Supplementary Information (SI) for RSC Advances.

Electronic Supporting Information (ESI)

Strategies for oxidative synthesis of N-triflyl sulfoximines

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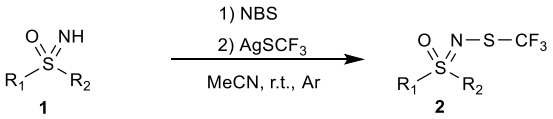
General Information

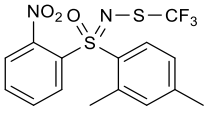
Chemicals and solvents were obtained from commercial sources. TLC was performed on Merck-60-F254 plates using mixtures of petroleum ether (PE), hexane, dichloromethane (DCM), diethyl ether, ethyl acetate, and methanol. For flash chromatography, silica gel (63−200µm, 70−230 mesh ASTM; Fluka) was used. Products were characterized by ^{1}H,^{13}C, and ^{19}F NMR spectroscopy, IR spectroscopy, HRMS, and melting points of solids. All NMR spectra were recorded in either $CDCl_3$ using Me_4Si as an internal standard or in DMSO-d_6. Chemical shifts are reported in δ (ppm) values relative to δ = 0 ppm (Me_4Si) or 2.50 ppm (DMSO) for ^{1}H NMR, and to the central line of $CDCl_3$(δ = 77.16 ppm) for ^{13}C NMR. ^{19}F spectra were referenced to $CFCl_3$ as an external standard at δ = 0.00 ppm. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded with a Bruker Avance III 500 instrument at 500, 126, and 471 MHz, respectively. IR spectra were recorded with a Bruker FTIR Alpha Platinum spectrophotometer. LC-HRMS analyses were performed on a Shimadzu LCMS-IT-TOF system (Kyoto, Japan), composed of a liquid chromatograph Nexera XR hyphenated to a mass spectrometer with an ion trap and time-of-flight tube equipped with an electrospray ionization (ESI) source. The melting points were determined with an OptiMelt MPA100.

Preparation of N-trifluoromethylthio sulfoximines



Prepared according to a known procedure.[1] A dried flask was charged with sulfoximine **1** and equipped with a septum and argon balloon. Dry MeCN (0.1 M) and *N*-bromosuccinimide (NBS) (1.0 equiv.) were added and the reaction mixture was stirred for 30 min. In another dried flask a solution of $AgSCF_3$ (0.1 M) was prepared and slowly transferred to the *in-situ* formed *N*-bromo sulfoximine using a syringe. After complete consumption of the reactant (checked with TLC, DCM) the solvent was removed using reduced pressure and the residue was purified using flash chromatography (DCM).

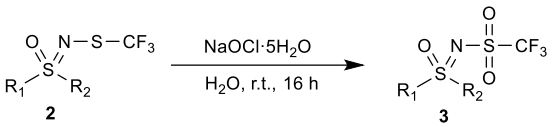
Characterization of unknown *N*-trifuoromethylthio sulfoximines 2



N-trifluoromethylthio-*S*-(2,4-dimethylphenyl)-*S*-(2-nitrophenyl) sulfoximine (**2ab**). Orange solid (84%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.27 – 8.19 (m, 1H), 7.85 (d, J = 8.3 Hz, 1H), 7.83 – 7.75 (m, 3H), 7.22 – 7.16 (m, 1H), 7.12 (s, 1H), 2.43 (s, 3H), 2.39 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −50.75. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 149.30, 145.57, 138.25, 134.99, 134.01, 133.20, 132.46, 132.14, 132.01, 130.63, 130.3 (C-F, $^1J_{C\text{-}F}$ = 312.6 Hz), 127.27, 125.49, 21.51, 20.35. **IR (neat)**: ν 3094, 2959, 2927, 2860, 1601, 1541, 1440, 1362, 1283, 1228, 1105, 1053, 963, 881, 850, 818, 780, 731, 661, 639, 622 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{14}F_3N_2O_3S_2$ 391.0392; Found 391.0389. Mp = 56.7 – 58.6 °C.

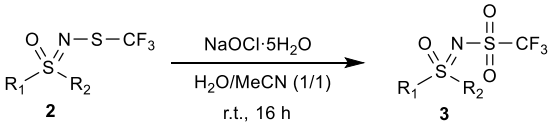
Preparation of *N*-triflyl sulfoximines 3

General procedure 1 (GP1)



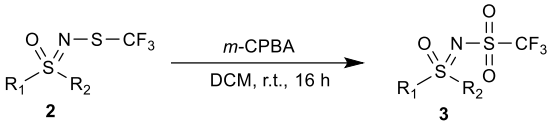
A flask was charged with *N*-trifluoromethylthio sulfoximine **2a–2j** (0.3 mmol), water (1 mL), $NaOCl{\cdot}5H_2O$ (2.5 equiv.) and the reaction mixture was stirred at r.t. for 16 h. The reaction mixture was then extracted twice with EtOAc and the organic phase was dried under anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure yielded the product **3a–3j**.

General procedure 2 (GP2)



A flask was charged with *N*-trifluoromethylthio sulfoximine **2k–2u** (0.3 mmol), water (0.5 mL), MeCN (0.5 mL), $NaOCl{\cdot}5H_2O$ (2.5 equiv.) and the reaction mixture was stirred at r.t. for 16 h. The reaction mixture was then extracted twice with EtOAc and the organic phase was dried under anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure yielded the product **3k–3u**.

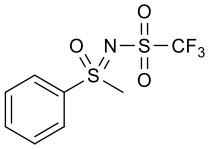
General procedure 3 (GP3)



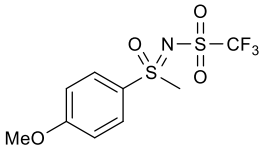
2 3

A flask was charged with *N*-trifluoromethylthio sulfoximine **2v–2ag** (0.3 mmol), DCM (1 mL), *m*-CPBA (2.5 equiv.) and the reaction mixture was stirred at r.t. for 16 h. Saturated $NaHCO_3$ solution was added to the reaction mixture and stirred until the organic phase became transparent. The product was extracted twice with DCM and the organic phase was dried under anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure yielded the product **3v–3ag**.

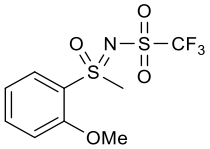
Characterization of synthesized *N*-triflyl sulfoximines 3



N-(triflyl)-*S*-phenyl-*S*-methyl sulfoximine (**3a**).[2] **2a** (0.3 mmol; 77 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP1: White solid (60 mg, 73%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.13 – 7.98 (m, 3H), 7.80 (td, J = 7.4, 1.4 Hz, 2H), 7.73 – 7.60 (m, 3H), 3.52 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.24. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 137.26, 135.53, 130.30, 127.43, 119.33, (C-F, $^1J_{C\text{-}F}$ = 321.0 Hz), 46.86. **IR (neat)**: ν 3020, 2925, 1582, 1452, 1409, 1354, 1341, 1319, 1254, 1196, 1175, 1134, 1093, 1049, 989, 974, 851, 795, 739, 686, 679, 619 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_9F_3NO_3S_2$ 287.997; Found 287.9965. Mp = 77.5 – 80.1 °C.

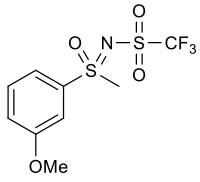


N-(triflyl)-*S*-(4-methoxyphenyl)-*S*-methyl sulfoximine (**3b**). **2b** (0.3 mmol; 86 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP1: White semi solid (90%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.99 – 7.92 (m, 2H), 7.15 – 7.09 (m, 2H), 3.93 (s, 3H), 3.49 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.28. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 165.23, 129.85, 127.94, 119.35 (C-F, $^1J_{C\text{-}F}$ = 320.9 Hz), 115.52, 56.15, 47.44. **IR (neat)**: ν 3034, 2935, 1591, 1496, 1443, 1347, 1324, 1259, 1219, 1174, 1135, 1092, 1038, 1021, 982, 961, 834, 804, 767, 739, 622 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_{11}F_3NO_4S_2$ 318.0076; Found 318.0072.

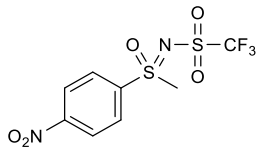


N-(triflyl)-*S*-(2-methoxyphenyl)-*S*-methyl sulfoximine (**3c**). **2c** (0.3 mmol; 86 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP1: White solid (68 mg, 81%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.00 (dd, J = 8.0, 1.7 Hz, 1H), 7.74 (ddd, J = 8.4, 7.4, 1.7 Hz, 1H), 7.21 (ddd, J =

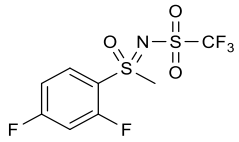
8.3, 7.5, 1.0 Hz, 1H), 7.15 (dd, *J* = 8.5, 1.0 Hz, 1H), 4.04 (s, 3H), 3.63 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.44. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 157.02, 137.70, 130.26, 123.80, 121.44, 119.40 (C-F, $^{1}J_{C\text{-}F}$ = 321.3 Hz), 113.11, 56.78, 44.44. **IR (neat)**: ν 3111, 3041, 3019, 2935, 1594, 1576, 1482, 1439, 1338, 1286, 1252, 1185, 1130, 1050, 1009, 968, 803, 769, 714, 669, 616 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_{11}F_3NO_4S_2$ 318.0076; Found 318.0053. Mp = 97.6 – 97.8 °C.



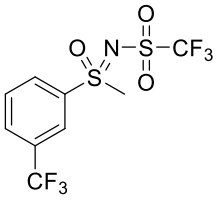
N-(triflyl)-*S*-(3-methoxyphenyl)-*S*-methyl sulfoximine (**3d**). **2d** (0.3 mmol; 86 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·5H_2O (0.75 mmol, 123 mg), GP1: Off white solid (85 mg, 89%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 7.63 – 7.55 (m, 1H), 7.53 – 7.46 (m, 1H), 7.31 – 7.27 (m, 1H), 3.91 (d, J = 2.2 Hz, 3H), 3.51 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.19 – (−79.30) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 160.63, 138.31, 131.28, 121.73, 119.30, 119.23 ((C-F, $^{1}J_{C\text{-}F}$ = 321.2 Hz), 111.87, 55.98, 46.80. **IR (neat)**: ν 3095, 3076, 3026, 3017, 2988, 2949, 2929, 2844, 1595, 1483, 1432, 1351, 1290, 1248, 1185, 1134, 1076, 1032, 985, 879, 854, 782, 764, 737, 679, 624 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_{11}F_3NO_4S_2$ 318.0076; Found 318.0077. Mp = 96.1 – 96.9 °C.



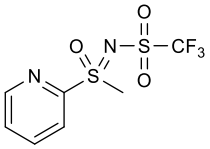
N-(triflyl)-*S*-(4-nitrophenyl)-*S*-methyl sulfoximine (**3e**). **2e** (0.3 mmol; 90 mg), 1 mL H_2O, 3.5 equiv. of NaOCl·5H_2O (1.05 mmol, 173 mg), GP1: Off white solid (88 mg, 88%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.53 (d, J = 9.0 Hz, 2H), 8.28 (d, J = 9.0 Hz, 2H), 3.59 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.06. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 151.85, 143.00, 129.28, 125.42, 119.17 (C-F, $^{1}J_{C\text{-}F}$ = 321.0 Hz), 46.54. **IR (neat)**: ν 3105, 3034, 3018, 2928, 1605, 1524, 1476, 1400, 1353, 1323, 1256, 1188, 1131, 1089, 1051, 993, 853, 797, 773, 740, 713, 624 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8F_3N_2O_5S_2$ 332.9821; Found 332.982. Mp = 97.2 – 98.6 °C.



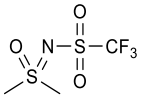
N-(triflyl)-*S*-(2,4-difluorophenyl)-*S*-methyl sulfoximine (**3f**). **2f** (0.3 mmol; 87 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·5H_2O (0.75 mmol, 123 mg), GP1: White solid (86 mg, 89%). Column chromatography (EtoAc:hexane) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.12 – 8.02 (m, 1H), 7.20 (dddd, J = 8.8, 7.4, 2.4, 1.1 Hz, 1H), 7.13 (ddd, J = 10.4, 8.1, 2.4 Hz, 1H), 3.64 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.07 – (−79.49) (m), −94.66 – (−94.90), (−101.91 – (−102.23) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 168.91 (d, C-F, $^{1}J_{C\text{-}F}$ = 11.9 Hz), 166.82 (d, C-F, $^{1}J_{C\text{-}F}$ = 11.8 Hz), 160.67 (d, C-F, $^{1}J_{C\text{-}F}$ = 13.2 Hz), 158.60 (d, C-F, $^{1}J_{C\text{-}F}$ = 13.3 Hz), 132.41 (d, C-F, $^{1}J_{C\text{-}F}$ = 11.1 Hz), 121.23 – 120.85 (m), 119.09 (C-F, $^{1}J_{C\text{-}F}$ = 321.2 Hz), 115.26, 113.38 (dd, C-F, $^{1}J_{C\text{-}F}$ = 22.3, 3.6 Hz), 106.63 (dd, C-F, $^{1}J_{C\text{-}F}$ = 26.5, 24.3 Hz), 45.56 (d, C-F, $^{1}J_{C\text{-}F}$ = 3.7 Hz). **IR (neat)**: ν 3111, 3019, 1601, 1474, 1434, 1340, 1282, 1256, 1189, 1132, 1079, 991, 976, 854, 826, 800, 770, 743, 618 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_7F_5NO_3S_2$ 323.9782; Found 323.9781. Mp = 53.2 – 56.7 °C.



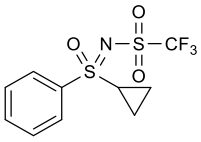
N-(triflyl)-*S*-(3-trifluoromethylphenyl)-*S*-methyl sulfoximine (**3g**). **2g** (0.3 mmol; 97 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP1: White solid (93 mg, 87%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.32 – 8.24 (m, 2H), 8.09 – 8.02 (m, 1H), 7.92 – 7.85 (m, 1H), 3.58 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −63.37 – (−63.46 (m)), −79.06 – (−79.24 (m)). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 138.80 – 138.58 (m), 132.29, 131.33, 130.90, 124.73, 122.78 (C-F, $^1J_{C\text{-}F}$ = 273.9 Hz), 119.23 (C-F, $^1J_{C\text{-}F}$ = 320.9 Hz), 46.81. **IR (neat)**: ν 3078, 3032, 2936, 1609, 1437, 1350, 1326, 1285, 1262, 1198, 1173, 1031, 1106, 1093, 1045, 990, 977, 932, 915, 826, 808, 791, 764, 742, 693, 649, 631, 610 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_8F_6NO_3S_2$ 355.9855; Found 355.985. Mp = 81.7 – 83.9 °C.



N-(triflyl)-*S*-(2-pyridyl)-*S*-methyl sulfoximine (**3h**). **2h** (0.3 mmol; 77 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP1: Off white solid (83 mg, 96%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.80 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 8.25 (dt, *J* = 8.0, 1.0 Hz, 1H), 8.09 (td, *J* = 7.8, 1.7 Hz, 1H), 7.70 (ddd, *J* = 7.8, 4.7, 1.1 Hz, 1H), 3.66 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.24. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 155.21, 150.68, 139.08, 128.93, 122.97, 119.26 (C-F, $^1J_{C\text{-}F}$ = 321.2 Hz), 41.58. **IR (neat)**: ν 3022, 2936, 1580, 1454, 1425, 1346, 1322, 1251, 1193, 1155, 1133, 1084, 1047, 987, 801, 765, 749, 698, 611 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_7H_8F_3N_2O_3S_2$ 288.9923; Found 288.9924. Mp = 70.4 – 71.5 °C.

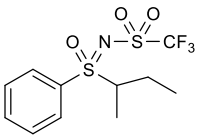


N-(triflyl)-*S,S*-dimethyl sulfoximine (**3i**).[3] **2i** (0.3 mmol; 58 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP1: Off white solid (52 mg, 77%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 3.46 (s, 6H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.17. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 119.31 (C-F, $^1J_{C\text{-}F}$ = 320.8 Hz), 44.50. **IR (neat)**: ν 3034, 2936, 1421, 1392, 1337, 1316, 1250, 1173, 1134, 1057, 1027, 947, 784, 751, 676, 624 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_3H_7F_3NO_3S_2$ 225.9814; Found 225.9812. Mp = 56.0 – 57.5 °C.

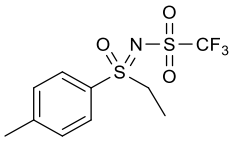


N-(triflyl)-*S*-phenyl-*S*-cyclopropyl sulfoximine (**3j**). **2j** (0.3 mmol; 84 mg), 1 mL H_2O, 3.5 equiv. of NaOCl·$5H_2O$ (1.05 mmol, 173 mg), GP1: White solid (78 mg, 83%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.00 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 2H), 2.87 –

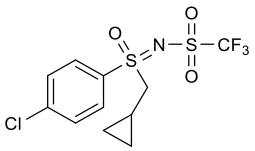
2.78 (m, 1H), 1.80 – 1.71 (m, 1H), 1.46 – 1.31 (m, 2H), 1.22 – 1.12 (m, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.27. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 137.89, 135.12, 130.13, 127.58, 119.35 (C-F, $^{1}J_{C\text{-}F}$ = 321.0 Hz), 35.71, 7.93, 7.10. **IR (neat)**: ν 3074, 1446, 1341, 1253, 1189, 1130, 1037, 902, 880, 837, 785, 757, 728, 687, 622 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{10}H_{11}F_3NO_3S_2$ 314.0127; Found 314.0123. Mp = 87.8 – 89.3 °C.



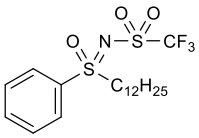
N-(triflyl)-*S*-phenyl-*S*-(*sec*-butyl) sulfoximine (**3k**). **2k** (0.3 mmol; 94 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (84 mg, 85%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.02 – 7.94 (m, 2H), 7.82 – 7.75 (m, 1H), 7.71 – 7.65 (m, 2H), 3.47 – 3.32 (m, 1H), 2.27 – 1.94 (m, 1H), 1.65 – 1.46 (m, 1H), 1.45 – 1.28 (m, 3H), 1.07 – 0.97 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.30 – (−79.34) (m). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.24, 134.27, 129.92, 129.02, 128.98, 119.18 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz), 65.20, 64.97, 22.09, 21.87, 12.03, 11.90, 10.88. **IR (neat)**: ν 2982, 2944, 2884, 1449, 1352, 1250, 1186, 1137, 1091, 1045, 997, 789, 753, 721, 686, 621 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_{15}F_3NO_3S_2$ 330.044; Found 330.0443. Mp = 41.5 – 41.9 °C.



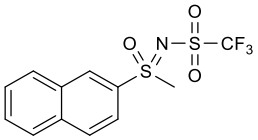
N-(triflyl)-*S*-(*p*-tolyl)-*S*-ethyl sulfoximine (**3l**). **2l** (0.3 mmol; 90 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (77 mg, 82%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 8.2 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 3.62 (dq, J = 14.7, 7.4 Hz, 1H), 3.51 (dq, J = 14.6, 7.3 Hz, 1H), 2.50 (s, 3H), 1.34 (t, J = 7.3 Hz, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.34. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 147.05, 131.87, 130.83, 128.31, 119.30 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz), 53.74, 21.86, 7.18. **IR (neat)**: ν 2989, 2955, 1591, 1346, 1259, 1192, 1134, 1093, 1050, 1012, 819, 777, 728, 622 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{10}H_{13}F_3NO_3S_2$ 316.0283; Found 316.0279. Mp = 79.5 – 80.3 °C.



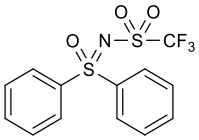
N-(triflyl)-*S*-(4-chlorophenyl)-*S*-cyclopropylmethyl sulfoximine (**3m**). **2m** (0.3 mmol; 99 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (99 mg, 91%). Flash chromatography for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.99 – 7.92 (m, 2H), 7.70 – 7.62 (m, 2H), 3.61 – 3.47 (m, 2H), 1.07 – 0.94 (m, 1H), 0.74 – 0.59 (m, 2H), 0.25 (ddq, *J* = 58.8, 10.4, 5.1 Hz, 2H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.29. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.51, 134.02, 130.30, 129.91, 119.13 (C-F, $^{1}J_{C\text{-}F}$ = 321.0 Hz), 64.34, 4.74, 4.55, 4.29. **IR (neat)**: ν 3096, 3021, 2980, 2927, 1574, 1472, 1400, 1357, 1249, 1217, 1188, 1135, 1057, 1008, 976, 919, 828, 766, 620 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_{12}ClF_3NO_3S_2$ 361.9894; Found 361.9893. Mp = 86.5 – 87.4 °C.



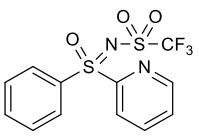
N-(triflyl)-*S*-phenyl-*S*-dodecyl sulfoximine (**3n**). **2n** (0.3 mmol; 123 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (76 mg, 57%). Column chromatography for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.04 – 7.98 (m, 2H), 7.82 – 7.76 (m, 1H), 7.72 – 7.66 (m, 2H), 3.59 (ddd, *J* = 14.1, 11.2, 5.1 Hz, 1H), 3.45 (ddd, *J* = 14.1, 11.1, 5.0 Hz, 1H), 1.84 – 1.62 (m, 2H), 1.42 – 1.14 (m, 18H), 0.87 (t, *J* = 7.2 Hz, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.30. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.90, 135.39, 130.19, 128.19, 119.30 (C-F, $^1J_{C\text{-}F}$ = 321.1 Hz), 58.76, 32.02, 29.68, 29.64, 29.50, 29.43, 29.25, 28.96, 27.87, 22.81, 22.33, 14.25. **IR (neat)**: ν 2917, 2850, 1471, 1451, 1347, 1241, 76, 1186, 1136, 1091, 1044, 806, 772, 742, 681, 631 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{19}H_{31}F_3NO_3S_2$ 442.1692; Found 442.1692. Mp = 53.0 – 55.8 °C.



N-(triflyl)-*S*-naphthalenyl-*S*-methyl sulfoximine (**3o**). **2o** (0.3 mmol; 92 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (74 mg, 73%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.64 (d, *J* = 2.0 Hz, 1H), 8.12 (d, *J* = 8.8 Hz, 1H), 8.06 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.99 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.94 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.77 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.71 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 3.59 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.16. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.97, 133.82, 132.20, 130.93, 130.67, 130.04, 129.85, 128.73, 128.33, 121.10, 119.40 (C-F, $^1J_{C\text{-}F}$ = 321.1 Hz), 47.01. **IR (neat)**: ν 3056, 3020, 2930, 1503, 1349, 1317, 1271, 1255, 1191, 1125, 1080, 1054, 981, 942, 926, 860, 799, 761, 746, 704, 641, 628, 616 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{11}F_3NO_3S_2$ 338.0127; Found 338.0123. Mp = 104.1 – 104.7 °C.

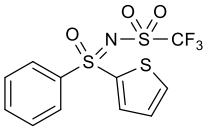


N-(triflyl)-*S,S*-diphenyl sulfoximine (**3p**).[3] **2p** (0.3 mmol; 95 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (87 mg, 83%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.06 – 8.00 (m, 4H), 7.72 – 7.67 (m, 2H), 7.64 – 7.58 (m, 4H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.40. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 138.93, 134.89, 130.12, 127.67, 119.27 (C-F, $^1J_{C\text{-}F}$ = 321.0 Hz). **IR (neat)**: ν 3069, 1579, 1474, 1450, 1358, 1250, 1216, 1189, 1134, 1086, 1049, 995, 792, 760, 727, 677, 628 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{13}H_{11}F_3NO_3S_2$ 350.0127; Found 350.0128. Mp = 67.7 – 70.0 °C.

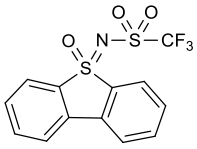


N-(triflyl)-*S*-phenyl-*S*-(2-pyridyl) sulfoximine (**3q**). **2q** (0.3 mmol; 95 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: White solid (85 mg, 81%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.72 – 8.67 (m, 1H), 8.36 – 8.30 (m, 1H), 8.16 (ddd, *J* = 8.5, 2.5, 1.2

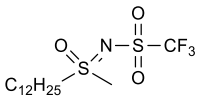
Hz, 2H), 8.02 (td, *J* = 7.8, 1.7 Hz, 1H), 7.77 – 7.70 (m, 1H), 7.63 (td, *J* = 7.9, 7.4, 1.4 Hz, 2H), 7.56 (ddd, *J* = 7.7, 4.6, 1.1 Hz, 1H).**^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.31. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 156.81, 151.02, 138.88, 135.37, 135.28, 129.81, 129.21, 128.14, 123.22, 119.28 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz). **IR (neat)**: ν 3097, 3061, 3014, 1582, 1557, 1453, 1427, 1348, 1256, 1193, 1118, 1087, 1054, 992, 798, 740, 729, 701, 681, 636 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{12}H_{10}F_3N_2O_3S_2$ 351.0079; Found 351.0075. Mp = 90.6 – 91.1 °C.



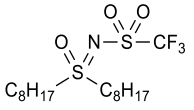
N-(triflyl)-*S*-(phenyl)-*S*-(2-thienyl) sulfoximine (**3r**). **2r** (0.3 mmol; 107 mg), 1 mL H_2O/MeCN (1:1), 3.5 equiv. of NaOCl·5H_2O (1.05 mmol, 173 mg), GP2: White solid (88 mg, 83%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.11 – 8.06 (m, 2H), 7.83 (ddd, *J* = 5.4, 4.4, 1.4 Hz, 2H), 7.73 – 7.68 (m, 1H), 7.64 – 7.59 (m, 2H), 7.18 (dd, *J* = 5.0, 3.9 Hz, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.37. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 139.70, 138.96, 136.80, 135.32, 134.84, 130.00, 128.81, 127.20, 119.09 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz). **IR (neat)**: ν 3107, 1449, 1397, 1358, 1252, 1189, 1136, 1089, 1047, 855, 786, 724, 679, 627 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{11}H_9F_3NO_3S_3$ 355.9691; Found 355.9693. Mp = 48.2 – 51.3 °C.



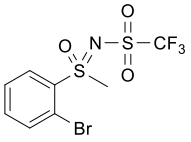
N-(triflyl)-dibenzo[b,d]thienyl sulfoximine (**3s**). **2s** (0.3 mmol; 95 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·5H_2O (0.75 mmol, 123 mg), GP2: White solid (93 mg, 89%). **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 8.15 (ddt, *J* = 8.3, 3.2, 1.6 Hz, 2H), 7.89 – 7.85 (m, 2H), 7.78 (tdt, *J* = 7.7, 2.6, 1.2 Hz, 2H), 7.63 (tdt, *J* = 7.7, 3.0, 1.4 Hz, 2H). **^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −78.80. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 135.98, 135.86, 132.73, 131.38, 125.28, 122.25, 119.45 (C-F, $^{1}J_{C\text{-}F}$ = 321.7 Hz). **IR (neat)**: ν 3096, 2921, 1590, 1578, 1482, 1451, 1351, 1287, 1251, 1184, 1124, 1068, 1034, 954, 795, 760, 743, 705, 686, 625 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{13}H_9F_3NO_3S_2$ 347.997; Found 347.9974. Mp = 137.6 – 140.5 °C.



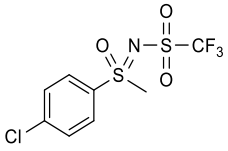
N-(triflyl)-*S*-dodecyl-*S*-methyl sulfoximine (**3t**). **2t** (0.3 mmol; 104 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·5H_2O (0.75 mmol, 123 mg), GP2: White solid (86 mg, 76%). Column chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) *δ* 3.50 – 3.32 (m, 5H), 2.00 – 1.86 (m, 2H), 1.53 – 1.45 (m, 2H), 1.40 – 1.20 (m, 13H), 0.88 (t, *J* = 6.9 Hz, 3H).**^{19}F NMR** (471 MHz, Chloroform-*d*) *δ* −79.15. **^{13}C NMR** (126 MHz, Chloroform-*d*) *δ* 119.35 (C-F, $^{1}J_{C\text{-}F}$ = 321.0 Hz) 56.96, 41.78, 32.03, 29.71, 29.67, 29.55, 29.45, 29.30, 29.03, 28.07, 22.82, 22.40, 14.26. **IR (neat)**: ν 3022, 2953, 2873, 2852, 2921, 1468, 1344, 1240, 1185, 1140, 1067, 973, 806, 769, 727, 691, 618 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{14}H_{29}F_3NO_3S_2$ 380.1535; Found 380.1536. Mp = 68.6 – 69.7 °C.



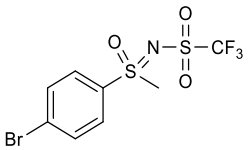
N-(triflyl)-*S,S*-dioctyl sulfoximine (**3u**). **2u** (0.3 mmol; 125 mg), 1 mL H_2O/MeCN (1:1), 2.5 equiv. of NaOCl·$5H_2O$ (0.75 mmol, 123 mg), GP2: Colorless oil (115 mg, 91%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 3.55 – 3.26 (m, 4H), 1.91 (dtd, *J* = 13.6, 8.4, 7.9, 5.5 Hz, 4H), 1.54 – 1.43 (m, 4H), 1.40 – 1.23 (m, 16H), 0.91 – 0.85 (m, 6H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.11. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 119.22 (C-F, $^1J_{C\text{-}F}$ = 321.1 Hz), 54.15, 31.61, 28.87, 28.85, 28.05, 22.56, 22.17, 14.04. **IR (neat)**: ν 2956, 2927, 2858, 1405, 1349, 1188, 1138, 1058, 790, 723, 616 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{17}H_{35}F_3NO_3S_2$ 422.2005; Found 422.201.



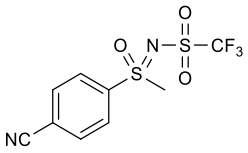
N-(triflyl)-*S*-(2-bromophenyl)-*S*-methyl sulfoximine (**3v**). **2v** (0.3 mmol; 100 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: White solid (106 mg, 96%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.31 – 8.25 (m, 1H), 7.88 (dd, J = 7.5, 1.6 Hz, 1H), 7.67 – 7.59 (m, 2H), 3.76 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.15. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 136.57, 136.43, 136.28, 131.63, 120.47, 119.23 (C-F, $^1J_{C\text{-}F}$ = 320.9 Hz), 44.08. **IR (neat)**: ν 3108, 3028, 3012, 2878, 1570, 1446, 1348, 1261, 1183, 1126, 1051, 979, 791, 758, 746, 2, 704, 641, 614 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8BrF_3NO_3S_2$ 365.9076; Found 365.9073. Mp = 107.3 – 107.8 °C.



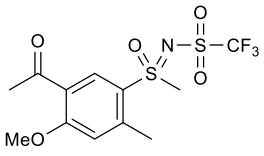
N-(triflyl)-*S*-(4-chlorophenyl)-*S*-methyl sulfoximine (**3w**). **2w** (0.3 mmol; 87 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: White semi solid (81 mg, 84%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.99 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 8.7 Hz, 2H), 3.53 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.19. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.74, 135.65, 130.69, 128.99, 119.25 (C-F, $^1J_{C\text{-}F}$ = 320.9 Hz), 46.97. **IR (neat)**: ν 3034, 2937, 1579, 1476, 1397, 1351, 1253, 1209, 1187, 1133, 1085, 1055, 1010, 970, 836, 826, 793, 775, 754, 725, 623 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8ClF_3NO_3S_2$ 321.9581; Found 321.9578. Mp = 91.5 – 93.0 °C.



