Supplemental information

Diastereoselective Synthesis of 1,3-disubstituted Isoindolines and Sultams via Brønsted Acid-Catalyzed Intramolecular Hydroamidation of Sulfonamides

Ye Tao and Scott R. Gilbertson

Department of Chemistry, University of Houston, Houston TX 77204-5003

srgilbe2@central.uh.edu

Table of Contents:

29th January 2020

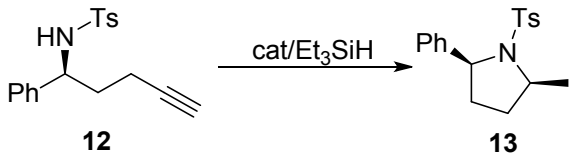
Note added after first publication: This Supplementary Information file replaces that originally published on 11th September 2018, in which the intermediates **21** and **23**, **25**, **26**, **27**, **28** and **29** were incorrectly identified as alkynes, rather than cyclized 5-member rings with an exocyclic double bond.

General Procedure:

All reagents were purchased from Sigma-Aldrich, Oakwood Chemicals, Combi-Blocks and used without purification. Thin layer chromatography (TLC) was performed on silica gel 60 F254 pre-coated plates (0.25 mm) from Silicycle and components were visualized by UV light (254 nm) and/or 10% phosphomolybdic acid in ethanol stain. Column Chromatography was performed on Silicycle silica gel 230-400 (particle size 40-63 μm) mesh with solvents specified below. ^{1}H and ^{13}C NMR were obtained on JEOL ECX-500 NMR spectrometer (500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR) in chloroform-d at ambient temperature. ^{1}H NMR chemical shifts are reported in terms of chemical shift (δ, ppm) relative to the singlet at δ 7.26 ppm for chloroform or δ 0.00 ppm for tetramethylsilane as an internal standard. Splitting patterns are designated as follows: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet. Coupling constants are reported in Hz. ^{13}C NMR spectra were fully decoupled and are reported in terms of chemical shift (δ, ppm) relative to the triplet at δ 77.0 ppm for $CDCl_3$. High resolution mass spectral data were recorded on an High-resolution Orbitrap MS equipped with a TriVersa NanoMate nano-electrospray (nESI) source from University of Houston, Mass Spectrometry Laboratory (MSL) of the Department of Chemistry.

Experimental Procedures:

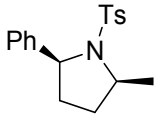
Cyclization of terminal alkyne **12** to **13**



12 **13**

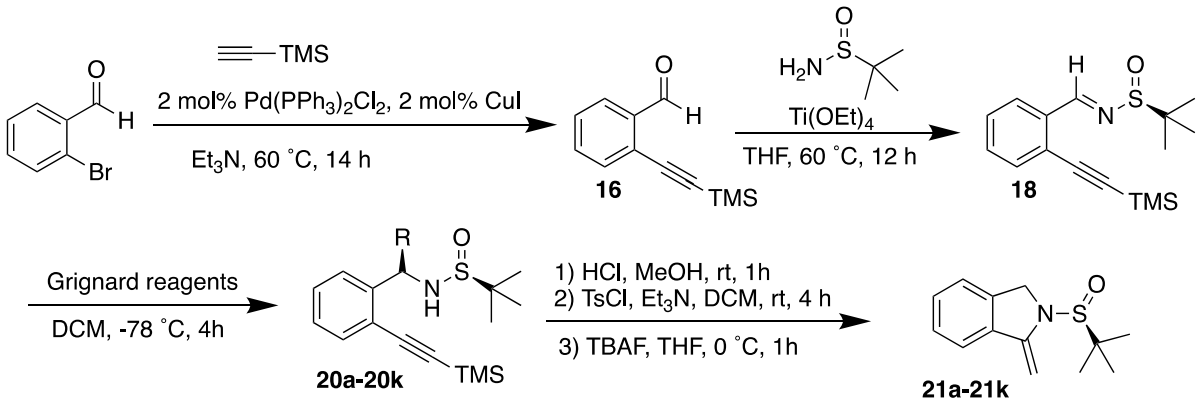
To a solution of compound **12** (0.2 mmol) in ACS reagent 1,2-DCE (2.0 ml) was added Tf_2NH (11.2 mg, 0.04 mmol, 20 mol%) and Et_3SiH (64 µl, 0.4 mmol, 2 equiv) sequentially under open air. The reaction mixture was stirred for at 50 ^oC until the reaction was completed via TLC following. After completion of reaction, the solvent was removed under reduced pressure and purified by flash column chromatography over silicone gel (EtOAc/hexane = 15:85) to produce **13** solid.

(2S,5S)-2-methyl-5-phenyl-1-tosylpyrrolidine (known compound **13**)



Yield: 42%, white solid.^{1}H NMR (500 MHz, Chloroform-d) δ 7.69 (d, J = 8.2 Hz, 2H), 7.37 (d, J = 7.4 Hz, 2H), 7.34 – 7.26 (m, 4H), 7.23 (q, J = 6.9 Hz, 1H), 4.72 (t, J = 6.6 Hz, 1H), 3.91 (h, J = 6.3 Hz, 1H), 2.42 (s, 3H), 1.93 – 1.79 (m, 2H), 1.76 – 1.63 (m, 1H), 1.46-1.52 (m, 4H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.4, 142.9, 135.2, 129.66, 128.4, 127.7, 127.1, 126.4, 65.0, 58.0, 34.5, 32.2, 22.9, 21.6.

Preparation and Characterization **21a-21k18**



The 2-acetylene benzaldehyde **16** was prepared according to the literature.[1] To a mixture of 2-bromobenzaldehyde (1.16 ml, 10.0 mmol), $PdCl_2(PPh_3)_2$ (140 mg, 0.2 mmol, 2 mol%) and CuI (39 mg, 0.2 mmol, 2 mol%) under N_2 atmosphere, Et_3N (20 ml) and ethynyltrimethylsilane (1.67 ml, 12.0 mmol, 1.2 equiv) was added sequentially. The system was stirred at 80 °C for overnight. After the reaction was completed, the mixture was filtered through a short pad of Celite®, washed with ethyl acetate. The filtrate was concentrated under reduced pressure and the residue was purified by flash column chromatography over silicone gel (EtOAc/hexane = 5:95) to give **16** as yellow solid.

The 2-acetylene t-butylsulfinyl imine **18** was prepared according to the literature with slight modification.[2] To a mixture of **16** (1.73 g, 8.6 mmol), (S)-(-)-t-butylsulfinamide (1.04 g, 8.6 mmol) in 18 ml THF, $Ti(OEt)_4$ (3.6 ml, 17.2 mmol) was added. The result yellow solution was stirred at 60 °C for 12 hours. At this time, saturated aqueous brine was added until white titanium salts precipitate. The suspension was filtered through a short pad of Celite® washing with small portions of ethyl acetate. The filtrate was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under vacuum and purified by means of flash chromatography on silica gel (EtOAc/hexane = 6:94) to give **18** as yellow oil.

The compound **20a-20k** was prepared according to literature reported method with slight modification.[3] Grinard reagent (1.5 eq) was added dropwise to the solution of **18** (0.84 mmol) in DCM (8 mL) under N_2 atmosphere at -78 ^oC. After the completion of addition, the solution was increased to -40 ^oC for 4 hours. After the reaction was completed (determined by TLC analysis), the reaction mixture was quenched by saturated aqueous NH_4Cl solution. Then the aqueous layer was extracted with DCM (3 × 5 mL) and then dried over anhydrous Na_2SO_4. The solution was evaporated under reduced pressure and the product **20a-20k** was used directly in next step without further purification. The diastereoselectivity is excellent (dr > 99:1) in most cases which was determined by crude ^1H-NMR.

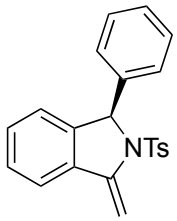
To a solution of compound **20a-20k** (0.8 mmol) in 2 ml MeOH, was slowly added HCl (in iPrOH, 1.6 mmol) under N_2 atmosphere at 0 ^oC. Then the mixture was run at room temperature for 1 hour and tracked by TLC until all starting material is gone. The resulting mixture was neutralized by NH_4OH (28%) aqueous solution. The solvent was removed under reduced pressure and the crude product was used for next tosylation without purification. The crude amine was redissolved in 4 ml DCM, Et_3N (0.12 ml, 0.8 mmol) was added to the solution. The mixture was cooled to 0 ^oC, then TsCl (193 mg, 1.0 mmol) was added portions. Then the mixture was run at room temperature for 4 hours. After the reaction was completed (determined by TLC analysis), the reaction mixture was washed with water and 1 N citric acid sequentially, dried over anhydrous Na_2SO_4, and concentrated under vacuum and purified by flash chromatography on silica gel (EtOAc/hexane = 15:85) to give tosylate products as yellow oil.

To the solution of tosylate compound (0.65 mmol) from previous step in 6.5 ml THF cooled to 0 ^oC, was added TBAF (0.7 ml, 1 N in THF) slowly. The mixture was run at this temperature for 1 hours. After the reaction was completed

(determined by TLC analysis), the reaction mixture was concentrated under vacuum and purified by flash chromatography on silica gel (EtOAc/hexane = 15:85) to give **21a-21k** as light yellow to black, purple solid in 28%-42% overall yield.

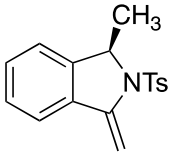
Characterization Data

(R)-N-((2-ethynylphenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (**21a**)



Purple solid, M.P.: 102.2-105.8 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.20 (m, 7H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 7.4 Hz, 1H), 6.17 (s, 1H), 5.32 (d, *J* = 1.7 Hz, 1H), 5.06 (d, *J* = 1.8 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 144.2, 143.9, 141.1, 140.7, 135.7, 134.0, 129.7, 129.5, 128.7, 128.24, 128.1, 127.6, 127.5, 123.4, 120.6, 88.0, 70.4, 21.6. HRMS ($^{+}$ESI) calculated for $C_{22}H_{20}NO_2S$ $[M+H]^+$ 362.1215, found 362.1250.

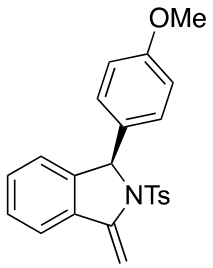
(R)-N-(1-(2-ethynylphenyl)ethyl)-4-methylbenzenesulfonamide (**21b**)



Light purple solid, M.P.: 97.7-101.8 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 6.9 Hz, 1H), 7.27 – 7.20 (m, 3H), 7.18 (d, *J* = 7.6 Hz, 1H), 5.33 (d, *J* = 1.6 Hz, 1H), 5.20 (q, *J* = 6.4 Hz, 1H), 5.00 (d, *J* = 1.7 Hz, 1H), 2.35 (s, 3H), 1.72 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR

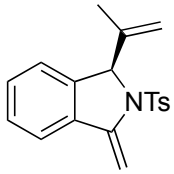
(126 MHz, Chloroform-d) δ 143.9, 143.9, 141.4, 135.2, 133.9, 129.5, 129.3, 127.9, 127.4, 122.1, 120.6, 88.8, 63.3, 24.0, 21.5. HRMS ($^+$ESI) calculated for $C_{17}H_{18}NO_2S$ $[M+H]^+$ 300.1058, found 300.1087.

(R)-N-((2-ethynylphenyl)(4-methoxyphenyl)methyl)-4-methylbenzenesulfonamide (**21c**)



Brown solid, M.P.: 82.4-85.7 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 1H), 7.29 – 7.21 (m, 2H), 7.18 – 7.12 (m, 4H), 6.97 (d, *J* = 7.4 Hz, 1H), 6.81 (d, *J* = 8.7 Hz, 2H), 6.16 (s, 1H), 5.29 (d, *J* = 1.8 Hz, 1H), 5.05 (d, *J* = 1.9 Hz, 1H), 3.79 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 159.4, 143.9, 143.7, 140.7, 135.8, 133.9, 133.2, 129.6, 129.3, 128.8, 128.1, 127.4, 123.3, 120.4, 113.9, 87.8, 69.9, 55.3, 21.5. HRMS ($^+$ESI) calculated for $C_{23}H_{22}NO_3S$ $[M+H]^+$ 392.1320, found 392.1358.

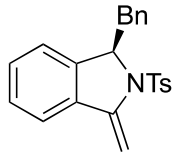
(R)-N-(1-(2-ethynylphenyl)-2-methylallyl)-4-methylbenzenesulfonamide (**21d**)



Green solid, M.P.: 81.1-84.4 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.39 (m, 1H), 7.30 – 7.22 (m, 4H), 7.14 (dd, *J* = 5.3, 3.1 Hz, 1H), 5.58 (s, 1H), 5.36 (d, *J* = 1.7 Hz, 1H), 5.28 (s, 1H), 5.06 – 5.02 (m, 1H), 5.00 (d, *J* = 1.8 Hz, 1H), 2.37 (s, 3H), 1.44 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 144.4, 144.2, 143.9, 138.3, 135.4, 134.7, 129.5, 129.4, 128.4,

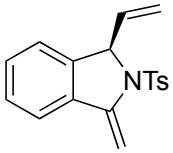
127.5, 122.6, 120.4, 114.1, 88.0, 72.8, 21.6, 16.1. HRMS ($^+$ESI) calculated for $C_{19}H_{20}NO_2S$ $[M+H]^+$ 326.1215, found 326.1247.

(R)-N-(1-(2-ethynylphenyl)-2-phenylethyl)-4-methylbenzenesulfonamide (**21e**)



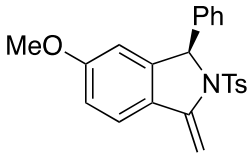
Black solid, M.P.: 73.6-77.7 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.11 (m, 10H), 6.69 (d, *J* = 7.4 Hz, 1H), 5.39 (dd, *J* = 8.2, 3.2 Hz, 1H), 5.30 (d, *J* = 1.6 Hz, 1H), 4.91 (d, *J* = 1.7 Hz, 1H), 3.63 (dd, *J* = 13.3, 3.2 Hz, 1H), 3.18 (dd, *J* = 13.3, 8.3 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.8, 139.1, 136.1, 135.1, 134.7, 130.3, 129.5, 128.6, 128.1, 127.9, 127.4, 126.6, 123.0, 120.4, 89.3, 67.6, 43.5, 21.5. HRMS ($^+$ESI) calculated for $C_{23}H_{22}NO_2S$ $[M+H]^+$ 376.1371, found 376.1409.

(R)-N-(1-(2-ethynylphenyl)allyl)-4-methylbenzenesulfonamide (**21f**)



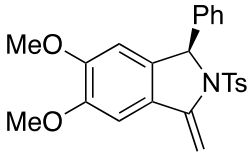
Black oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.39 (m, 1H), 7.32 – 7.27 (m, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.16 (d, *J* = 7.2 Hz, 1H), 5.91 (ddd, *J* = 17.3, 10.0, 7.6 Hz, 1H), 5.58 (d, *J* = 7.6 Hz, 1H), 5.50 (d, *J* = 17.0 Hz, 1H), 5.31 – 5.26 (m, 2H), 5.00 (d, *J* = 1.8 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 144.1, 143.9, 138.409, 137.3, 135.6, 134.3, 129.6, 129.5, 128.5, 127.7, 123.4, 120.7, 117.3, 88.6, 69.5, 21.7. HRMS ($^+$ESI) calculated for $C_{18}H_{18}NO_2S$ $[M+H]^+$ 312.1058, found 312.1088.

(R)-N-((2-ethynyl-5-methoxyphenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (**21g**)



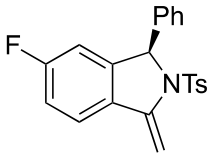
Purple solid, M.P.: 84.1-88.4 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.55 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.6 Hz, 1H), 7.33 – 7.23 (m, 4H), 7.16 (d, J = 8.1 Hz, 2H), 6.82 (dd, J = 8.6, 2.2 Hz, 1H), 6.44 (d, J = 2.0 Hz, 1H), 6.12 (s, 1H), 5.21 (d, J = 1.6 Hz, 1H), 4.91 (d, J = 1.8 Hz, 1H), 3.69 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 161.2, 143.9, 142.35, 141.1, 129.5, 128.7, 128.2, 127.5, 126.7, 121.8, 115.7, 107.3, 86.2, 70.3, 55.6, 21.6. HRMS ($^{+}$ESI) calculated for $C_{23}H_{22}NO_3S$ $[M+H]^+$ 392.1320, found 392.1359.

(R)-N-((2-ethynyl-4,5-dimethoxyphenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (**21h**)



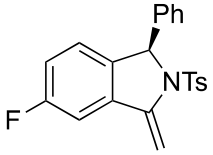
Purple solid, M.P.: 80.1-84.4 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.31 – 7.28 (m, 3H), 7.26 – 7.23 (m, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 6.87 (s, 1H), 6.39 (s, 1H), 6.09 (s, 1H), 5.22 (d, *J* = 1.8 Hz, 1H), 4.87 (d, *J* = 1.9 Hz, 1H), 3.88 (s, 3H), 3.74 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 151.2, 149.8, 144.4, 143.7, 141.0, 135.7, 133.3, 129.4, 128.6, 128.1, 127.5, 127.5, 127.4, 126.2, 105.0, 102.2, 86.1, 70.2, 56.1, 21.5. HRMS ($^{+}$ESI) calculated for $C_{24}H_{24}NO_4S$ $[M+H]^+$ 422.1426, found 422.1466.

(R)-N-((2-ethynyl-5-fluorophenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (**21i**)



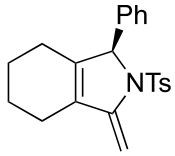
Brown solid, M.P.: 73.3-76.7 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.43 (dd, *J* = 8.6, 4.8 Hz, 1H), 7.30 (m, 3H), 7.23 (m, 2.4 Hz, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 6.97 (td, *J* = 8.7, 2.3 Hz, 1H), 6.66 (dd, *J* = 8.1, 2.0 Hz, 1H), 6.14 (s, 1H), 5.29 (d, *J* = 1.9 Hz, 1H), 4.99 (d, *J* = 2.0 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.9, 143.2, 140.4, 135.5, 129.9, 129.4, 128.8, 128.3, 127.4, 127.3, 122.3, 122.2, 116.2, 116.0, 110.4, 110.2, 87.7, 69.9, 21.5. HRMS ($^+$ESI) calculated for $C_{22}H_{19}FNO_2S$ $[M+H]^+$ 380.1121, found 380.1161.

(R)-N-((2-ethynyl-4-fluorophenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (**21j**)



Brown solid, M.P.: 73.5-77.0 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.27 (m, 3H), 7.25 – 7.21 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 1H), 6.96 – 6.90 (m, 2H), 6.13 (s, 1H), 5.35 (d, *J* = 2.0 Hz, 1H), 5.02 (d, *J* = 2.0 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 144.0, 140.7, 135.5, 129.4, 128.7, 128.2, 127.4, 127.3, 125.0, 124.9, 117.4, 117.2, 107.2, 107.0, 89.0, 69.8, 21.5. HRMS ($^+$ESI) calculated for $C_{22}H_{19}FNO_2S$ $[M+H]^+$ 380.1121, found 380.1159.

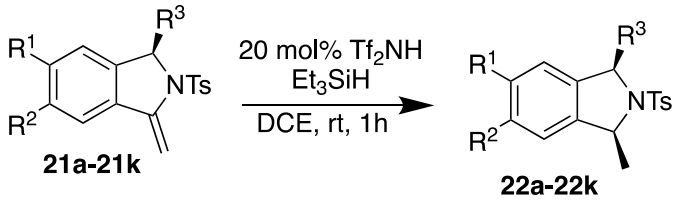
(R)-N-((2-ethynylcyclohex-1-en-1-yl)(phenyl)methyl)-4-methylbenzenesulfonamide (**21k**)



Yellow solid, M.P.: 106.8-110.0 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.47 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.29 (m, 2H), 7.24 – 7.13 (m, 5H), 5.47 (s, 1H), 4.94

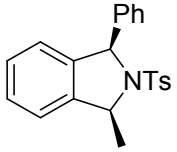
(s, 1H), 4.28 (s, 1H), 2.36 (s, 3H), 2.12 (d, J = 17.1 Hz, 1H), 1.90 (d, J = 18.1 Hz, 1H), 1.66 – 1.50 (m, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 148.5, 143.5, 140.9, 139.1, 136.1, 131.2, 131.1, 129.4, 129.3, 128.6, 128.1, 127.6, 127.5, 127.3, 126.6, 85.2, 73.4, 22.6, 22.2, 21.8, 21.6, 20.9. HRMS ($^+$ESI) calculated for $C_{22}H_{24}NO_2S$ $[M+H]^+$ 366.1528, found 366.1568.

General procedure for the synthesis of 1,3-disubstituted isoindolines from sulfonamides



To a solution of compound **21a-21k** (0.125 mmol) in ACS reagent 1,2-DCE (1.25 ml) was added Tf_2NH (7 mg, 0.025 mmol, 20 mol%) and Et_3SiH (40 μl, 0.25 mmol, 2 equiv) sequentially under open air. The reaction mixture was stirred for 1-2 hour at room temperature until the reaction was completed via TLC following. After completion of reaction, the solvent was removed under reduced pressure and purified by flash column chromatography over silicone gel (EtOAc/hexane = 10:90-15:85) to produce 1,3-disubstituted isoindolines **22a-22k** as oil or solid.

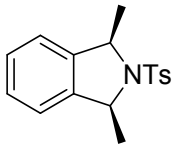
(1S,3R)-1-methyl-3-phenyl-2-tosylisoindoline (**22a**)



Yield: 95%, pink oil. 96% ee (determined by HPLC: Chiralcel OD-H Column, 3/97 i-PrOH /hexane, 0.9 mL/min, 254 nm; TR = 14.03 min (major), 15.83 min (minor)). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.63 (d, J = 8.2 Hz, 2H), 7.34 – 7.27 (m, 4H), 7.26 – 7.20 (m, 2H), 7.16 (dd, J = 17.5, 7.3 Hz, 4H), 6.87 (d, J =

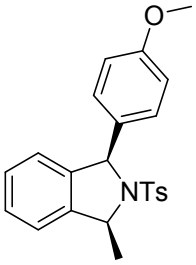
8.0 Hz, 1H), 5.88 (s, 1H), 5.13 (q, *J* = 6.4 Hz, 1H), 2.33 (s, 3H), 1.77 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 143.5, 142.6, 140.6, 139.6, 135.6, 129.7, 128.6, 128.2, 128.1, 127.8, 127.7, 127.7, 123.7, 122.3, 69.8, 62.1, 24.8, 21.6. HRMS ($^{+}$ESI) calculated for $C_{22}H_{22}NO_2S$ $[M+H]^+$ 364.1371, found 364.1386.

(1R,3S)-1,3-dimethyl-2-tosylisoindoline (**22b**)



Yield: 97%, white solid, M.P.: 122.3-125.6 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 (d, J = 8.2 Hz, 2H), 7.26 – 7.20 (m, 4H), 7.08 (dd, J = 5.4, 3.3 Hz, 2H), 4.88 (q, J = 6.5 Hz, 2H), 2.35 (s, 3H), 1.66 (d, J = 6.5 Hz, 6H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.5, 140.7, 135.0, 129.8, 127.9, 127.6, 122.4, 62.0, 25.9, 21.6. HRMS ($^{+}$ESI) calculated for $C_{17}H_{20}NO_2S$ $[M+H]^+$ 302.1214, found 302.1230.

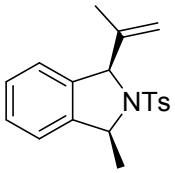
(1R,3S)-1-(4-methoxyphenyl)-3-methyl-2-tosylisoindoline (**22c**)



Yield: 77%, white solid, M.P.: 141.0-143.4 °C. 89% ee (determined by HPLC: Chiralcel OD-H Column, 3/97 i-PrOH /hexane, 0.9 mL/min, 254 nm; TR = 20.68 min (major), 26.35 min (minor)). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.63 (d, J = 8.2 Hz, 2H), 7.28 – 7.11 (m, 7H), 6.87 (d, J = 7.6 Hz, 1H), 6.83 (d, J = 8.6 Hz, 2H), 5.84 (s, 1H), 5.11 (q, J = 6.4 Hz, 1H), 3.79 (s, 3H), 2.35 (s, 3H), 1.75 (d, J = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 159.2, 143.4, 140.6, 139.8, 135.7, 134.8, 129.6, 129.0, 128.1, 127.7, 123.7, 122.2, 113.9, 69.3, 61.9,

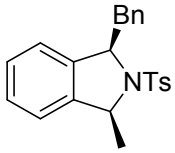
55.4, 24.8, 21.6. HRMS ($^+$ESI) calculated for $C_{23}H_{24}NO_3S$ $[M+H]^+$ 394.1476, found 394.1496.

(1S,3R)-1-methyl-3-(prop-1-en-2-yl)-2-tosylisoindoline (**22d**)



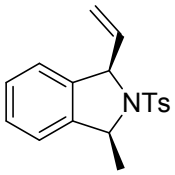
Yield: 80%, colorless oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.75 (d, J = 8.2 Hz, 2H), 7.31 – 7.18 (m, 4H), 7.10 (d, J = 7.4 Hz, 1H), 7.02 (d, J = 7.4 Hz, 1H), 5.24 (s, 1H), 5.17 (s, 1H), 5.05 – 4.97 (m, 2H), 2.38 (s, 3H), 1.72 (d, J = 6.4 Hz, 3H), 1.55 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 145.0, 143.6, 141.1, 137.4, 135.1, 129.8, 128.4, 127.9, 127.8, 122.8, 122.2, 114.1, 72.3, 62.2, 24.6, 21.6, 17.1. HRMS ($^+$ESI) calculated for $C_{19}H_{22}NO_2S$ $[M+H]^+$ 328.1371, found 328.1390.

(1R,3S)-1-benzyl-3-methyl-2-tosylisoindoline (**22e**)



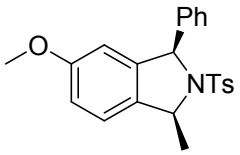
Yield: 92%, colorless oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.74 (d, J = 8.3 Hz, 2H), 7.30 – 7.21 (m, 2H), 7.17 (m, 5H), 7.04 (dd, J = 7.5, 1.6 Hz, 2H), 6.96 – 6.91 (m, 1H), 6.91 – 6.86 (m, 1H), 5.14 (dd, J = 7.2, 2.6 Hz, 1H), 4.75 (q, J = 6.5 Hz, 1H), 3.40 (dd, J = 13.4, 2.7 Hz, 1H), 3.30 (dd, J = 13.4, 7.3 Hz, 1H), 2.35 (s, 3H), 1.05 (d, J = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.5, 141.5, 138.1, 136.7, 135.0, 130.9, 129.9, 127.9, 127.5, 127.4, 126.6, 123.2, 122.2, 66.9, 62.1, 43.8, 24.2, 21.6. HRMS ($^+$ESI) calculated for $C_{23}H_{23}NO_2SNa$ $[M+Na]^+$ 400.1347, found 400.1370.

(1S,3R)-1-methyl-2-tosyl-3-vinylisoindoline (**22f**)



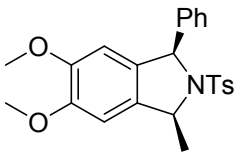
Yield: 53%, white solid, M.P.: 90.3-93.1 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.74 (d, J = 8.3 Hz, 2H), 7.30 – 7.19 (m, 4H), 7.14 – 7.03 (m, 2H), 5.93 (ddd, J = 17.2, 10.1, 7.4 Hz, 1H), 5.41 (d, J = 16.8 Hz, 1H), 5.25 (d, J = 7.3 Hz, 1H), 5.20 (d, J = 10.2 Hz, 1H), 4.98 (q, J = 6.4 Hz, 1H), 2.37 (s, 3H), 1.64 (d, J = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.6, 141.0, 139.5, 137.8, 135.5, 129.8, 128.3, 127.9, 127.6, 123.4, 122.4, 116.2, 68.3, 62.1, 25.3, 21.6. HRMS ($^{+}$ESI) calculated for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.1214, found 314.1214.

(1S,3R)-5-methoxy-1-methyl-3-phenyl-2-tosylisoindoline (**22g**)



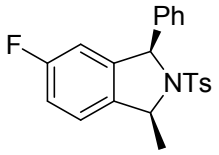
Yield: 67%, purple oil. 97% ee (determined by HPLC: Chiralcel OD-H Column, 3/97 i-PrOH /hexane, 0.9 mL/min, 254 nm; TR = 21.86 min (major), 24.58 min (minor)). ^{1}H NMR (500 MHz, Chloroform-d) δ 7.62 (d, J = 8.2 Hz, 2H), 7.36 – 7.22 (m, 5H), 7.18 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.4 Hz, 1H), 6.78 (dd, J = 8.4, 2.1 Hz, 1H), 6.35 (d, J = 1.8 Hz, 1H), 5.81 (s, 1H), 5.06 (q, J = 6.3 Hz, 1H), 3.65 (s, 3H), 2.35 (s, 3H), 1.73 (d, J = 6.3 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 159.8, 143.4, 142.4, 140.9, 135.6, 132.8, 129.6, 128.6, 127.8, 127.7, 123.1, 114.9, 108.2, 69.7, 61.7, 55.5, 24.9, 21.6. HRMS ($^{+}$ESI) calculated for $C_{23}H_{24}NO_3S$ $[M+H]^+$ 394.1477, found 394.1514.

(1S,3R)-5,6-dimethoxy-1-methyl-3-phenyl-2-tosylisoindoline (**22h**)



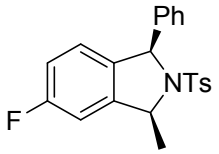
Yield: 60%, green solid, M.P.: 91.5-93.5 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.62 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 4.3 Hz, 4H), 7.28 – 7.24 (m, 1H), 7.19 (d, J = 8.1 Hz, 2H), 6.60 (s, 1H), 6.30 (s, 1H), 5.81 (s, 1H), 5.06 (q, J = 6.3 Hz, 1H), 3.85 (s, 3H), 3.69 (s, 3H), 2.35 (s, 3H), 1.73 (d, J = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 149.7, 149.6, 143.4, 142.5, 135.7, 132.4, 131.1, 129.6, 128.6, 127.8, 127.8, 127.7, 105.9, 104.5, 69.8, 62.2, 56.1, 24.9, 21.6. HRMS ($^{+}$ESI) calculated for $C_{24}H_{25}NO_4SNa$ $[M+Na]^+$ 446.1402, found 446.1440.

(1S,3R)-5-fluoro-1-methyl-3-phenyl-2-tosylisoindoline (**22i**)



Yield: 92%, yellow oil. 98% ee (determined by HPLC: Chiralcel OD-H Column, 3/97 i-PrOH /hexane, 0.9 mL/min, 254 nm; TR = 18.99 min (major), 23.20 min (minor)). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.23 (m, 5H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.09 (dd, *J* = 8.4, 4.8 Hz, 1H), 6.93 (td, *J* = 8.6, 2.3 Hz, 1H), 6.56 (dd, *J* = 8.5, 2.1 Hz, 1H), 5.84 (s, 1H), 5.10 (q, *J* = 6.4 Hz, 1H), 2.35 (s, 3H), 1.74 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 163.8, 161.8, 143.6, 141.8, 141.6 (d, J = 8.2 Hz), 136.1, 135.5, 129.7, 128.7, 128.0, 127.7, 127.6, 123.7 (d, J = 9.0 Hz), 115.7 (d, J = 23.0 Hz), 110.7 (d, J = 23.5 Hz), 69.5, 61.6, 24.8, 21.6. HRMS ($^{+}$ESI) calculated for $C_{22}H_{21}FNO_2S$ $[M+H]^+$ 382.1277, found 382.1300.

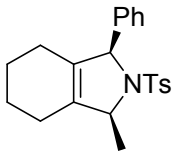
(1R,3S)-5-fluoro-3-methyl-1-phenyl-2-tosylisoindoline (**22j**)



Yield: 90%, pink solid, M.P.: 105.5-109.0 °C. 98% ee (determined by HPLC: Chiralcel OD-H Column, 3/97 i-PrOH /hexane, 0.9 mL/min, 254 nm; TR = 18.92

min (major), 23.20 min (minor)). ^{1}H NMR (500 MHz, Chloroform-d) δ 7.61 (d, J = 8.3 Hz, 2H), 7.41 – 7.22 (m, 5H), 7.19 (d, J = 8.1 Hz, 2H), 6.91 – 6.76 (m, 3H), 5.84 (s, 1H), 5.11 (q, J = 6.4 Hz, 1H), 2.35 (s, H),1.74 (d, J = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 163.9, 161.9, 143.6, 142.7, 142.2, 135.5, 135.2, 129.7, 128.7, 127.9, 127.7, 127.6, 125.2 (d, J = 9.0 Hz), 115.6 (d, J = 23.0 Hz), 109.3 (d, J = 23.3 Hz), 69.2, 61.8, 24.6, 21.6. HRMS ($^{+}$ESI) calculated for $C_{22}H_{21}FNO_2S$ $[M+H]^+$ 382.1277, found 382.1301.

(1S,3R)-1-methyl-3-phenyl-2-tosyl-2,3,4,5,6,7-hexahydro-1H-isoindole (**22k**)



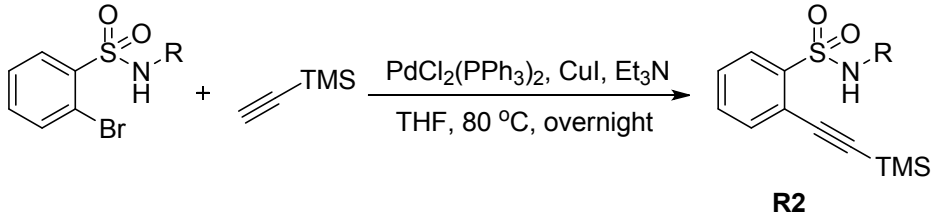
Yield: 80%, white solid, M.P.: 122.3-124.4 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.56 (d, J = 8.2 Hz, 2H), 7.32 – 7.14 (m, 7H), 5.17 (s, 1H), 4.55 – 4.41 (m, 1H), 2.38 (s, 3H), 1.97-2.01 (m, 1H), 1.83-1.86 (m, 1H), 1.69-1.72 (m, 1H), 1.49-1.60 (m, 4H), 1.43-1.47 (m, 4H). ^{13}C NMR (126 MHz, Chloroform-d) δ 143.0, 140.9, 136.2, 134.2, 132.3, 129.5, 128.4, 127.7, 127.6, 127.5, 72.9, 64.9, 22.4, 22.2, 22.0, 21.6. HRMS ($^{+}$ESI) calculated for $C_{22}H_{26}NO_2S$ $[M+H]^+$ 368.1684, found 368.1705.

Preparation and Characterization of Substrates:

R1

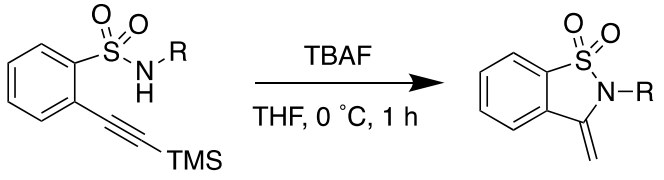
To a mixture of 2-bromobenzenesulfonylchloride (511 mg, 2.0 mmol) in DCM (6 ml) and Et_3N (0.3 ml, 2.2 mmol) was added free amine (2.2 mmol) in one portion at room temperature and the mixture was stirred for 1-4 hours by following the reaction via TLC. After the reaction done, concentrated under

reduced pressure. The residue was purified by flash column chromatography over silicone gel (EtOAc/hexane = 5:95-10:90) to give sulfonamides **R1** as solid.



R2

To a mixture of **R1** (0.92 mmol), $PdCl_2(PPh_3)_2$ (33 mg, 0.046 mmol, 5 mol%) and CuI (9 mg, 0,046, 5 mol%) in THF (2 ml) under N_2 atmosphere, Et_3N (3 ml) and ethynyltrimethylsilane (153 µl, 1.1 mmol, 1.2 equiv) was added sequentially. The system was stirred at 80 °C for overnight. After the reaction was completed, the mixture was filtered through a short pad of Celite®, washed with ethyl acetate. The filtrate was concentrated under reduced pressure and the residue was purified by flash column chromatography over silicone gel (EtOAc/hexane = 5:95-10:90) to give **R2** as yellow oil.

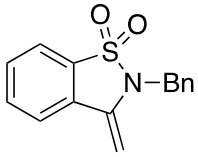


23a-23o, 25-29

To a solution of **R2** (0.45 mmol) in THF (4.5 ml) was added TBAF (1 M in THF, 0.5 ml, 0.5 mmol) slowly at 0 °C, the mixture was stirred for another 60 min at this temperature. The solvent was removed, residue was purified by flash column chromatography over silicone gel (EtOAc/hexane = 5:95-10:90) to give desired substrates **23a-23o, 25-29** as yellow solid or oil in 40%-72% overall yield.

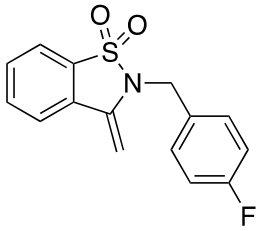
Characterization Data

N-benzyl-2-ethynylbenzenesulfonamide (**23a**)



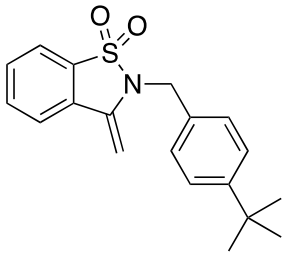
Yellow solid, M.P.: 129.1-132.1 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.91 – 7.84 (m, 1H), 7.72 – 7.68 (m, 1H), 7.65 (td, *J* = 7.6, 1.3 Hz, 1H), 7.61 (td, *J* = 7.5, 1.3 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 4.90 (d, *J* = 2.9 Hz, 1H), 4.82 (s, 2H), 4.33 (d, *J* = 2.9 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.5, 135.1, 133.1, 131.7, 130.4, 130.2, 128.8, 127.8, 127.2, 121.5, 121.1, 86.1, 44.3. HRMS ($^{+}$ESI) calculated for $C_{15}H_{14}NO_2S$ $[M+H]^+$ 272.0745, found 272.0773.

2-ethynyl-N-(4-fluorobenzyl)benzenesulfonamide (**23b**)



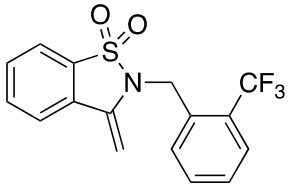
Yellow solid, M.P.: 125.1-127.3 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.5 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.63 (dtd, *J* = 22.8, 7.4, 1.0 Hz, 2H), 7.45 – 7.38 (m, 2H), 7.07 – 7.01 (m, 2H), 4.91 (d, *J* = 2.9 Hz, 1H), 4.79 (s, 2H), 4.31 (d, *J* = 2.9 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.4, 161.4, 137.5, 133.3, 131.8, 130.9, 130.9, 130.6, 130.2, 129.1, 129.1, 121.6, 121.3, 115.9, 115.7, 86.2, 43.7. HRMS ($^{+}$ESI) calculated for $C_{15}H_{13}FNO_2S$ $[M+H]^+$ 290.0651, found 290.0681.

N-(4-(tert-butyl)benzyl)-2-ethynylbenzenesulfonamide (**23c**)



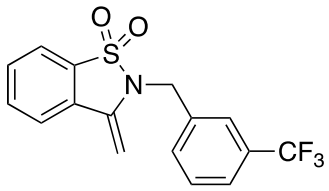
Yellow solid, M.P.: 124.5-128.1 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.66 – 7.57 (m, 2H), 7.37 (s, 4H), 4.90 (d, *J* = 2.8 Hz, 1H), 4.79 (s, 2H), 4.38 (d, *J* = 2.8 Hz, 1H), 1.30 (s, 9H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.8, 137.6, 133.2, 132.1, 131.9, 130.5, 130.4, 127.1, 125.8, 121.5, 121.2, 86.2, 44.1, 34.6, 31.4. HRMS ($^{+}$ESI) calculated for $C_{19}H_{22}NO_2S$ $[M+H]^+$ 328.1371, found 328.1408.

2-ethynyl-N-(2-(trifluoromethyl)benzyl)benzenesulfonamide (**23d**)



Yellow solid, M.P.: 140.1-142.3 °C. ^{1}H NMR (500 MHz,) δ 7.90 (d, *J* = 7.6 Hz, 1H), 7.79 – 7.59 (m, 5H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 5.04 (s, 2H), 4.93 (d, *J* = 3.0 Hz, 1H), 4.22 (d, *J* = 3.1 Hz, 1H). ^{13}C NMR (126 MHz,) δ 136.7, 132.9, 132.6, 131.9, 131.1, 129.9, 129.3, 127.2, 127.0, 126.8, 126.6, 125.4, 125.3, 124.8, 120.9, 120.5, 85.5, 76.6, 76.4, 76.1, 40.2, 40.2. HRMS ($^{+}$ESI) calculated for $C_{16}H_{13}F_3NO_2S$ $[M+H]^+$ 340.0619, found 340.0660.

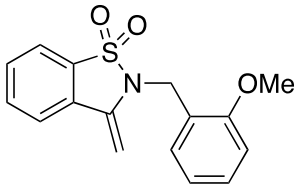
2-ethynyl-N-(3-(trifluoromethyl)benzyl)benzenesulfonamide (**23e**)



Yellow solid, M.P.: 99.1-101.5 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.69 – 7.61 (m, 4H), 7.56 (d, *J* = 7.7

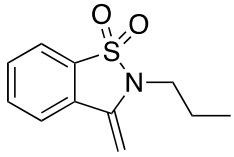
Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 1H), 4.93 (d, *J* = 3.0 Hz, 1H), 4.87 (s, 2H), 4.28 (d, *J* = 3.0 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.5, 136.4, 133.4, 131.7, 131.4, 131.1, 130.7, 130.7, 130.1, 129.5, 124.9, 124.8, 124.0, 124.0, 122.9, 121.6, 121.3, 86.2, 43.9. HRMS ($^{+}$ESI) calculated for $C_{16}H_{13}F_3NO_2S$ $[M+H]^+$ 340.0619, found 340.0657.

2-ethynyl-N-(2-methoxybenzyl)benzenesulfonamide (**23f**)



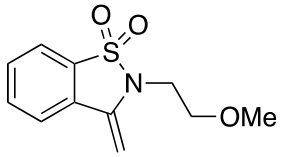
Off-white solid, M.P.: 137.2-139.5 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.63 – 7.57 (m, 1H), 7.37 (d, *J* = 7.4 Hz, 1H), 7.26 (m, 1H), 6.98 – 6.85 (m, 2H), 4.91 (d, *J* = 2.8 Hz, 1H), 4.87 (s, 2H), 4.39 (d, *J* = 2.8 Hz, 1H), 3.91 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.6, 133.0, 130.3, 128.62, 128.0, 123.0, 121.4, 121.1, 120.8, 110.0, 85.7, 55.4, 38.8. HRMS ($^{+}$ESI) calculated for $C_{16}H_{16}NO_3S$ $[M+H]^+$ 302.0851, found 302.0855.

2-ethynyl-N-propylbenzenesulfonamide (**23g**)



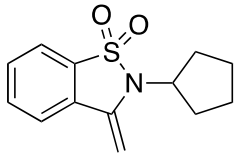
Yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.60 – 7.55 (m, 1H), 4.99 (d, *J* = 2.8 Hz, 1H), 4.48 (d, *J* = 2.8 Hz, 1H), 3.62 – 3.55 (m, 2H), 1.86 (h, *J* = 7.4 Hz, 2H), 1.03 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.9, 133.0, 132.0, 130.5, 130.4, 121.5, 121.0, 84.4, 42.5, 21.0. HRMS ($^{+}$ESI) calculated for $C_{11}H_{14}NO_2S$ $[M+H]^+$ 224.0745, found 224.0771.

2-ethynyl-N-(2-methoxyethyl)benzenesulfonamide (**23h**)



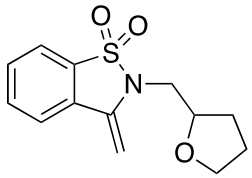
Yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 5.02 (d, *J* = 2.8 Hz, 1H), 4.69 (d, *J* = 2.8 Hz, 1H), 3.83 (t, J = 6.2 Hz, 2H), 3.74 (q, J = 6.4 Hz, 2H), 3.41 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 138.2, 133.2, 130.4, 125.3, 121.6, 121.1, 85.3, 70.0, 59.2, 40.4. HRMS ($^{+}$ESI) calculated for $C_{11}H_{14}NO_3S$ $[M+H]^+$ 240.0694, found 240.0721.

N-cyclopentyl-2-ethynylbenzenesulfonamide (**23i**)



Yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.65 – 7.59 (m, 1H), 7.56 (t, J = 7.3 Hz, 1H), 5.02 (d, J = 2.5 Hz, 1H), 4.51 (d, J = 2.7 Hz, 1H), 4.24 (p, J = 8.5 Hz, 1H), 2.28 – 2.14 (m, 4H), 1.97 – 1.86 (m, 2H), 1.62-1.74 (m, 2H). ^{13}C NMR (126 MHz, Chloroform-d) δ 137.3, 134.3, 132.9, 130.3, 121.3, 120.8, 85.7, 55.6, 32.0, 29.5, 28.6, 24.2. HRMS ($^{+}$ESI) calculated for $C_{13}H_{16}NO_2S$ $[M+H]^+$ 250.0902, found 250.0930.

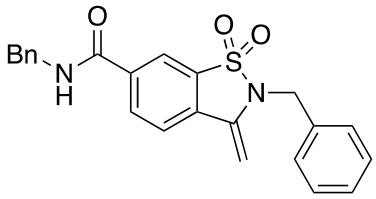
2-ethynyl-N-((tetrahydrofuran-2-yl)methyl)benzenesulfonamide (**23j**)



Yellow oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.82 (d, J = 7.6 Hz, 1H), 7.73 (d, J = 7.7 Hz, 1H), 7.64 (t, J = 7.4 Hz, 1H), 7.58 (t, J = 7.8 Hz, 1H), 5.03 (d, J = 2.7 Hz, 1H), 4.82 (d, J = 2.7 Hz, 1H), 4.31 (p, J = 6.4 Hz, 1H), 3.94 (q, J = 7.2

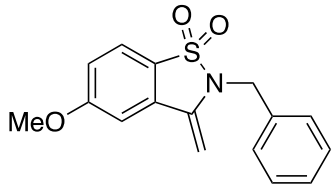
Hz, 1H), 3.86 – 3.72 (m, 2H), 3.65 (dd, J = 15.5, 5.8 Hz, 1H), 2.16 – 2.03 (m, 1H), 2.04 – 1.76 (m, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 138.8, 133.2, 131.7, 130.5, 130.4, 121.5, 121.1, 86.0, 68.6, 45.5, 29.7, 25.7. HRMS ($^{+}$ESI) calculated for $C_{13}H_{16}NO_3S$ $[M+H]^+$ 266.0851, found 266.0883.

N-benzyl-3-(N-benzylsulfamoyl)-4-ethynylbenzamide (**23k**)



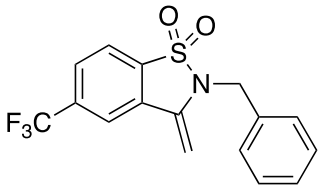
Yellow solid, M.P.: 175.3-179.0 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 1.2 Hz, 1H), 8.15 (d, *J* = 1.6 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 1H), 7.43 – 7.29 (m, 10H), 6.56 (t, *J* = 5.1 Hz, 1H), 4.97 (d, *J* = 3.0 Hz, 1H), 4.79 (s, 2H), 4.66 (d, *J* = 5.6 Hz, 2H), 4.42 (d, *J* = 3.1 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.9, 137.5, 136.9, 136.7, 134.8, 132.8, 132.5, 132.1, 129.1, 128.9, 128.1, 128.1, 128.0, 127.3, 122.0, 119.6, 88.2, 44.6, 44.5. HRMS ($^{+}$ESI) calculated for $C_{23}H_{21}N_2O_3S$ $[M+H]^+$ 405.1273, found 405.1299.

N-benzyl-2-ethynyl-4-methoxybenzenesulfonamide (**23l**)



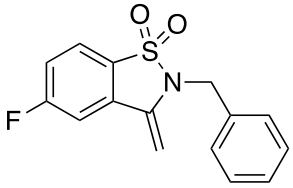
Yellow solid, M.P.: 109.5-111.9 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 8.6 Hz, 1H), 7.44 (d, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.13 – 7.08 (m, 2H), 4.84 (d, *J* = 2.8 Hz, 1H), 4.80 (s, 2H), 4.30 (d, *J* = 2.9 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.7, 137.7, 135.3, 132.7, 128.8, 127.8, 127.3, 124.2, 122.8, 117.6, 105.3, 85.9, 56.0, 44.5. HRMS ($^{+}$ESI) calculated for $C_{16}H_{16}NO_3S$ $[M+H]^+$ 302.0851, found 302.0884.

N-benzyl-2-ethynyl-4-(trifluoromethyl)benzenesulfonamide (**23m**)



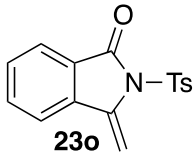
Yellow solid, M.P.: 149.1-152.3 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 8.2 Hz, 1H), 7.94 (s, 1H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 5.01 (d, *J* = 3.3 Hz, 1H), 4.84 (s, 2H), 4.46 (d, *J* = 3.3 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 136.5, 135.6, 135.3, 134.7, 134.6, 131.1, 129.0, 128.1, 127.3, 124.2, 122.3, 122.0, 119.0, 119.0, 88.0, 44.6. HRMS ($^+$ESI) calculated for $C_{16}H_{12}F_3NO_2SNa$ $[M+Na]^+$ 362.0438, found 362.0475.

N-benzyl-2-ethynyl-4-fluorobenzenesulfonamide (**23n**)



Yellow solid, M.P.: 140.3-143.5 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (dd, *J* = 8.6, 4.7 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 2H), 7.39 – 7.27 (m, 5H), 4.86 (d, *J* = 3.1 Hz, 1H), 4.81 (s, 2H), 4.38 (d, *J* = 3.1 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.7, 164.7, 136.8, 136.74, 134.9, 133.4, 133.3, 128.9, 128.0, 127.3, 123.8, 123.7, 118.6, 118.5, 108.8, 108.6, 87.3, 44.6. HRMS ($^+$ESI) calculated for $C_{15}H_{13}FNO_2S$ $[M+H]^+$ 290.0651, found 290.0685.

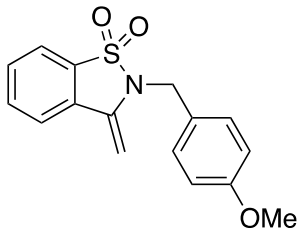
2-ethynyl-N-tosylbenzamide (**23o**)



Yellow solid, M.P.: 160.8-163.0 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 7.9 Hz, 2H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.73 – 7.60 (m, 2H), 7.49 (t, *J* = 7.4

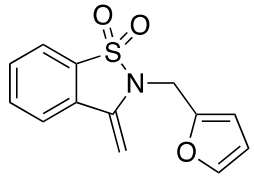
Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 6.20 (d, *J* = 1.5 Hz, 1H), 5.55 (d, *J* = 1.6 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 145.4, 134.1, 130.1, 129.7, 128.1, 124.4, 120.1, 96.7, 21.7. HRMS ($^{+}$ESI) calculated for $C_{16}H_{14}NO_3S$ $[M+H]^+$ 300.0694, found 300.0727.

2-ethynyl-N-(4-methoxybenzyl)benzenesulfonamide (**25**)



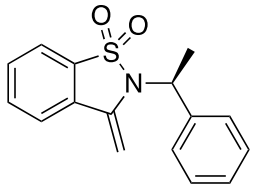
Yellow solid, M.P.: 91.7-94.1 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.37 (d, *J* = 8.6 Hz, 2H), 6.88 (d, *J* = 8.6 Hz, 2H), 4.90 (d, *J* = 2.7 Hz, 1H), 4.76 (s, 2H), 4.36 (d, *J* = 2.7 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 133.1, 130.4, 128.7, 127.0, 121.4, 121.1, 114.1, 86.0, 55.3, 43.8. HRMS ($^{+}$ESI) calculated for $C_{16}H_{16}NO_3S$ $[M+H]^+$ 302.0851, found 302.0889.

2-ethynyl-N-(furan-2-ylmethyl)benzenesulfonamide (**26**)



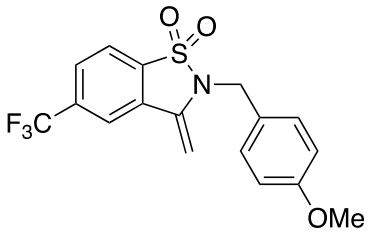
Yellow solid, M.P.: 99.1-101.5 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.65 (td, *J* = 7.7, 1.0 Hz, 1H), 7.62 – 7.57 (m, 1H), 7.39 (d, *J* = 1.4 Hz, 1H), 6.42 (d, *J* = 3.0 Hz, 1H), 6.35 (dd, *J* = 3.1, 1.9 Hz, 1H), 5.01 (d, *J* = 2.9 Hz, 1H), 4.80 (s, 2H), 4.67 (d, *J* = 3.0 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 148.9, 142.6, 137.5, 133.2, 130.5, 121.5, 121.2, 110.9, 109.4, 85.9, 37.3. HRMS ($^{+}$ESI) calculated for $C_{13}H_{12}NO_3S$ $[M+H]^+$ 262.0538, found 262.0559.

(S)-2-ethynyl-N-(1-phenylethyl)benzenesulfonamide (**27**)



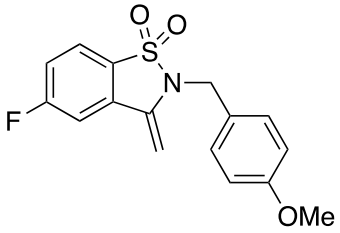
Yellow solid, M.P.: 88.2-90.1 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 – 7.54 (m, 3H), 7.46-7.50 (m, 2H), 7.34-7.38 (m, 3H), 7.26-7.30 (m, 1H), 5.37 (q, J = 7.1 Hz, 1H), 4.82 (d, J = 2.6 Hz, 1H), 4.14 (d, J = 2.6 Hz, 1H), 1.99 (d, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 139.7, 135.1, 133.0, 130.3, 128.8, 127.7, 126.8, 121.3, 121.0, 87.6, 52.2, 17.0. HRMS ($^{+}$ESI) calculated for $C_{16}H_{16}NO_3S$ $[M+H]^+$ 302.0851, found. HRMS ($^{+}$ESI) calculated for $C_{16}H_{16}NO_2S$ $[M+H]^+$ 286.0902, found 286.0935.

2-ethynyl-N-(4-methoxybenzyl)-4-(trifluoromethyl)benzenesulfonamide (**28**)



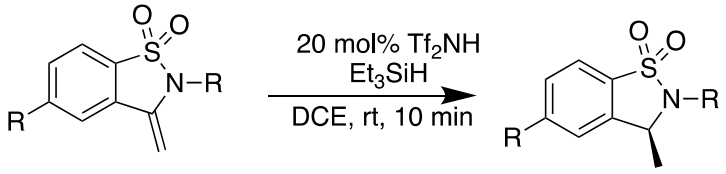
Yellow solid, M.P.: 153.3-155.0 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.00 (d, *J* = 8.1 Hz, 1H), 7.93 (s, 1H), 7.85 (d, *J* = 8.9 Hz, 1H), 7.36 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.6 Hz, 2H), 5.00 (d, *J* = 3.2 Hz, 1H), 4.78 (s, 2H), 4.49 (d, *J* = 3.1 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.4, 136.4, 135.5, 135.2, 134.7, 131.2, 127.4, 127.4, 126.5, 124.2, 122.3, 119.0, 119.0, 114.3, 88.0, 55.4, 44.1. HRMS ($^{+}$ESI) calculated for $C_{17}H_{14}F_3NO_3SNa$ $[M+Na]^+$ 392.0544, found 392.0570.

2-ethynyl-4-fluoro-N-(4-methoxybenzyl)benzenesulfonamide (**29**)



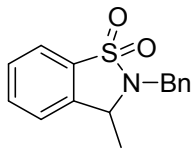
Yellow solid, M.P.: 141.7-143.1 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.86 (dd, *J* = 8.6, 4.7 Hz, 1H), 7.38 – 7.27 (m, 4H), 6.89 (d, *J* = 8.7 Hz, 2H), 4.86 (d, *J* = 2.9 Hz, 1H), 4.75 (s, 2H), 4.41 (d, *J* = 3.0 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.3, 136.7, 128.8, 126.7, 123.7, 123.7, 118.6, 118.4, 114.3, 108.7, 108.5, 87.3, 55.4, 44.1. HRMS ($^{+}$ESI) calculated for $C_{16}H_{15}FNO_3S$ $[M+H]^+$ 320.0757, found 320.0791.

General procedure for the synthesis of sultams from sulfonamides



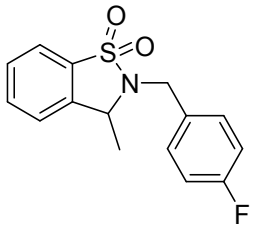
To a solution of compound **23a-23o** (0.125 mmol) in ACS reagent 1,2-DCE (1.25 ml) was added Tf_2NH (7 mg, 0.025 mmol, 20 mol%) and Et_3SiH (40 μl, 0.25 mmol, 2 equiv) sequentially under open air. The reaction mixture was stirred for 10-20 min at room temperature until the reaction was completed via TLC following. After completion of reaction, the solvent was removed under reduced pressure and purified by flash column chromatography over silicone gel (EtOAc/hexane = 10:90-30:70) to produce sultam **24a-24o** as oil or solid.

2-benzyl-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24a**)



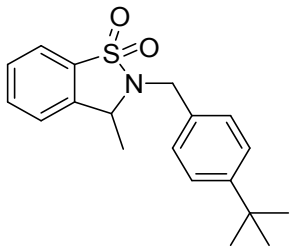
Yield: 90%, white solid, M.P.: 110.1-113.2 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.7 Hz, 1H), 7.60 (td, *J* = 7.6, 1.2 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.47 (d, *J* = 7.4 Hz, 2H), 7.39 – 7.30 (m, 4H), 4.65 (d, *J* = 15.5 Hz, 1H), 4.50 – 4.35 (m, 2H), 1.43 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.2, 135.6, 134.2, 133.0, 129.3, 128.9, 128.7, 128.1, 123.9, 121.4, 55.9, 44.9, 19.3. HRMS ($^{+}$ESI) calculated for $C_{15}H_{16}NO_2S$ $[M+H]^+$ 274.0901, found 274.0917.

2-(4-fluorobenzyl)-3-methyl-2,3-dihydrobenzo[d]isothiazole-1,1-dioxide (**24b**)



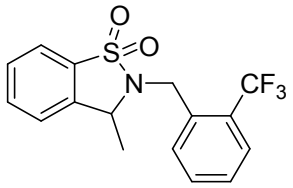
Yield: 98%, white oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.83 (d, J = 7.8 Hz, 1H), 7.61 (td, J = 7.5, 0.9 Hz, 1H), 7.54 (t, J = 7.5 Hz, 1H), 7.45 (dd, J = 8.5, 5.5 Hz, 2H), 7.34 (d, J = 7.5 Hz, 1H), 7.05 (t, J = 8.7 Hz, 1H), 4.60 (d, J = 15.5 Hz, 1H), 4.44 – 4.34 (m, 2H), 1.44 (d, J = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 163.6, 161.6, 139.1, 134.1, 133.0, 131.4, 130.4, 130.4, 123.9, 121.4, 115.8, 115.7, 56.0, 44.3, 19.3. HRMS ($^{+}$ESI) calculated for $C_{15}H_{15}FNO_2S$ $[M+H]^+$ 292.0807, found 292.0825.

2-(4-(tert-butyl)benzyl)-3-methyl-2,3-dihydrobenzo[d]isothiazole-1,1-dioxide (**24c**)



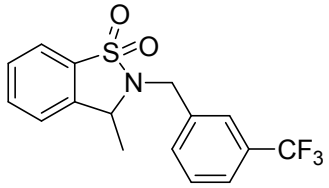
Yield: 76%, white solid, M.P.: 132.1-135.3 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.83 (d, J = 7.7 Hz, 1H), 7.59 (td, J = 7.5, 0.9 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.38 (d, J = 3.5 Hz, 4H), 7.32 (d, J = 7.7 Hz, 1H), 4.66 (d, J = 15.4 Hz, 1H), 4.40 (q, J = 6.5 Hz, 1H), 4.34 (d, J = 15.4 Hz, 1H), 1.45 (d, J = 6.5 Hz, 3H), 1.31 (s, 9H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 151.1, 139.3, 134.3, 132.3, 129.2, 128.5, 125.8, 123.9, 121.4, 55.6, 44.3, 34.7, 31.4, 19.3. HRMS ($^{+}$ESI) calculated for $C_{19}H_{24}NO_2S$ $[M+H]^+$ 330.1527, found 330.1545.

3-methyl-2-(2-(trifluoromethyl)benzyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24d**)



Yield: 81%, white solid, M.P.: 65.5-67.7 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.85 (t, J = 8.3 Hz, 2H), 7.72 – 7.60 (m, 2H), 7.55 (dt, J = 12.7, 7.7 Hz, 2H), 7.38 (dd, J = 13.0, 7.8 Hz, 2H), 4.83 (d, J = 17.3 Hz, 1H), 4.64 (d, J = 17.3 Hz, 1H), 4.52 (q, J = 6.6 Hz, 1H), 1.38 (d, J = 6.5 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 139.0, 134.0, 133.2, 132.4, 130.0, 129.4, 127.7, 125.9, 125.9, 123.9, 121.5, 57.6, 41.5, 19.5. HRMS ($^{+}$ESI) calculated for $C_{16}H_{15}F3NO_2S$ $[M+H]^+$ 342.0775, found 342.0796.

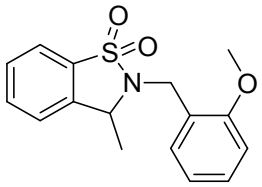
3-methyl-2-(3-(trifluoromethyl)benzyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24e**)



Yield: 82%, white solid, M.P.: 80.6-83.3 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.85 (d, J = 7.8 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.63 (td, J = 7.4, 0.8 Hz, 1H),

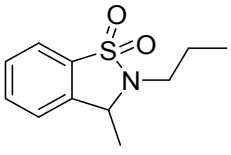
7.57 (q, J = 7.6 Hz, 2H), 7.50 (t, J = 7.9 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 4.63 (d, J = 15.9 Hz, 1H), 4.53 (d, J = 15.9 Hz, 1H), 4.42 (q, J = 6.6 Hz, 1H), 1.45 (d, J = 6.5 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 138.9, 137.0, 134.0, 133.2, 132.0, 131.1, 129.5, 129.4, 125.1, 125.1, 125.1, 125.0, 125.0, 125.0, 121.5, 56.5, 19.4. HRMS ($^{+}$ESI) calculated for $C_{16}H_{15}F3NO_2S$ $[M+H]^+$ 342.0775, found 342.0797.

2-(4-methoxybenzyl)-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24f**)



Yield: 75%, white solid, M.P.: 67.3-68.5 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.59 (td, *J* = 7.6, 1.1 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 2H), 7.34 (d, J = 8.4 Hz, 1H), 7.32 – 7.23 (m, 1H), 6.95 (td, J = 7.5, 0.9 Hz, 1H), 6.90 (d, J = 8.2 Hz, 1H), 4.67 (d, J = 15.9 Hz, 1H), 4.52 (d, J = 15.9 Hz, 1H), 4.47 (q, J = 6.5 Hz, 1H), 3.88 (s, 3H), 1.48 (d, J = 6.6 Hz, 3H). 13C NMR (126 MHz, Chloroform-d) δ 157.5, 139.5, 134.4, 132.8, 130.5, 129.2, 129.1, 124.1, 123.8, 121.4, 120.9, 110.4, 56.7, 55.5, 39.0, 19.5. HRMS ($^{+}$ESI) calculated for $C_{16}H_{18}NO_3S$ $[M+H]^+$ 304.1007, found 304.1028.

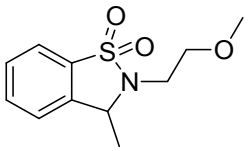
3-methyl-2-propyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24g**)



Yield: 68%, yellow-dish oil. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 (d, J = 7.8 Hz, 1H), 7.61 (td, J = 7.5, 0.8 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.39 (d, J = 7.9 Hz, 1H), 4.50 (q, J = 6.5 Hz, 1H), 3.33 (ddd, J = 14.1, 8.1, 6.1 Hz, 1H), 3.28 – 3.20 (m, 1H), 1.81 (hd, J = 7.2, 2.2 Hz, 2H), 1.55 (d, J = 6.5 Hz, 3H), 1.02 (t, J

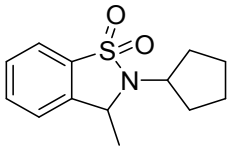
= 7.4 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 139.3, 134.6, 132.9, 129.2, 123.8, 121.3, 56.8, 43.8, 21.8, 19.3. HRMS ($^{+}$ESI) calculated for $C_{11}H_{15}NO_2SNa$ $[M+Na]^+$ 248.0721, found 248.0736.

2-(2-methoxyethyl)-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24h**)



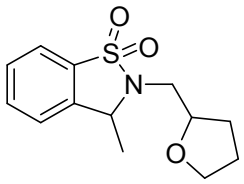
Yield: 87%, colorless oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 7.7 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 4.71 (q, 1H), 3.79 – 3.73 (m, 1H), 3.68 (dt, *J* = 10.0, 4.8 Hz, 1H), 3.55 (t, *J* = 5.4 Hz, 2H), 3.39 (s, 3H), 1.57 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.6, 134.2, 132.9, 129.1, 123.8, 121.3, 71.9, 59.1, 57.6, 41.1, 19.2. HRMS ($^{+}$ESI) calculated for $C_{11}H_{16}NO_3S$ $[M+H]^+$ 242.0850, found 242.0865.

2-cyclopentyl-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24i**)



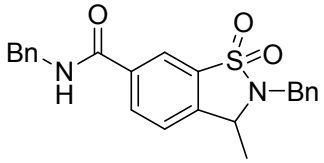
Yield: 83%, white solid, M.P.: 78.1-80.8 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 7.8 Hz, 1H), 7.63 – 7.57 (m, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 4.63 (q, *J* = 6.5 Hz, 1H), 3.85 (ddd, *J* = 16.0, 8.8, 7.2 Hz, 1H), 2.22 – 2.10 (m, 2H), 2.09 – 1.99 (m, 1H), 1.91 – 1.75 (m, 3H), 1.70 – 1.61 (m, 2H), 1.58 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.7, 135.1, 132.8, 129.1, 123.7, 121.2, 56.7, 56.2, 31.2, 29.8, 23.6, 22.8, 21.2. HRMS ($^{+}$ESI) calculated for $C_{13}H_{18}NO_2S$ $[M+H]^+$ 252.1058, found 252.1071.

3-methyl-2-((tetrahydrofuran-2-yl)methyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24j**)



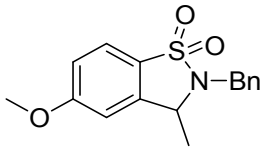
Yield: 48%, colorless oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 4.91 (q, *J* = 6.5 Hz, 1H), 4.24 (qd, *J* = 7.4, 3.3 Hz, 1H), 3.92 (q, *J* = 7.4 Hz, 1H), 3.79 (q, *J* = 7.5 Hz, 1H), 3.58 (dd, *J* = 11.1, 5.0 Hz, 1H), 3.27 (dd, *J* = 15.1, 7.8 Hz, 1H), 2.14 – 2.07 (m, 1H), 2.00 – 1.84 (m, 2H), 1.69 – 1.60 (m, 1H), 1.56 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.9, 134.1, 132.8, 129.0, 123.9, 121.2, 78.9, 68.6, 57.0, 44.8, 29.8, 25.5, 18.9. HRMS ($^{+}$ESI) calculated for $C_{13}H_{18}NO_3S$ $[M+H]^+$ 268.1007, found 268.1023.

N,2-dibenzyl-3-methyl-2,3-dihydrobenzo[d]isothiazole-6-carboxamide 1,1-dioxide (**24k**)



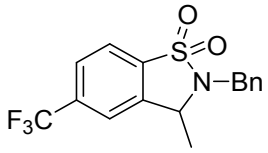
Yield: 87%, white foam. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 1.1 Hz, 1H), 8.15 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.43 – 7.29 (m, 9H), 7.28 – 7.21 (m, 1H), 7.11 (t, *J* = 5.6 Hz, 1H), 4.62 (d, *J* = 5.6 Hz, 2H), 4.52 (d, *J* = 15.5 Hz, 1H), 4.40 (q, *J* = 6.6 Hz, 1H), 4.29 (d, *J* = 15.5 Hz, 1H), 1.40 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.3, 142.1, 137.9, 135.9, 135.2, 134.4, 132.8, 128.9, 128.9, 128.6, 128.2, 127.9, 127.7, 124.4, 119.6, 55.9, 44.8, 44.3, 19.1. HRMS ($^{+}$ESI) calculated for $C_{23}H_{23}N_2O_3S$ $[M+H]^+$ 407.1429, found 407.1451.

2-benzyl-5-methoxy-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24l**)



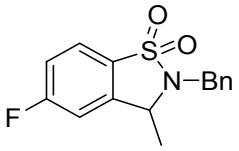
Yield: 92%, white solid, M.P.: 112.3-115.1 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.6 Hz, 1H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.36 (dd, *J* = 8.0, 6.5 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.03 (dd, *J* = 8.7, 2.2 Hz, 1H), 6.74 (d, *J* = 2.1 Hz, 1H), 4.60 (d, *J* = 15.4 Hz, 1H), 4.40 (d, *J* = 15.4 Hz, 1H), 4.34 (q, *J* = 6.6 Hz, 1H), 3.85 (s, 3H), 1.41 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.4, 141.7, 135.7, 128.8, 128.0, 126.3, 123.0, 115.8, 108.3, 55.9, 55.9, 45.1, 19.4. HRMS ($^+$ESI) calculated for $C_{16}H_{18}NO_3S$ $[M+H]^+$ 304.1007, found 304.1039.

2-benzyl-3-methyl-5-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24m**)



Yield: 98%, colorless oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.81 (d, *J* = 8.3 Hz, 1H), 7.60 (s, 1H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.40 – 7.31 (m, 3H), 4.68 (d, *J* = 15.4 Hz, 1H), 4.48 – 4.39 (m, 2H), 1.48 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.2, 137.7, 135.1, 135.0, 134.8, 129.0, 128.7, 128.3, 126.5, 124.3, 122.4, 122.1, 121.3, 55.7, 44.9, 19.1. HRMS ($^+$ESI) calculated for $C_{16}H_{14}F_3NO_2SNa$ $[M+Na]^+$ 364.0595, found 364.0626.

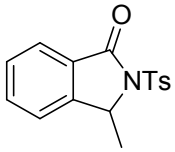
2-benzyl-5-fluoro-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**24n**)



Yield: 85%, white solid, M.P.: 113.7-116.0 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.83 (dd, *J* = 8.6, 4.8 Hz, 1H), 7.46 (d, *J* = 7.3 Hz, 2H), 7.39 – 7.30 (m, 3H), 7.23 (td, *J* = 8.6, 2.2 Hz, 1H), 7.00 (dd, *J* = 8.2, 2.1 Hz, 1H), 4.63 (d, *J* = 15.4 Hz, 1H), 4.43 – 4.34 (m, 2H), 1.42 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (126 MHz,

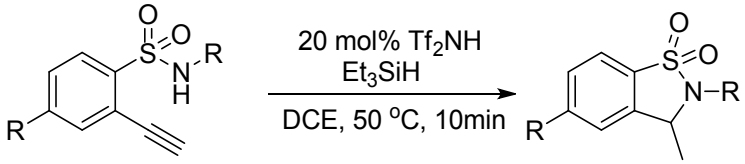
Chloroform-*d*) δ 166.4, 164.4, 142.4, 142.3, 135.3, 130.3, 128.9, 128.7, 128.2, 123.9, 123.8, 117.2, 111.3, 111.1, 55.6, 45.1, 19.2. HRMS ($^+$ESI) calculated for $C_{15}H_{15}FNO_2S$ $[M+H]^+$ 292.0808, found 292.0829.

3-methyl-2-tosylisoindolin-1-one (**24o**)



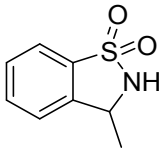
Yield: 90%, white solid, M.P.: 132.0-131.7 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.04 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.45 (dd, *J* = 17.7, 7.6 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 5.31 (q, *J* = 6.5 Hz, 1H), 2.42 (s, 3H), 1.79 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.4, 147.4, 145.0, 136.2, 134.0, 129.6, 128.8, 128.2, 124.9, 122.5, 58.7, 21.7, 21.5. HRMS ($^+$ESI) calculated for $C_{16}H_{16}NO_3S$ $[M+H]^+$ 302.0851, found 302.0879.