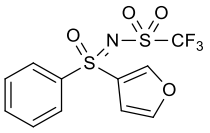
N-(triflyl)-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**3x**).[3] **2x** (0.3 mmol; 100 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: White solid (91 mg, 83%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.92 – 7.89 (m, 2H), 7.85 – 7.81 (m, 2H), 3.52 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.18. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 136.25, 133.69, 131.38, 128.96, 119.24 (C-F, $^1J_{C\text{-}F}$ = 321.0 Hz), 46.92. **IR (neat)**: ν 3025, 2931, 1571, 1392, 1351, 1253, 1208, 1188, 1134, 1091, 1055, 1007, 969, 823, 792, 772, 750, 712, 624 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_8H_8BrF_3NO_3S_2$ 365.9076; Found 365.9079. Mp = 113.1 – 114.7°C.



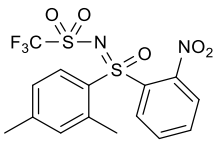
N-(triflyl)-*S*-(4-cyanophenyl)-*S*-methyl sulfoximine (**3y**).[3] **2y** (0.3 mmol; 84 mg), 1 mL DCM, 3.5 equiv. of *m*-CPBA (1.05 mmol, 182 mg), GP3: White solid (58 mg, 62%). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.29 (d, J = 1.7 Hz, 4H), 4.00 (s, 3H).**^{19}F NMR** (471 MHz, DMSO-d_6) δ −78.76. **^{13}C NMR** (126 MHz, DMSO-d_6) δ 141.47, 133.95, 128.37, 118. 28 (C-F, $^1J_{C\text{-}F}$ = 321.5 Hz), 117.56, 117.30, 44.14. **IR (neat)**: ν 3095, 3046, 3026, 2937, 2240, 1523, 1393, 1341, 1253, 1188, 1130, 1087, 1055, 990, 840, 801, 733, 622 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_9H_8F_3N_2O_2S_2$ 312.9923; Found 312.9925. Mp = 180.0 – 180.5 °C.



N-(triflyl)-*S*-(5-acetyl-4-methoxy-2-methylphenyl)-*S*-methyl sulfoximine (**3z**). **2z** (0.3 mmol; 102 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: White solid (91 mg, 81%). Column chromatography for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.42 (s, 1H), 6.99 (s, 1H), 4.04 (s, 3H), 3.55 (s, 3H), 2.79 (s, 3H), 2.62 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.24. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 196.65, 163.03, 144.30, 132.74, 127.30, 126.95, 119.26 (C-F, $^1J_{C\text{-}F}$ = 321.2 Hz), 116.80, 56.59, 45.87, 31.79, 21.35. **IR (neat)**: ν 3024, 3007, 2923, 2852, 1678, 1594, 1547, 1486, 1473, 1416, 1388, 1345, 1331, 1262, 1247, 1229, 1187, 1137, 1086, 1042, 974, 924, 862, 794, 769, 735, 709, 639, 611 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{15}F_3NO_5S_2$ 374.0338; Found 374.0334. Mp = 163.9 – 167.7 °C (decomposition).

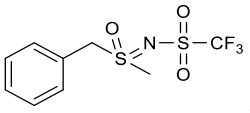


N-(triflyl)-*S*-phenyl-*S*-(3-furyl) sulfoximine (**3aa**). **2aa** (0.3 mmol; 92 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: Colourless oil (88 mg, 95%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 1.6, 0.9 Hz, 1H), 8.09 – 8.02 (m, 2H), 7.77 – 7.71 (m, 1H), 7.68 – 7.61 (m, 2H), 7.56 (t, *J* = 1.8 Hz, 1H), 6.68 (dd, *J* = 2.1, 0.9 Hz, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.38. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 147.80, 146.25, 138.74, 135.17, 130.16, 127.45, 126.92, 119.24 (C-F, $^1J_{C\text{-}F}$ = 321.0 Hz), 108.46. **IR (neat)**: ν 3150, 1543, 1498, 1449, 1355, 1263, 1189, 1134, 1050, 945, 870, 788, 726, 682, 643 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^+$ Calcd for $C_{11}H_9F_3NO_4S_2$ 339.992; Found 339.9922.

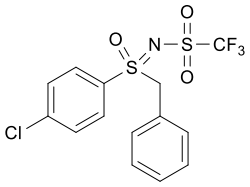


N-(triflyl)-*S*-(2,4-dimethylphenyl)-*S*-(2-nitrophenyl) sulfoximine (**3ab**). **2ab** (0.3 mmol; 117 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: Brown solid (108 mg,

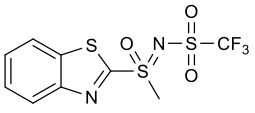
85%). Column chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.59 – 8.54 (m, 1H), 8.03 – 7.89 (m, 4H), 7.29 – 7.26 (m, 1H), 7.16 – 7.13 (m, 1H), 2.43 (s, 3H), 2.40 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.21. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 147.86, 146.96, 137.89, 136.05, 134.32, 133.14, 132.37, 132.28, 132.23, 130.40, 127.65, 126.30, 119.08 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz), 21.54, 20.03. **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{14}F_3N_2O_5S_2$ 423.0291; Found 423.0286. Mp = 106.9 – 107.5°C.



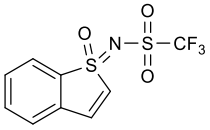
N-(triflyl)-*S*-benzyl-*S*-methyl sulfoximine (**3ac**). **2ac** (0.3 mmol; 81 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: White solid (57 mg, 63%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.54 – 7.42 (m, 5H), 4.84 – 4.66 (m, 2H), 3.17 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.09. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 131.25, 130.62, 129.67, 125.19, 119.22 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz), 63.11, 39.85. **IR (neat)**: ν 3033, 3004, 2979, 2924, 1412, 1347, 1248, 1187, 1135, 1072, 984, 929, 885, 774, 729, 698, 664, 616 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_{11}F_3NO_3S_2$ 302.0132; Found 302.0129. Mp = 99.0 – 99.8 °C.



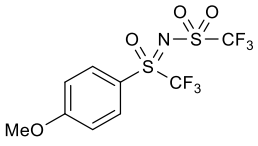
N-(triflyl)-*S*-(4-chlorophenyl)-*S*-benzyl sulfoximine (**3ad**). **2ad** (0.3 mmol; 110 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: White solid (106 mg, 89%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.61 – 7.57 (m, 2H), 7.52 – 7.47 (m, 2H), 7.42 – 7.37 (m, 1H), 7.30 (dd, *J* = 8.5, 7.0 Hz, 2H), 7.07 – 7.03 (m, 2H), 4.81 (dd, *J* = 87.2, 14.0 Hz, 2H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.16. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 142.68, 132.47, 131.57, 130.41, 130.27, 130.06, 129.22, 125.05, 119.26 (C-F, $^{1}J_{C\text{-}F}$ = 321.2 Hz), 65.61. **IR (neat)**: ν 3109, 3065, 2983, 2931, 1568, 1495, 1471, 1396, 1347, 1248, 1194, 1126, 1088, 1056, 1007, 822, 761, 739, 693, 627. (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{12}ClF_3NO_3S_2$ 397.9894; Found 397.9885. Mp = 133.7 – 134.9 °C.



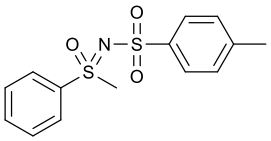
N-(triflyl)-*S*-(benzo[*d*]thiazol-2-yl)-*S*-methyl sulfoximine (**3ae**). **2ae** (0.22 mmol; 70 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.55 mmol, 95 mg), GP3: Off white solid (67 mg, 87%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.28 – 8.23 (m, 1H), 8.08 – 8.03 (m, 1H), 7.74 – 7.65 (m, 2H), 3.86 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −78.93. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 162.83, 152.44, 137.75, 129.24, 128.49, 125.98, 122.58, 119.21 (C-F, $^{1}J_{C\text{-}F}$ = 321.1 Hz), 44.38. **IR (neat)**: ν 3045, 3007, 2914, 1552, 1463, 1415, 1358, 1320, 1252, 1211, 1186, 1138, 1090, 1065, 1025, 973, 857, 793, 764, 724, 696, 621 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_8F_3N_2O_3S_3$ 344.9644; Found 344.9645. Mp = 106.1 – 107.6 °C.



N-(triflyl)-*S*-(benzo[*b*]thienyl) sulfoximine (**3af**). **2af** (0.3 mmol; 80 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: Colorless oil (72 mg, 85%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.03 (d, *J* = 7.6 Hz, 1H), 7.70 (dtd, *J* = 32.6, 7.6, 1.1 Hz, 2H), 7.52 (ddd, *J* = 20.9, 7.0, 1.0 Hz, 2H), 7.24 (d, *J* = 6.7 Hz, 1H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −78.78. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.76, 135.70, 135.05, 132.02, 131.94, 129.42, 126.44, 124.38, 119.37 (C-F, $^{1}J_{C\text{-}F}$ = 321.5 Hz). **IR (neat)**: ν 3118, 3095, 1548, 1464, 1354, 1296, 1251, 1186, 1129, 1082, 1031, 870, 795, 760, 684, 607 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_9H_7F_3NO_3S_2$ 297.9801; Found 297.9805.



N-(triflyl)-*S*-(4-methoxyphenyl)-*S*-trifluoromethyl sulfoximine (**3ag**). **2ag** (0.3 mmol; 102 mg), 1 mL DCM, 2.5 equiv. of *m*-CPBA (0.75 mmol, 130 mg), GP3: Colorless oil (89 mg, 80%). Column chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.09 – 8.04 (m, 2H), 7.23 – 7.18 (m, 2H), 3.99 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −76.81, −79.11. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.67, 133.47, 120.02 (C-F, $^{1}J_{C\text{-}F}$ = 327.5 Hz), 119.05 (C-F, $^{1}J_{C\text{-}F}$ = 320.5 Hz), 118.48, 116.33, 56.49. **IR (neat)**: ν 3108, 2952, 2906, 2804, 1588, 1496, 1464, 1443, 1374, 1277, 1198, 1165, 1128, 1089, 1045, 837, 809, 785, 752, 678, 658, 630 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_9H_8F_6NO_4S_2$ 371.9793; Found 371.979.



N-(tosyl)-*S*-phenyl-*S*-methyl sulfoximine (**7**).[4] **6** (0.3 mmol; 83 mg), 1 mL H_2O, 2.5 equiv. of NaOCl·5H_2O (0.75 mmol, 123 mg), GP1: White solid (86 mg, 92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.05 – 7.97 (m, 2H), 7.88 – 7.82 (m, 2H), 7.73 – 7.67 (m, 1H), 7.63 – 7.57 (m, 2H), 7.28 – 7.23 (m, 2H), 3.43 (s, 3H), 2.40 (s, 3H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 143.02, 140.73, 138.47, 134.51, 129.83, 129.41, 127.61, 126.77, 46.77, 21.65. **IR (neat)**: ν 3020, 2921, 1597, 1479, 1448, 1403, 1313, 1226, 1145, 1087, 1060, 980, 809, 790, 742, 705, 683, 652 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: [M + H]$^{+}$ Calcd for $C_{14}H_{16}NO_3S_2$ 310.0566; Found 310.0563. Mp = 96.4 – 98.1 °C.

References:

1) C. Bohnen and C. Bolm, *Org. Lett.*, 2015, **17**, 3011–3013.

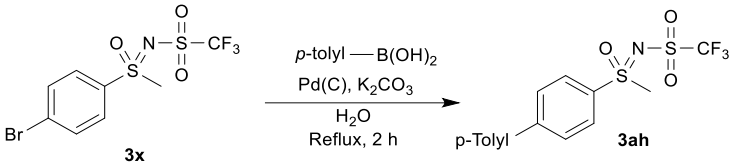
2) D. Craig, N. J. Geach, C. J. Pearson, A. M. Z. Slawin, A. J. P. White and D. J. Williams, Tetrahedron 1995, **51**, 6071-60983.

3) M. Ochiai, M. Naito, K. Miyamoto, S. Hayashi and W. Nakanishi, *Chem. Eur. J.*, 2010, **16**, 8713–8718.

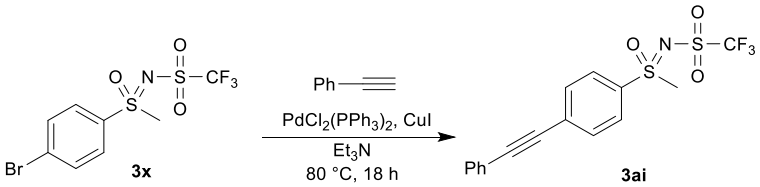
4) G. Y. Cho and C. Bolm, *Org. Lett.*, 2005, **7**, 4983.

Post-modification reactions

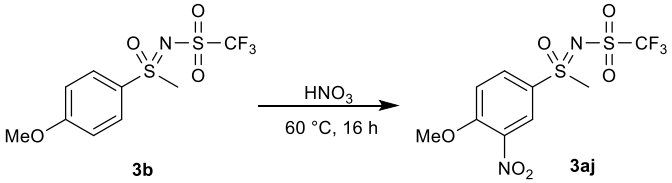
Post-modification reaction procedures



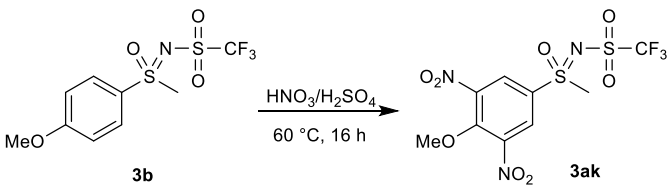
A round bottom flask was charged with *N*-(trifluoromethylsulfaneylidene)-*S*-(4- bromophenyl)-*S*-methyl sulfoximine (**3x**) (183 mg, 0.5 mmol), 4-methylphenyl boronic acid (1.33 equiv.) and K_2CO_3 (3 equiv.). Water (15 mL) was added along with palladium on carbon (tip of the spatula) and the reaction mixture was stirred under reflux for 2 h. After 2 h the reaction mixture was cooled to room temperature and extracted with EtOAc. The solvent was removed under reduced pressure and the residue was purified by column chromatography (DCM) yielding **3ah** (165 mg, 88%).



A dried flask was charged with *N*-(trifluoromethylsulfaneylidene)-*S*-(4-bromophenyl)- *S*-methyl sulfoximine (**3x**) (73 mg, 0.2 mmol) and Et_3N (2 mL). To this solution $PdCl_2(PPh_3)_2$ (4 mg, 3 mol%) and CuI (1 mg, 3 mol%) were added and the reaction mixture was stirred for 5 min under an inert atmosphere, followed by addition of phenylacetylene (26 µL, 1.2 equiv.). The resulting mixture was then heated under an inert atmosphere at 80 °C for 18 h. The mixture was cooled to room temperature, and solvent removed under reduced pressure. The crude product was purified by column chromatography yielding **3ai** as an off white solid (64 mg, 83%).

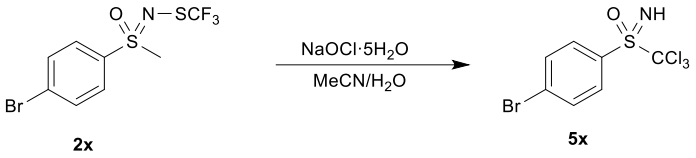


To a flask charged with *N*-(triflyl)-*S*-(4-methoxyphenyl)-*S*-methyl sulfoximine (**3b**) (32 mg, 0.1 mmol) was added 1 mL of a mixture of aqueous HNO_3 (68%) and H_2SO_4 (98%) (2:1 (V/V)). The reaction mixture was heated to 60 °C and stirred for 16 h. The acid was neutralised by addition of saturated aqueous $NaHCO_3$ solution and extracted with DCM. The organic phase was dried and the solvent was removed under reduced pressure and the residue was purified using flash chromatography (EtOAc and hexane 1/1) yielding **3aj** as a colorless semi solid (28 mg, 78%).



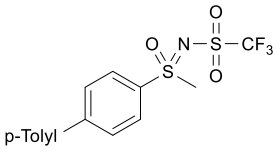
To a flask charged with *N*-(triflyl)-*S*-(4-methoxyphenyl)-*S*-methyl sulfoximine (**3b**) (40 mg, 0.13 mmol) was added 1 mL of a mixture aqueous HNO_3 (68%) and H_2SO_4 (98%) (1:2 (V/V)). The reaction mixture was heated to 60 °C and stirred for 16 h. The acid was neutralised by addition of saturated aqueous

$NaHCO_3$ solution and extracted with EtOAc. The organic phase was dried and the solvent was removed under reduced pressure and the residue was purified using flash chromatography (DCM) yielding **3ak** as a yellow solid (33 mg, 65%).

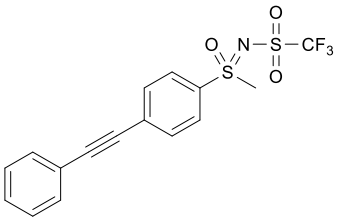


A flask was charged with *N*-trifluoromethylthio-*S*-(4-bromophenyl)-*S*-methyl sulfoximine (**2x**) (100 mg, 0.3 mmol), water (0.5 mL), MeCN (0.5 mL), $NaOCl{\cdot}5H_2O$ (4 equiv.) and the reaction mixture was stirred at r.t. for 2 h. The reaction mixture was then extracted twice with EtOAc and the organic phase was dried under anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure yielded the product **5x** as a white solid (98 mg, 97%). Some minor impurities are present which could not be removed due to the decomposition of the product during chromatography separation.

Characterization of post-modification products

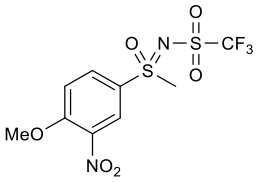


N-(triflyl)-*S*-(4'-methyl-[1,1'-biphenyl]-4-yl)-*S*-methyl sulfoximine (**3ah**). **2y** (0.5 mmol; 183 mg), 1.33 equiv. 4-methylphenyl boronic acid (0.665 mmol, 90 mg), 3 equiv. K_2CO_3 (1.5 mmol, 207 mg), catalytic amount of Pd/C: White solid (165 mg, 88%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.11 – 8.04 (m, 2H), 7.88 – 7.82 (m, 2H), 7.57 – 7.50 (m, 2H), 7.35 – 7.29 (m, 2H), 3.55 (s, 3H), 2.43 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.20. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 148.63, 139.66, 135.54, 135.11, 130.16, 128.51, 128.02, 127.45, 119.36 (C-F, $^1J_{C\text{-}F}$ = 321.1 Hz), 47.16, 21.38. **IR (neat)**: ν 3020, 2931, 1589, 1484, 1396, 1347, 1251, 1190, 1133, 1095, 1049, 969, 849, 810, 792, 771, 752, 724, 630 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{14}F_3NO_3S_2$ 378.044; Found 378.0437. Mp = 153.0 – 153.4 °C.

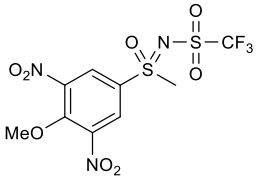


N-(triflyl)- *S*-(4-(phenylethynyl)phenyl)-*S*-methyl sulfoximine (**3ai**). **2y** (0.2 mmol; 73 mg), 1.2 equiv. phenylacetylene (0.24 mmol, 24 mg), 3 mol% $PdCl_2(PPh_3)_2$ (0.006 mmol, 4 mg), 3 mol% CuI (0.006 mmol, 1 mg): Off white solid (64 mg, 83%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.05 – 7.97 (m, 2H), 7.81 – 7.75 (m, 2H), 7.60 – 7.54 (m, 2H), 7.45 – 7.37 (m, 3H), 3.54 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.17. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 135.89, 133.02, 132.09, 131.36, 129.65, 128.73, 127.53, 121.94, 119.32 (C-F, $^1J_{C\text{-}F}$ = 321.0 Hz), 95.37, 87.16, 46.98. **IR (neat)**: ν 3030, 2933, 2219, 1585, 1493, 1442, 1399, 1347, 1257, 1221, 1202, 1183, 1136, 1088, 1043, 1013, 989, 957, 838, 795, 763, 750, 720, 693,

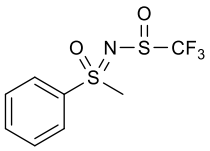
629 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{13}F_3NO_3S_2$ 388.0283; Found 388.0282. Mp = 150.8 – 151.8 °C.



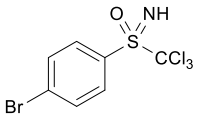
N-(triflyl)-*S*-(4-methoxy-3-nitrophenyl)-*S*-methyl sulfoximine (**3aj**). **3b** (0.1 mmol; 32 mg), 1 mL HNO_3 (68%): Colorless semi solid (28 mg, 78%). Flash chromatography (DCM) for purification **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.49 (d, *J* = 2.5 Hz, 1H), 8.21 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.38 (d, *J* = 9.0 Hz, 1H), 4.12 (s, 3H), 3.56 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −79.13. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 157.99, 139.82, 133.35, 128.62, 125.91, 119.20 (C-F, $^1J_{C\text{-}F}$ = 321.1 Hz), 115.25, 57.73, 47.18. **IR (neat)**: ν 3028, 2932, 1605, 1573, 1534, 1492, 1463, 1441, 1350, 1289, 1254, 1184, 1135, 1051, 1005, 980, 889, 824, 798, 764, 738, 681, 618 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_{10}F_3N_2O_6S_2$ 362.9927; Found 362.9921.



N-(triflyl)-*S*-(4-methoxy-3,5-dinitrophenyl)-*S*-methyl sulfoximine (**3ak**). **3b** (0.13 mmol; 40 mg), 1 mL (HNO_3 (68%):H_2SO_4 (98%) = 1:2): Yellow solid (33 mg, 65%). Flash chromatography (DCM) for purification. **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.64 (s, 2H), 4.20 (s, 3H), 3.64 (s, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −78.88. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 152.62, 145.35, 132.54, 128.19, 118.92 (C-F, $^1J_{C\text{-}F}$ = 320.9 Hz), 65.40, 46.69. **IR (neat)**: ν 3033, 2941, 1613, 1544, 1478, 1342, 1292, 1255, 1191, 1136, 1095, 1065, 969, 921, 884, 809, 787, 764, 740, 714, 683, 618 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_9H_9F_3N_3O_8S_2$ 407.9778; Found 407.9785. Mp = 127.4 – 129.0 °C.

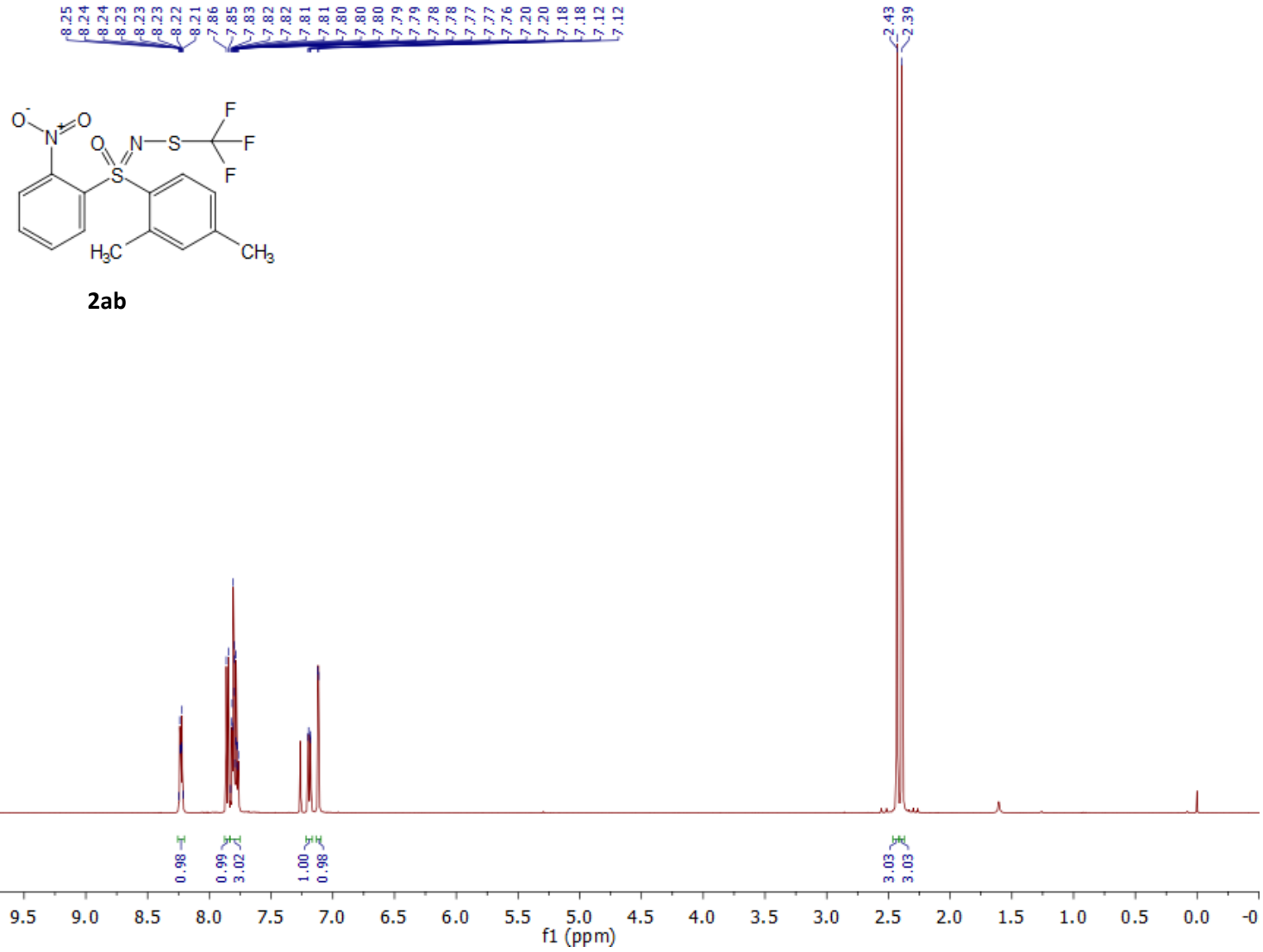


N-(trifluoromethylsulfaneylidene)-*S*-phenyl-*S*-methyl sulfoximine (**4a**). **2a** (0.3 mmol; 86 mg), 1 mL EtOAc, 1.1 equiv. of $NaOCl{\cdot}5H_2O$ (0.3 mmol, 49 mg): Colorless oil (92%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.09 – 7.97 (m, 2H), 7.79 – 7.62 (m, 3H), 3.47 – 3.36 (m, 3H). **^{19}F NMR** (471 MHz, Chloroform-*d*) δ −80.54, −80.89. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 138.39, 137.83, 135.21, 135.00, 130.23, 130.09, 128.32, 127.54, 124.08 (C-F, $^1J_{C\text{-}F}$ = 333.8 Hz), 47.46, 47.16. **IR (neat)**: ν 3067, 3015, 1582, 1448, 1405, 1325, 1231, 1175, 1151, 1090, 1030, 1013, 993, 786, 738, 683 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_8H_9F_3NO_2S_2$ 272.0021; Found 272.0016.



S-(4-bromophenyl)-*S*-trichloromethyl sulfoximine (**5x**). **2x** (0.3 mmol; 199 mg), 1 mL H_2O, 4 equiv. of $NaOCl{\cdot}5H_2O$ (1.2 mmol, 197 mg), GP1: White solid (98 mg, 97%). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.05 – 8.00 (m, 2H), 7.80 – 7.76 (m, 2H). Unknown minor impurities are present due to decomposition and the inability to purify the product with chromatographic means. **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 132.94, 132.84, 132.15, 128.93, 127.82. **IR (neat)**: ν 3094, 1579, 1393, 1352, 1324, 1298, 1202, 1168, 1136, 1088, 1067, 1012, 820, 786, 754, 727, 700, 643 (cm^{-1}). **HRMS (ESI-TOF)** *m/z*: $[M + H]^+$ Calcd for $C_7H_6BrCl_3NOS$ 335.8414; Found 335.8415. Mp = 168.7 – 171.9 °C (decomposition – changes to a dark-brown solid).

Copies of ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra



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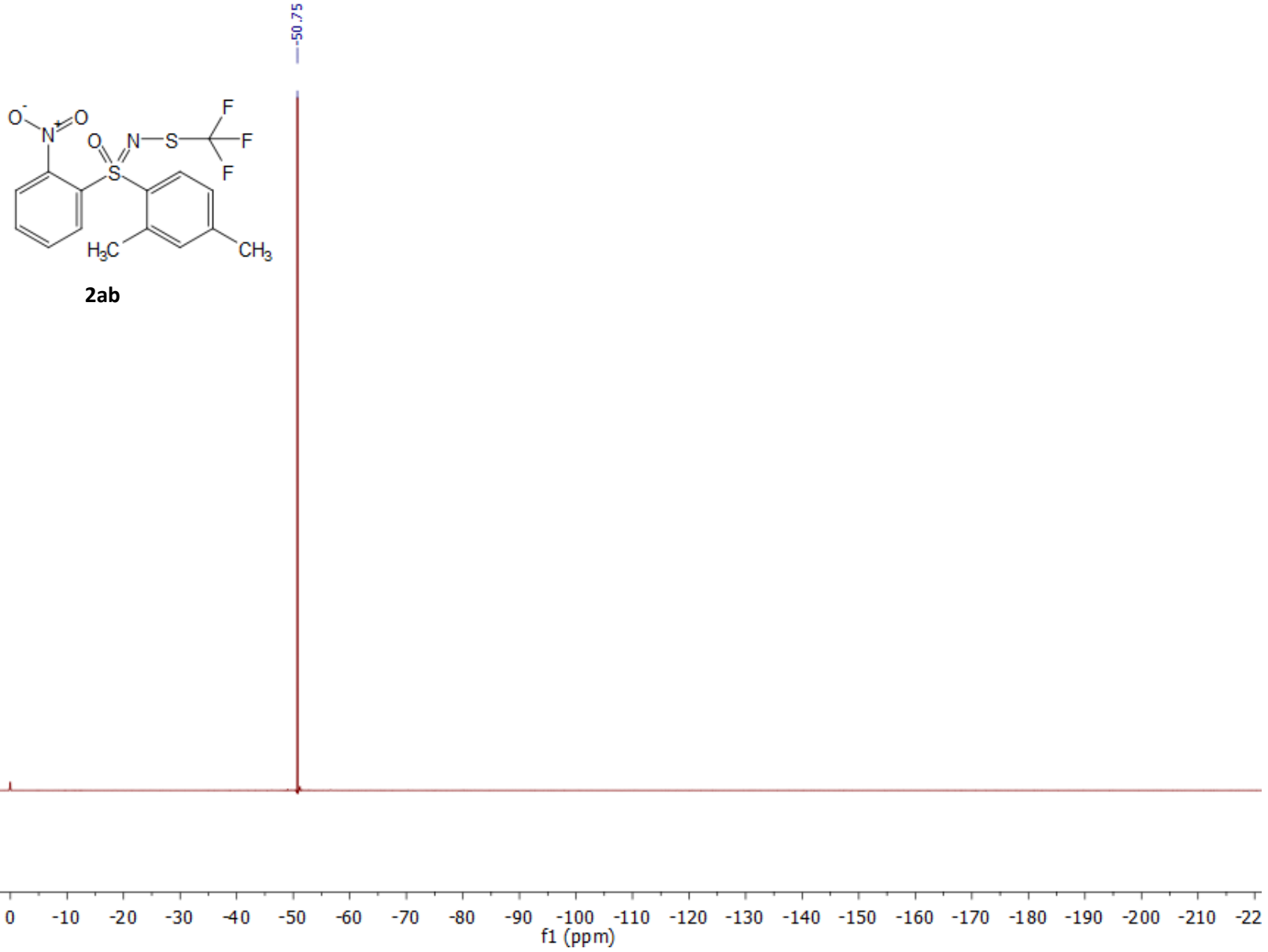
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F
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F
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H3C
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-60
-70
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-90
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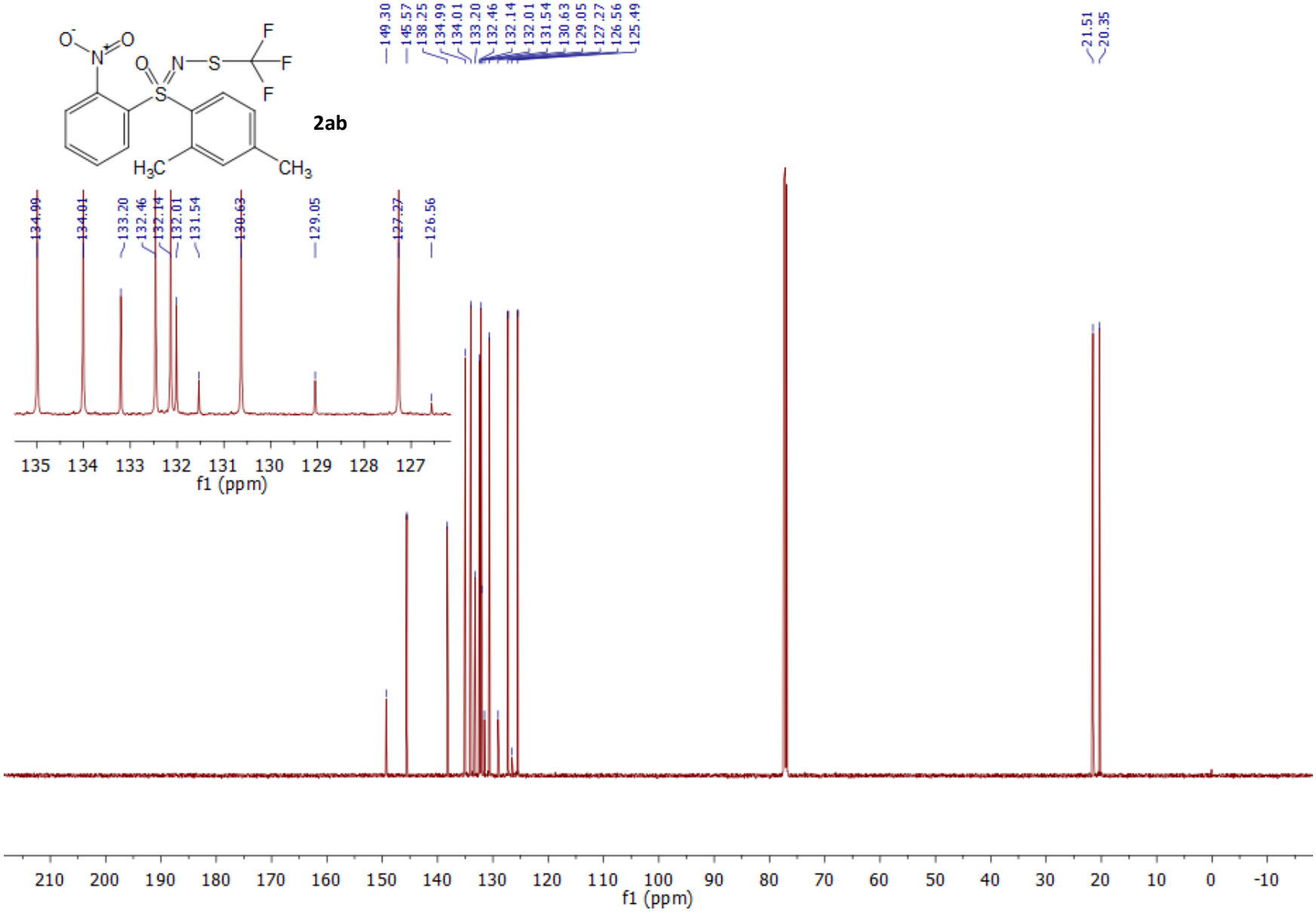
-22
f1 (ppm)

2ab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134.01
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132.01
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129.05
127.27
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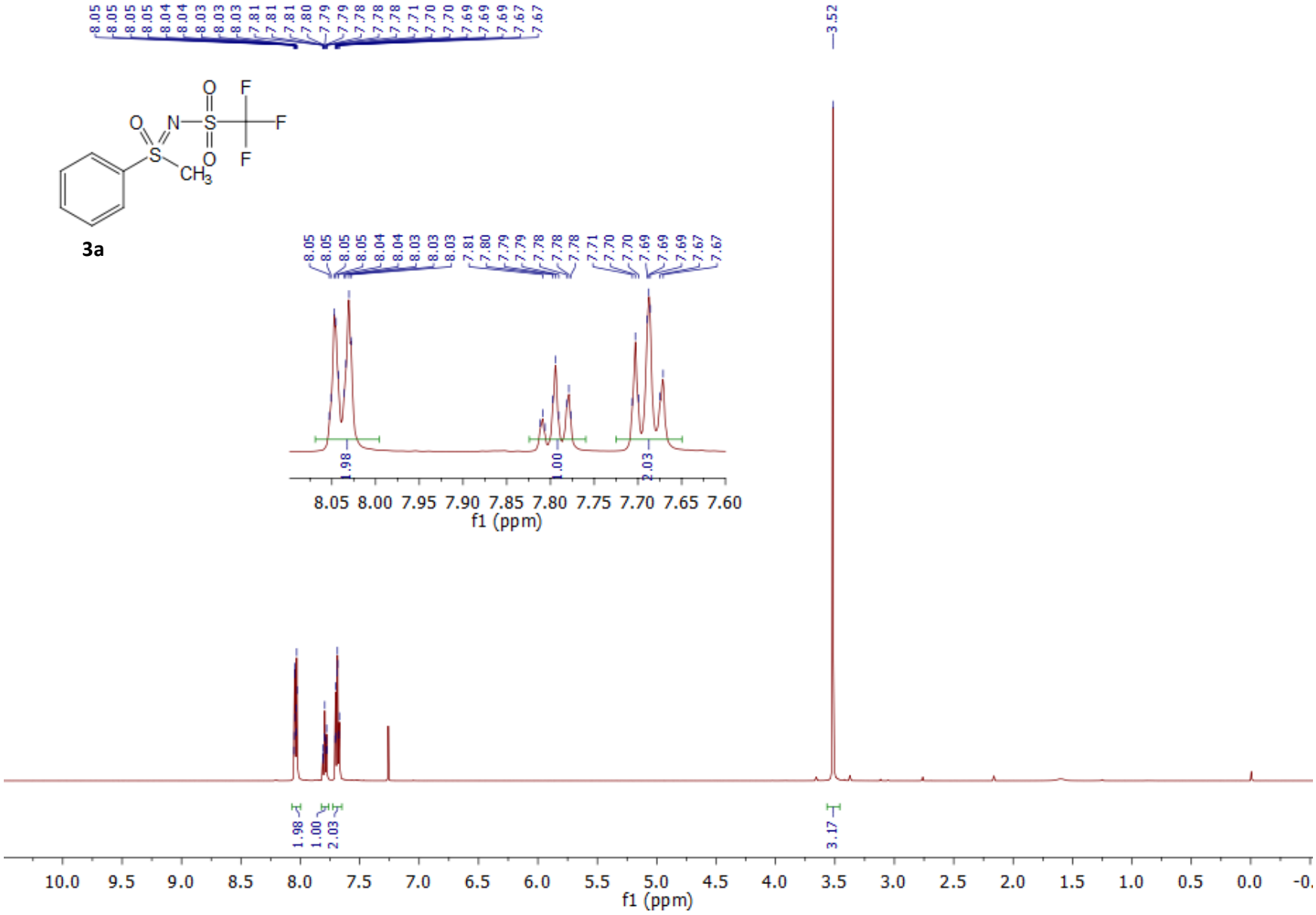
125.49
21.51
20.35
f1 (ppm)
f1 (ppm)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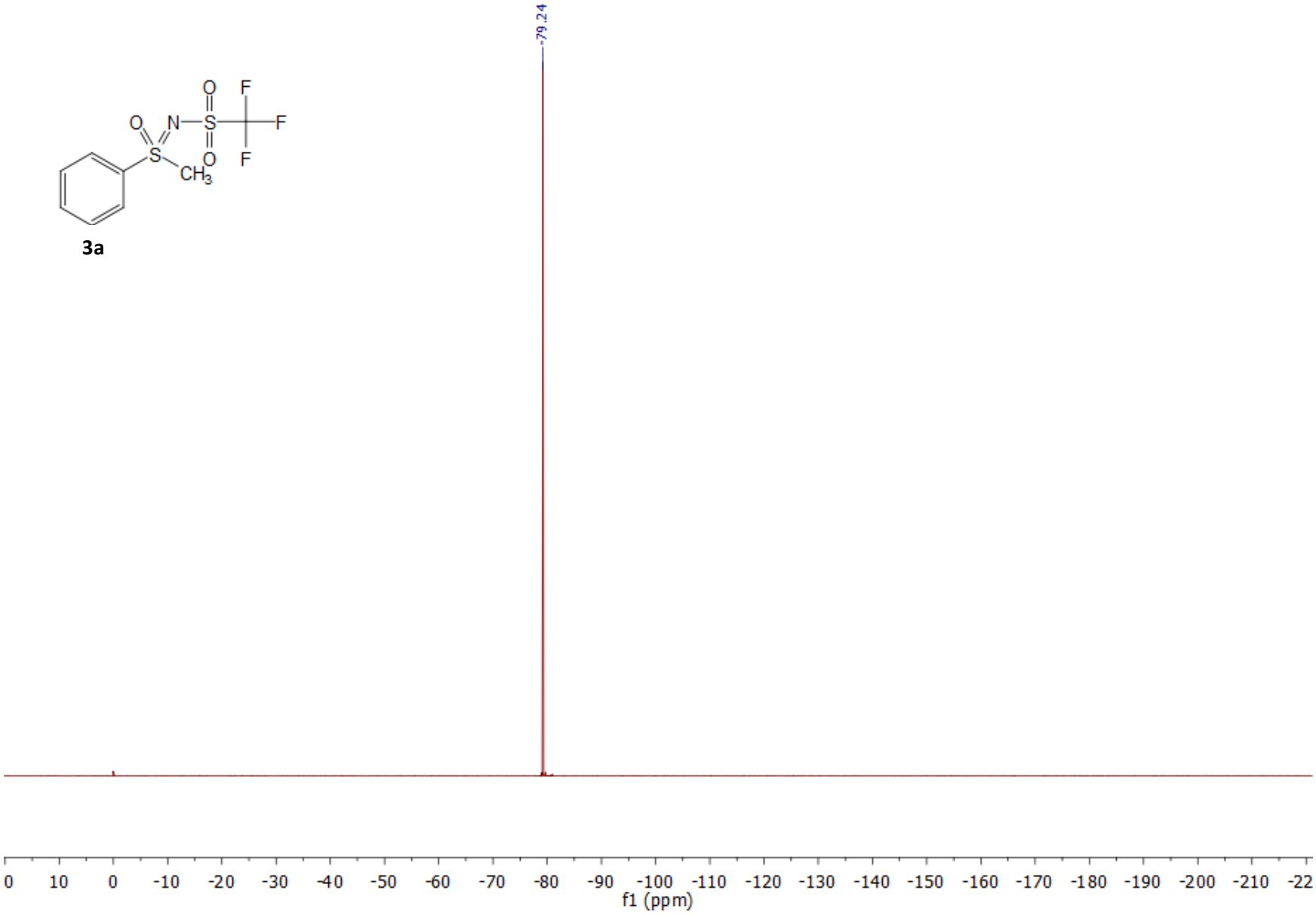
3.52
O F
O N S F
S
O F
CH3
3a
1.98
1.00
2.03
8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60
f1 (ppm)
1.98
1.00
2.03
3.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3a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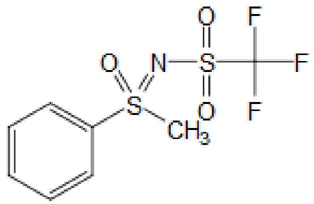
-22
f1 (ppm)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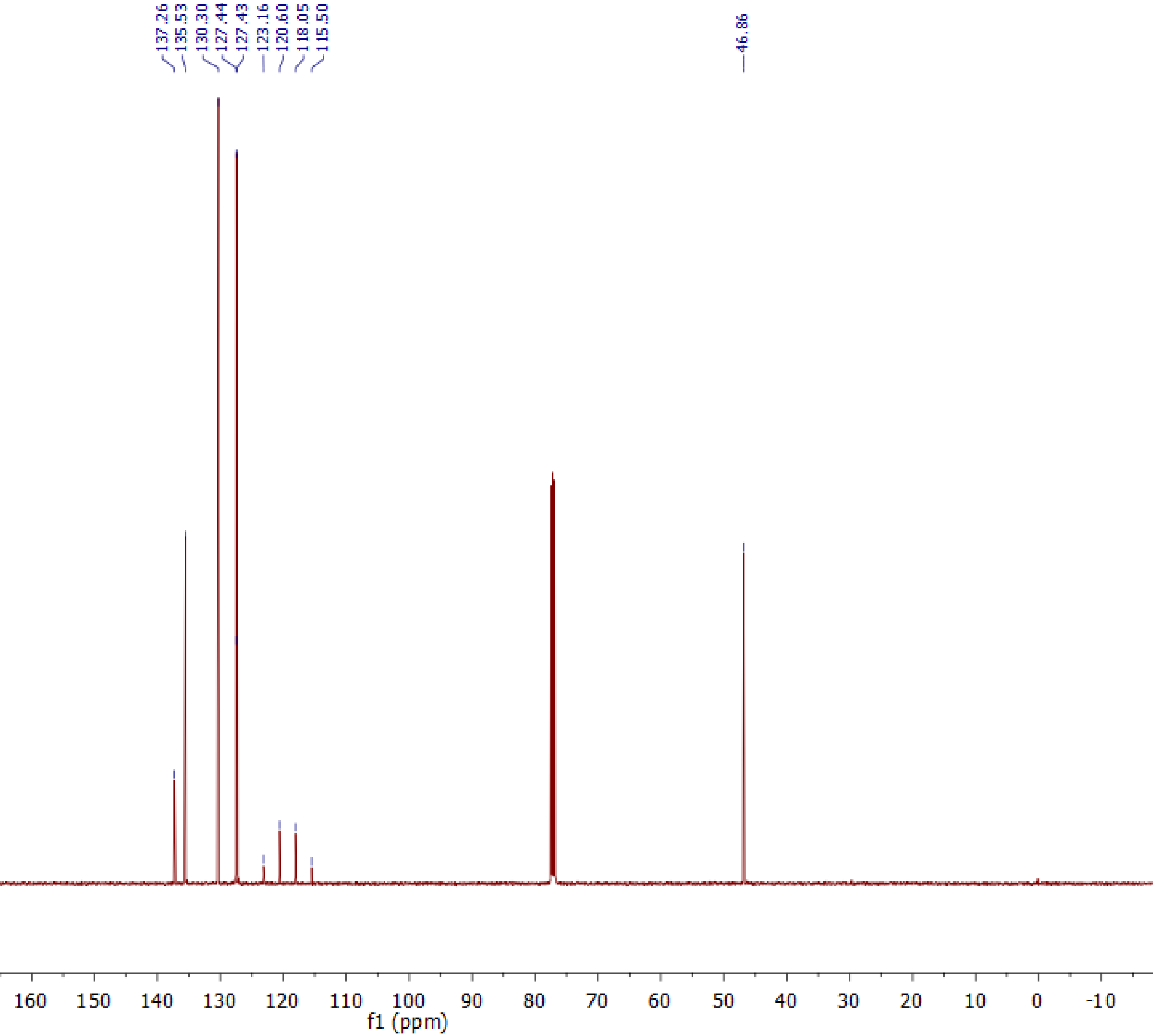
O
F
F
F
O
S
CH3

3a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118.05
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46.86
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170
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80
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50
40
30
20
10
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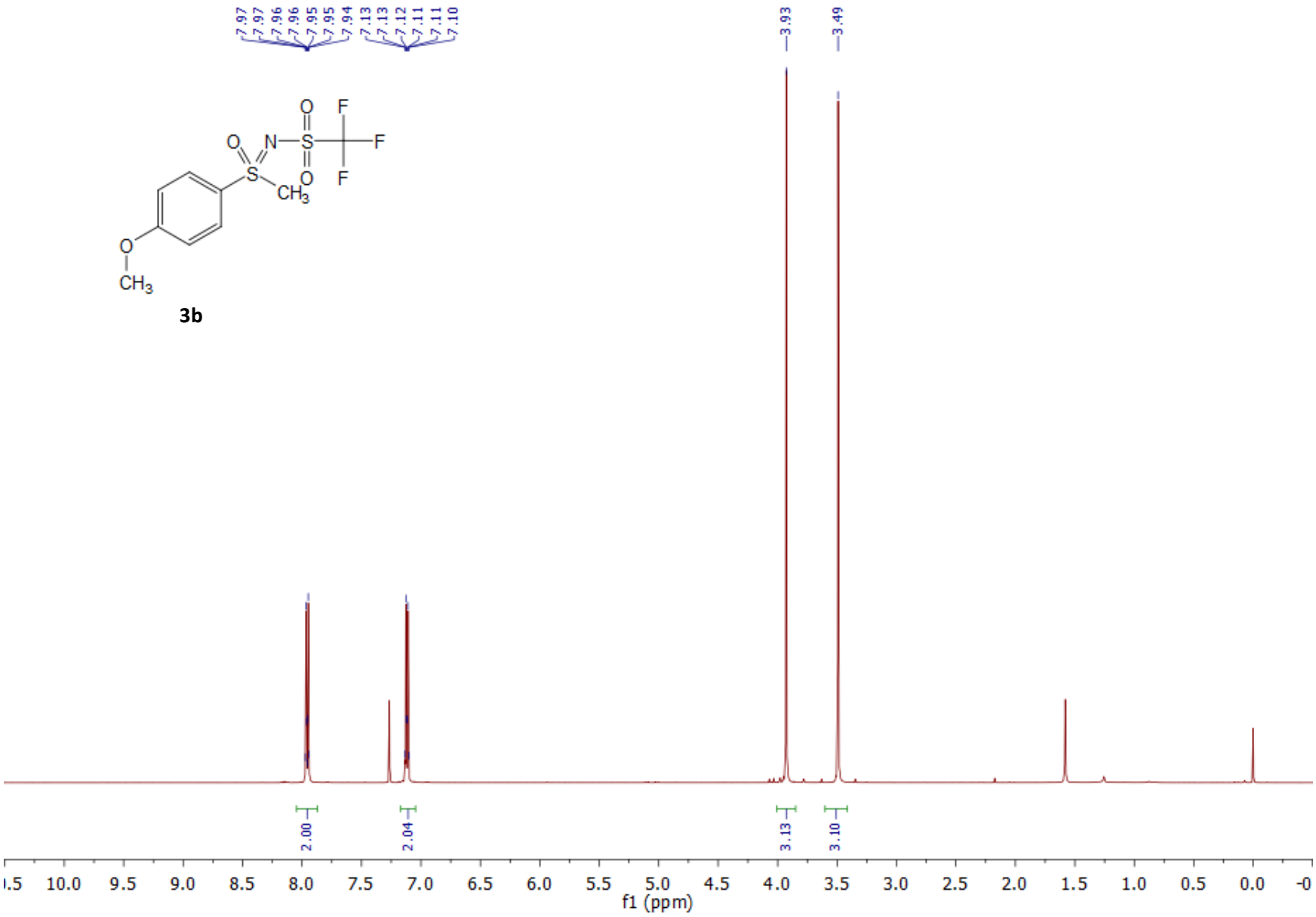
-10
f1 (ppm)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7.13
7.13
7.12
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7.11
7.10
3.93
3.49
O
F
O
N
S
F
S
F
O
CH3
O
CH3
2.00
2.04
3.13
3.10
f1 (ppm)

3b

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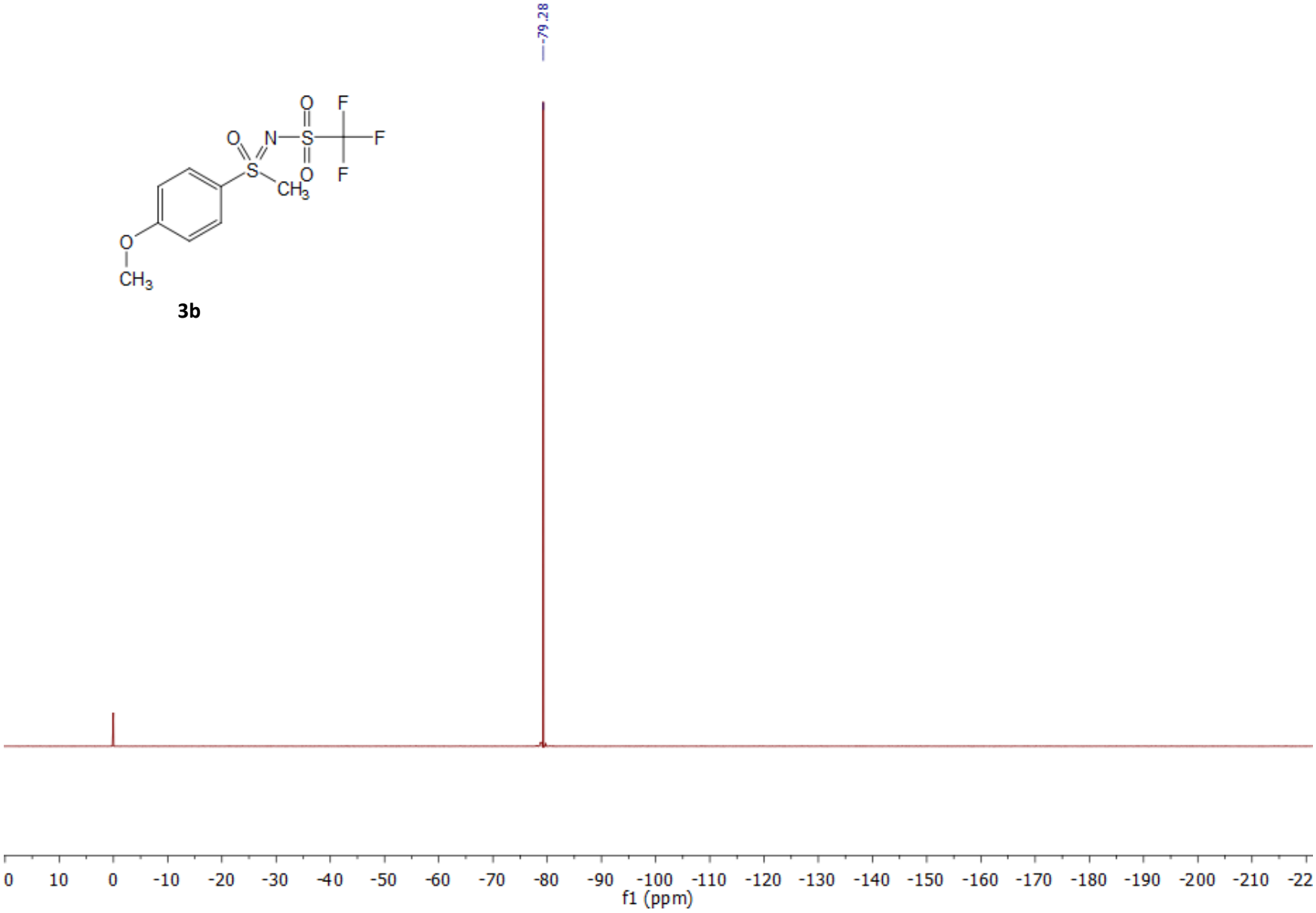
F
O
N
S
F
S
O
F
CH3
O
CH3

3b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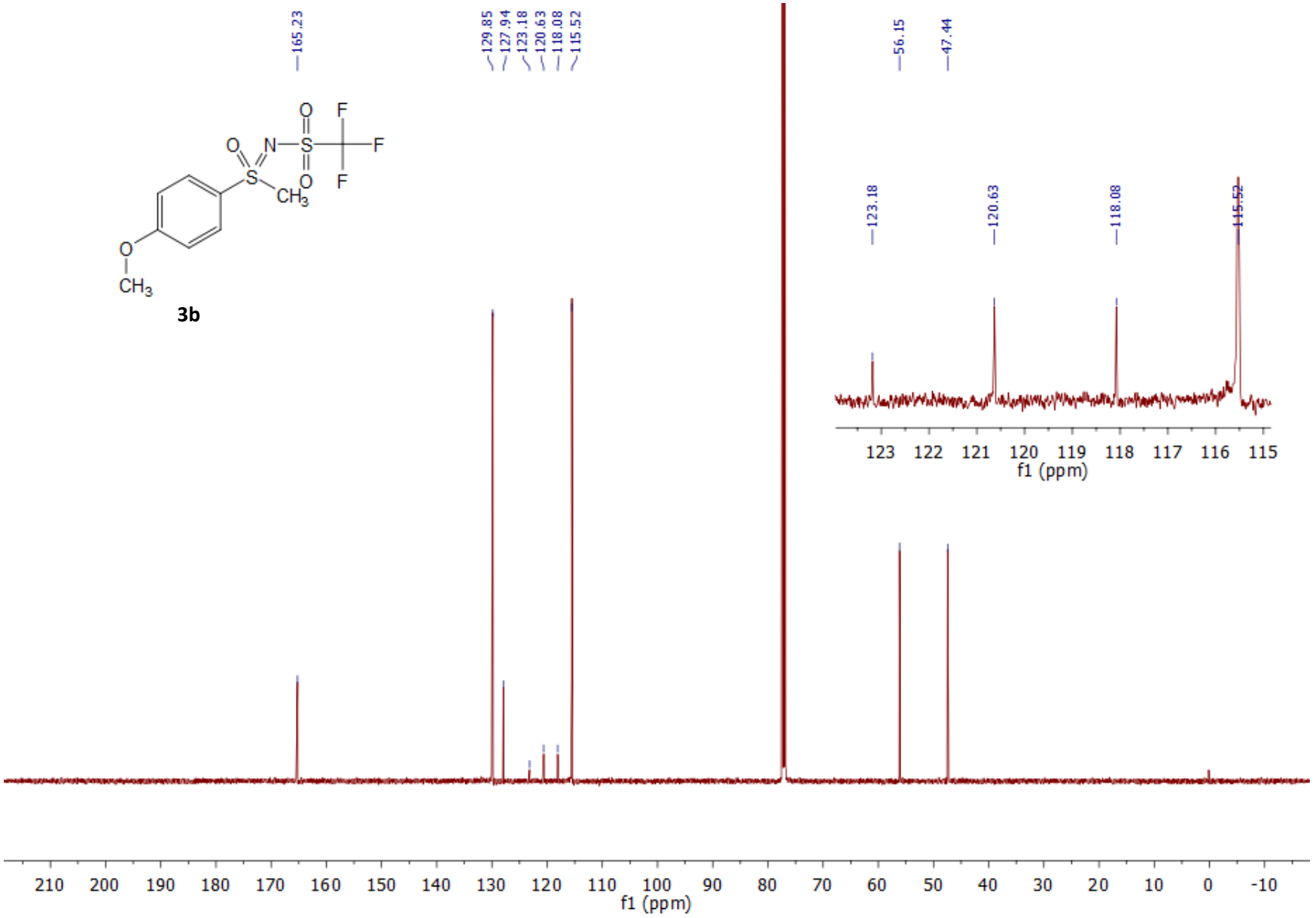
-200
-210
-22
f1 (ppm)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56.15
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N
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F
S
F
O
CH3
O
CH3
3b
123.18
120.63
118.08
115.52
123 122 121 120 119 118 117 116 115
f1 (ppm)
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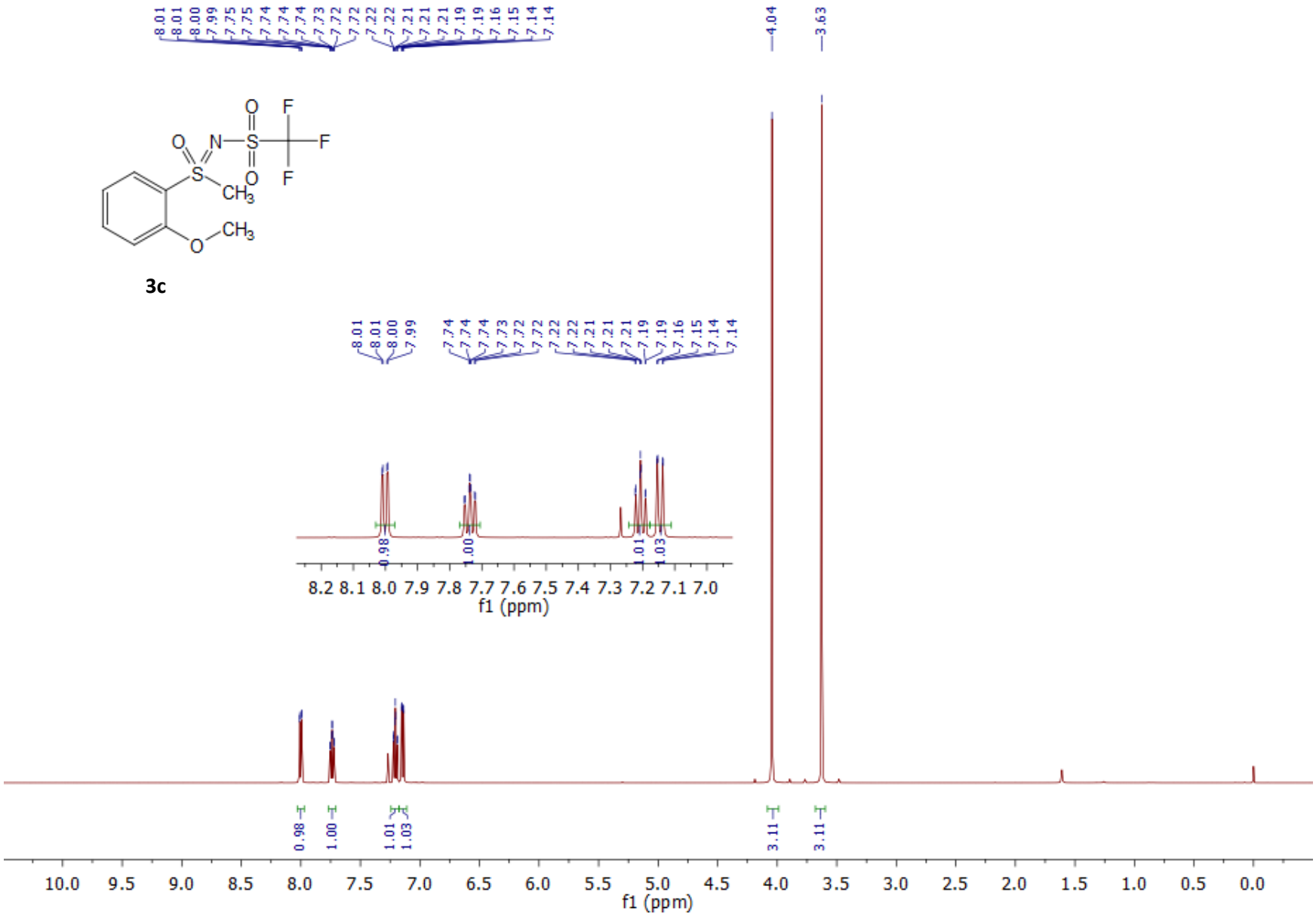
f1 (ppm)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7.21
7.19
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7.16
7.15
7.14
7.14
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1.01
1.03
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f1 (ppm)
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1.01
1.03
3.11
3.11
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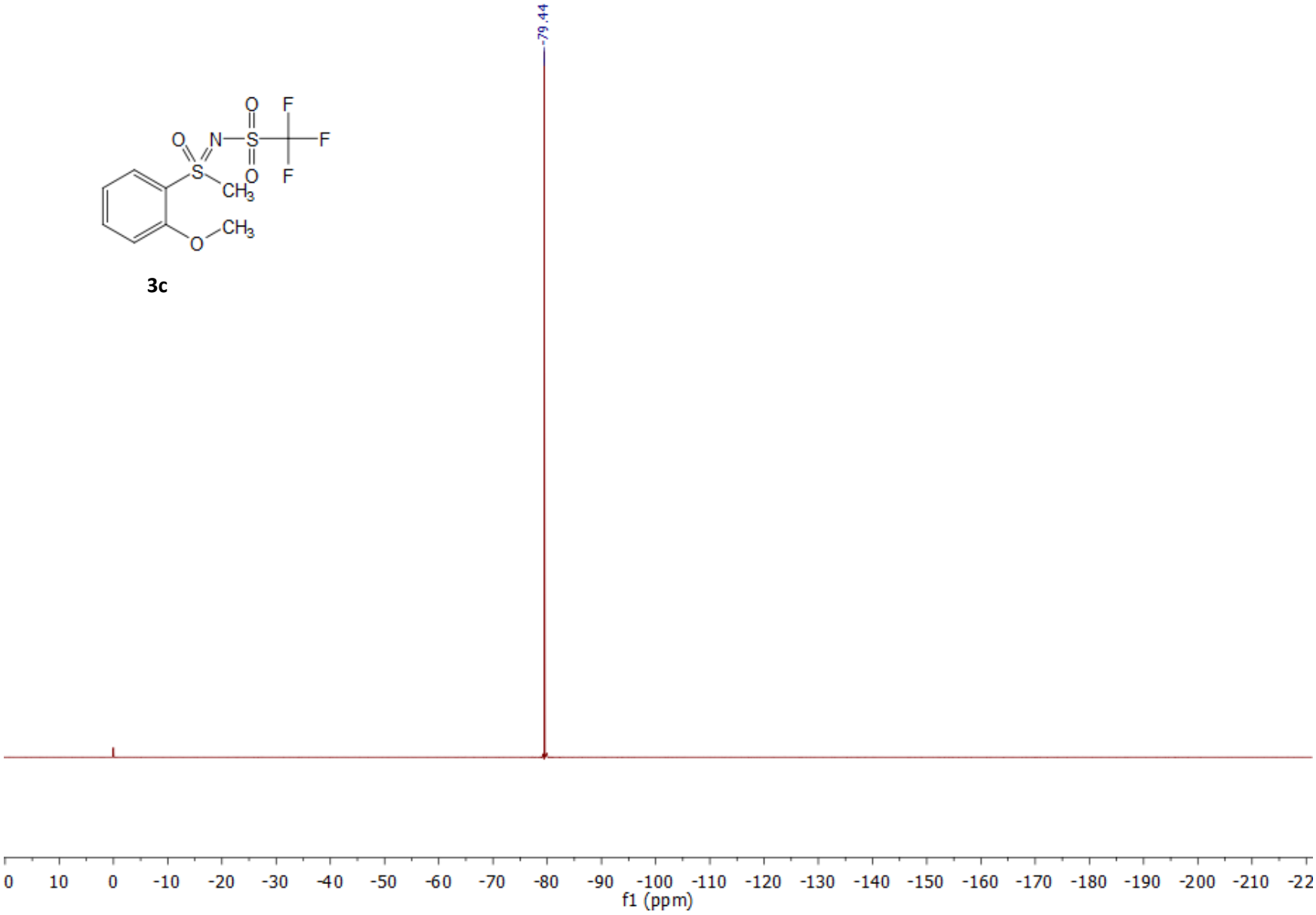
f1 (ppm)