General procedure for the synthesis of free amide sultams from sulfonamides



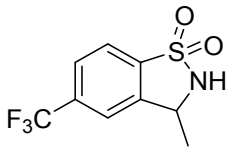
To a solution of compound **19-24** (0.125 mmol) in ACS reagent 1,2-DCE (1.25 ml) was added Tf_2NH (7 mg, 0.025 mmol, 20 mol%) and Et_3SiH (40 μl, 0.25 mmol, 2 equiv) sequentially under open air. The reaction mixture was stirred for 10-20 min at 50 ^{o}C until the reaction was completed via TLC following. After completion of reaction, the solvent was removed under reduced pressure and purified by flash column chromatography over silicone gel (EtOAc/hexane = 10:90-30:70) to produce sultam **25-27** as oil or solid.

3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (know compound **30**)



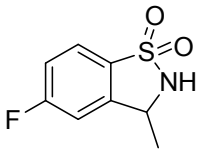
Yield: 67-98%, white solid, M.P.: 63.0-65.2 °C. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 (d, J = 7.8 Hz, 1H), 7.63 (td, J = 7.6, 1.1 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.42 – 7.38 (m, 1H), 4.87 (s, 1H), 4.80 (p, J = 6.5 Hz, 1H), 1.62 (d, J = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 141.8, 135.6, 133.3, 129.3, 124.0, 121.3, 53.5, 21.5.

3-methyl-5-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**31**)



Yield: 96%, white solid, M.P.: 116.4-118.7 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.1 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.67 (s, 1H), 5.00 (s, 1H), 4.85 (p, J = 6.5 Hz, 1H), 1.67 (d, J = 6.8 Hz, 3H). 13C NMR (126 MHz, Chloroform-d) δ 142.8, 139.0, 129.5, 126.68, 122.3, 121.4, 114.3, 53.4, 21.3. HRMS ($^{+}$ESI) calculated for $C_9H_8F_3NO_2SNa$ $[M+Na]^+$ 274.0126, found 274.0152.

5-fluoro-3-methyl-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide (**32**)



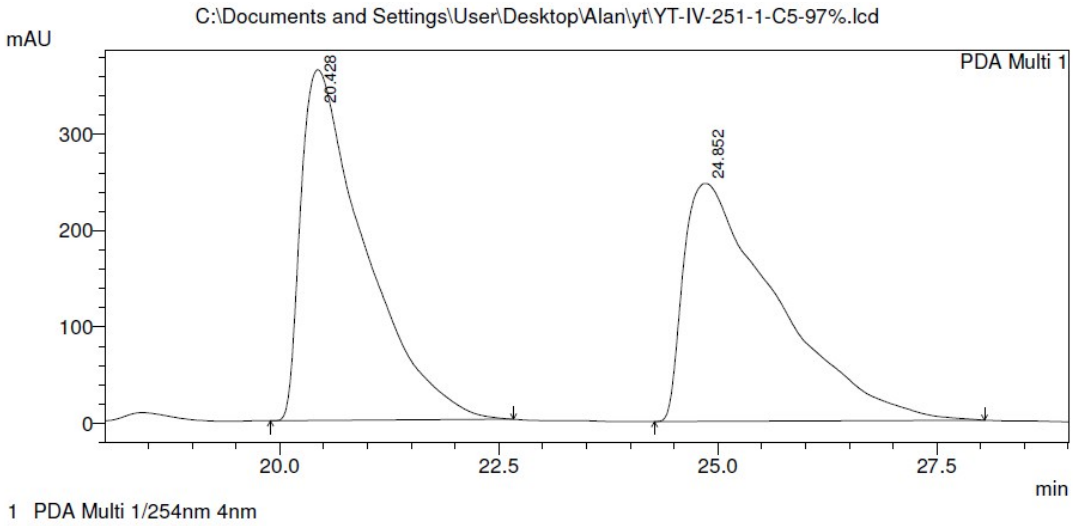
Yield: 90%, white solid, M.P.: 106.1-108.1 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 (dd, *J* = 8.6, 4.8 Hz, 1H), 7.22 (td, *J* = 8.5, 2.2 Hz, 1H), 7.07 (dd, *J* = 8.2, 2.0 Hz, 1H), 5.00 (s, 1H), 4.81 – 4.72 (m, 1H), 1.61 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.7 (d, *J* = 255.1 Hz), 145.1 (d, *J* = 8.8 Hz), 131.7 (d, *J* = 1.9 Hz), 123.7 (d, *J* = 9.8 Hz), 117.3 (d, *J* = 24.4 Hz), 111.2 (d, *J* =

23.7 Hz), 53.1 (d, J = 1.6 Hz), 21.4. HRMS ($^{+}$ESI) calculated for $C_8H_9FNO_2S$ $[M+H]^+$ 202.0338, found 202.0359.

References:

1) Zhang, S.; Cheng, B.; Wang, S-A.; Zhou, L.; Tung, C-H.; Wang, J.; Xu, Z. *Org. Lett*. **2017**, *19*, 1072-1075.
2) Fustero, S.; Moscardo, J.; Sanchez-Rosello, M.; Rodriguez, Elsa.; Barrio, P. *Org. Lett*. **2010**, *12*, 5494-5497.
3) Liu, G.; Cogan, D. A.; Ellman, J. A. *J. Am. Chem. Soc*. **1997**, *119*, 9913-9914.

Compound **22c**

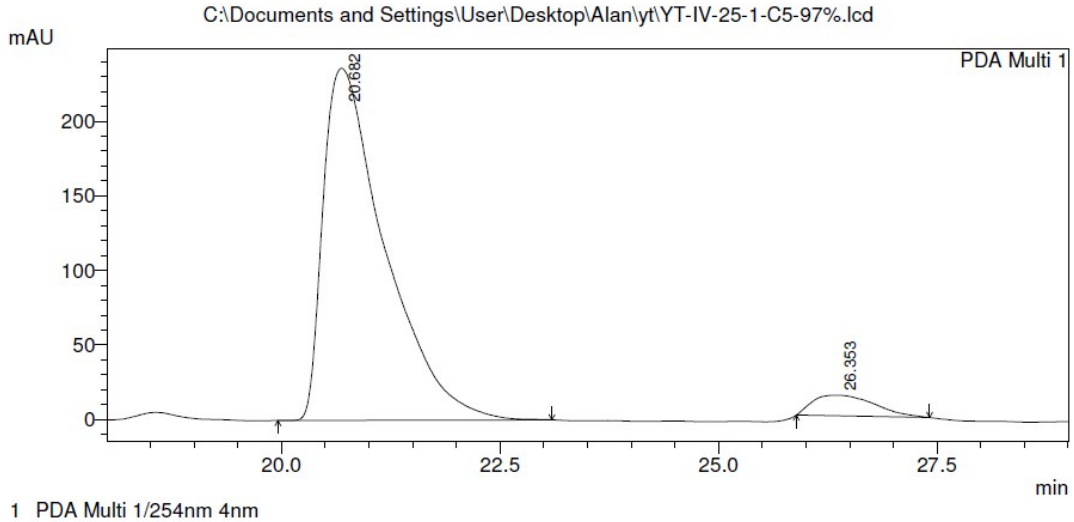


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.428	18577047	363987	50.331	59.566
2	24.852	18332894	247079	49.669	40.434
Total		36909941	611066	100.000	100.000



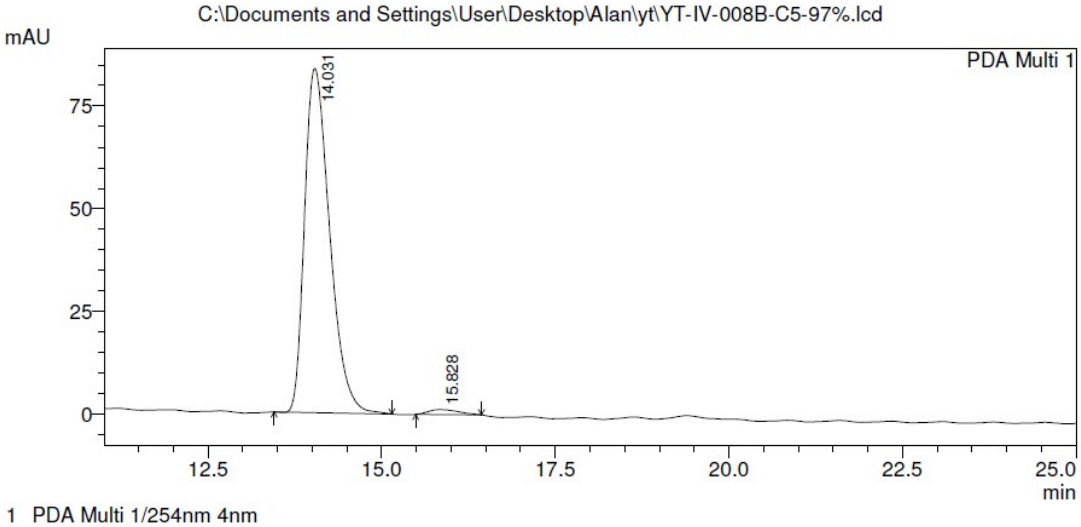
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.682	11611729	236201	94.439	94.462
2	26.353	683757	13847	5.561	5.538
Total		12295486	250048	100.000	100.000

Compound **22a**



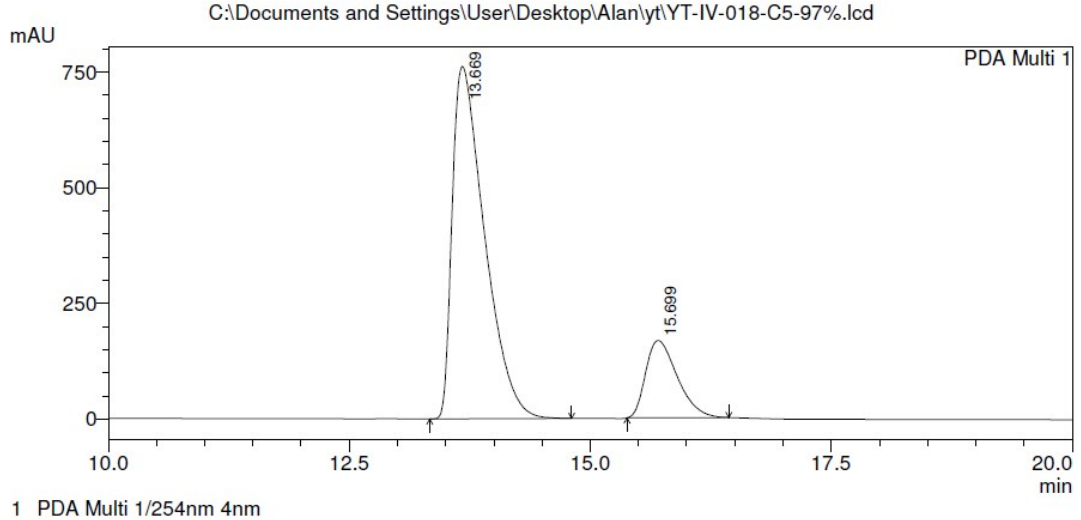
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.031	2108201	83772	97.962	98.143
2	15.828	37196	1254	1.728	1.469
3	29.726	6674	331	0.310	0.388
Total		2152071	85357	100.000	100.000

Compound **22b**



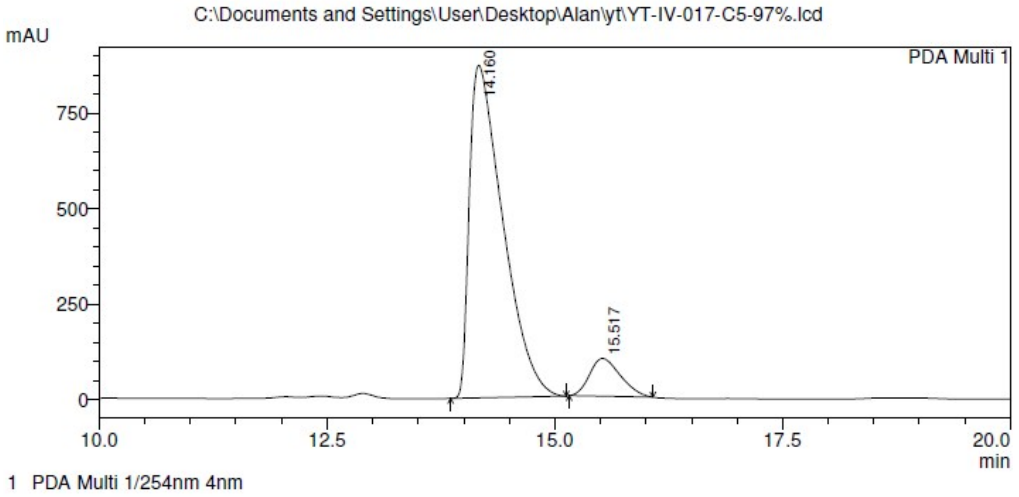
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.669	17750290	761320	82.300	81.990
2	15.699	3817577	167230	17.700	18.010
Total		21567867	928550	100.000	100.000

Compound **22f**

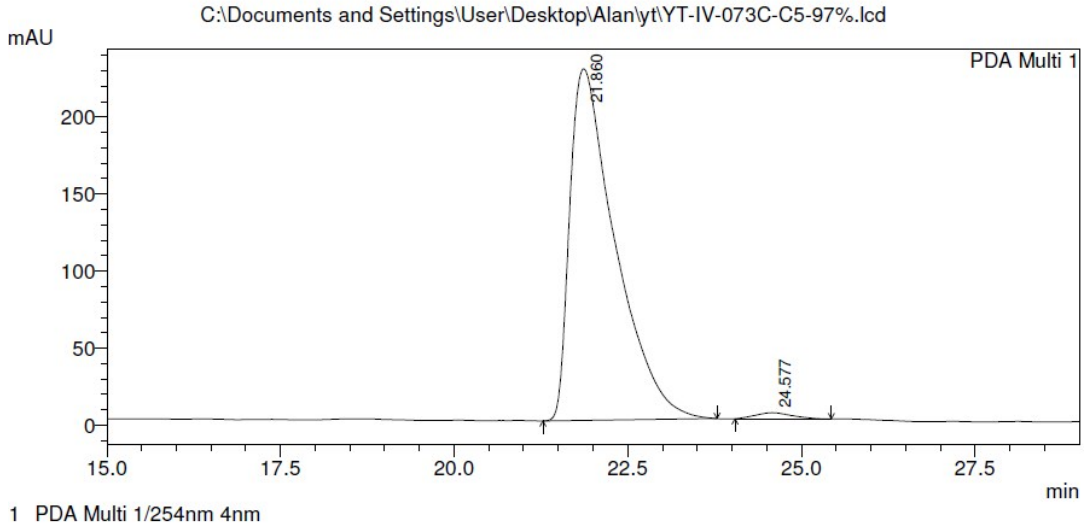


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.160	22239902	870133	90.467	89.780
2	15.517	2343630	99054	9.533	10.220
Total		24583532	969187	100.000	100.000

Compound **22g**

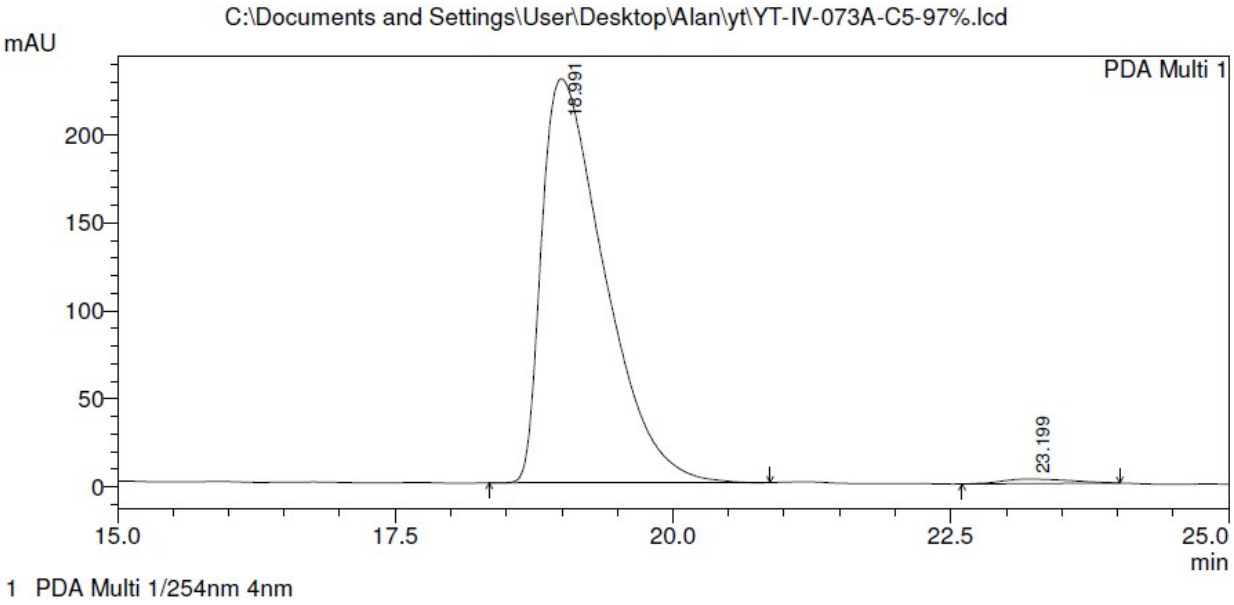


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.860	10397195	228038	98.693	98.349
2	24.577	137703	3827	1.307	1.651
Total		10534898	231865	100.000	100.000

Compound **22i**

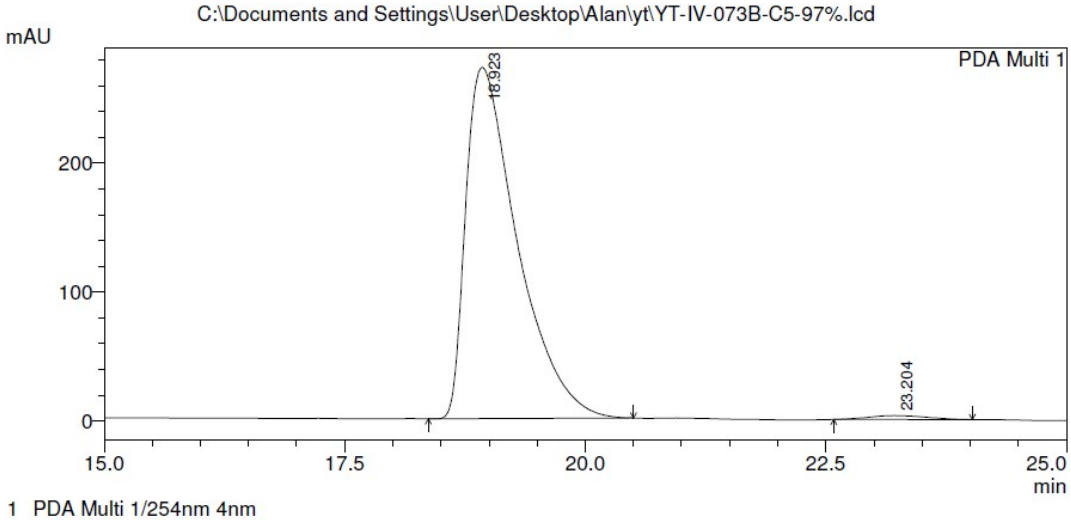


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.991	9005841	229760	98.796	98.848
2	23.199	109761	2679	1.204	1.152
Total		9115602	232438	100.000	100.000

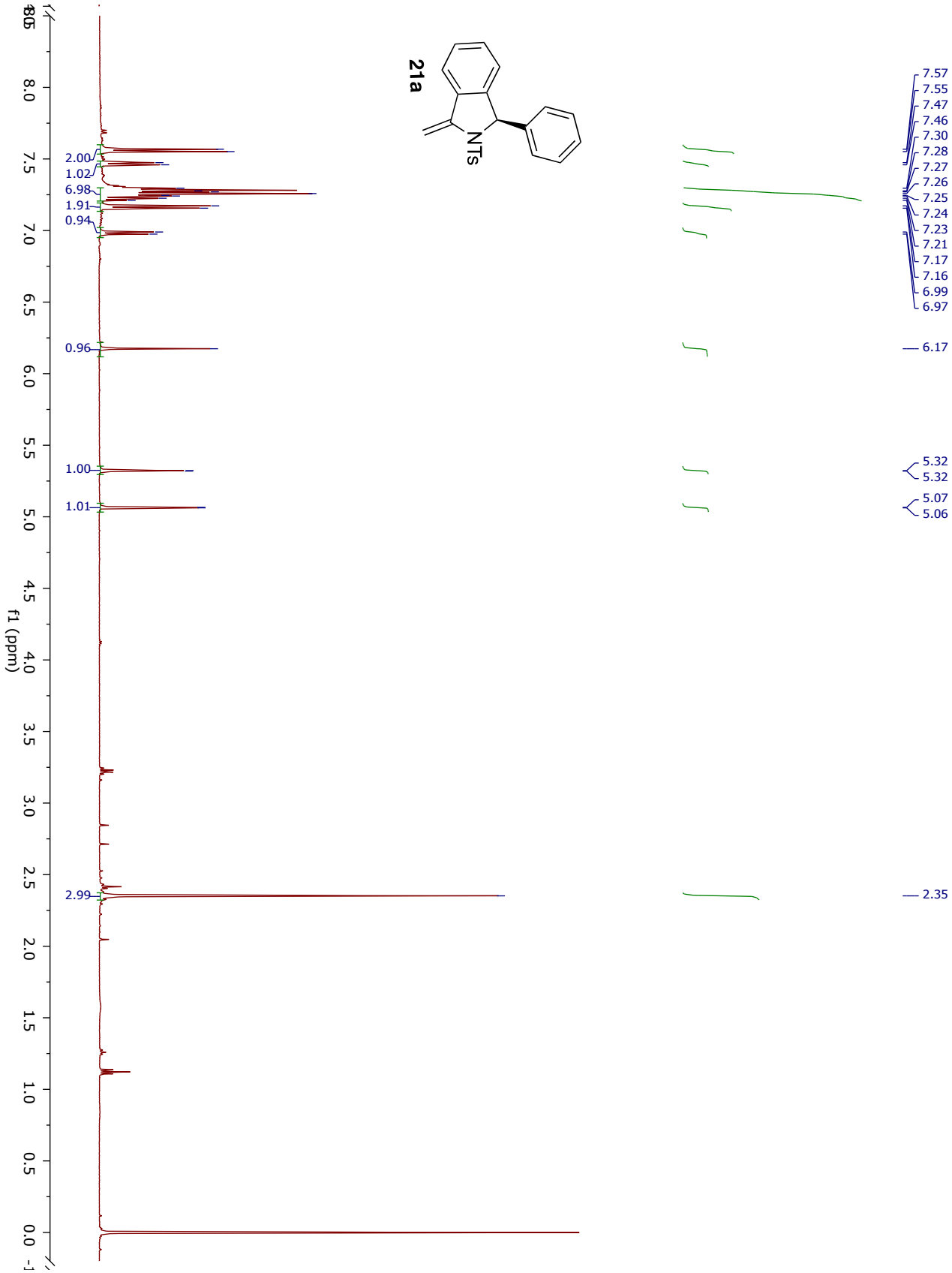
Compound **22j**

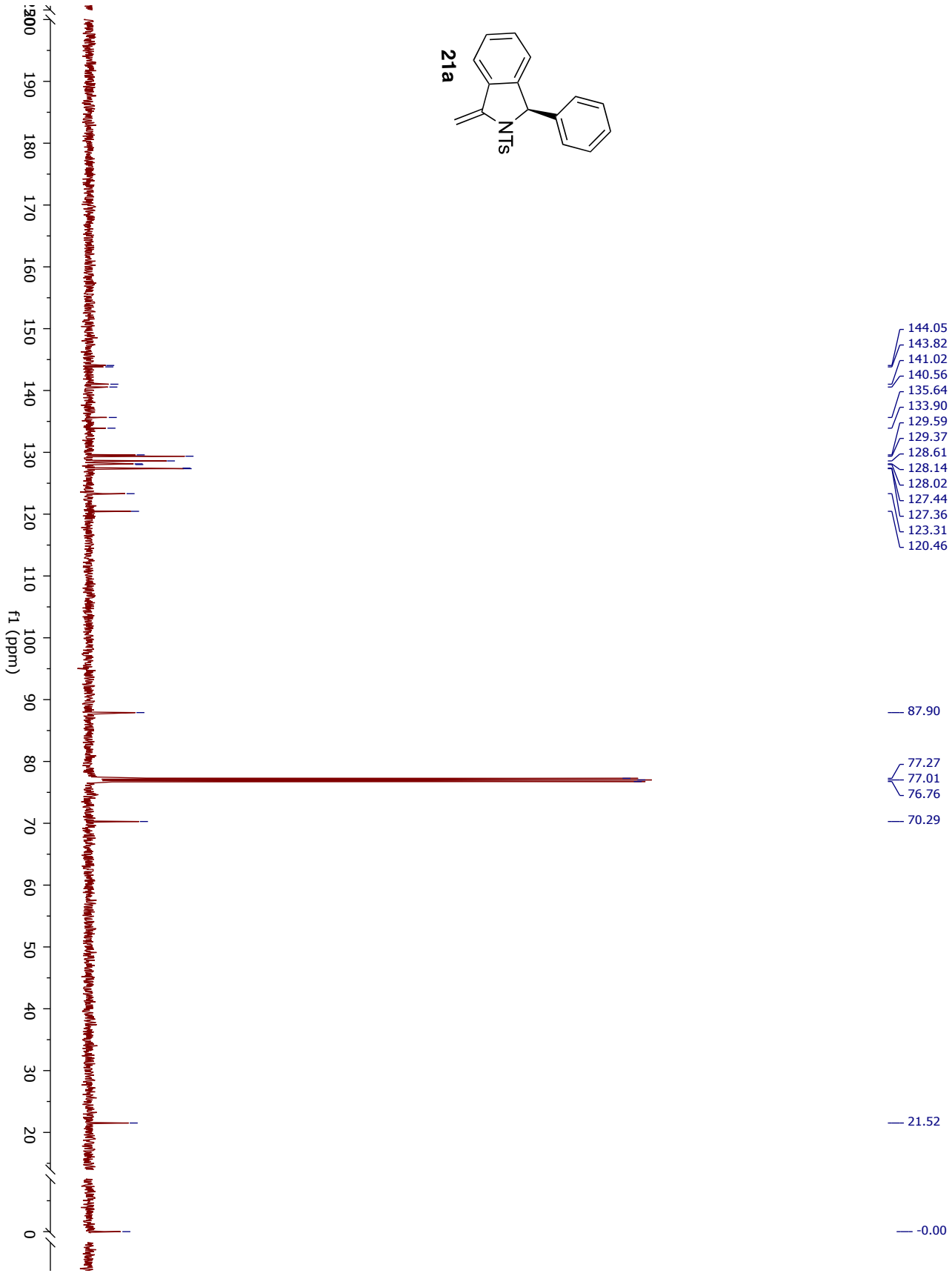


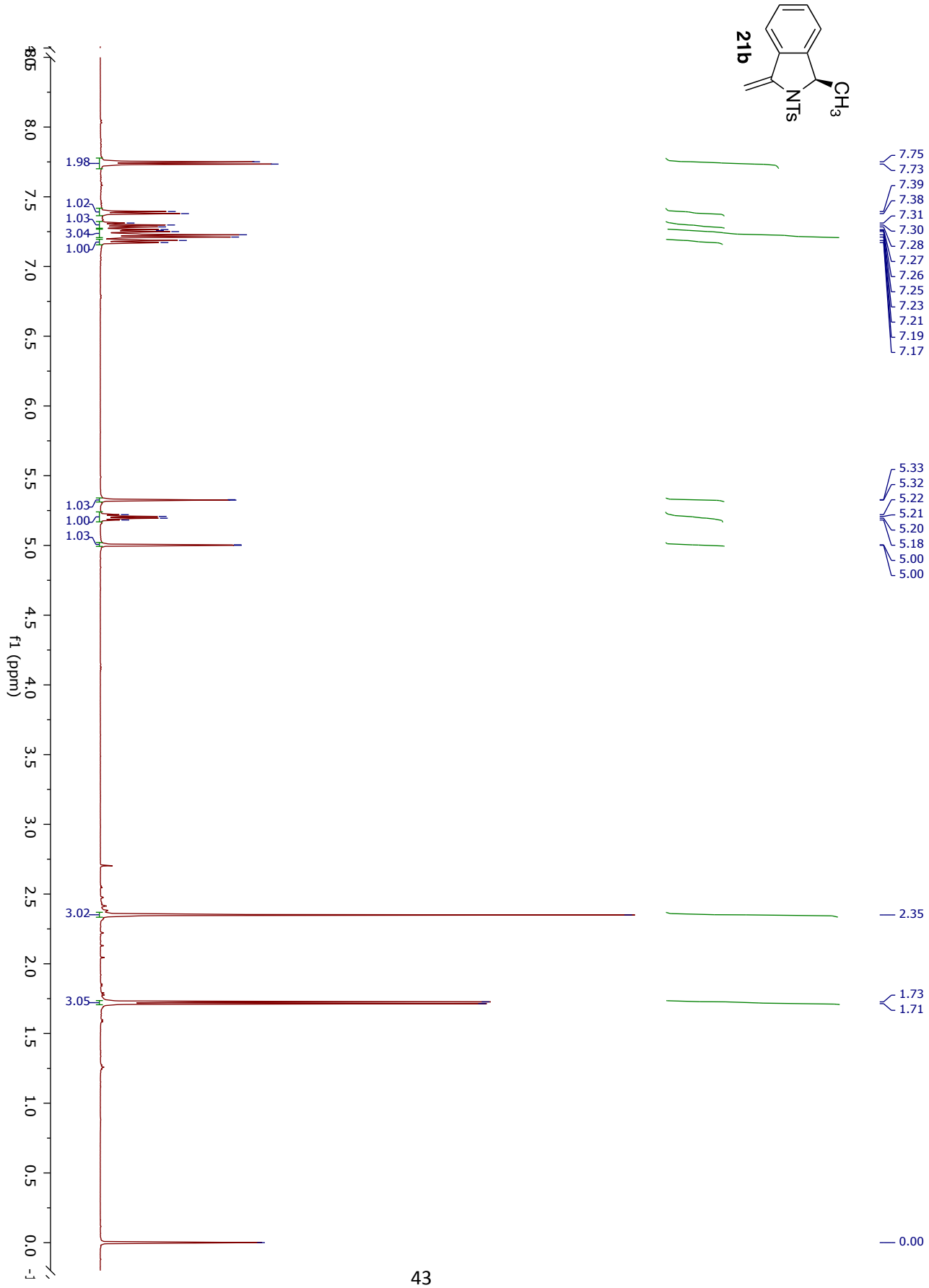
PeakTable

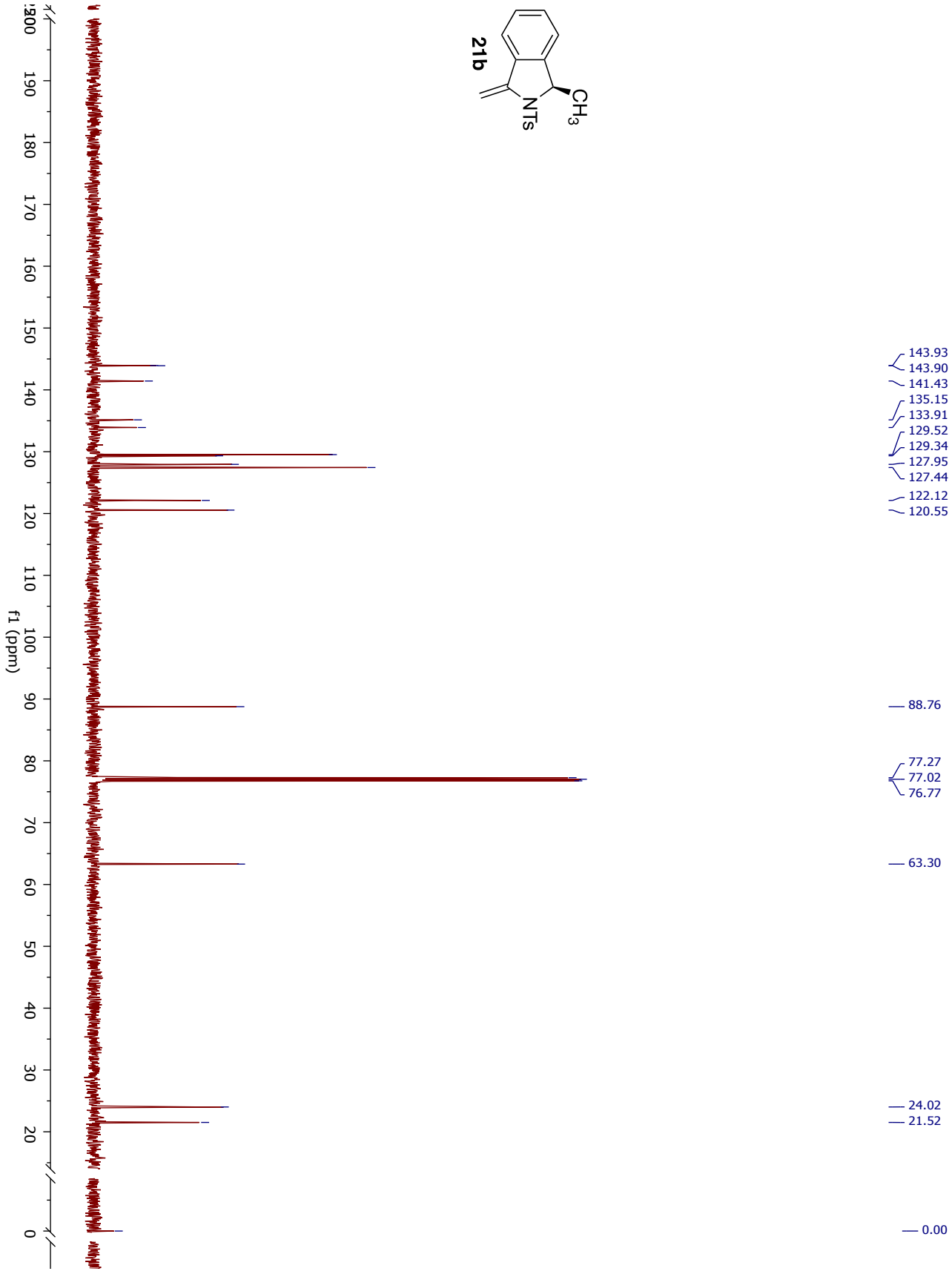
PDA Ch1 254nm 4nm

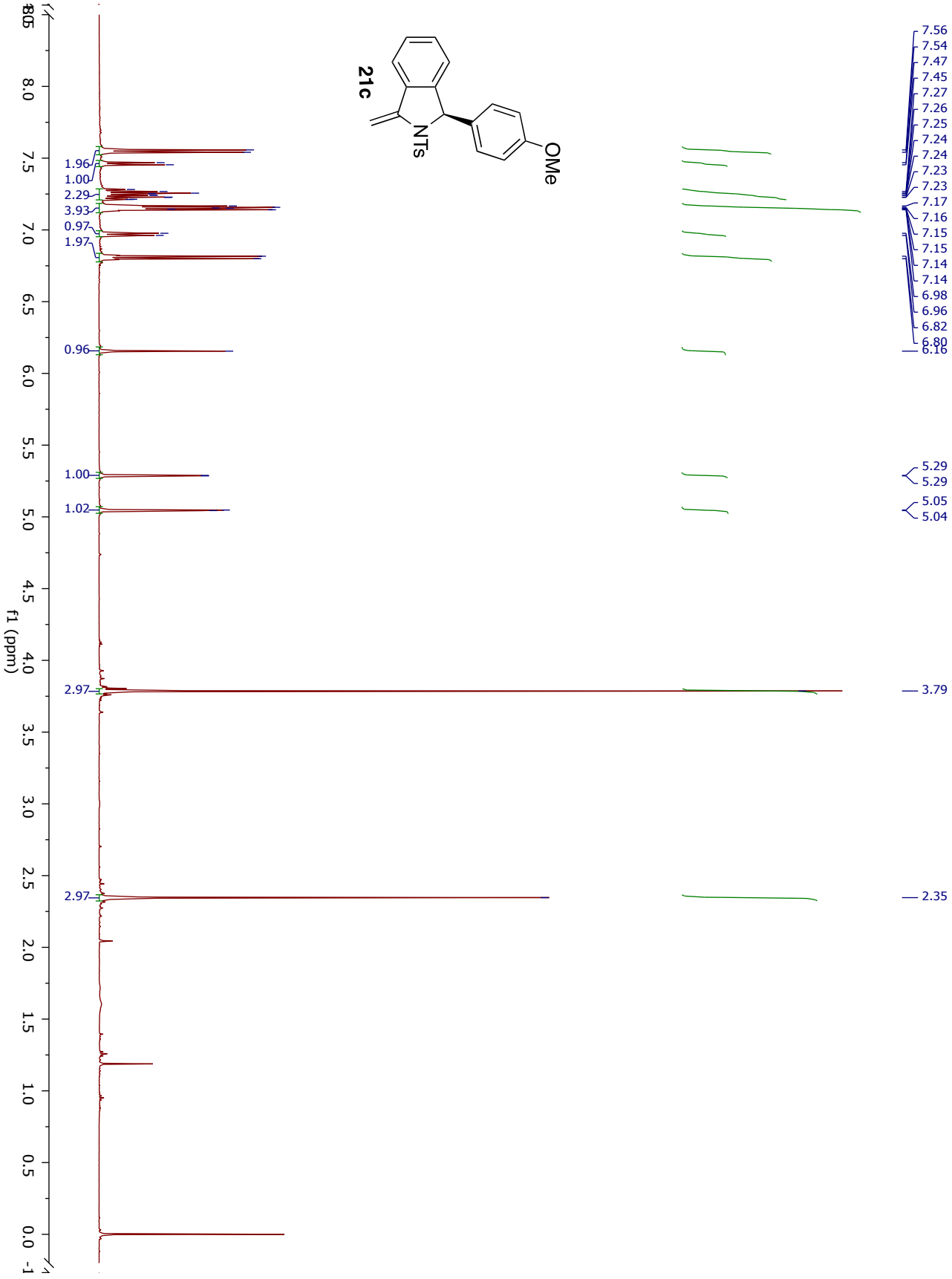
Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.923	10182403	272408	98.791	98.921
2	23.204	124589	2971	1.209	1.079
Total		10306992	275379	100.000	100.000

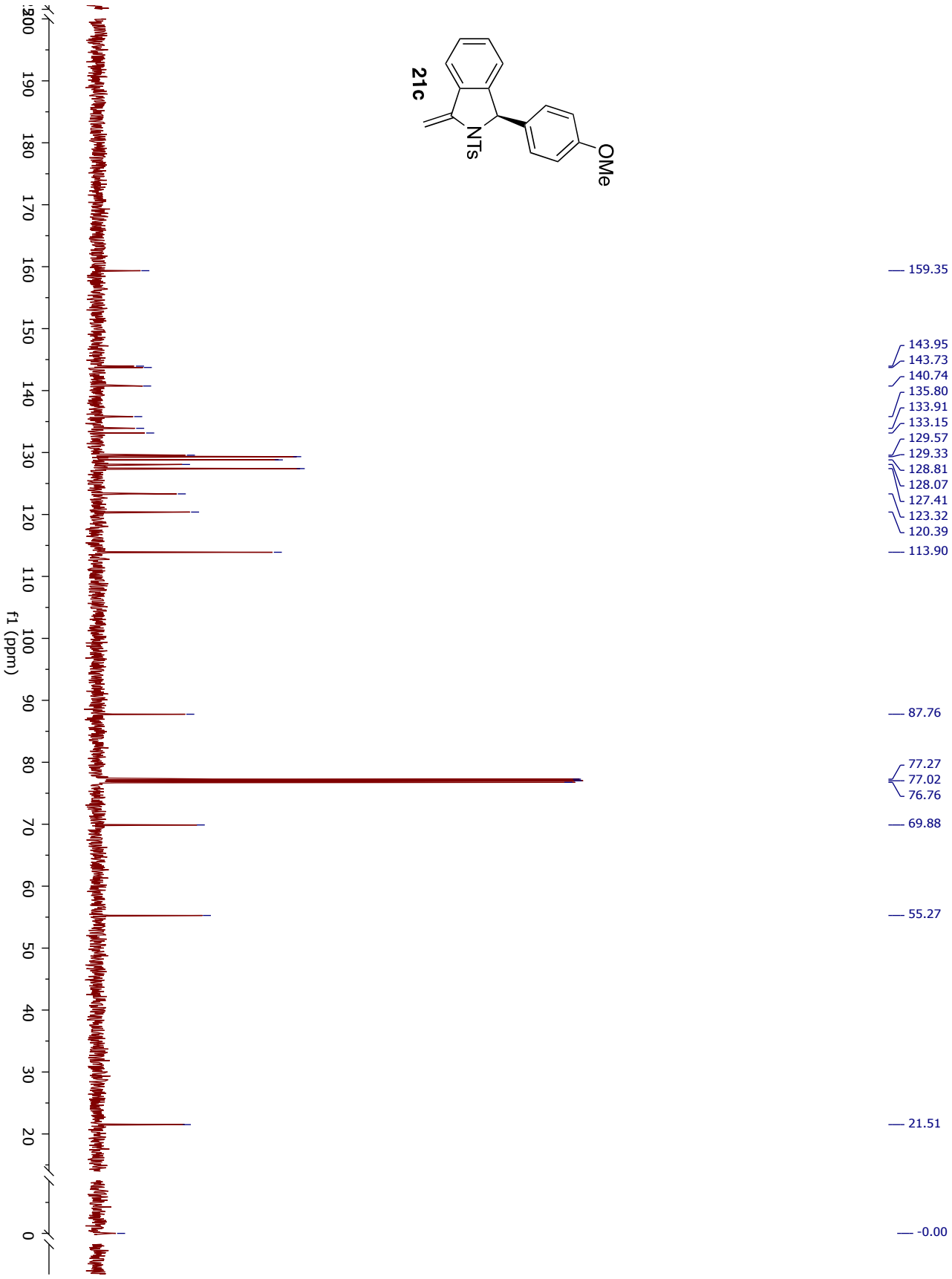

21a
NTs
2.00
1.02
6.98
1.91
0.94
0.96
1.00
1.01
2.99
7.57
7.55
7.47
7.46
7.30
7.28
7.27
7.26
7.25
7.24
7.23
7.21
7.17
7.16
6.99
6.97
6.17
5.32
5.32
5.07
5.06
2.35
f1 (ppm)

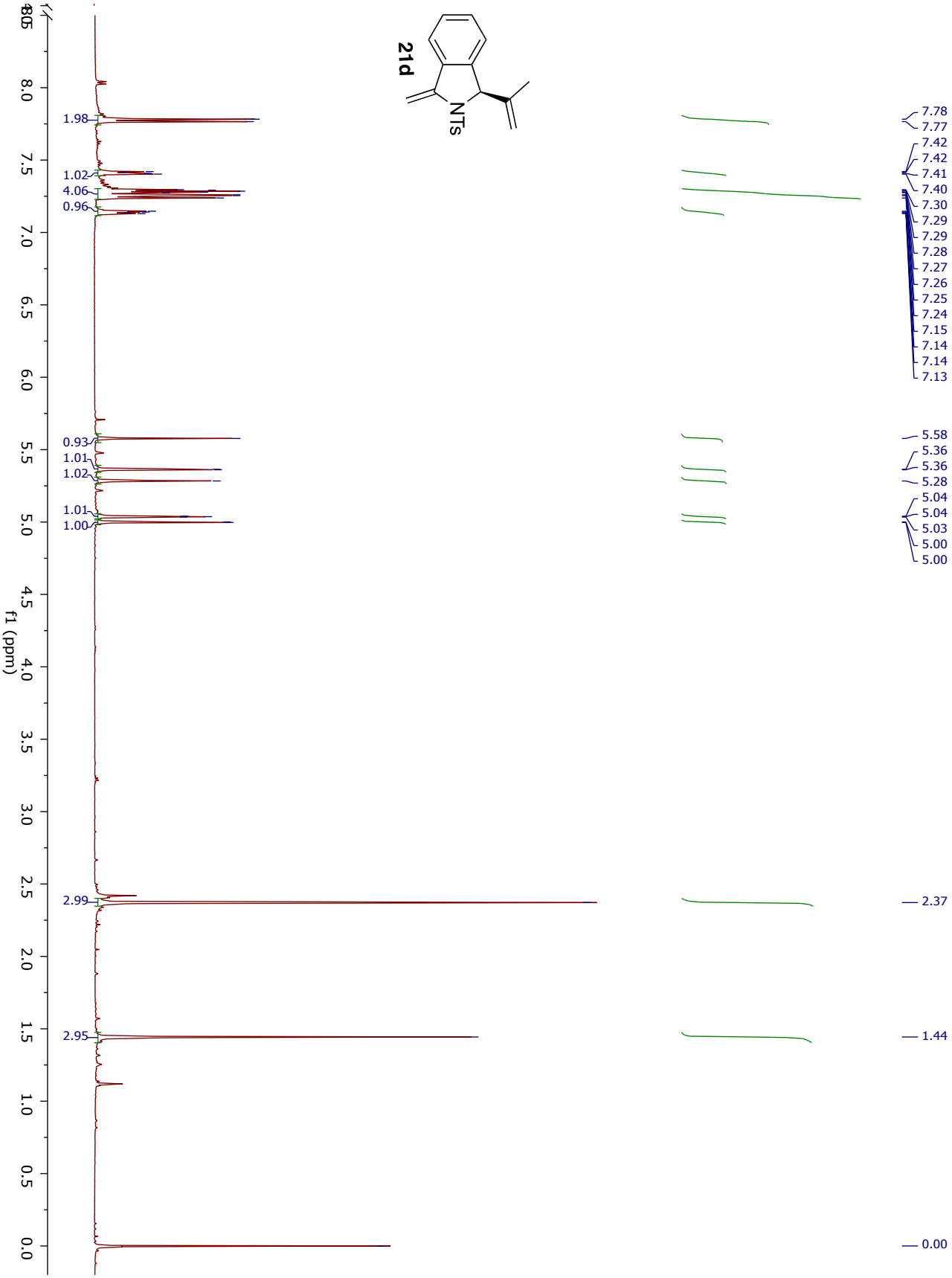

21a
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
144.05
143.82
141.02
140.56
135.64
133.90
129.59
129.37
128.61
128.14
128.02
127.44
127.36
123.31
120.46
87.90
77.27
77.01
76.76
70.29
21.52
-0.00

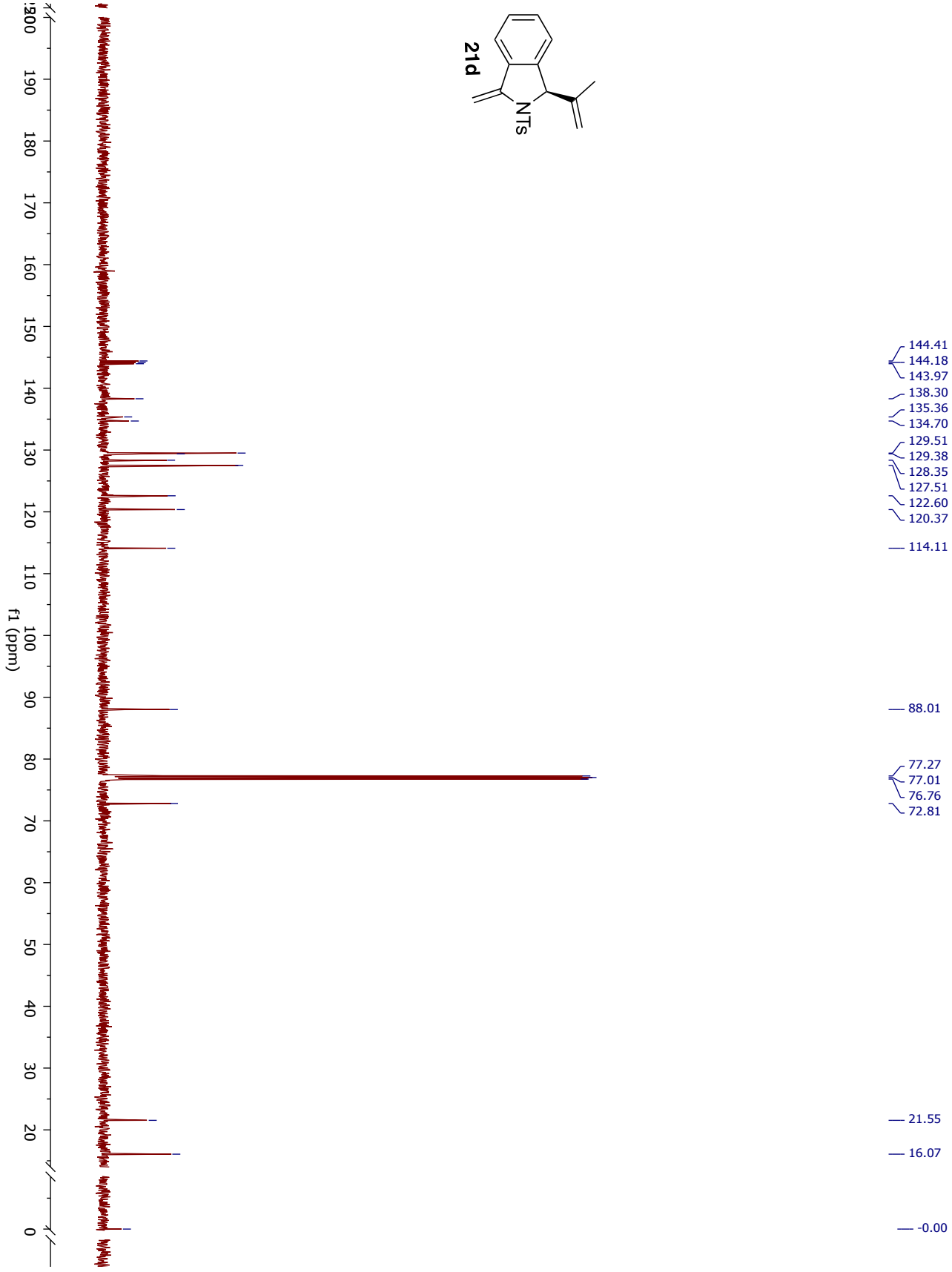

21b
NTs
CH3
f1 (ppm)
1.98
1.02
1.03
3.04
1.00
1.03
1.00
1.03
3.02
3.05
7.75
7.73
7.39
7.38
7.31
7.30
7.28
7.27
7.26
7.25
7.23
7.21
7.19
7.17
5.33
5.32
5.22
5.21
5.20
5.18
5.00
5.00
2.35
1.73
1.71
0.00

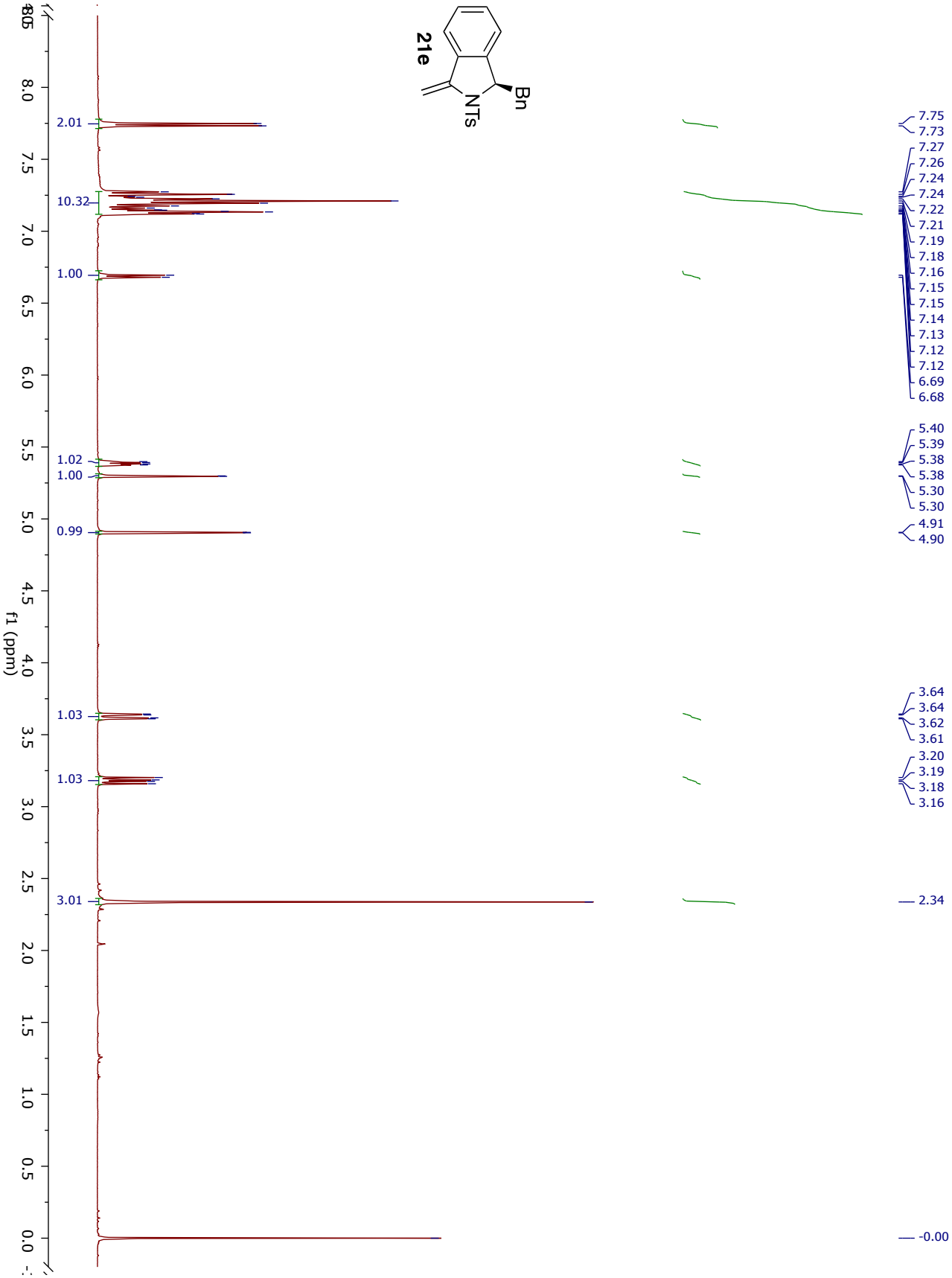

21b
NTs
CH3
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
143.93
143.90
141.43
135.15
133.91
129.52
129.34
127.95
127.44
122.12
120.55
88.76
77.27
77.02
76.77
63.30
24.02
21.52
0.00

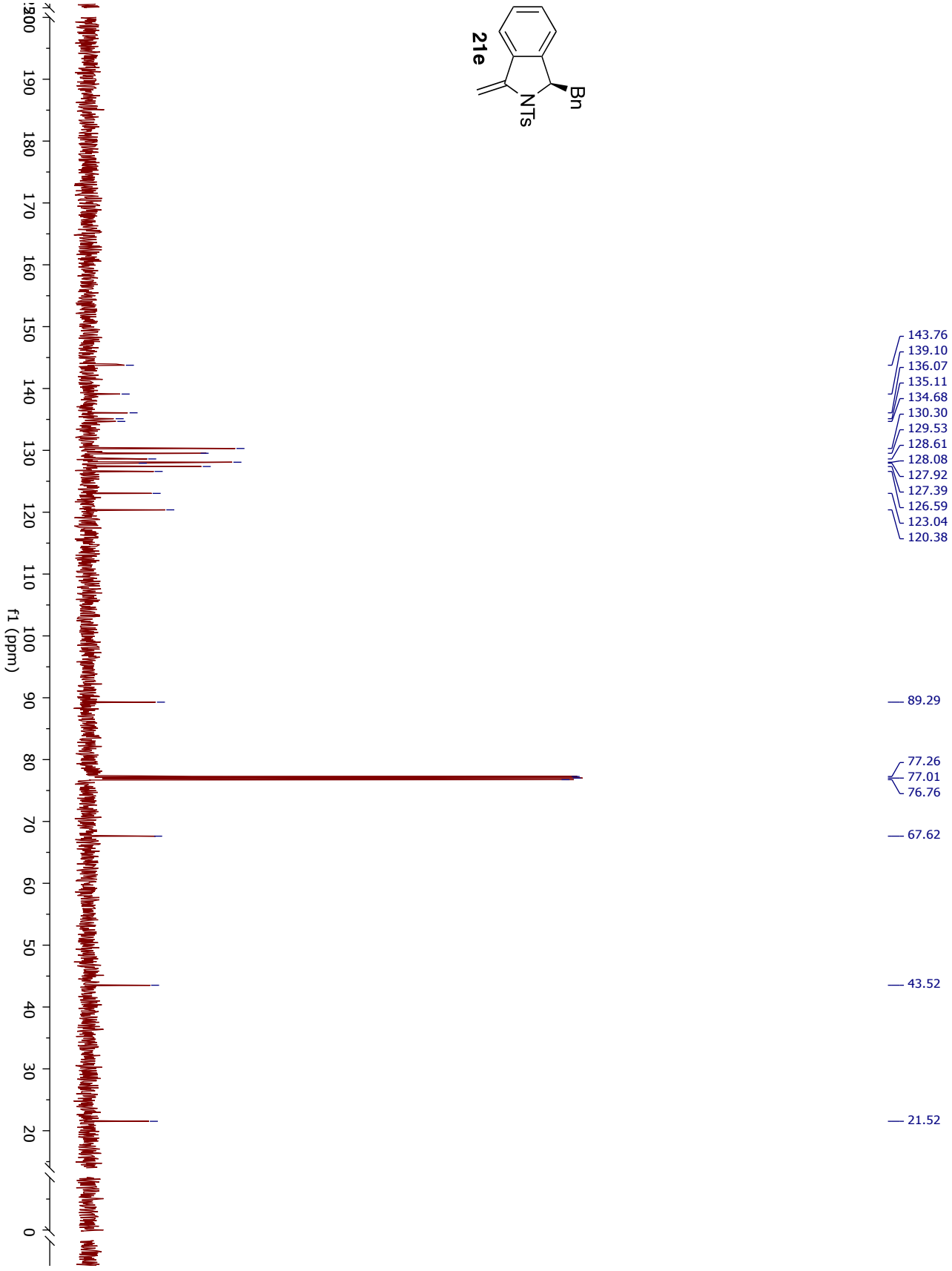

21c
NTs
OMe
f1 (ppm)
1.96
1.00
2.29
3.93
0.97
1.97
0.96
1.00
1.02
2.97
2.97
7.56
7.54
7.47
7.45
7.27
7.26
7.25
7.24
7.24
7.23
7.23
7.17
7.16
7.15
7.15
7.14
7.14
6.98
6.96
6.82
6.80
6.16
5.29
5.29
5.05
5.04
3.79
2.35

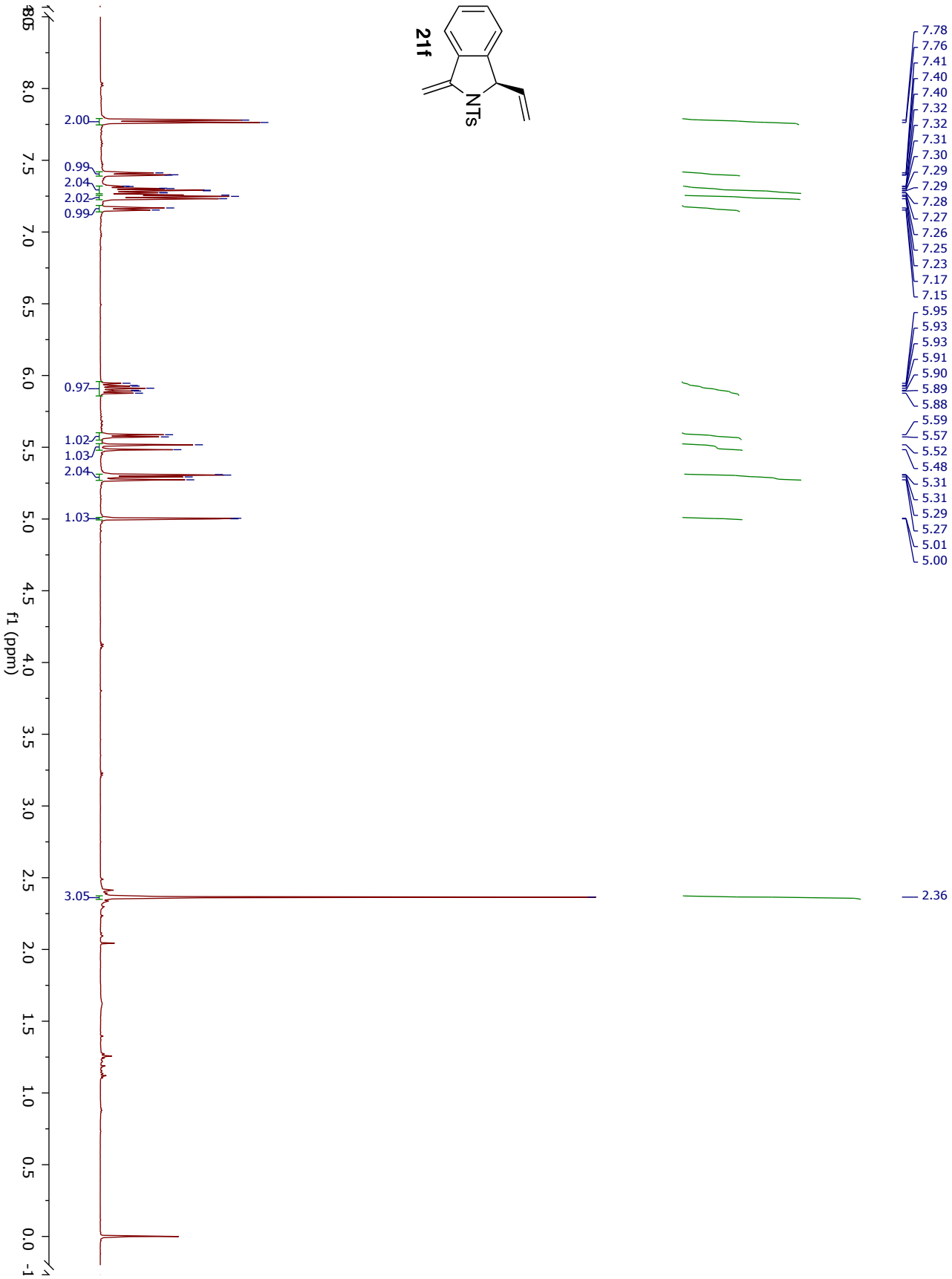

21c
NTs
OMe
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
159.35
143.95
143.73
140.74
135.80
133.91
133.15
129.57
129.33
128.81
128.07
127.41
123.32
120.39
113.90
87.76
77.27
77.02
76.76
69.88
55.27
21.51
-0.00

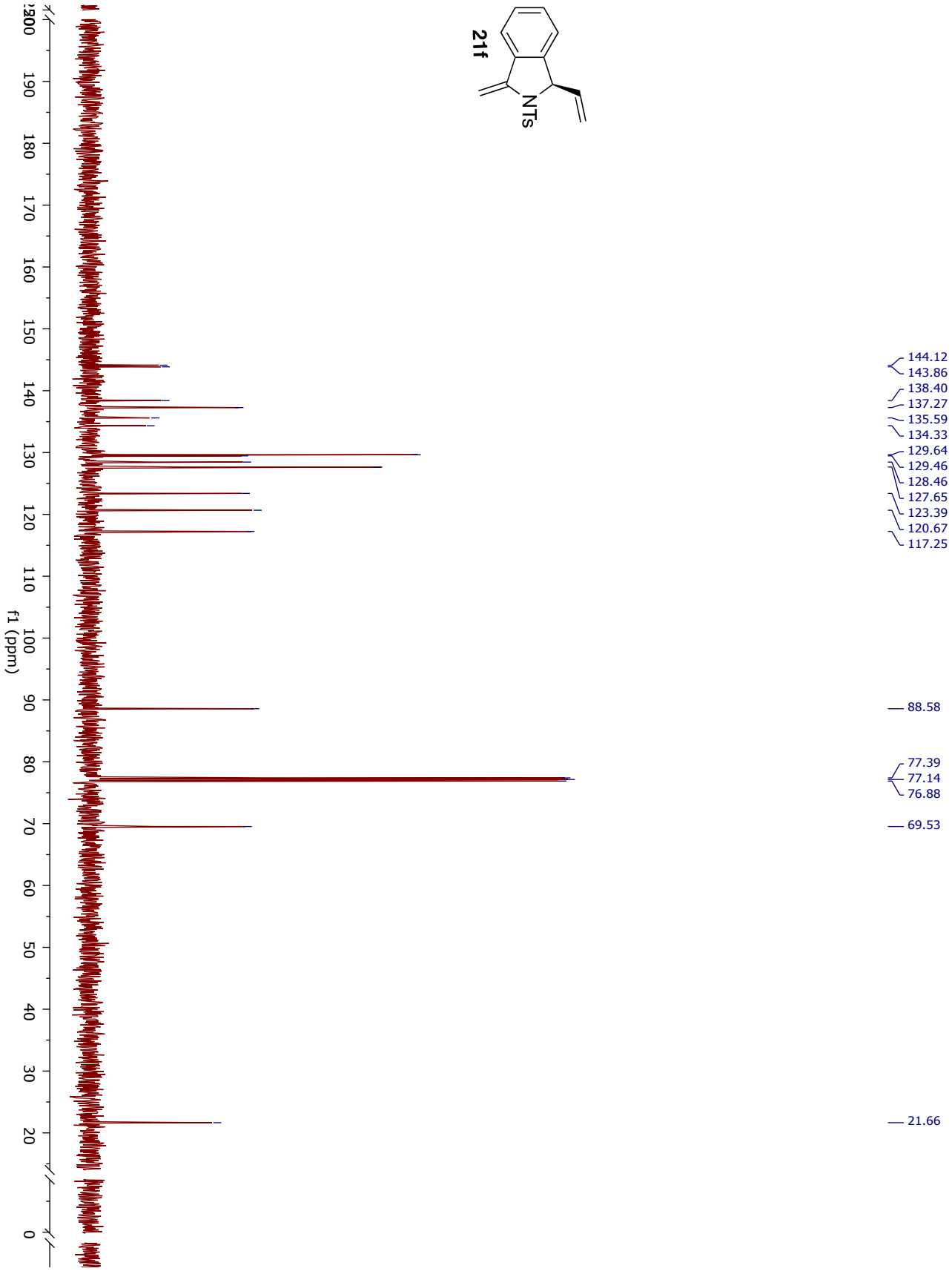

21d
NTs
f1 (ppm)
1.98
1.02
4.06
0.96
0.93
1.01
1.02
1.01
1.00
2.99
2.95
7.78
7.77
7.42
7.42
7.41
7.40
7.30
7.29
7.29
7.28
7.27
7.26
7.25
7.24
7.15
7.14
7.14
7.13
5.58
5.36
5.36
5.28
5.04
5.04
5.03
5.00
5.00
2.37
1.44
0.00

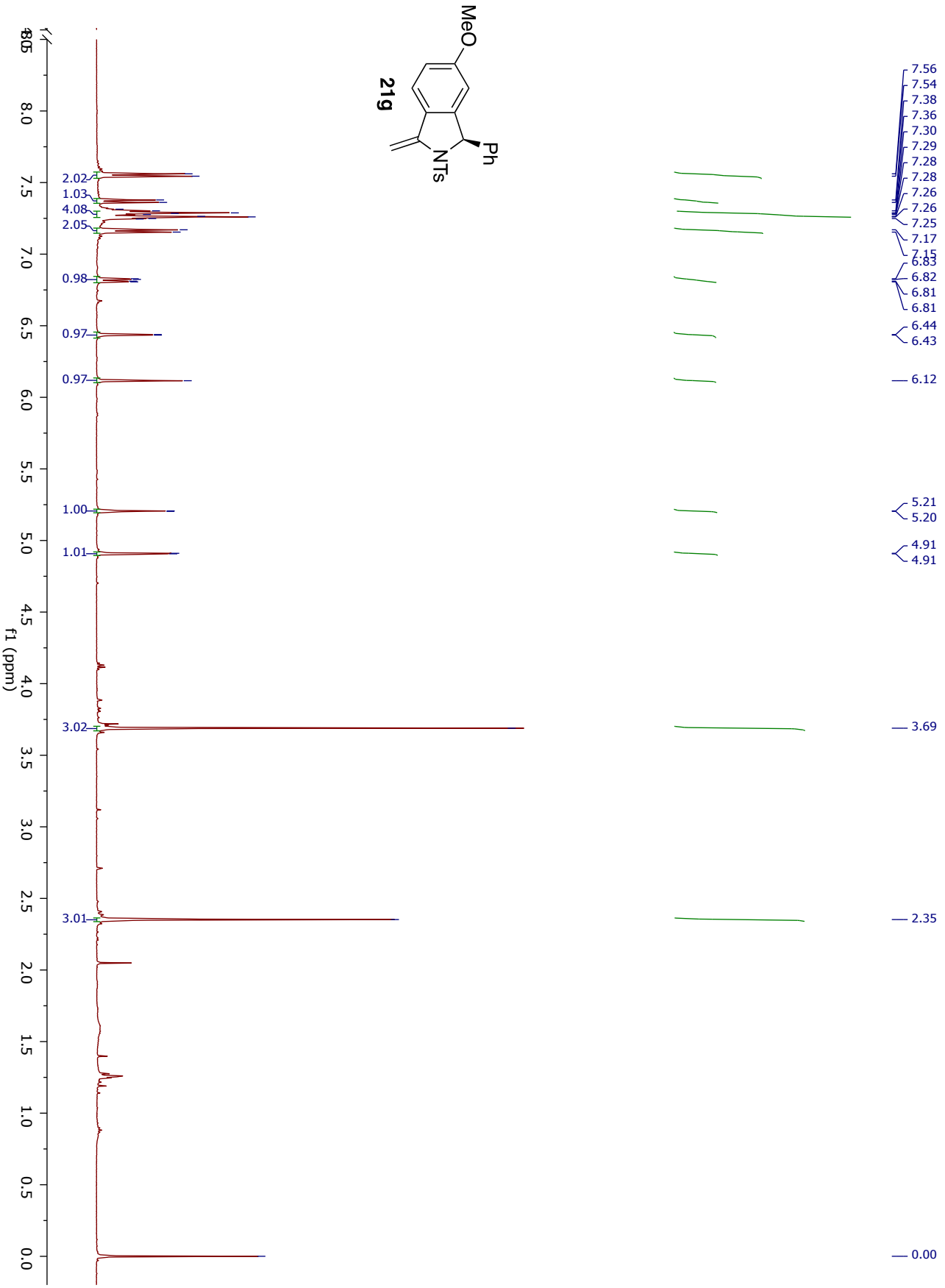

21d
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
144.41
144.18
143.97
138.30
135.36
134.70
129.51
129.38
128.35
127.51
122.60
120.37
114.11
88.01
77.27
77.01
76.76
72.81
21.55
16.07
-0.00

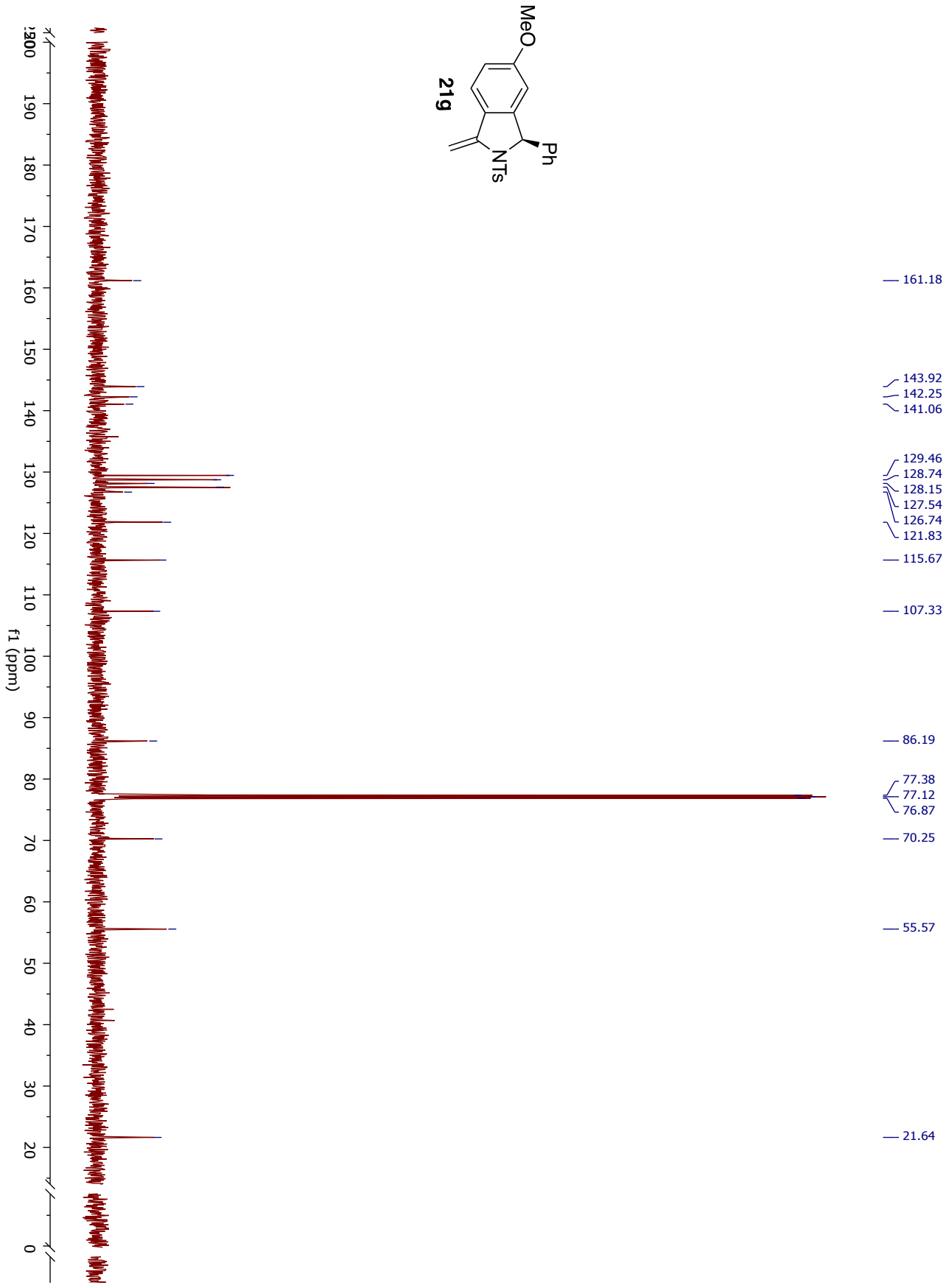

21e
Bn
NTs
f1 (ppm)
2.01
10.32
1.00
1.02
1.00
0.99
1.03
1.03
3.01
7.75
7.73
7.27
7.26
7.24
7.24
7.22
7.21
7.19
7.18
7.16
7.15
7.15
7.14
7.13
7.12
7.12
6.69
6.68
5.40
5.39
5.38
5.38
5.30
5.30
4.91
4.90
3.64
3.64
3.62
3.61
3.20
3.19
3.18
3.16
2.34
-0.00