3c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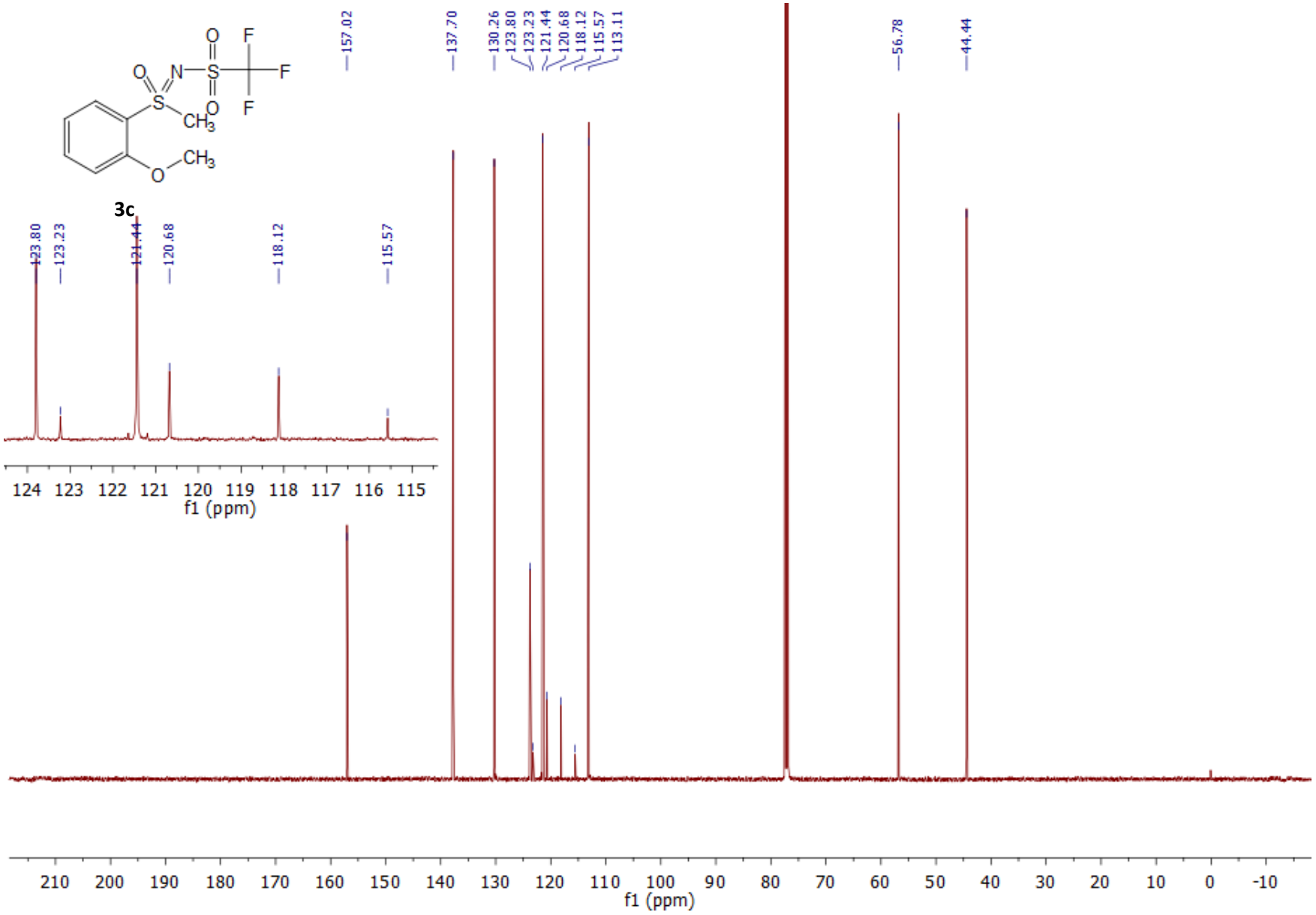
-210
-22
f1 (ppm)


3c
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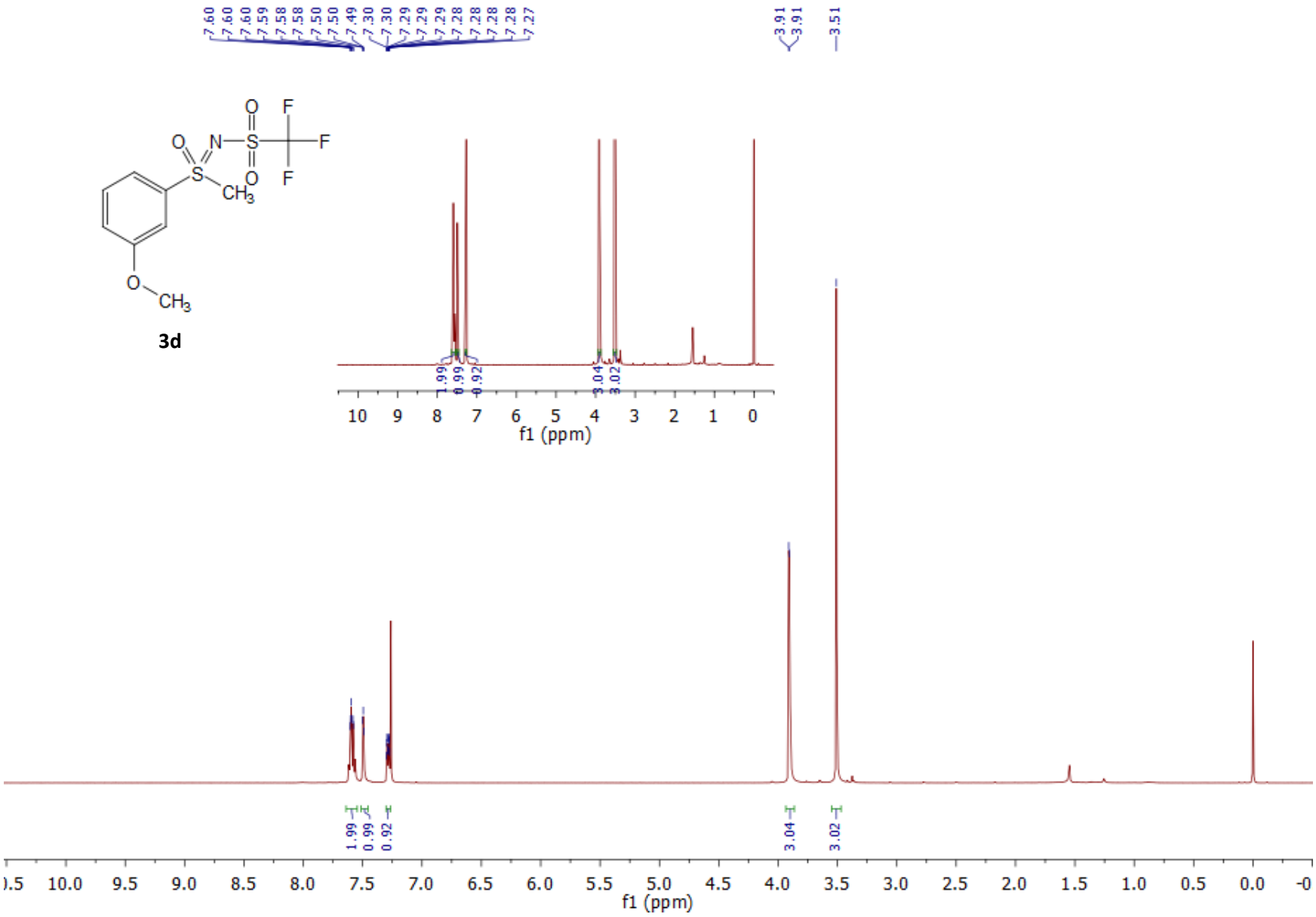
f1 (ppm)
f1 (ppm)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3.02
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0.99
0.92
3.04
3.02
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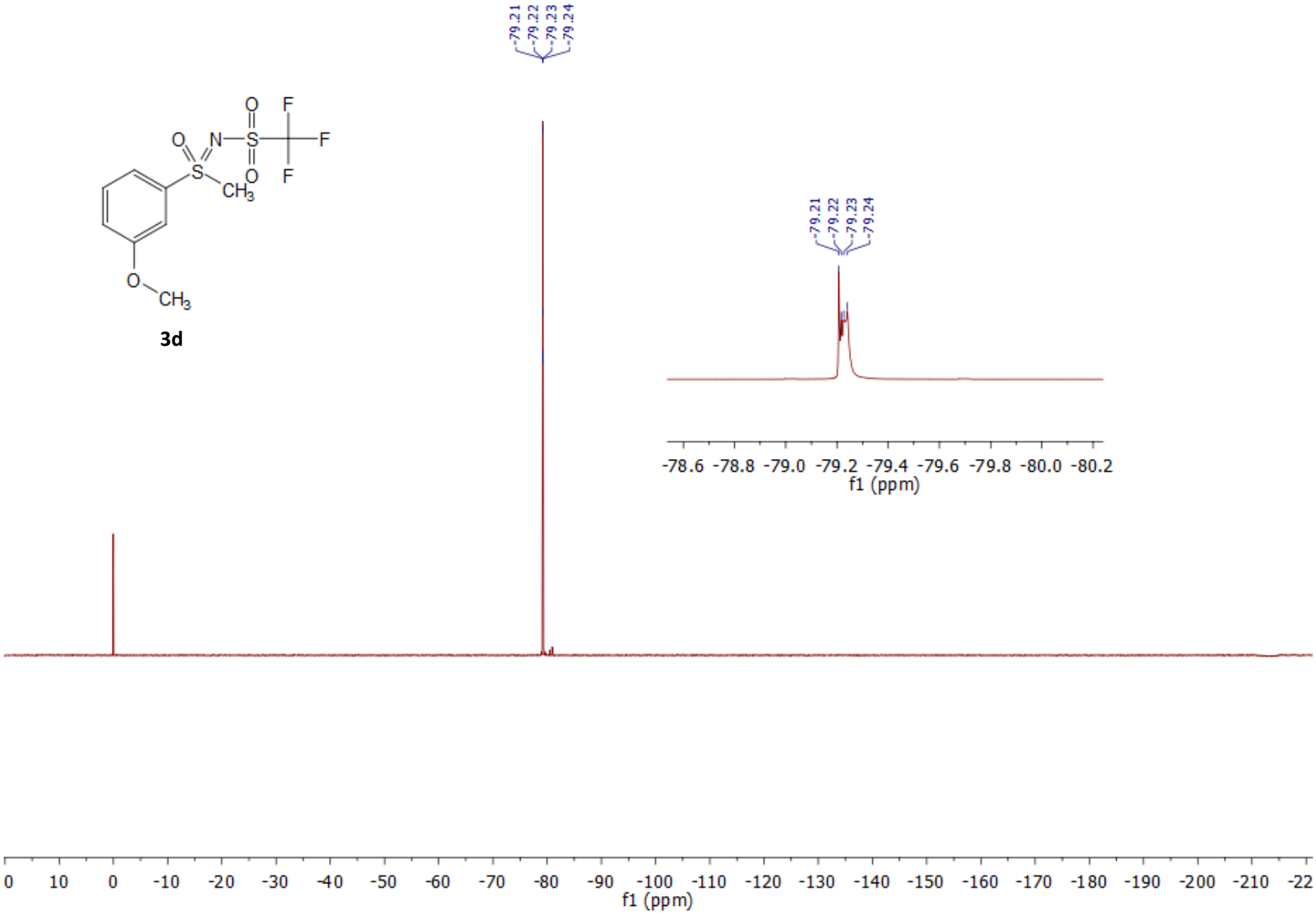
f1 (ppm)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-79.22
-79.23
-79.24
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f1 (ppm)
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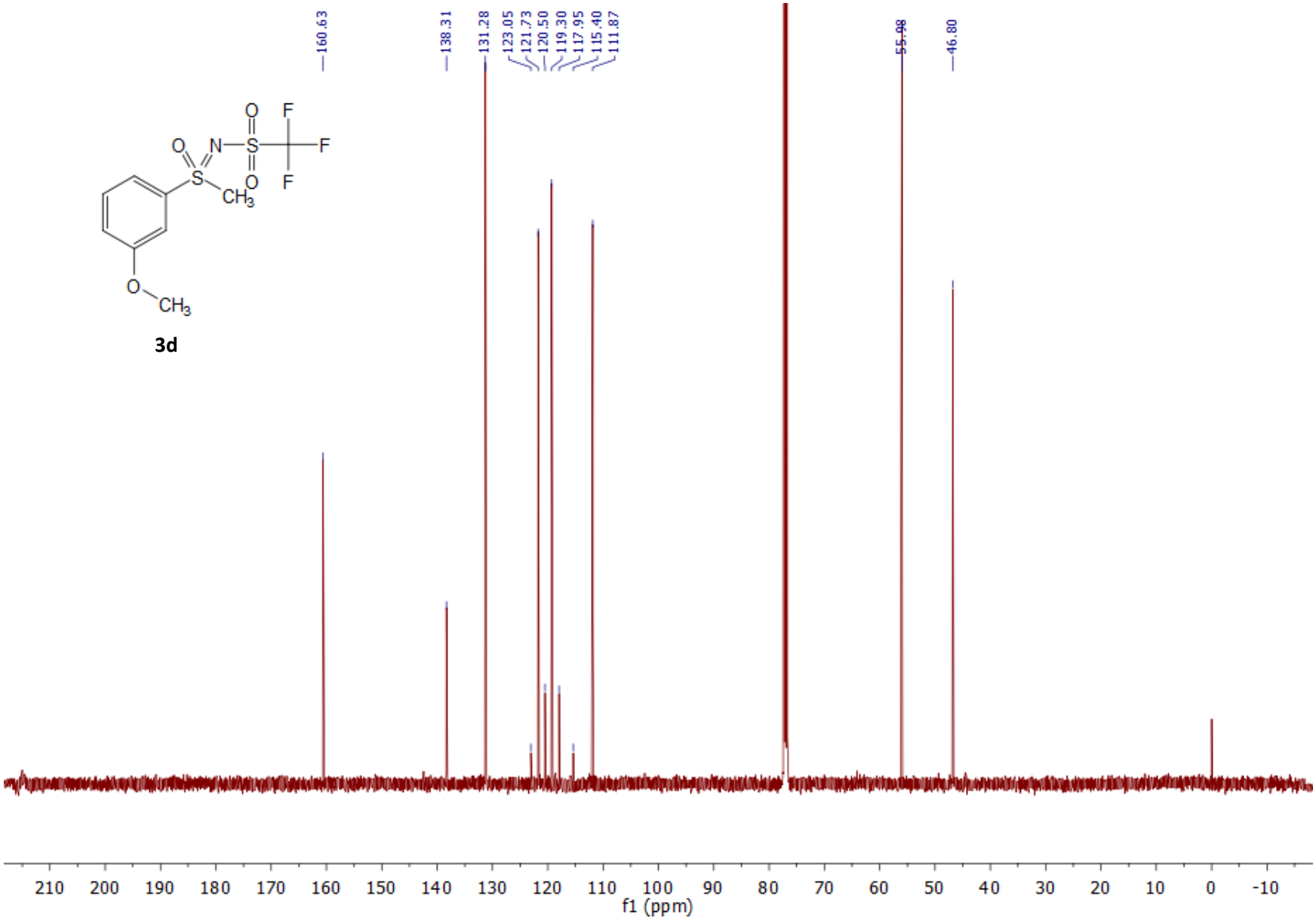
f1 (ppm)

3d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S
O
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O
CH3
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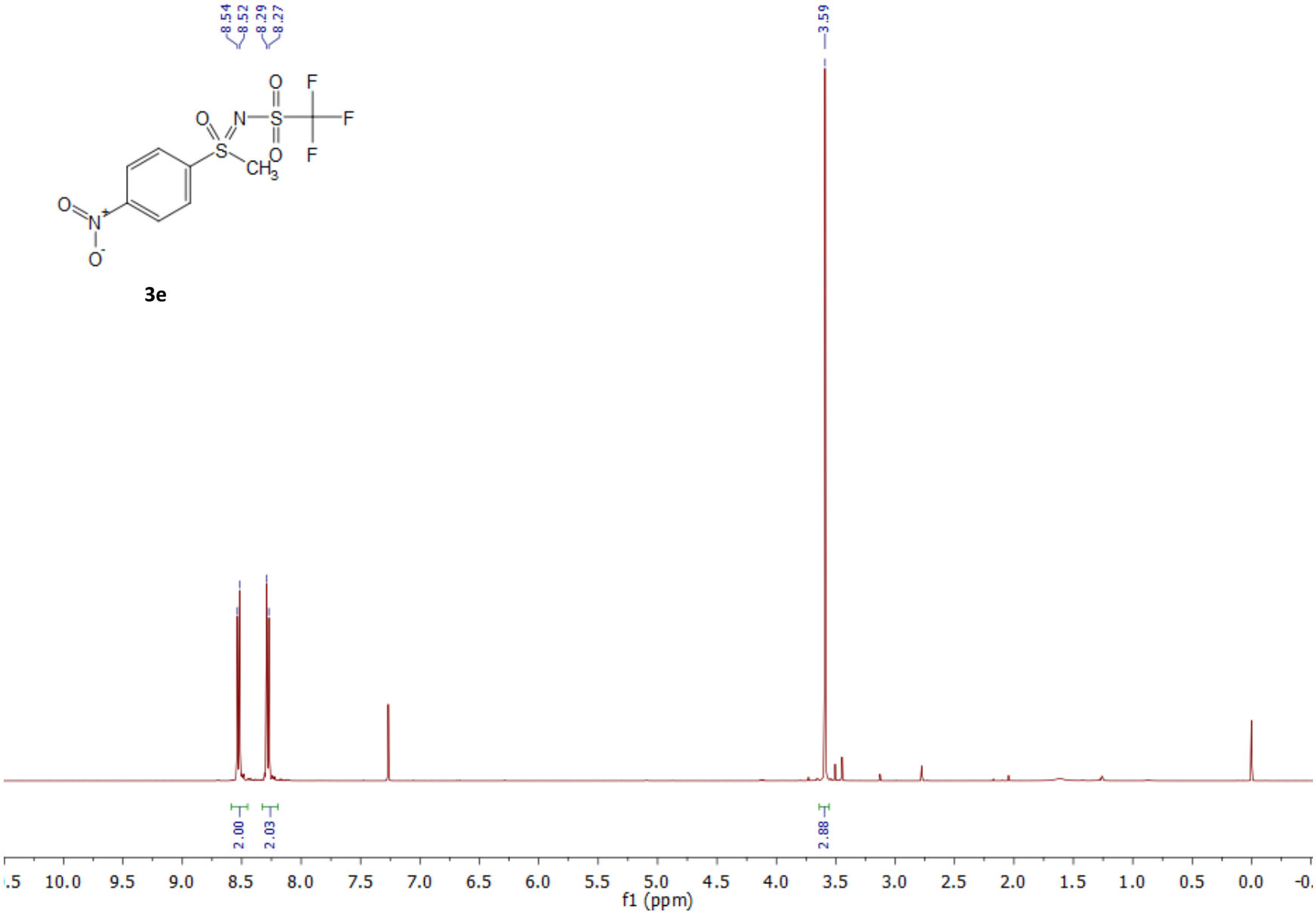
f1 (ppm)

3d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O
S
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N+
O-
2.00
2.03
2.88
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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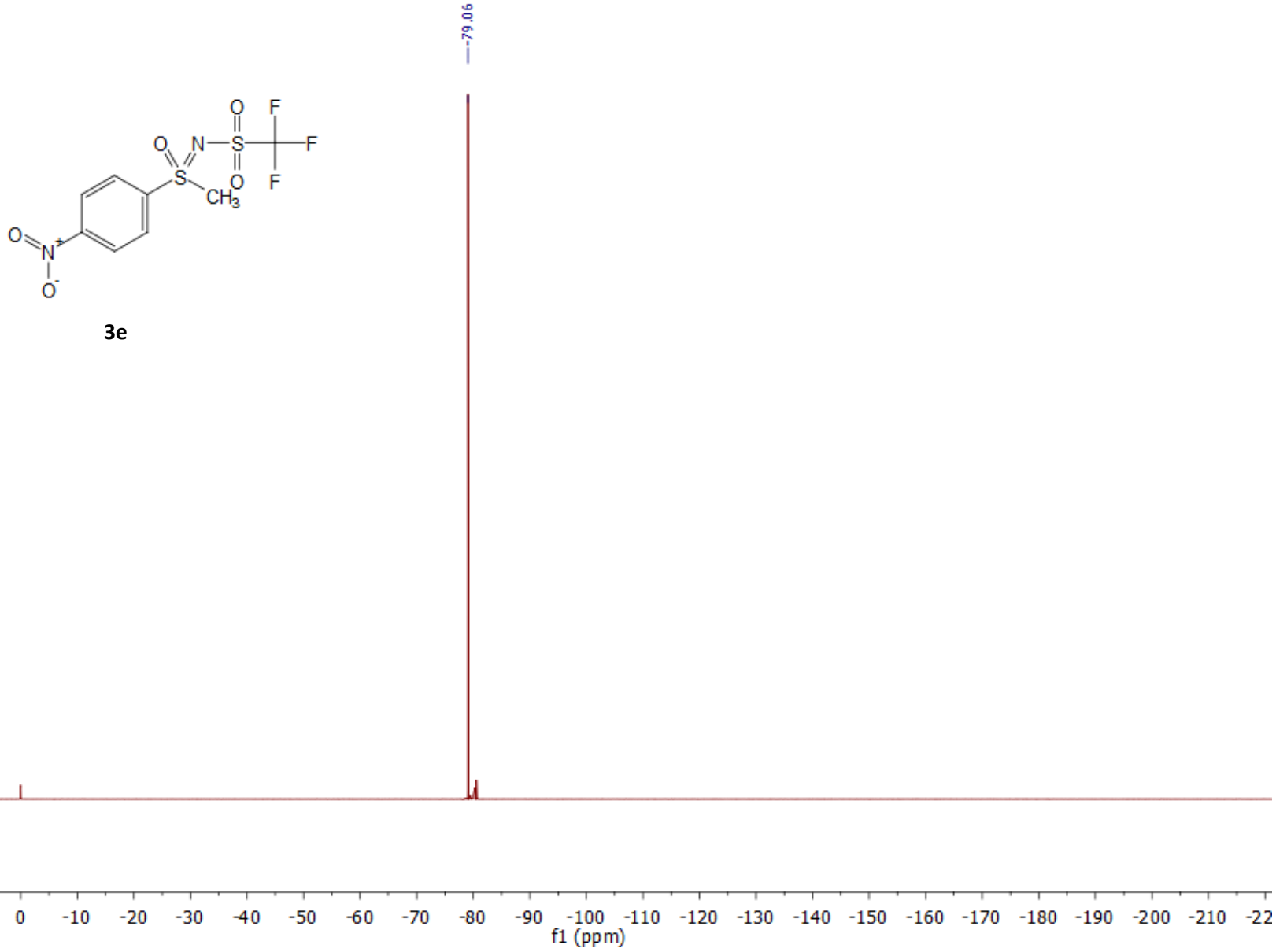
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3e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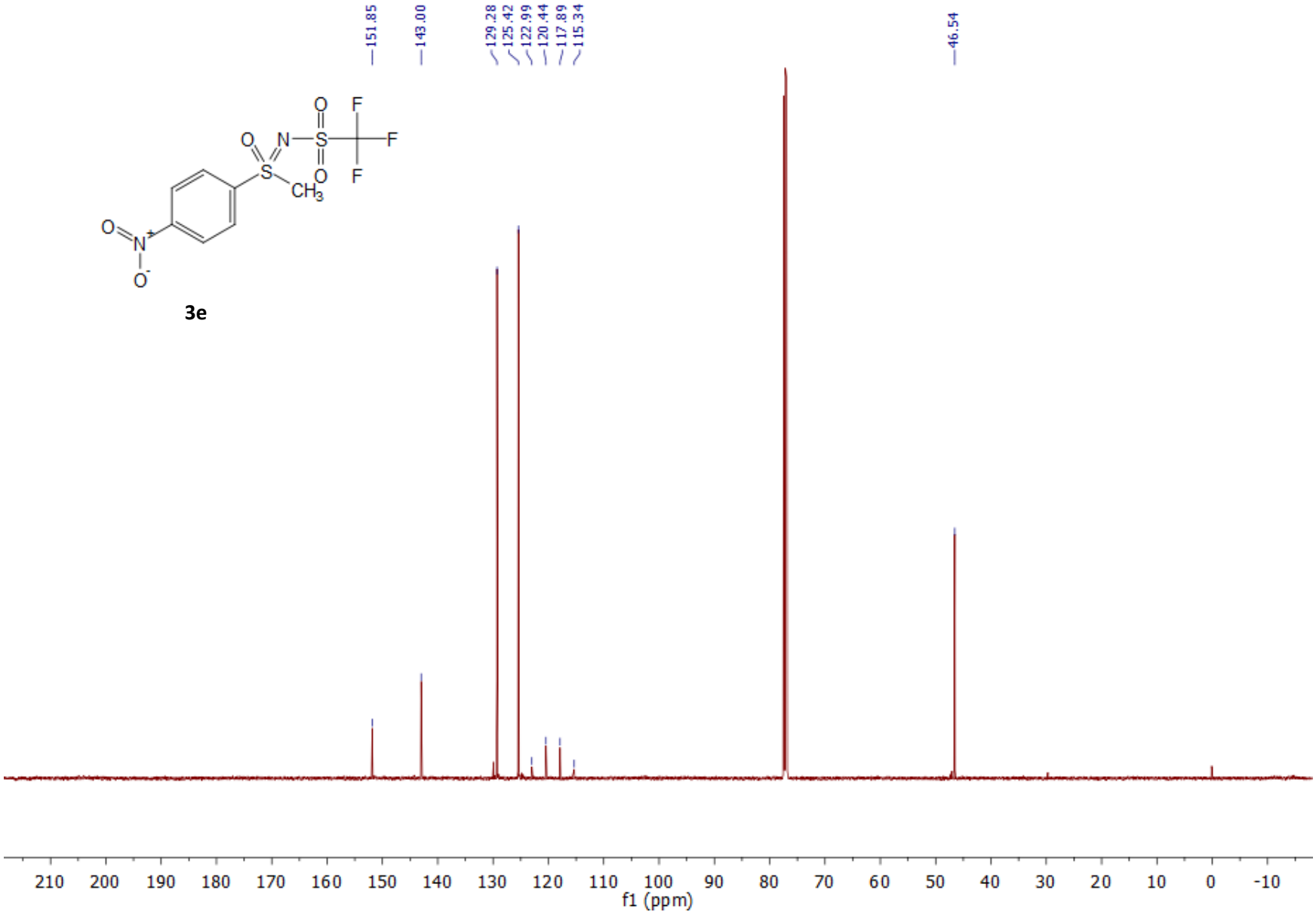
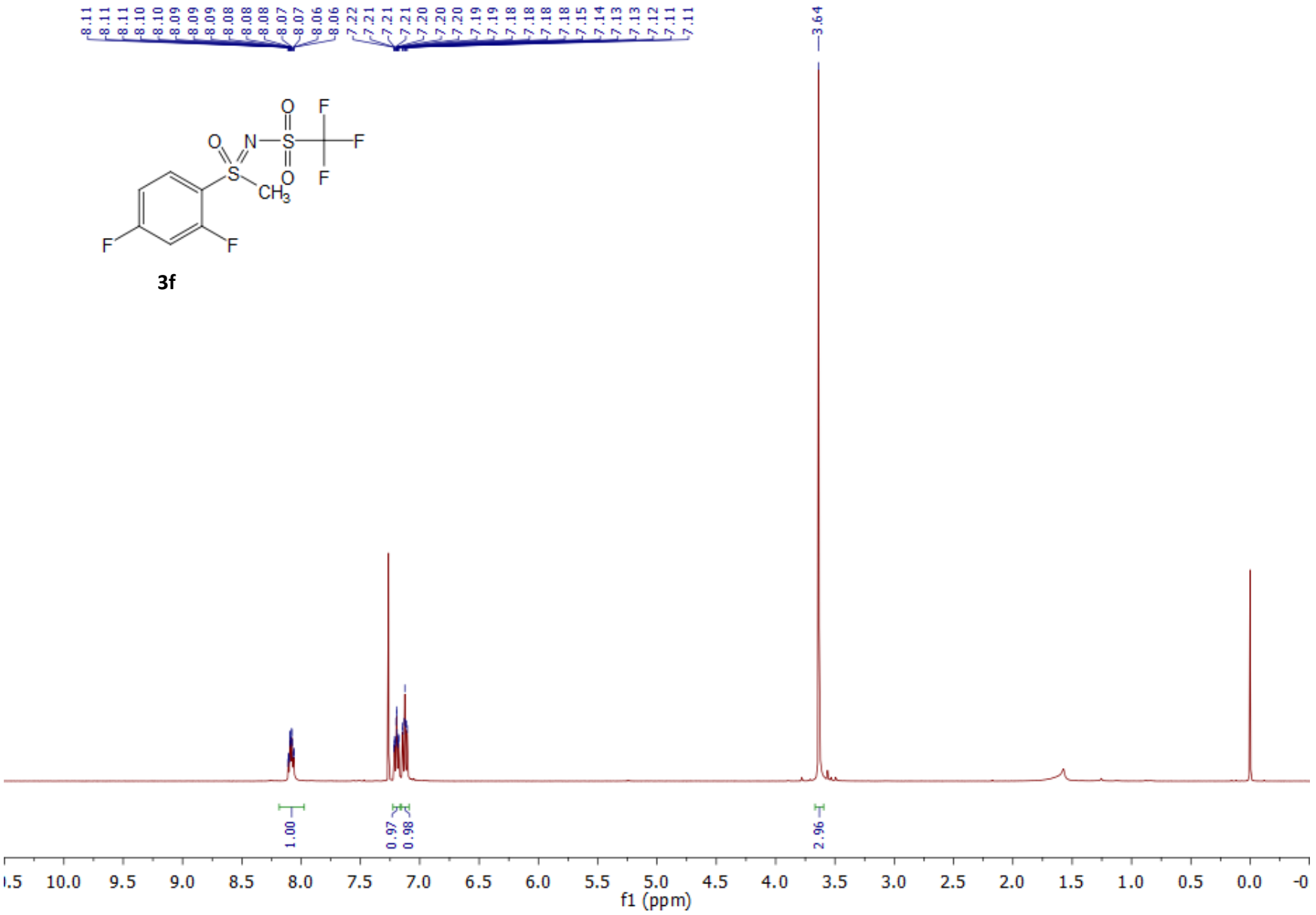
-210
-22
f1 (ppm)

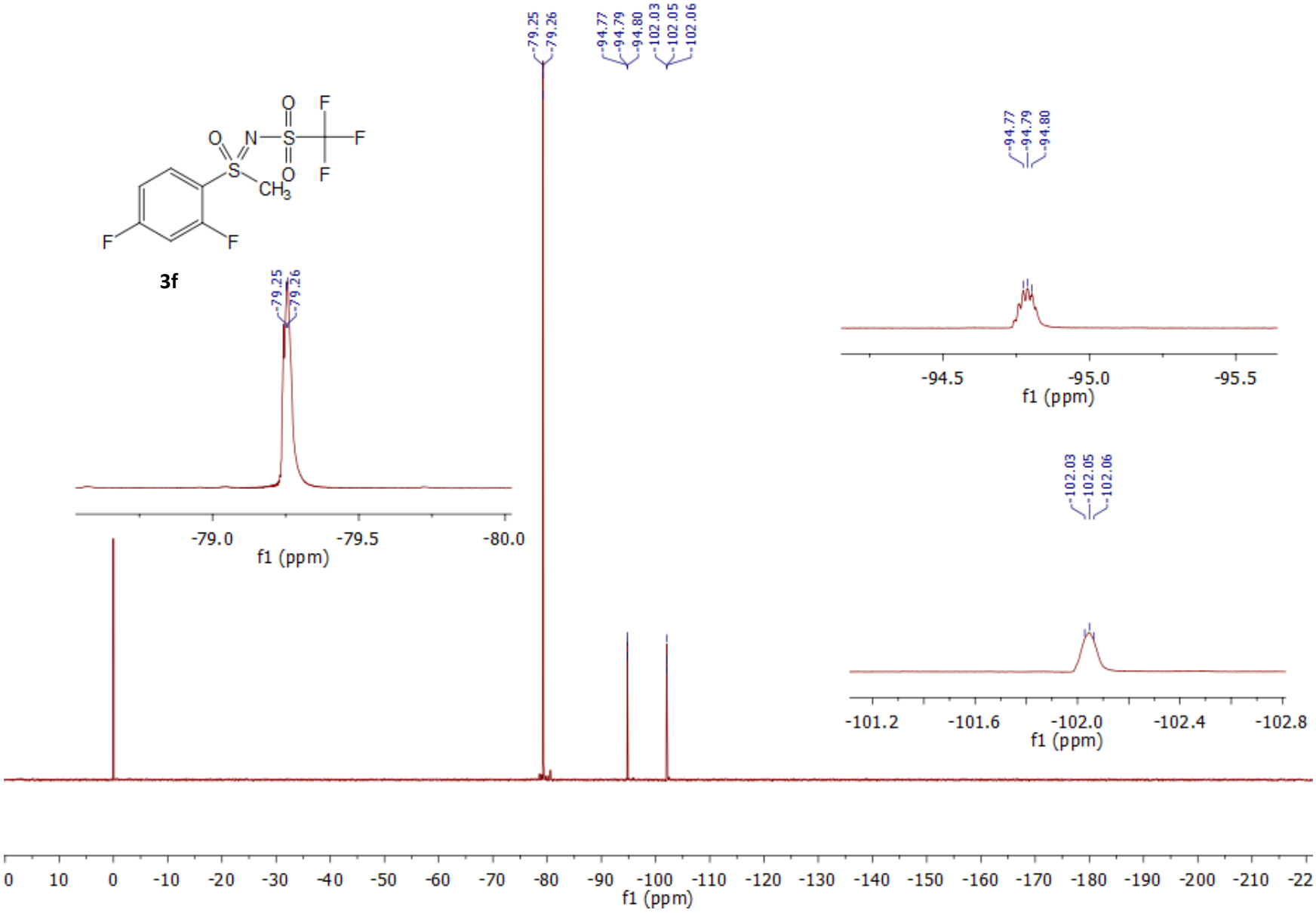
3e

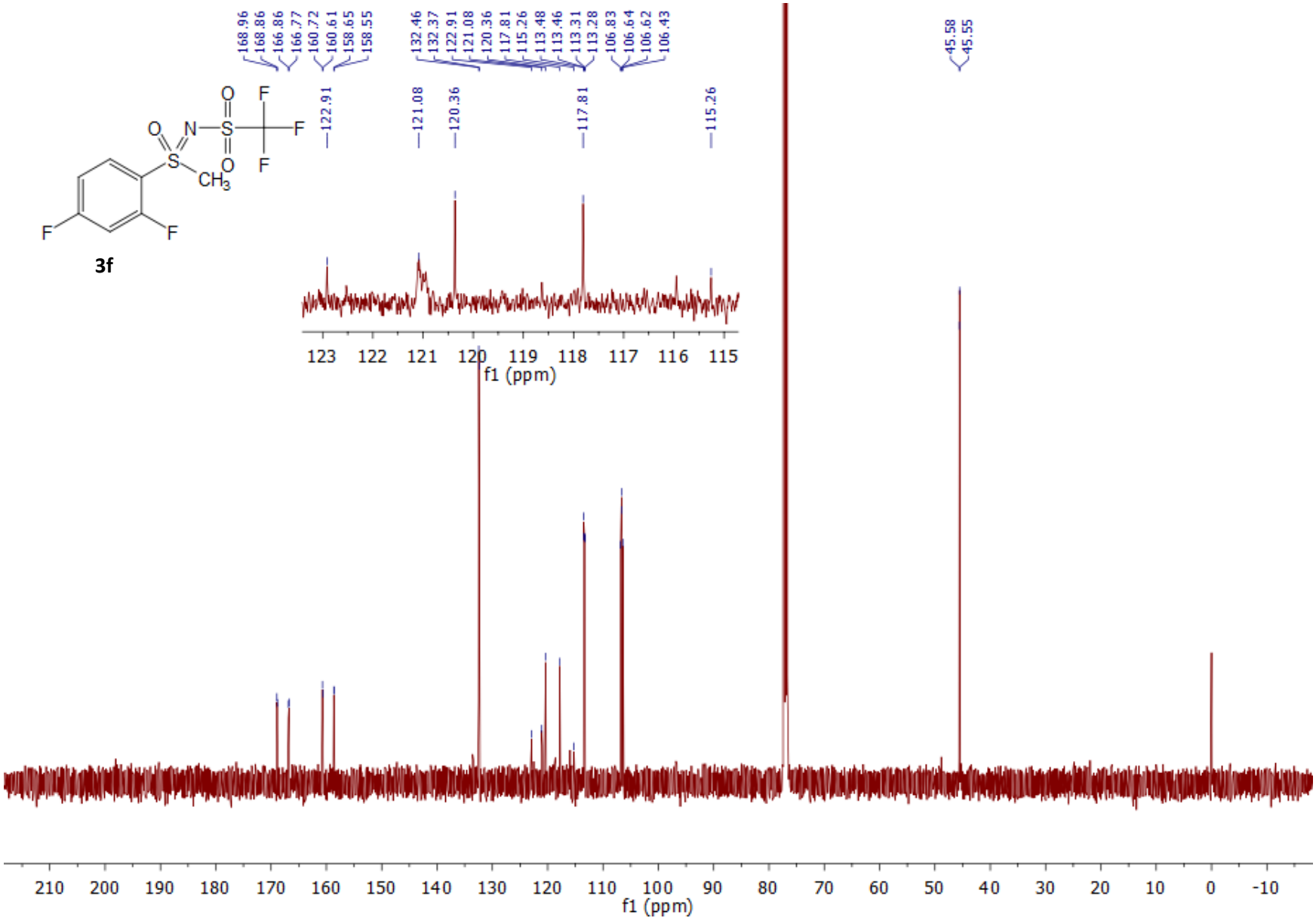

151.85
143.00
129.28
125.42
122.99
120.44
117.89
115.34
46.54
O
F
O
N
S
F
S
O
F
CH3
O
N+
O-
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

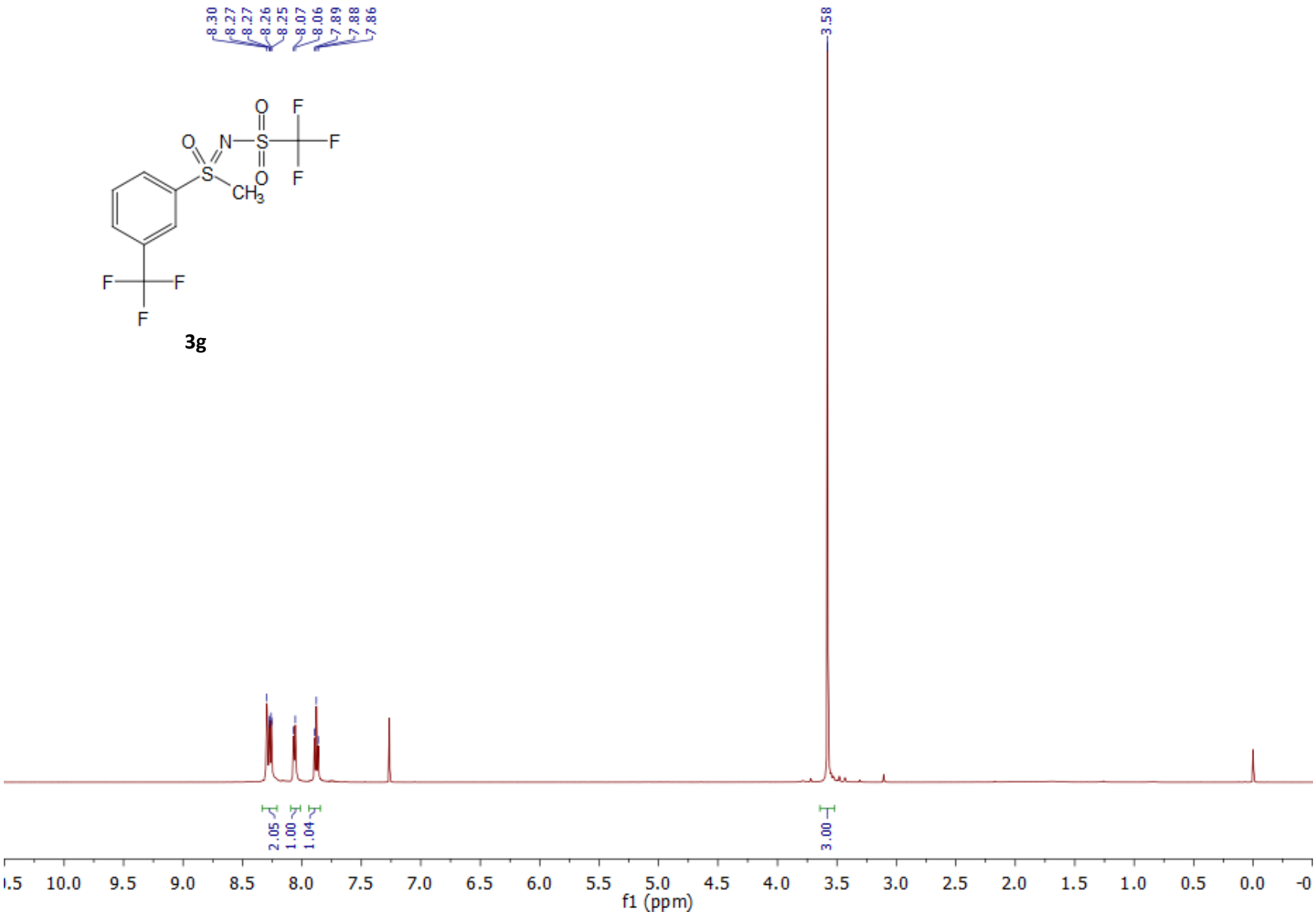
3e


8.11
8.11
8.11
8.10
8.09
8.09
8.09
8.08
8.08
8.08
8.07
8.07
8.06
8.06
7.22
7.21
7.21
7.21
7.20
7.20
7.20
7.19
7.19
7.18
7.18
7.18
7.18
7.15
7.14
7.13
7.13
7.12
7.11
7.11
3.64
O
F
O
N
S
F
S
F
O
CH3
F
F
1.00
0.97
0.98
2.96
f1 (ppm)

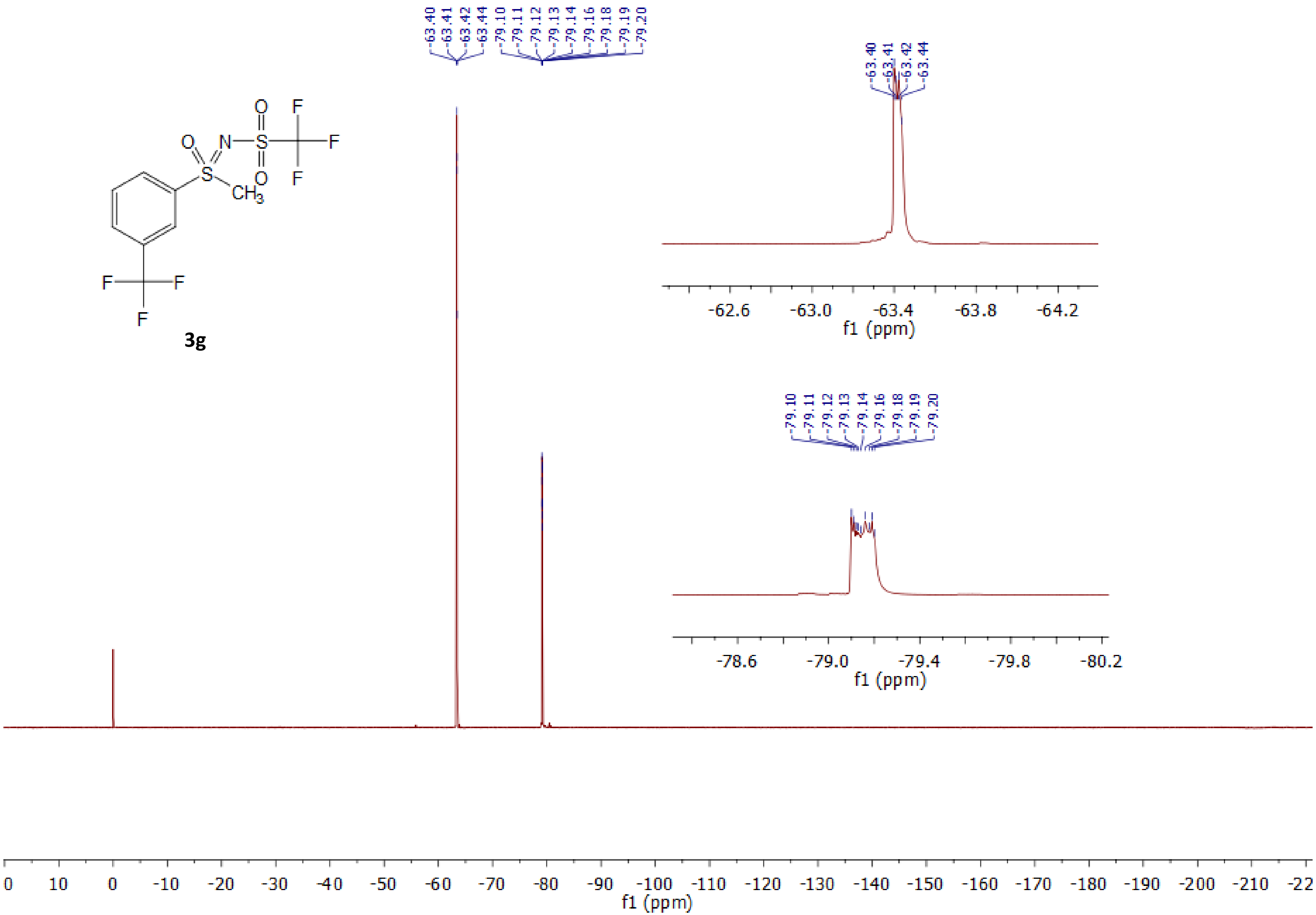
3f

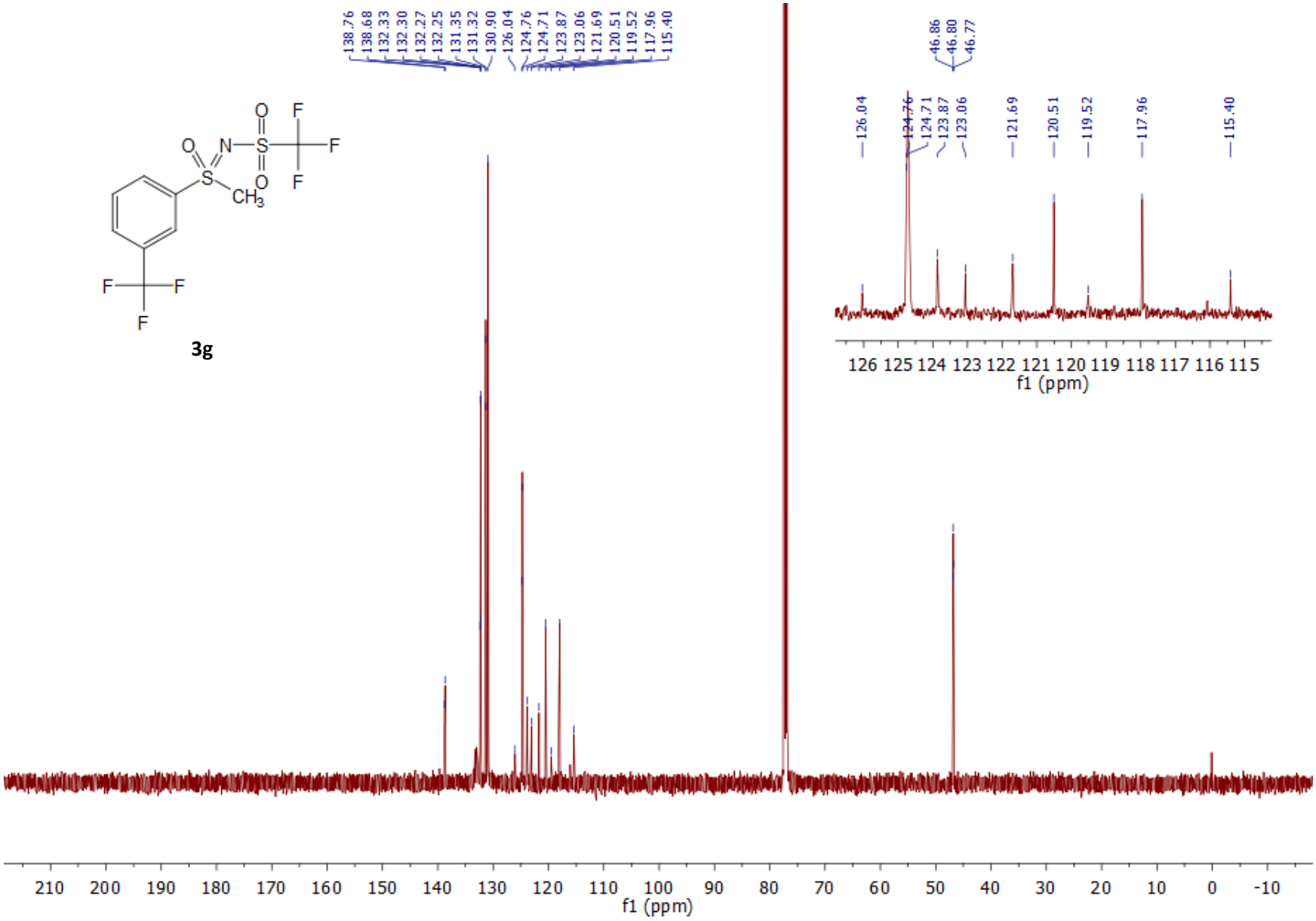

-79.25
-79.26
-94.77
-94.79
-94.80
-102.03
-102.05
-102.06
3f
f1 (ppm)
f1 (ppm)
f1 (ppm)
f1 (ppm)


168.96
168.86
166.86
166.77
160.72
160.61
158.65
158.55
132.46
132.37
122.91
121.08
120.36
117.81
115.26
113.48
113.46
113.31
113.28
106.83
106.64
106.62
106.43
45.58
45.55
O
N
S
F
CH3
3f
123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

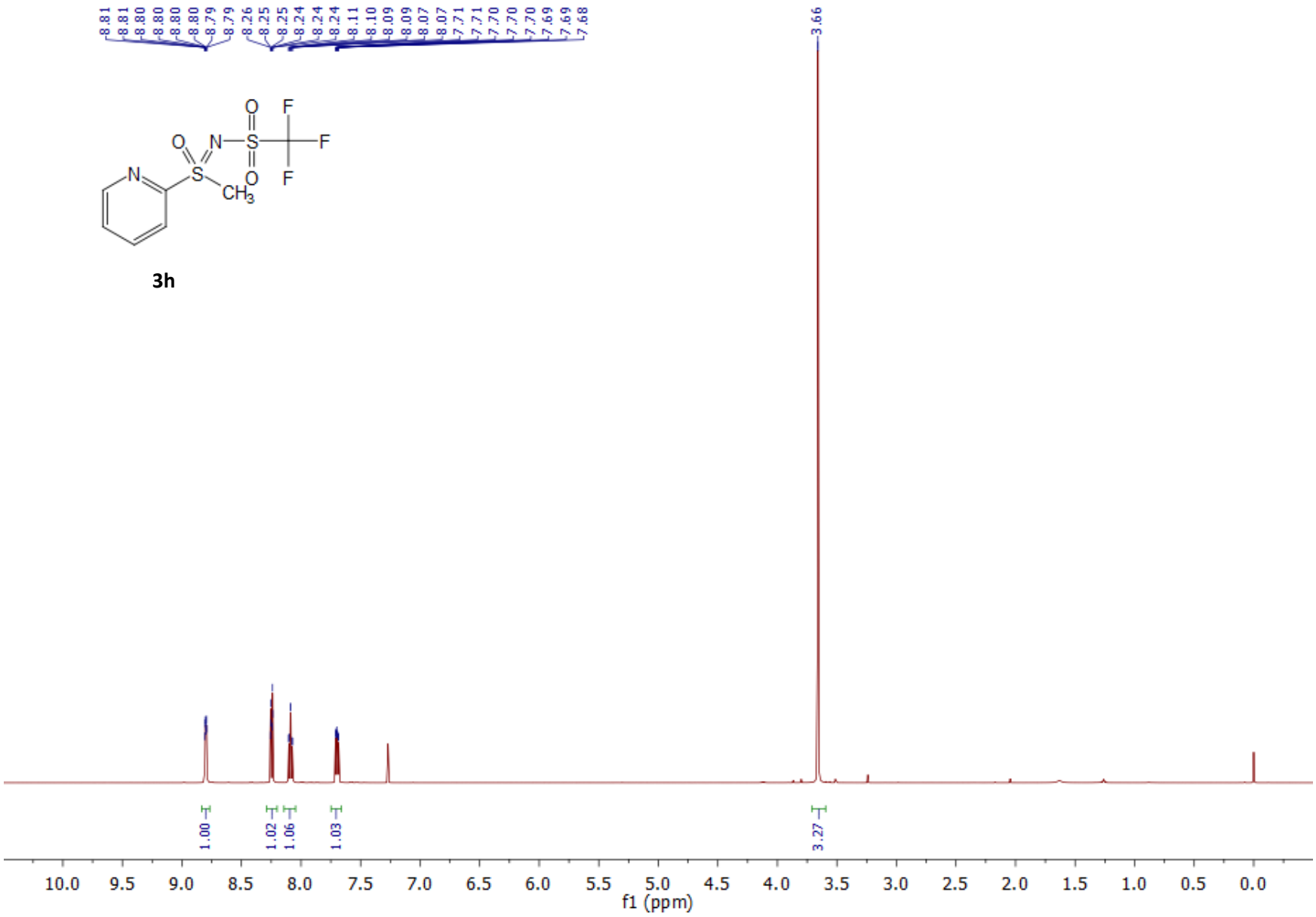

8.30
8.27
8.27
8.26
8.25
8.07
8.06
7.89
7.88
7.86
3.58
2.05
1.00
1.04
3.00
f1 (ppm)

3g


3g
-63.40
-63.41
-63.42
-63.44
-79.10
-79.11
-79.12
-79.13
-79.14
-79.16
-79.18
-79.19
-79.20
f1 (ppm)


138.76
138.68
132.33
132.30
132.27
132.25
131.35
131.32
130.90
126.04
124.76
124.71
123.87
123.06
121.69
120.51
119.52
117.96
115.40
46.86
46.80
46.77
126.04
124.76
124.71
123.87
123.06
121.69
120.51
119.52
117.96
115.40
126 125 124 123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

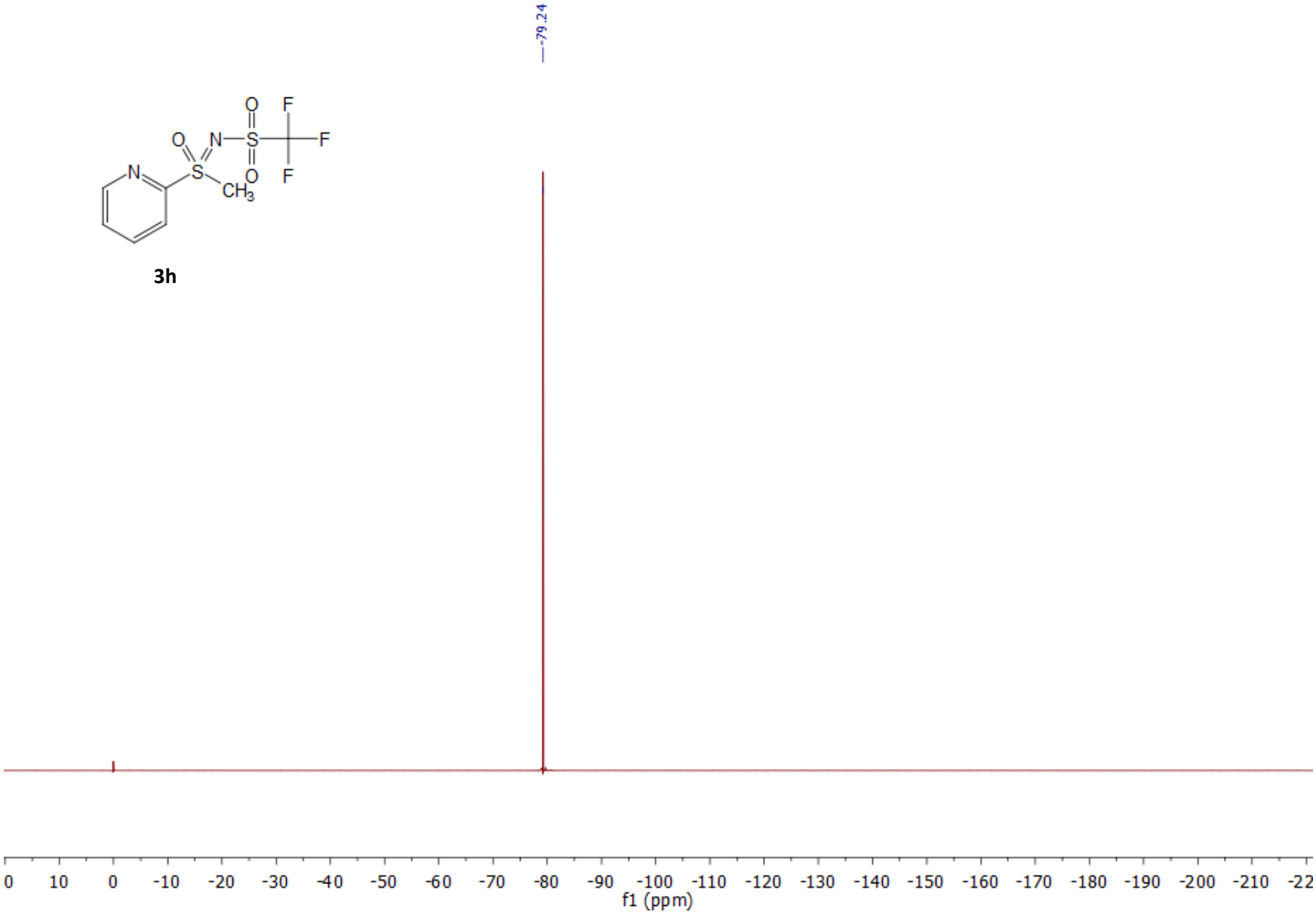
3g

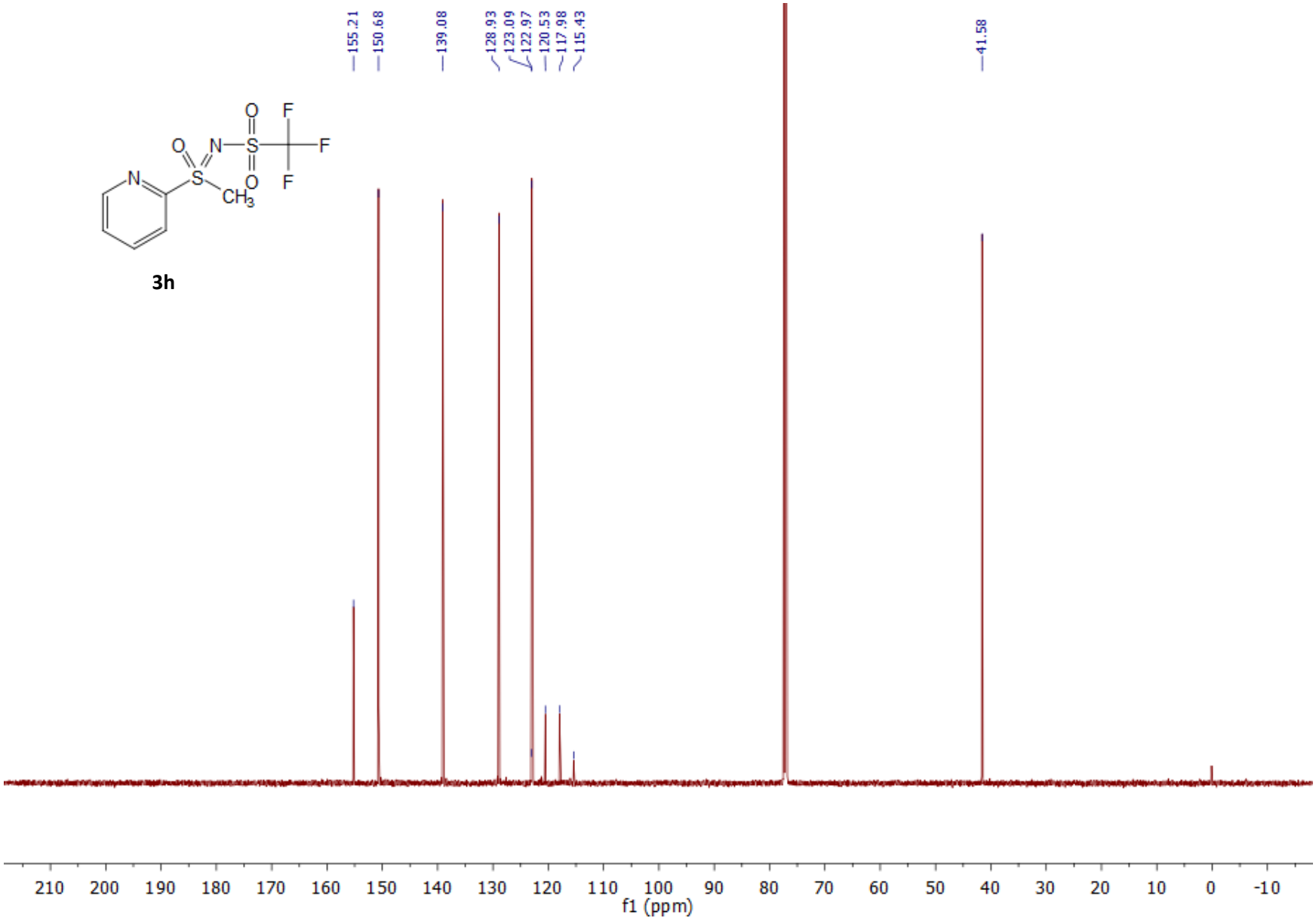

8.81
8.81
8.80
8.80
8.80
8.79
8.79
8.26
8.25
8.25
8.24
8.24
8.24
8.11
8.10
8.09
8.09
8.07
8.07
7.71
7.71
7.70
7.70
7.70
7.69
7.69
7.68
3.66
O
F
O
N
S
F
N
S
F
O
CH3
1.00
1.02
1.06
1.03
3.27
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3h