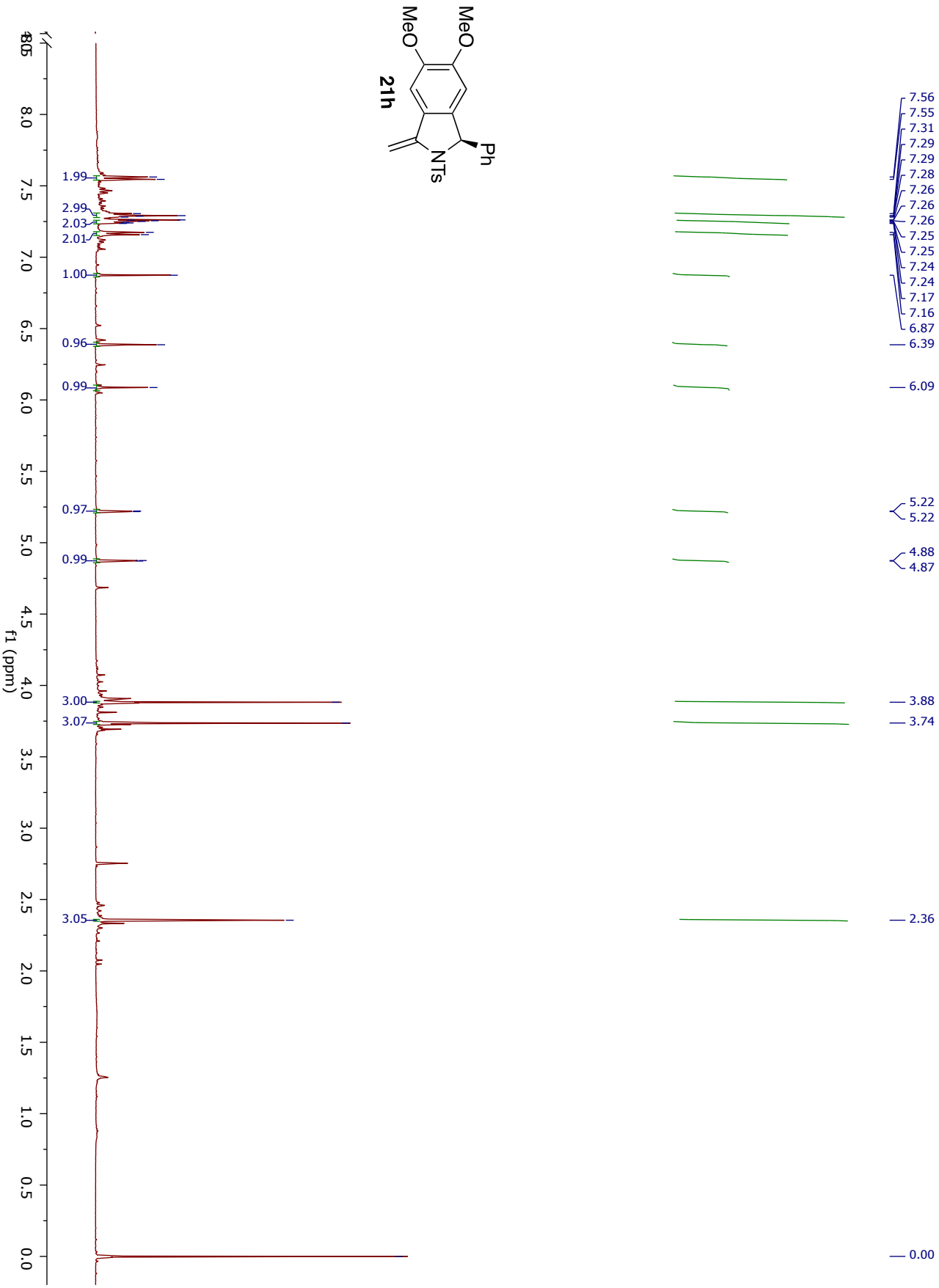

21e
Bn
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
143.76
139.10
136.07
135.11
134.68
130.30
129.53
128.61
128.08
127.92
127.39
126.59
123.04
120.38
89.29
77.26
77.01
76.76
67.62
43.52
21.52

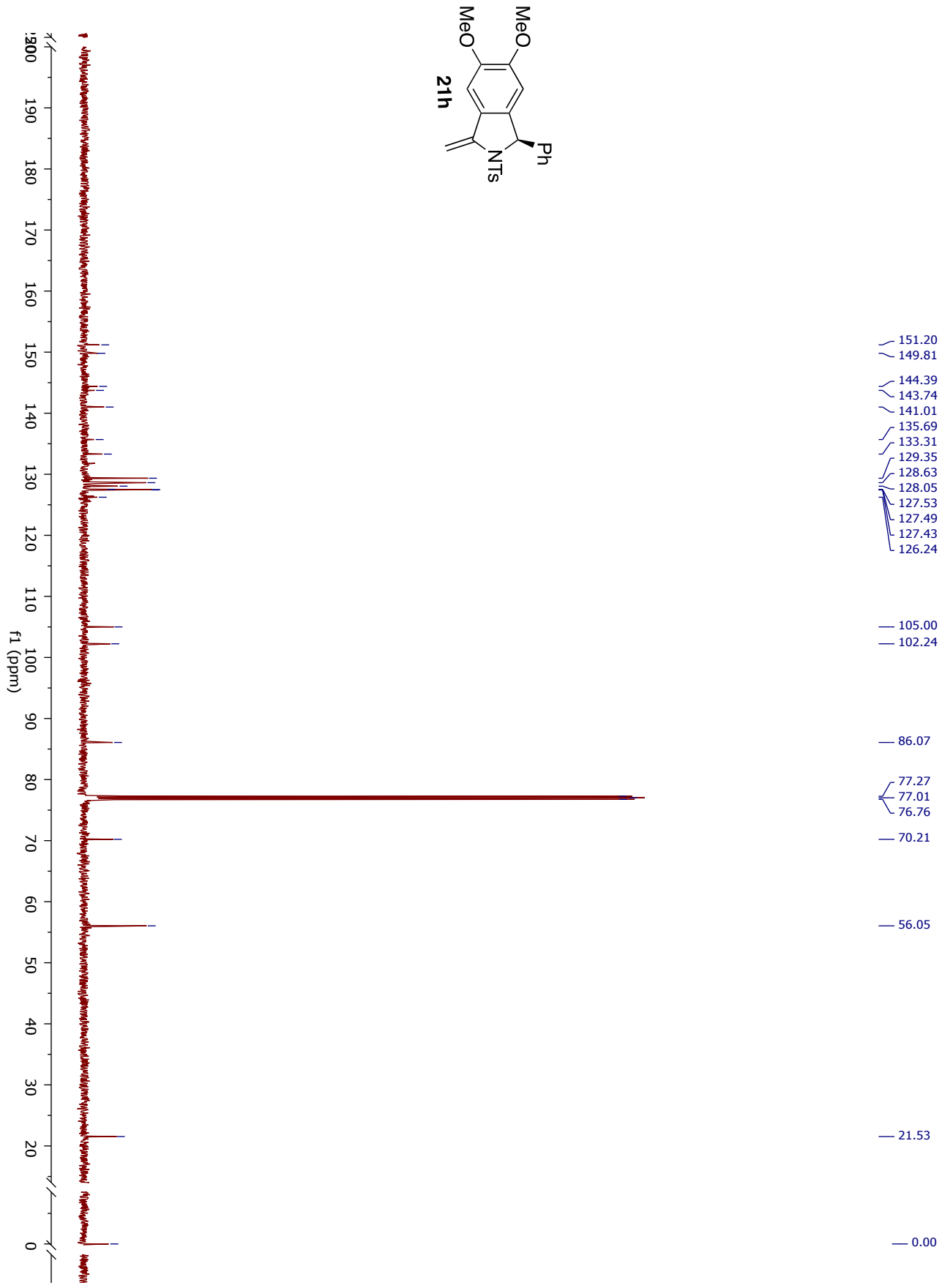

21f
NTs
f1 (ppm)
2.00
0.99
2.04
2.02
0.99
0.97
1.02
1.03
2.04
1.03
3.05
7.78
7.76
7.41
7.40
7.40
7.32
7.32
7.31
7.30
7.29
7.29
7.28
7.27
7.26
7.25
7.23
7.17
7.15
5.95
5.93
5.93
5.91
5.90
5.89
5.88
5.59
5.57
5.52
5.48
5.31
5.31
5.29
5.27
5.01
5.00
2.36

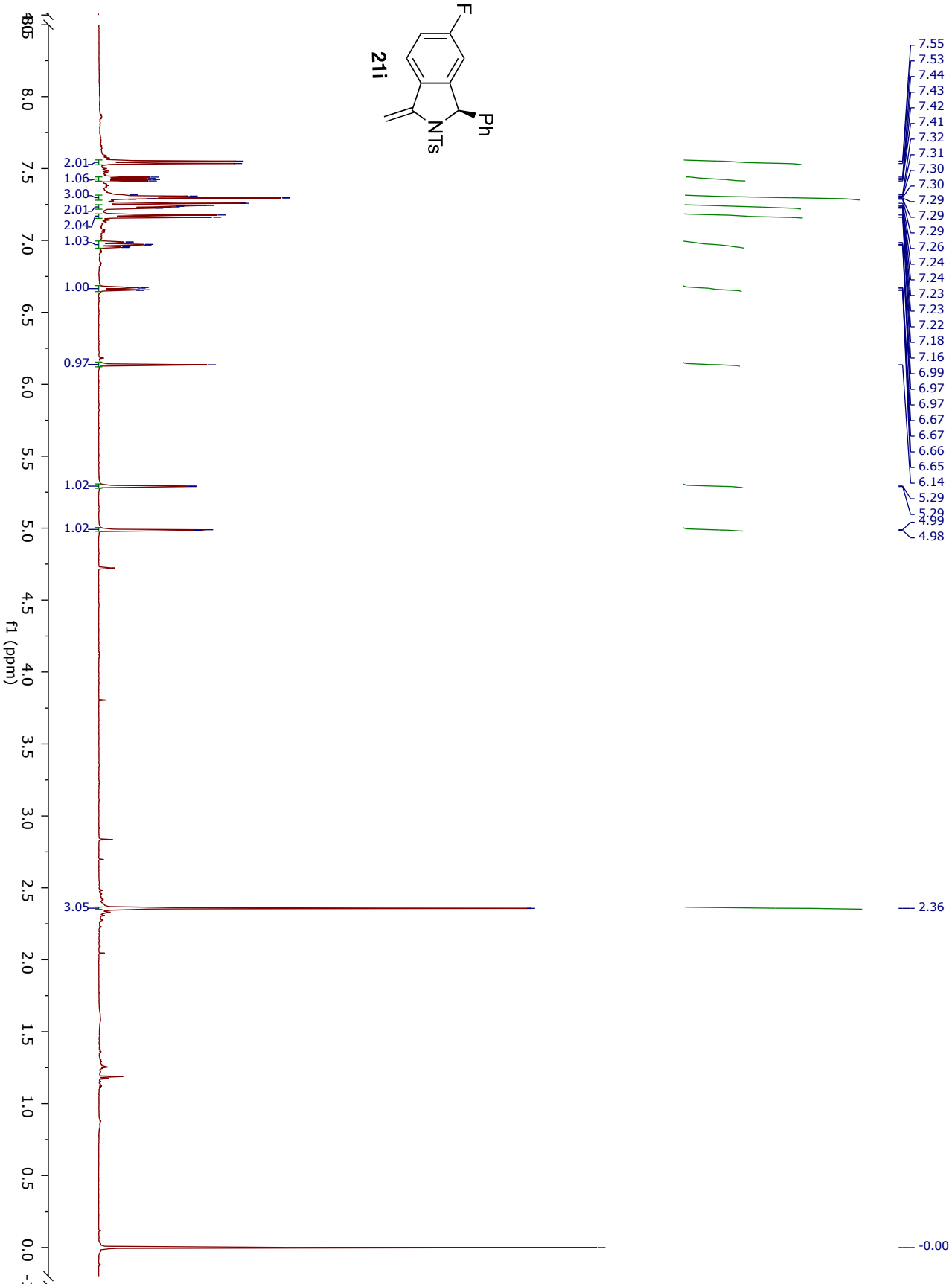

21f
NTs
144.12
143.86
138.40
137.27
135.59
134.33
129.64
129.46
128.46
127.65
123.39
120.67
117.25
88.58
77.39
77.14
76.88
69.53
21.66
f1 (ppm)

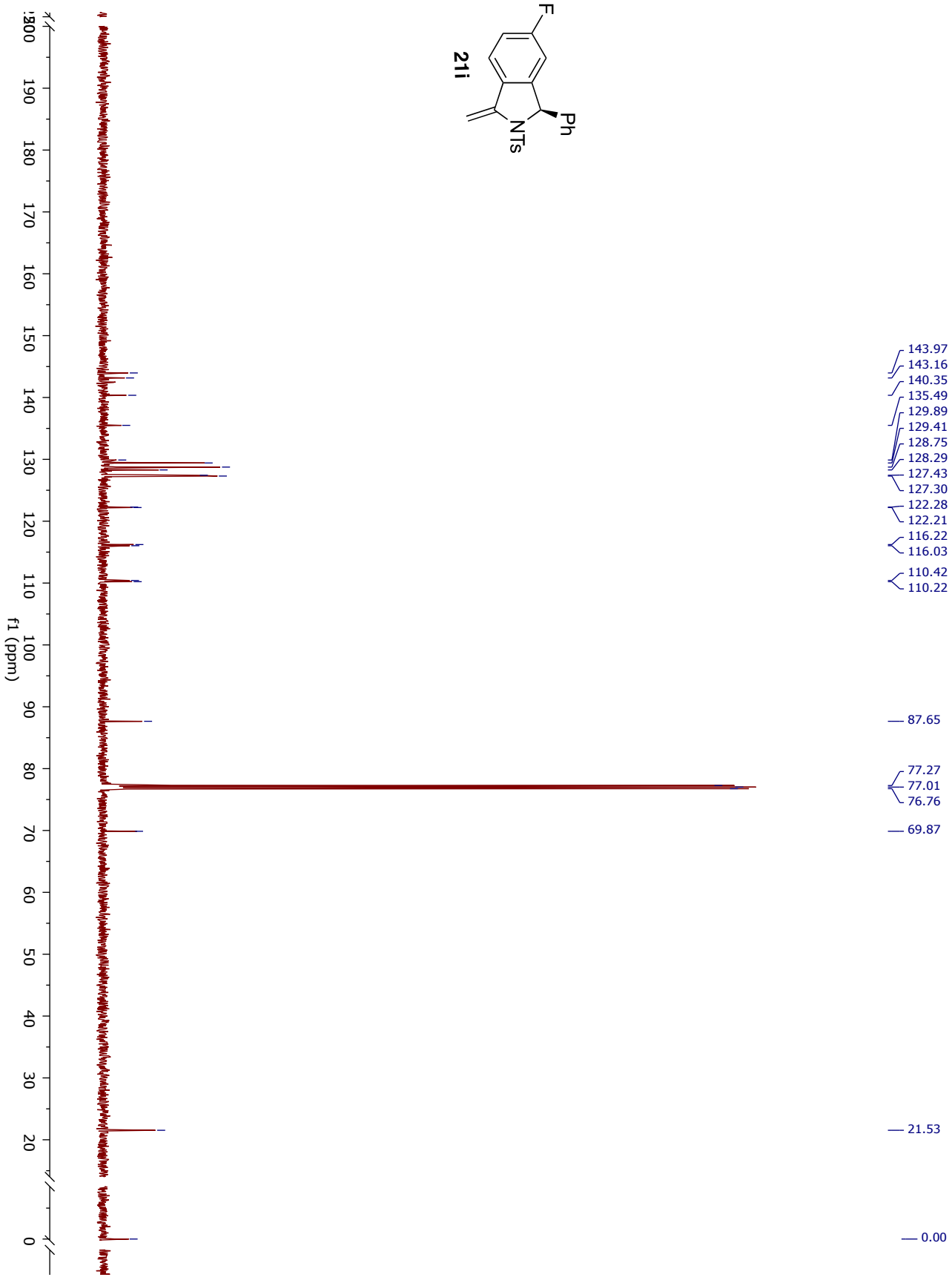

MeO
21g
Ph
NTs
f1 (ppm)
2.02
1.03
4.08
2.05
0.98
0.97
0.97
1.00
1.01
3.02
3.01
7.56
7.54
7.38
7.36
7.30
7.29
7.28
7.28
7.26
7.26
7.25
7.17
7.15
6.83
6.82
6.81
6.81
6.44
6.43
6.12
5.21
5.20
4.91
4.91
3.69
2.35
0.00

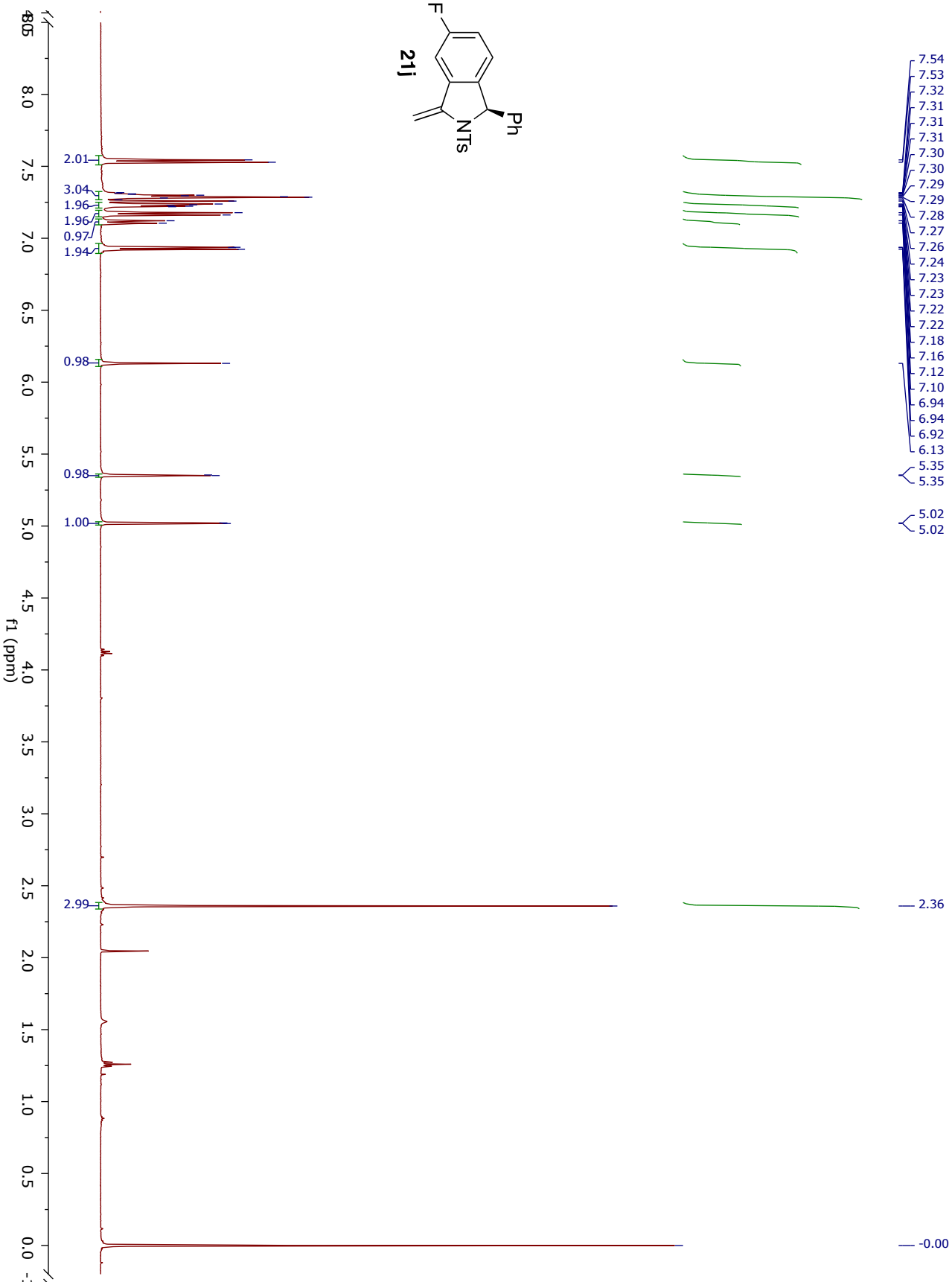

MeO
21g
Ph
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
161.18
143.92
142.25
141.06
129.46
128.74
128.15
127.54
126.74
121.83
115.67
107.33
86.19
77.38
77.12
76.87
70.25
55.57
21.64

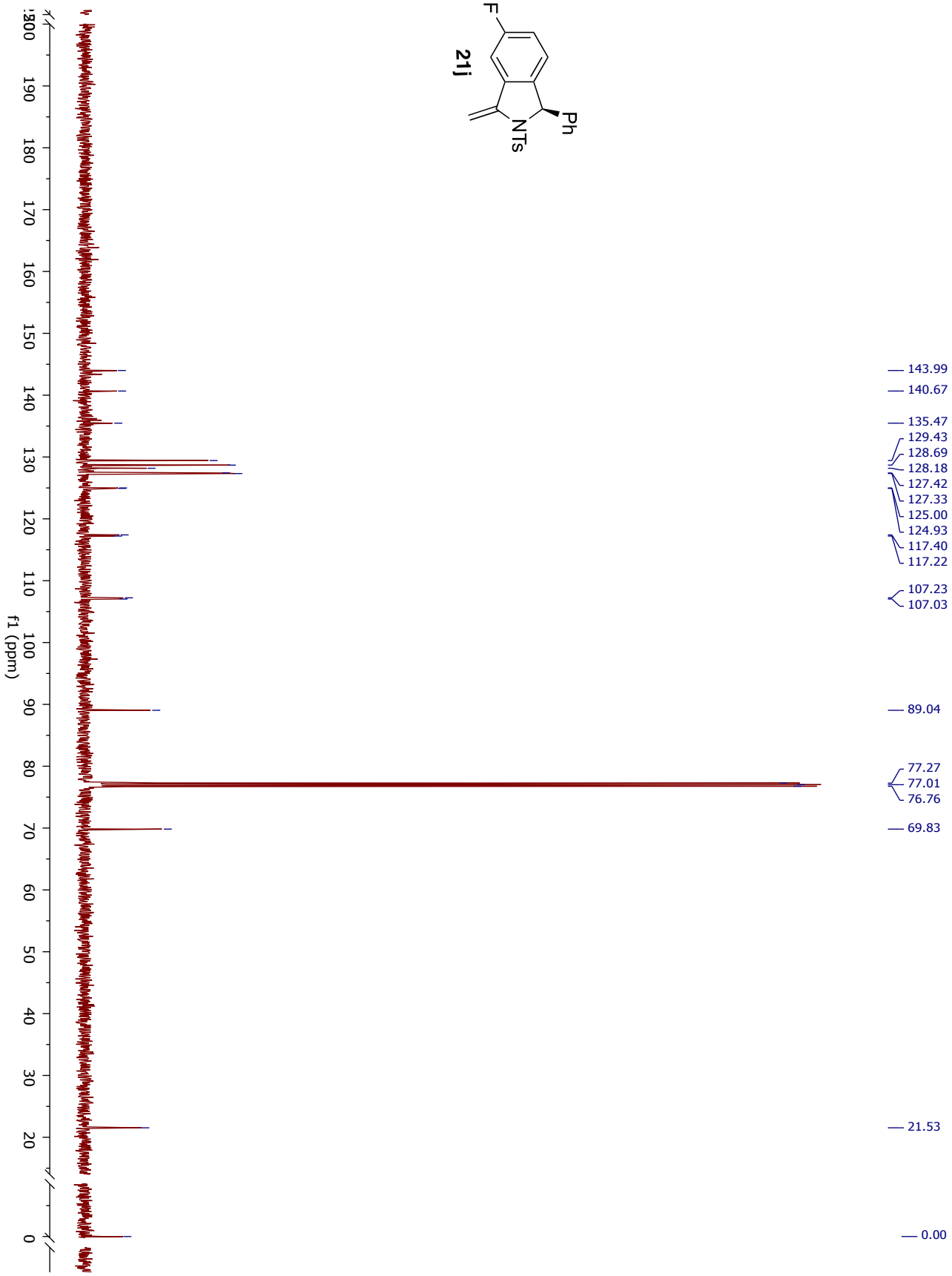

MeO
MeO
21h
Ph
NTs
f1 (ppm)
1.99
2.99
2.03
2.01
1.00
0.96
0.99
0.97
0.99
3.00
3.07
3.05
7.56
7.55
7.31
7.29
7.29
7.28
7.26
7.26
7.26
7.25
7.25
7.24
7.24
7.17
7.16
6.87
6.39
6.09
5.22
5.22
4.88
4.87
3.88
3.74
2.36
0.00

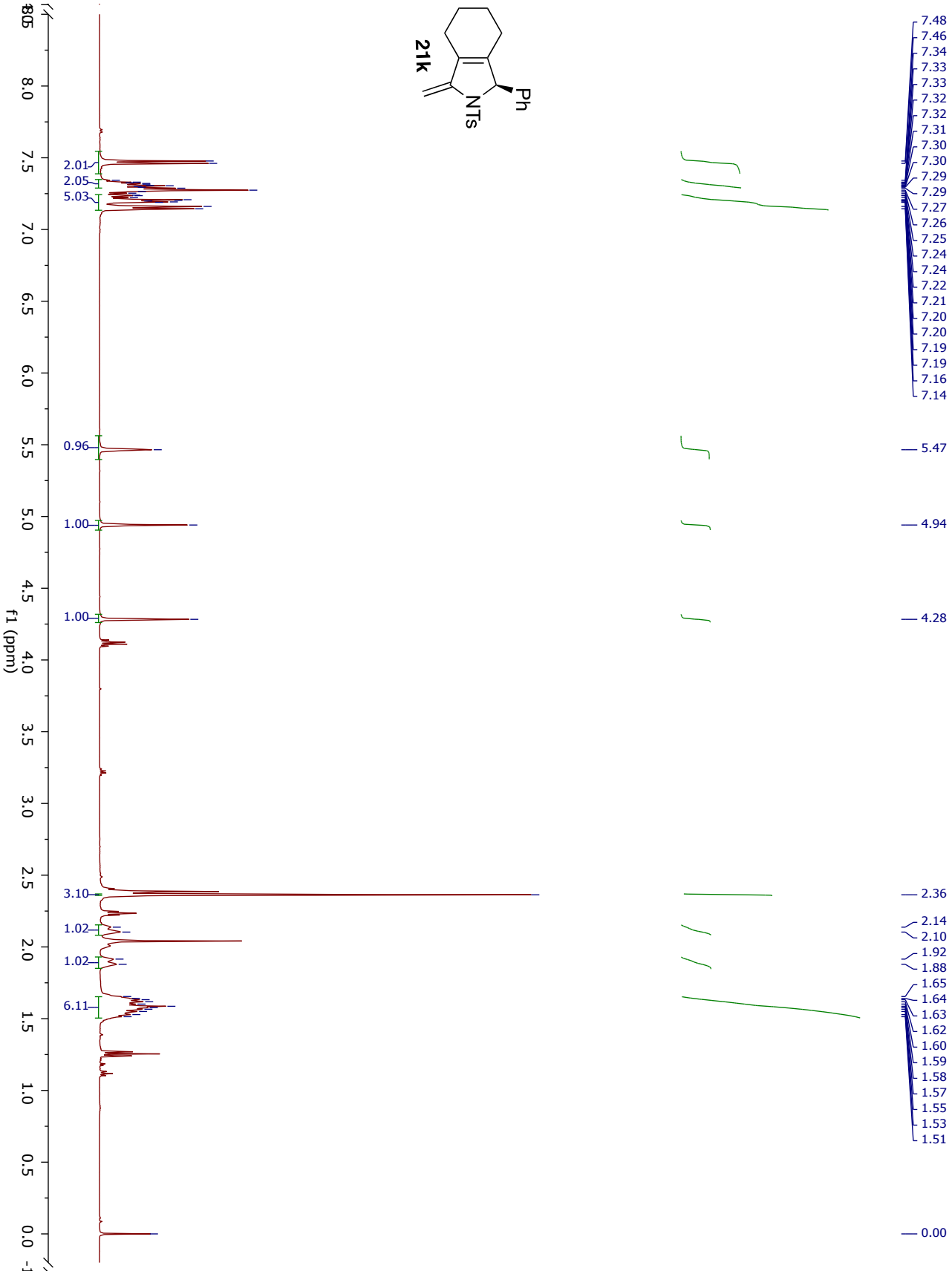

MeO
MeO
21h
Ph
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
151.20
149.81
144.39
143.74
141.01
135.69
133.31
129.35
128.63
128.05
127.53
127.49
127.43
126.24
105.00
102.24
86.07
77.27
77.01
76.76
70.21
56.05
21.53
0.00

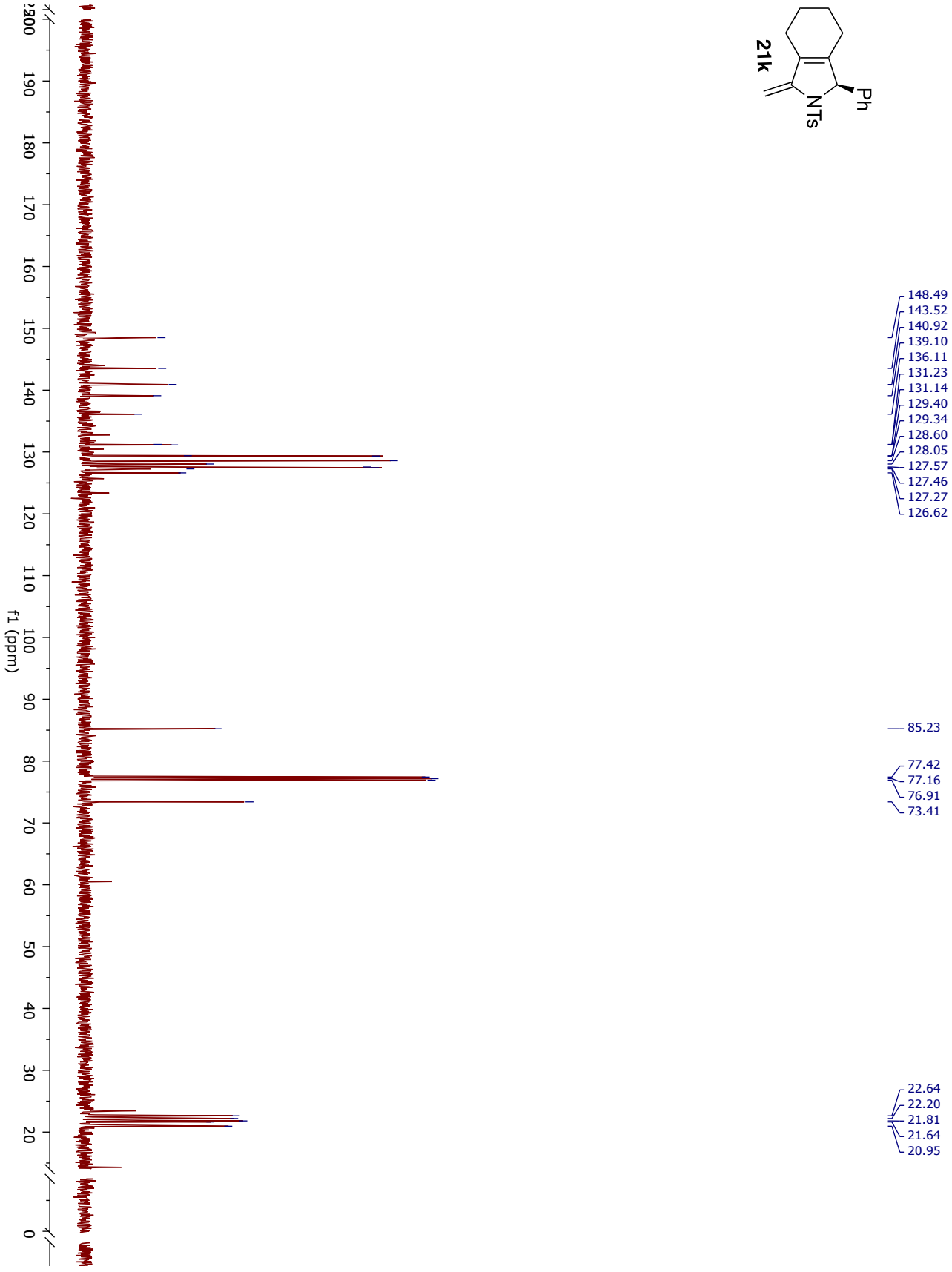

21i
F
Ph
NTs
f1 (ppm)
2.01
1.06
3.00
2.01
2.04
1.03
1.00
0.97
1.02
1.02
3.05
7.55
7.53
7.44
7.43
7.42
7.41
7.32
7.31
7.30
7.30
7.29
7.29
7.29
7.26
7.24
7.24
7.23
7.23
7.22
7.18
7.16
6.99
6.97
6.97
6.67
6.67
6.66
6.65
6.14
5.29
4.99
4.98
2.36
-0.00

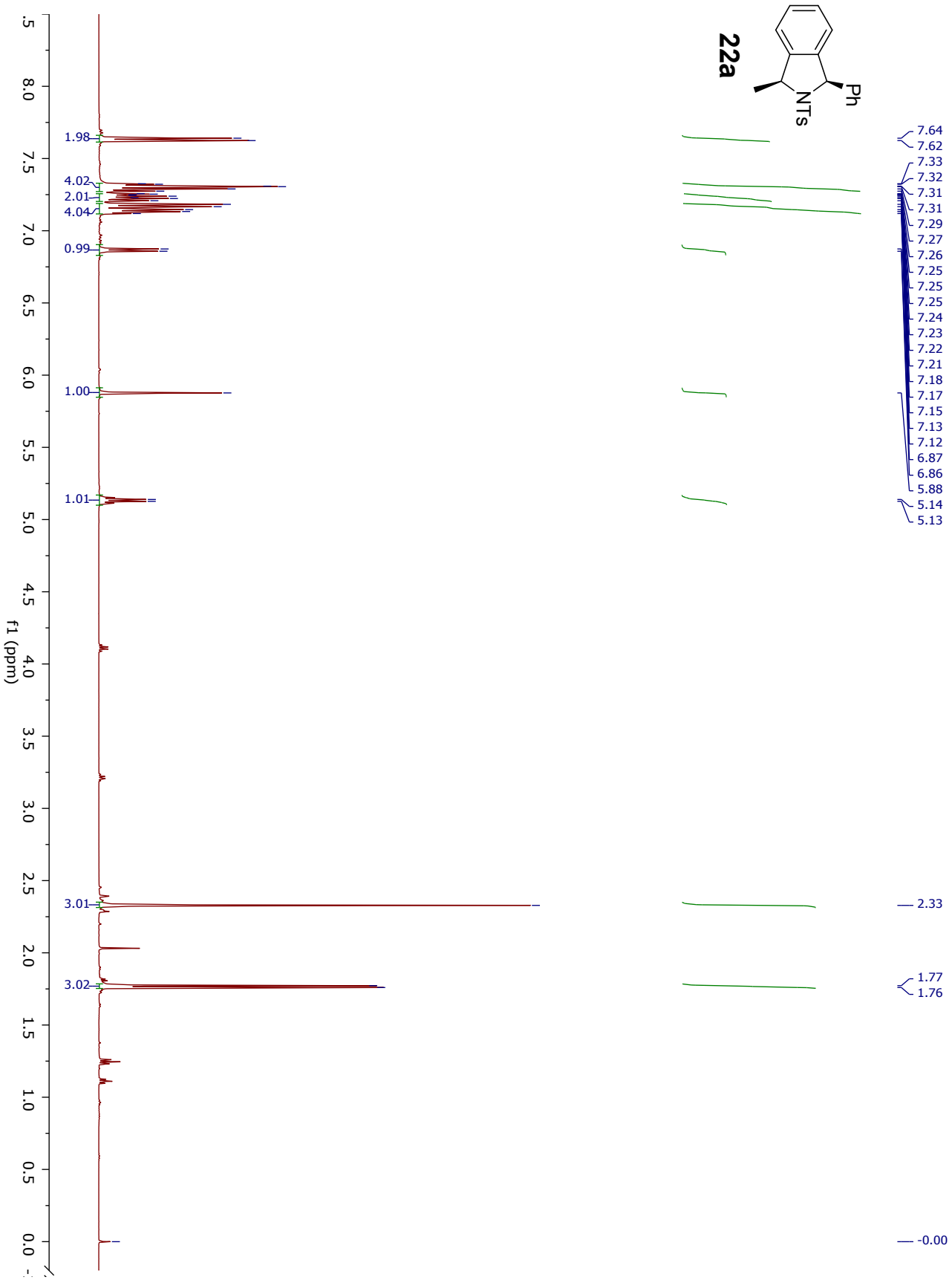

F
21i
Ph
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
143.97
143.16
140.35
135.49
129.89
129.41
128.75
128.29
127.43
127.30
122.28
122.21
116.22
116.03
110.42
110.22
87.65
77.27
77.01
76.76
69.87
21.53
0.00

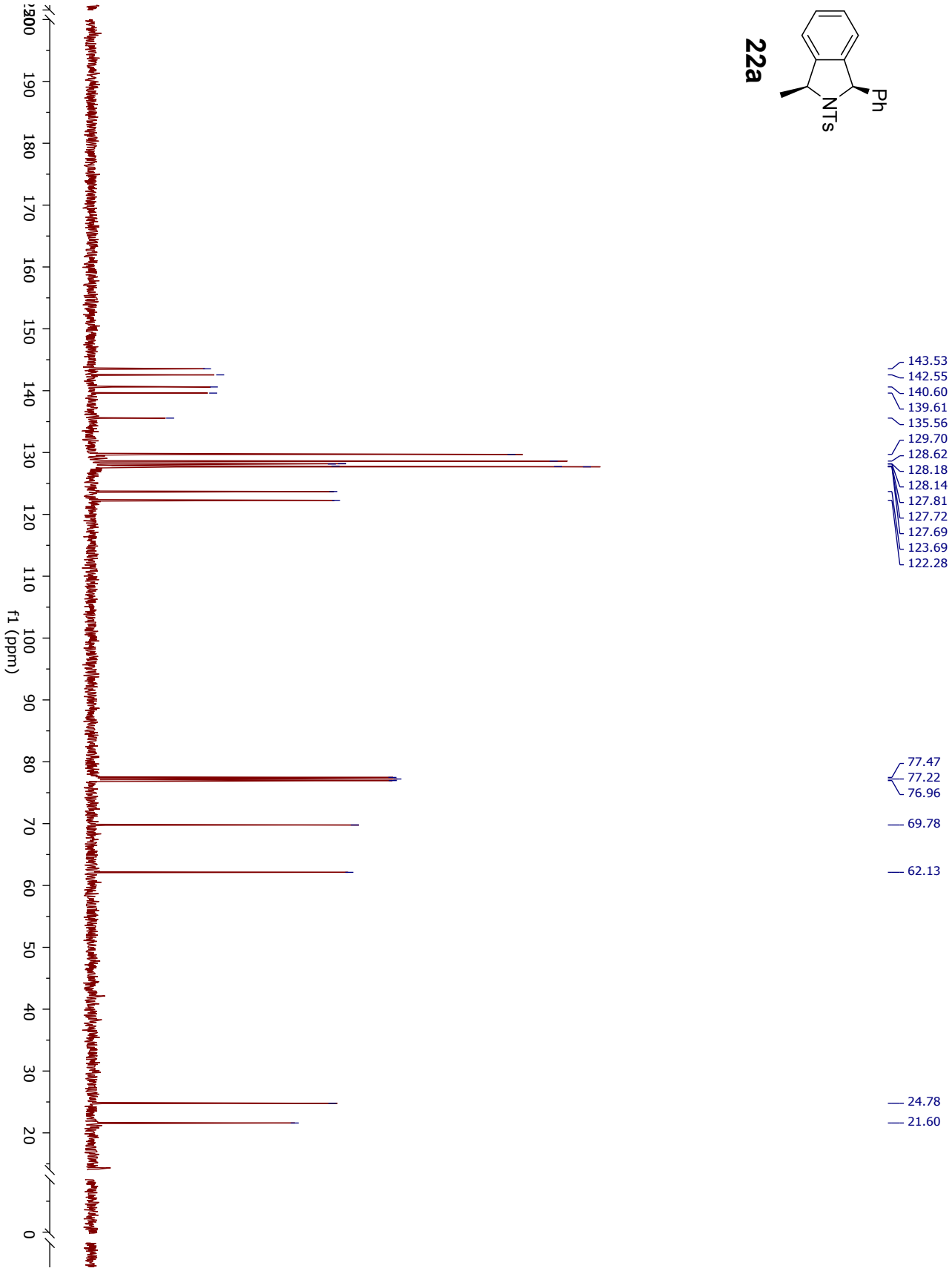

F
21j
Ph
NTs
2.01
3.04
1.96
1.96
0.97
1.94
0.98
0.98
1.00
2.99
7.54
7.53
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.26
7.24
7.23
7.23
7.22
7.22
7.18
7.16
7.12
7.10
6.94
6.94
6.92
6.13
5.35
5.35
5.02
5.02
2.36
-0.00
f1 (ppm)

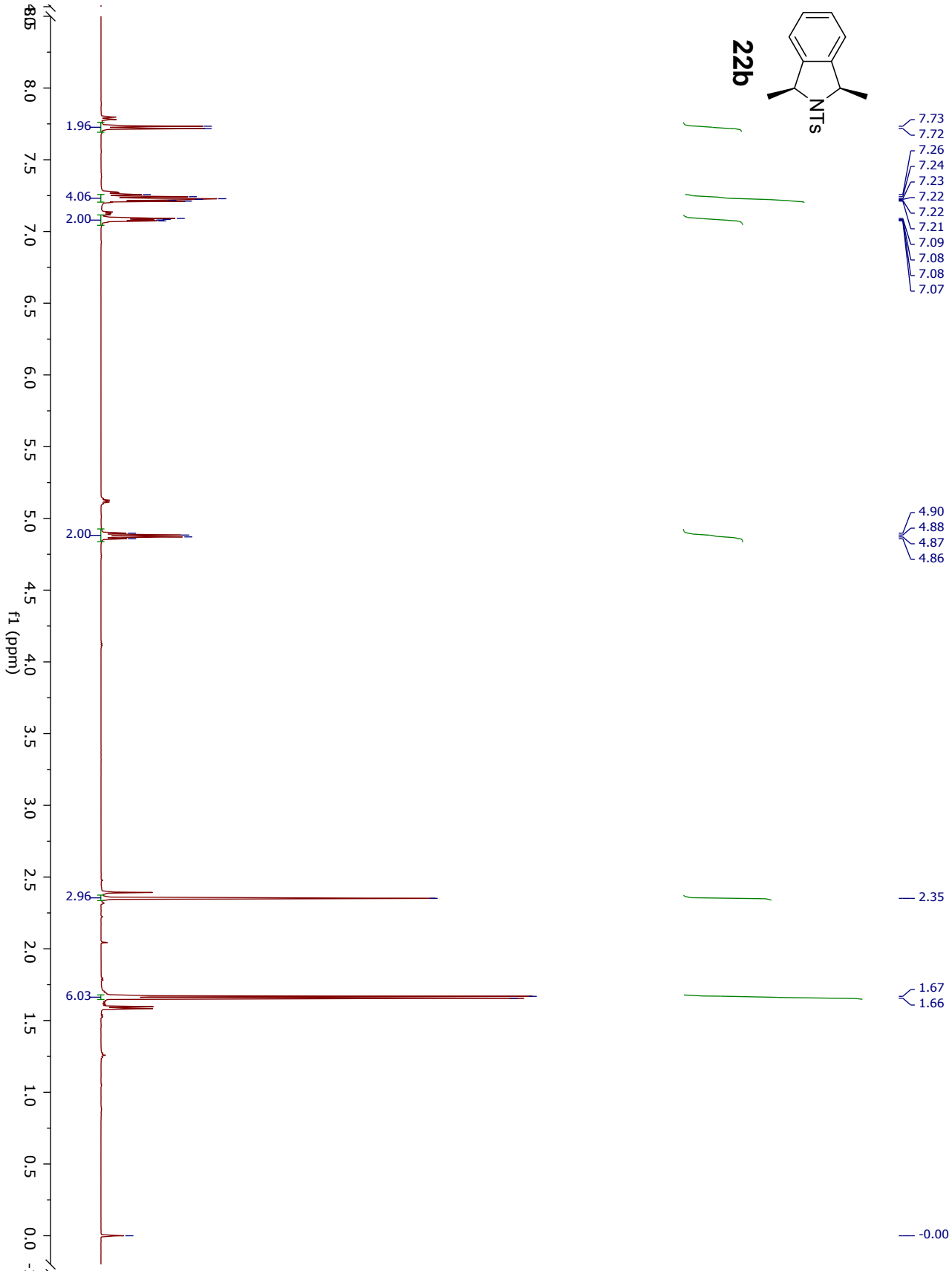

F
21j
Ph
NTs
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
143.99
140.67
135.47
129.43
128.69
128.18
127.42
127.33
125.00
124.93
117.40
117.22
107.23
107.03
89.04
77.27
77.01
76.76
69.83
21.53
0.00

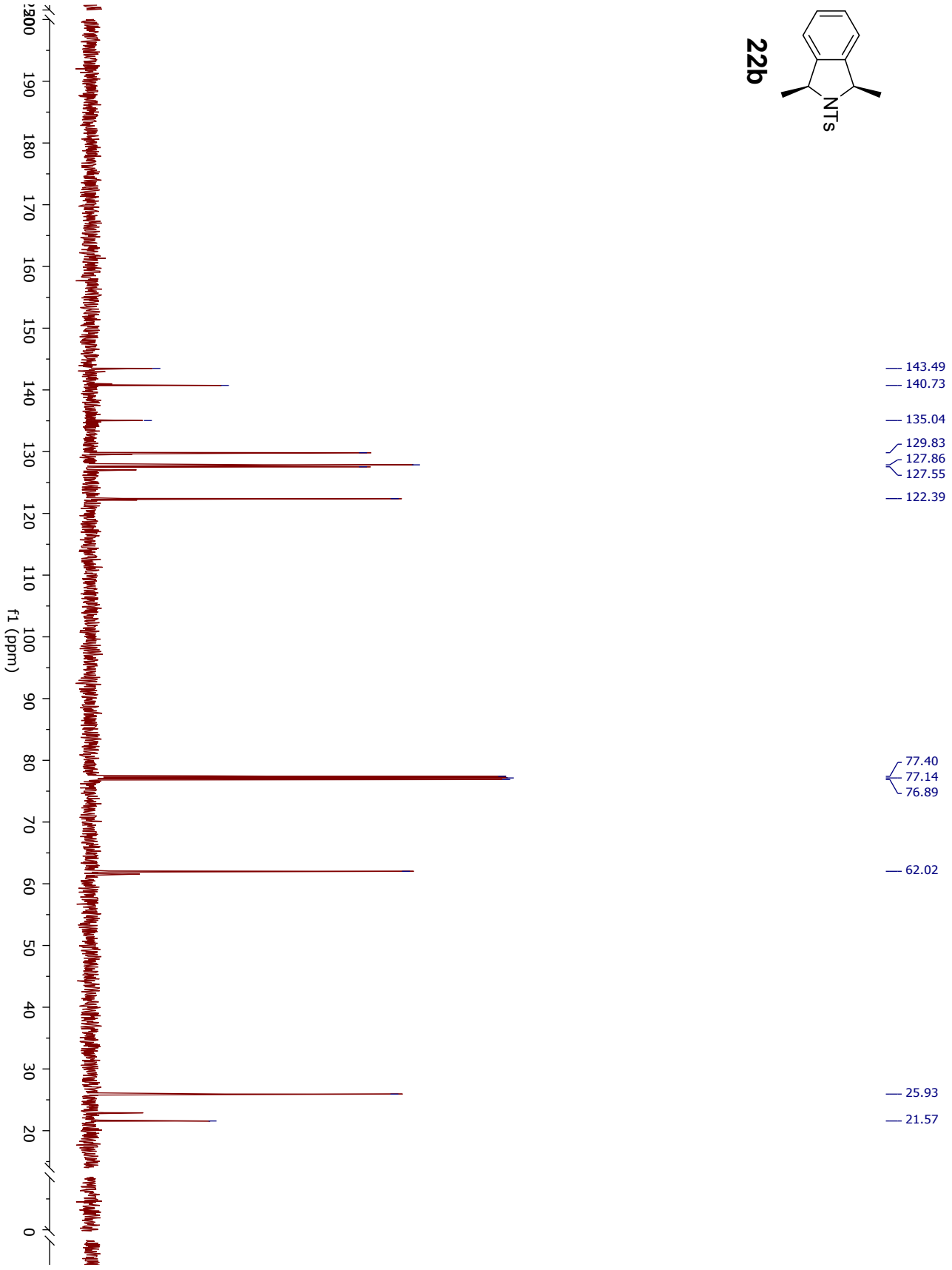

21k
Ph
NTs
f1 (ppm)
2.01
2.05
5.03
0.96
1.00
1.00
3.10
1.02
1.02
6.11
7.48
7.46
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.27
7.26
7.25
7.24
7.24
7.22
7.21
7.20
7.20
7.19
7.19
7.16
7.14
5.47
4.94
4.28
2.36
2.14
2.10
1.92
1.88
1.65
1.64
1.63
1.62
1.60
1.59
1.58
1.57
1.55
1.53
1.51
0.00

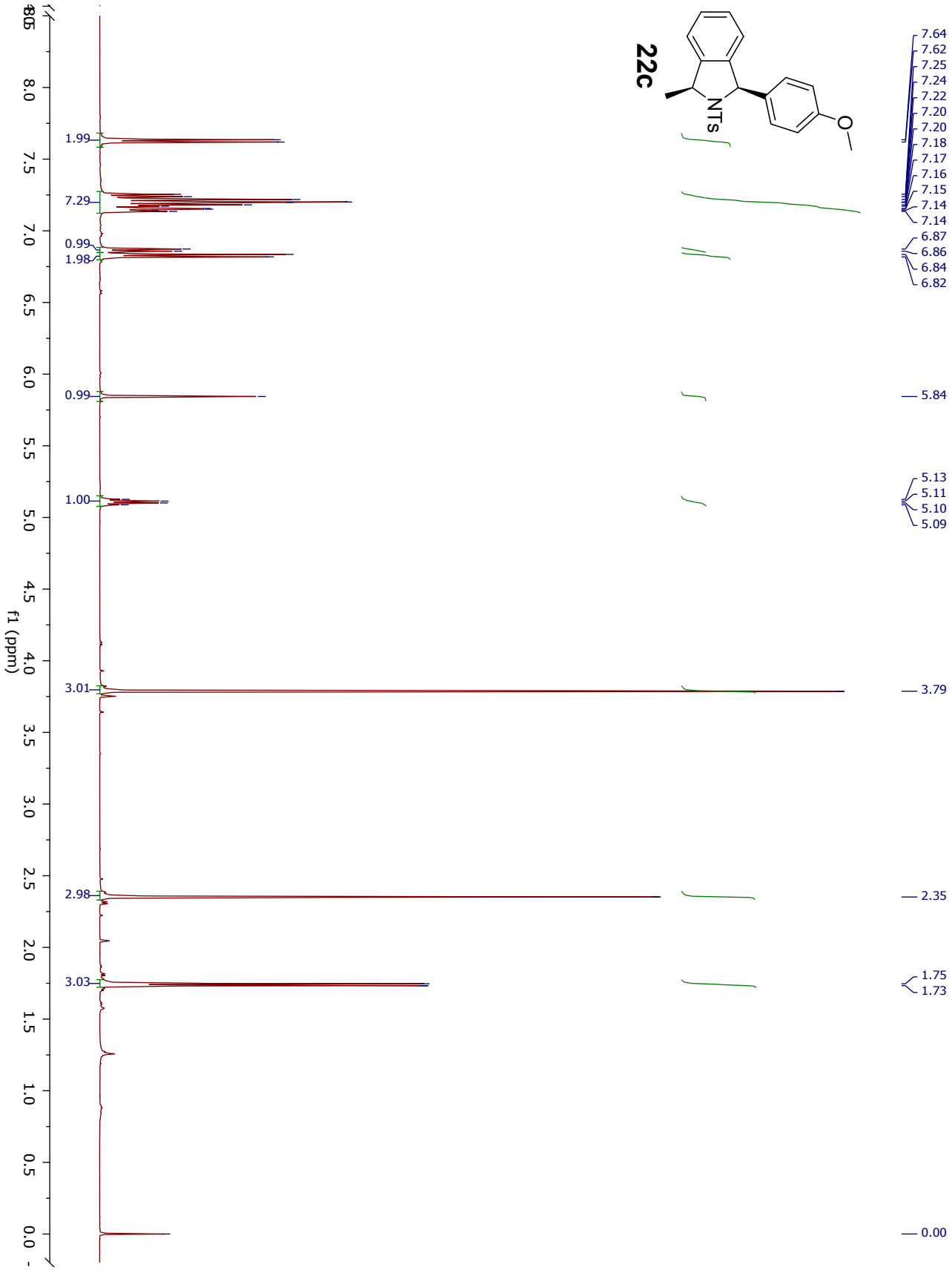

21k
Ph
NTs
148.49
143.52
140.92
139.10
136.11
131.23
131.14
129.40
129.34
128.60
128.05
127.57
127.46
127.27
126.62
85.23
77.42
77.16
76.91
73.41
22.64
22.20
21.81
21.64
20.95
f1 (ppm)

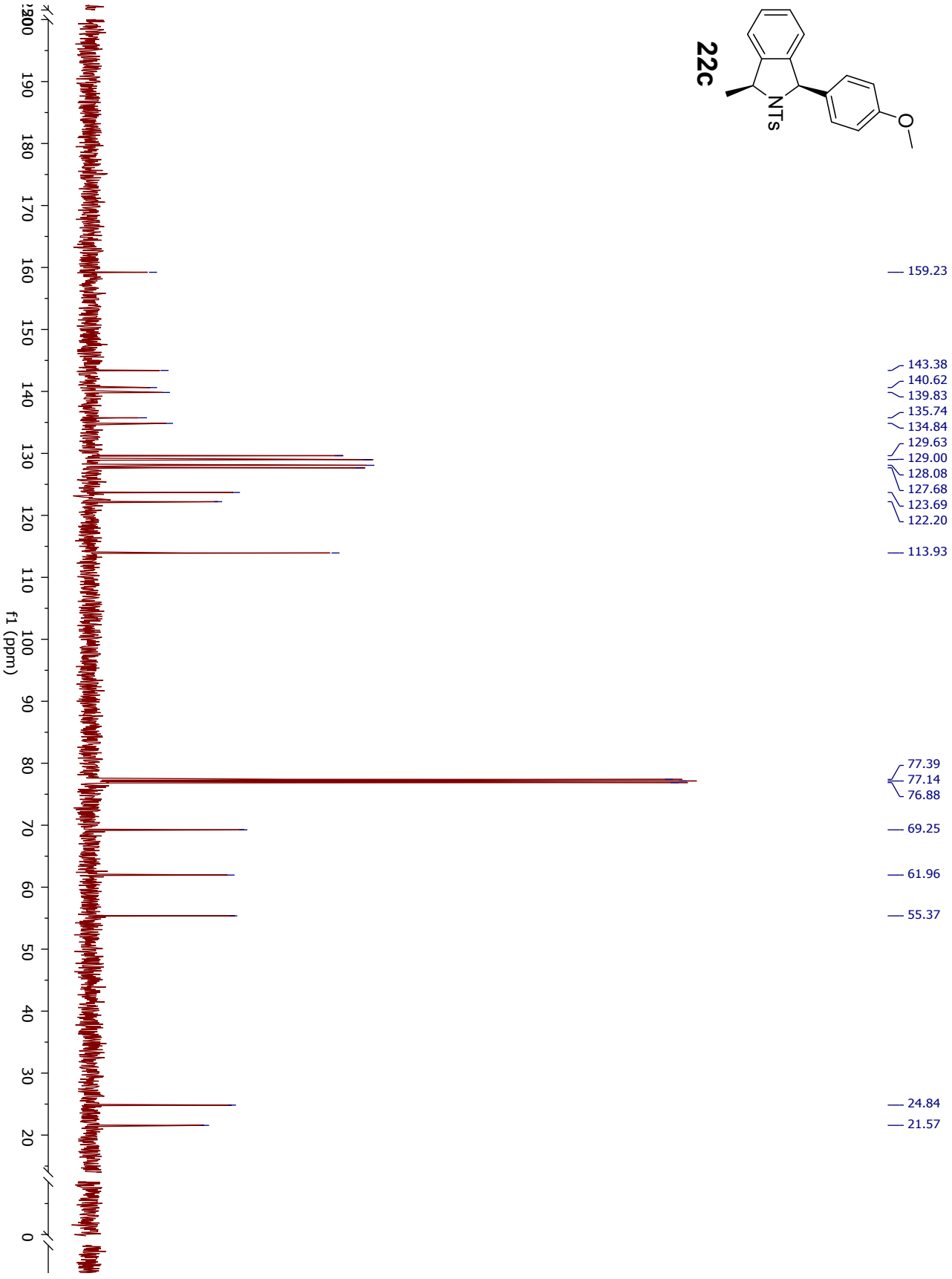

22a
Ph
NTs
f1 (ppm)
1.98
4.02
2.01
4.04
0.99
1.00
1.01
3.01
3.02
7.64
7.62
7.33
7.32
7.31
7.31
7.29
7.27
7.26
7.25
7.25
7.25
7.24
7.23
7.22
7.21
7.18
7.17
7.15
7.13
7.12
6.87
6.86
5.88
5.14
5.13
2.33
1.77
1.76
-0.00

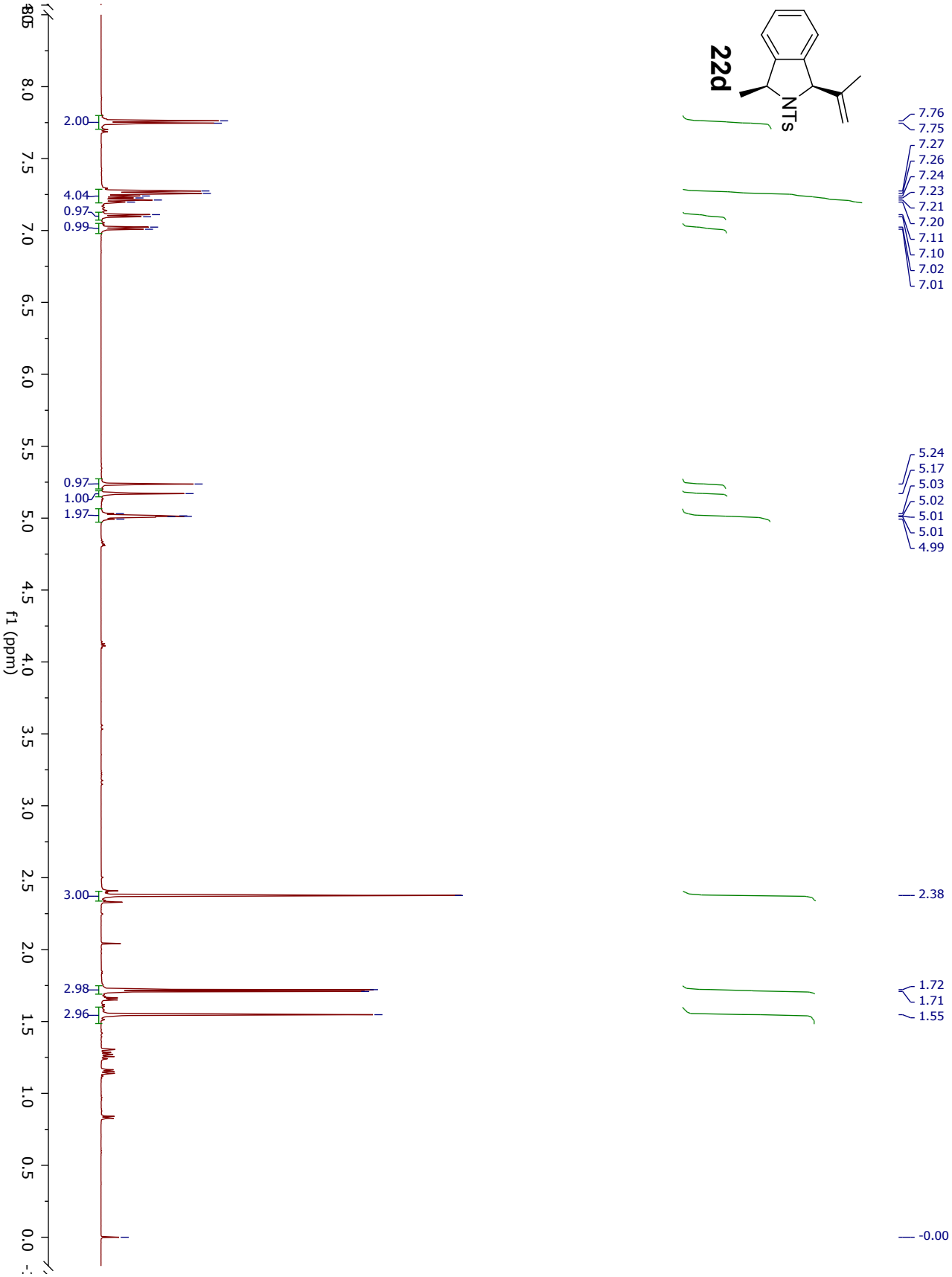

22a
Ph
NTs
143.53
142.55
140.60
139.61
135.56
129.70
128.62
128.18
128.14
127.81
127.72
127.69
123.69
122.28
77.47
77.22
76.96
69.78
62.13
24.78
21.60
f1 (ppm)

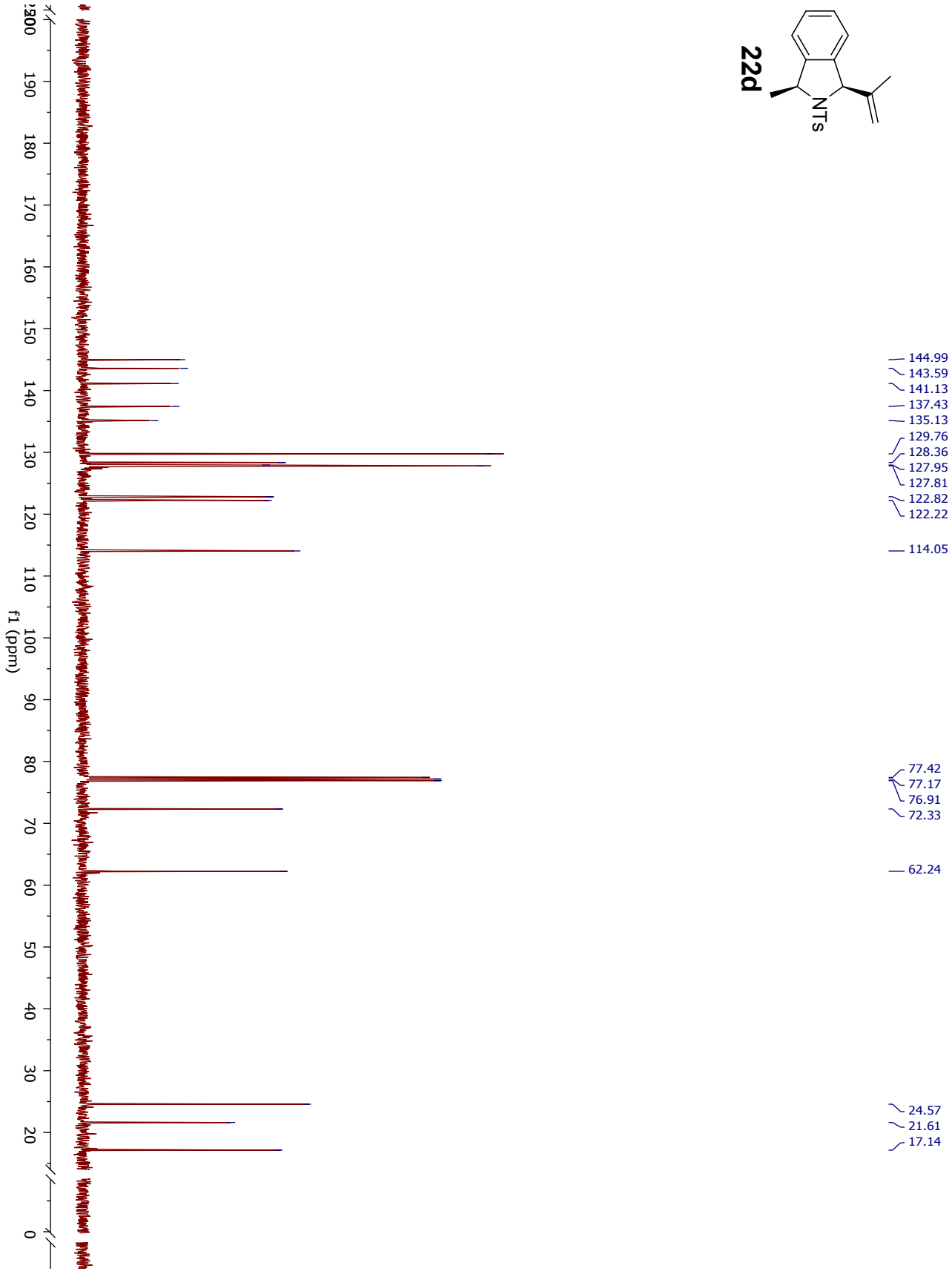

22b
NTs
1.96
4.06
2.00
2.00
2.96
6.03
7.73
7.72
7.26
7.24
7.23
7.22
7.22
7.21
7.09
7.08
7.08
7.07
4.90
4.88
4.87
4.86
2.35
1.67
1.66
-0.00
f1 (ppm)

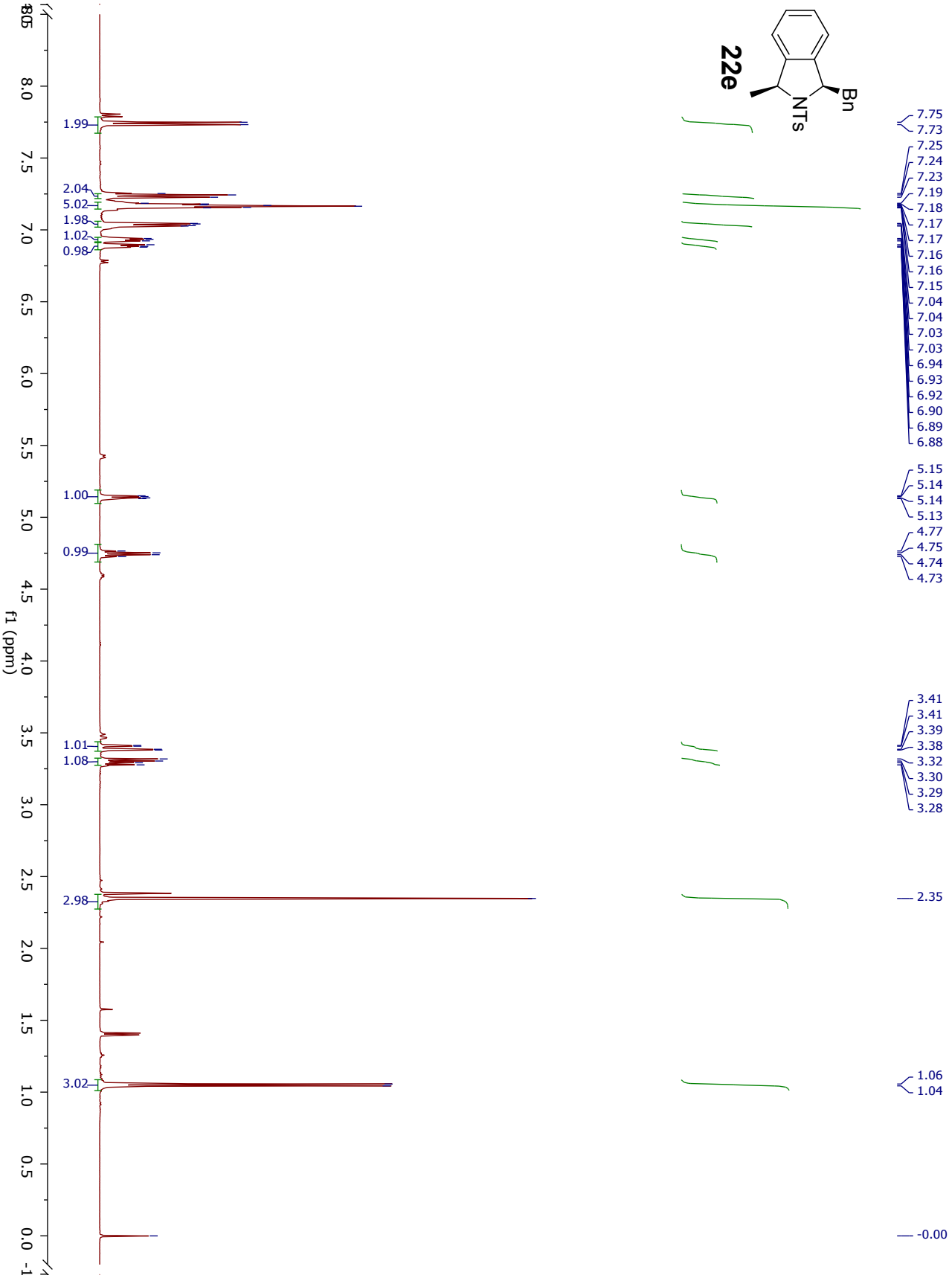

22b
NTs
143.49
140.73
135.04
129.83
127.86
127.55
122.39
77.40
77.14
76.89
62.02
25.93
21.57
f1 (ppm)

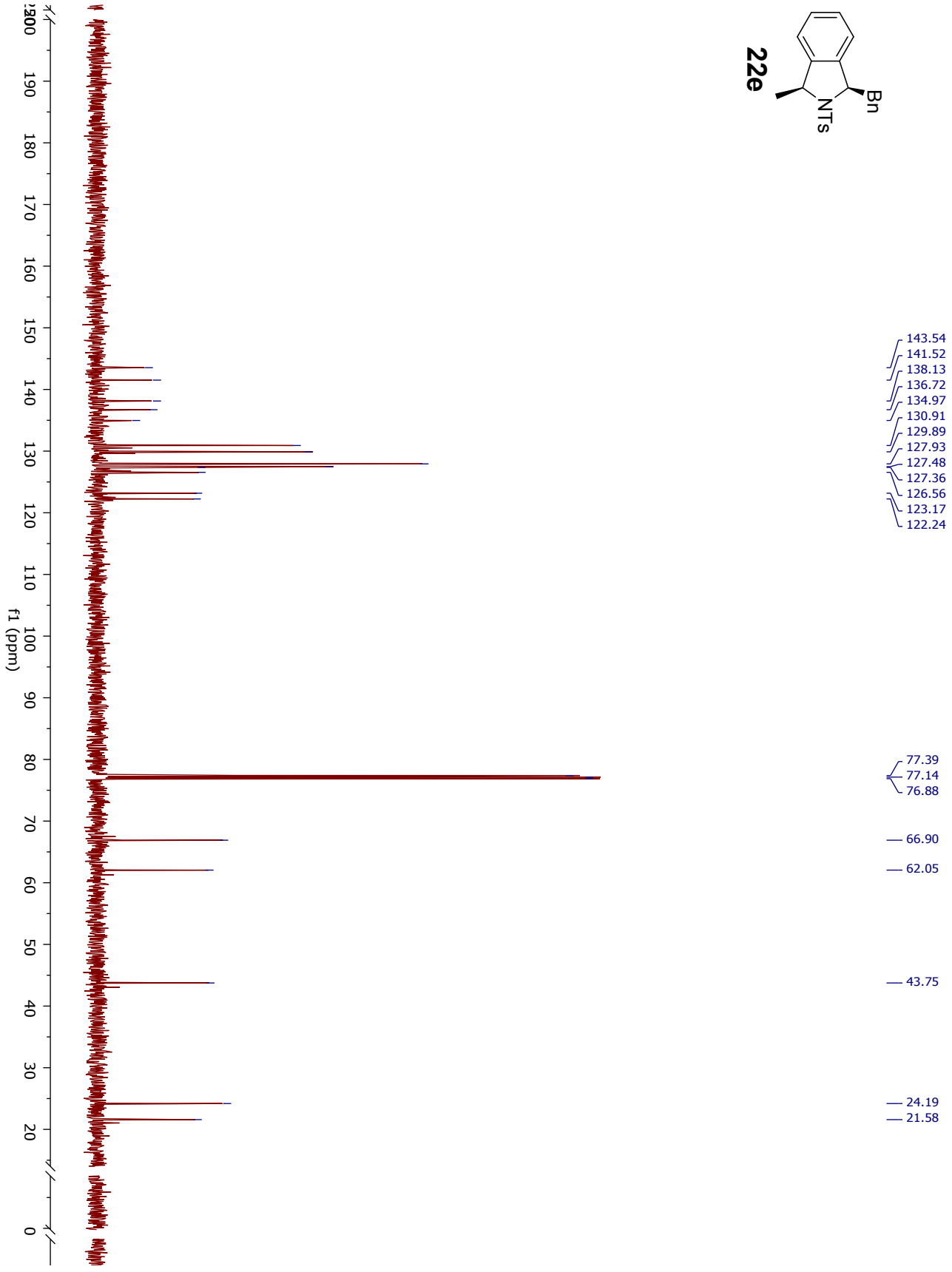

22c
NTs
O
f1 (ppm)
1.99
7.29
0.99
1.98
0.99
1.00
3.01
2.98
3.03
7.64
7.62
7.25
7.24
7.22
7.20
7.20
7.18
7.17
7.16
7.15
7.14
7.14
6.87
6.86
6.84
6.82
5.84
5.13
5.11
5.10
5.09
3.79
2.35
1.75
1.73
0.00

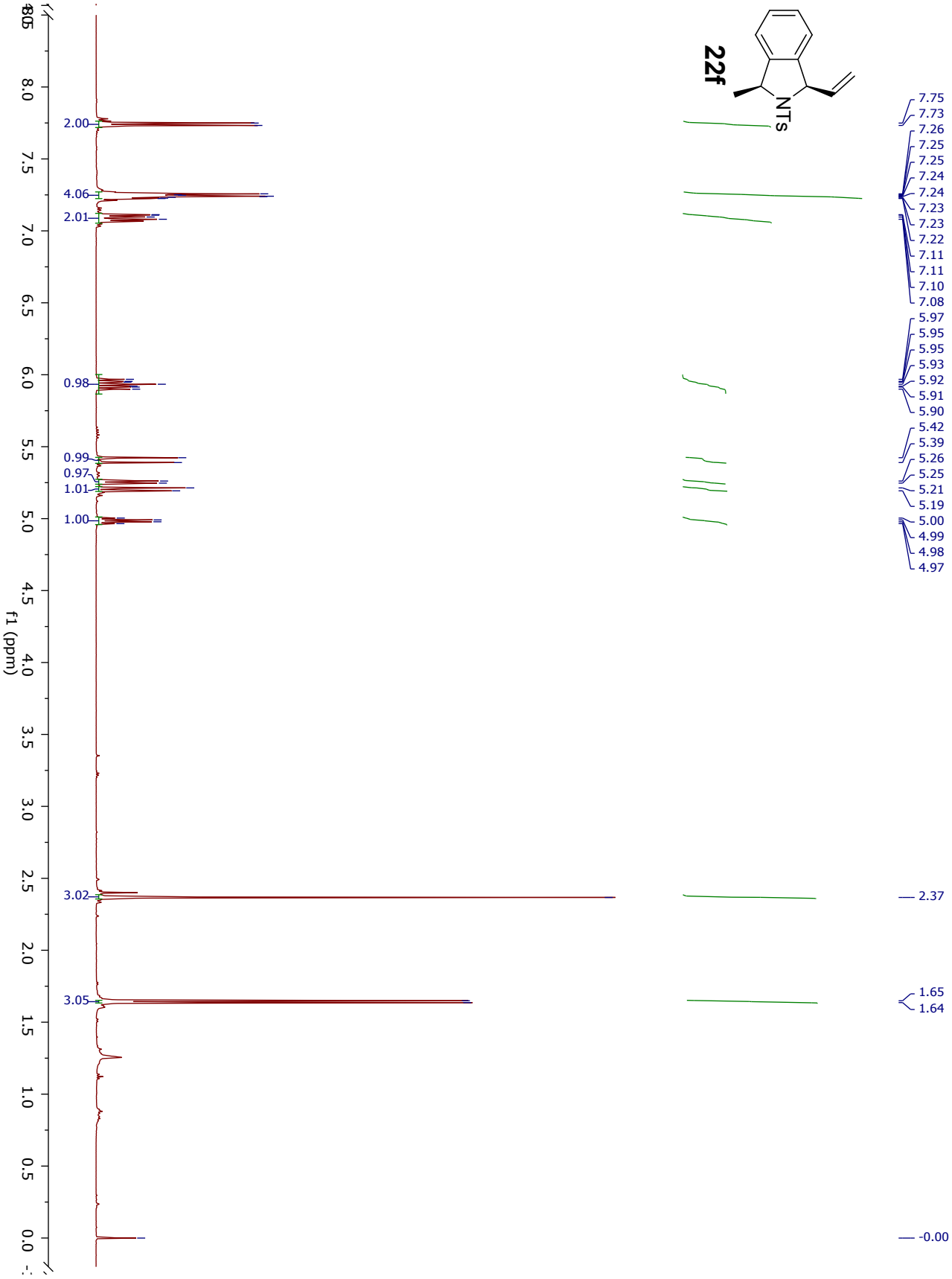

22c
NTs
O
159.23
143.38
140.62
139.83
135.74
134.84
129.63
129.00
128.08
127.68
123.69
122.20
113.93
77.39
77.14
76.88
69.25
61.96
55.37
24.84
21.57
f1 (ppm)

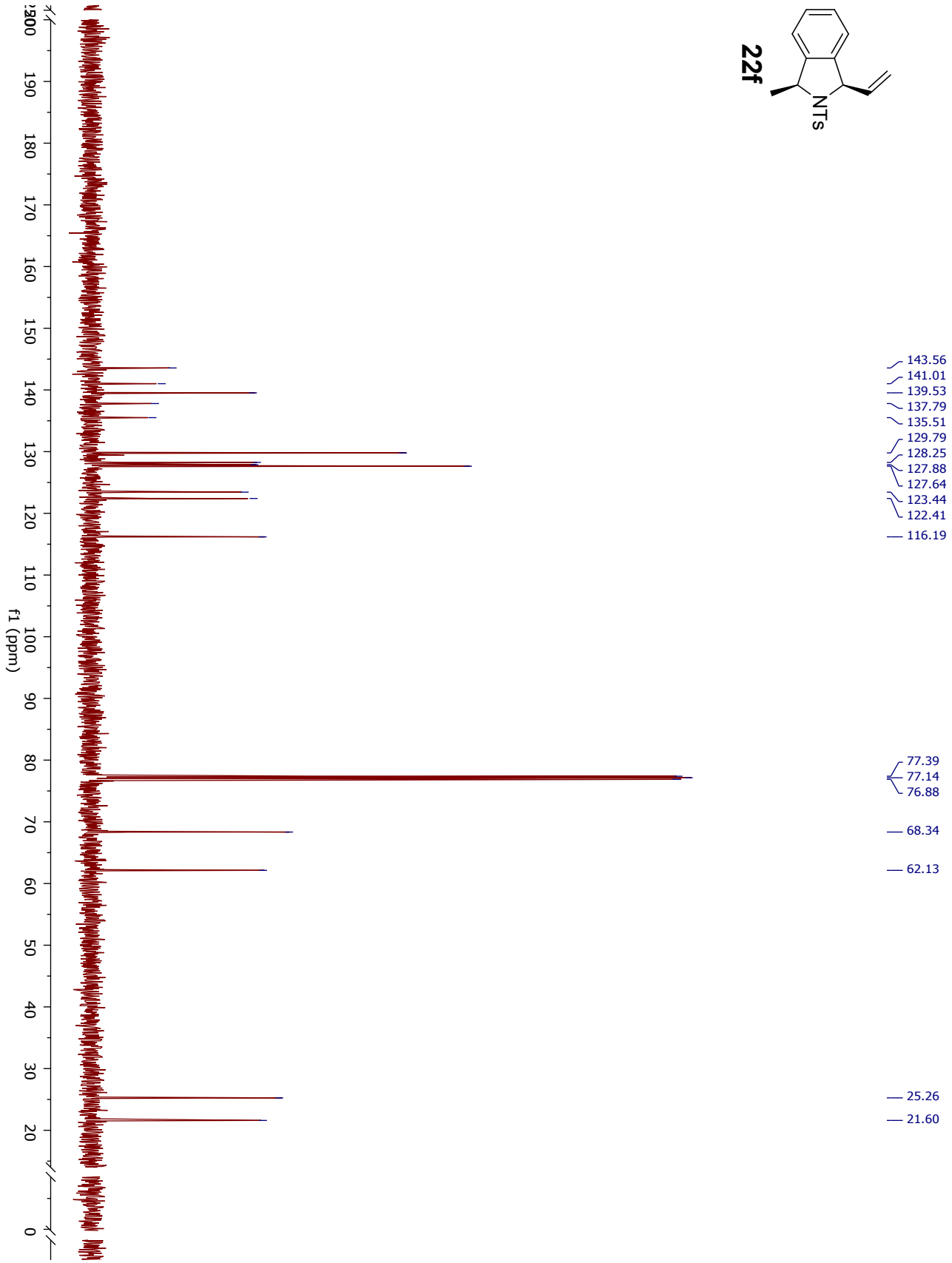

22d
NTs
f1 (ppm)
2.00
4.04
0.97
0.99
0.97
1.00
1.97
3.00
2.98
2.96
7.76
7.75
7.27
7.26
7.24
7.23
7.21
7.20
7.11
7.10
7.02
7.01
5.24
5.17
5.03
5.02
5.01
5.01
4.99
2.38
1.72
1.71
1.55
-0.00

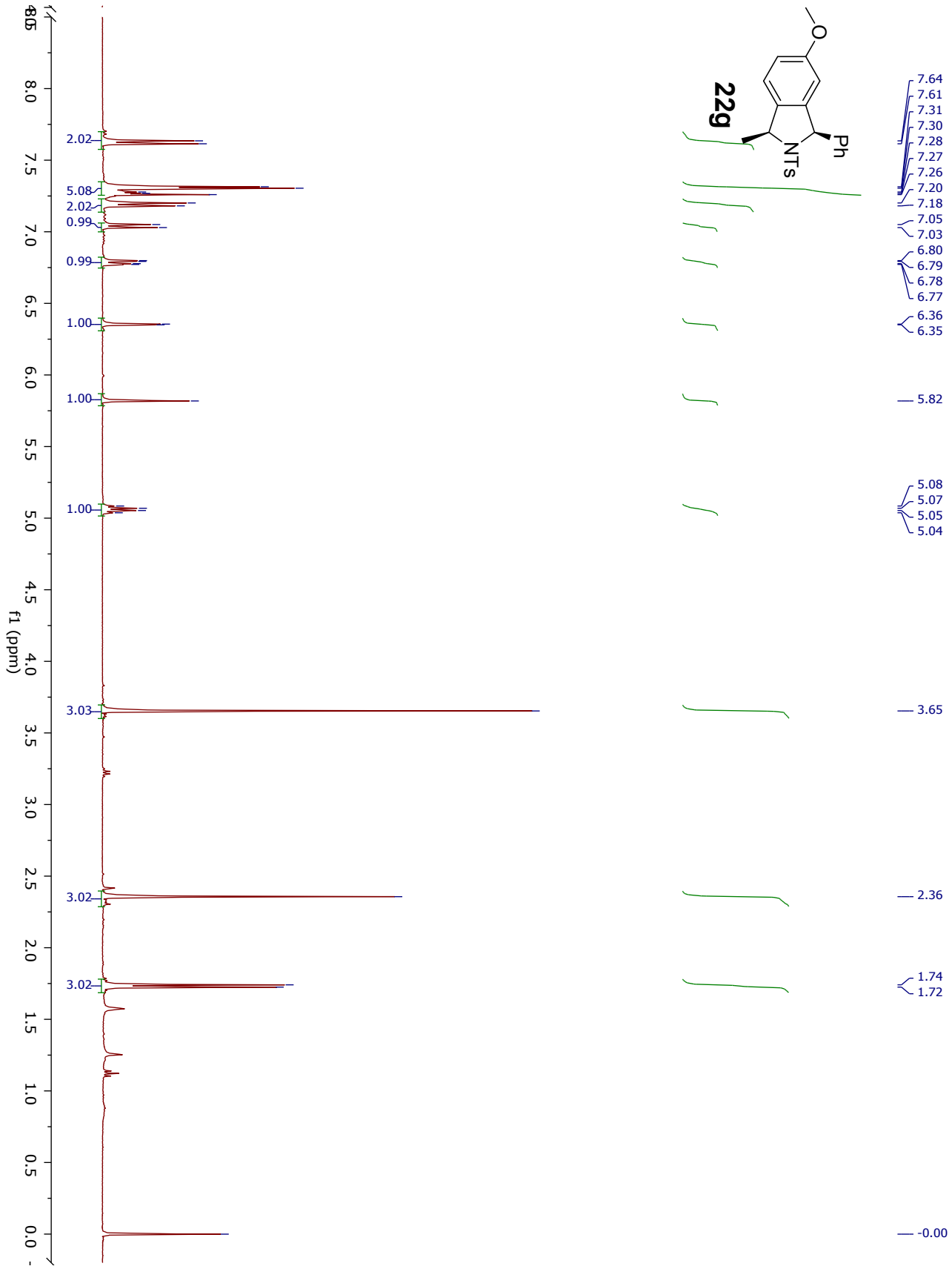

22d
NTs
144.99
143.59
141.13
137.43
135.13
129.76
128.36
127.95
127.81
122.82
122.22
114.05
77.42
77.17
76.91
72.33
62.24
24.57
21.61
17.14
f1 (ppm)

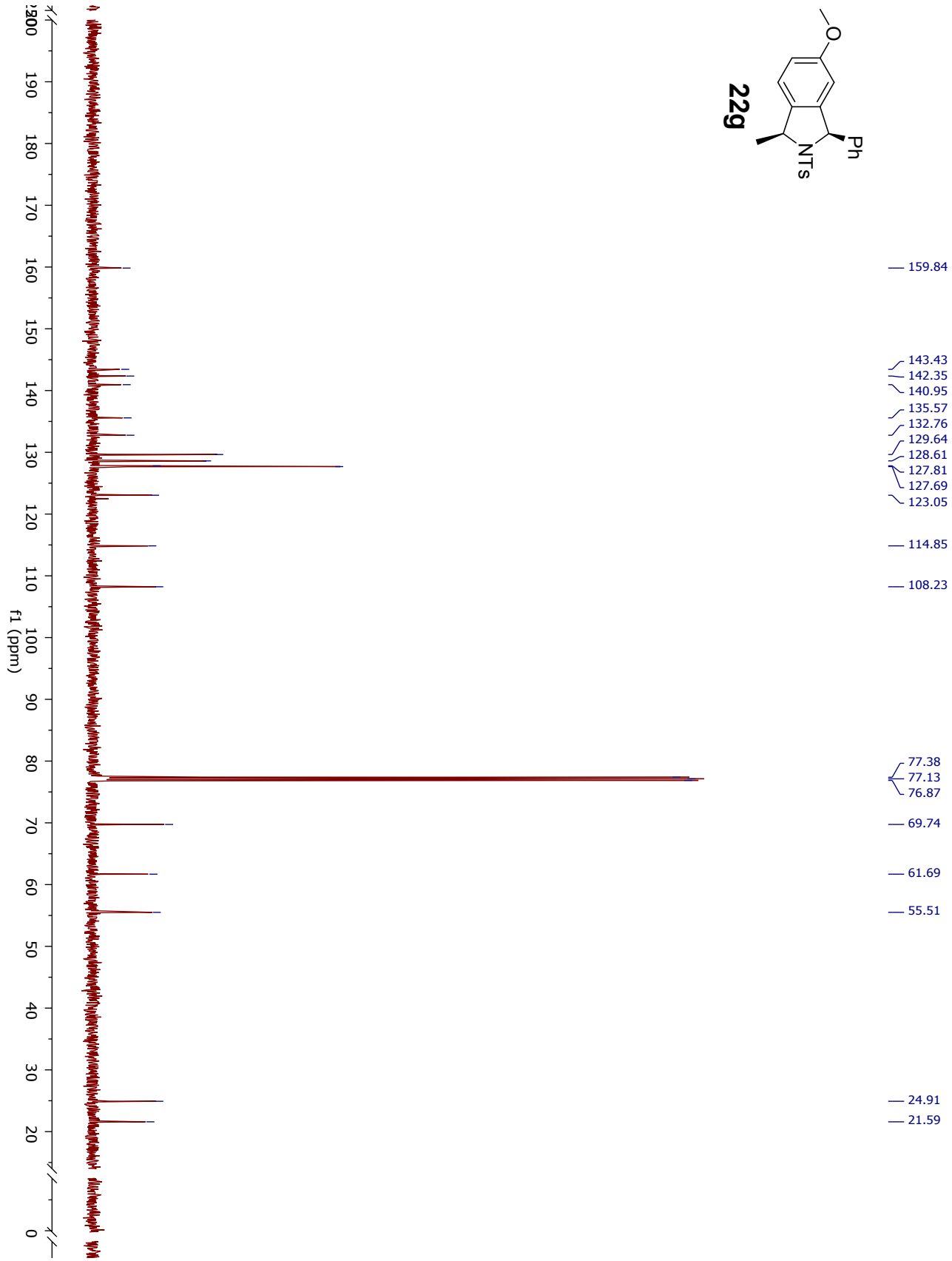

22e
Bn
NTs
f1 (ppm)
1.99
2.04
5.02
1.98
1.02
0.98
1.00
0.99
1.01
1.08
2.98
3.02
7.75
7.73
7.25
7.24
7.23
7.19
7.18
7.17
7.17
7.16
7.16
7.15
7.04
7.04
7.03
7.03
6.94
6.93
6.92
6.90
6.89
6.88
5.15
5.14
5.14
5.13
4.77
4.75
4.74
4.73
3.41
3.41
3.39
3.38
3.32
3.30
3.29
3.28
2.35
1.06
1.04
-0.00

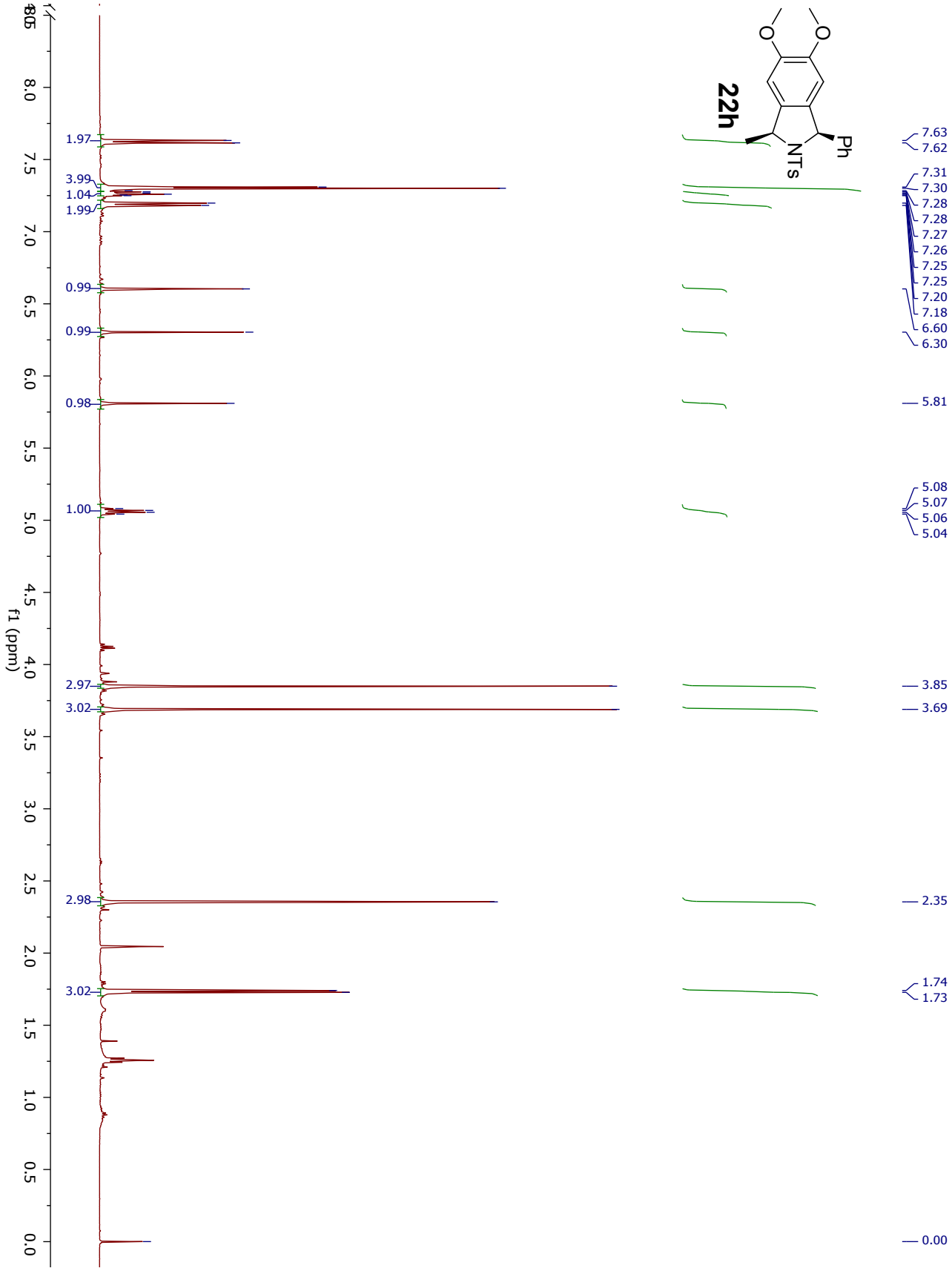

22e
Bn
NTs
143.54
141.52
138.13
136.72
134.97
130.91
129.89
127.93
127.48
127.36
126.56
123.17
122.24
77.39
77.14
76.88
66.90
62.05
43.75
24.19
21.58
f1 (ppm)

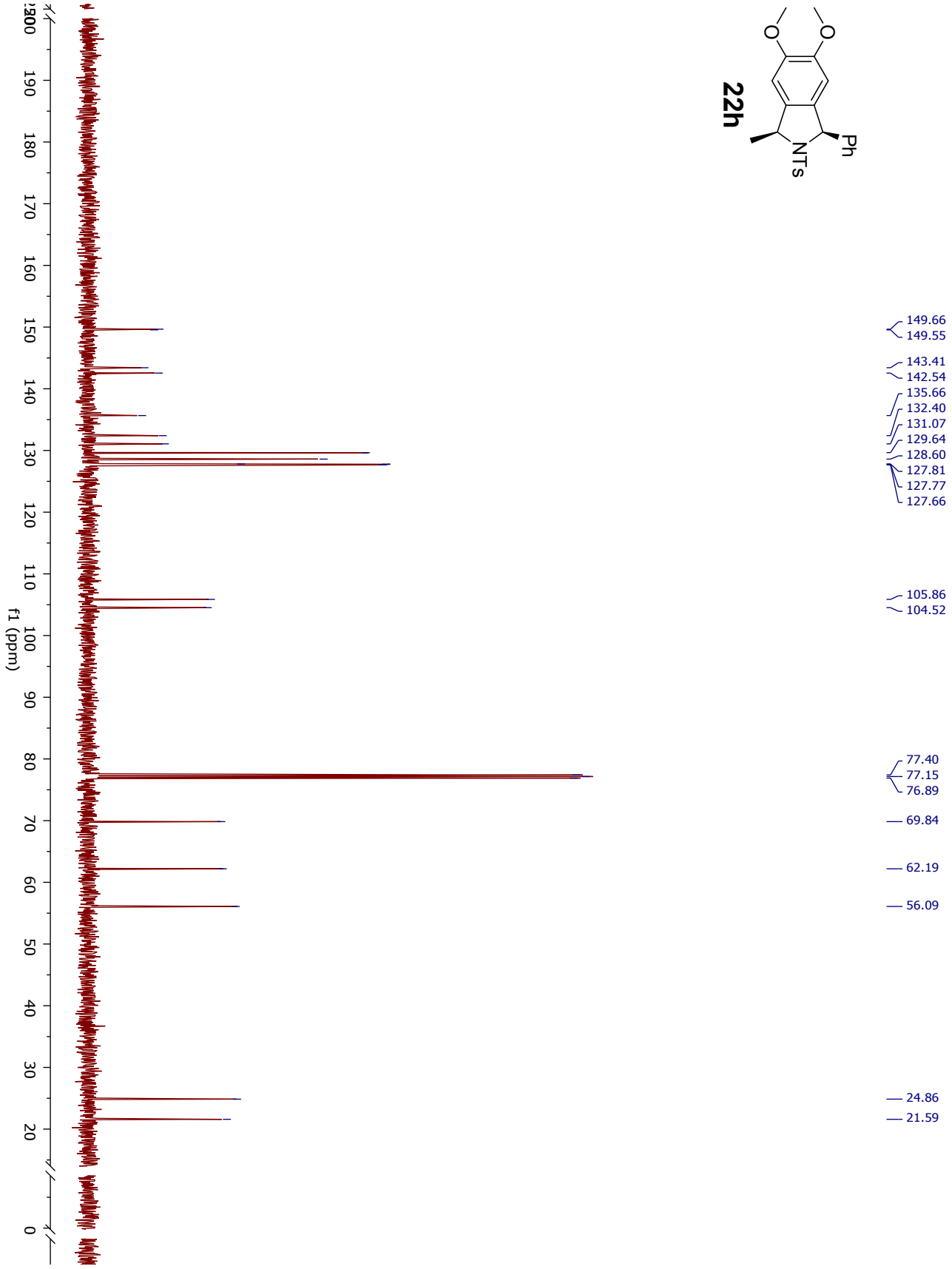

22f
NTs
f1 (ppm)
2.00
4.06
2.01
0.98
0.99
0.97
1.01
1.00
3.02
3.05
7.75
7.73
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.11
7.11
7.10
7.08
5.97
5.95
5.95
5.93
5.92
5.91
5.90
5.42
5.39
5.26
5.25
5.21
5.19
5.00
4.99
4.98
4.97
2.37
1.65
1.64
-0.00

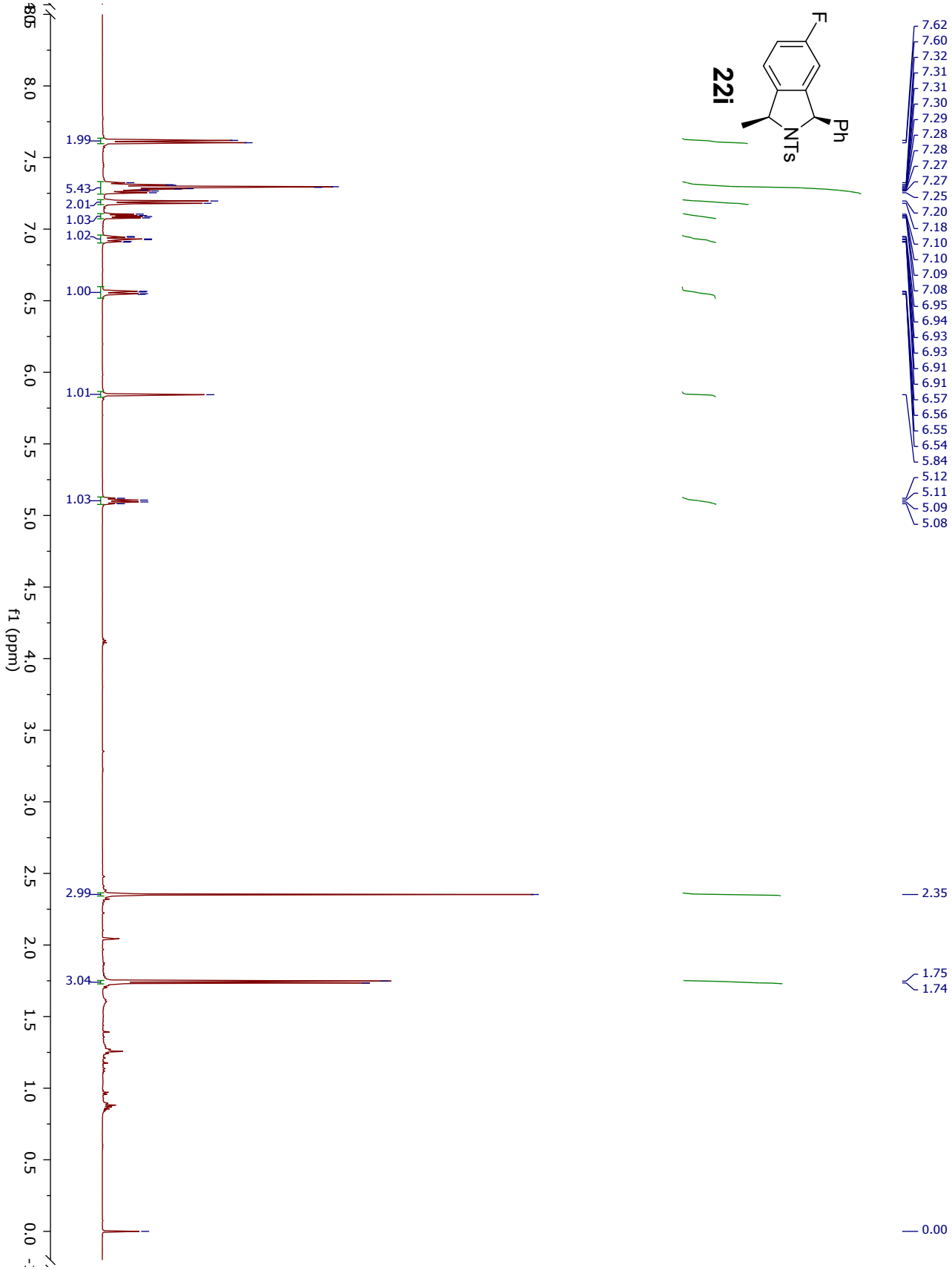

22f
NTs
143.56
141.01
139.53
137.79
135.51
129.79
128.25
127.88
127.64
123.44
122.41
116.19
77.39
77.14
76.88
68.34
62.13
25.26
21.60
f1 (ppm)

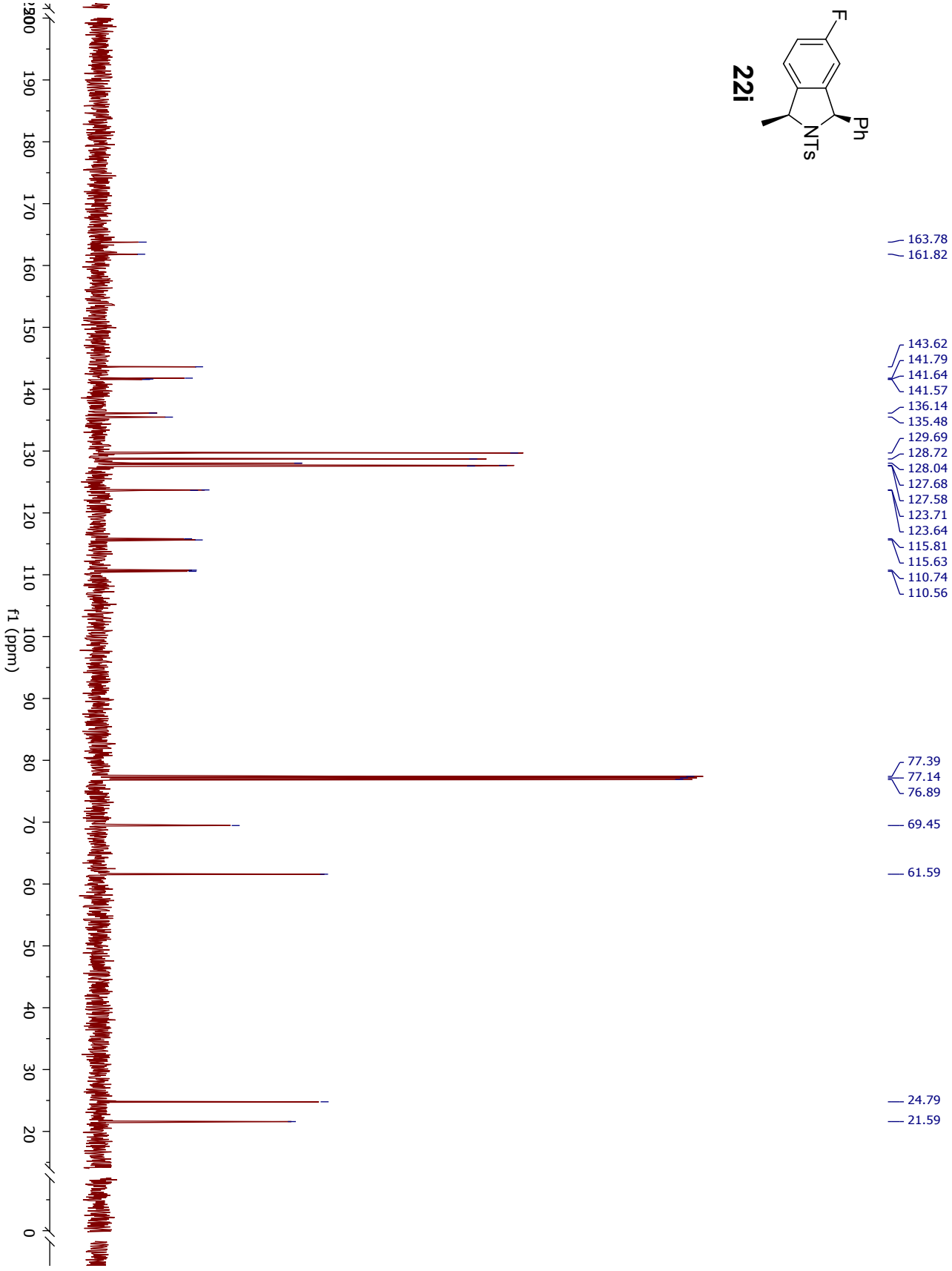

22g
O
NTs
Ph
f1 (ppm)
2.02
5.08
2.02
0.99
0.99
1.00
1.00
1.00
3.03
3.02
3.02
7.64
7.61
7.31
7.30
7.28
7.27
7.26
7.20
7.18
7.05
7.03
6.80
6.79
6.78
6.77
6.36
6.35
5.82
5.08
5.07
5.05
5.04
3.65
2.36
1.74
1.72
-0.00

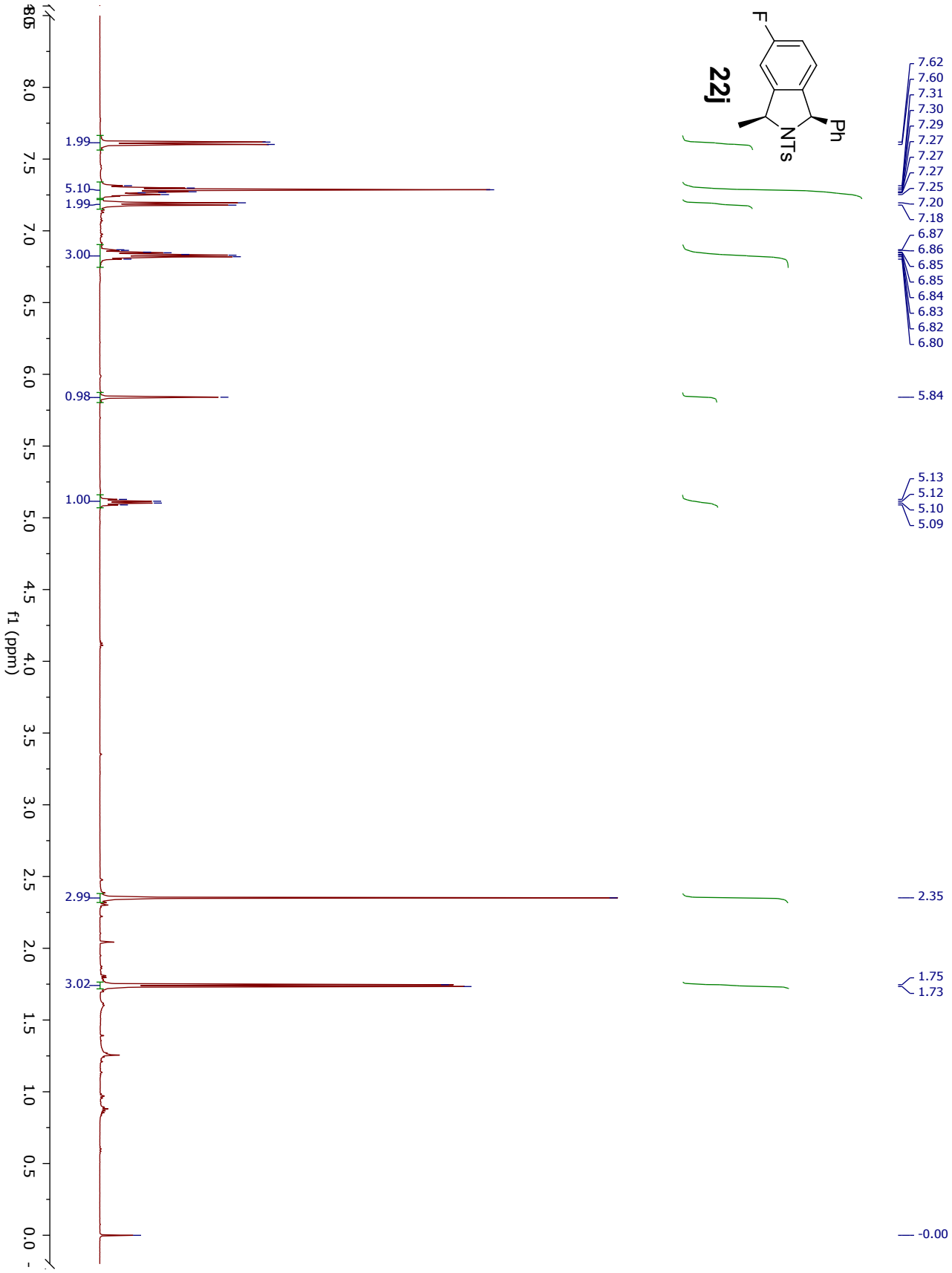

22g
O
Ph
NTs
159.84
143.43
142.35
140.95
135.57
132.76
129.64
128.61
127.81
127.69
123.05
114.85
108.23
77.38
77.13
76.87
69.74
61.69
55.51
24.91
21.59
f1 (ppm)

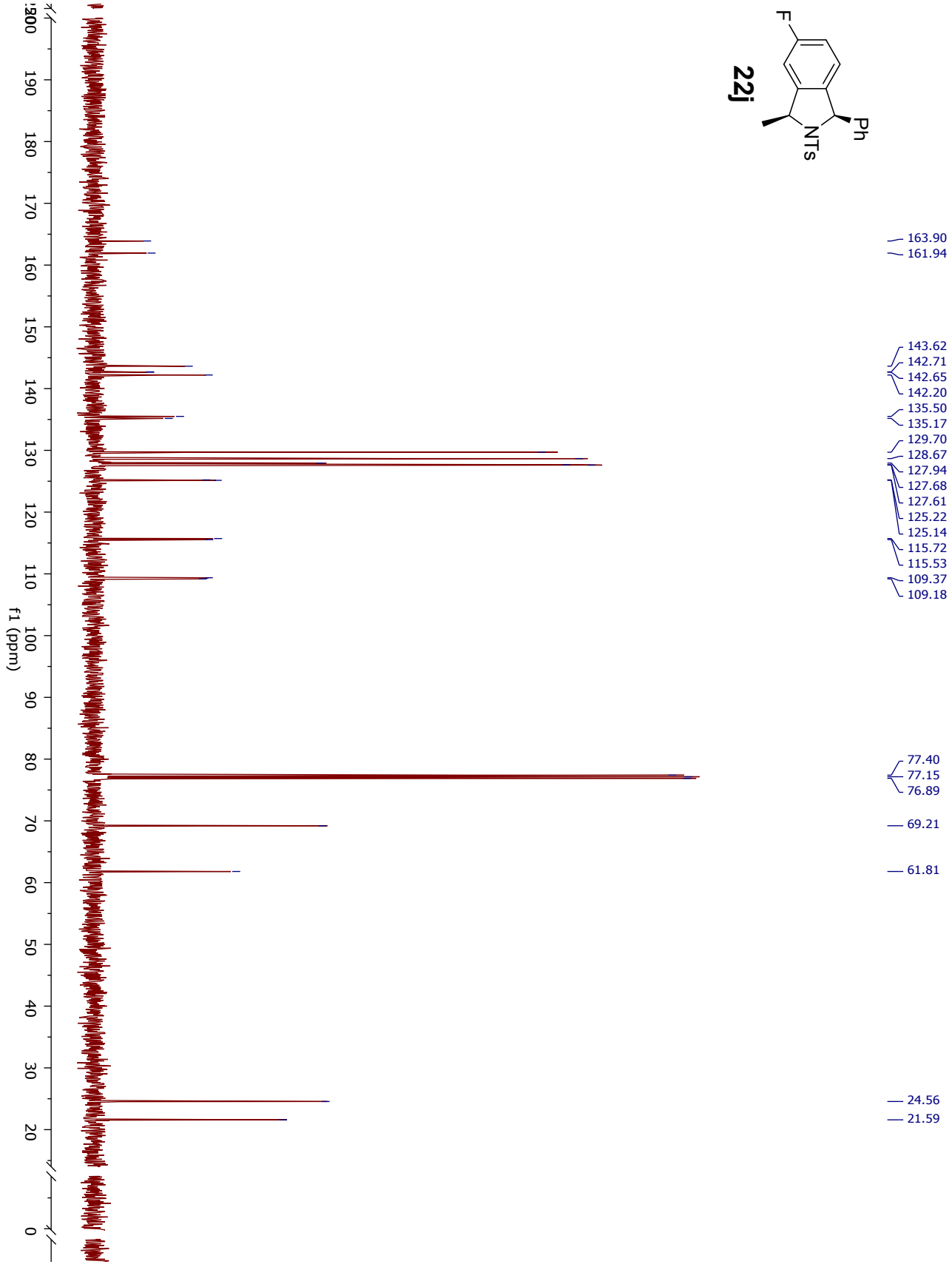

22h
O
O
Ph
NTs
1.97
3.99
1.04
1.99
0.99
0.99
0.98
1.00
2.97
3.02
2.98
3.02
7.63
7.62
7.31
7.30
7.28
7.28
7.27
7.26
7.25
7.25
7.20
7.18
6.60
6.30
5.81
5.08
5.07
5.06
5.04
3.85
3.69
2.35
1.74
1.73
0.00
f1 (ppm)

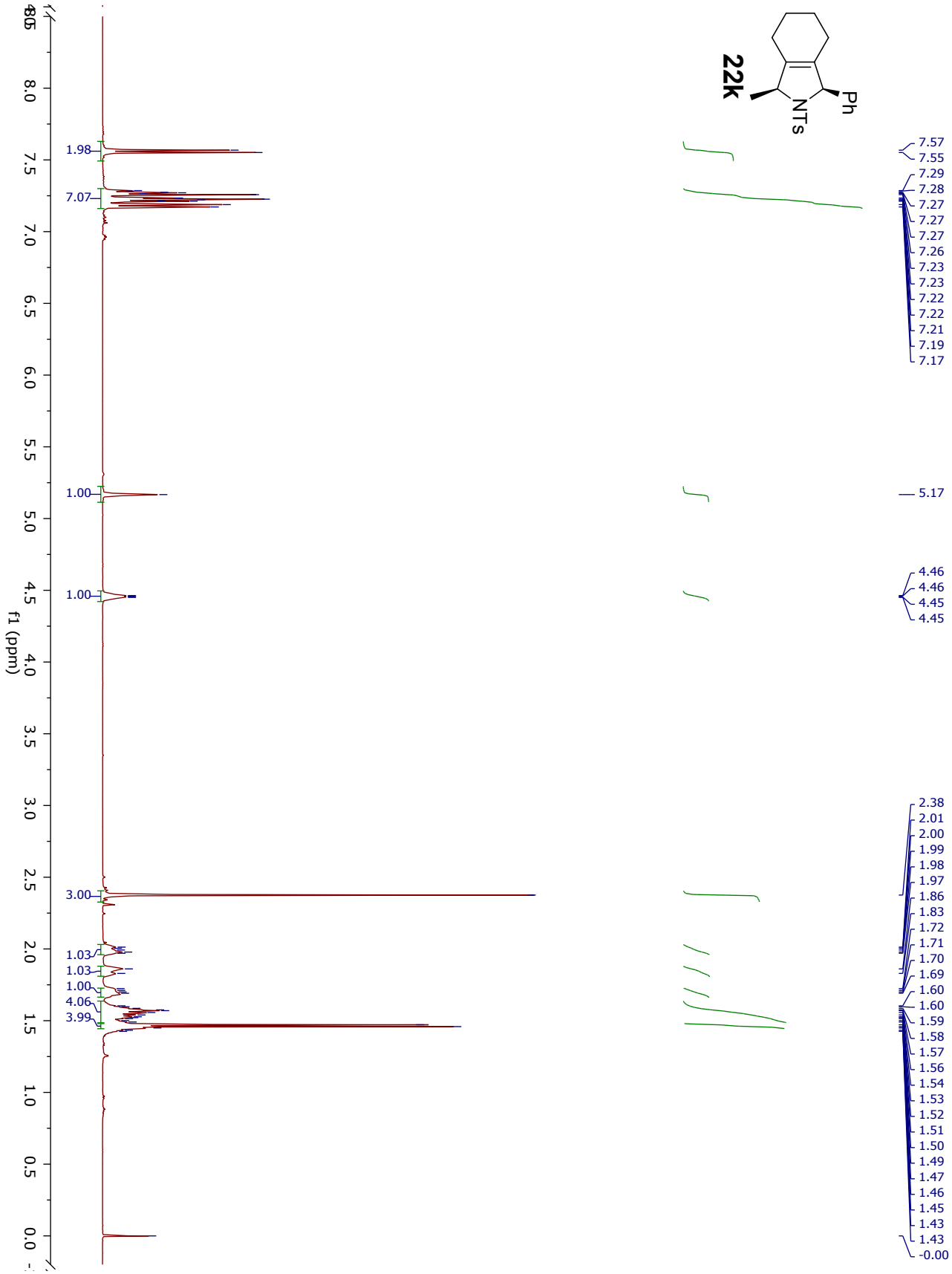

22h
O
O
Ph
NTs
149.66
149.55
143.41
142.54
135.66
132.40
131.07
129.64
128.60
127.81
127.77
127.66
105.86
104.52
77.40
77.15
76.89
69.84
62.19
56.09
24.86
21.59
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0

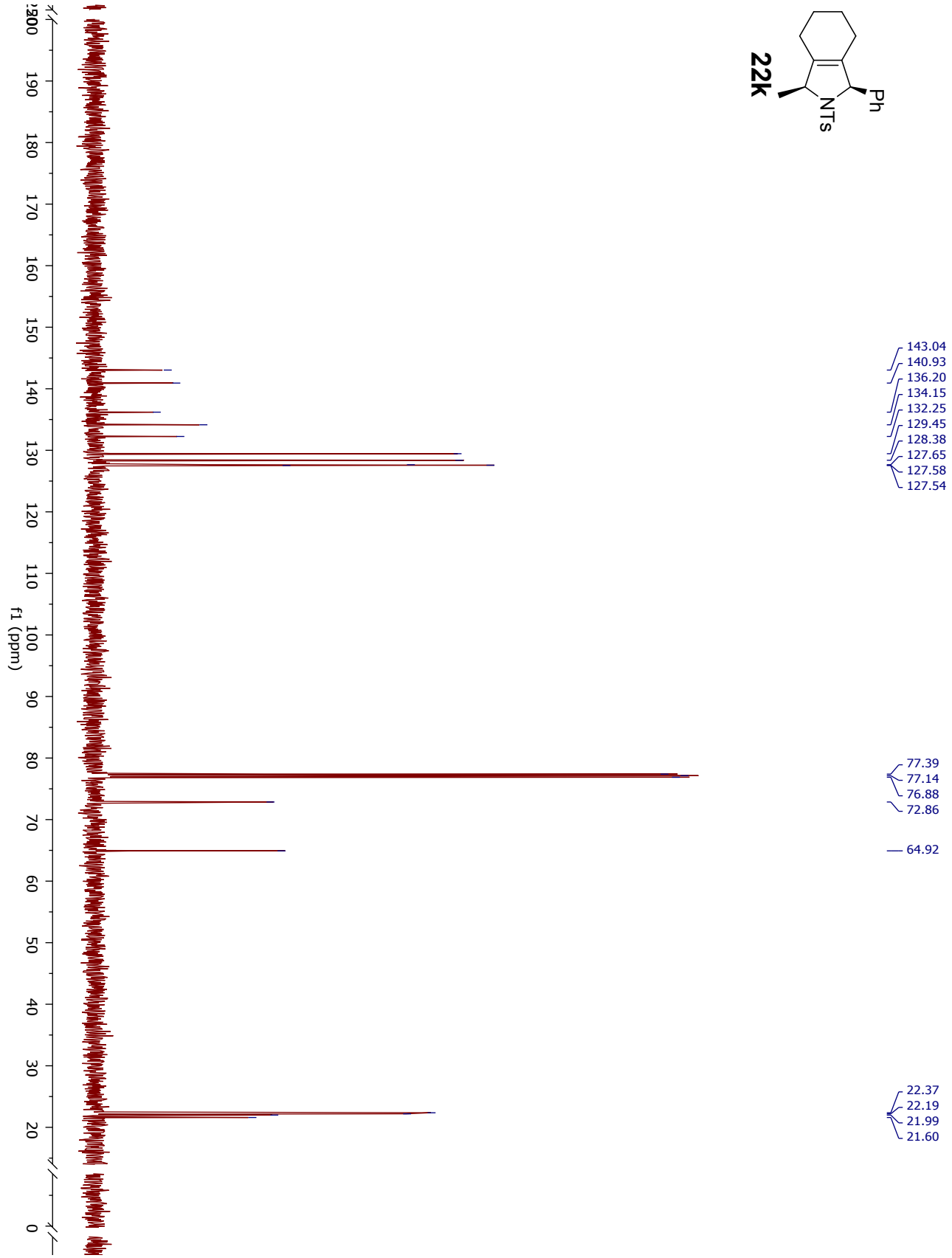

22i
F
Ph
NTs
f1 (ppm)
1.99
5.43
2.01
1.03
1.02
1.00
1.01
1.03
2.99
3.04
7.62
7.60
7.32
7.31
7.31
7.30
7.29
7.28
7.28
7.27
7.27
7.25
7.20
7.18
7.10
7.10
7.09
7.08
6.95
6.94
6.93
6.93
6.91
6.91
6.57
6.56
6.55
6.54
5.84
5.12
5.11
5.09
5.08
2.35
1.75
1.74
0.00

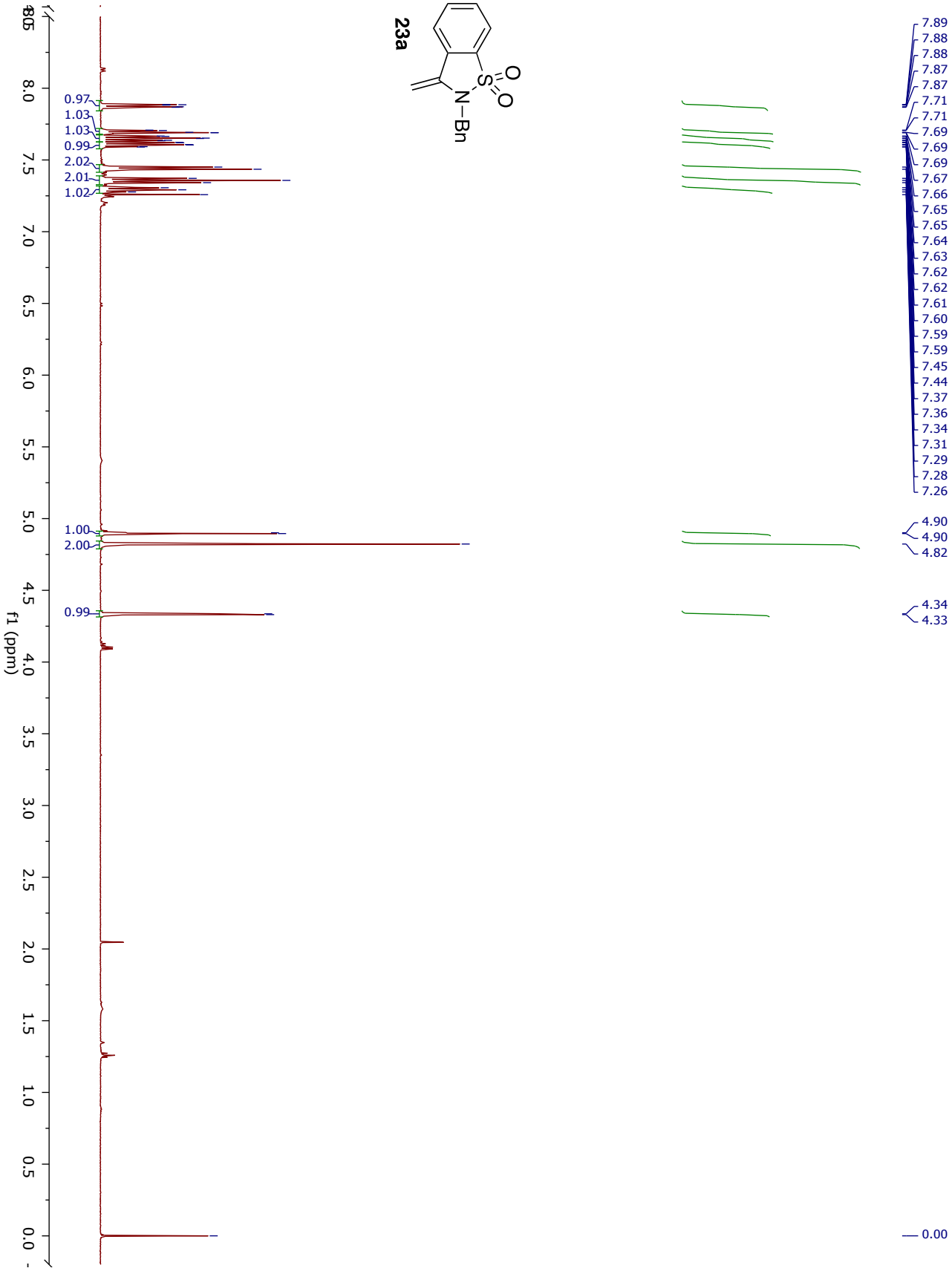

22i
F
Ph
NTs
163.78
161.82
143.62
141.79
141.64
141.57
136.14
135.48
129.69
128.72
128.04
127.68
127.58
123.71
123.64
115.81
115.63
110.74
110.56
77.39
77.14
76.89
69.45
61.59
24.79
21.59
f1 (ppm)

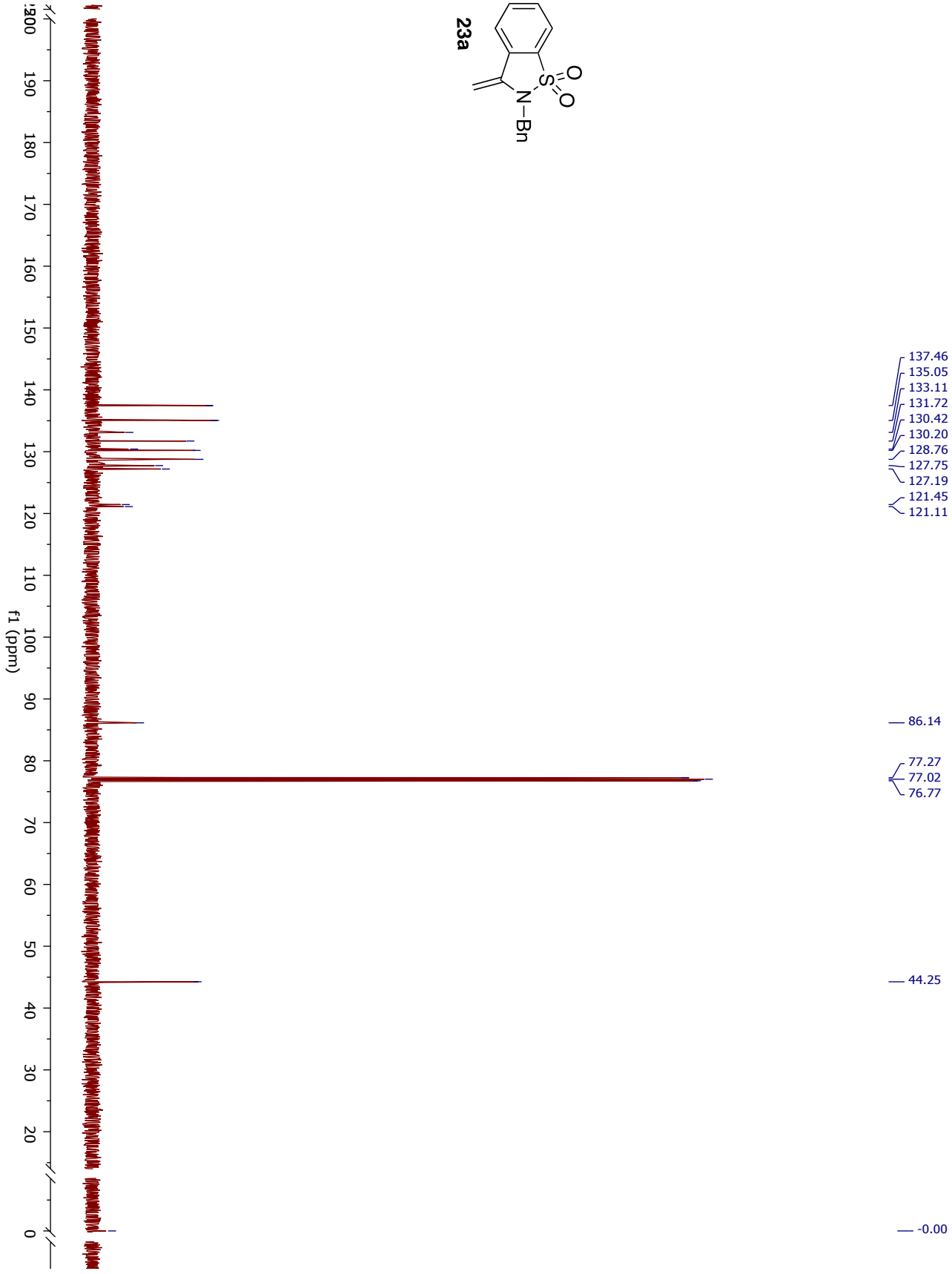

22j
F
Ph
NTs
f1 (ppm)
1.99
5.10
1.99
3.00
0.98
1.00
2.99
3.02
7.62
7.60
7.31
7.30
7.29
7.27
7.27
7.27
7.25
7.20
7.18
6.87
6.86
6.85
6.85
6.84
6.83
6.82
6.80
5.84
5.13
5.12
5.10
5.09
2.35
1.75
1.73
-0.00

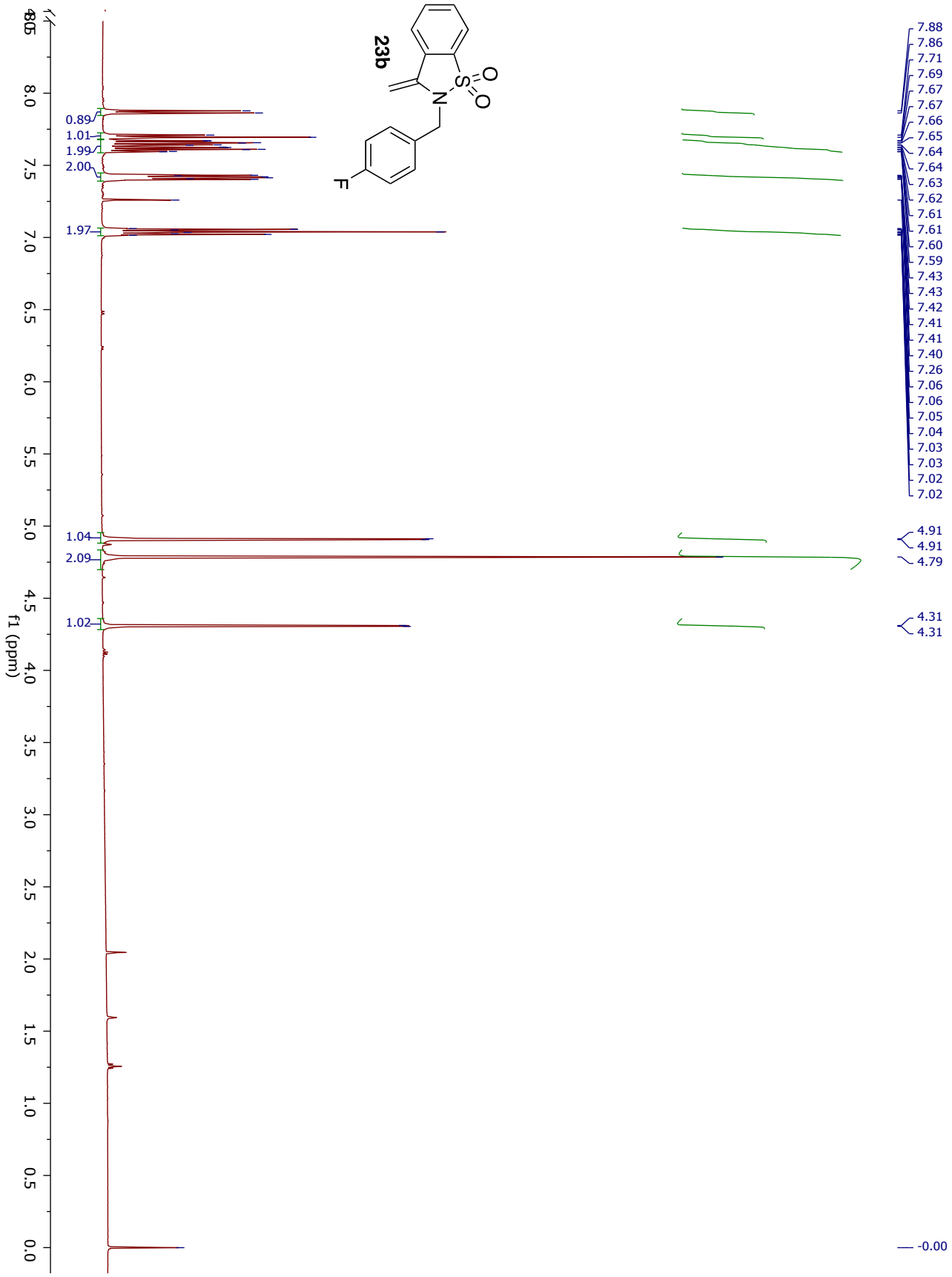

22j
F
Ph
NTs
163.90
161.94
143.62
142.71
142.65
142.20
135.50
135.17
129.70
128.67
127.94
127.68
127.61
125.22
125.14
115.72
115.53
109.37
109.18
77.40
77.15
76.89
69.21
61.81
24.56
21.59
f1 (ppm)

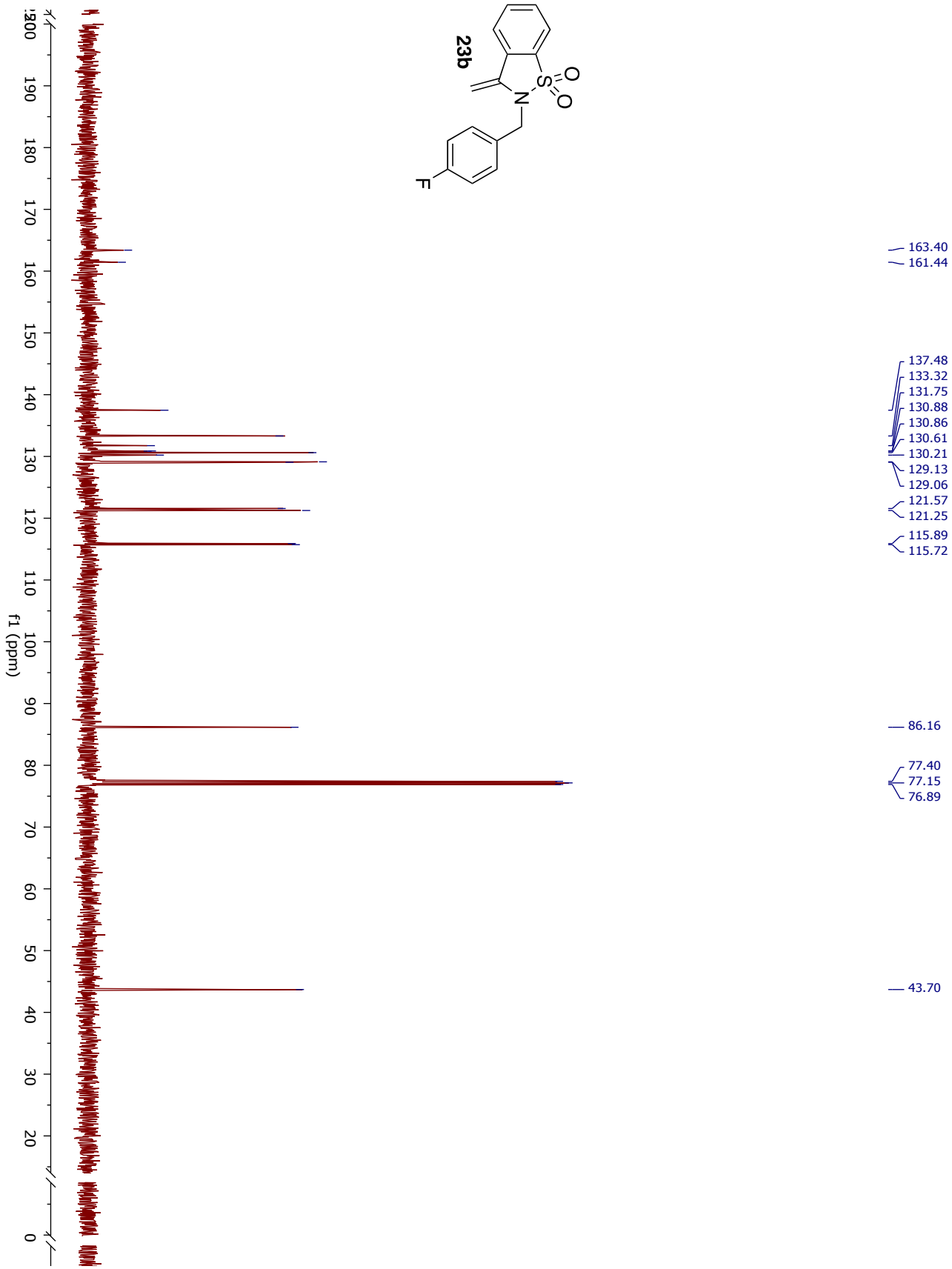

22k
Ph
NTs
f1 (ppm)
1.98
7.07
1.00
1.00
3.00
1.03
1.03
1.00
4.06
3.99
7.57
7.55
7.29
7.28
7.27
7.27
7.27
7.26
7.23
7.23
7.22
7.22
7.21
7.19
7.17
5.17
4.46
4.46
4.45
4.45
2.38
2.01
2.00
1.99
1.98
1.97
1.86
1.83
1.72
1.71
1.70
1.69
1.60
1.60
1.59
1.58
1.57
1.56
1.54
1.53
1.52
1.51
1.50
1.49
1.47
1.46
1.45
1.43
1.43
-0.00

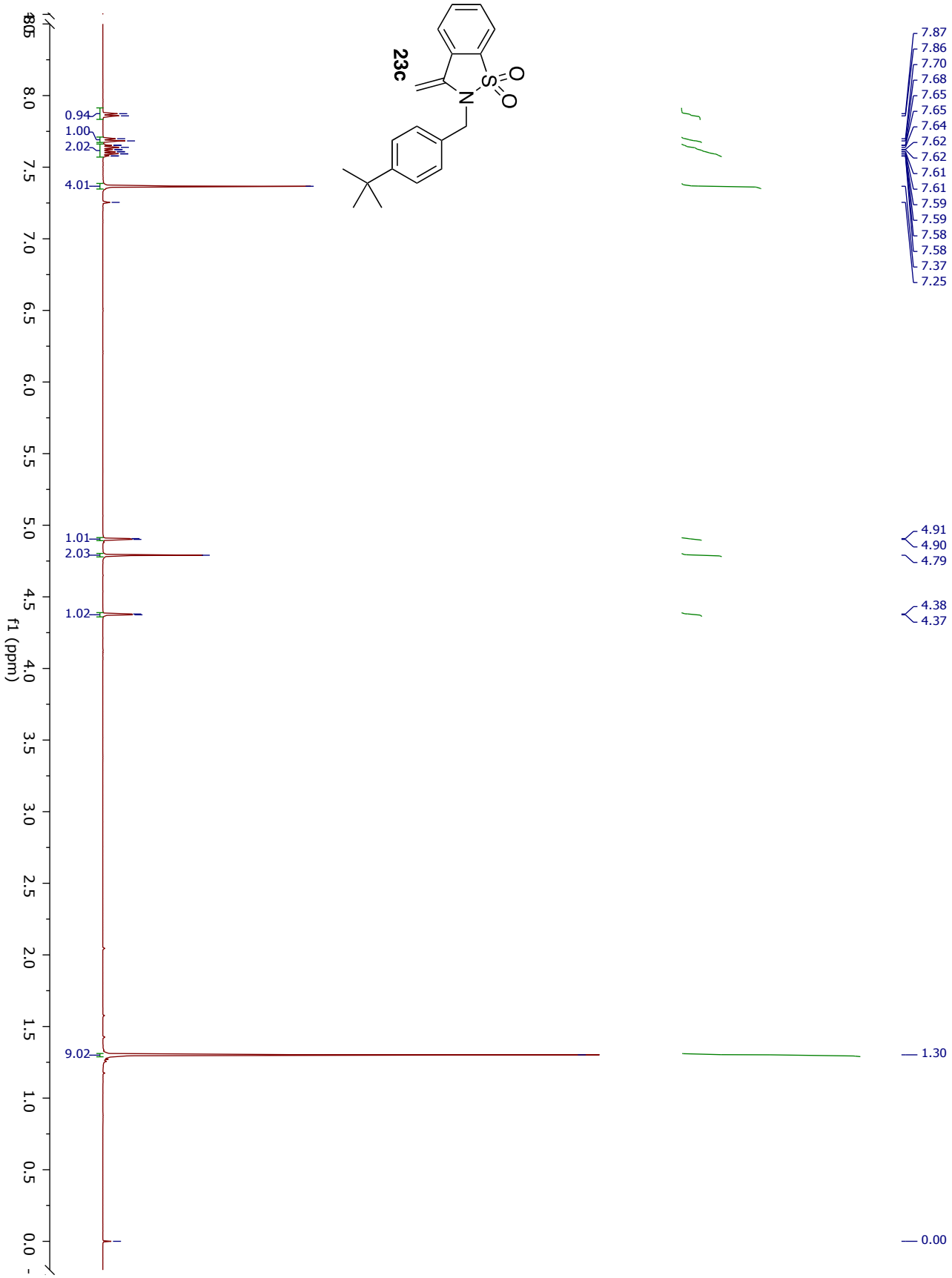

22k
NTs
Ph
143.04
140.93
136.20
134.15
132.25
129.45
128.38
127.65
127.58
127.54
77.39
77.14
76.88
72.86
64.92
22.37
22.19
21.99
21.60
f1 (ppm)