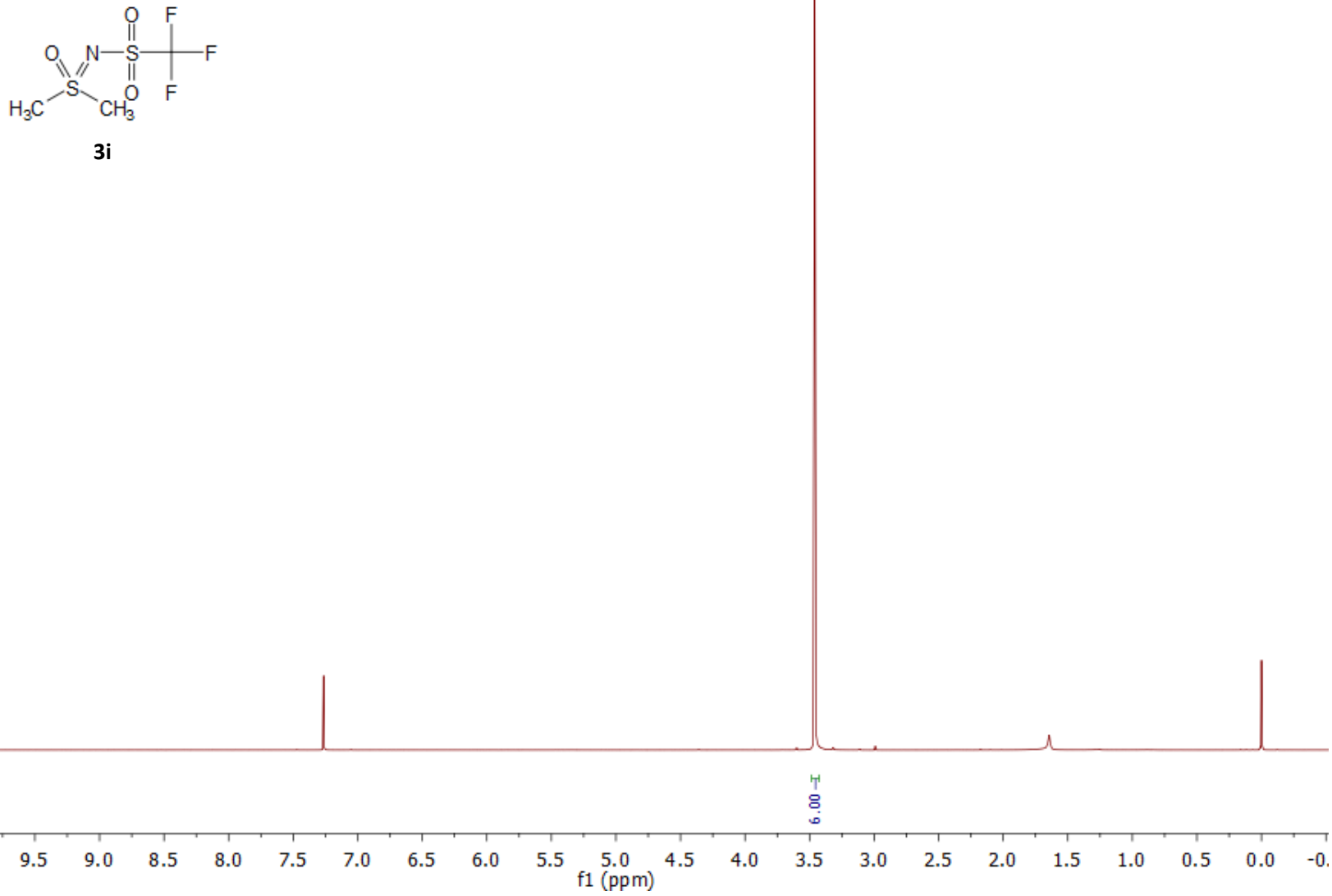
O
F
O
N
S
F
N
S
F
CH3

3h


-79.24
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


155.21
150.68
139.08
128.93
123.09
122.97
120.53
117.98
115.43
41.58
O
F
O
N
S
F
N
S
F
O
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

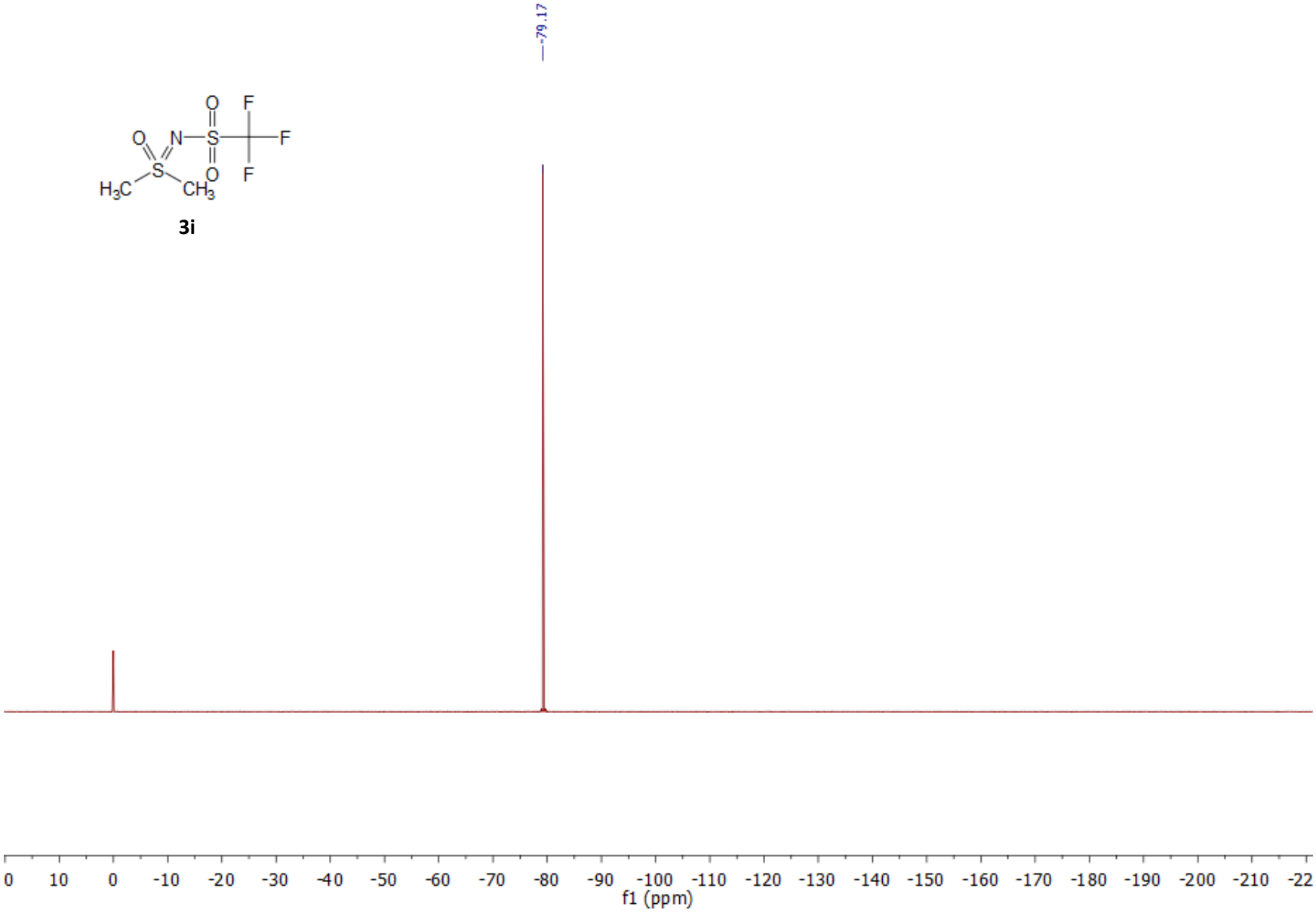
3h

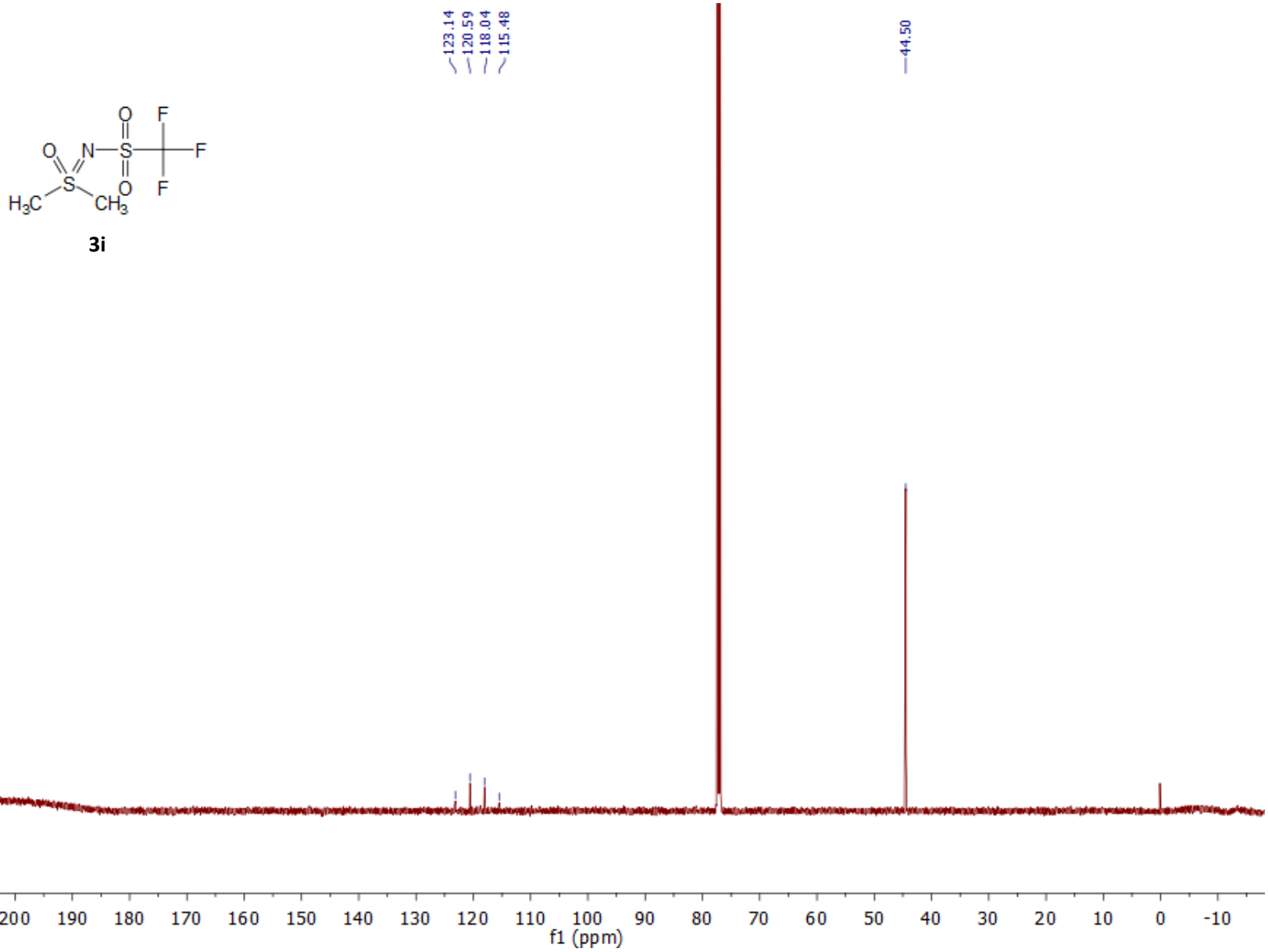

3.46
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3i

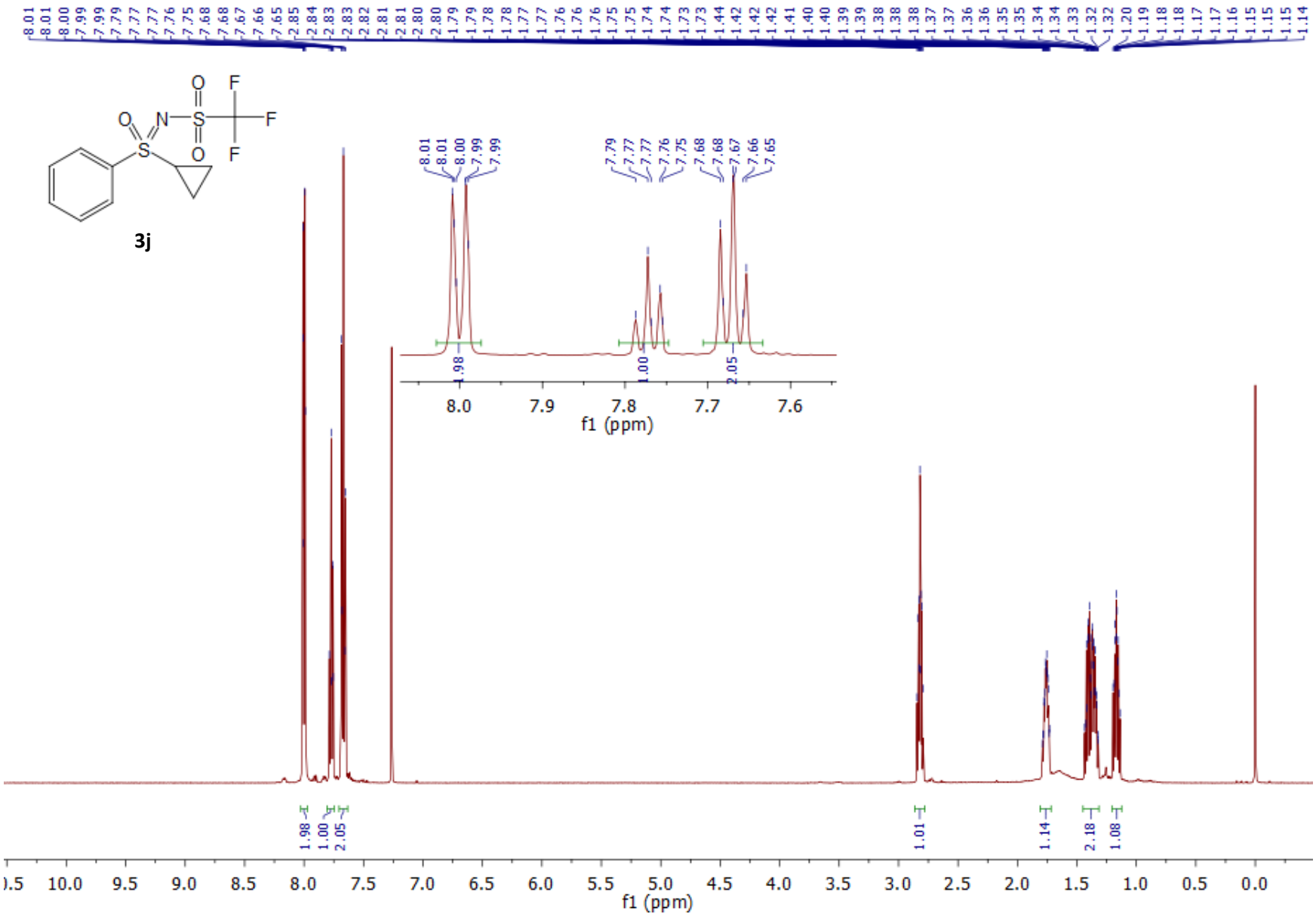
O
F
O
N
S
F
S
O
F
H3C
CH3

3i


-79.17
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

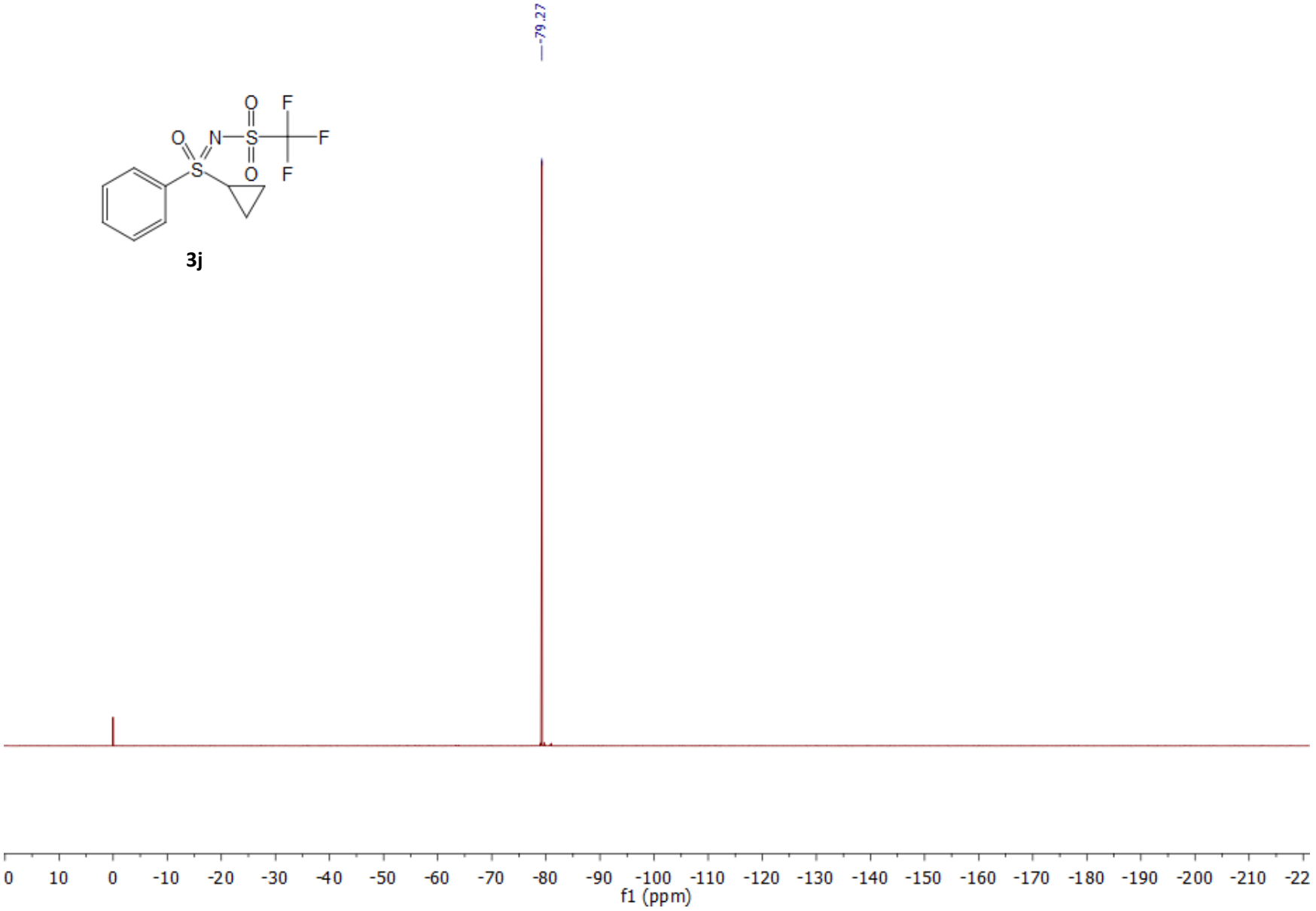

123.14
120.59
118.04
115.48
44.50
O
F
O
N
S
F
O
S
F
H3C
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

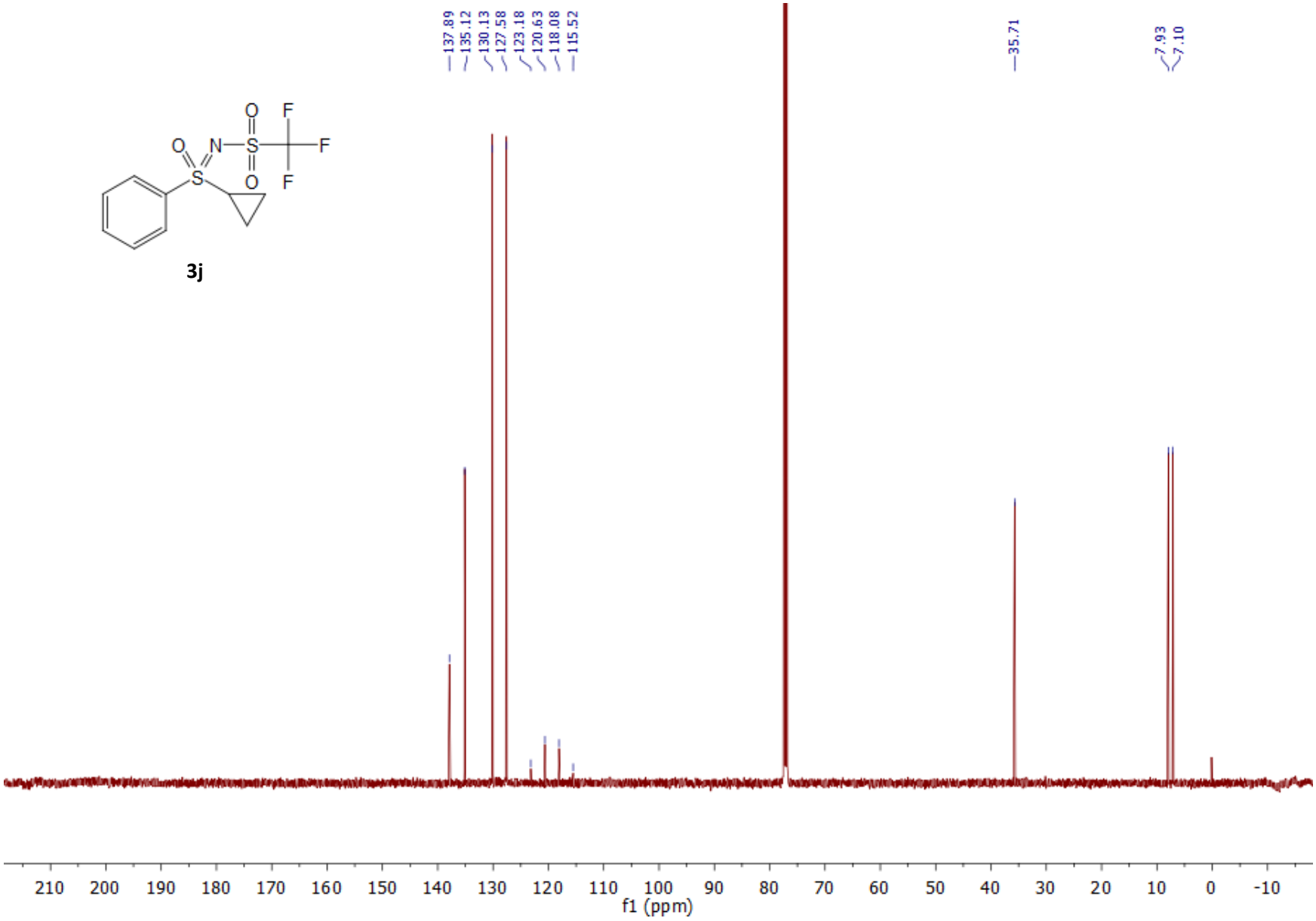
3i


3j
f1 (ppm)

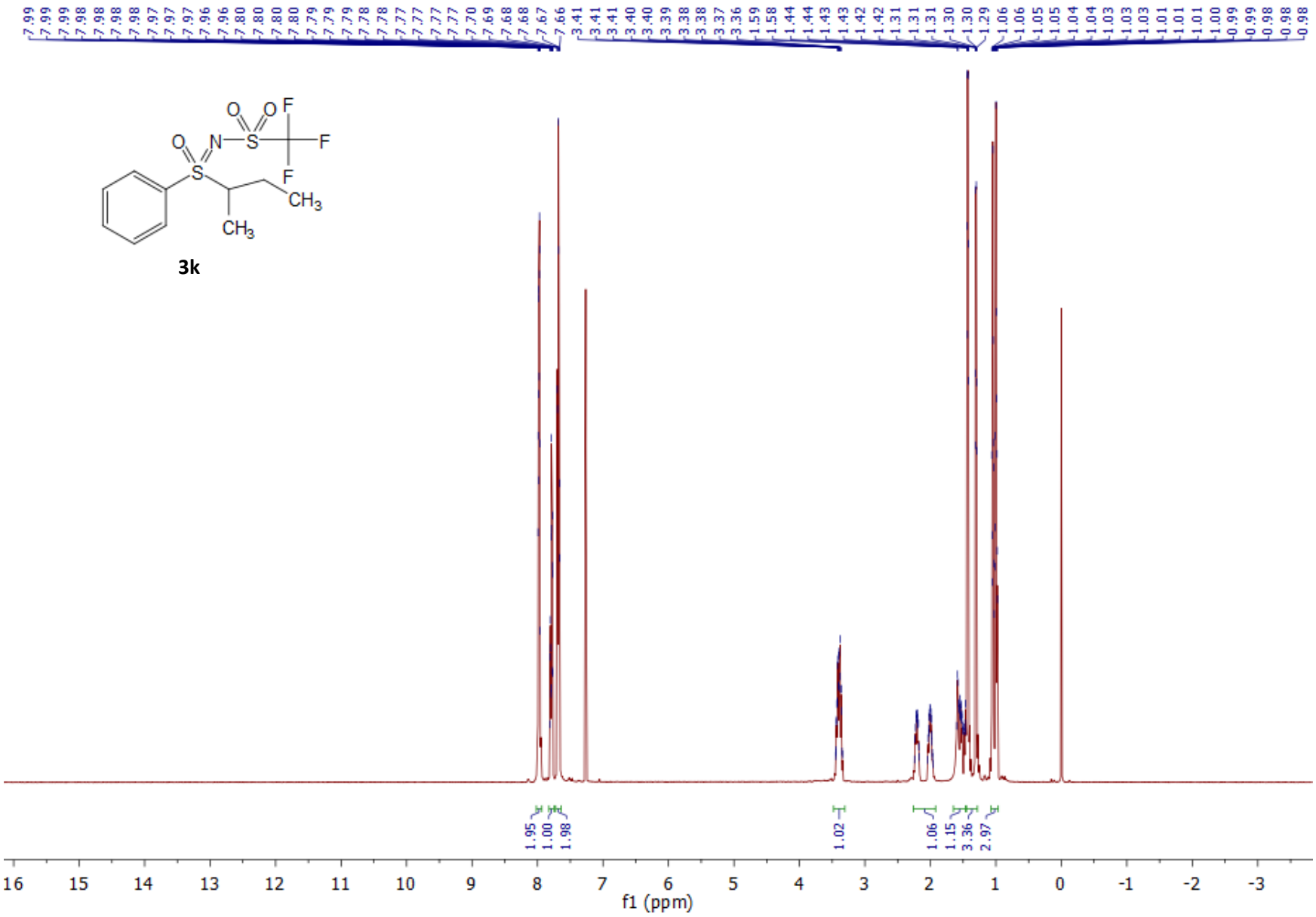
O
F
O
N
S
F
S
O
F

3j


-79.27
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

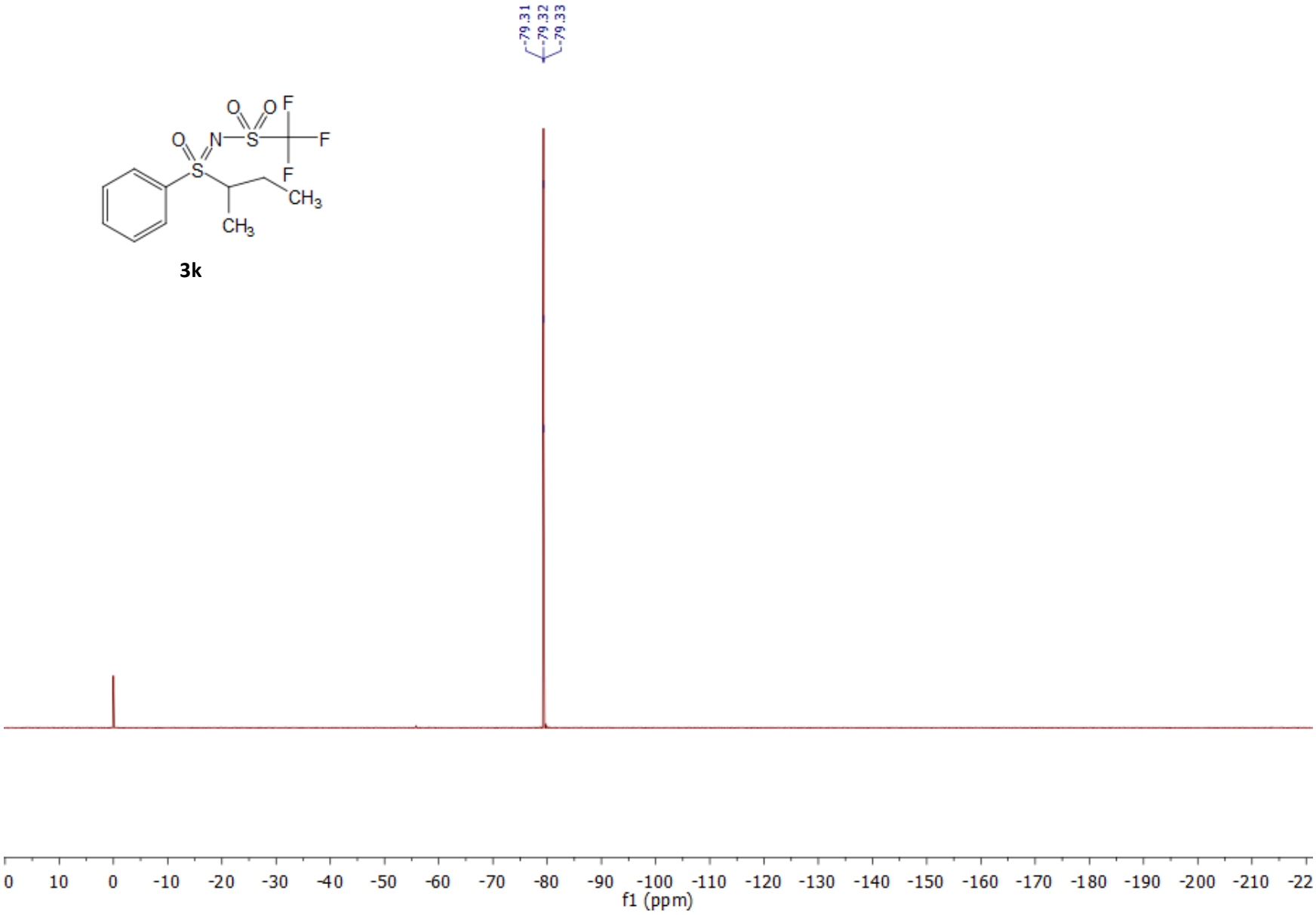

137.89
135.12
130.13
127.58
123.18
120.63
118.08
115.52
35.71
7.93
7.10
O
N
S
O
F
F
F
O
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