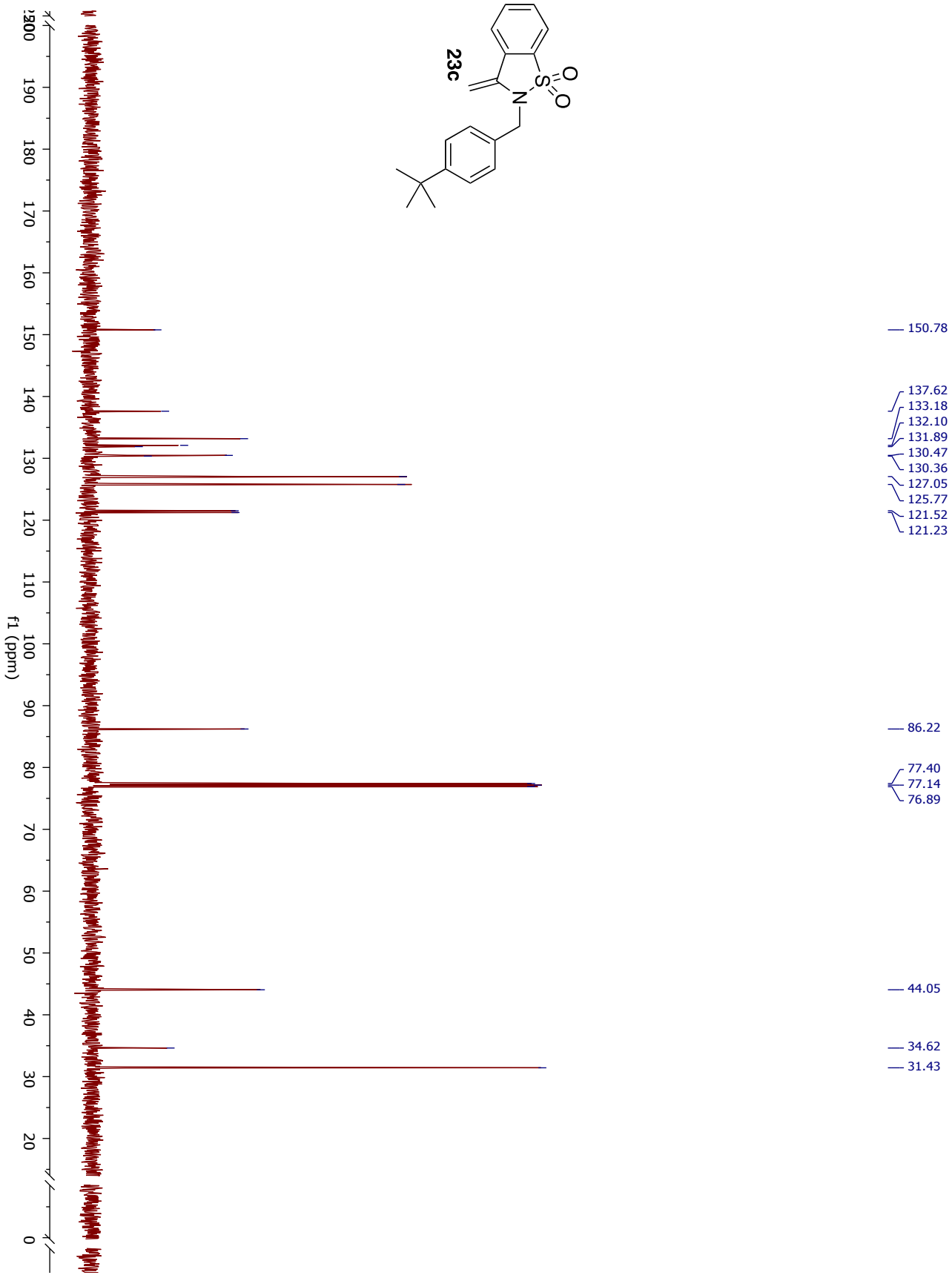

23a
O
S
O
N–Bn
0.97
1.03
1.03
0.99
2.02
2.01
1.02
1.00
2.00
0.99
7.89
7.88
7.88
7.87
7.87
7.71
7.71
7.69
7.69
7.69
7.67
7.66
7.65
7.65
7.64
7.63
7.62
7.62
7.61
7.60
7.59
7.59
7.45
7.44
7.37
7.36
7.34
7.31
7.29
7.28
7.26
4.90
4.90
4.82
4.34
4.33
0.00
f1 (ppm)

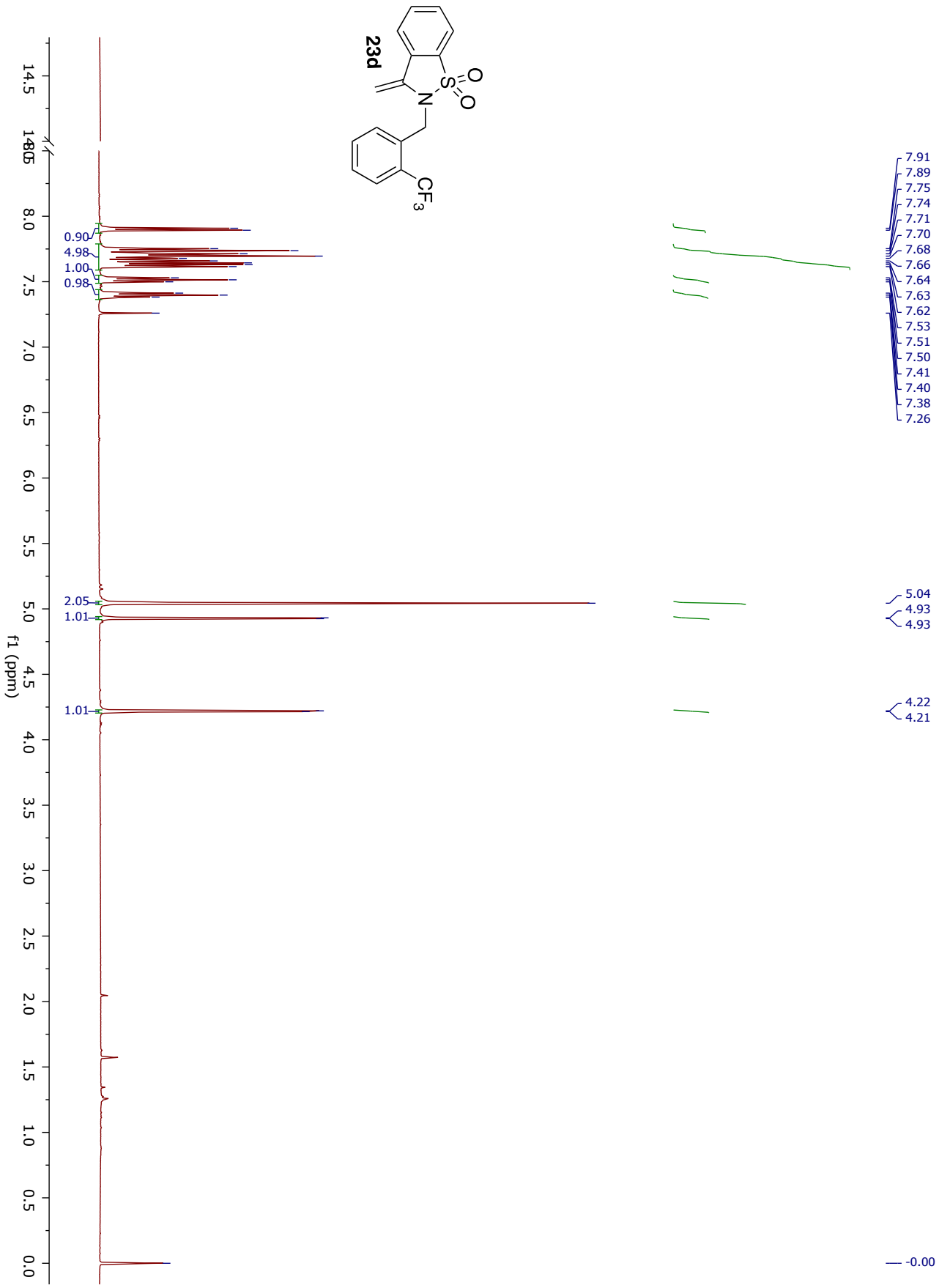

23a
O
S
O
N
Bn
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
137.46
135.05
133.11
131.72
130.42
130.20
128.76
127.75
127.19
121.45
121.11
86.14
77.27
77.02
76.77
44.25
-0.00

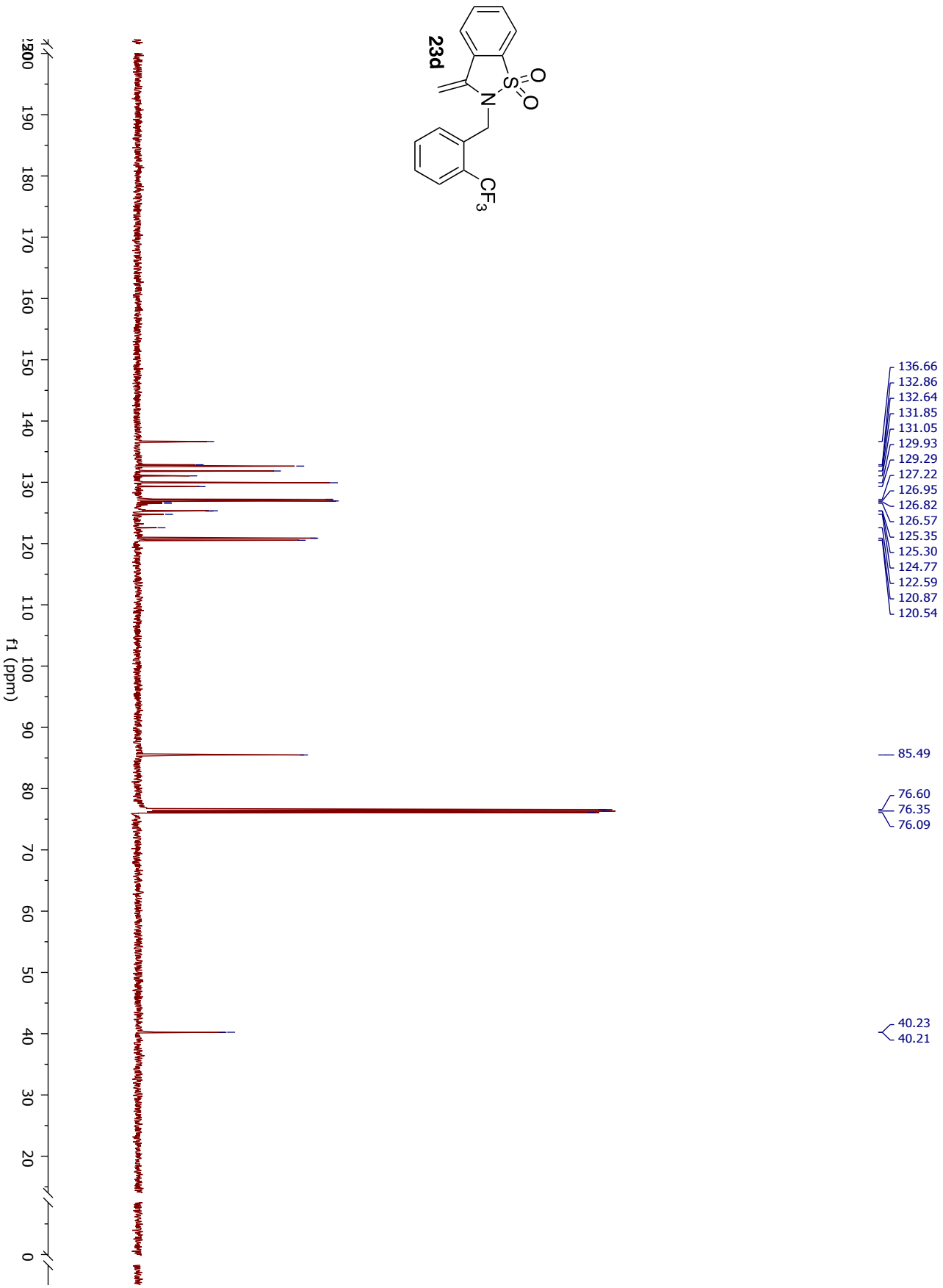

23b
O
S
O
N
F
0.89
1.01
1.99
2.00
1.97
1.04
2.09
1.02
7.88
7.86
7.71
7.69
7.67
7.67
7.66
7.65
7.64
7.64
7.63
7.62
7.61
7.61
7.60
7.59
7.43
7.43
7.42
7.41
7.41
7.40
7.26
7.06
7.06
7.05
7.04
7.03
7.03
7.02
7.02
4.91
4.91
4.79
4.31
4.31
-0.00
f1 (ppm)

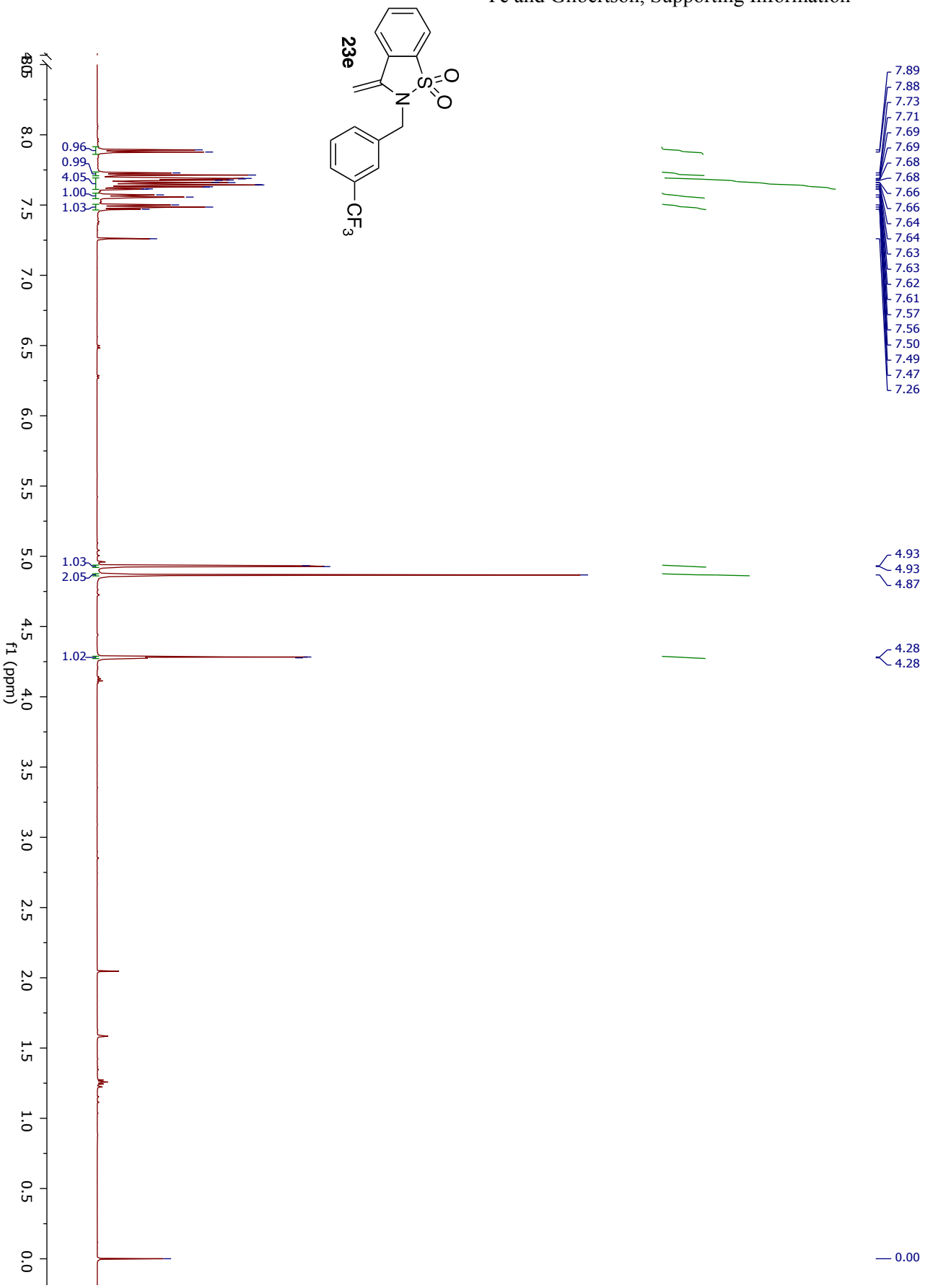

23b
O
S
O
N
F
163.40
161.44
137.48
133.32
131.75
130.88
130.86
130.61
130.21
129.13
129.06
121.57
121.25
115.89
115.72
86.16
77.40
77.15
76.89
43.70
f1 (ppm)

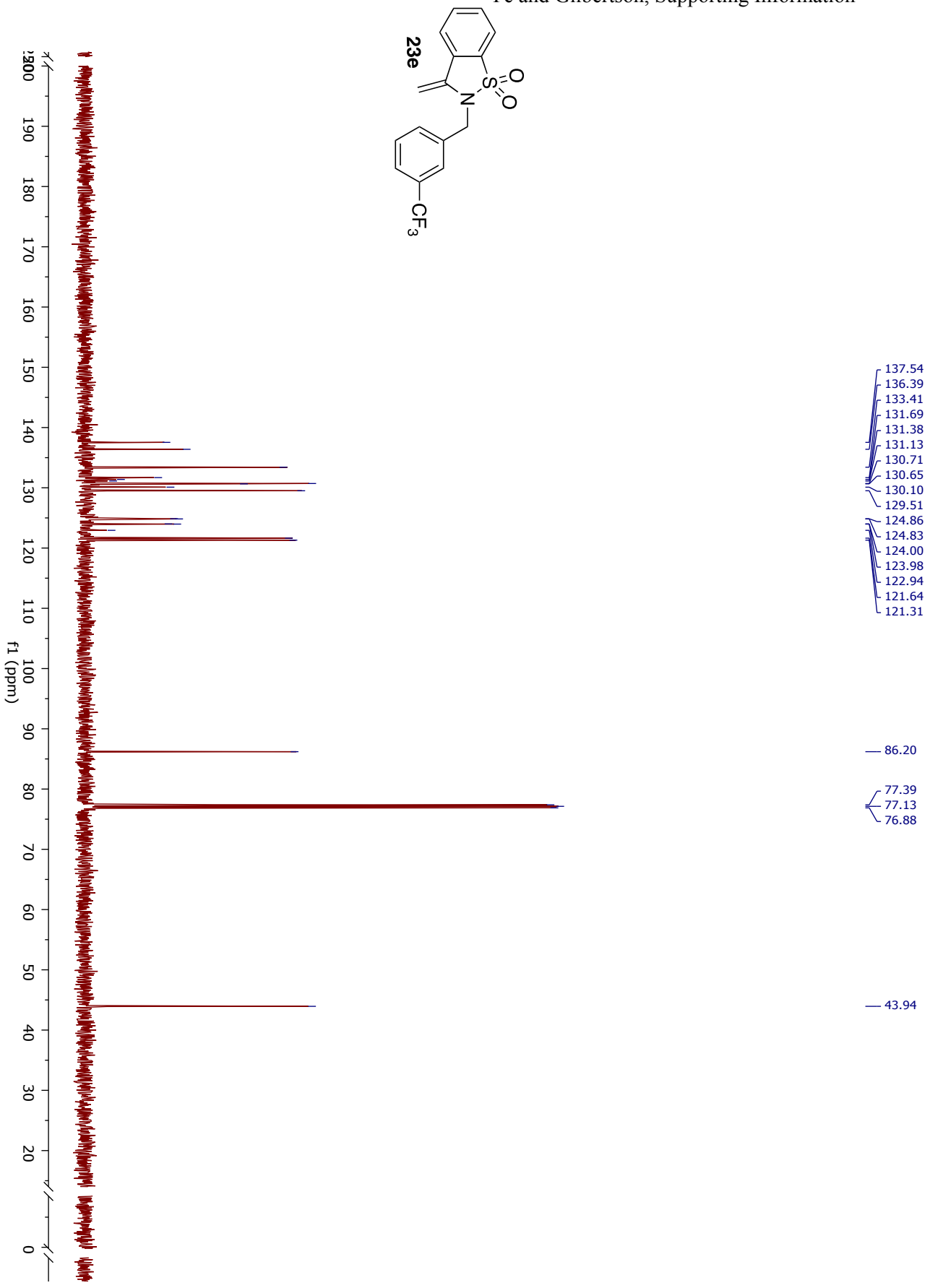

23c
O
S
O
N
0.94
1.00
2.02
4.01
1.01
2.03
1.02
9.02
7.87
7.86
7.70
7.68
7.65
7.65
7.64
7.62
7.62
7.61
7.61
7.59
7.59
7.58
7.58
7.37
7.25
4.91
4.90
4.79
4.38
4.37
1.30
0.00
f1 (ppm)

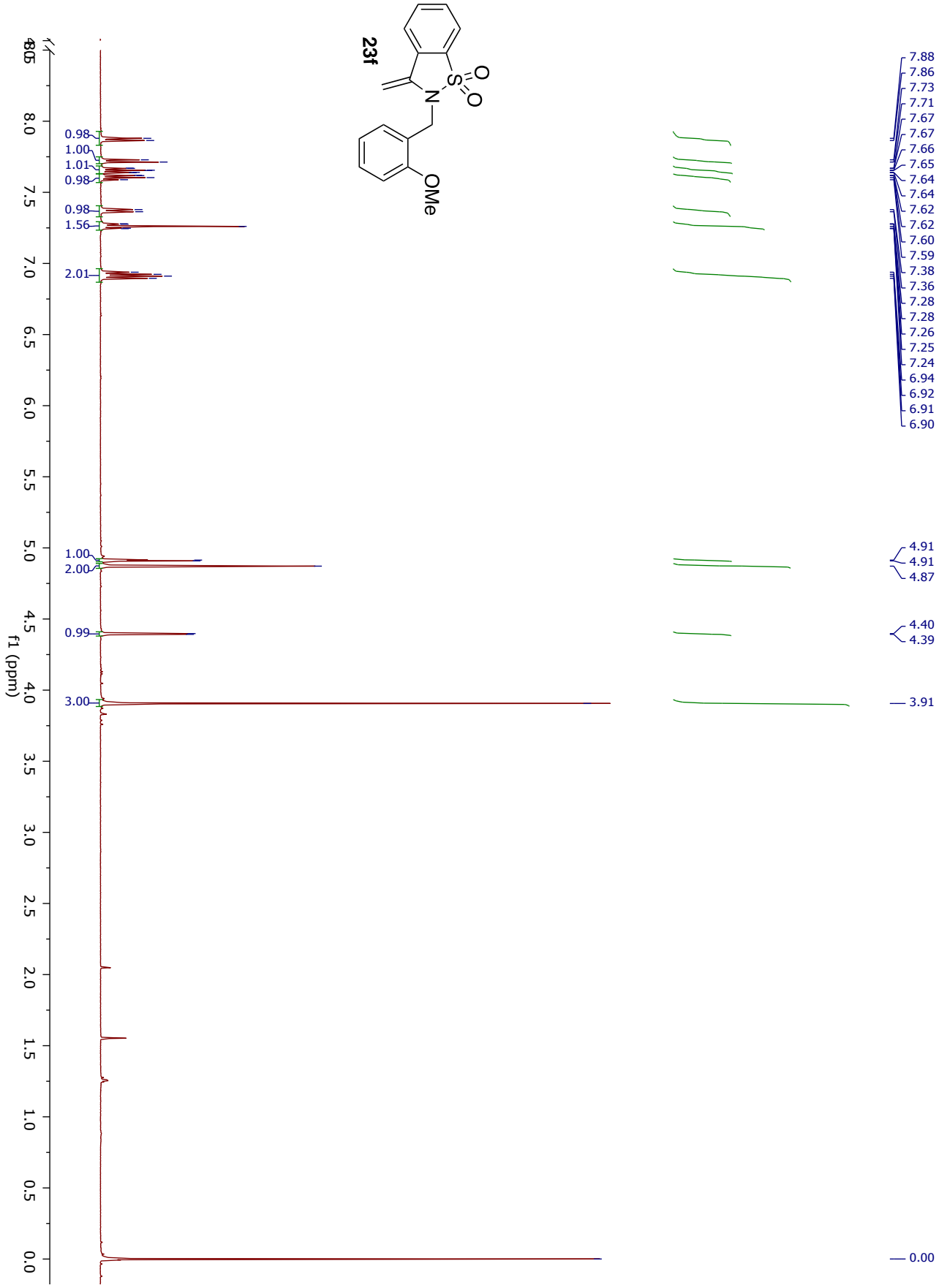

23c
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
150.78
137.62
133.18
132.10
131.89
130.47
130.36
127.05
125.77
121.52
121.23
86.22
77.40
77.14
76.89
44.05
34.62
31.43

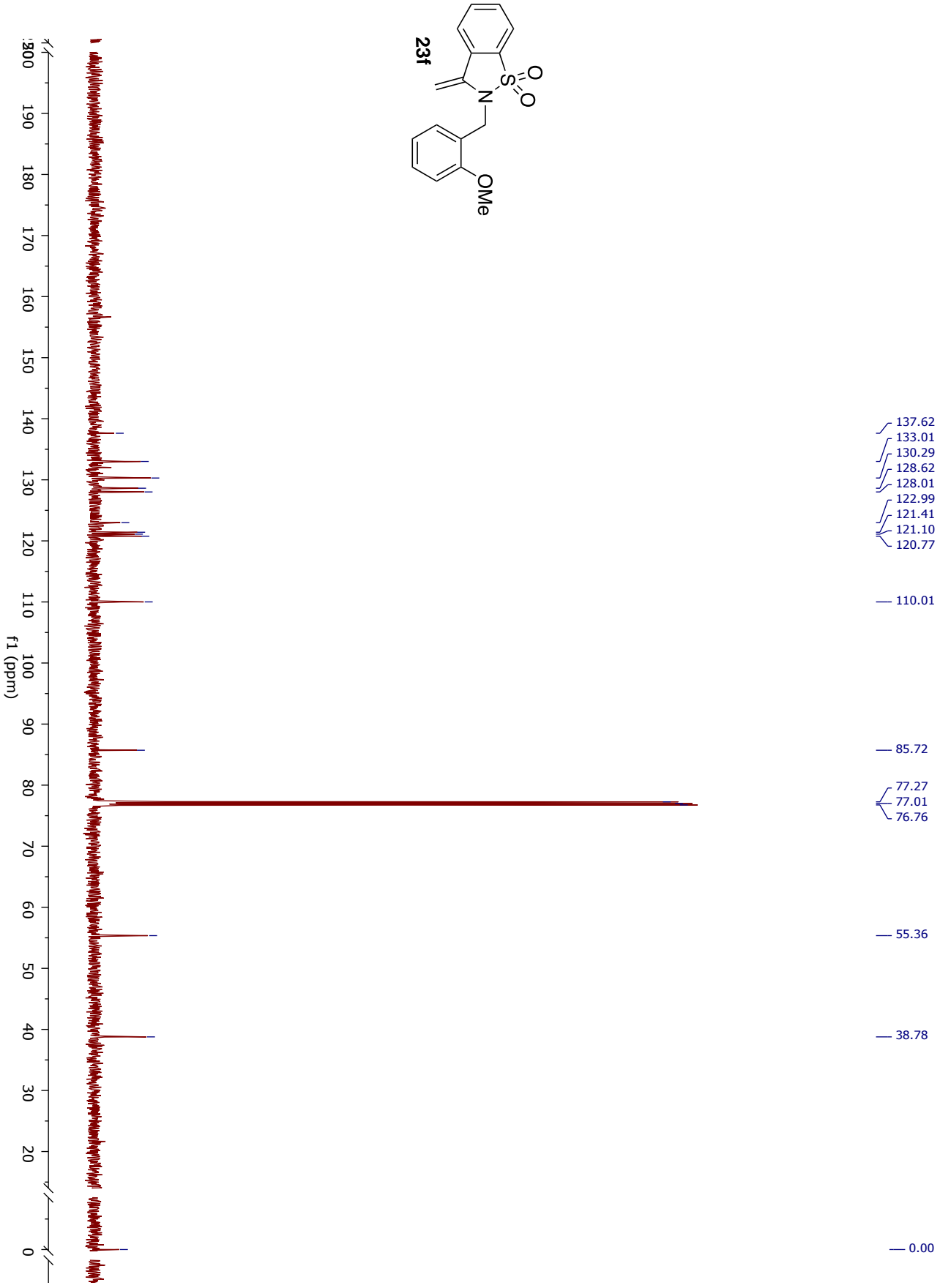

23d
O
S
O
N
CF3
f1 (ppm)
14.5
14.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.90
4.98
1.00
0.98
2.05
1.01
1.01
7.91
7.89
7.75
7.74
7.71
7.70
7.68
7.66
7.64
7.63
7.62
7.53
7.51
7.50
7.41
7.40
7.38
7.26
5.04
4.93
4.93
4.22
4.21
-0.00

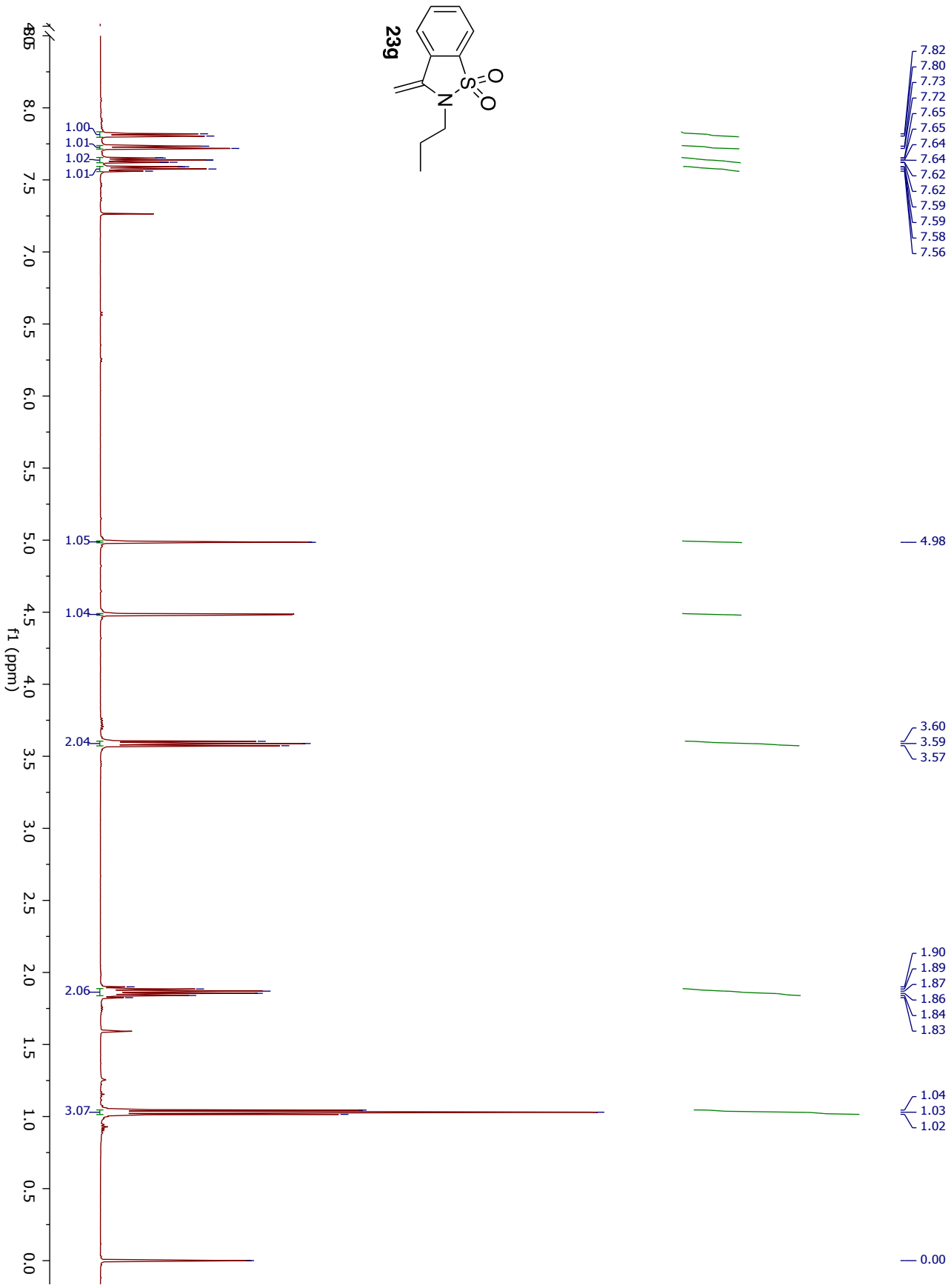

23d
O
S
O
N
CF3
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
136.66
132.86
132.64
131.85
131.05
129.93
129.29
127.22
126.95
126.82
126.57
125.35
125.30
124.77
122.59
120.87
120.54
85.49
76.60
76.35
76.09
40.23
40.21

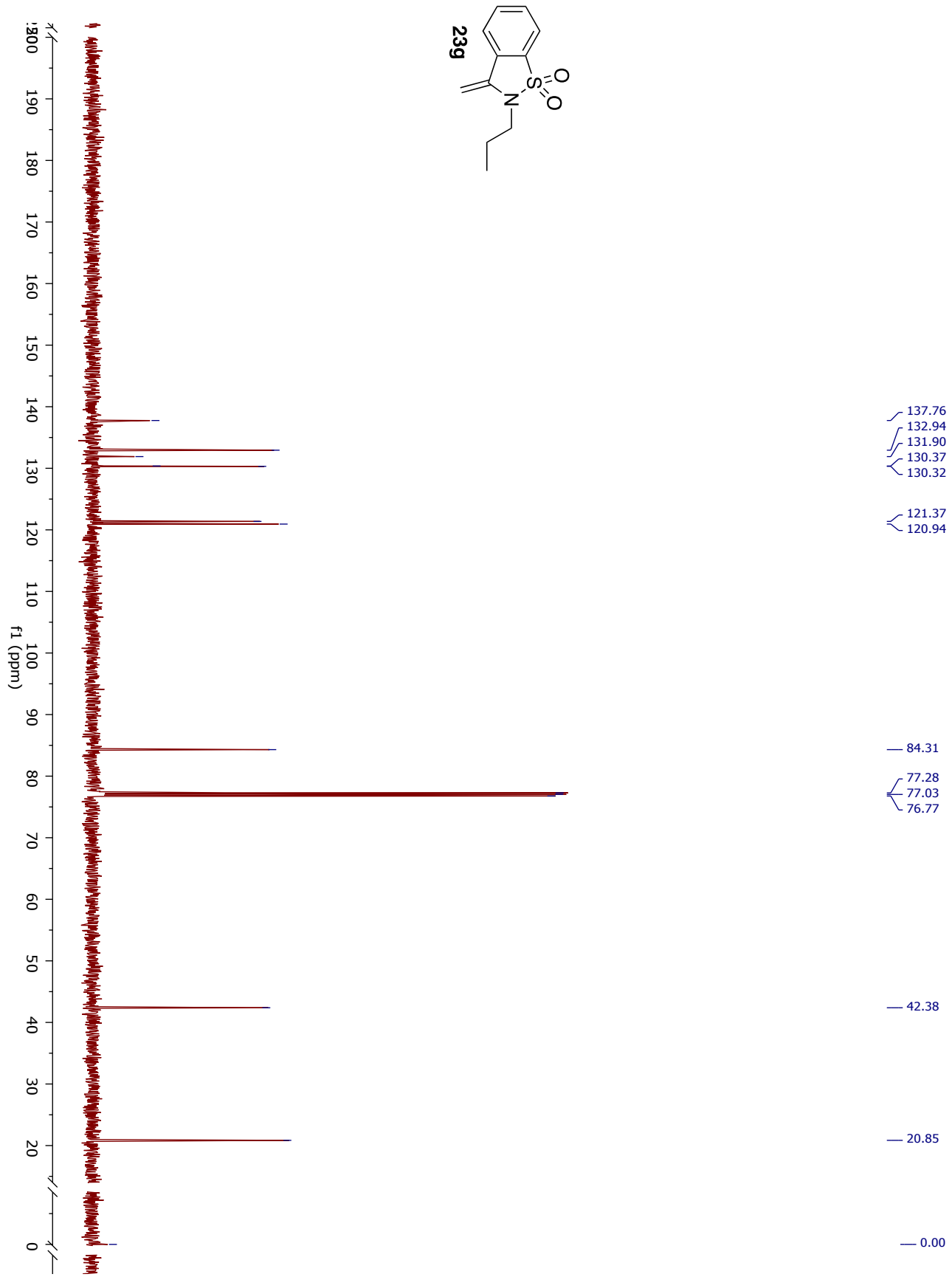

23e
O
S
O
N
CF3
0.96
0.99
4.05
1.00
1.03
1.03
2.05
1.02
7.89
7.88
7.73
7.71
7.69
7.69
7.68
7.68
7.66
7.66
7.64
7.64
7.63
7.63
7.62
7.61
7.57
7.56
7.50
7.49
7.47
7.26
4.93
4.93
4.87
4.28
4.28
0.00
f1 (ppm)

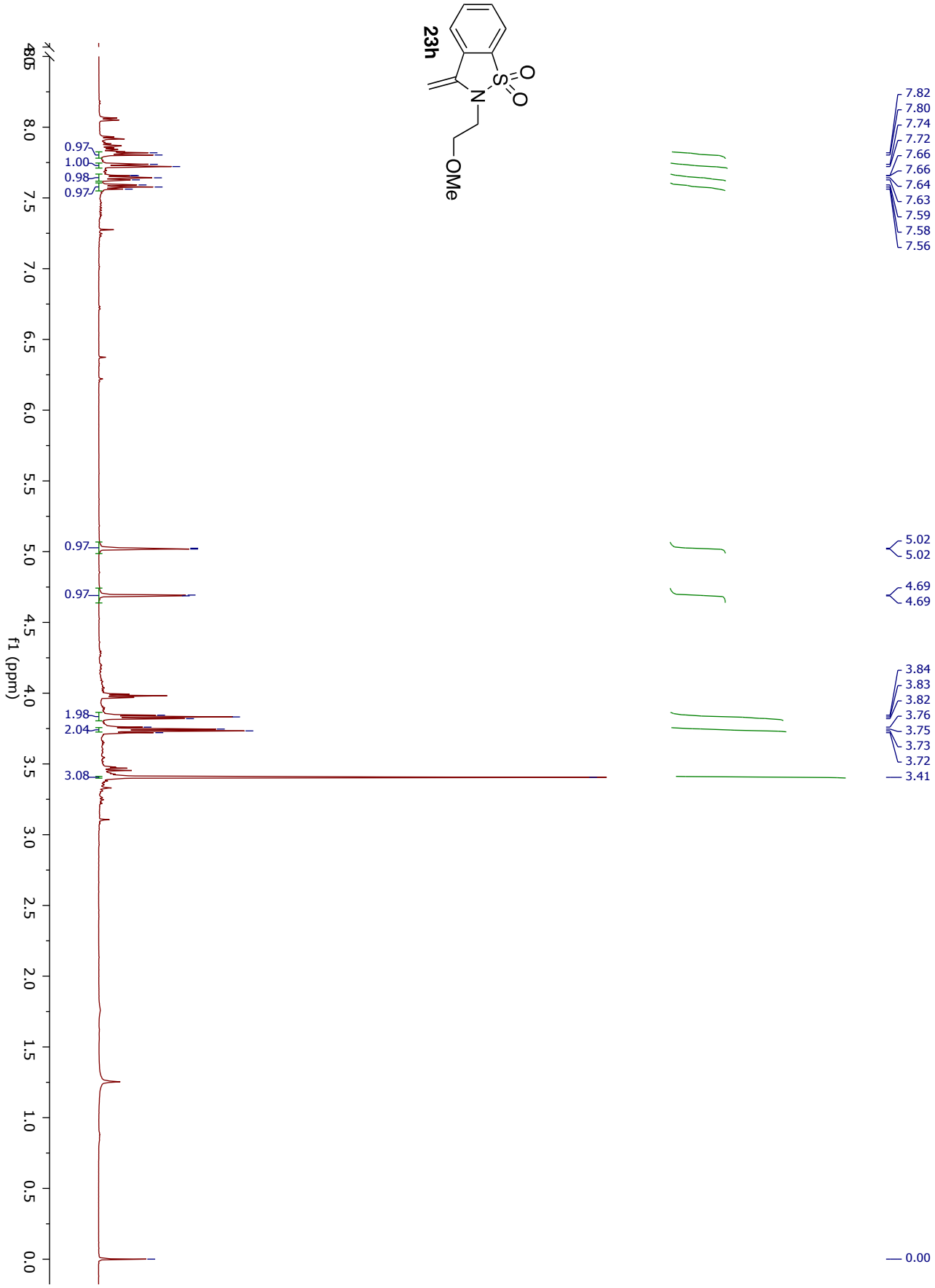

23e
O
S
O
N
CF3
137.54
136.39
133.41
131.69
131.38
131.13
130.71
130.65
130.10
129.51
124.86
124.83
124.00
123.98
122.94
121.64
121.31
86.20
77.39
77.13
76.88
43.94
f1 (ppm)

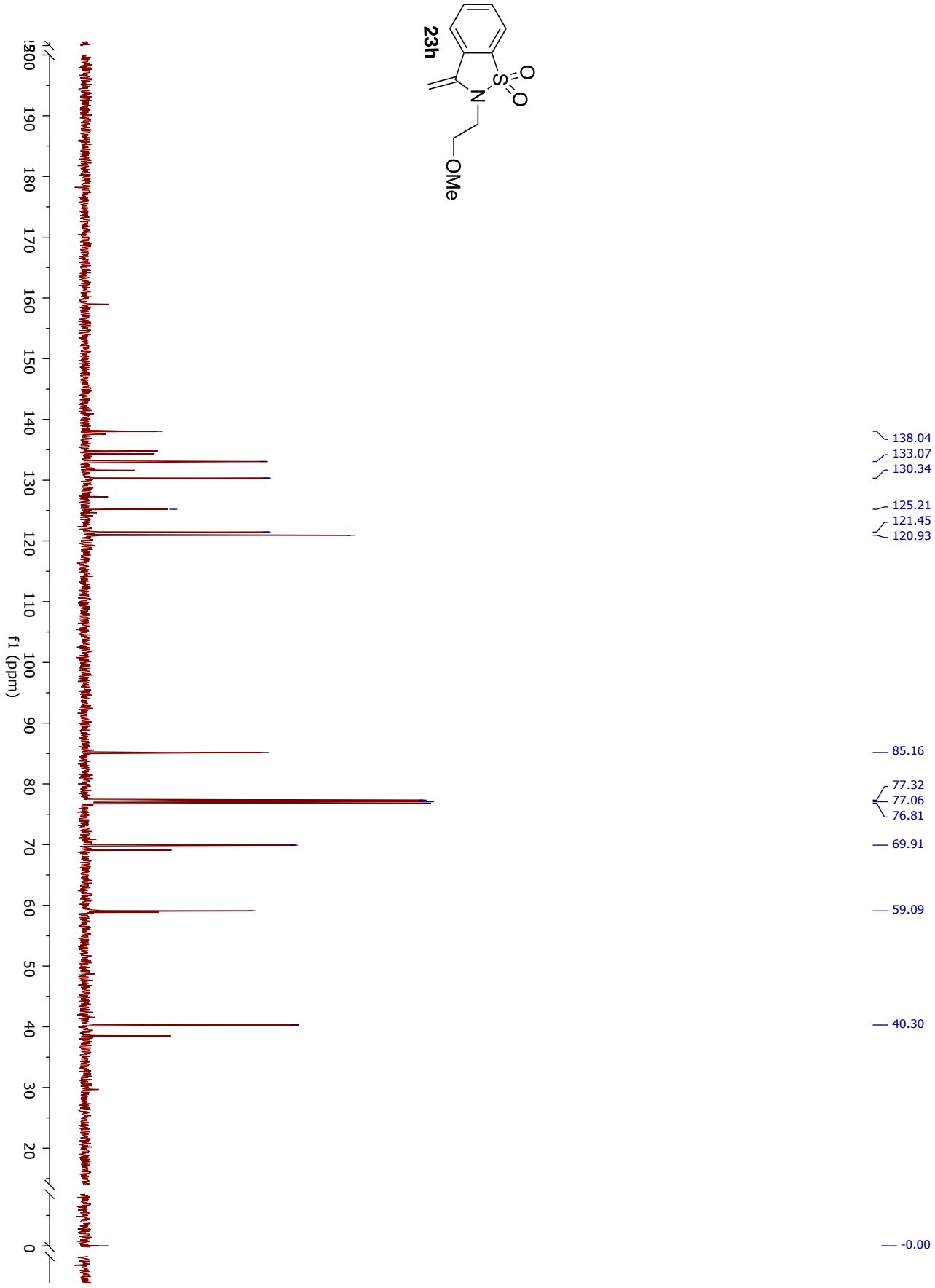

23f
O
S
O
N
OMe
f1 (ppm)
0.98
1.00
1.01
0.98
0.98
1.56
2.01
1.00
2.00
0.99
3.00
7.88
7.86
7.73
7.71
7.67
7.67
7.66
7.65
7.64
7.64
7.62
7.62
7.60
7.59
7.38
7.36
7.28
7.28
7.26
7.25
7.24
6.94
6.92
6.91
6.90
4.91
4.91
4.87
4.40
4.39
3.91
0.00

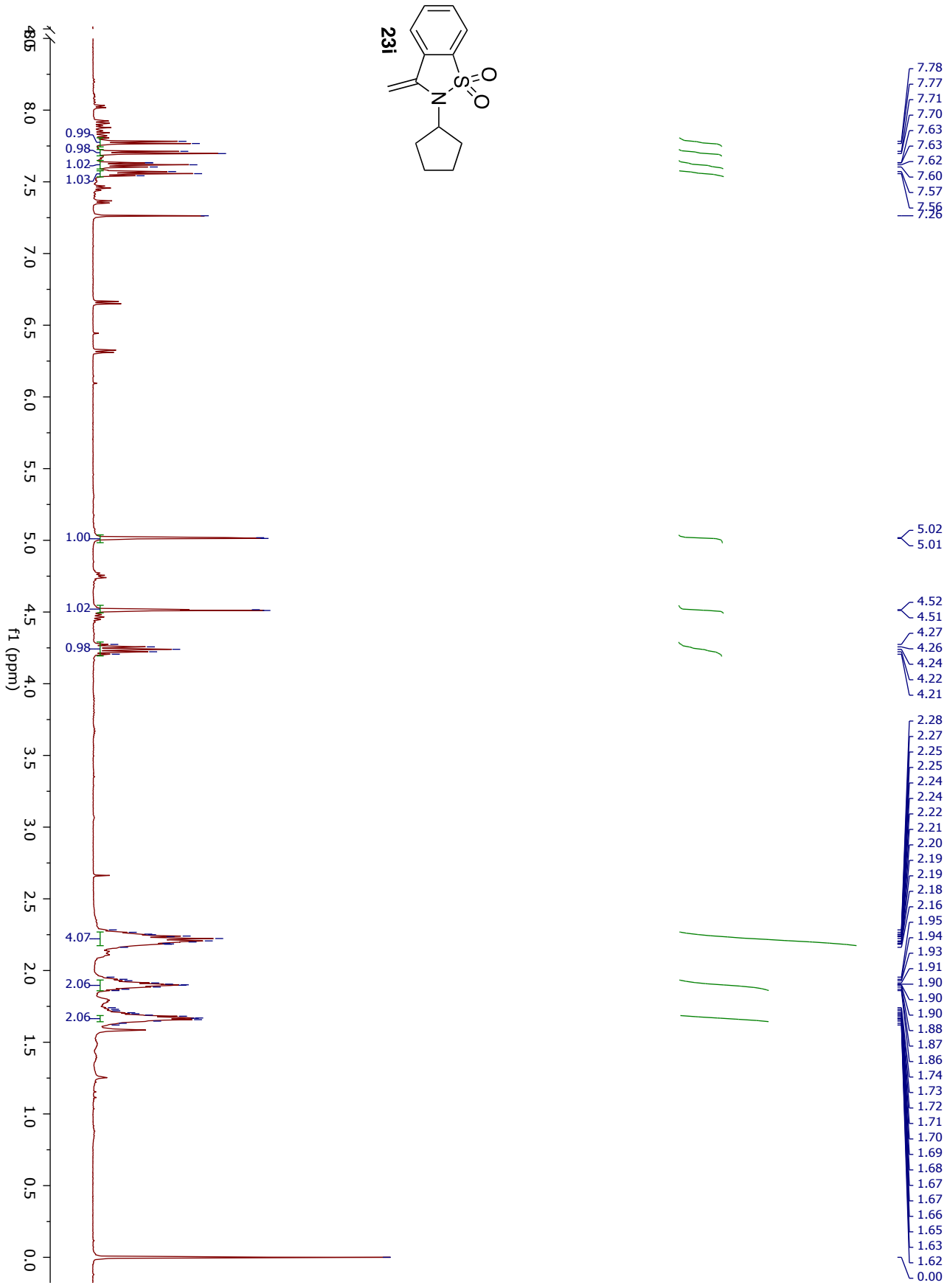

23f
O
S
O
N
OMe
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
137.62
133.01
130.29
128.62
128.01
122.99
121.41
121.10
120.77
110.01
85.72
77.27
77.01
76.76
55.36
38.78
0.00

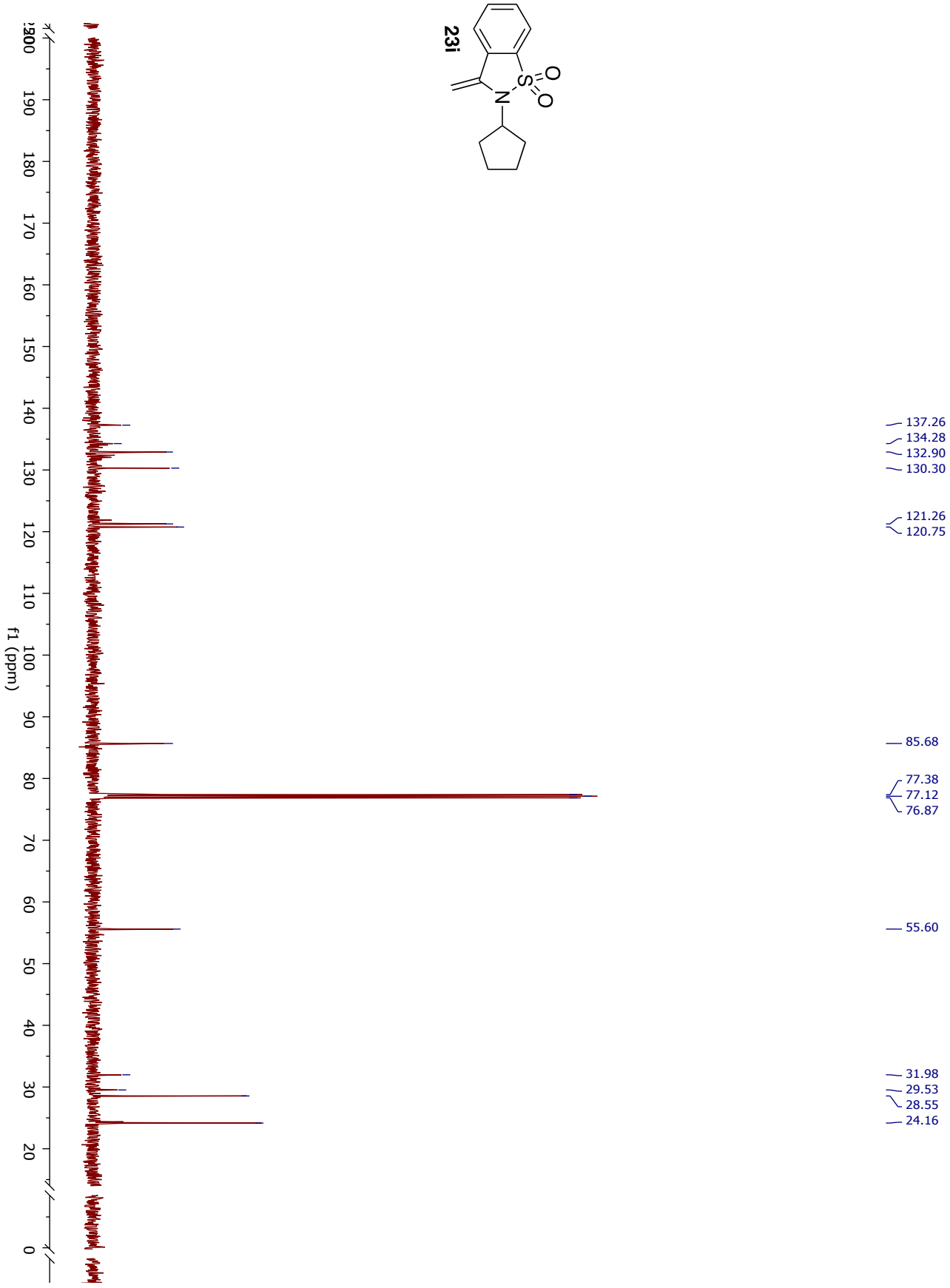

23g
O
S
O
N
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.00
1.01
1.02
1.01
1.05
1.04
2.04
2.06
3.07
7.82
7.80
7.73
7.72
7.65
7.65
7.64
7.64
7.62
7.62
7.59
7.59
7.58
7.56
4.98
3.60
3.59
3.57
1.90
1.89
1.87
1.86
1.84
1.83
1.04
1.03
1.02
0.00

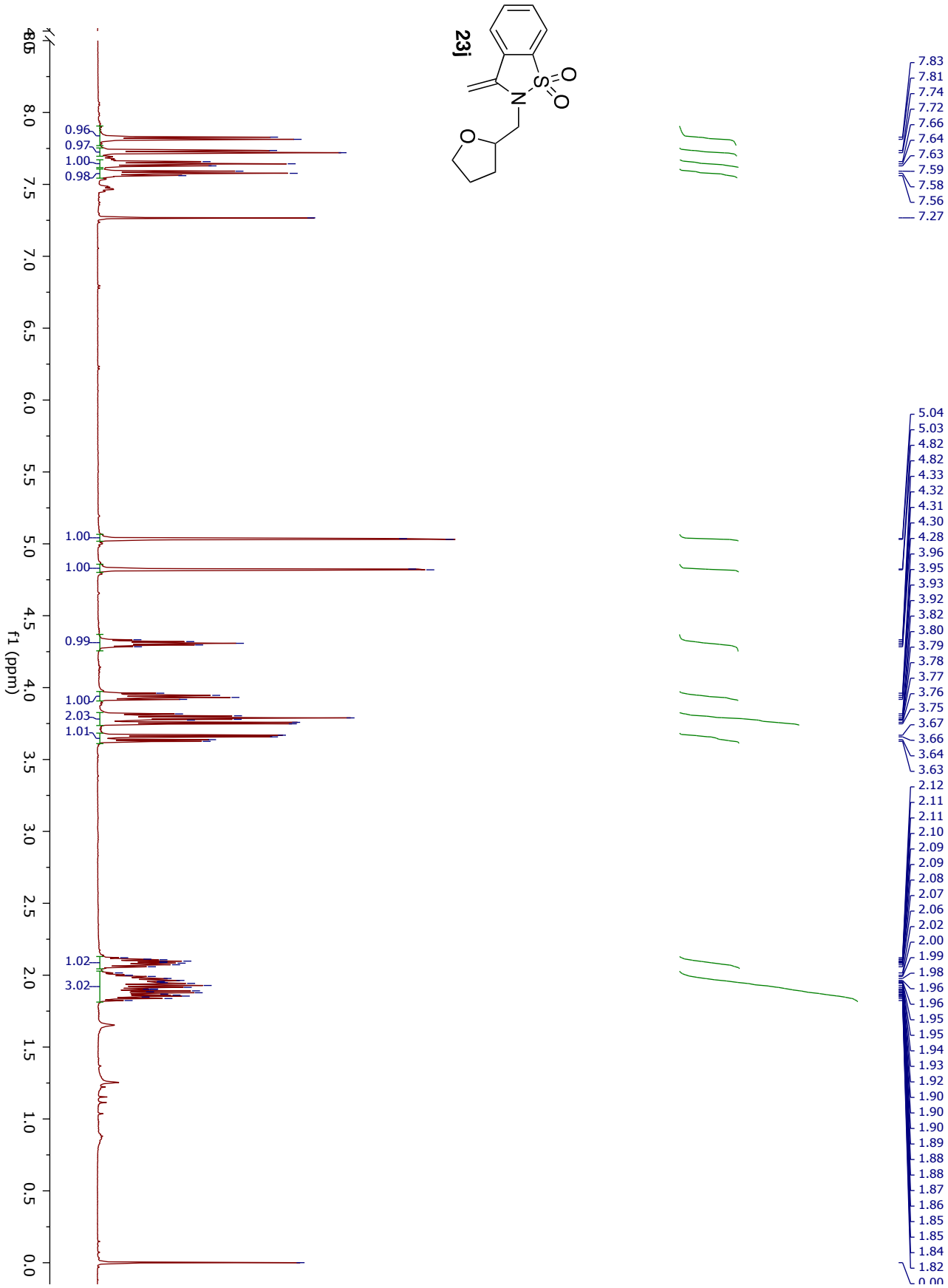

23g
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
137.76
132.94
131.90
130.37
130.32
121.37
120.94
84.31
77.28
77.03
76.77
42.38
20.85
0.00

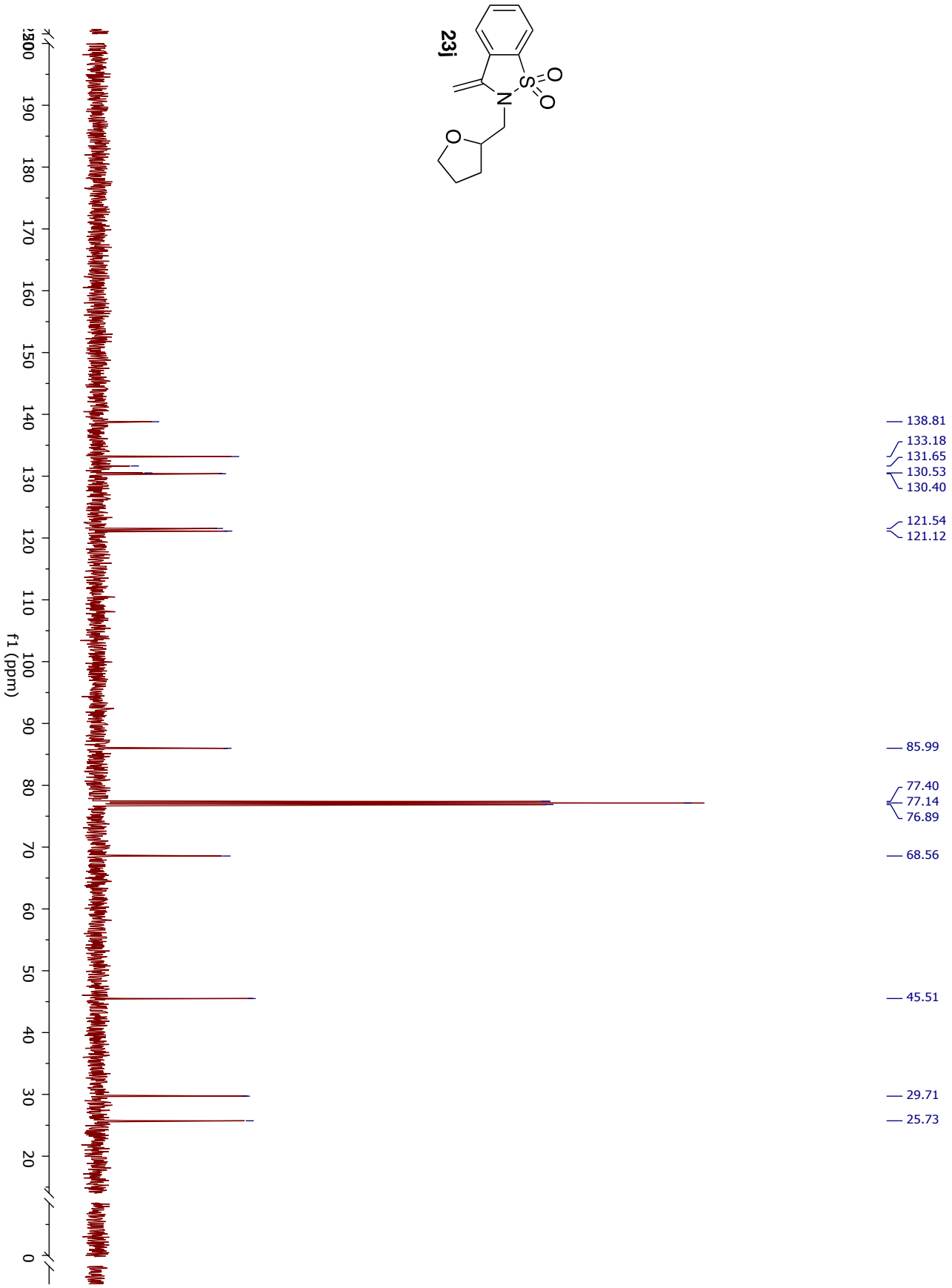

23h
O
S
O
N
OMe
f1 (ppm)
0.97
1.00
0.98
0.97
0.97
0.97
1.98
2.04
3.08
7.82
7.80
7.74
7.72
7.66
7.66
7.64
7.63
7.59
7.58
7.56
5.02
5.02
4.69
4.69
3.84
3.83
3.82
3.76
3.75
3.73
3.72
3.41
0.00

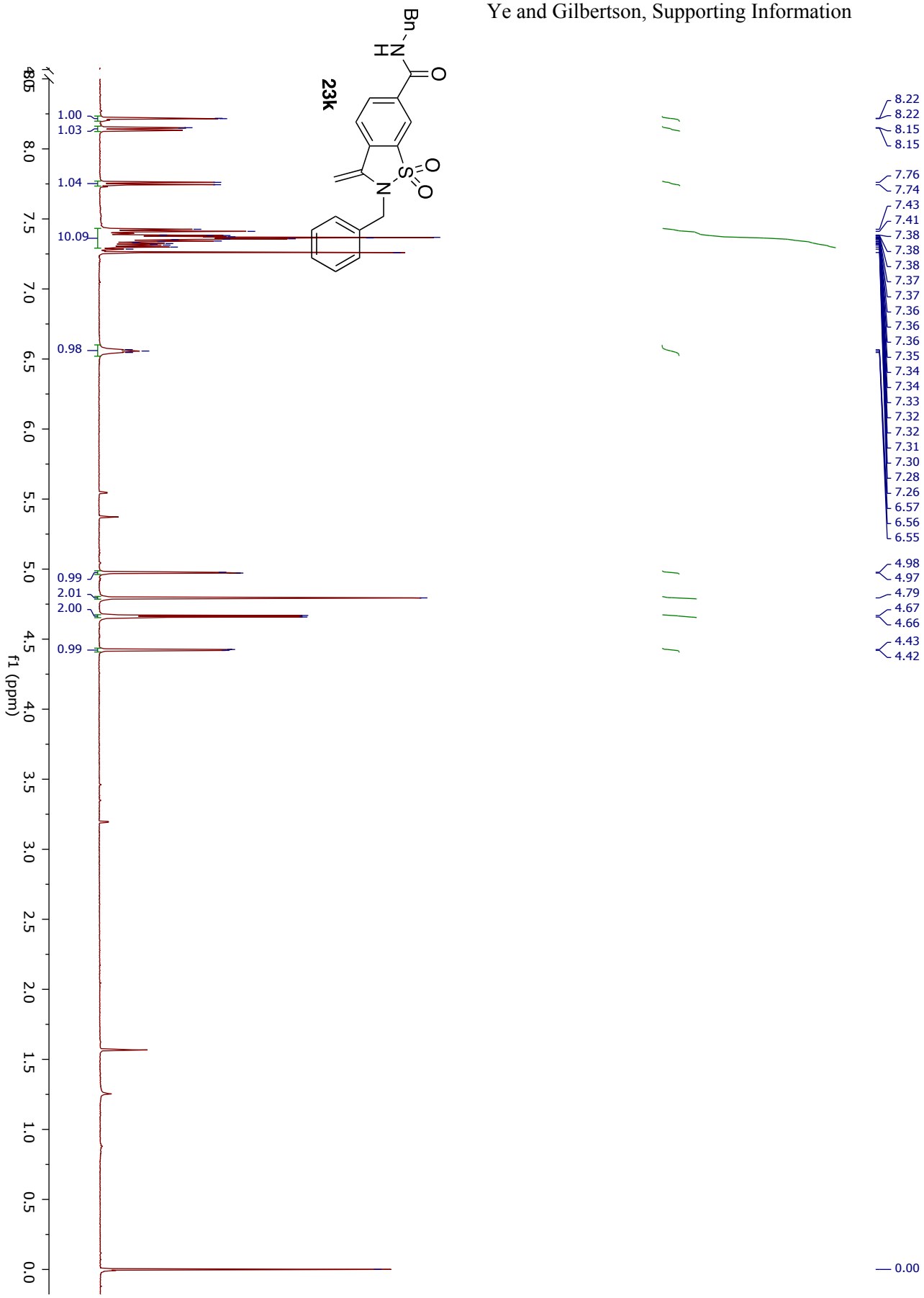

23h
O
S
O
N
OMe
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
138.04
133.07
130.34
125.21
121.45
120.93
85.16
77.32
77.06
76.81
69.91
59.09
40.30
-0.00

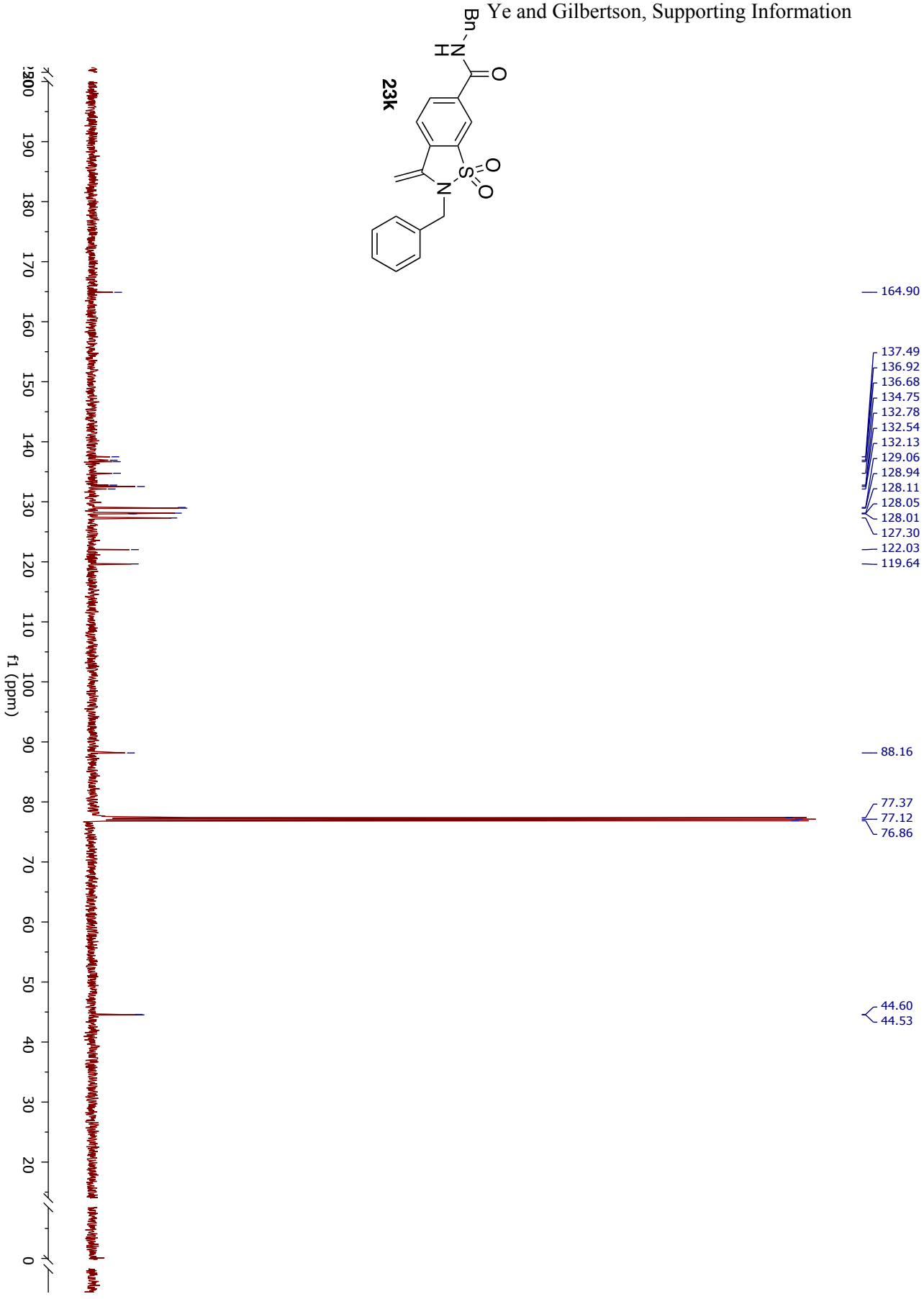

23i
O
S
O
N
f1 (ppm)
0.99
0.98
1.02
1.03
1.00
1.02
0.98
4.07
2.06
2.06
7.78
7.77
7.71
7.70
7.63
7.63
7.62
7.60
7.57
7.56
7.26
5.02
5.01
4.52
4.51
4.27
4.26
4.24
4.22
4.21
2.28
2.27
2.25
2.25
2.24
2.24
2.22
2.21
2.20
2.19
2.19
2.18
2.16
1.95
1.94
1.93
1.91
1.90
1.90
1.90
1.88
1.87
1.86
1.74
1.73
1.72
1.71
1.70
1.69
1.68
1.67
1.67
1.66
1.65
1.63
1.62
0.00

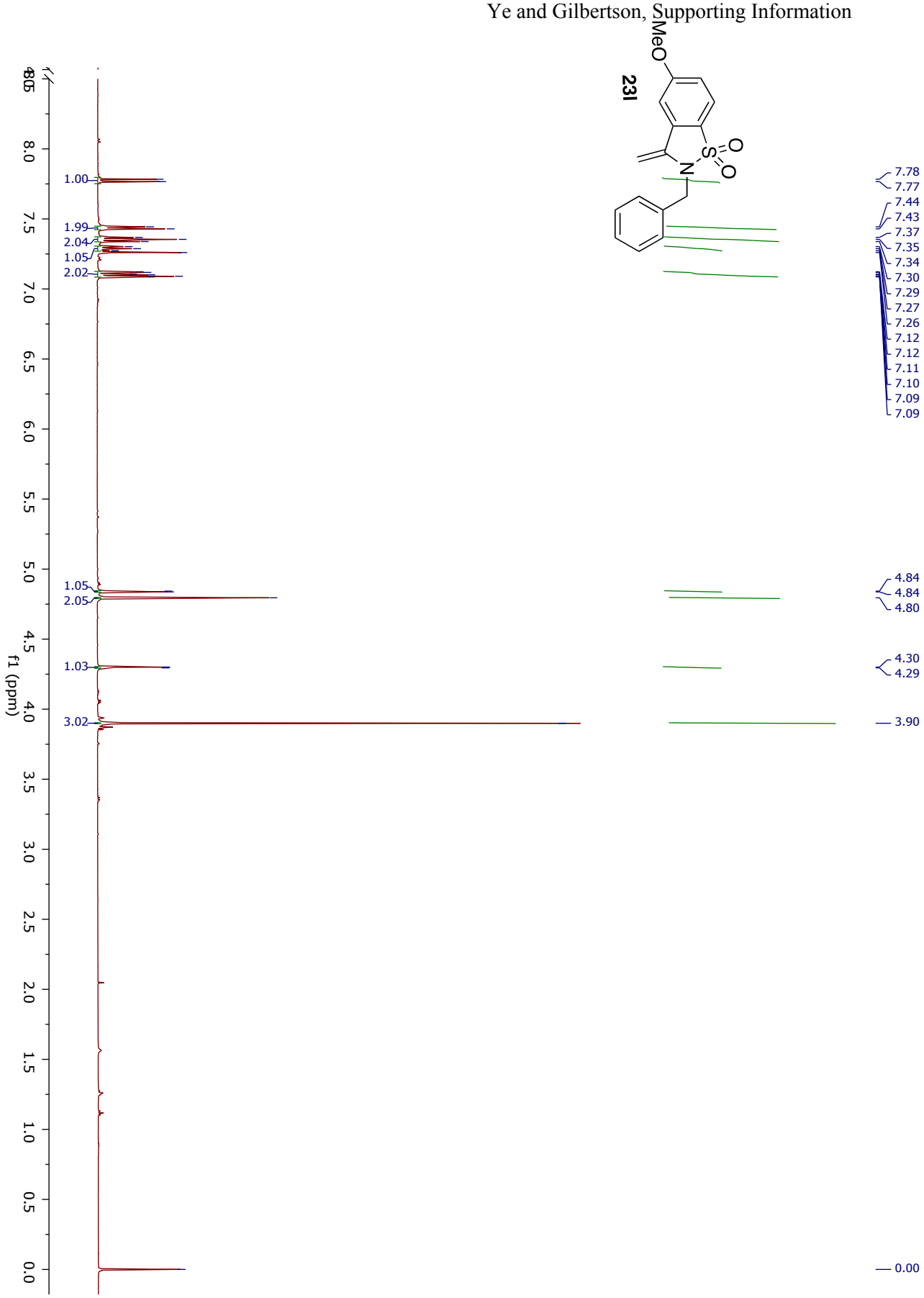

23i
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
137.26
134.28
132.90
130.30
121.26
120.75
85.68
77.38
77.12
76.87
55.60
31.98
29.53
28.55
24.16