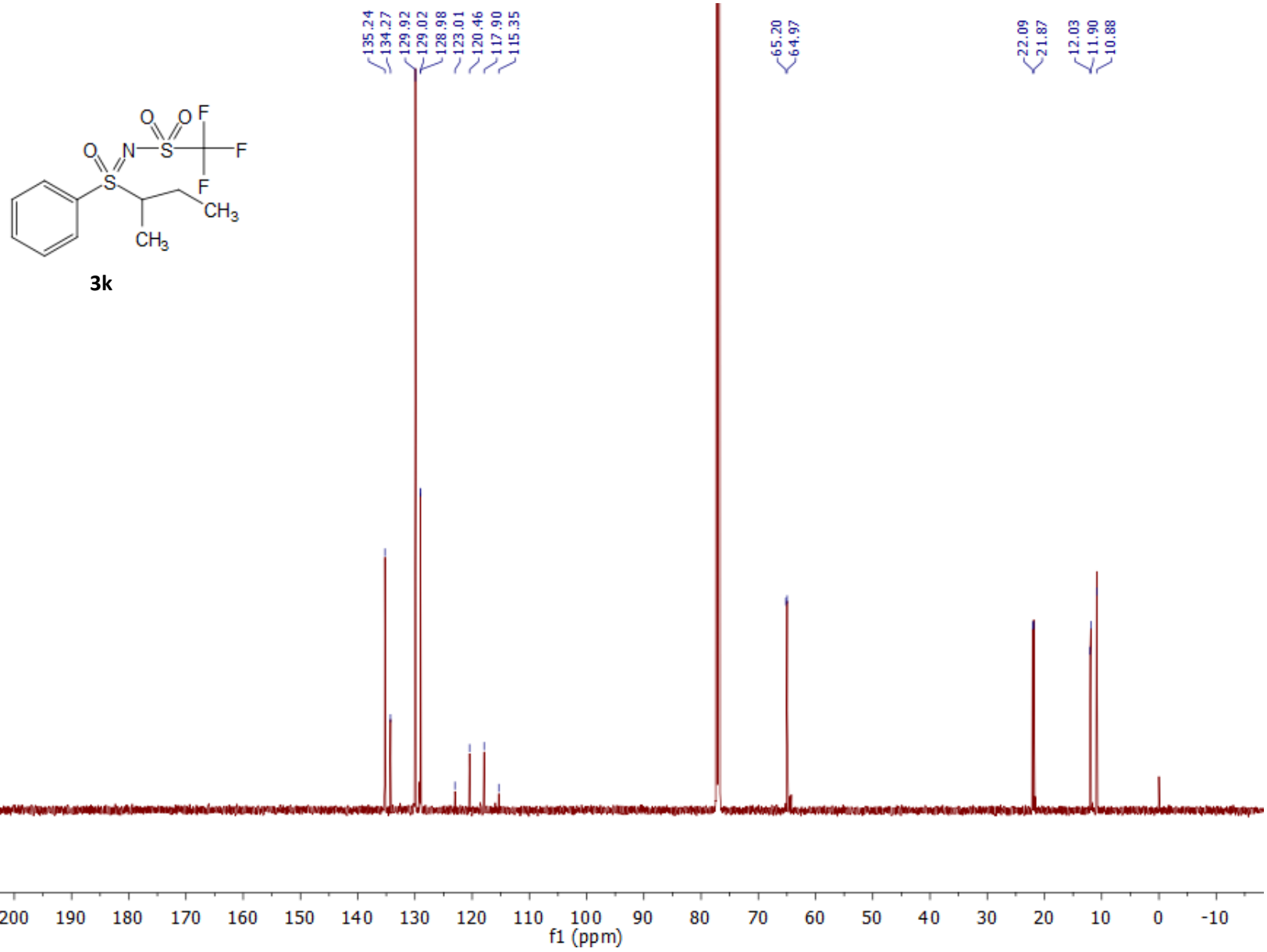
3j


7.99 7.99 7.99 7.98 7.98 7.98 7.98 7.97 7.97 7.97 7.96 7.96 7.80 7.80 7.80 7.80 7.79 7.79 7.79 7.78 7.78 7.77 7.77 7.77 7.77 7.70 7.69 7.68 7.68 7.67 7.66 3.41 3.41 3.41 3.40 3.40 3.39 3.38 3.38 3.37 3.36 1.59 1.58 1.44 1.44 1.43 1.43 1.42 1.42 1.31 1.31 1.31 1.30 1.30 1.29 1.06 1.06 1.05 1.05 1.04 1.04 1.03 1.03 1.03 1.01 1.01 1.01 1.00 0.99 0.99 0.98 0.98 0.98
O O F
O N S F
S F
CH3
CH3
3k
1.95 1.00 1.98 1.02 1.06 1.15 3.36 2.97
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

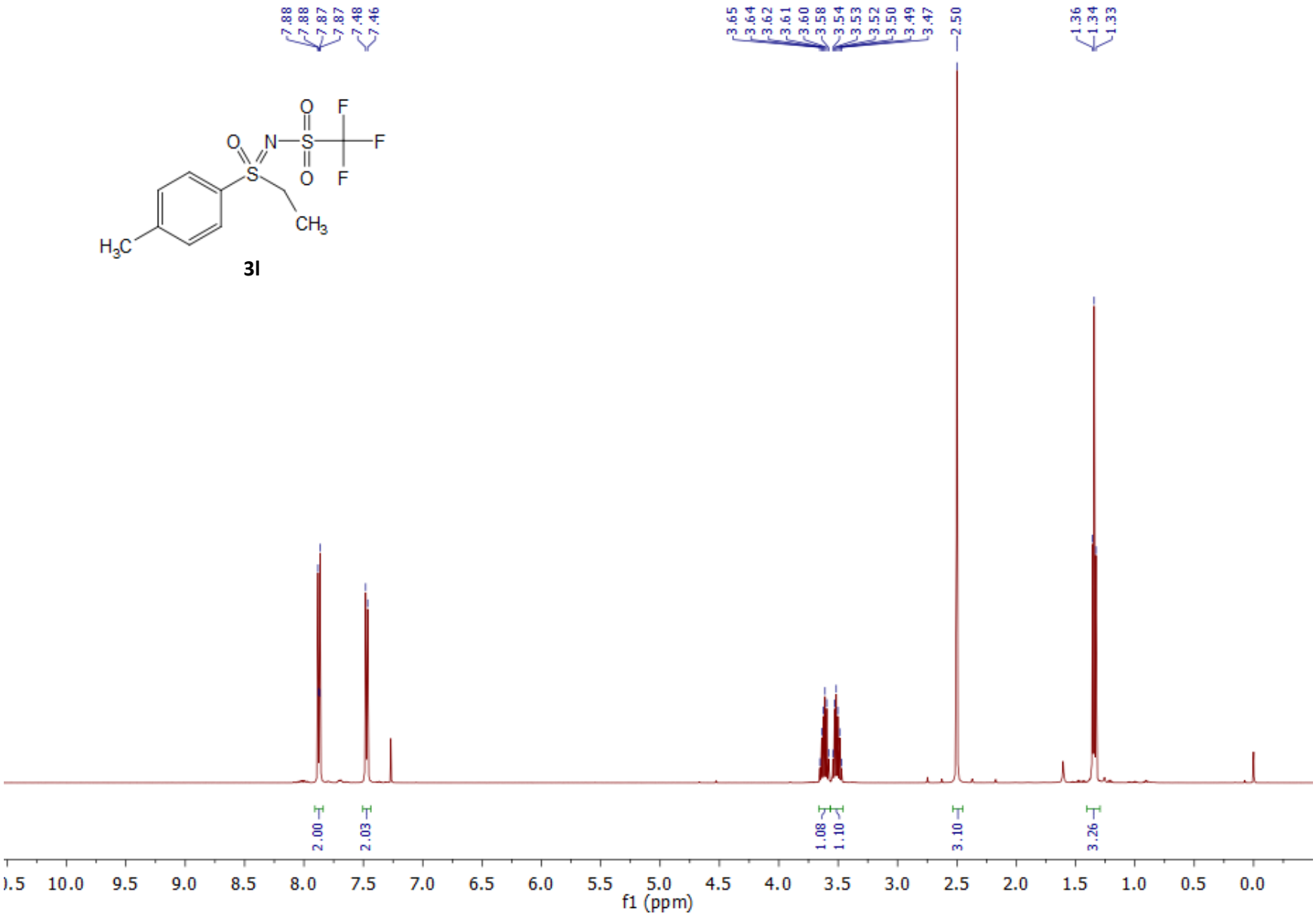
O
O
F
O
N
S
F
S
F
CH3
CH3

3k


-79.31
-79.32
-79.33
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


135.24
134.27
129.92
129.02
128.98
123.01
120.46
117.90
115.35
65.20
64.97
22.09
21.87
12.03
11.90
10.88
O
O
F
O
N
S
F
S
F
CH3
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

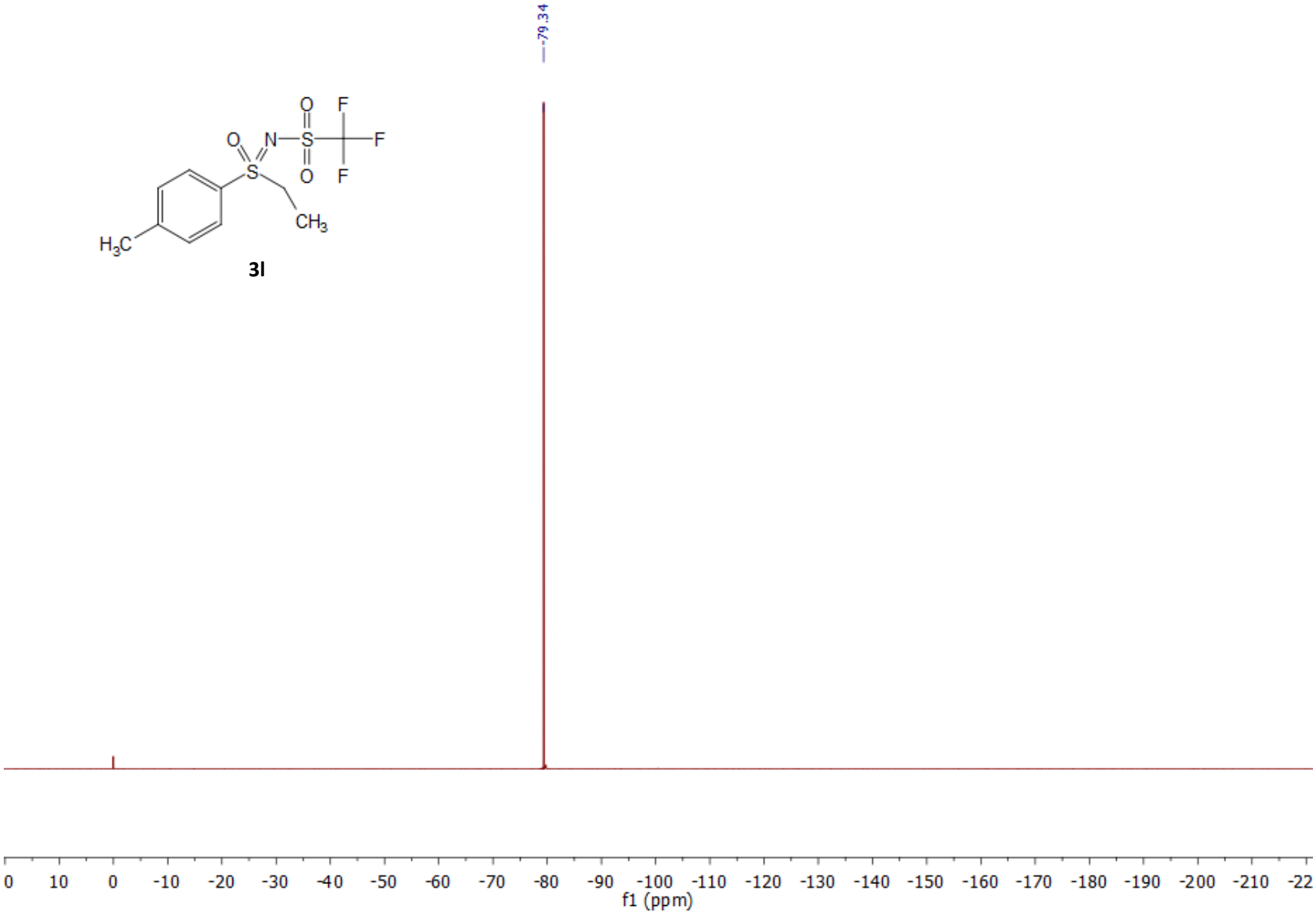
3k

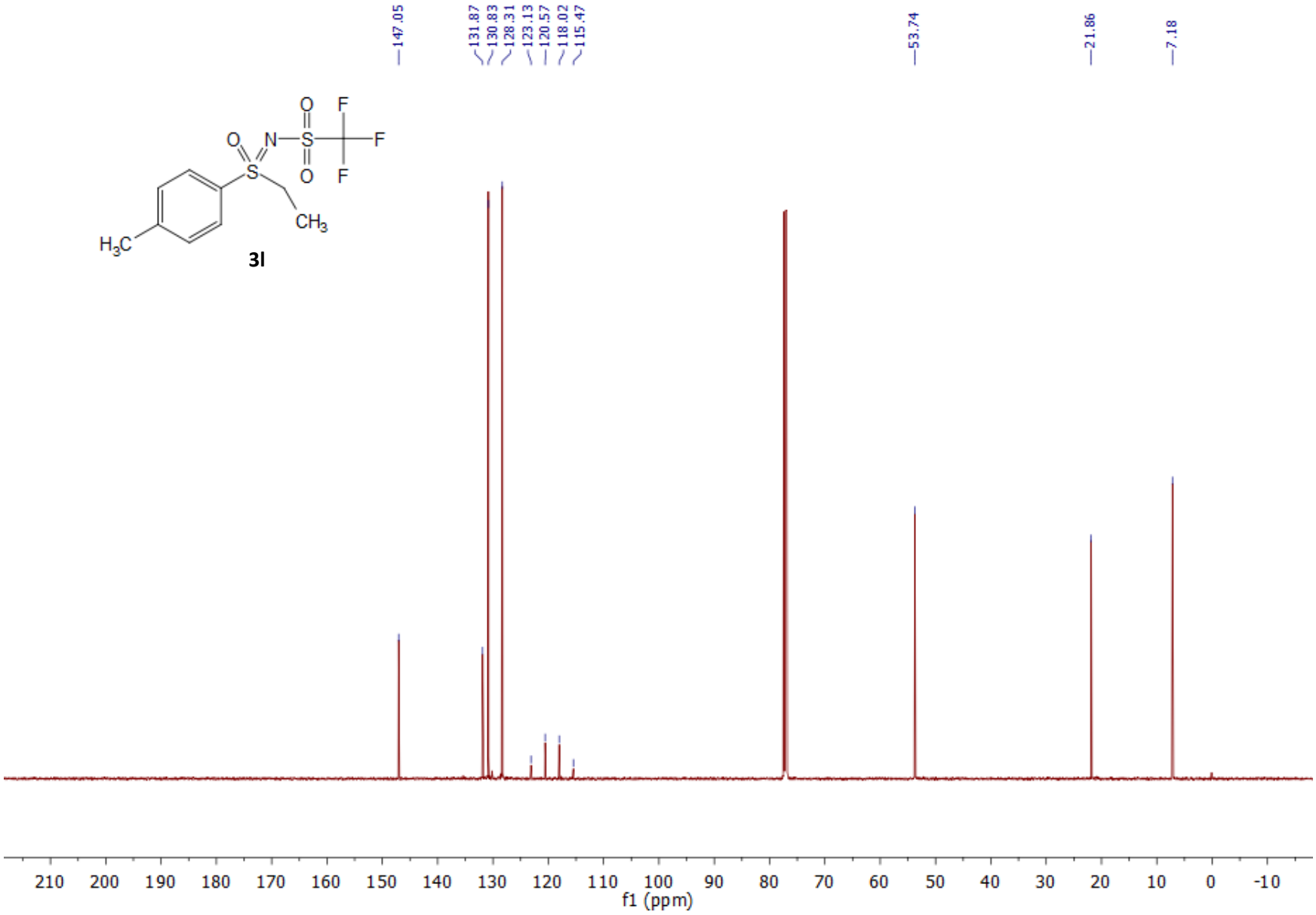

7.88
7.88
7.87
7.87
7.48
7.46
3.65
3.64
3.62
3.61
3.60
3.58
3.54
3.53
3.52
3.50
3.49
3.47
2.50
1.36
1.34
1.33
O
F
O
N
S
F
S
O
F
CH3
H3C
2.00
2.03
1.08
1.10
3.10
3.26
f1 (ppm)

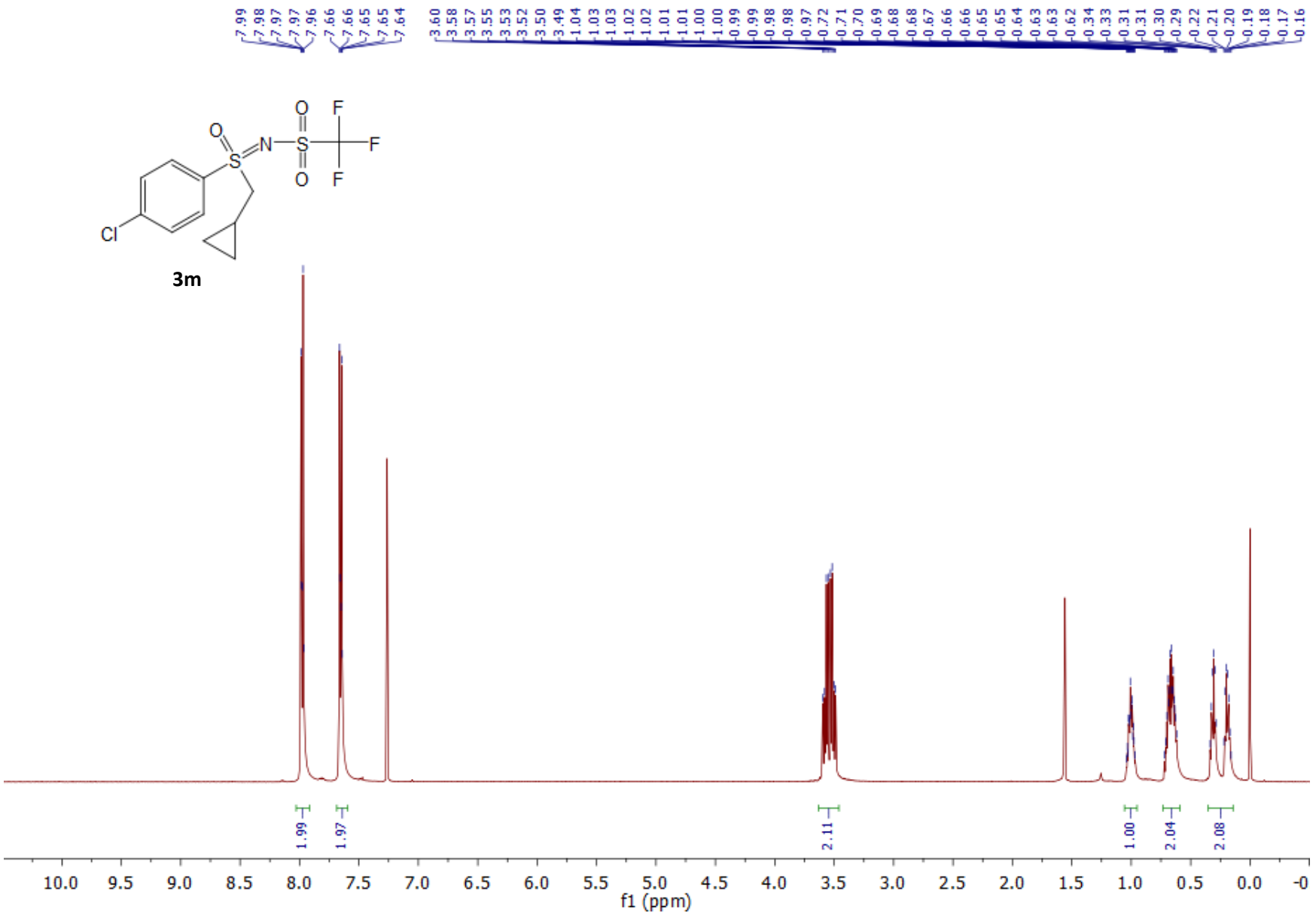
3l

O
F
O
N
S
F
S
O
F
CH3
H3C

3l


-79.34
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

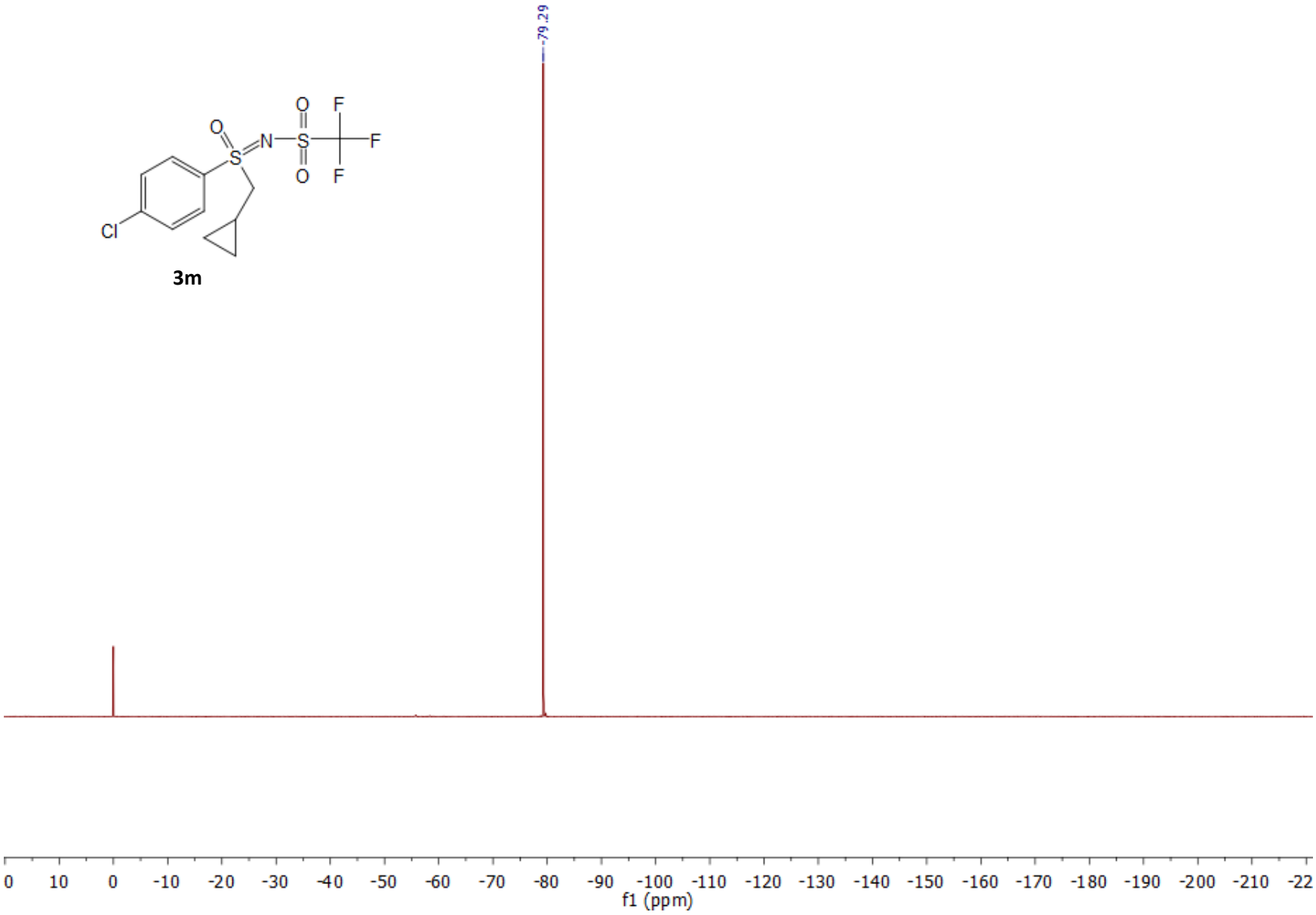

147.05
131.87
130.83
128.31
123.13
120.57
118.02
115.47
53.74
21.86
7.18
O
F
O
N
S
F
S
O
F
CH3
H3C
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

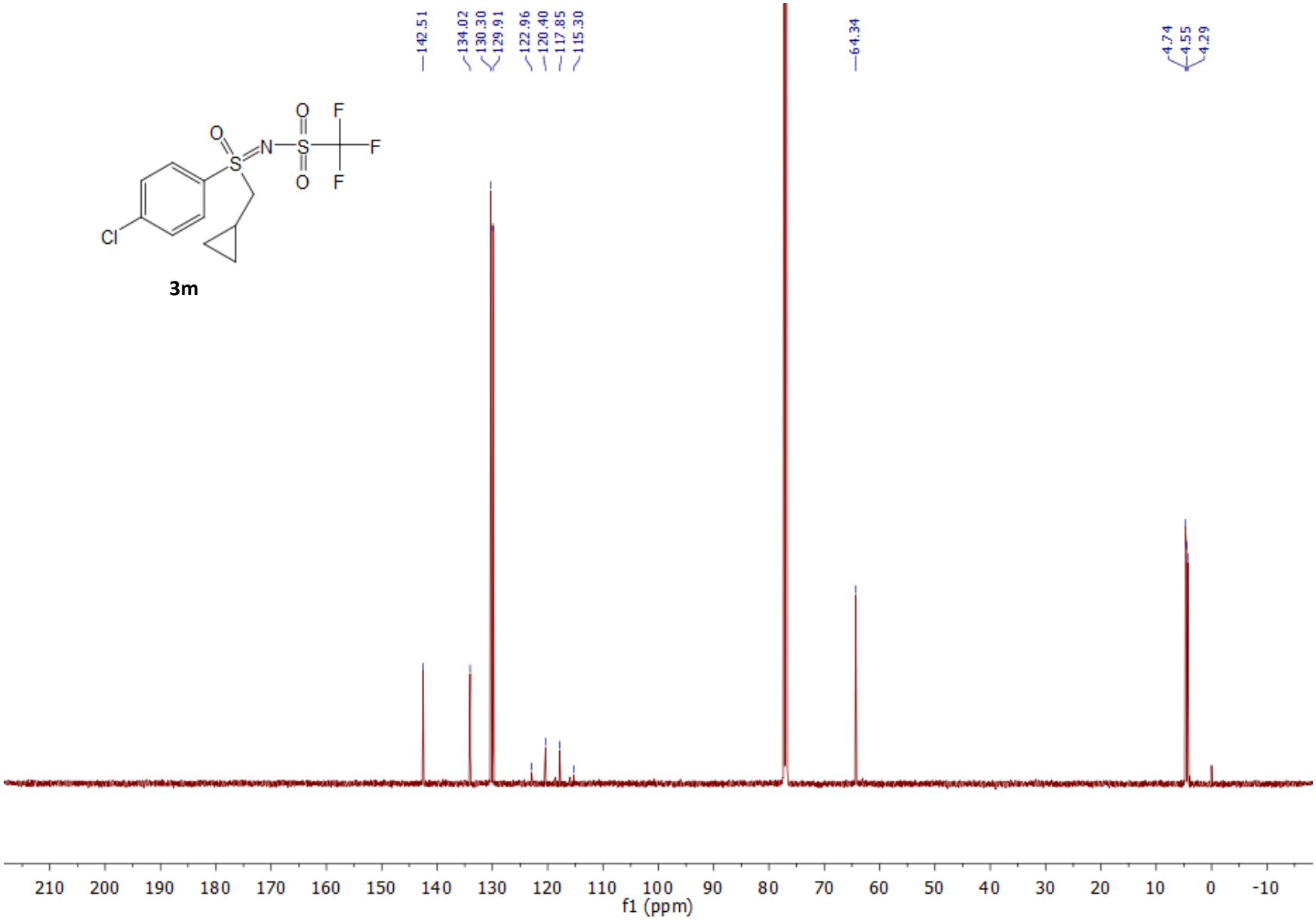

7.99
7.98
7.97
7.97
7.96
7.66
7.65
7.65
7.64
3.60
3.58
3.57
3.55
3.53
3.52
3.50
3.49
1.04
1.03
1.03
1.02
1.02
1.01
1.01
1.00
1.00
0.99
0.99
0.98
0.98
0.97
0.72
0.71
0.70
0.69
0.68
0.68
0.67
0.66
0.66
0.65
0.65
0.64
0.63
0.63
0.62
0.34
0.33
0.31
0.31
0.30
0.29
0.22
0.21
0.20
0.19
0.18
0.17
0.16
O
O
N
S
S
O
O
F
F
F
Cl
1.99
1.97
2.11
1.00
2.04
2.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