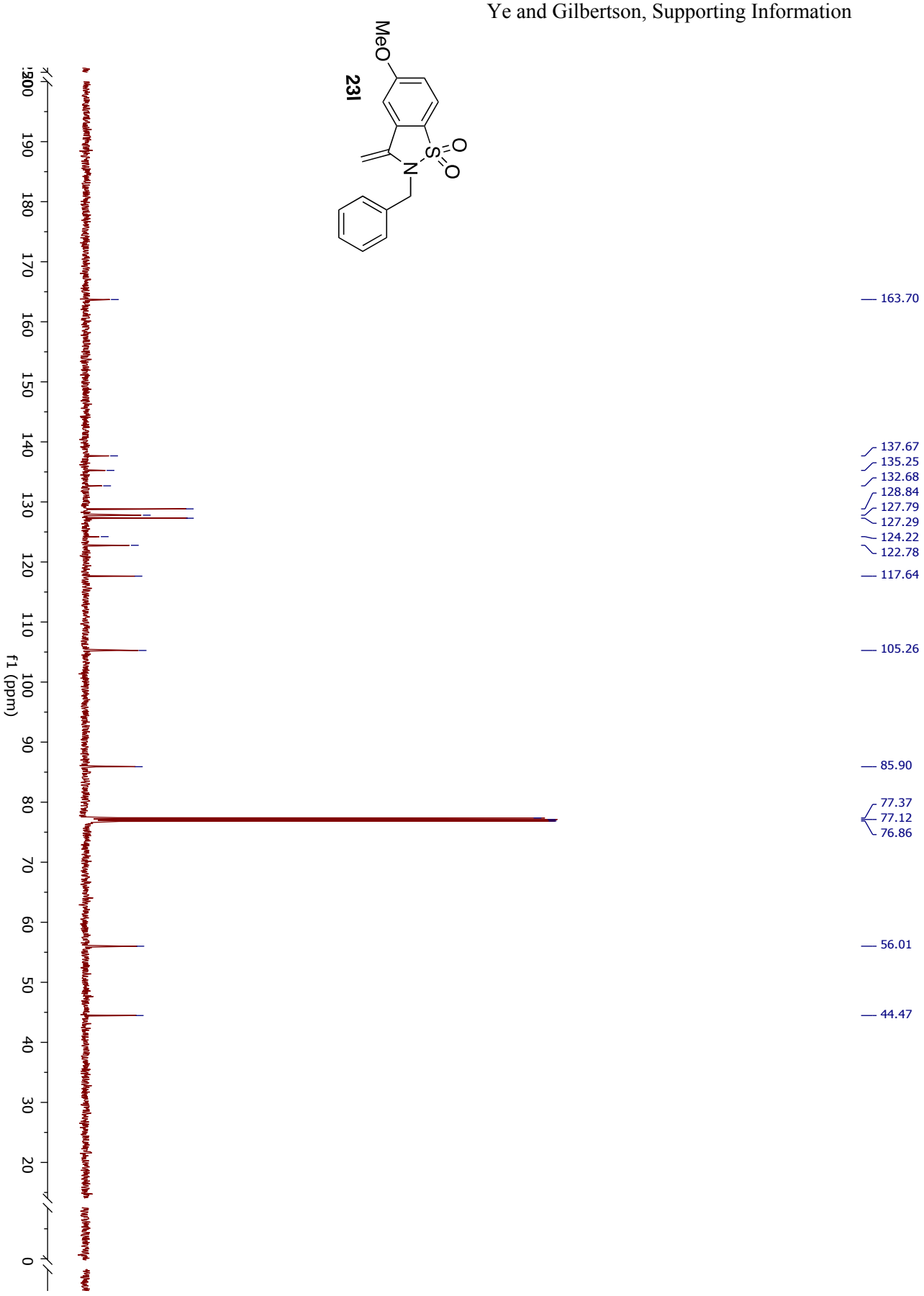

23j
O
S
O
N
O
0.96
0.97
1.00
0.98
1.00
1.00
0.99
1.00
2.03
1.01
1.02
3.02
f1 (ppm)
7.83
7.81
7.74
7.72
7.66
7.64
7.63
7.59
7.58
7.56
7.27
5.04
5.03
4.82
4.82
4.33
4.32
4.31
4.30
4.28
3.96
3.95
3.93
3.92
3.82
3.80
3.79
3.78
3.77
3.76
3.75
3.67
3.66
3.64
3.63
2.12
2.11
2.11
2.10
2.09
2.09
2.08
2.07
2.06
2.02
2.00
1.99
1.98
1.96
1.96
1.95
1.95
1.94
1.93
1.92
1.90
1.90
1.90
1.89
1.88
1.88
1.87
1.86
1.85
1.85
1.84
1.82

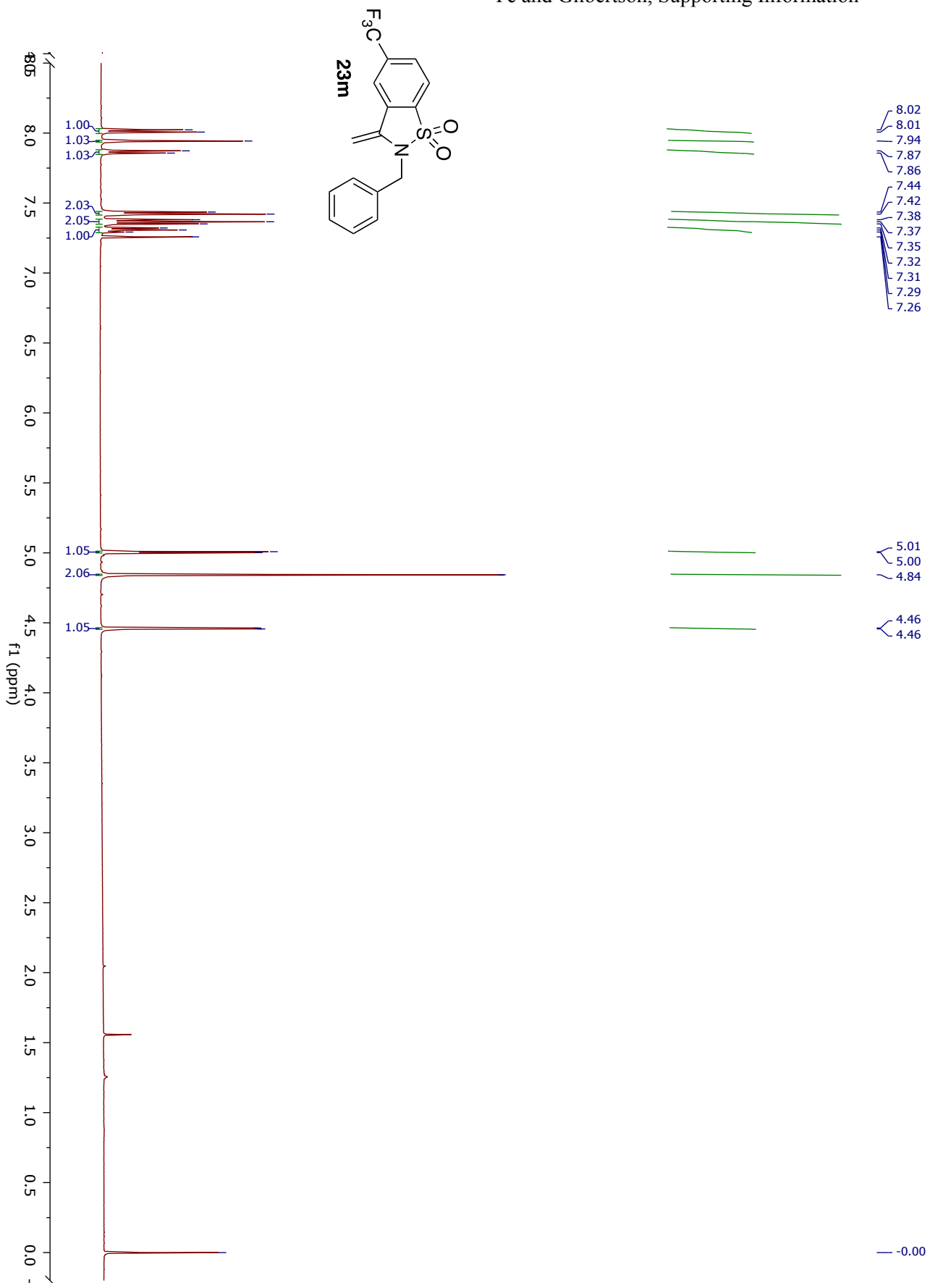

23j
O
S
O
N
O
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
138.81
133.18
131.65
130.53
130.40
121.54
121.12
85.99
77.40
77.14
76.89
68.56
45.51
29.71
25.73

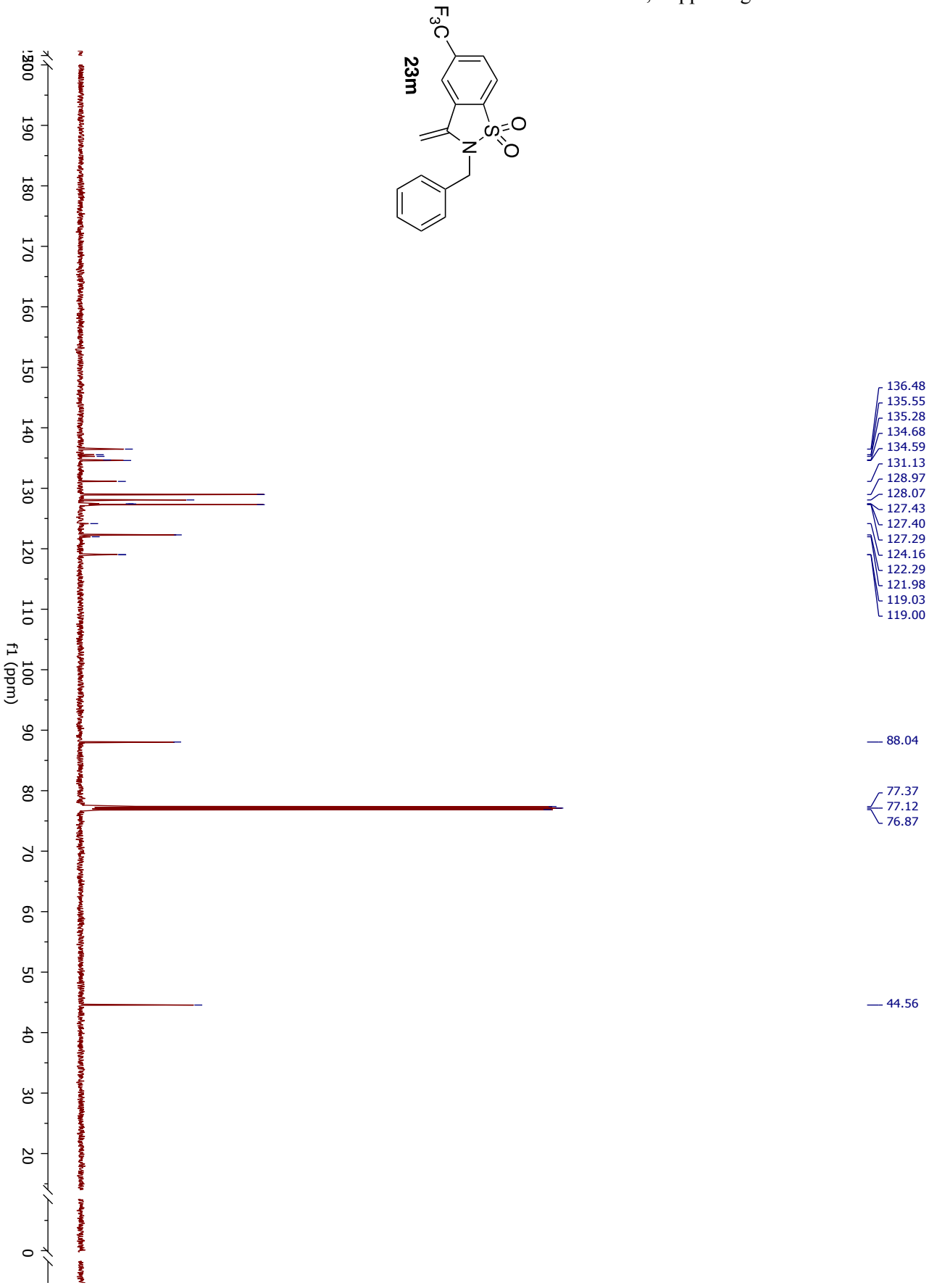

23k
Bn
H
N
O
S
O
O
N
1.00
1.03
1.04
10.09
0.98
0.99
2.01
2.00
0.99
8.22
8.22
8.15
8.15
7.76
7.74
7.43
7.41
7.38
7.38
7.38
7.37
7.37
7.36
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.28
7.26
6.57
6.56
6.55
4.98
4.97
4.79
4.67
4.66
4.43
4.42
0.00
f1 (ppm)

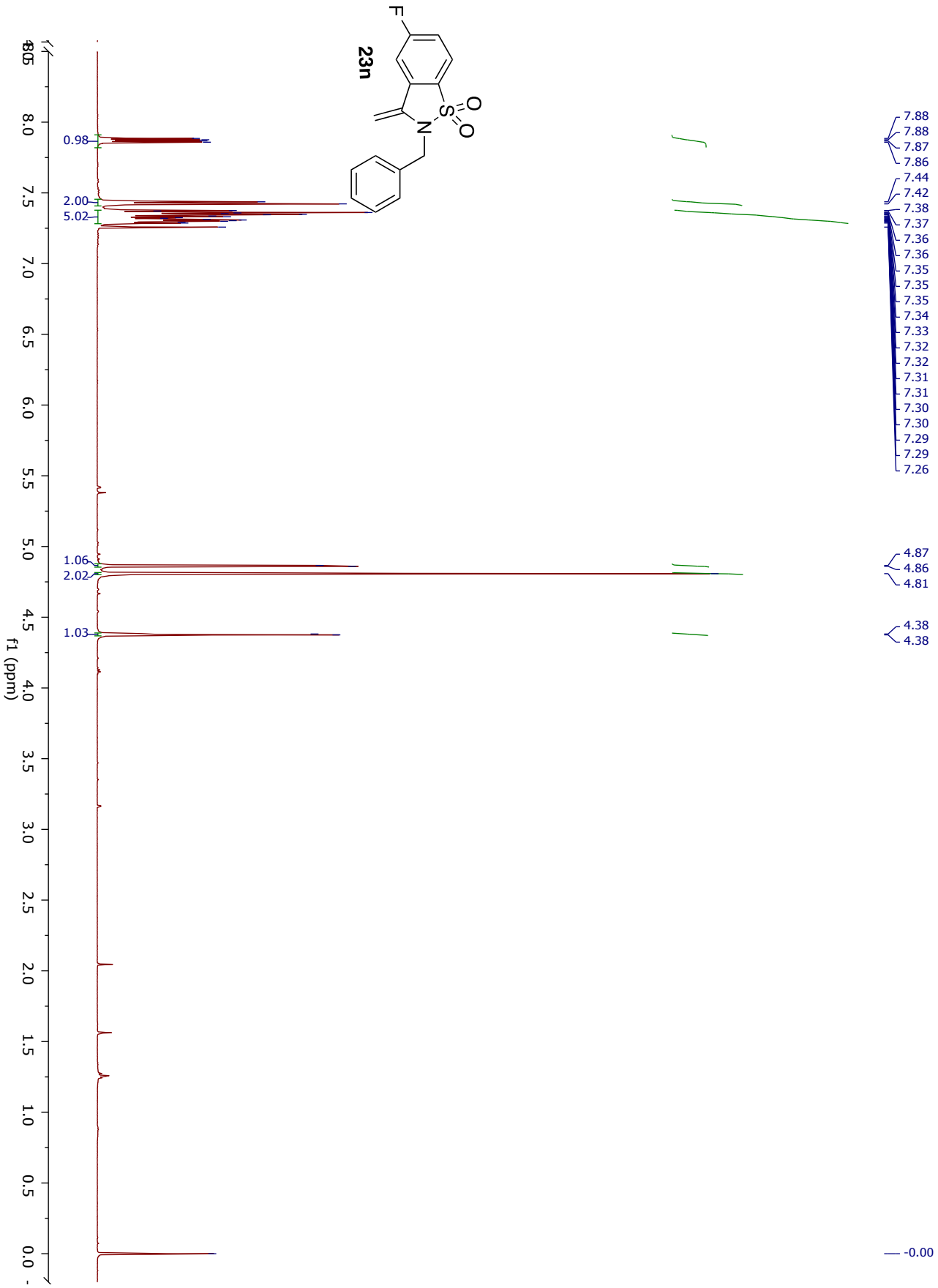

23k
Bn
H
N
O
S
O
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
164.90
137.49
136.92
136.68
134.75
132.78
132.54
132.13
129.06
128.94
128.11
128.05
128.01
127.30
122.03
119.64
88.16
77.37
77.12
76.86
44.60
44.53

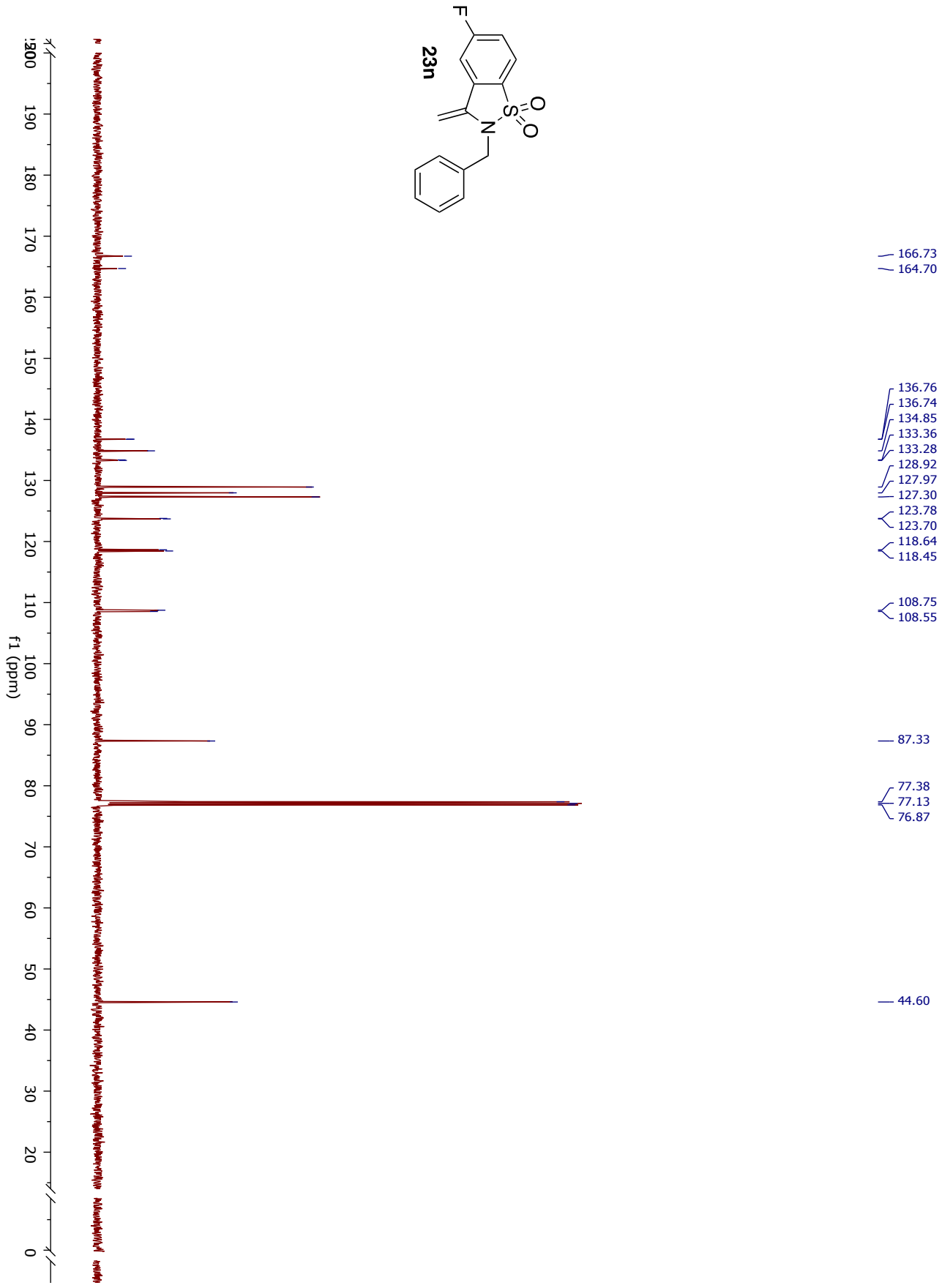

MeO
O
S
O
N
23l
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.00
1.99
2.04
1.05
2.02
1.05
2.05
1.03
3.02
7.78
7.77
7.44
7.43
7.37
7.35
7.34
7.30
7.29
7.27
7.26
7.12
7.12
7.11
7.10
7.09
7.09
4.84
4.84
4.80
4.30
4.29
3.90
0.00

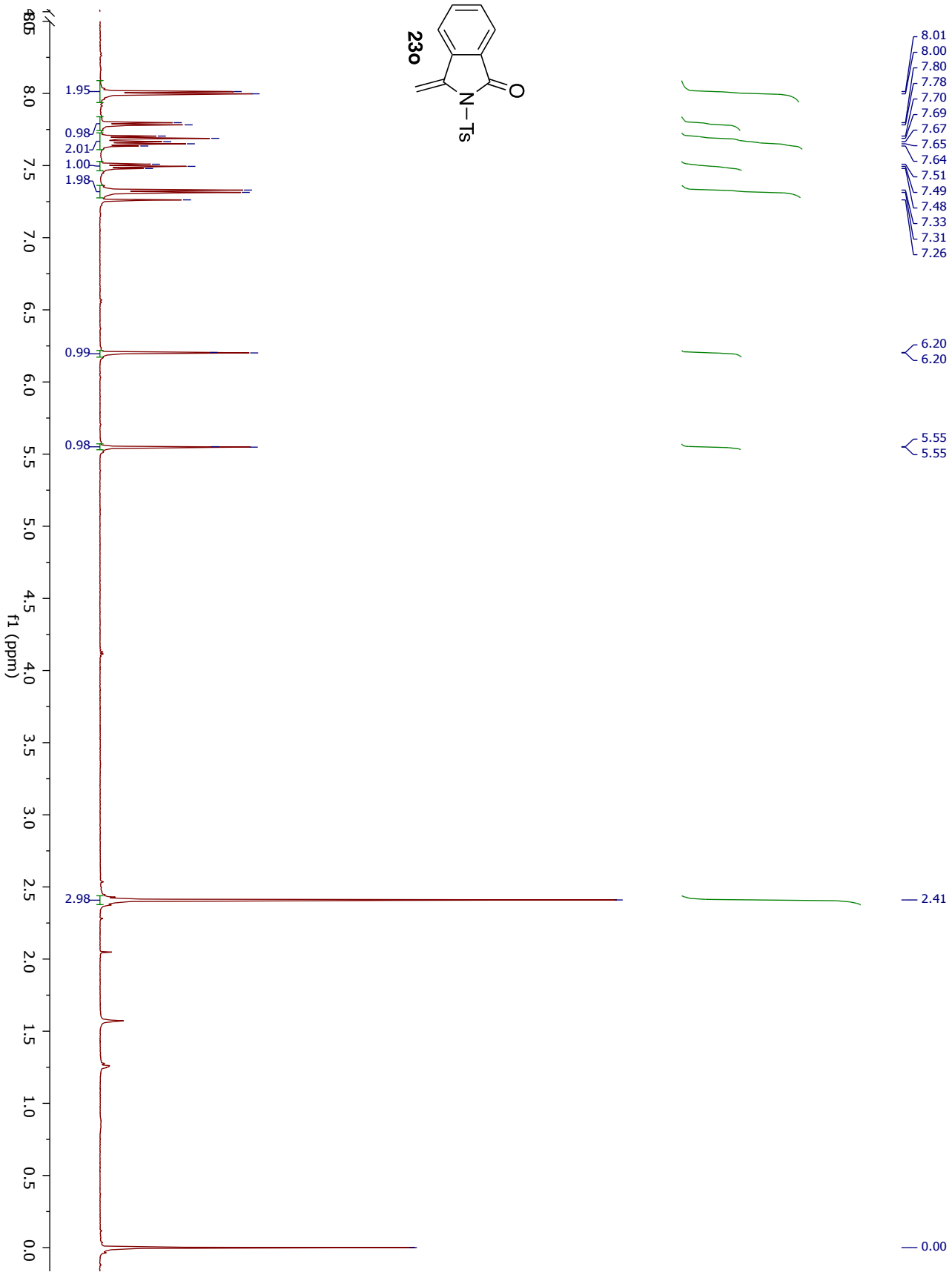

MeO
231
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
163.70
137.67
135.25
132.68
128.84
127.79
127.29
124.22
122.78
117.64
105.26
85.90
77.37
77.12
76.86
56.01
44.47

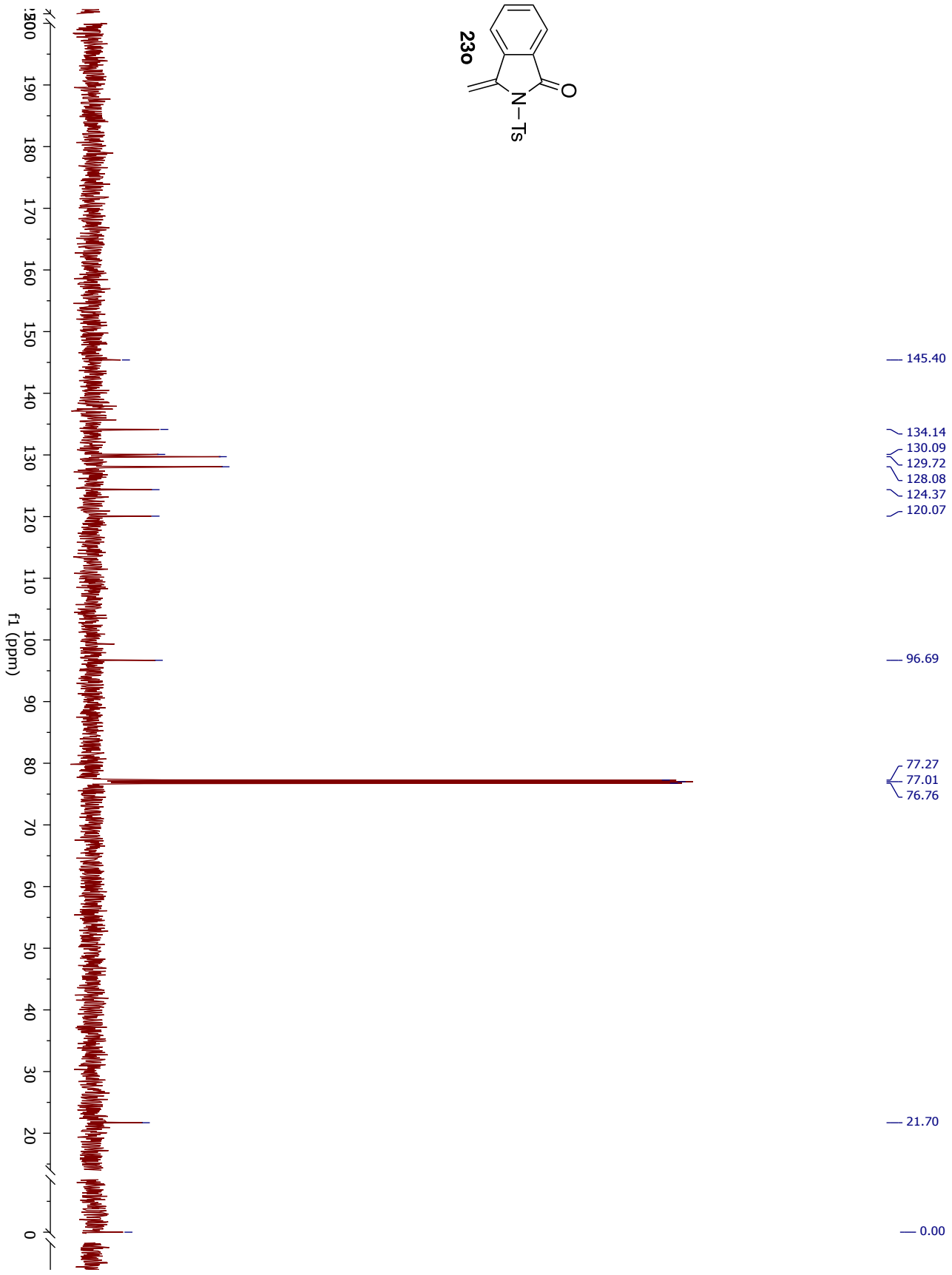

23m
F3C
O
O
S
N
1.00
1.03
1.03
2.03
2.05
1.00
1.05
2.06
1.05
8.02
8.01
7.94
7.87
7.86
7.44
7.42
7.38
7.37
7.35
7.32
7.31
7.29
7.26
5.01
5.00
4.84
4.46
4.46
-0.00
f1 (ppm)

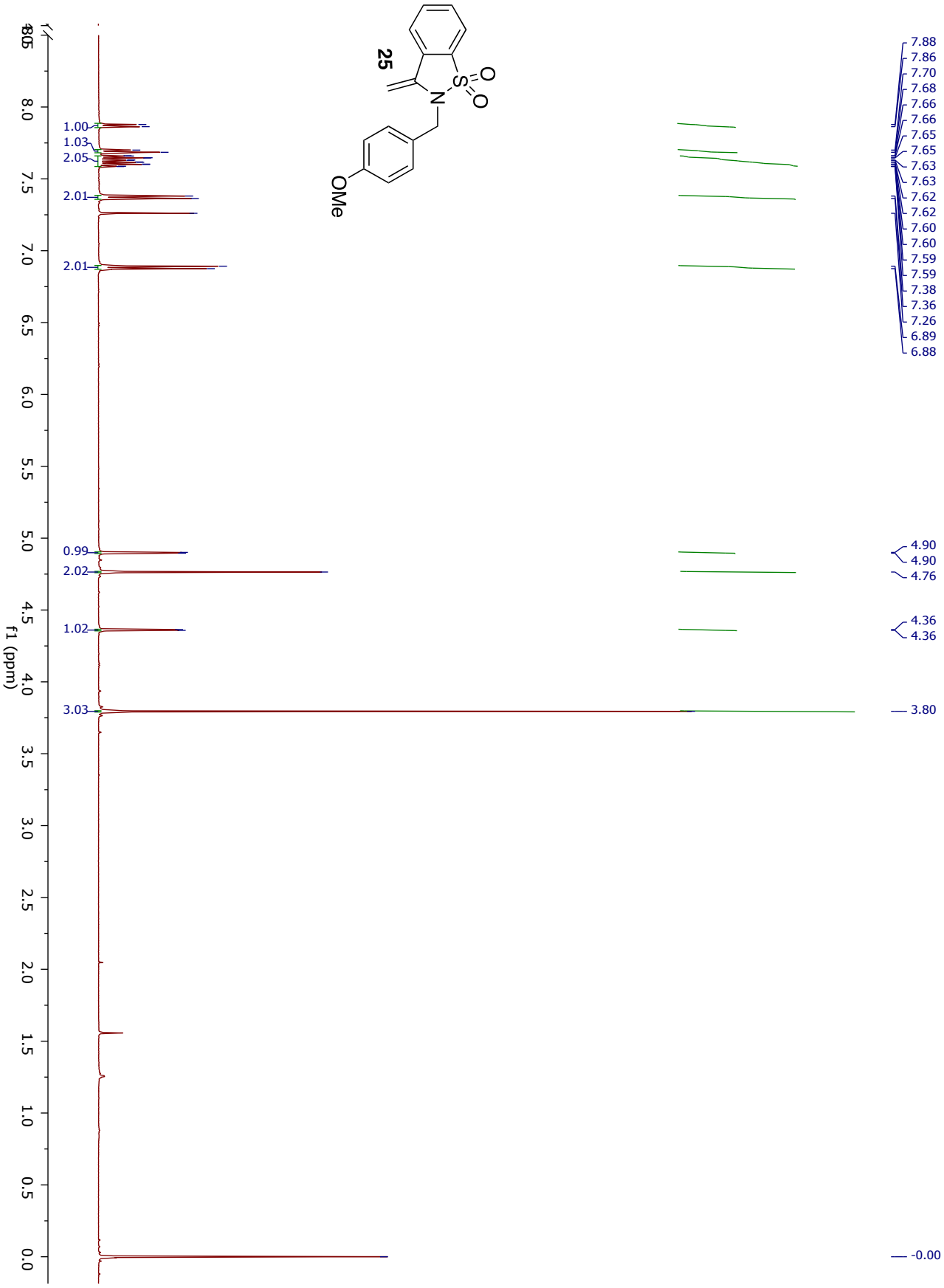

23m
F3C
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
136.48
135.55
135.28
134.68
134.59
131.13
128.97
128.07
127.43
127.40
127.29
124.16
122.29
121.98
119.03
119.00
88.04
77.37
77.12
76.87
44.56

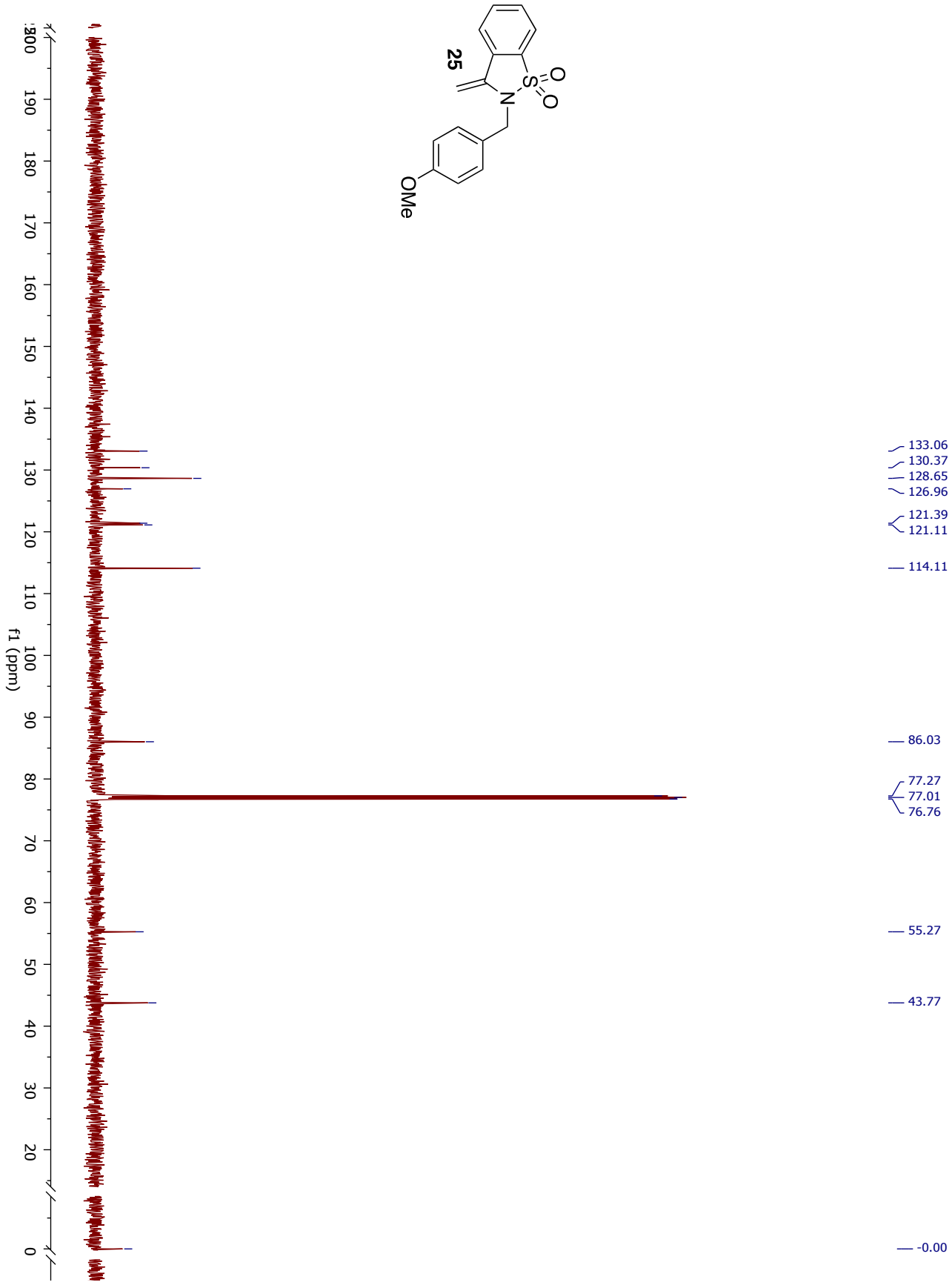

23n
F
O
O
S
N
0.98
2.00
5.02
1.06
2.02
1.03
7.88
7.88
7.87
7.86
7.44
7.42
7.38
7.37
7.36
7.36
7.35
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.26
4.87
4.86
4.81
4.38
4.38
-0.00
f1 (ppm)

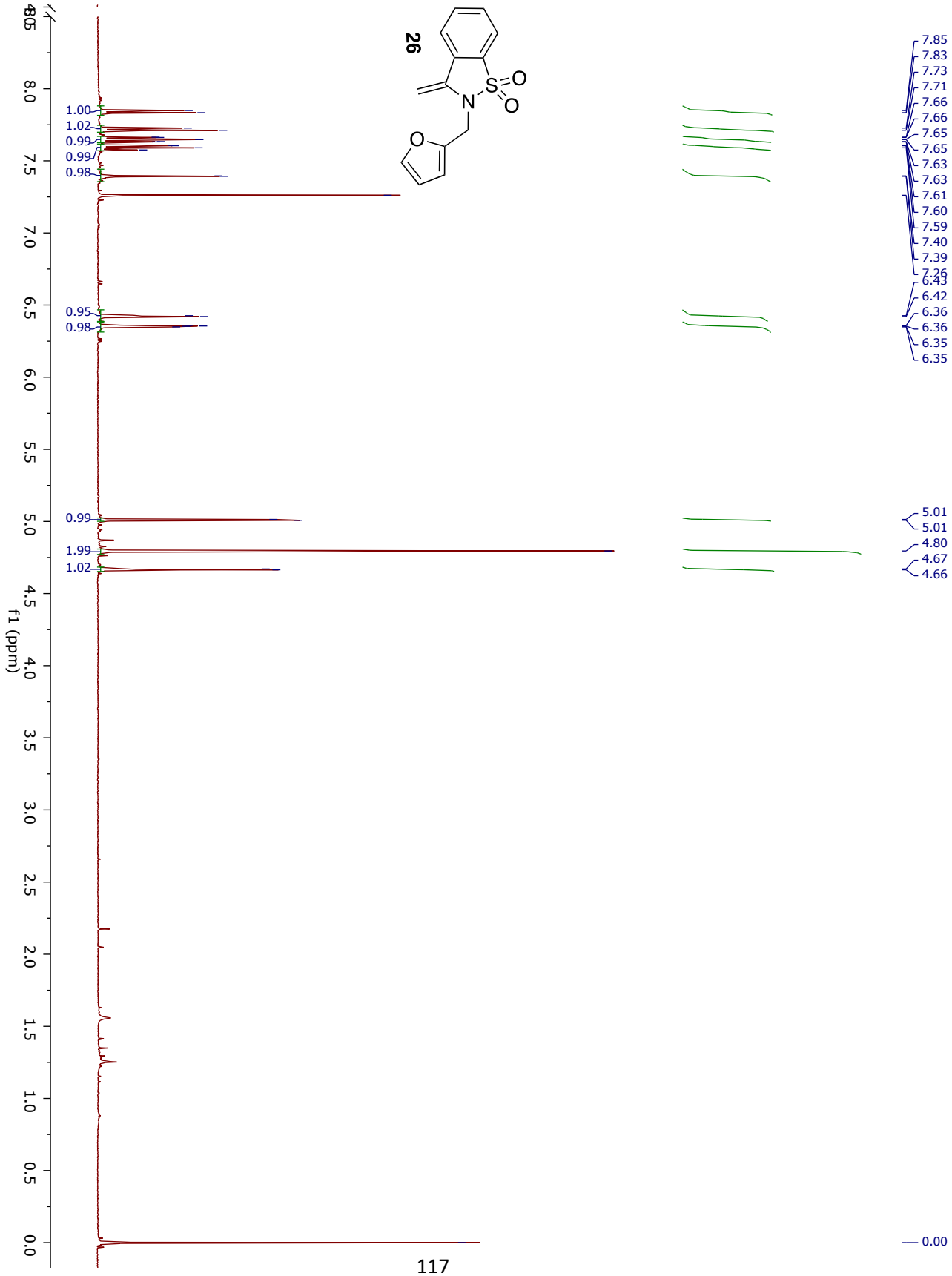

23n
F
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
166.73
164.70
136.76
136.74
134.85
133.36
133.28
128.92
127.97
127.30
123.78
123.70
118.64
118.45
108.75
108.55
87.33
77.38
77.13
76.87
44.60

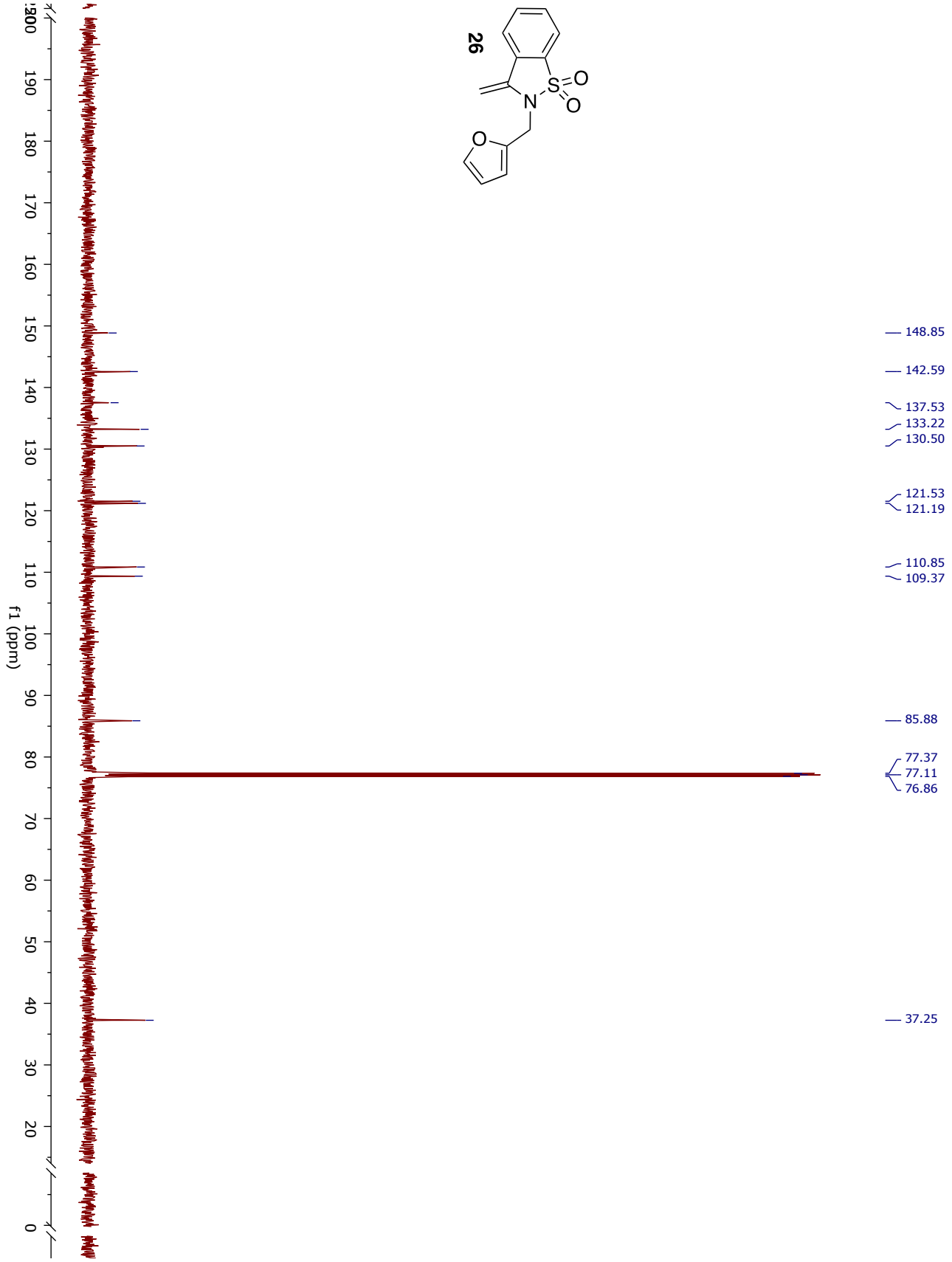

23o
N–Ts
O
f1 (ppm)
1.95
0.98
2.01
1.00
1.98
0.99
0.98
2.98
8.01
8.00
7.80
7.78
7.70
7.69
7.67
7.65
7.64
7.51
7.49
7.48
7.33
7.31
7.26
6.20
6.20
5.55
5.55
2.41
0.00

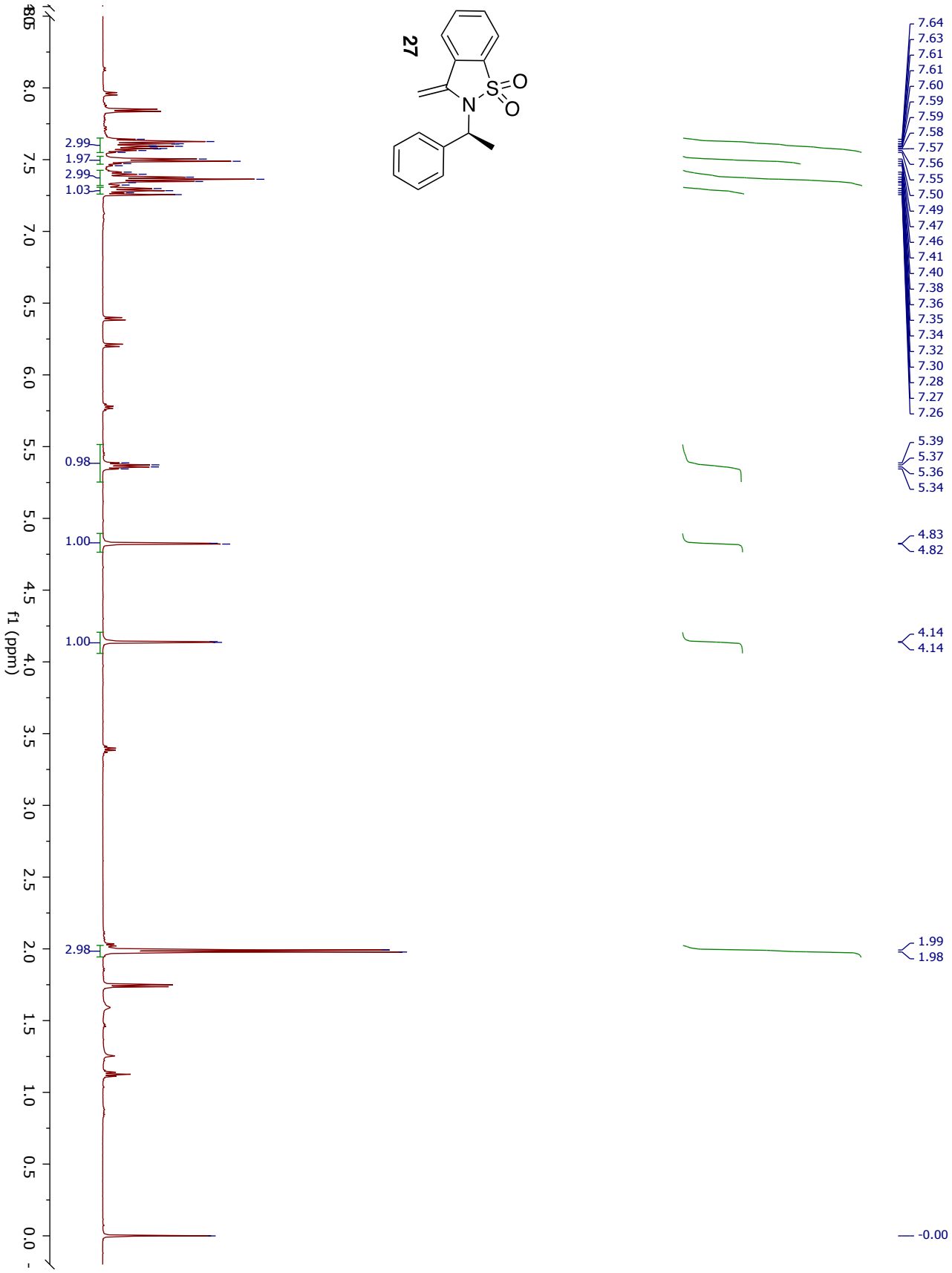

23o
O
N—Ts
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
145.40
134.14
130.09
129.72
128.08
124.37
120.07
96.69
77.27
77.01
76.76
21.70
0.00

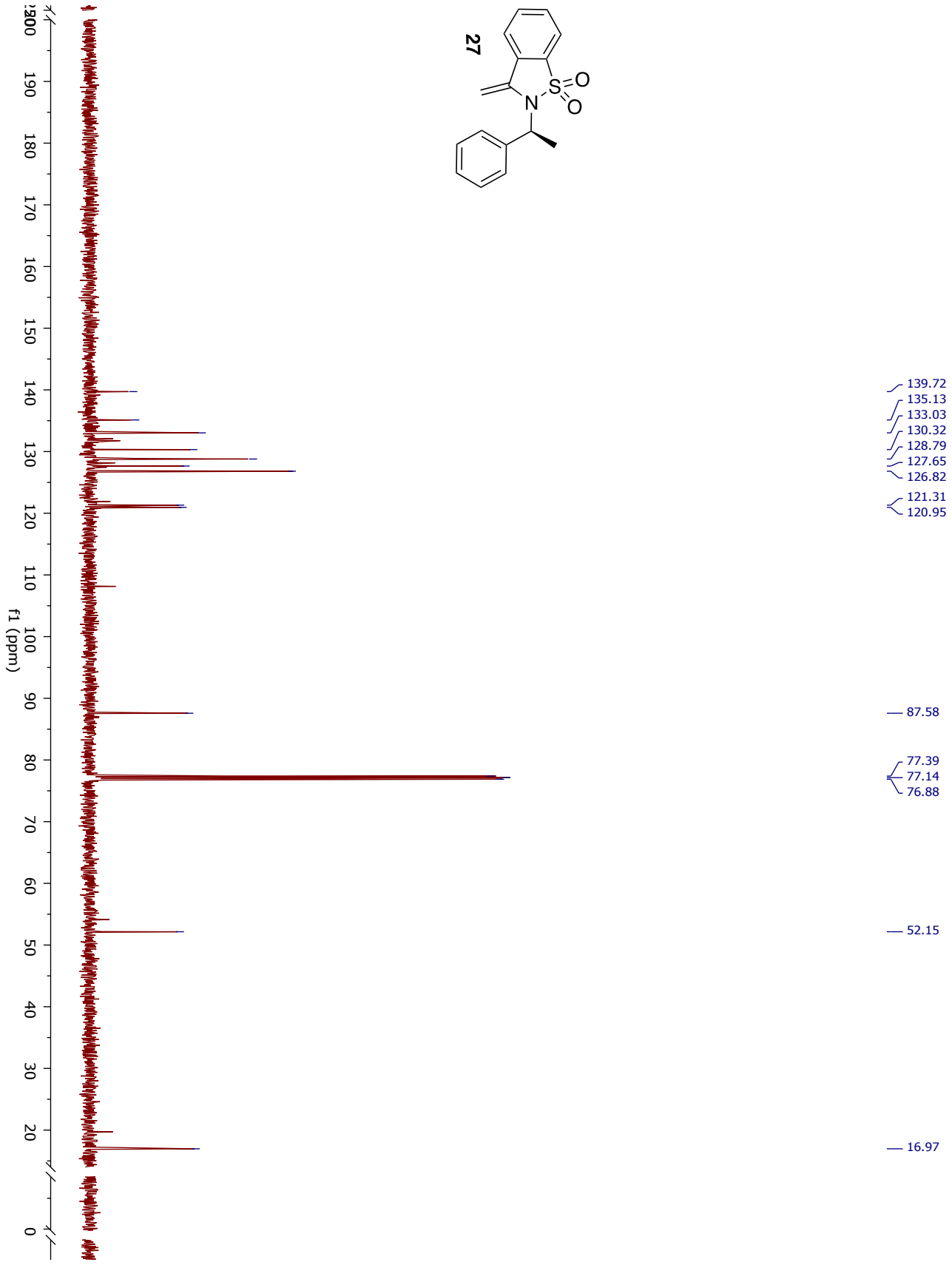

25
O
S
O
N
OMe
f1 (ppm)
1.00
1.03
2.05
2.01
2.01
0.99
2.02
1.02
3.03
7.88
7.86
7.70
7.68
7.66
7.66
7.65
7.65
7.63
7.63
7.62
7.62
7.60
7.60
7.59
7.59
7.38
7.36
7.26
6.89
6.88
4.90
4.90
4.76
4.36
4.36
3.80
-0.00

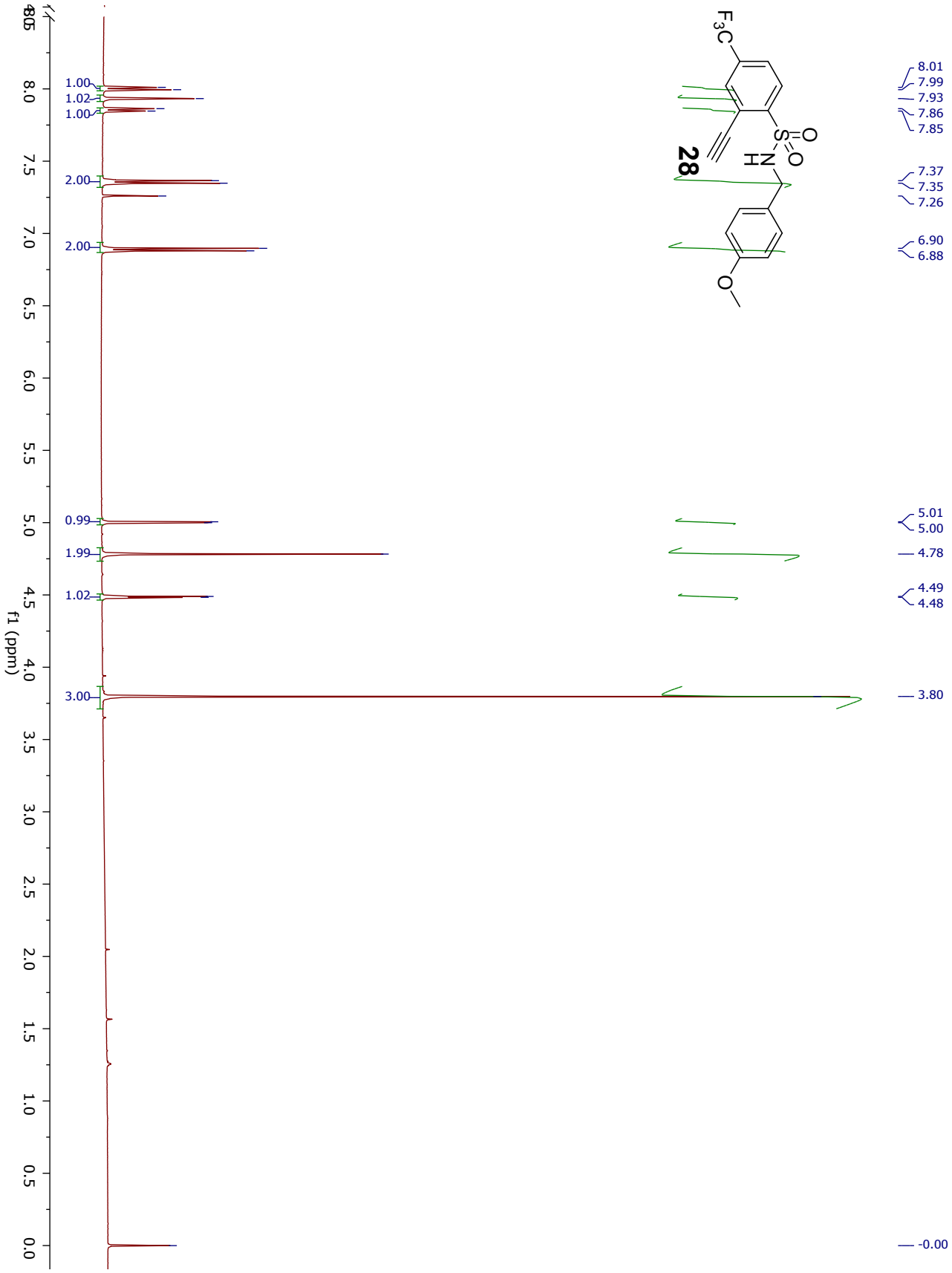

25
O
S
O
N
OMe
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
133.06
130.37
128.65
126.96
121.39
121.11
114.11
86.03
77.27
77.01
76.76
55.27
43.77
-0.00

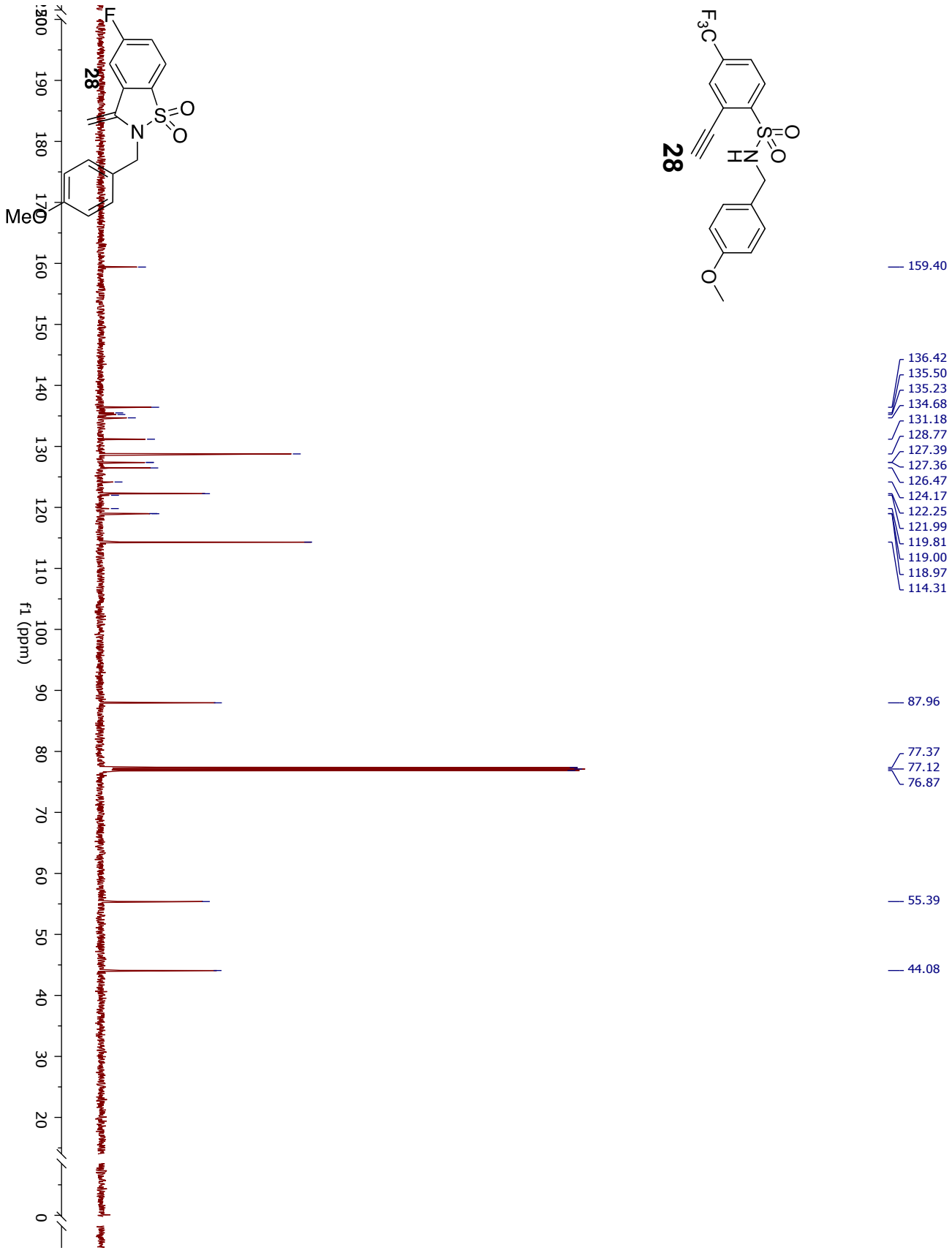

26
O
S
O
N
O
1.00
1.02
0.99
0.99
0.98
0.95
0.98
0.99
1.99
1.02
7.85
7.83
7.73
7.71
7.66
7.66
7.65
7.65
7.63
7.63
7.61
7.60
7.59
7.40
7.39
7.26
6.43
6.42
6.36
6.36
6.35
6.35
5.01
5.01
4.80
4.67
4.66
0.00
f1 (ppm)

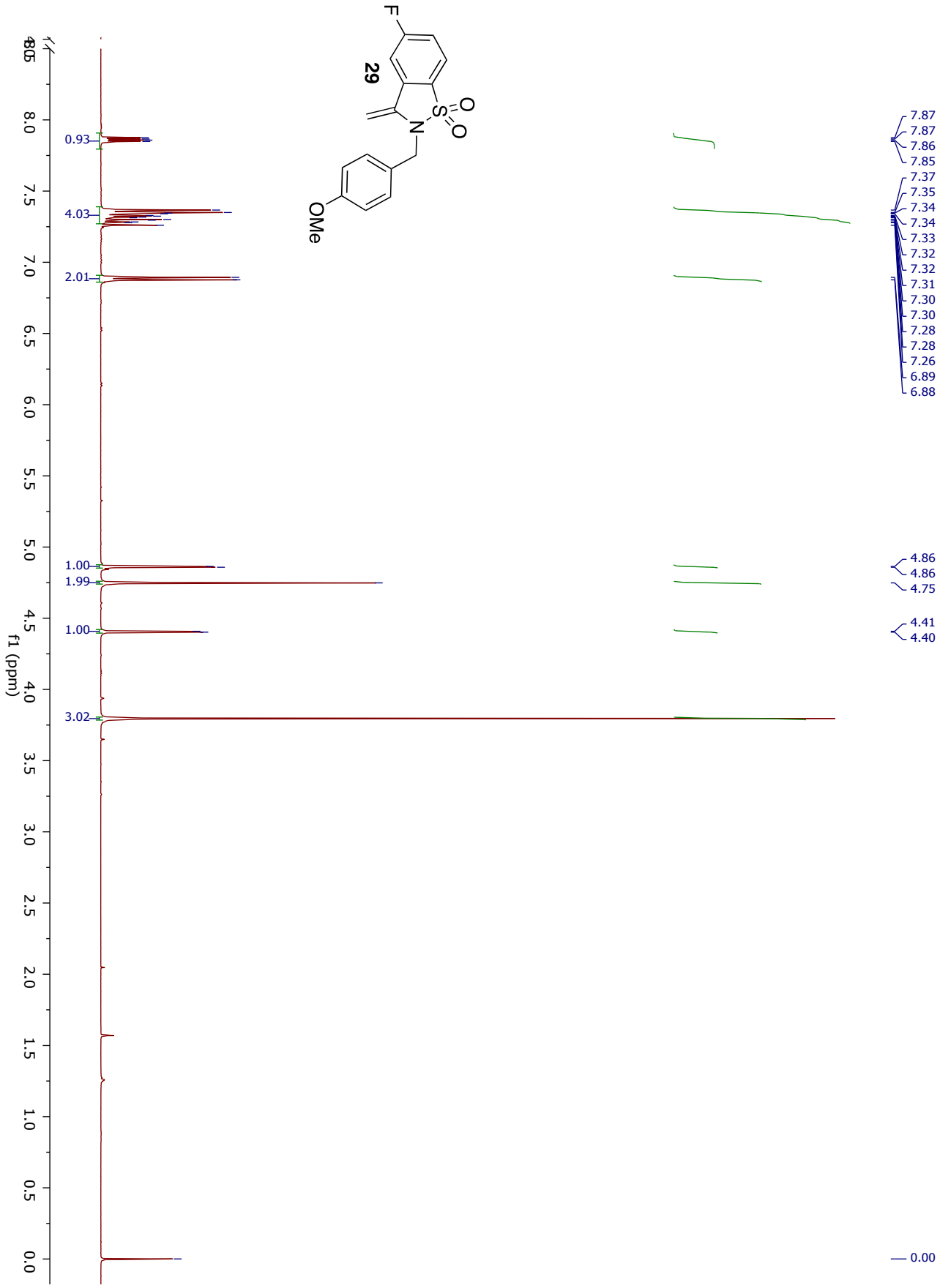

26
O
S
O
N
O
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
148.85
142.59
137.53
133.22
130.50
121.53
121.19
110.85
109.37
85.88
77.37
77.11
76.86
37.25

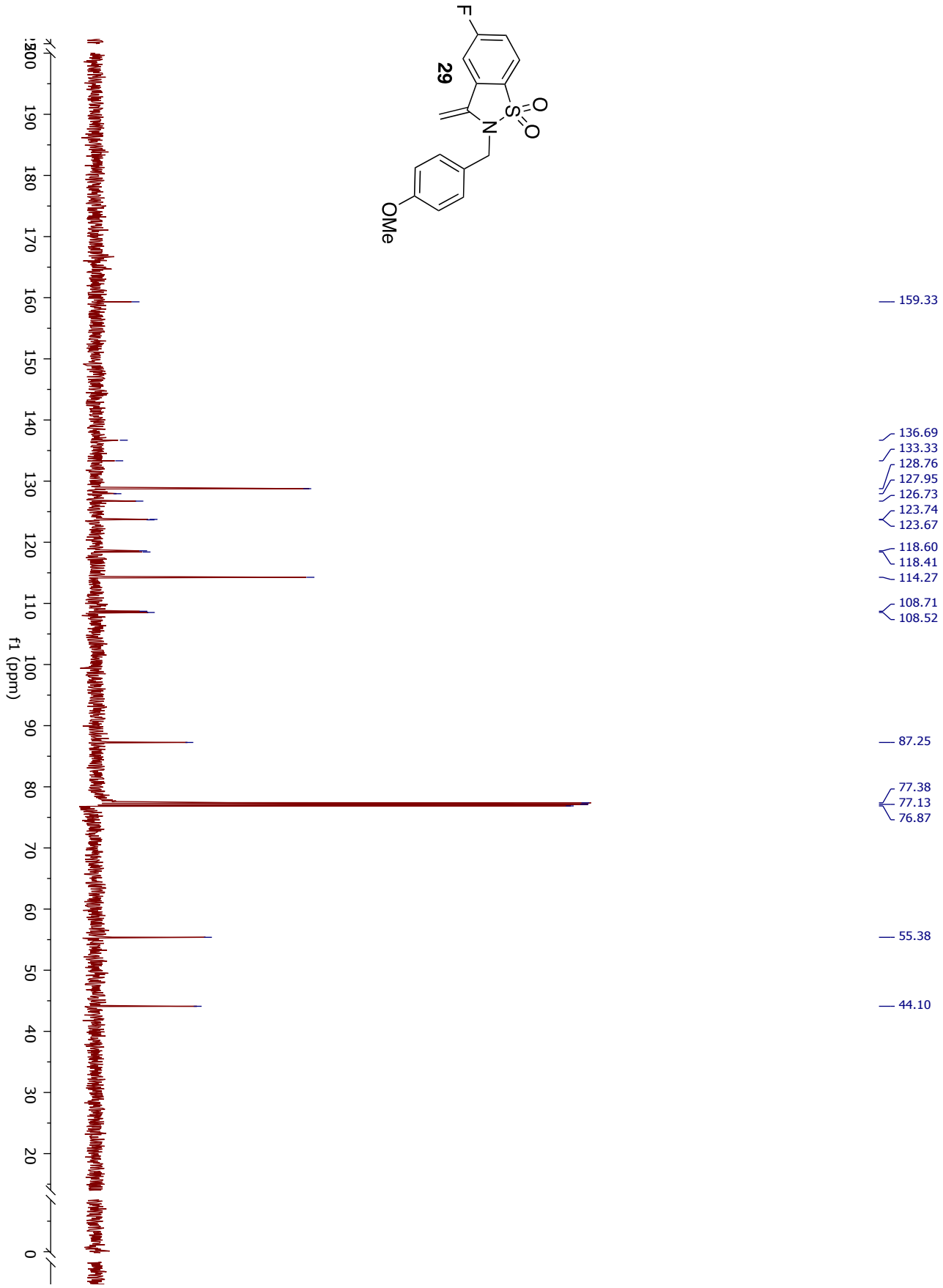

27
O
S
O
N
2.99
1.97
2.99
1.03
0.98
1.00
1.00
2.98
7.64
7.63
7.61
7.61
7.60
7.59
7.59
7.58
7.57
7.56
7.55
7.50
7.49
7.47
7.46
7.41
7.40
7.38
7.36
7.35
7.34
7.32
7.30
7.28
7.27
7.26
5.39
5.37
5.36
5.34
4.83
4.82
4.14
4.14
1.99
1.98
-0.00
f1 (ppm)

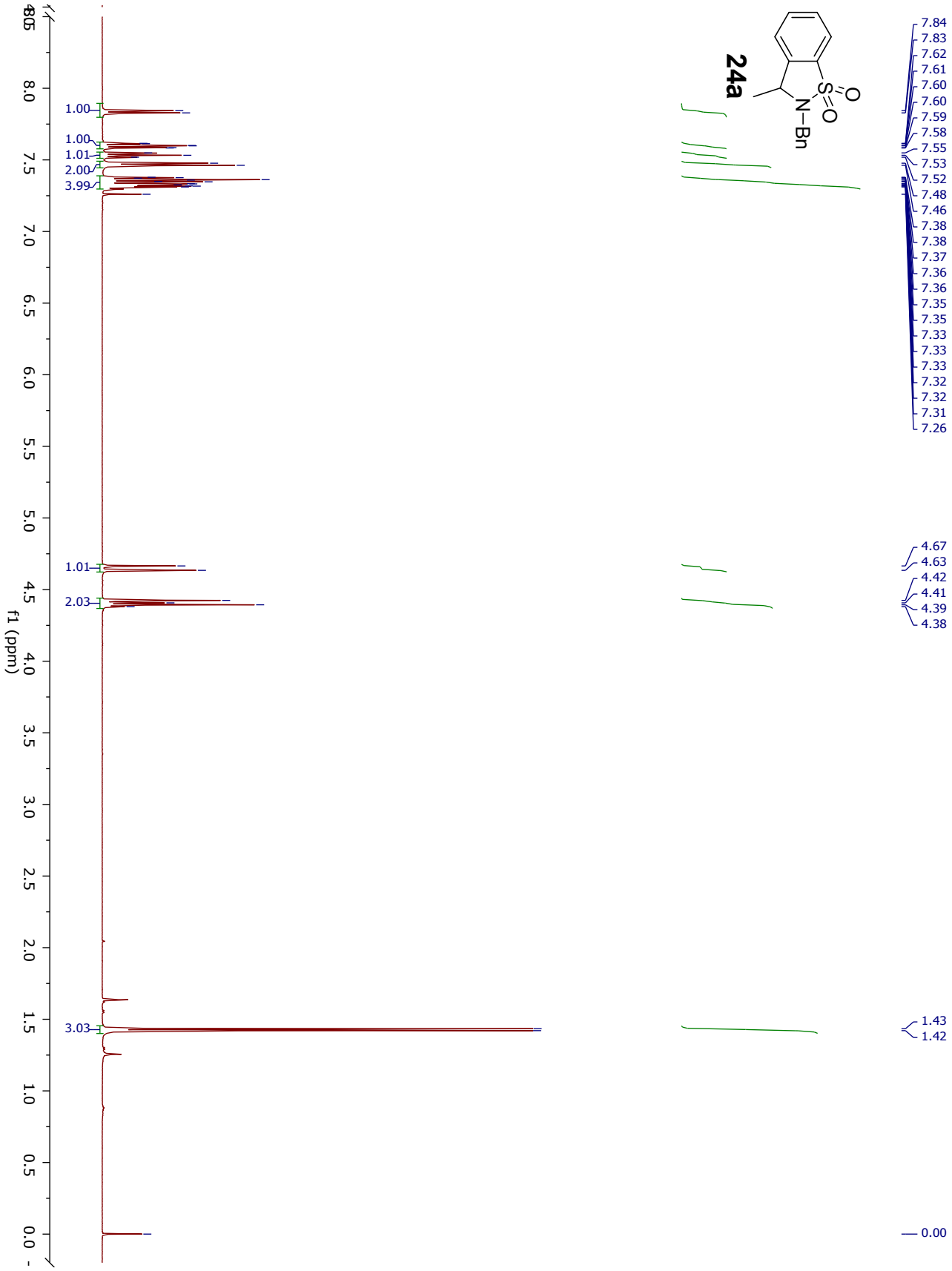

27
S
O
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
139.72
135.13
133.03
130.32
128.79
127.65
126.82
121.31
120.95
87.58
77.39
77.14
76.88
52.15
16.97

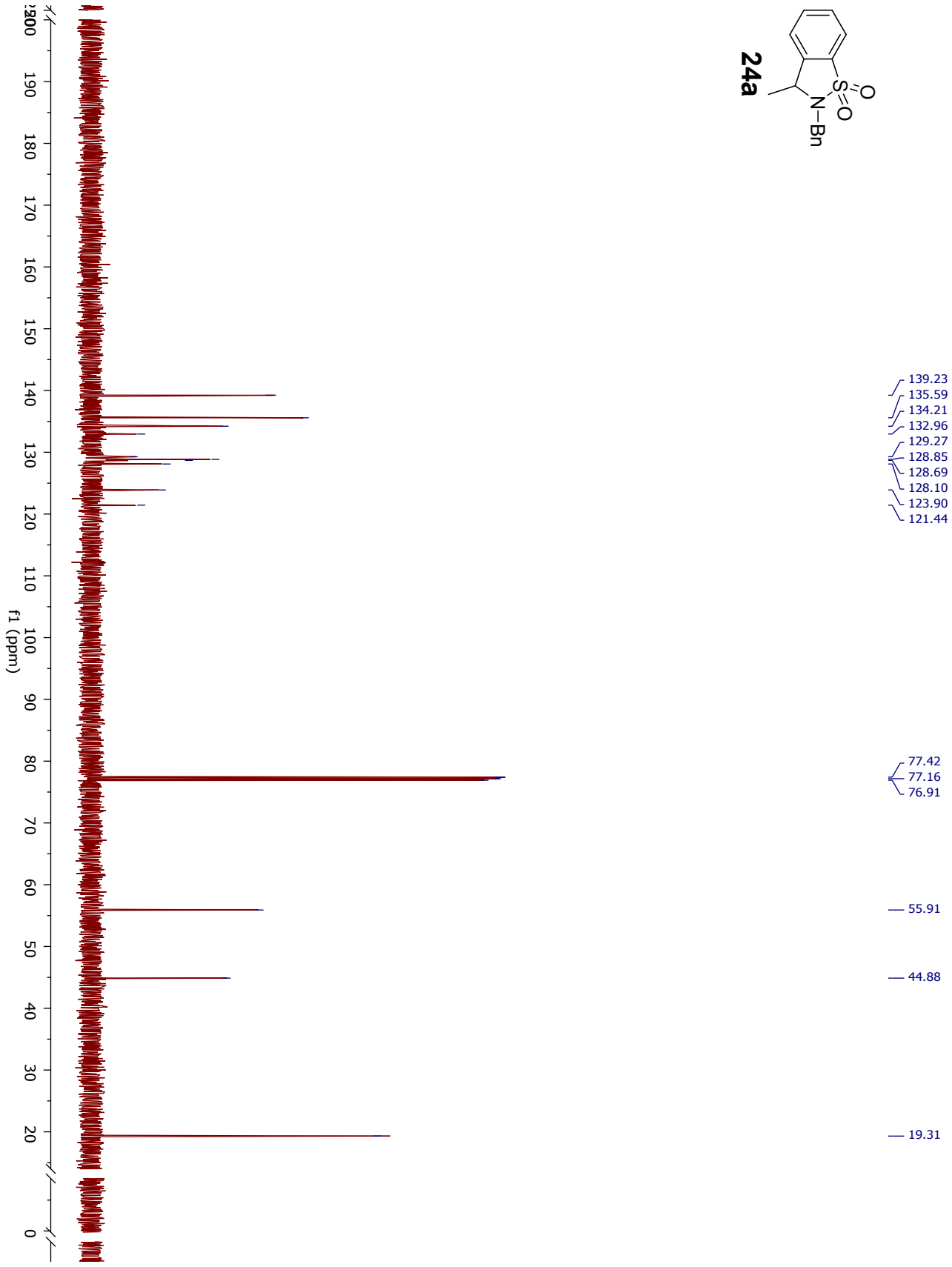

28
F3C
O
S
O
N
H
O
1.00
1.02
1.00
2.00
2.00
0.99
1.99
1.02
3.00
8.01
7.99
7.93
7.86
7.85
7.37
7.35
7.26
6.90
6.88
5.01
5.00
4.78
4.49
4.48
3.80
-0.00
f1 (ppm)

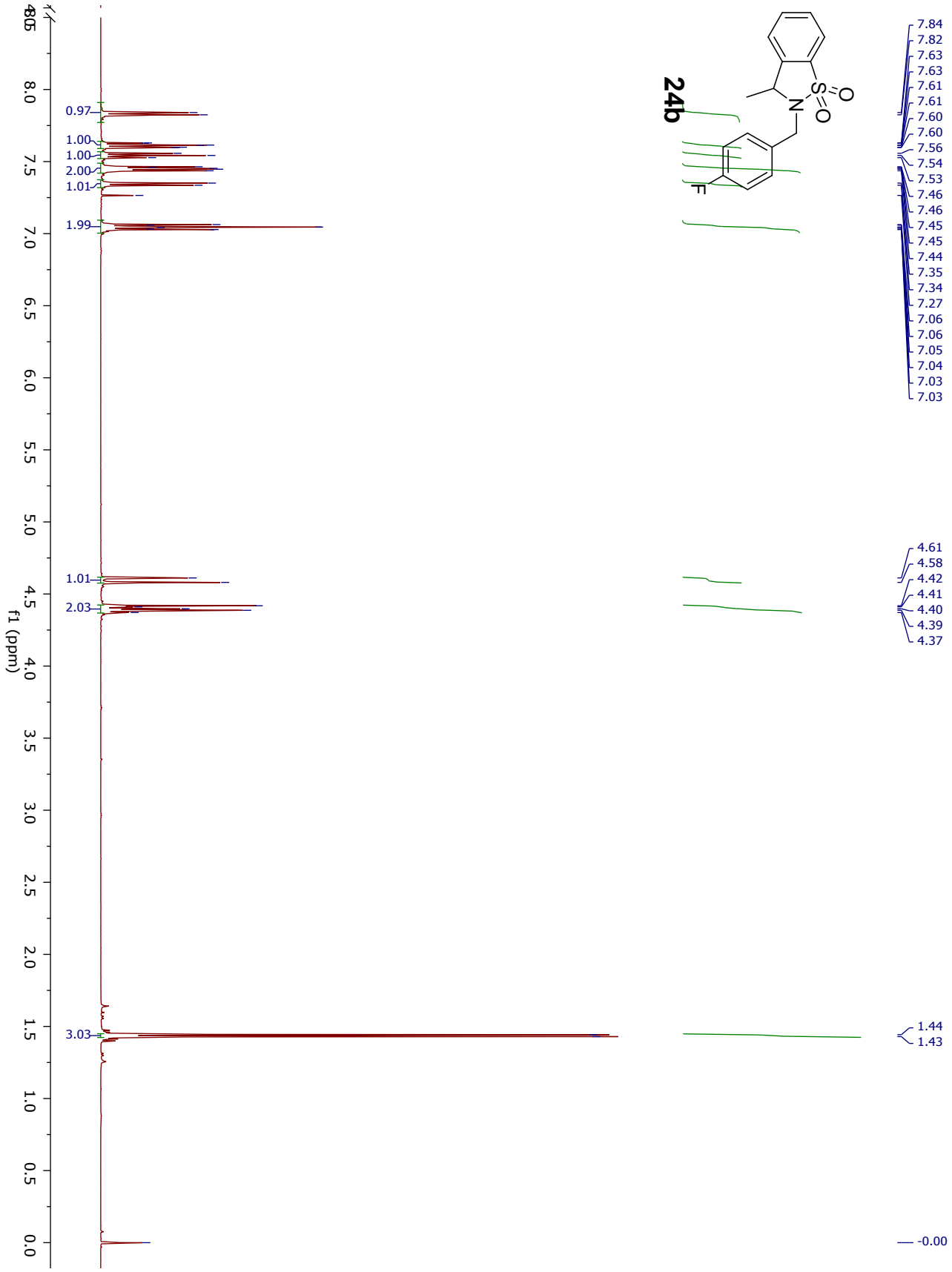

F
28
S
O
O
N
MeO
F3C
28
S
O
O
N
H
O
159.40
136.42
135.50
135.23
134.68
131.18
128.77
127.39
127.36
126.47
124.17
122.25
121.99
119.81
119.00
118.97
114.31
87.96
77.37
77.12
76.87
55.39
44.08
f1 (ppm)

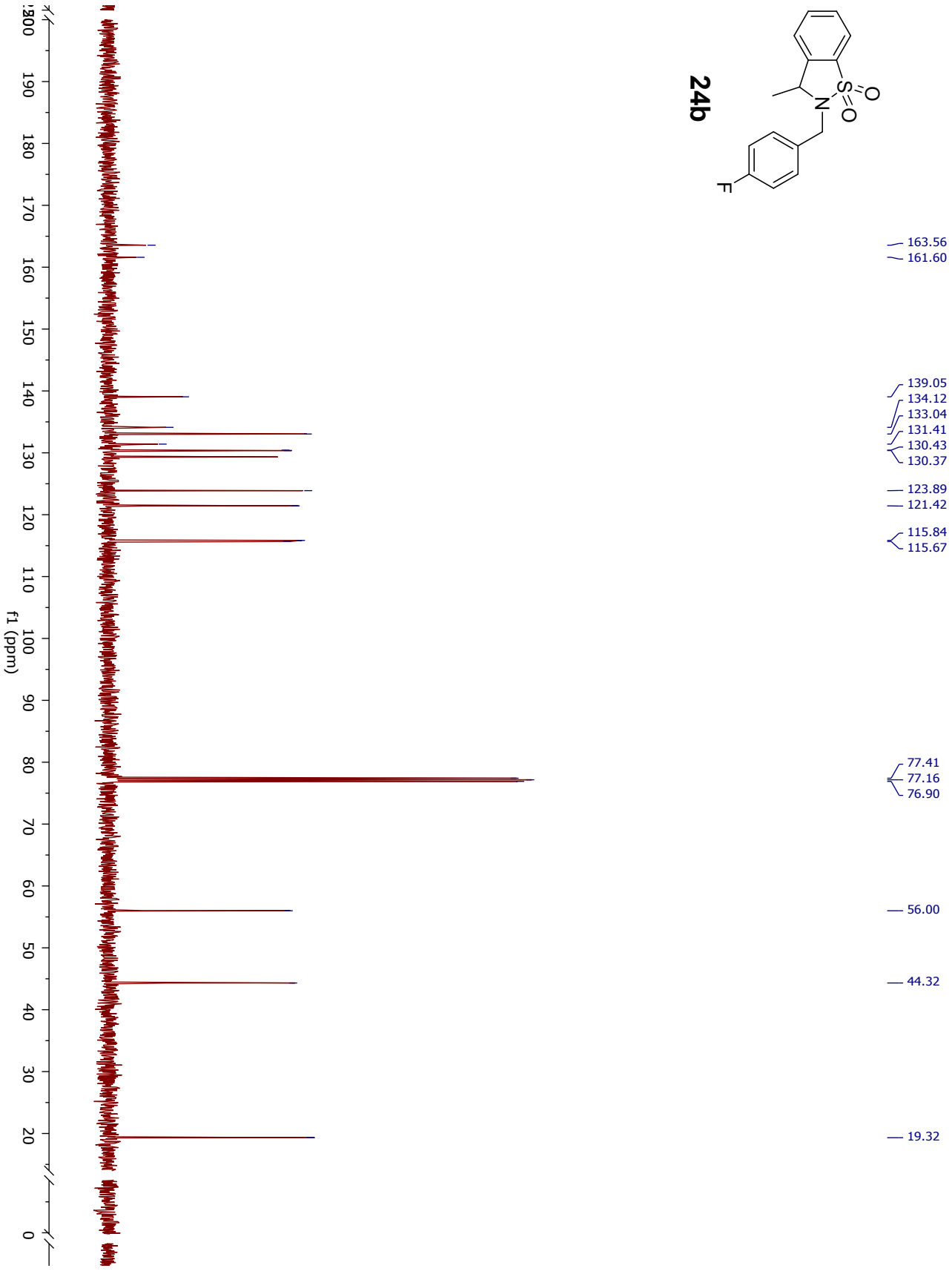

29
F
O
S
O
N
OMe
f1 (ppm)
0.93
4.03
2.01
1.00
1.99
1.00
3.02
7.87
7.87
7.86
7.85
7.37
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.28
7.28
7.26
6.89
6.88
4.86
4.86
4.75
4.41
4.40
0.00

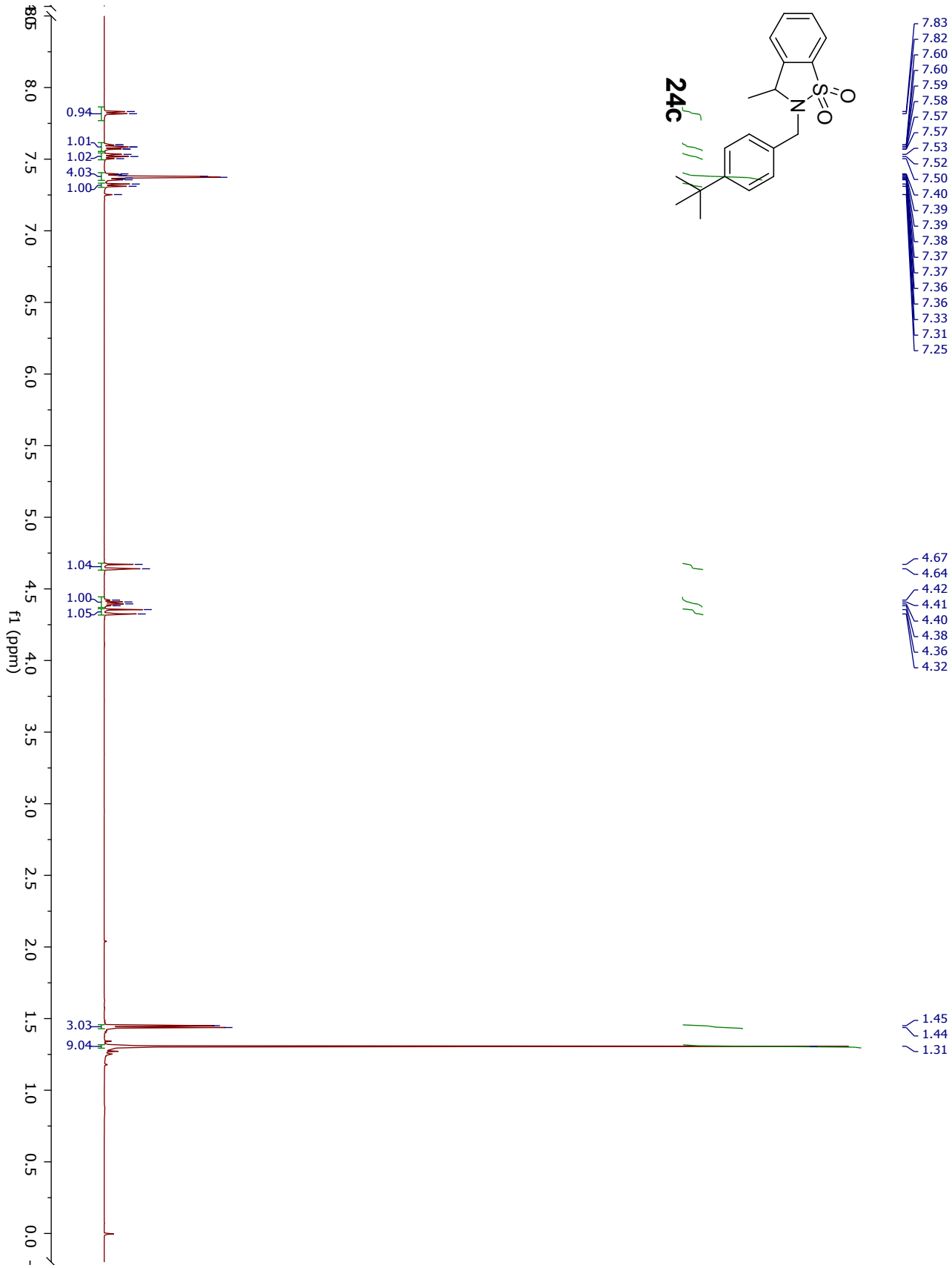

F
29
O
S
O
N
OMe
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
159.33
136.69
133.33
128.76
127.95
126.73
123.74
123.67
118.60
118.41
114.27
108.71
108.52
87.25
77.38
77.13
76.87
55.38
44.10

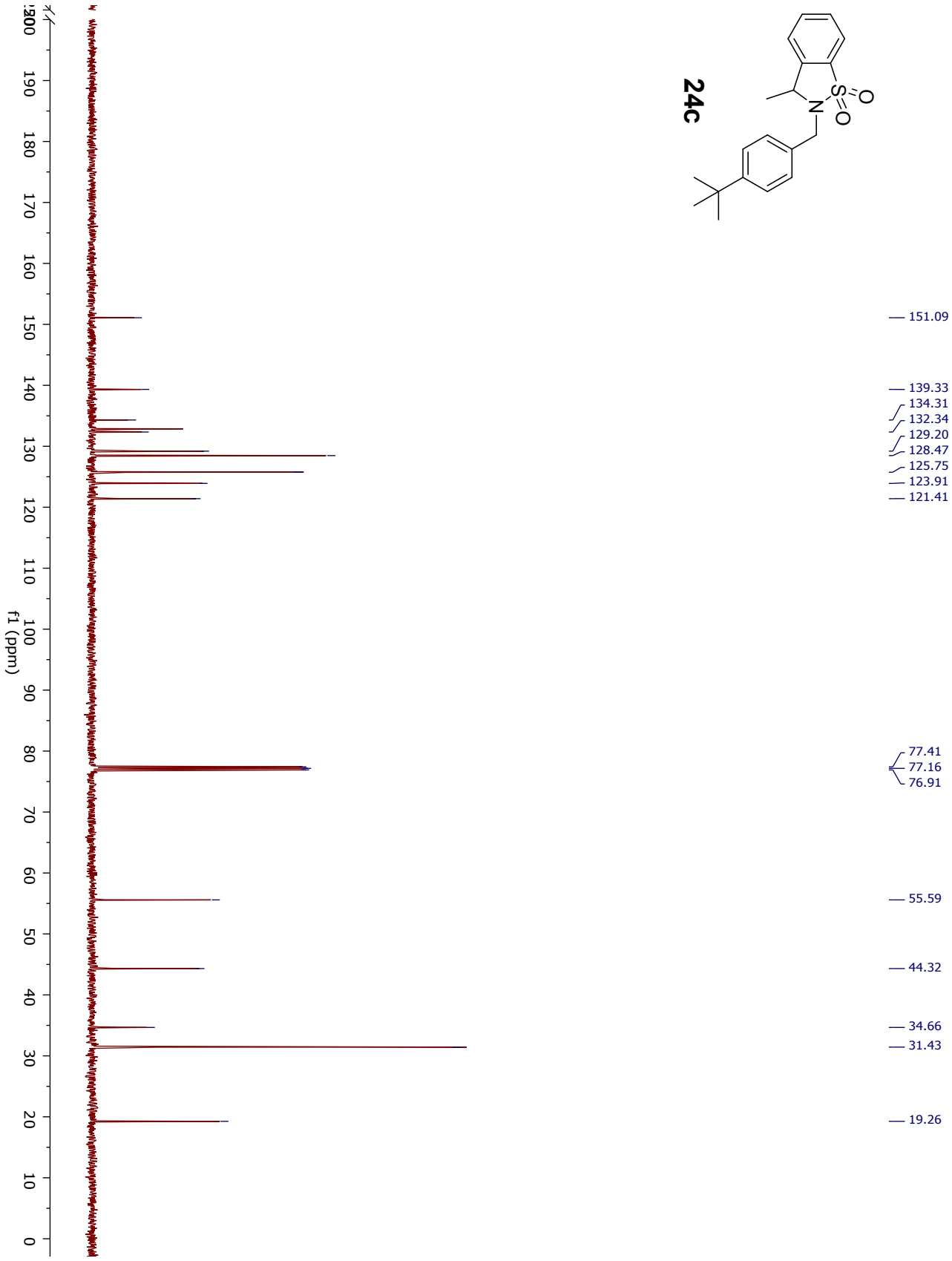

24a
O
S
O
N–Bn
f1 (ppm)
1.00
1.00
1.01
2.00
3.99
1.01
2.03
3.03
7.84
7.83
7.62
7.61
7.60
7.60
7.59
7.58
7.55
7.53
7.52
7.48
7.46
7.38
7.38
7.37
7.36
7.36
7.35
7.35
7.33
7.33
7.33
7.32
7.32
7.31
7.26
4.67
4.63
4.42
4.41
4.39
4.38
1.43
1.42
0.00

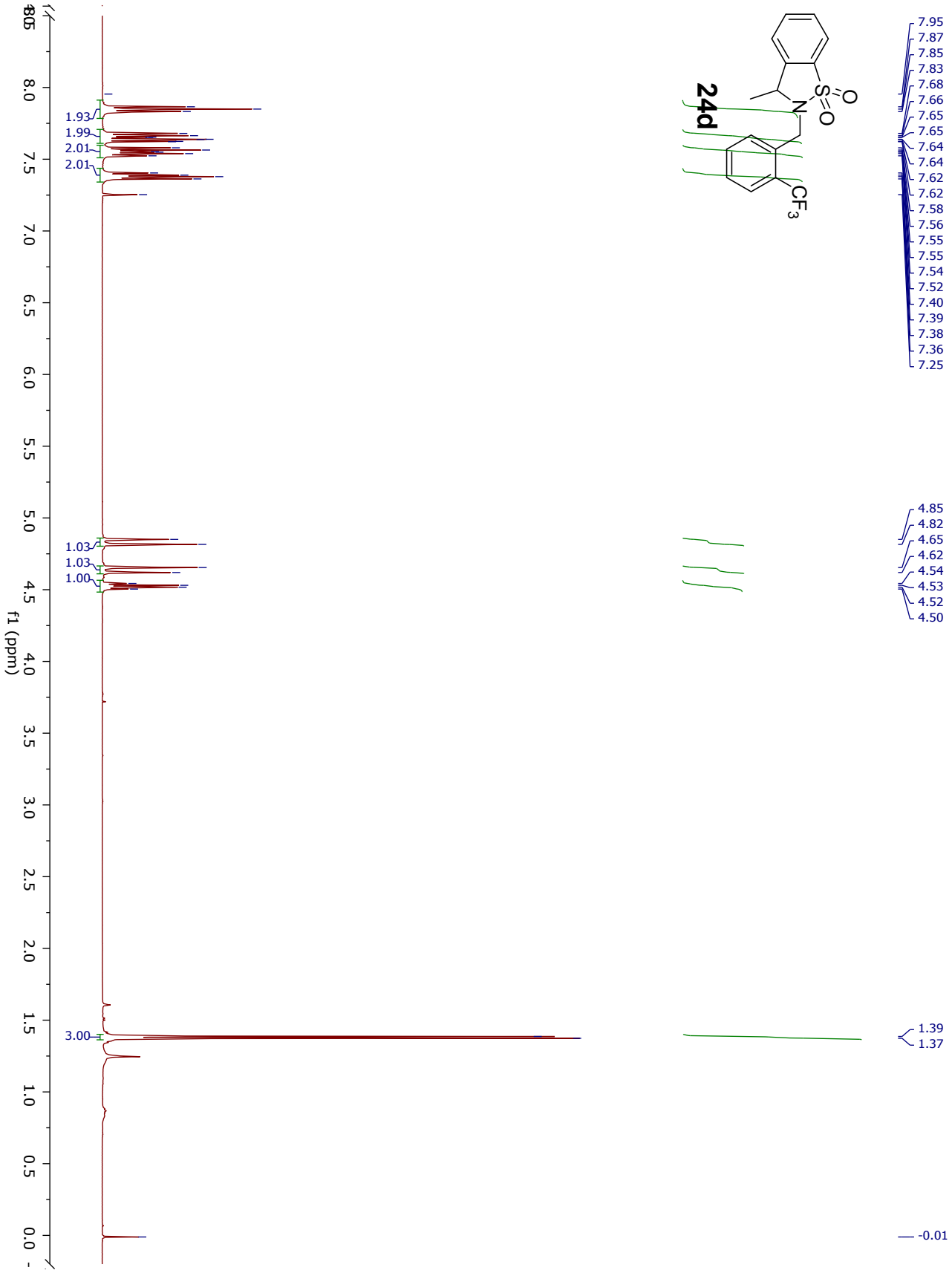

24a
O
S
O
N
Bn
139.23
135.59
134.21
132.96
129.27
128.85
128.69
128.10
123.90
121.44
77.42
77.16
76.91
55.91
44.88
19.31
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0

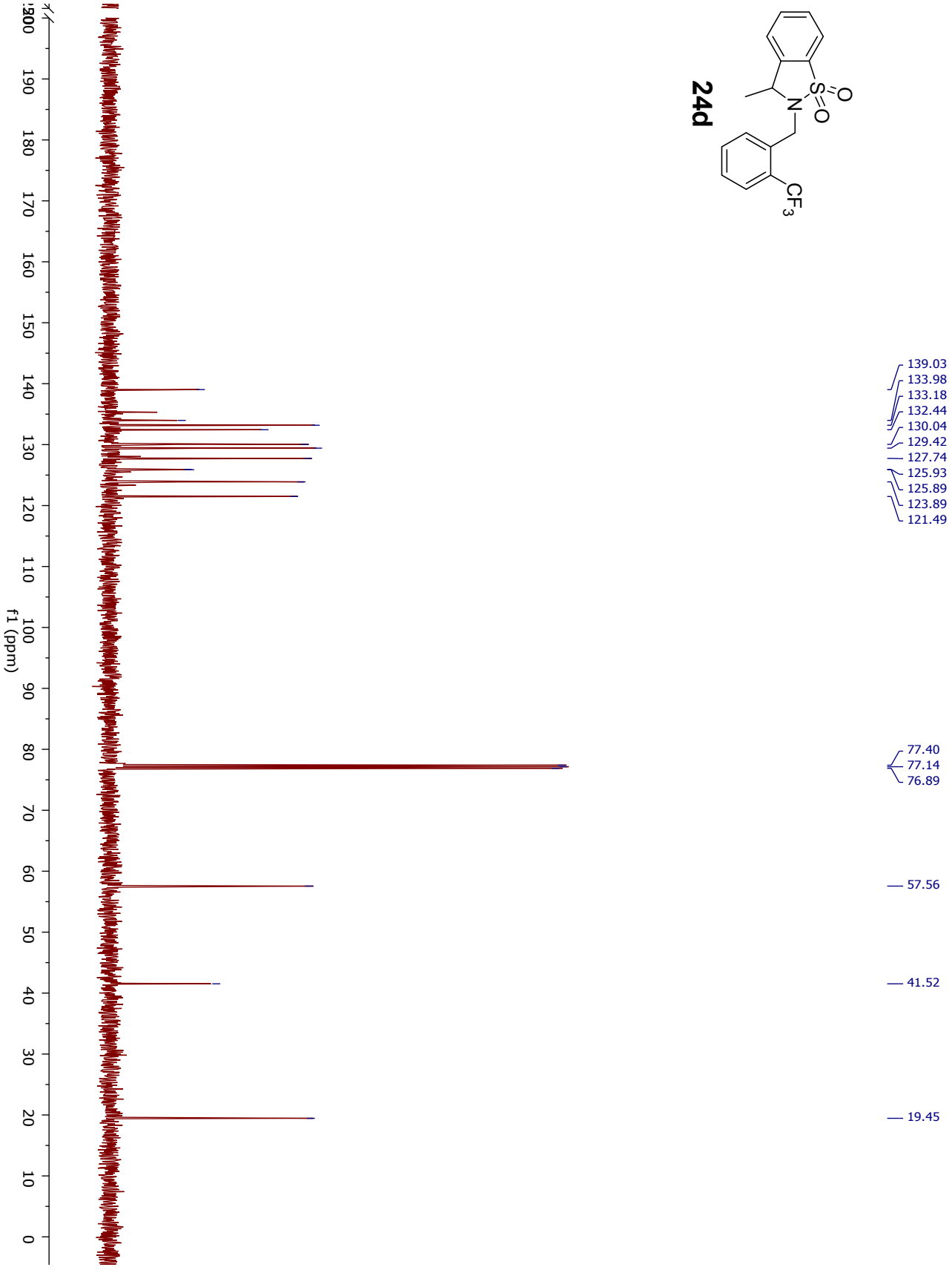

24b
O
S
O
N
F
0.97
1.00
1.00
2.00
1.01
1.99
1.01
2.03
3.03
7.84
7.82
7.63
7.63
7.61
7.61
7.60
7.60
7.56
7.54
7.53
7.46
7.46
7.45
7.45
7.44
7.35
7.34
7.27
7.06
7.06
7.05
7.04
7.03
7.03
4.61
4.58
4.42
4.41
4.40
4.39
4.37
1.44
1.43
-0.00
f1 (ppm)

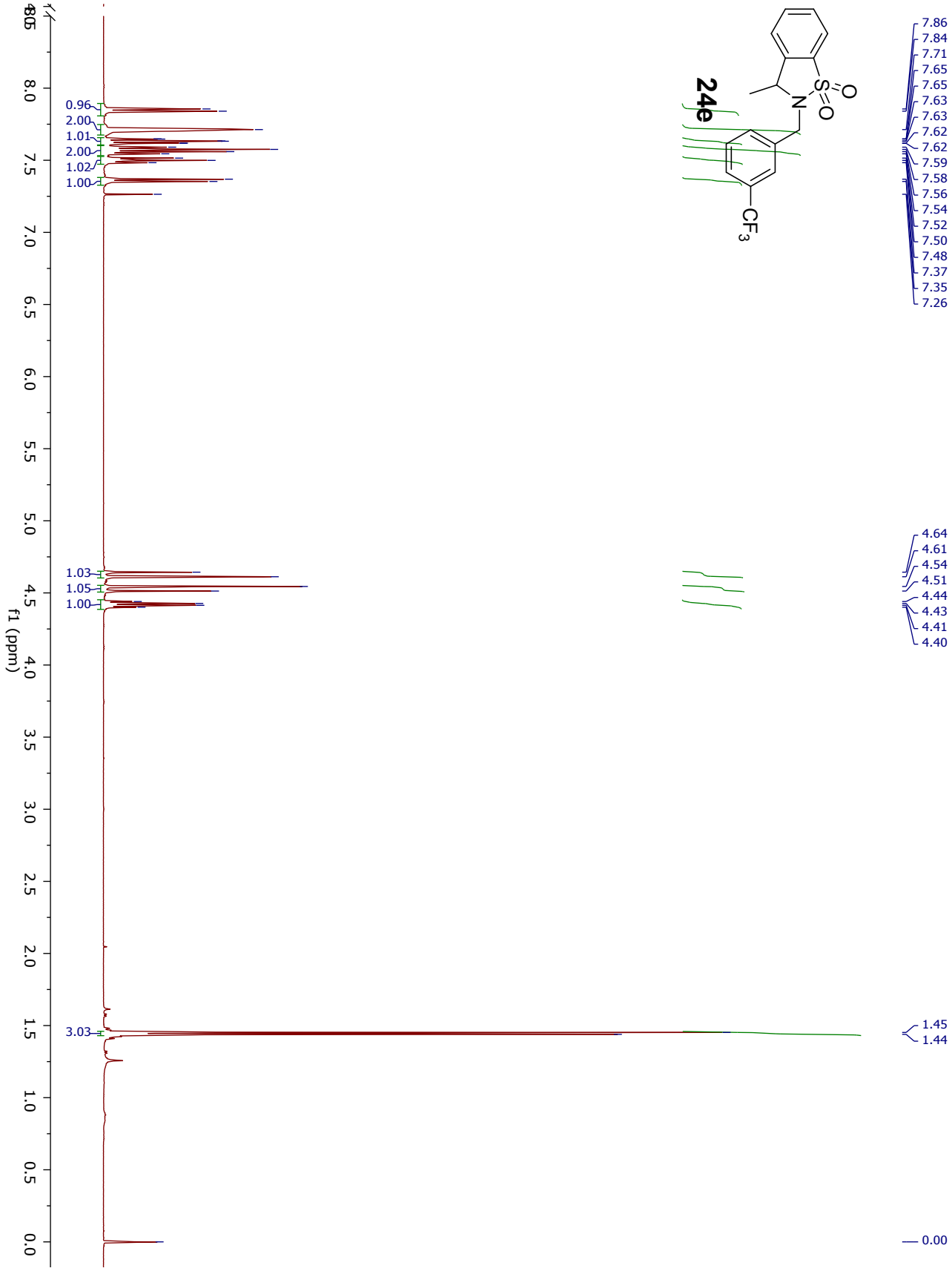

24b
O
S
O
N
F
163.56
161.60
139.05
134.12
133.04
131.41
130.43
130.37
123.89
121.42
115.84
115.67
77.41
77.16
76.90
56.00
44.32
19.32
f1 (ppm)

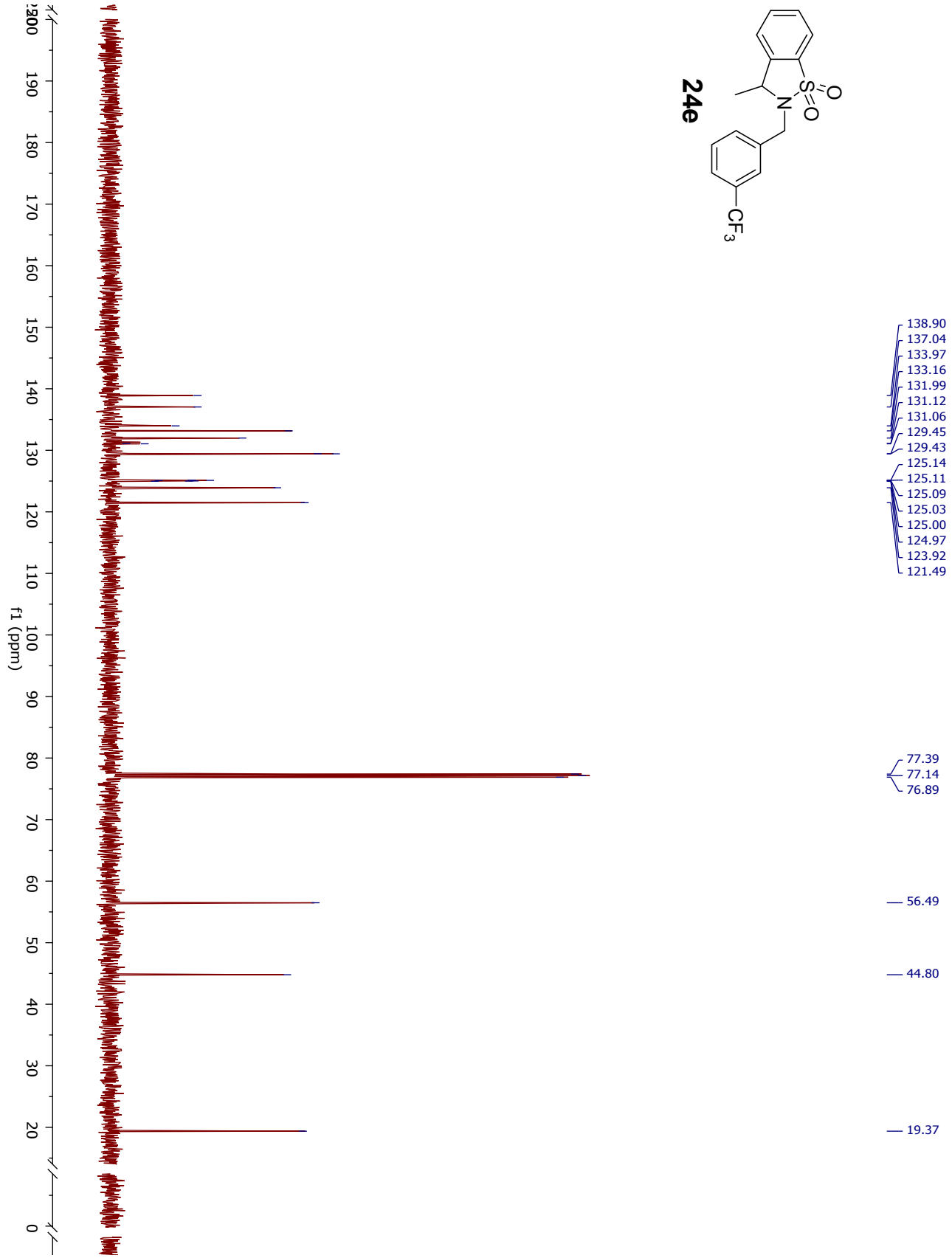

24c
O
S
O
N
7.83
7.82
7.60
7.60
7.59
7.58
7.57
7.57
7.53
7.52
7.50
7.40
7.39
7.39
7.38
7.37
7.37
7.36
7.36
7.33
7.31
7.25
4.67
4.64
4.42
4.41
4.40
4.38
4.36
4.32
1.45
1.44
1.31
0.94
1.01
1.02
4.03
1.00
1.04
1.00
1.05
3.03
9.04
f1 (ppm)

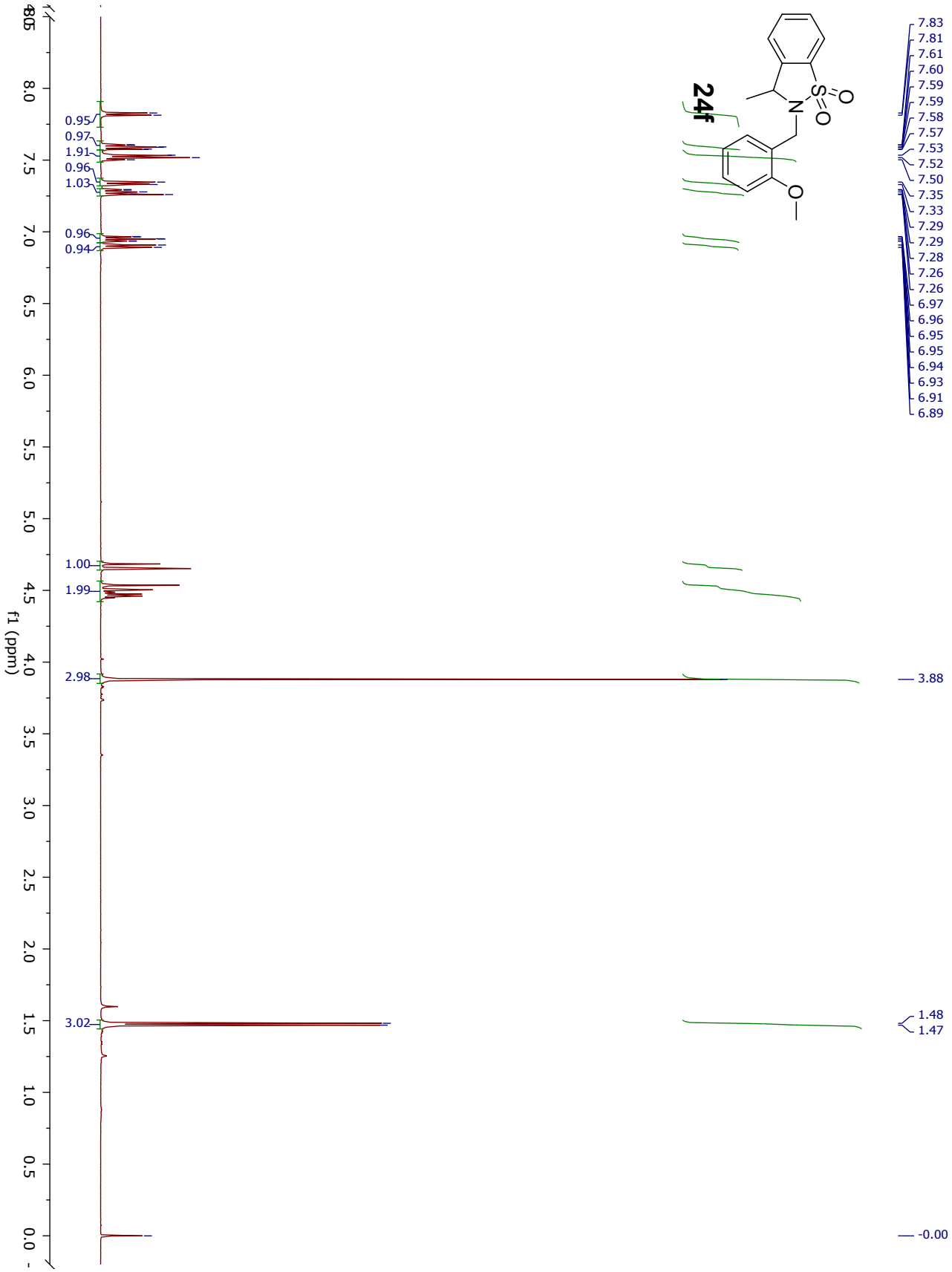

24c
151.09
139.33
134.31
132.34
129.20
128.47
125.75
123.91
121.41
77.41
77.16
76.91
55.59
44.32
34.66
31.43
19.26
f1 (ppm)

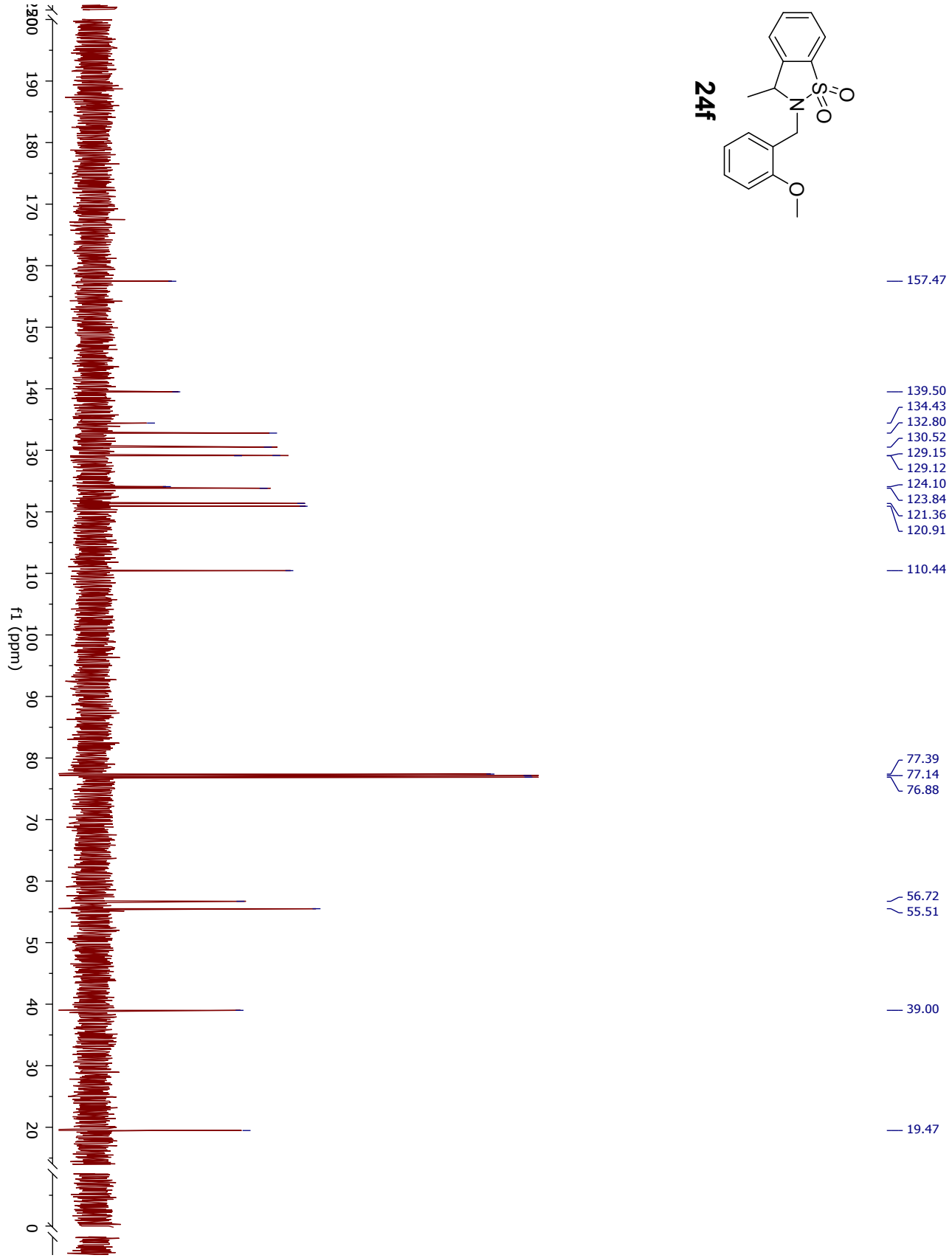

24d
O
S
O
N
CF3
f1 (ppm)
1.93
1.99
2.01
2.01
1.03
1.03
1.00
3.00
7.95
7.87
7.85
7.83
7.68
7.66
7.65
7.65
7.64
7.64
7.62
7.62
7.58
7.56
7.55
7.55
7.54
7.52
7.40
7.39
7.38
7.36
7.25
4.85
4.82
4.65
4.62
4.54
4.53
4.52
4.50
1.39
1.37
-0.01

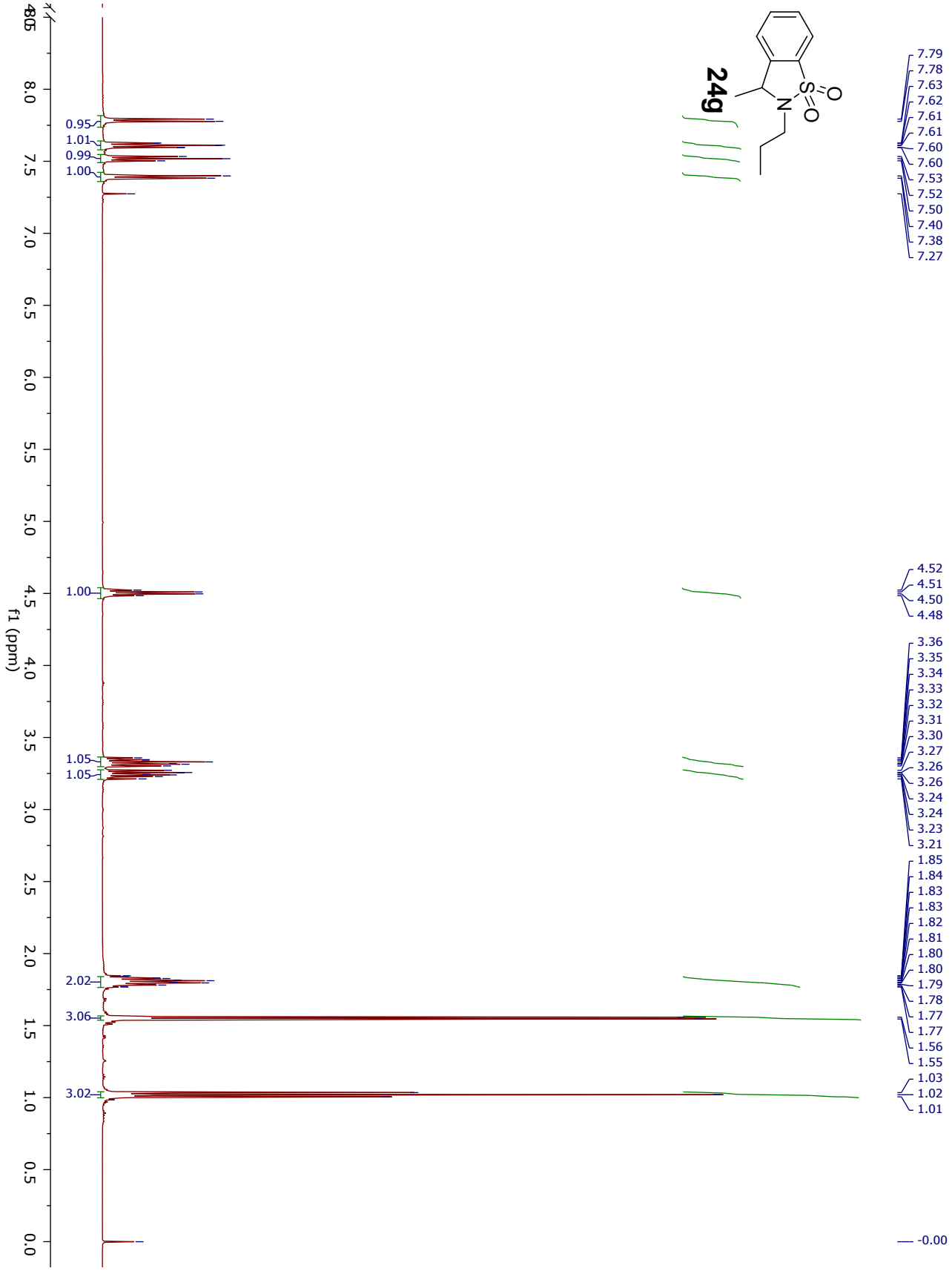

24d
O
S
O
N
CF3
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
139.03
133.98
133.18
132.44
130.04
129.42
127.74
125.93
125.89
123.89
121.49
77.40
77.14
76.89
57.56
41.52
19.45

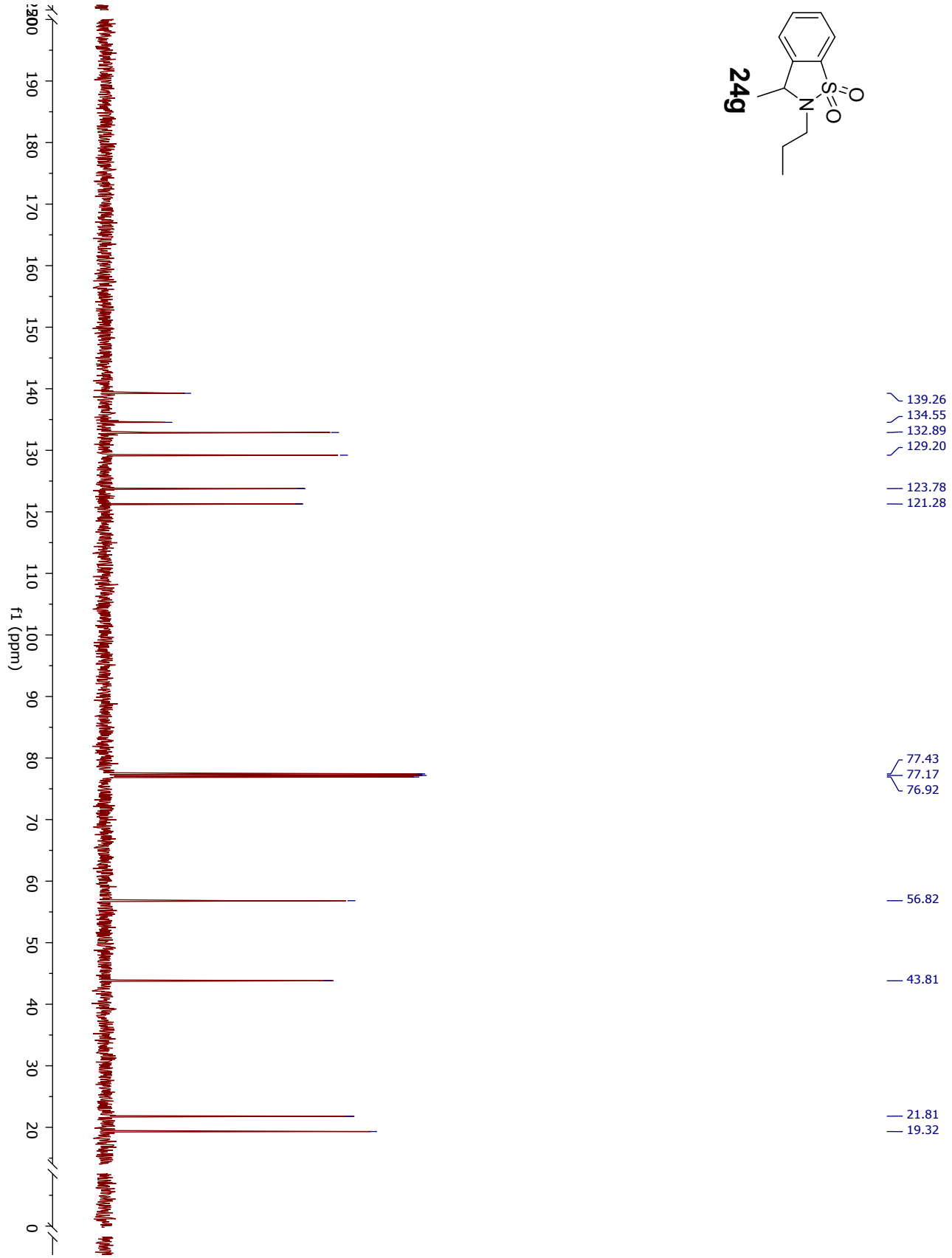

24e
O
S
O
N
CF3
0.96
2.00
1.01
2.00
1.02
1.00
1.03
1.05
1.00
3.03
7.86
7.84
7.71
7.65
7.65
7.63
7.63
7.62
7.62
7.59
7.58
7.56
7.54
7.52
7.50
7.48
7.37
7.35
7.26
4.64
4.61
4.54
4.51
4.44
4.43
4.41
4.40
1.45
1.44
0.00
f1 (ppm)

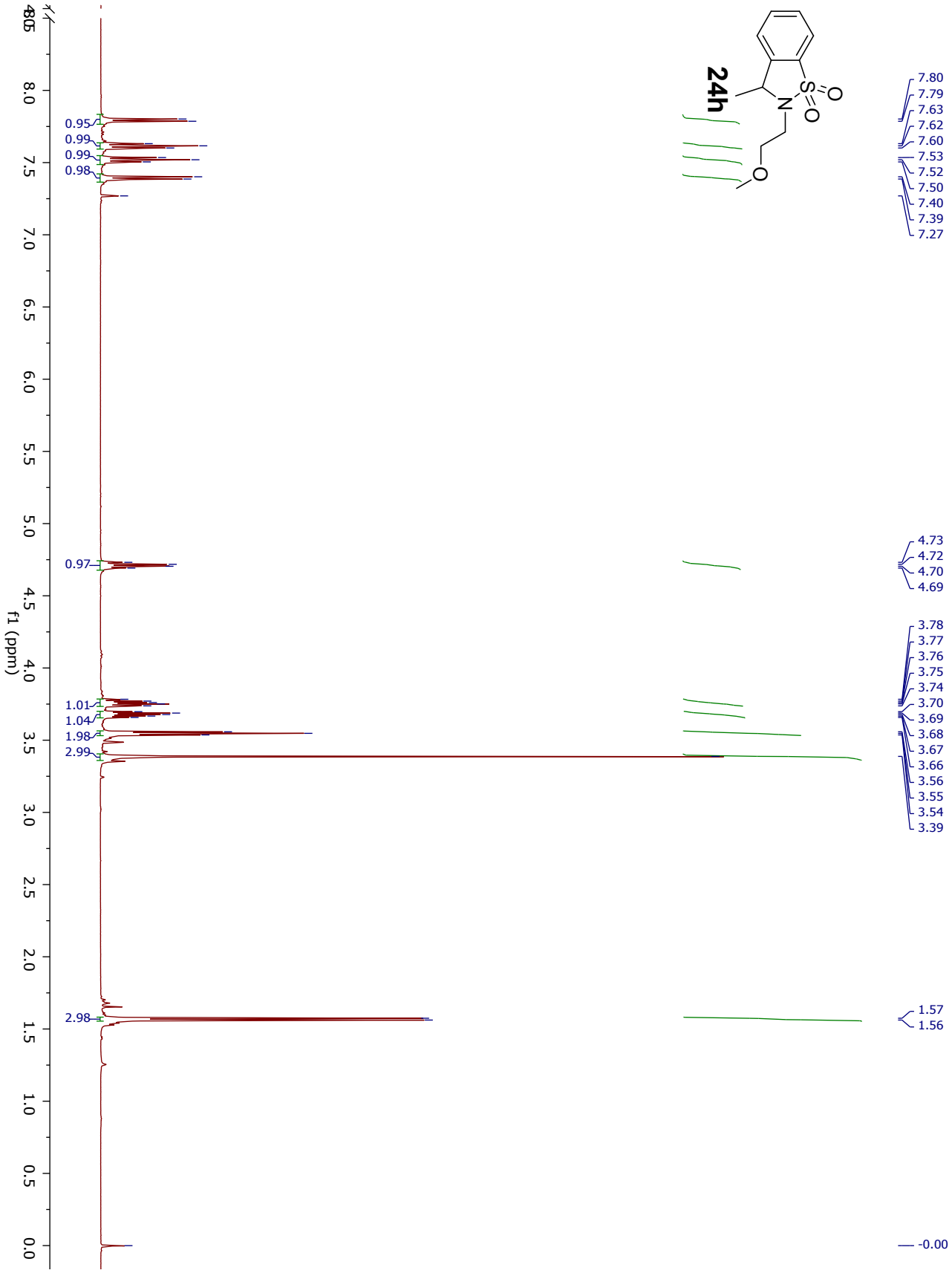

24e
O
S
O
N
CF3
138.90
137.04
133.97
133.16
131.99
131.12
131.06
129.45
129.43
125.14
125.11
125.09
125.03
125.00
124.97
123.92
121.49
77.39
77.14
76.89
56.49
44.80
19.37
f1 (ppm)

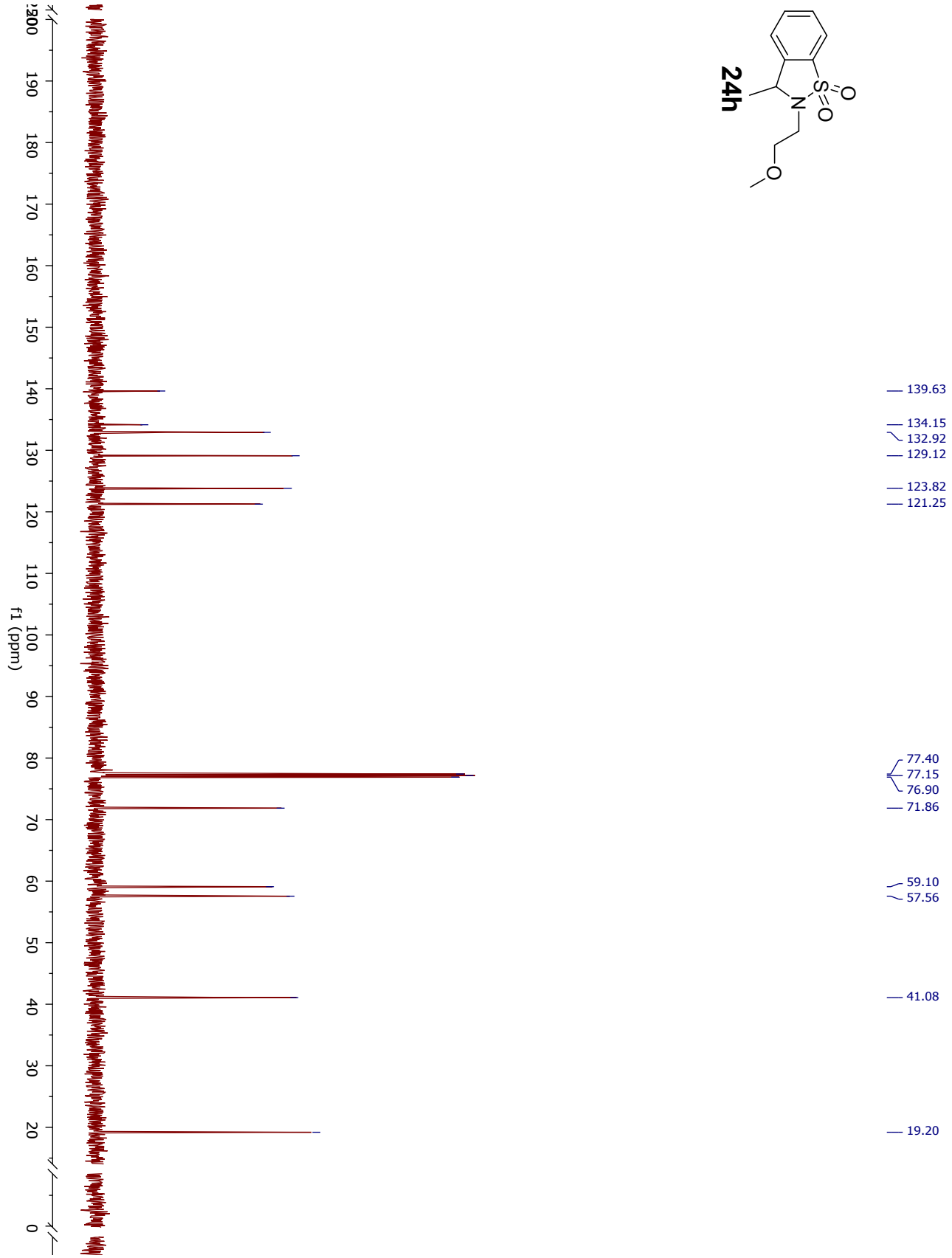

24f
f1 (ppm)
0.95
0.97
1.91
0.96
1.03
0.96
0.94
1.00
1.99
2.98
3.02
7.83
7.81
7.61
7.60
7.59
7.59
7.58
7.57
7.53
7.52
7.50
7.35
7.33
7.29
7.29
7.28
7.26
7.26
6.97
6.96
6.95
6.95
6.94
6.93
6.91
6.89
3.88
1.48
1.47
-0.00

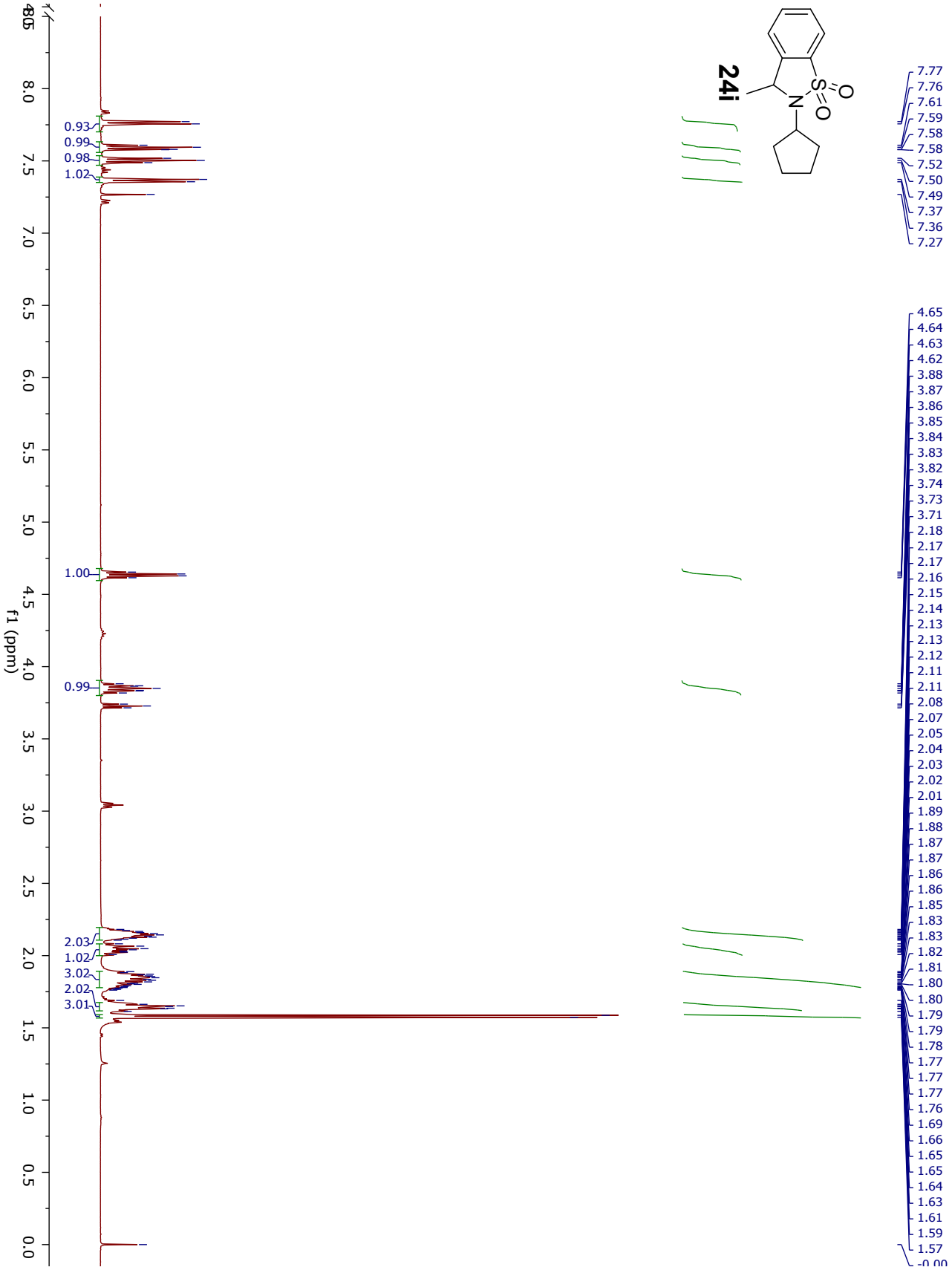

24f
157.47
139.50
134.43
132.80
130.52
129.15
129.12
124.10
123.84
121.36
120.91
110.44
77.39
77.14
76.88
56.72
55.51
39.00
19.47
f1 (ppm)

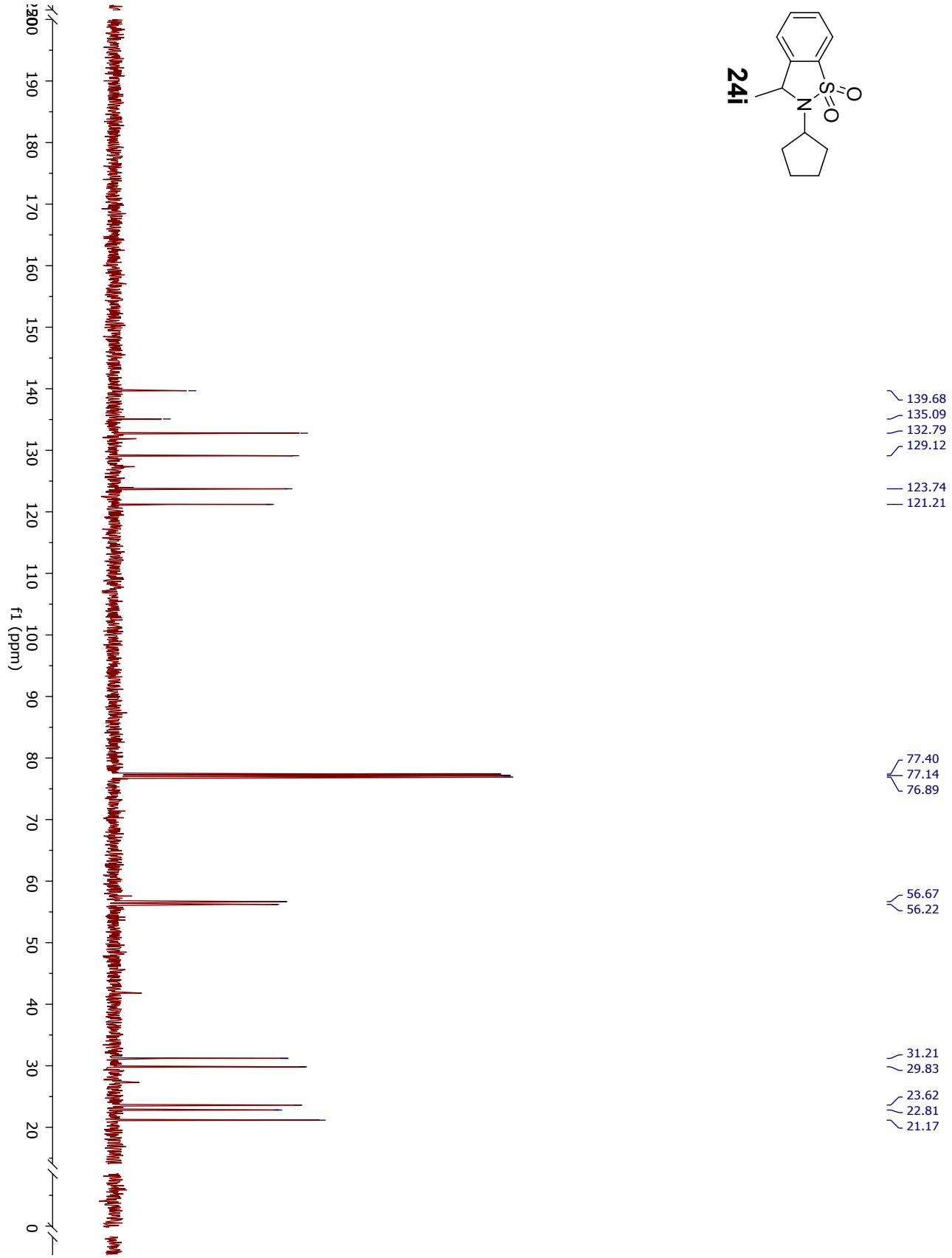

24g
f1 (ppm)
0.95
1.01
0.99
1.00
1.00
1.05
1.05
2.02
3.06
3.02
7.79
7.78
7.63
7.62
7.61
7.61
7.60
7.60
7.53
7.52
7.50
7.40
7.38
7.27
4.52
4.51
4.50
4.48
3.36
3.35
3.34
3.33
3.32
3.31
3.30
3.27
3.26
3.26
3.24
3.24
3.23
3.21
1.85
1.84
1.83
1.83
1.82
1.81
1.80
1.80
1.79
1.78
1.77
1.77
1.56
1.55
1.03
1.02
1.01
-0.00

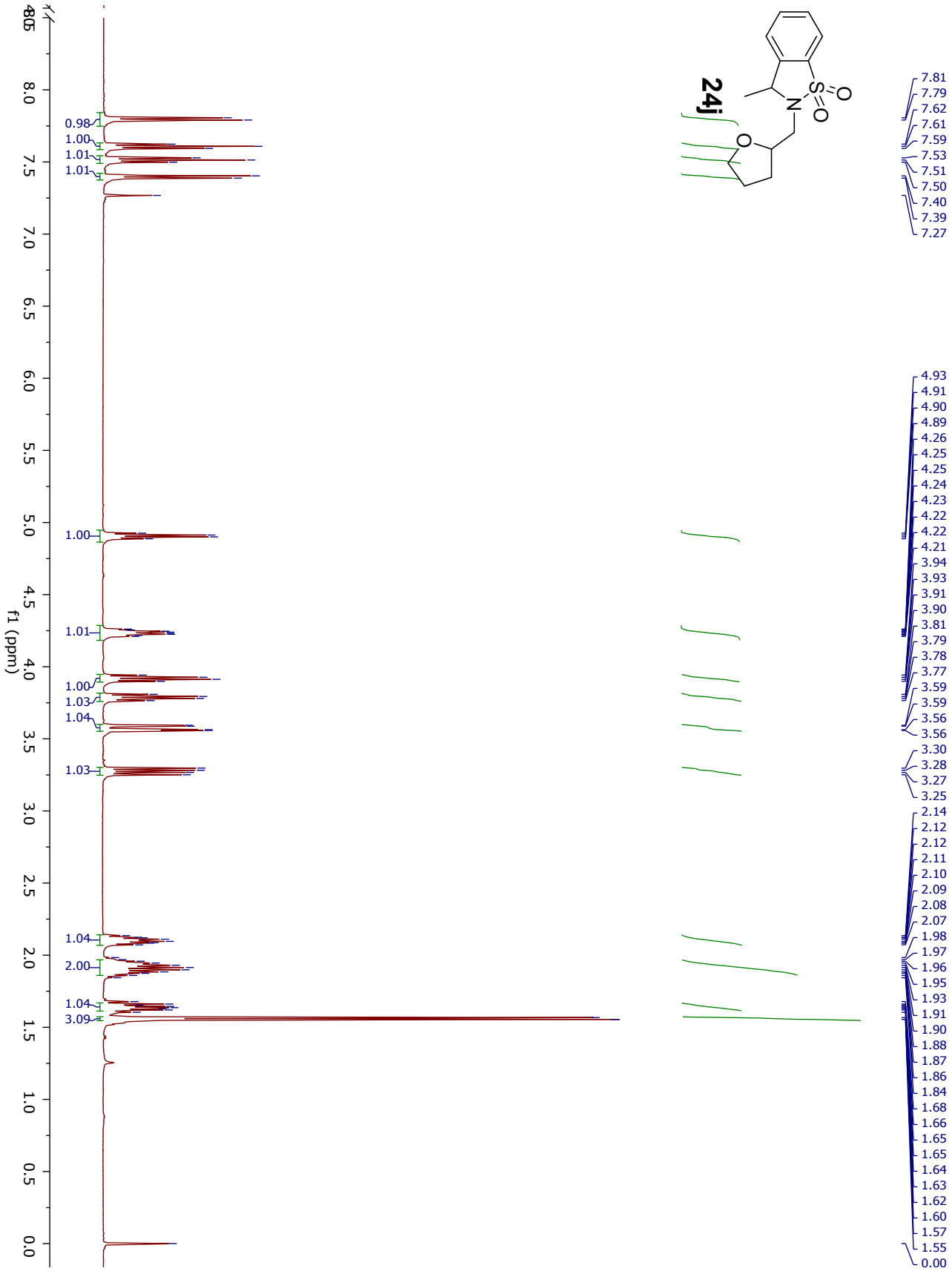

24g
O
S
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
f1 (ppm)
139.26
134.55
132.89
129.20
123.78
121.28
77.43
77.17
76.92
56.82
43.81
21.81
19.32

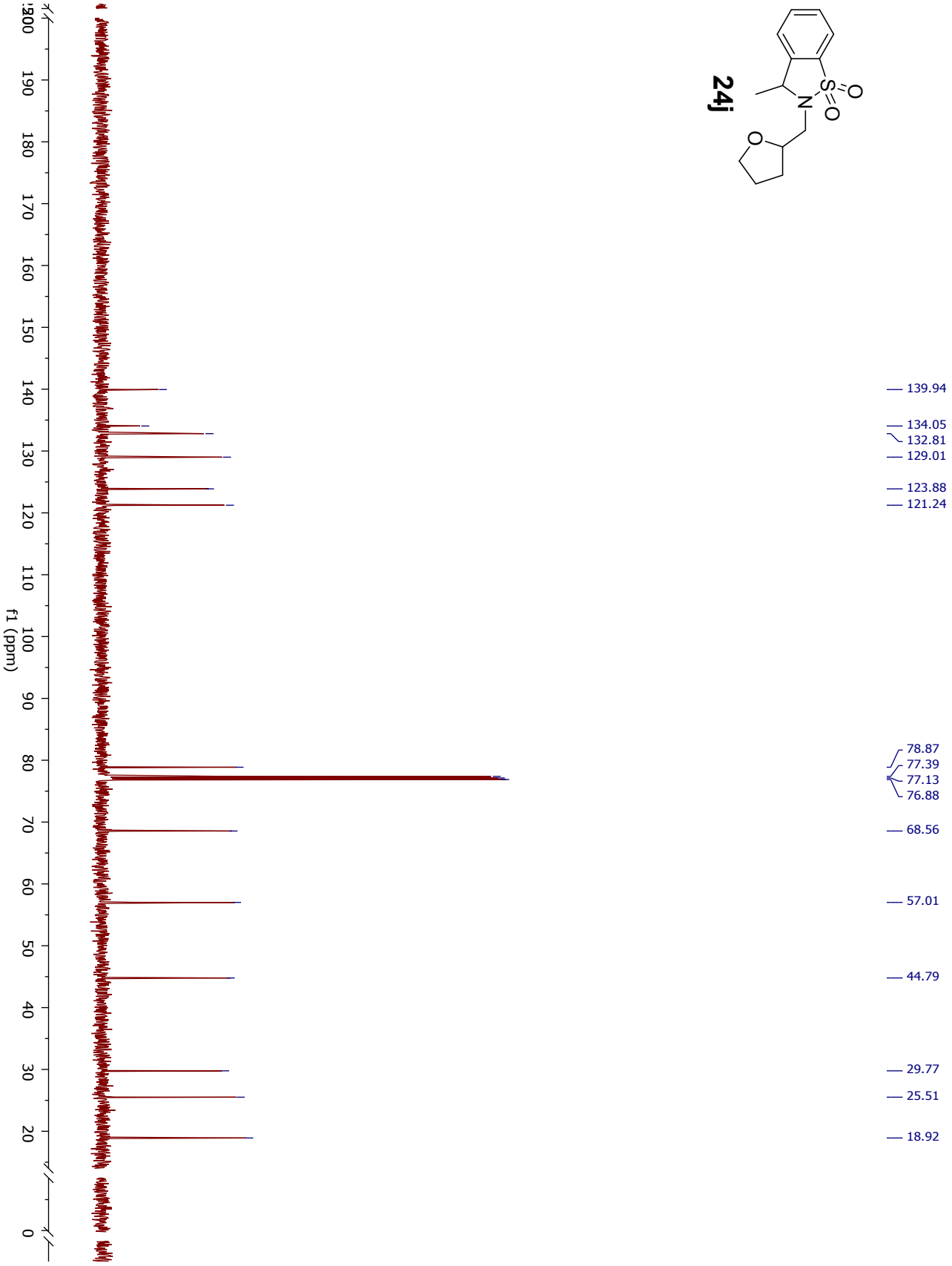

24h
O
S
O
N
O
7.80
7.79
7.63
7.62
7.60
7.53
7.52
7.50
7.40
7.39
7.27
4.73
4.72
4.70
4.69
3.78
3.77
3.76
3.75
3.74
3.70
3.69
3.68
3.67
3.66
3.56
3.55
3.54
3.39
1.57
1.56
-0.00
0.95
0.99
0.99
0.98
0.97
1.01
1.04
1.98
2.99
2.98
f1 (ppm)

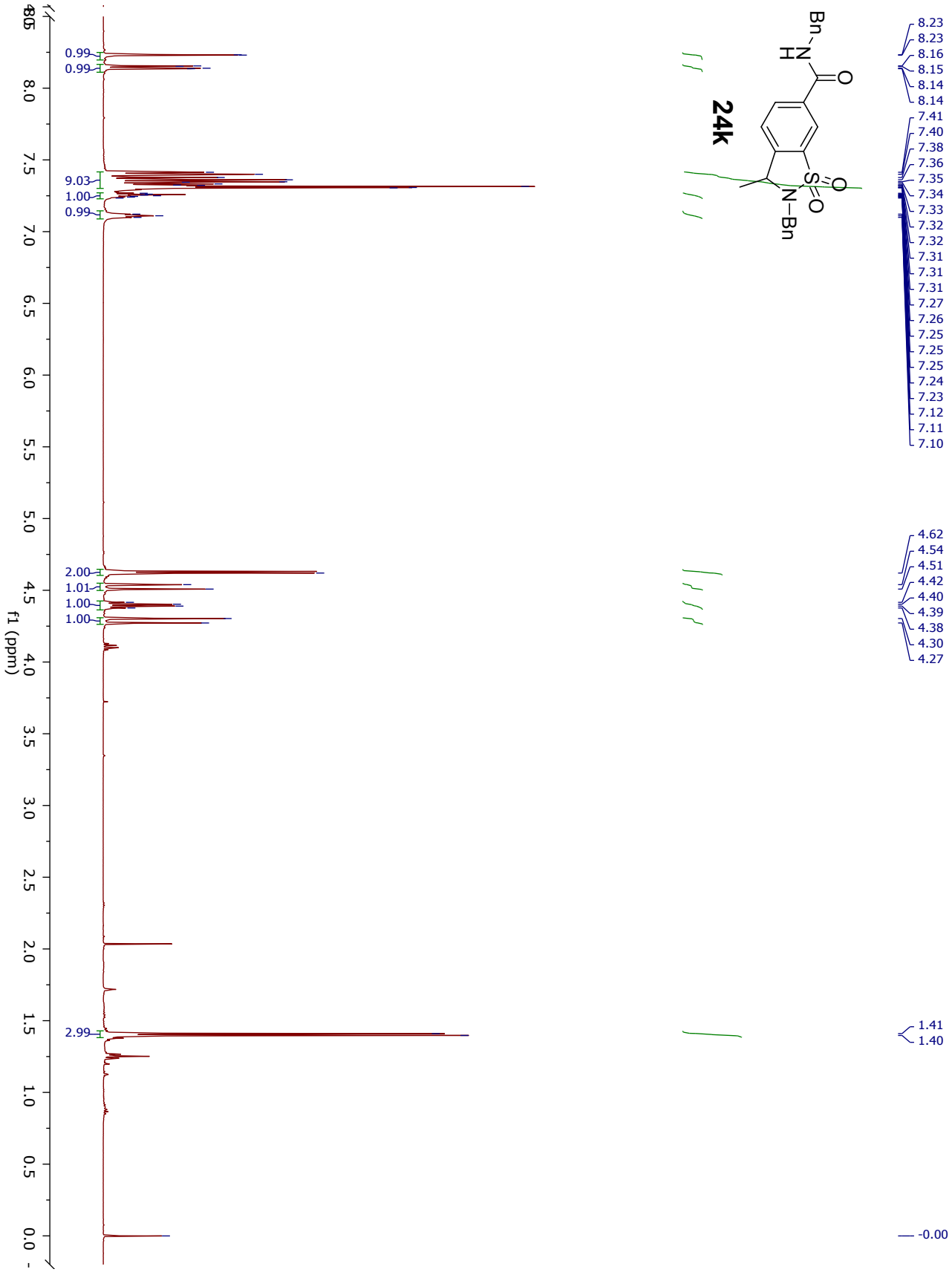

24h
O
S
O
N
O
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
139.63
134.15
132.92
129.12
123.82
121.25
77.40
77.15
76.90
71.86
59.10
57.56
41.08
19.20

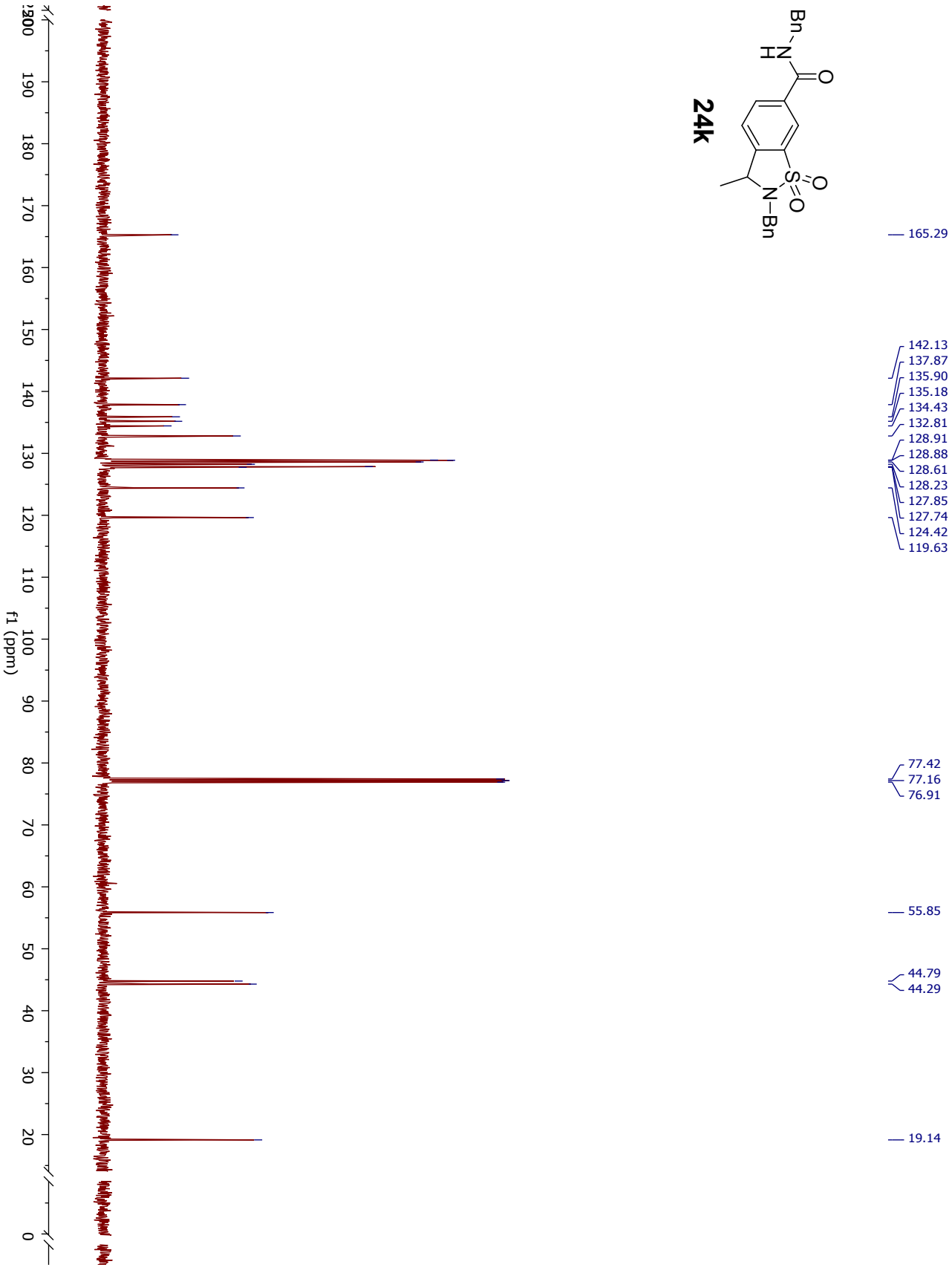

24i
f1 (ppm)
0.93
0.99
0.98
1.02
1.00
0.99
2.03
1.02
3.02
2.02
3.01
7.77
7.76
7.61
7.59
7.58
7.58
7.52
7.50
7.49
7.37
7.36
7.27
4.65
4.64
4.63
4.62
3.88
3.87
3.86
3.85
3.84
3.83
3.82
3.74
3.73
3.71
2.18
2.17
2.17
2.16
2.15
2.14
2.13
2.13
2.12
2.11
2.11
2.08
2.07
2.05
2.04
2.03
2.02
2.01
1.89
1.88
1.87
1.87
1.86
1.86
1.85
1.83
1.83
1.82
1.81
1.80
1.80
1.79
1.79
1.78
1.77
1.77
1.77
1.76
1.69
1.66
1.65
1.65
1.64
1.63
1.61
1.59
1.57

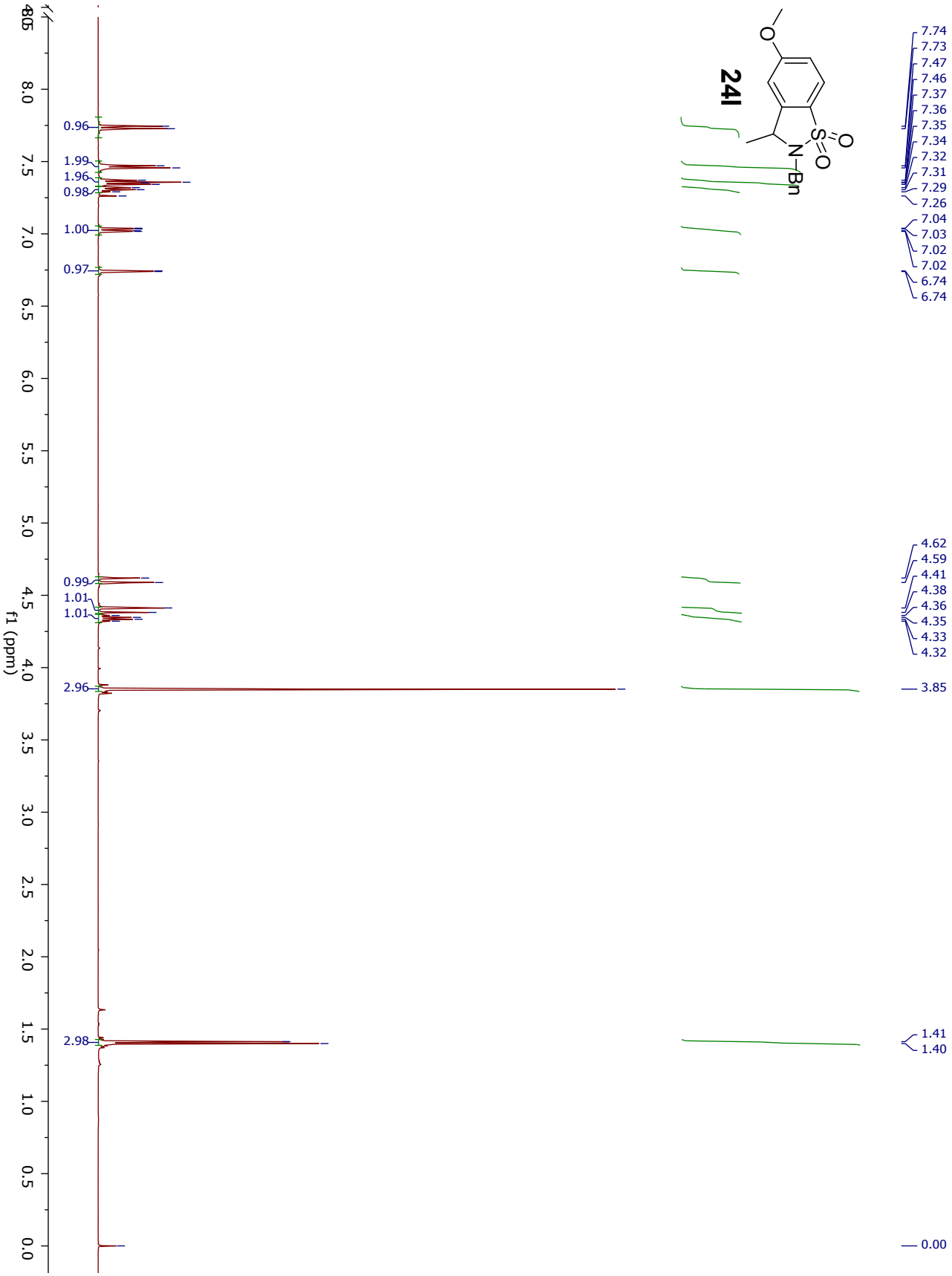

24i
O
S
O
N
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
139.68
135.09
132.79
129.12
123.74
121.21
77.40
77.14
76.89
56.67
56.22
31.21
29.83
23.62
22.81
21.17

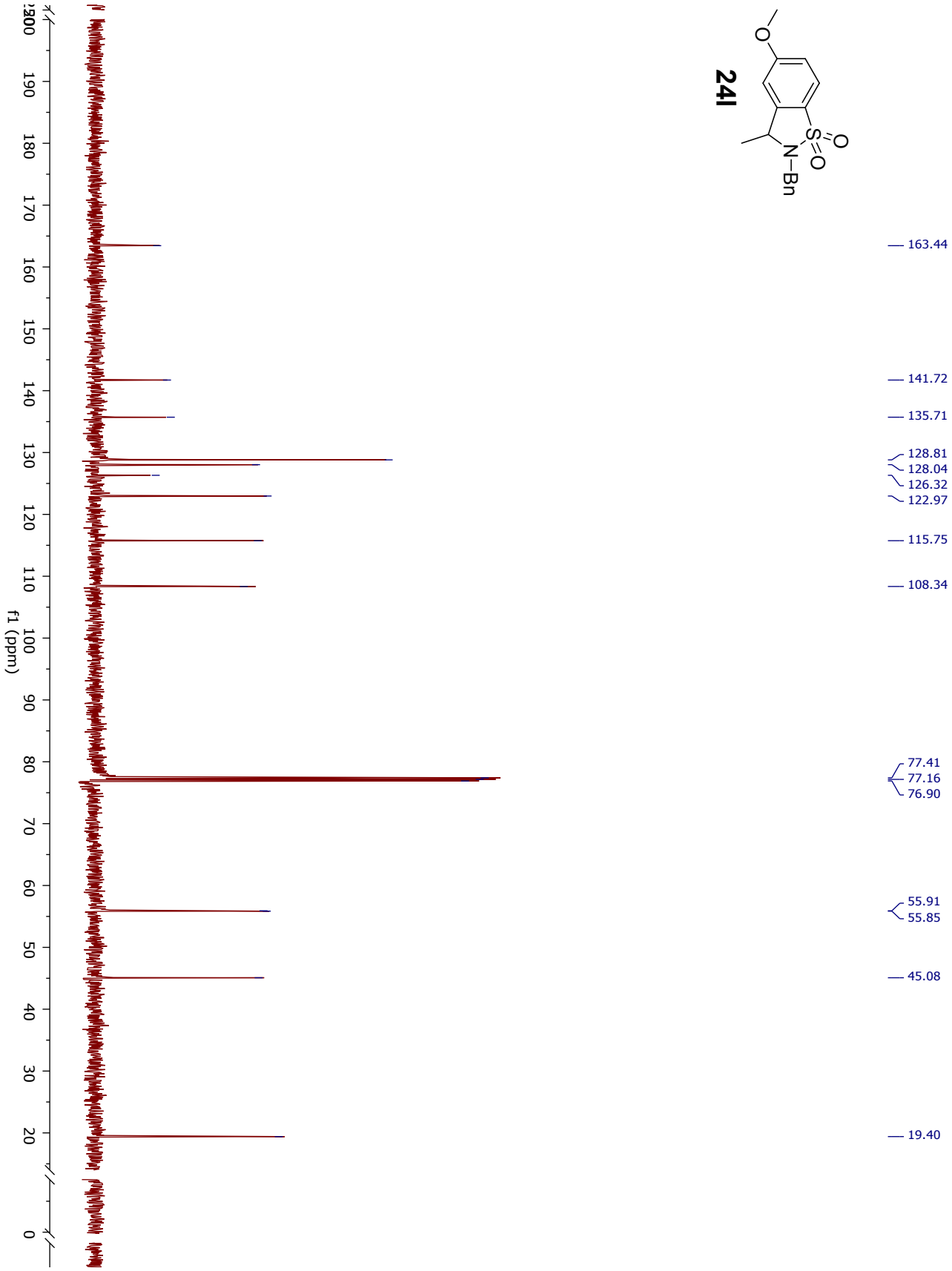

24j
f1 (ppm)
0.98
1.00
1.01
1.01
1.00
1.01
1.00
1.03
1.04
1.03
1.04
2.00
1.04
3.09
7.81
7.79
7.62
7.61
7.59
7.53
7.51
7.50
7.40
7.39
7.27
4.93
4.91
4.90
4.89
4.26
4.25
4.25
4.24
4.23
4.22
4.22
4.21
3.94
3.93
3.91
3.90
3.81
3.79
3.78
3.77
3.59
3.59
3.56
3.56
3.30
3.28
3.27
3.25
2.14
2.12
2.12
2.11
2.10
2.09
2.08
2.07
1.98
1.97
1.96
1.95
1.93
1.91
1.90
1.88
1.87
1.86
1.84
1.68
1.66
1.65
1.65
1.64
1.63
1.62
1.60
1.57
1.55
0.00

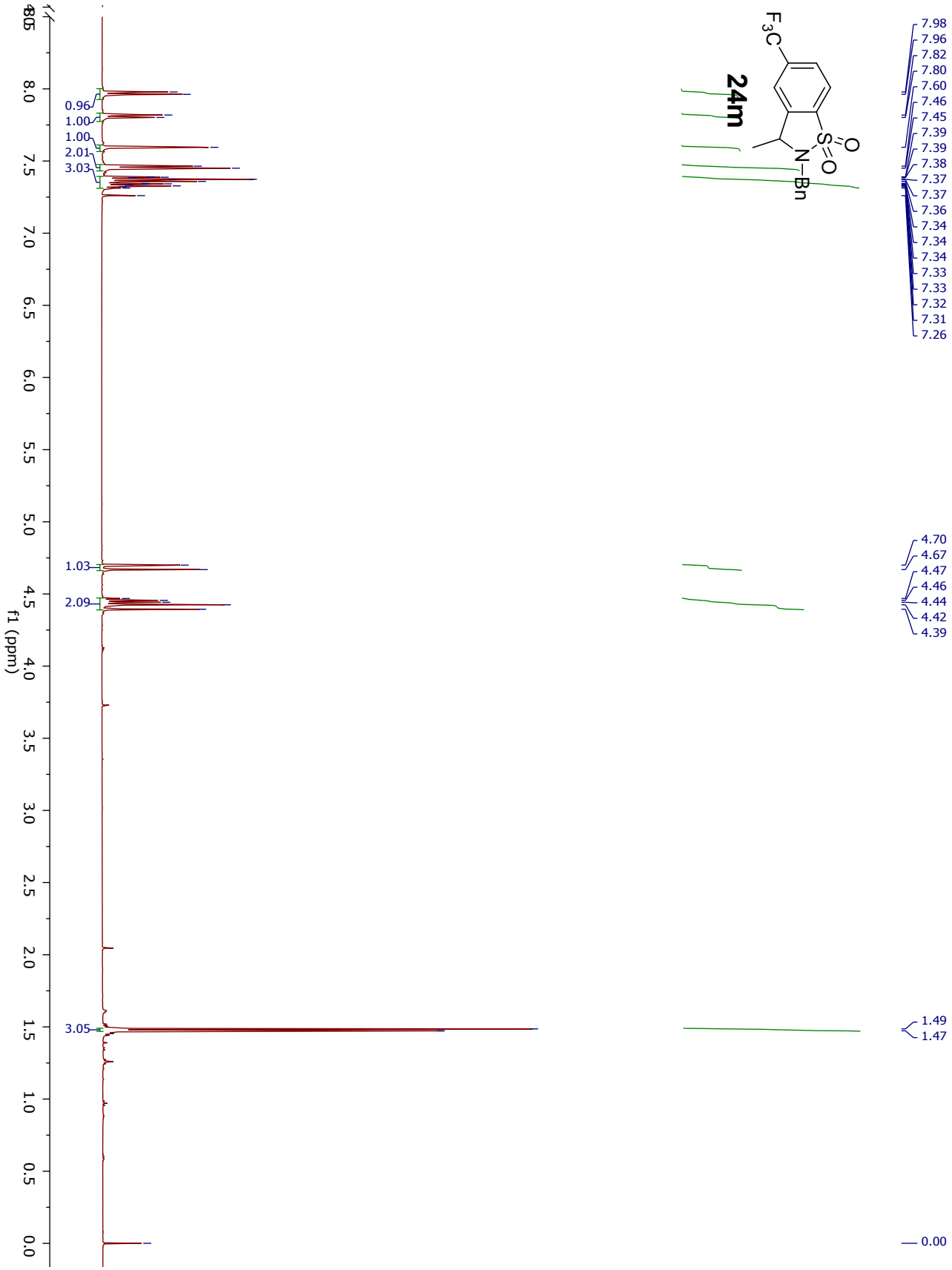

24j
O
S
O
N
O
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0
139.94
134.05
132.81
129.01
123.88
121.24
78.87
77.39
77.13
76.88
68.56
57.01
44.79
29.77
25.51
18.92

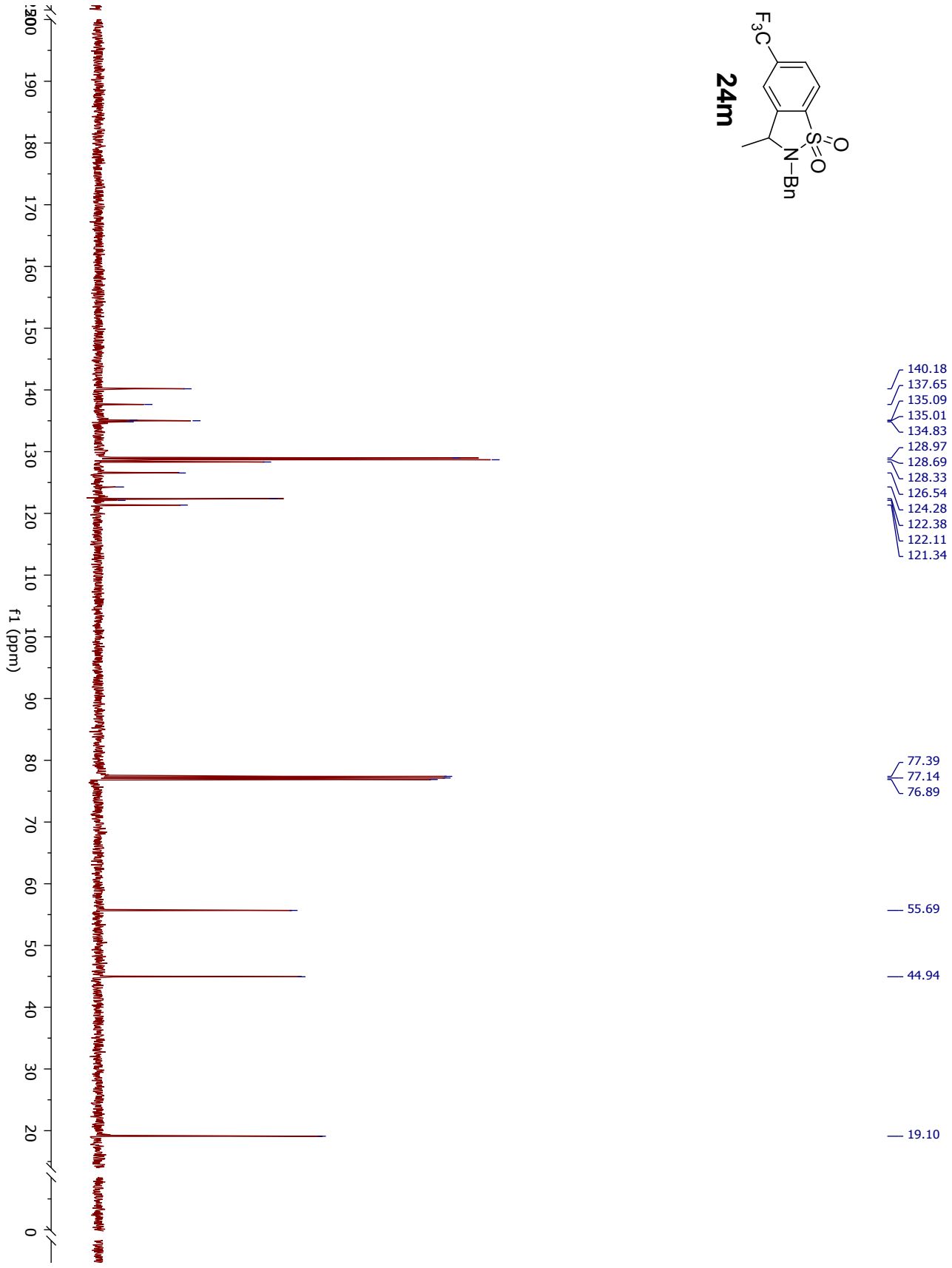

24k
f1 (ppm)
0.99
0.99
9.03
1.00
0.99
2.00
1.01
1.00
1.00
2.99
8.23
8.23
8.16
8.15
8.14
8.14
7.41
7.40
7.38
7.36
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.31
7.27
7.26
7.25
7.25
7.25
7.24
7.23
7.12
7.11
7.10
4.62
4.54
4.51
4.42
4.40
4.39
4.38
4.30
4.27
1.41
1.40
-0.00

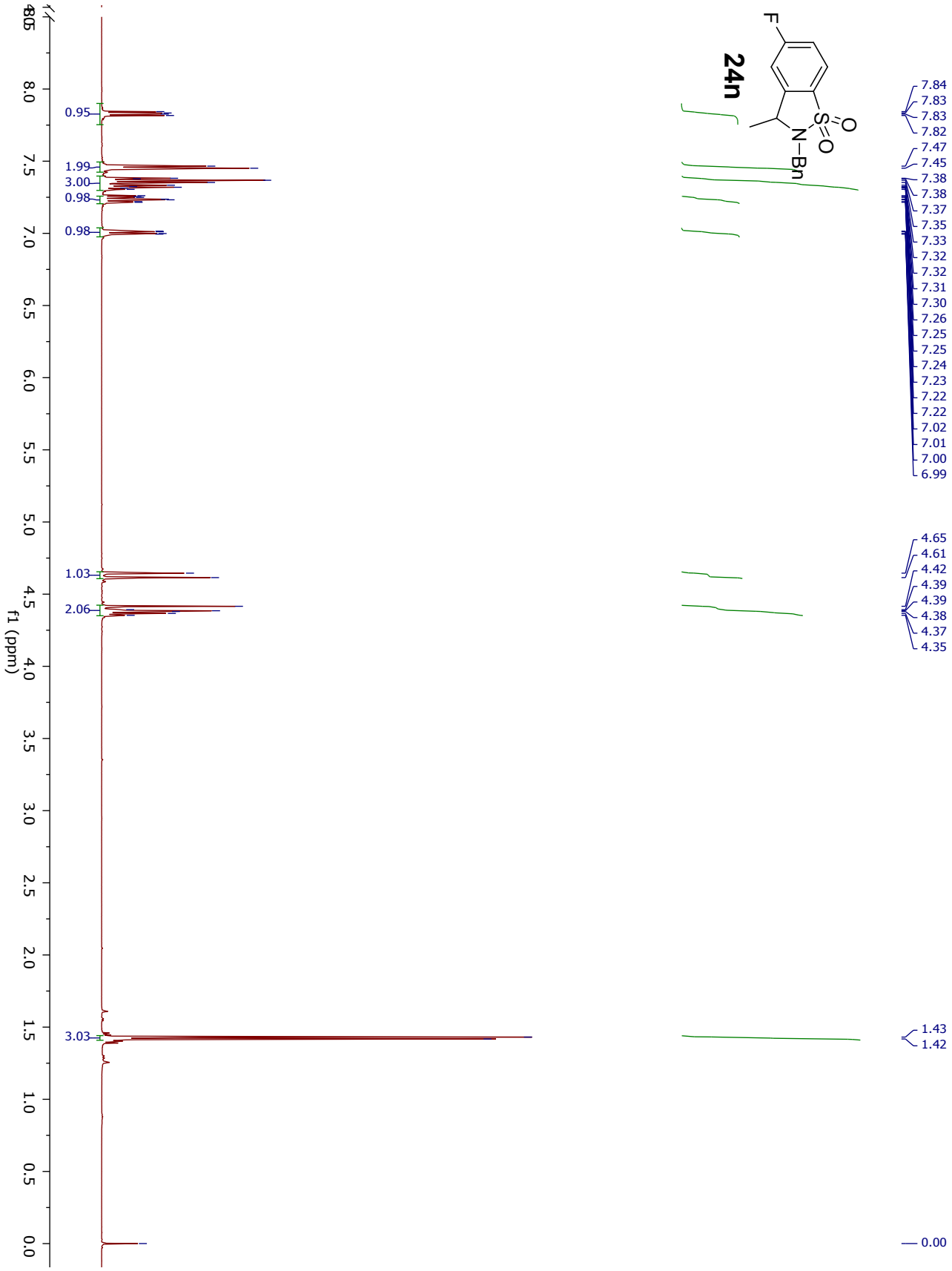

24k
Bn
N
H
O
O
S
O
N–Bn
165.29
142.13
137.87
135.90
135.18
134.43
132.81
128.91
128.88
128.61
128.23
127.85
127.74
124.42
119.63
77.42
77.16
76.91
55.85
44.79
44.29
19.14
f1 (ppm)

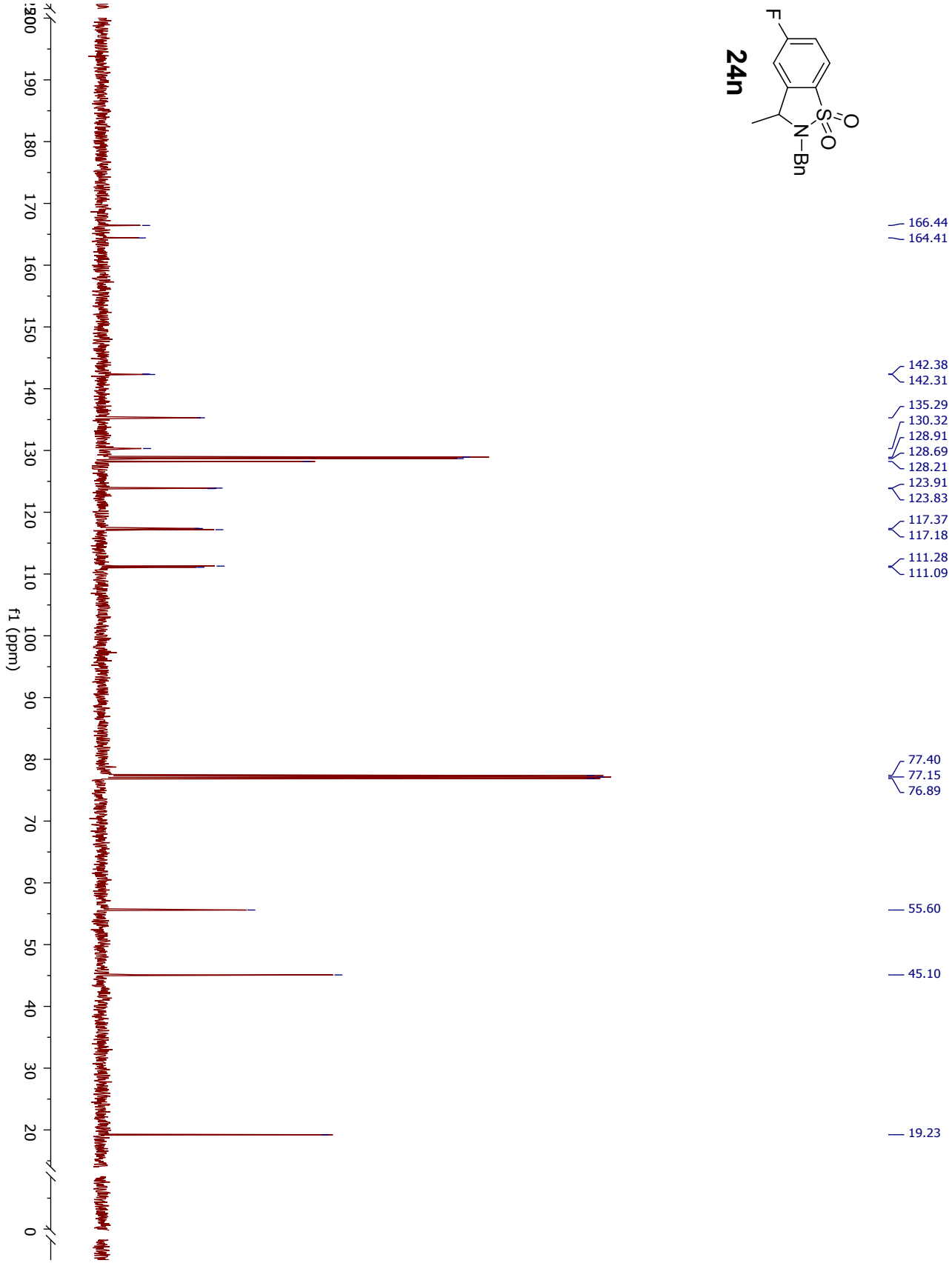

24l
f1 (ppm)
0.96
1.99
1.96
0.98
1.00
0.97
0.99
1.01
1.01
2.96
2.98
7.74
7.73
7.47
7.46
7.37
7.36
7.35
7.34
7.32
7.31
7.29
7.26
7.04
7.03
7.02
7.02
6.74
6.74
4.62
4.59
4.41
4.38
4.36
4.35
4.33
4.32
3.85
1.41
1.40
0.00

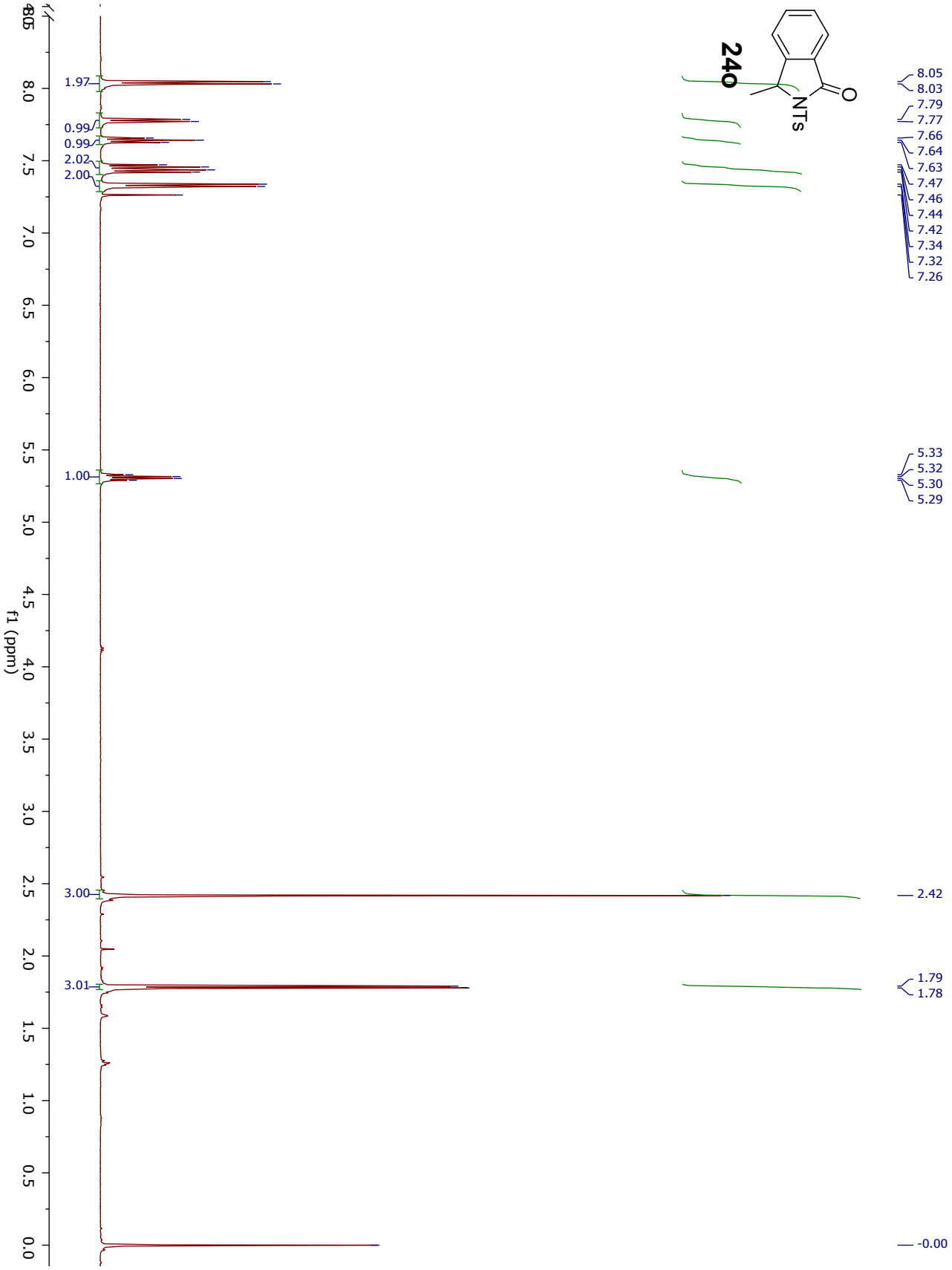

24l
O
S
O
O
N–Bn
163.44
141.72
135.71
128.81
128.04
126.32
122.97
115.75
108.34
77.41
77.16
76.90
55.91
55.85
45.08
19.40
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
0

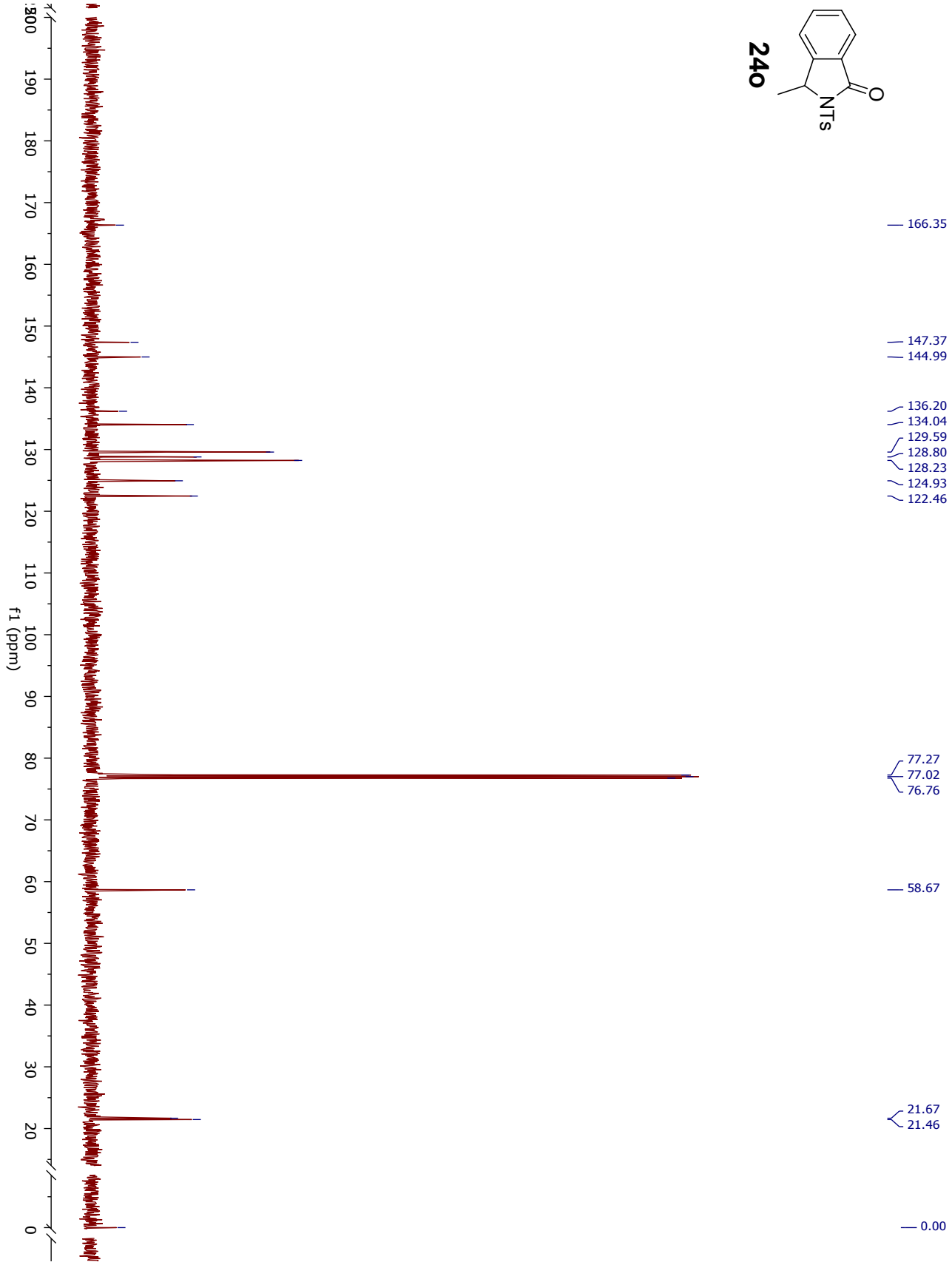

24m
F3C
O
S
O
N
Bn
0.96
1.00
1.00
2.01
3.03
1.03
2.09
3.05
7.98
7.96
7.82
7.80
7.60
7.46
7.45
7.39
7.39
7.38
7.37
7.37
7.36
7.34
7.34
7.34
7.33
7.33
7.32
7.31
7.26
4.70
4.67
4.47
4.46
4.44
4.42
4.39
1.49
1.47
0.00
f1 (ppm)

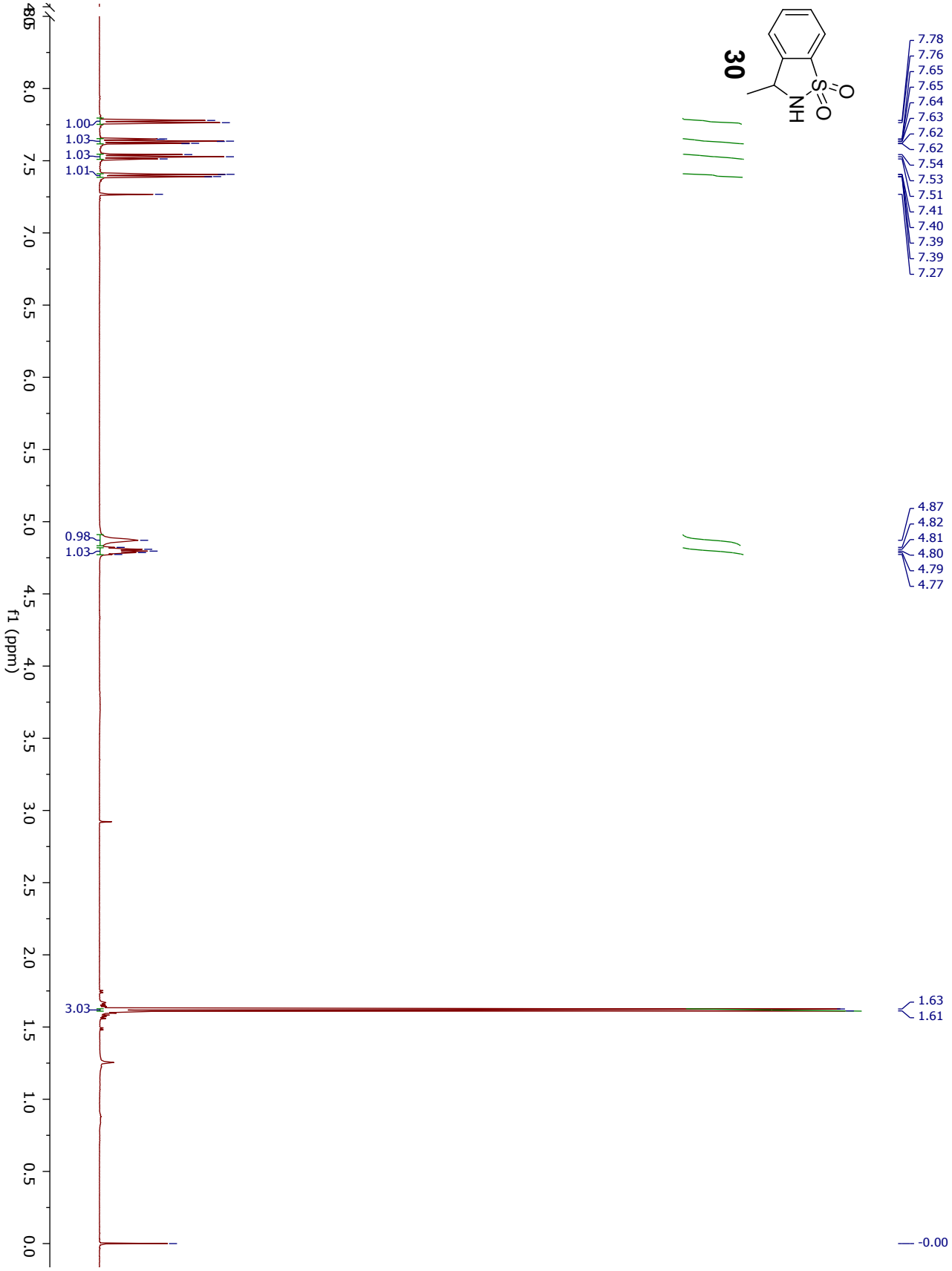

24m
F3C
S
O
O
N–Bn
140.18
137.65
135.09
135.01
134.83
128.97
128.69
128.33
126.54
124.28
122.38
122.11
121.34
77.39
77.14
76.89
55.69
44.94
19.10
f1 (ppm)

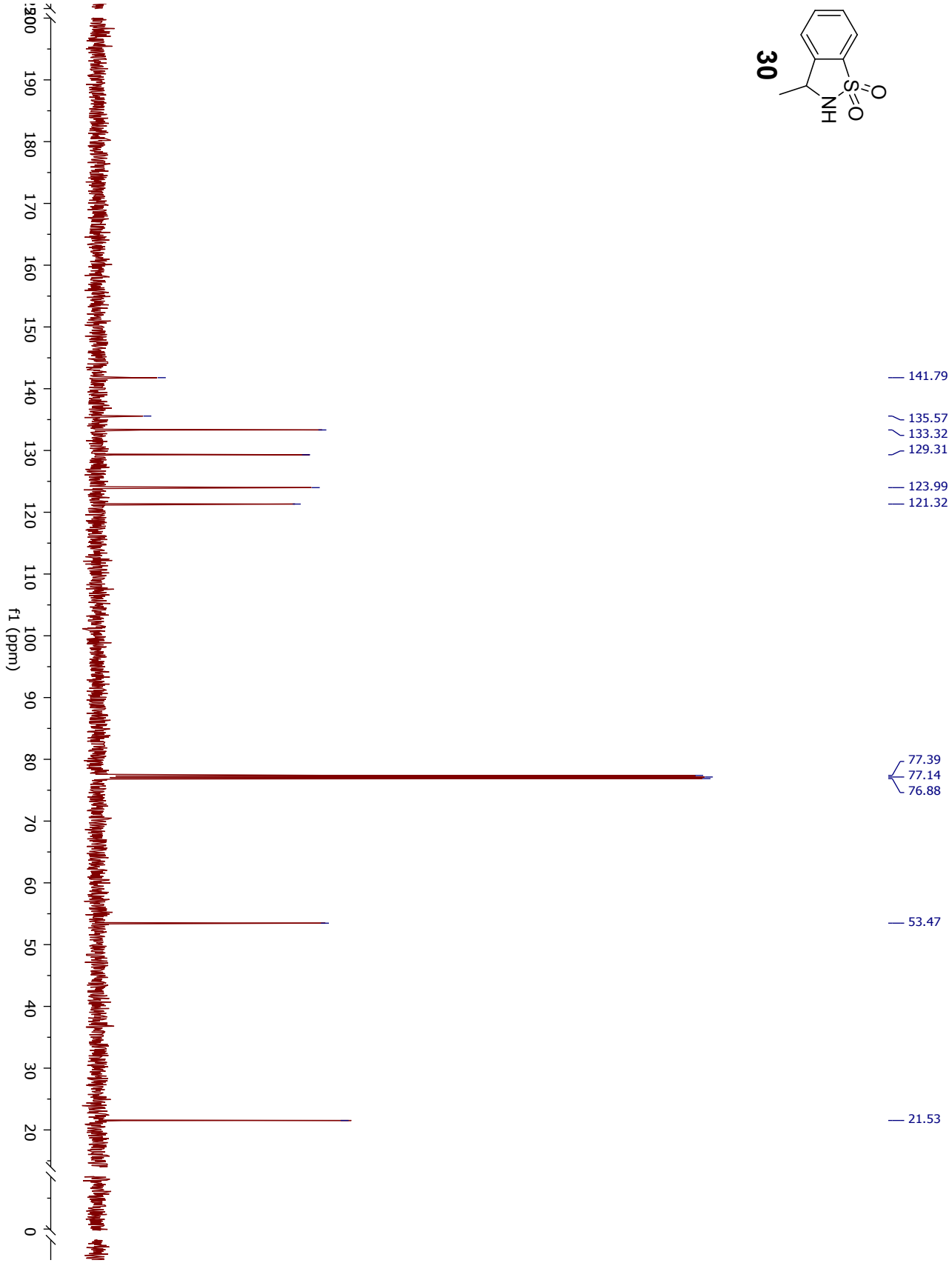

24n
F
O
S
O
N–Bn
0.95
1.99
3.00
0.98
0.98
1.03
2.06
3.03
7.84
7.83
7.83
7.82
7.47
7.45
7.38
7.38
7.37
7.35
7.33
7.32
7.32
7.31
7.30
7.26
7.25
7.25
7.24
7.23
7.22
7.22
7.02
7.01
7.00
6.99
4.65
4.61
4.42
4.39
4.39
4.38
4.37
4.35
1.43
1.42
0.00
f1 (ppm)

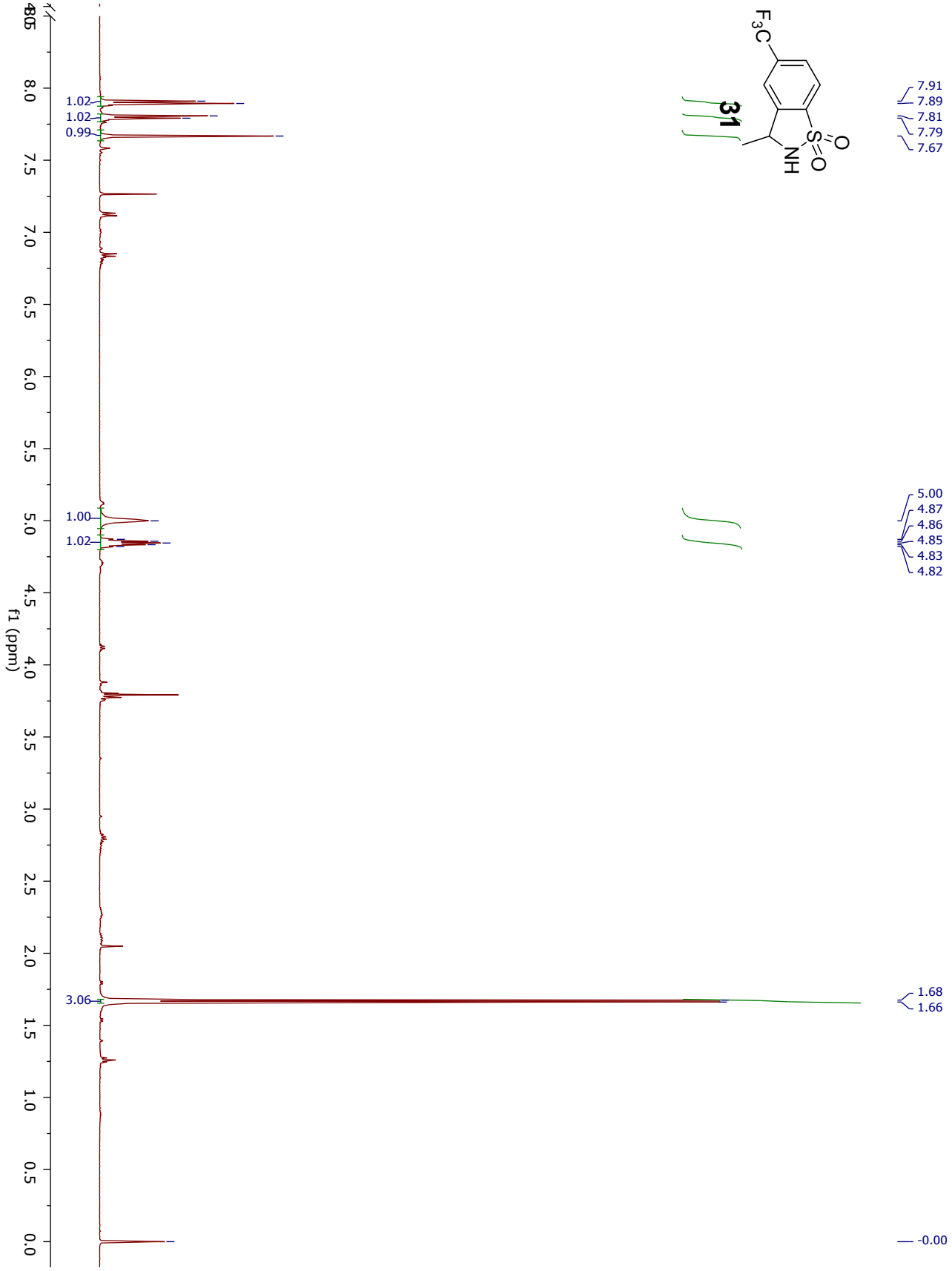

24n
F
O
S
O
N–Bn
166.44
164.41
142.38
142.31
135.29
130.32
128.91
128.69
128.21
123.91
123.83
117.37
117.18
111.28
111.09
77.40
77.15
76.89
55.60
45.10
19.23
f1 (ppm)

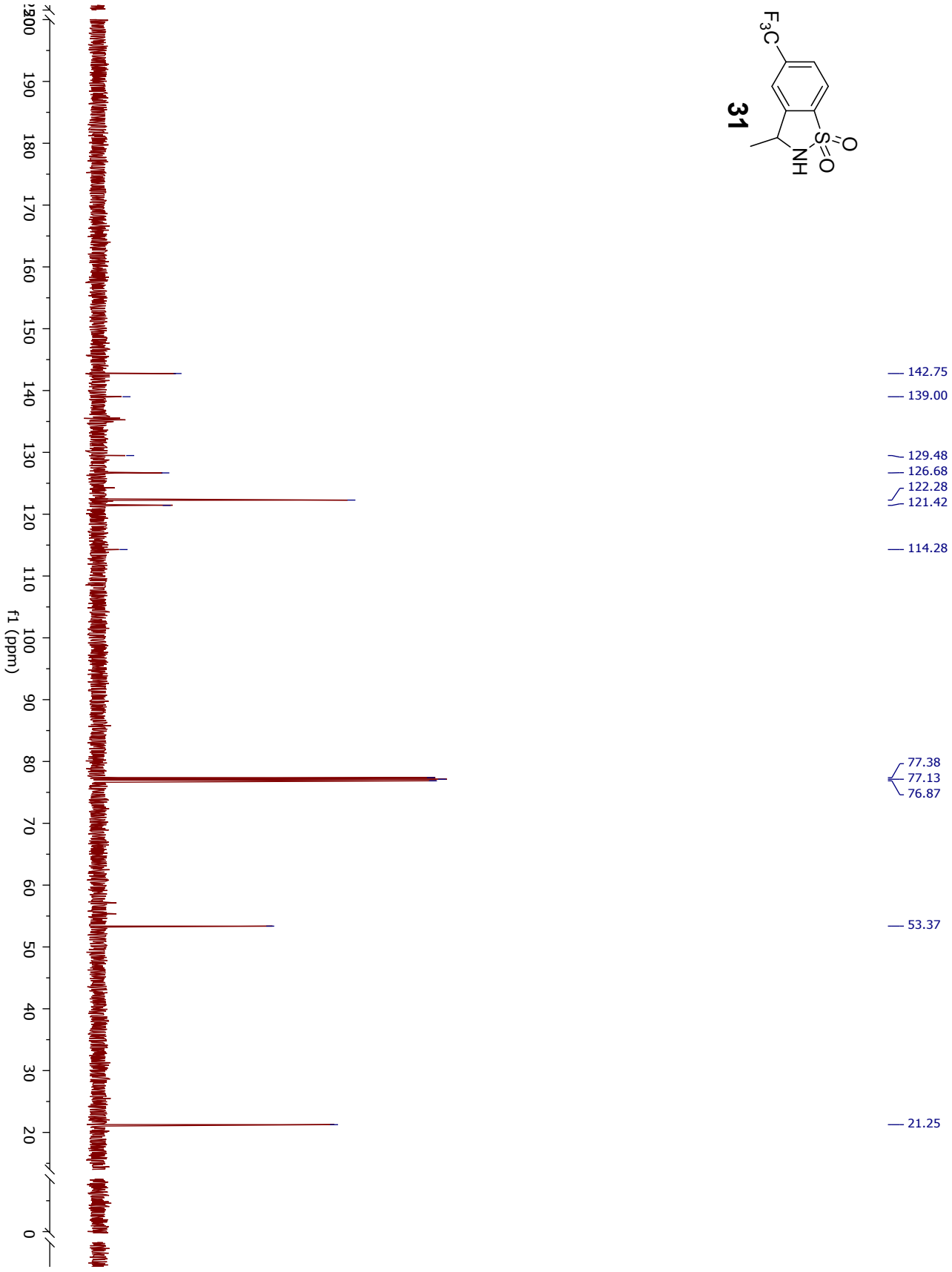

240
NTs
O
8.05
8.03
7.79
7.77
7.66
7.64
7.63
7.47
7.46
7.44
7.42
7.34
7.32
7.26
5.33
5.32
5.30
5.29
2.42
1.79
1.78
-0.00
1.97
0.99
0.99
2.02
2.00
1.00
3.00
3.01
f1 (ppm)

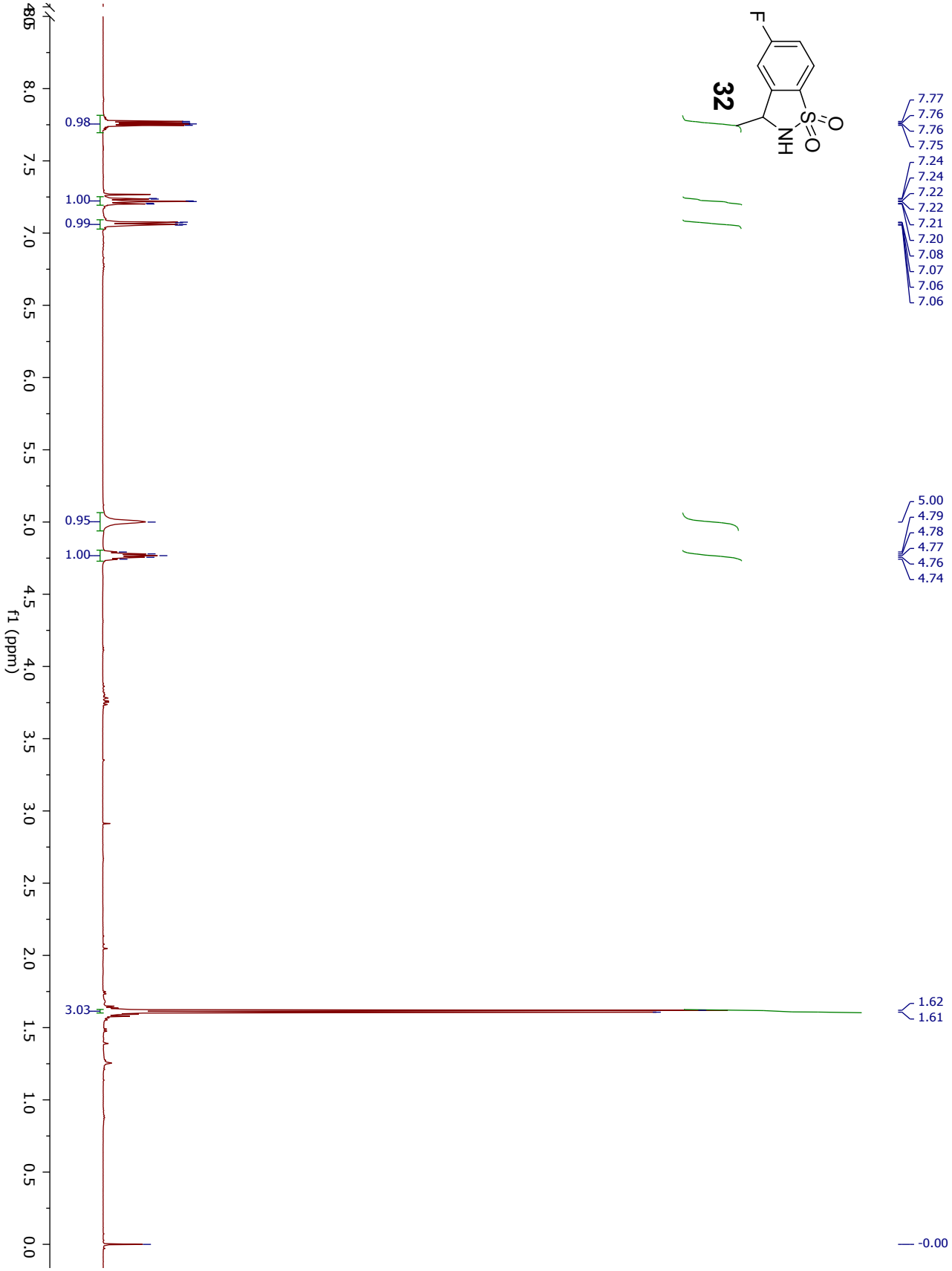

24o
NTs
O
166.35
147.37
144.99
136.20
134.04
129.59
128.80
128.23
124.93
122.46
77.27
77.02
76.76
58.67
21.67
21.46
0.00
f1 (ppm)

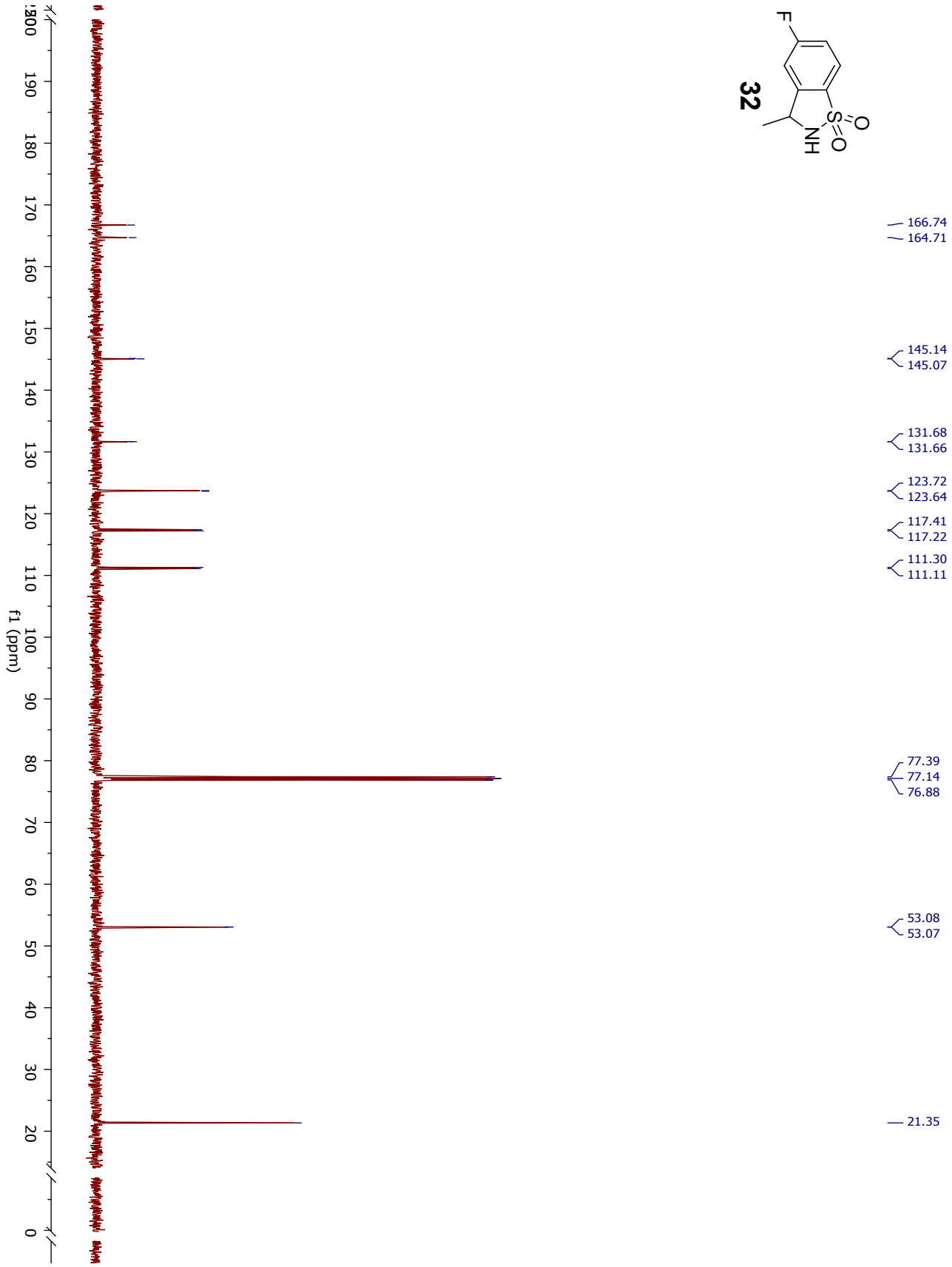

30
NH
S
O
O
7.78
7.76
7.65
7.65
7.64
7.63
7.62
7.62
7.54
7.53
7.51
7.41
7.40
7.39
7.39
7.27
4.87
4.82
4.81
4.80
4.79
4.77
1.63
1.61
-0.00
1.00
1.03
1.03
1.01
0.98
1.03
3.03
f1 (ppm)


30
141.79
135.57
133.32
129.31
123.99
121.32
77.39
77.14
76.88
53.47
21.53
f1 (ppm)


F3C
O
S
O
NH
31
7.91
7.89
7.81
7.79
7.67
5.00
4.87
4.86
4.85
4.83
4.82
1.68
1.66
-0.00
1.02
1.02
0.99
1.00
1.02
3.06
f1 (ppm)


F3C
O
S
O
NH
31
142.75
139.00
129.48
126.68
122.28
121.42
114.28
77.38
77.13
76.87
53.37
21.25
f1 (ppm)


32
F
S
O
O
NH
0.98
1.00
0.99
0.95
1.00
3.03
7.77
7.76
7.76
7.75
7.24
7.24
7.22
7.22
7.21
7.20
7.08
7.07
7.06
7.06
5.00
4.79
4.78
4.77
4.76
4.74
1.62
1.61
-0.00
f1 (ppm)


32
F
O
S
O
NH
166.74
164.71
145.14
145.07
131.68
131.66
123.72
123.64
117.41
117.22
111.30
111.11
77.39
77.14
76.88
53.08
53.07
21.35
f1 (ppm)