3m

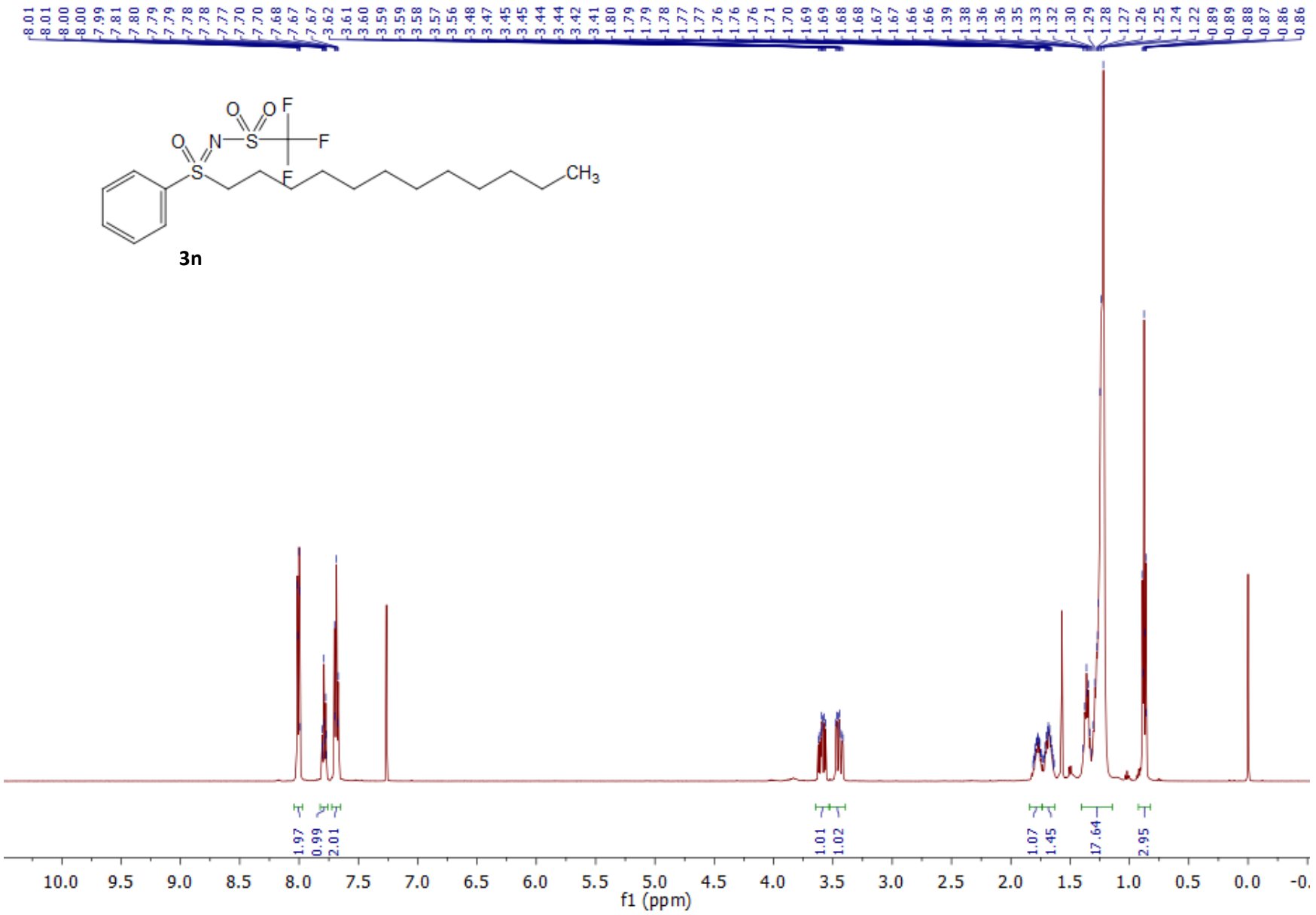
O
S
N
S
O
O
F
F
F
Cl

3m

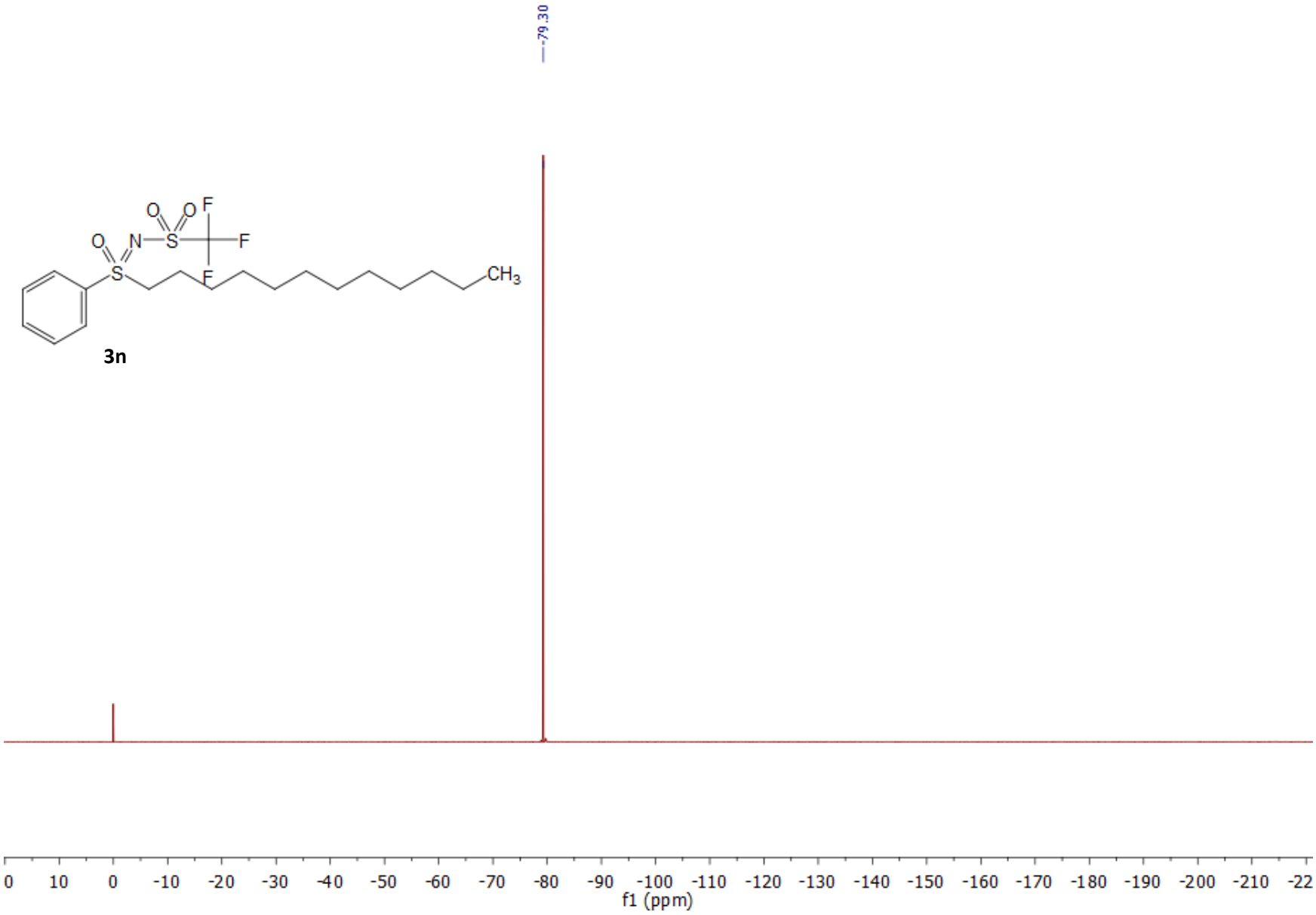

-79.29
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


142.51
134.02
130.30
129.91
122.96
120.40
117.85
115.30
64.34
4.74
4.55
4.29
O
O
N
S
S
O
O
F
F
F
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

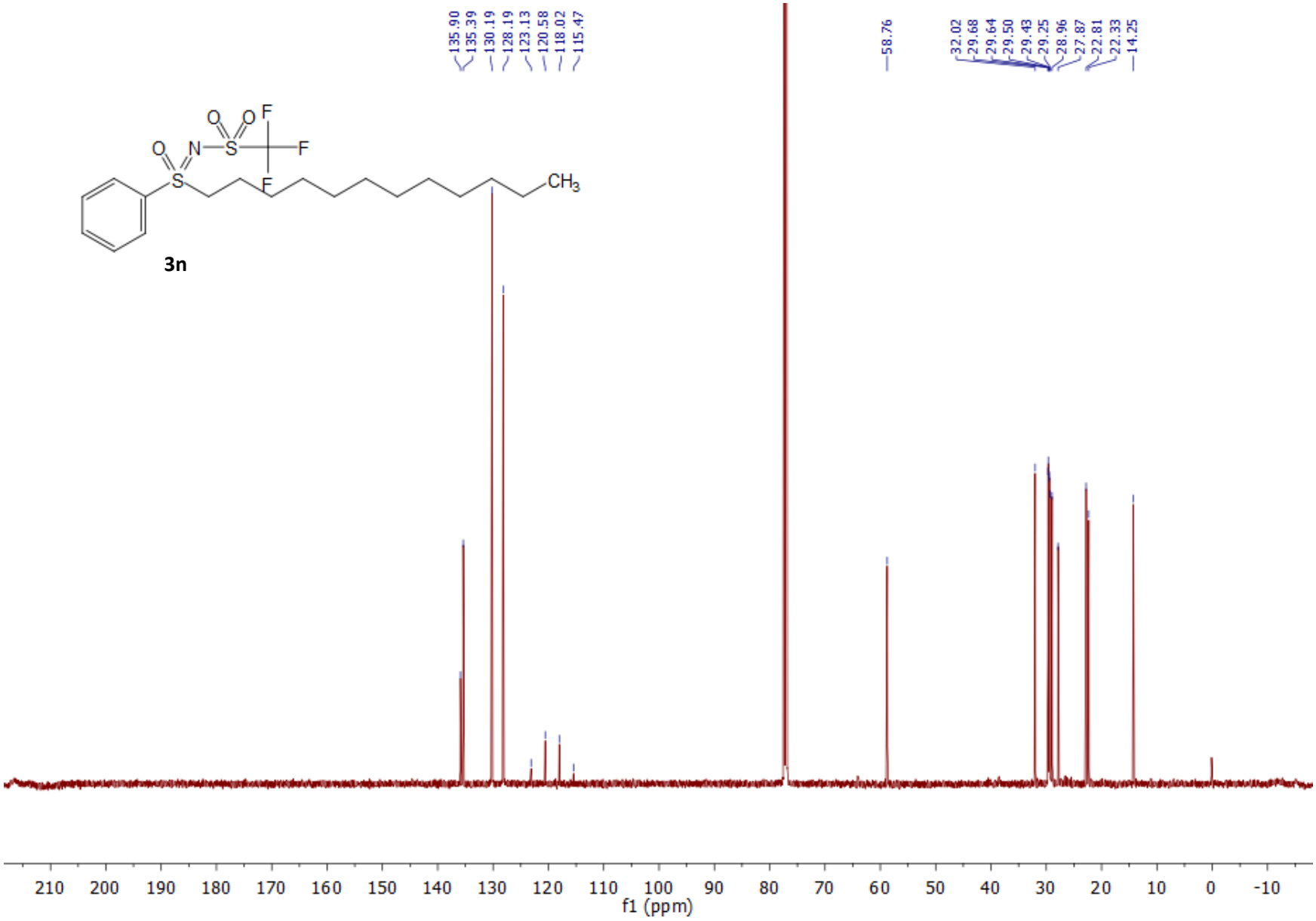
3m

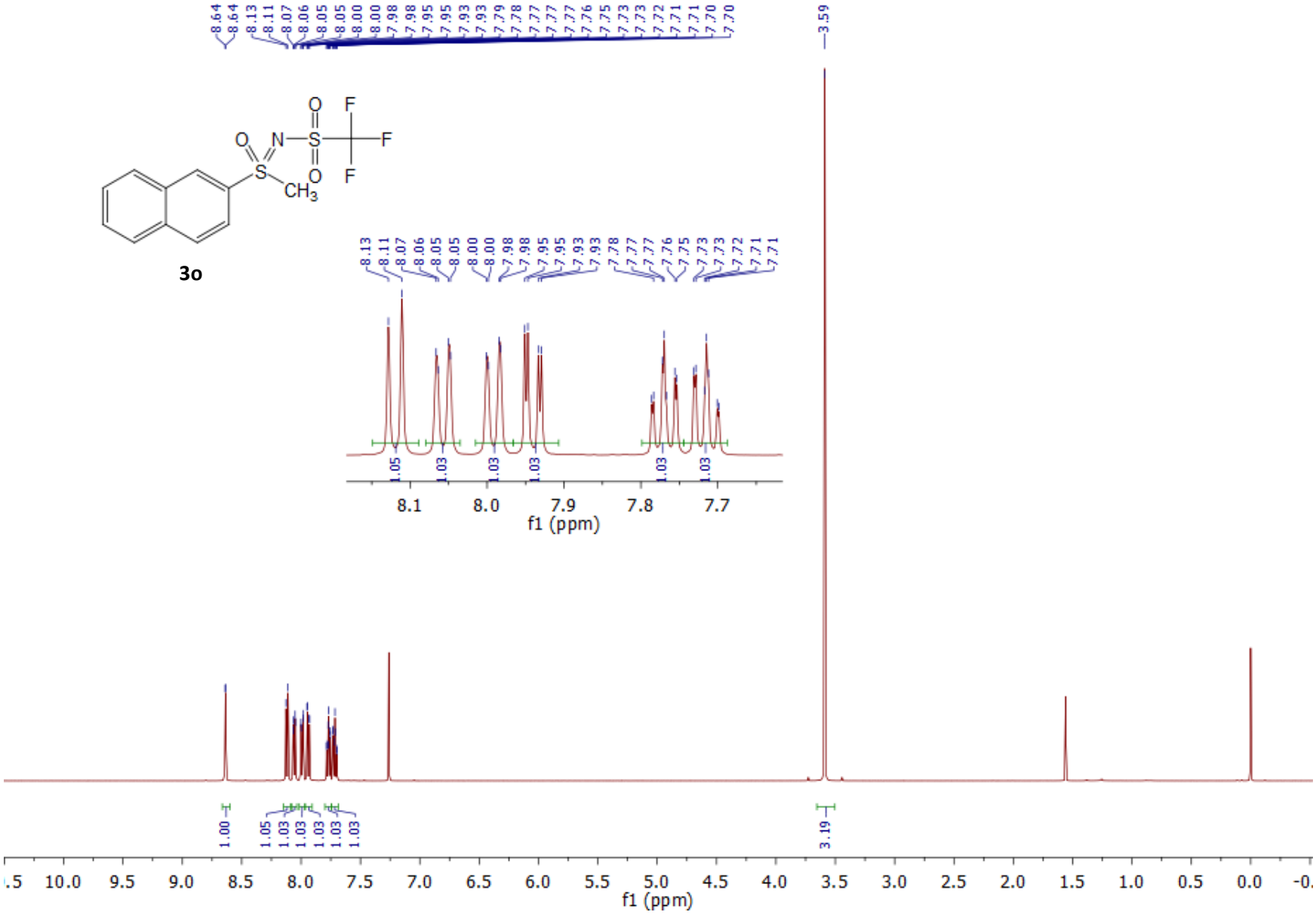

8.01 8.01 8.00 8.00 7.99 7.81 7.80 7.79 7.79 7.78 7.78 7.77 7.70 7.70 7.68 7.67 7.67 7.62 3.61 3.60 3.59 3.59 3.58 3.57 3.56 3.48 3.47 3.45 3.45 3.44 3.44 3.42 3.41 1.80 1.79 1.79 1.78 1.77 1.77 1.76 1.76 1.76 1.71 1.70 1.69 1.69 1.68 1.68 1.67 1.67 1.66 1.66 1.39 1.38 1.36 1.36 1.35 1.33 1.32 1.30 1.29 1.28 1.27 1.26 1.25 1.24 1.22 0.89 0.89 0.88 0.87 0.86 0.86
O
O
F
O
N
S
F
S
F
CH3
1.97
0.99
2.01
1.01
1.02
1.07
1.45
17.64
2.95
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3n


-79.30
O
O
F
O
N
S
F
S
F
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

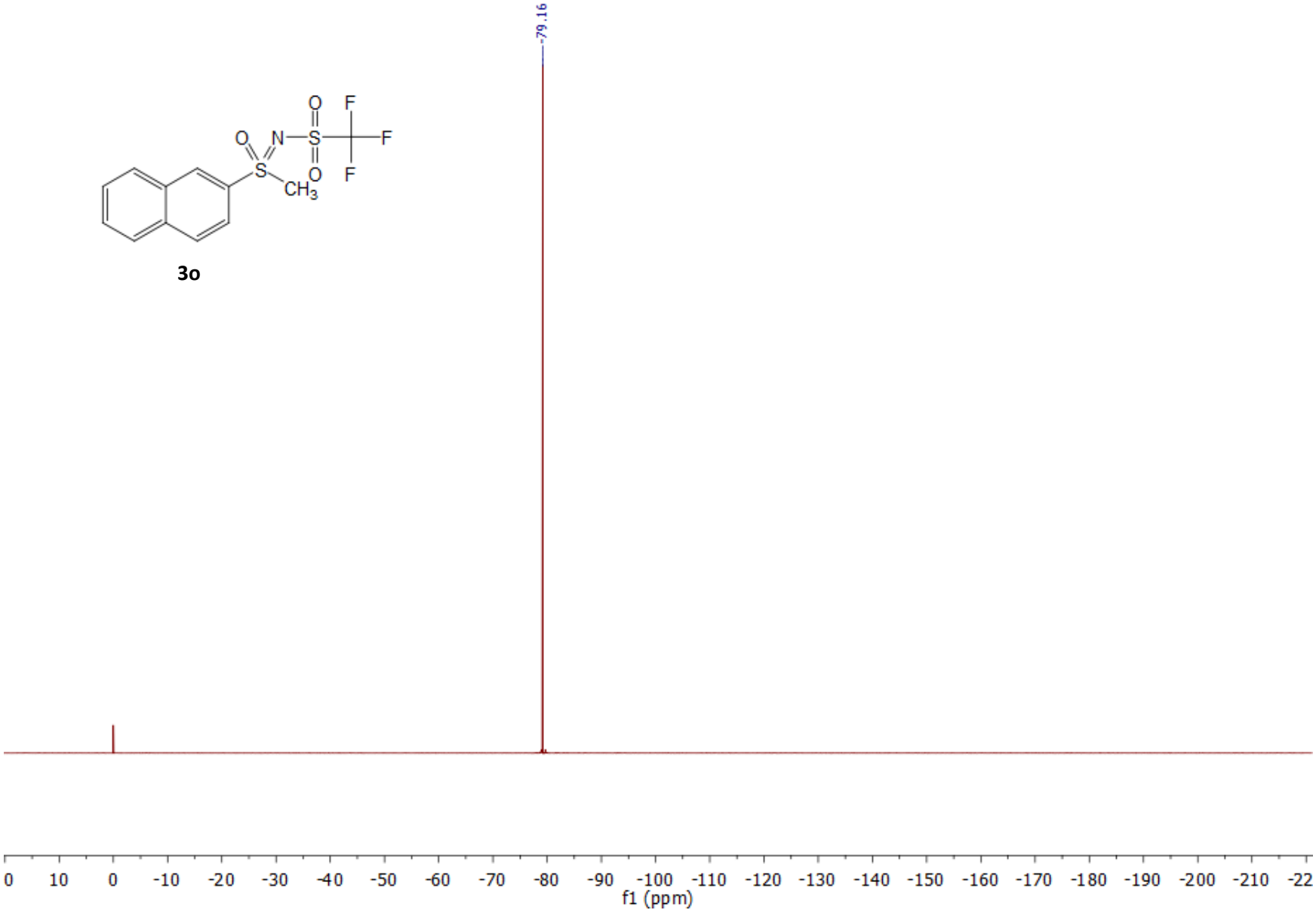
3n


135.90
135.39
130.19
128.19
123.13
120.58
118.02
115.47
58.76
32.02
29.68
29.64
29.50
29.43
29.25
28.96
27.87
22.81
22.33
14.25
O
O
F
O
N
S
F
S
F
CH3
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.64
8.64
8.13
8.11
8.07
8.06
8.05
8.05
8.00
8.00
7.98
7.98
7.95
7.95
7.93
7.93
7.79
7.78
7.77
7.77
7.77
7.76
7.75
7.73
7.73
7.72
7.71
7.71
7.70
7.70
3.59
O
F
O
N
S
F
O
S
F
CH3
3o
8.13
8.11
8.07
8.06
8.05
8.05
8.00
8.00
7.98
7.98
7.95
7.95
7.93
7.93
7.78
7.77
7.77
7.76
7.75
7.73
7.73
7.72
7.71
7.71
1.05
1.03
1.03
1.03
1.03
1.03
8.1
8.0
7.9
7.8
7.7
f1 (ppm)
1.00
1.05
1.03
1.03
1.03
1.03
1.03
3.19
.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

O
F
O
N
S
F
S
O
F
CH3

3o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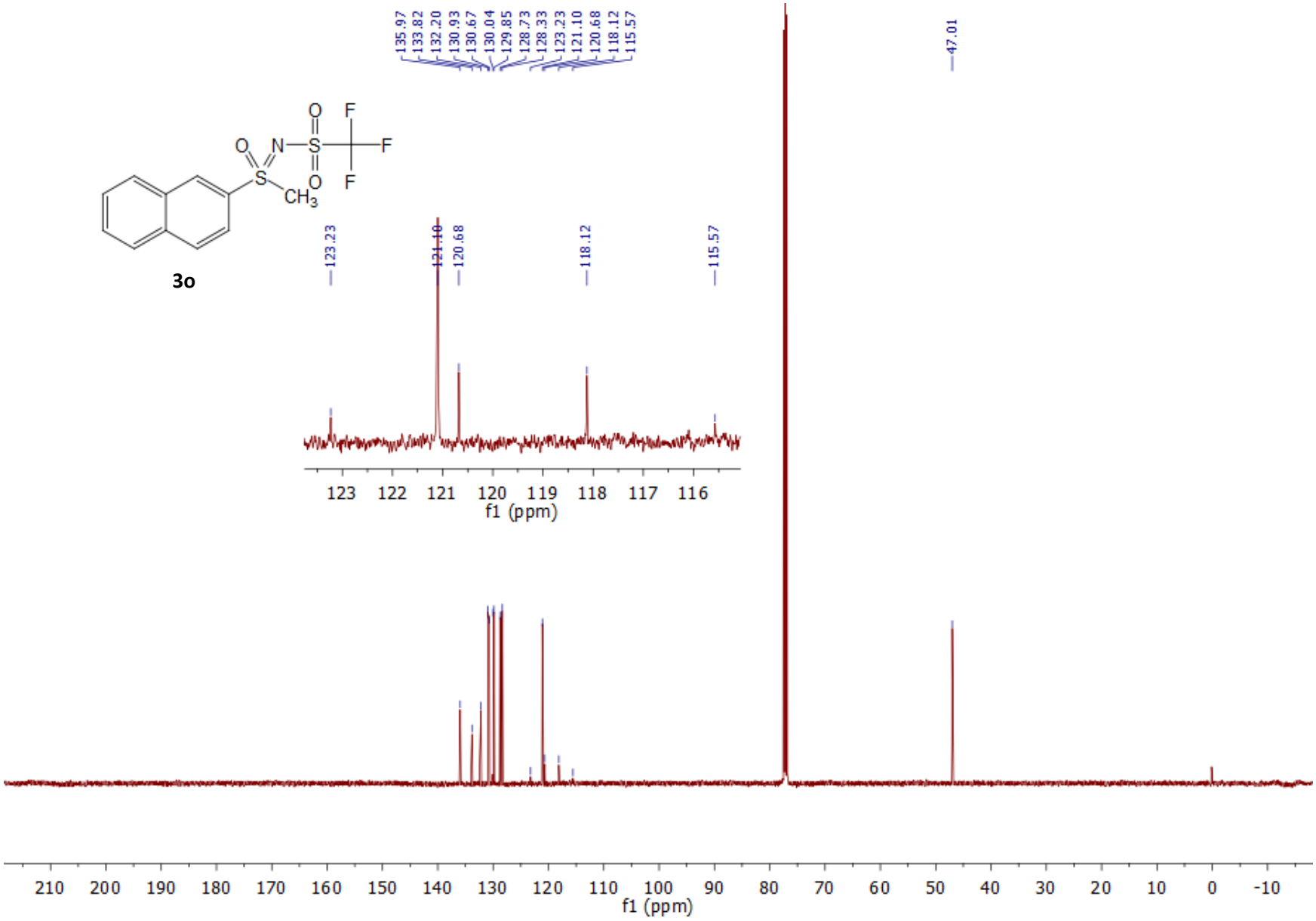
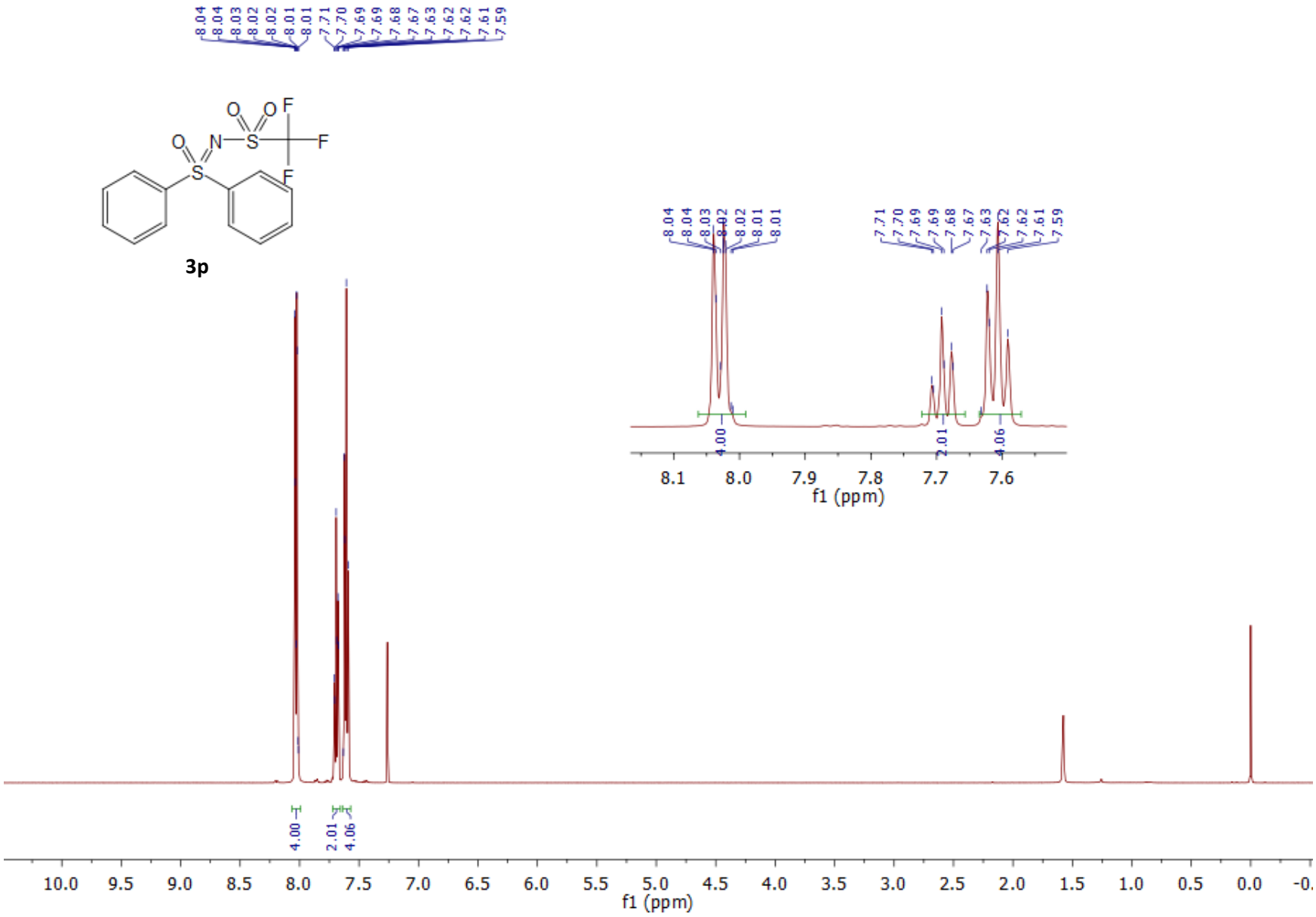
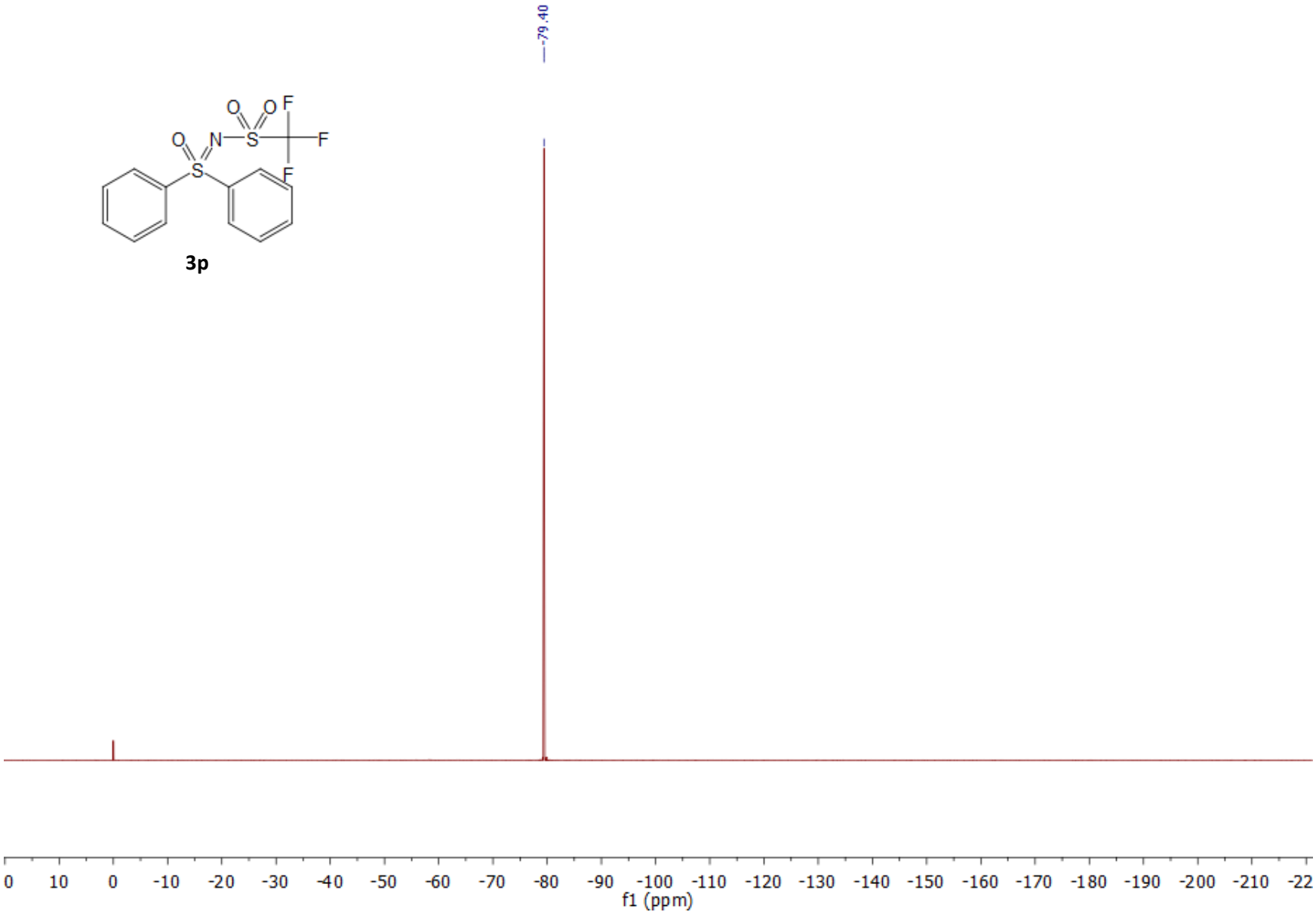
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


135.97
133.82
132.20
130.93
130.67
130.04
129.85
128.73
128.33
123.23
121.10
120.68
118.12
115.57
47.01
O
F
O
N
S
F
S
F
O
CH3
3o
123.23
121.10
120.68
118.12
115.57
123 122 121 120 119 118 117 116
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.04 8.04 8.03 8.02 8.02 8.01 8.01 7.71 7.70 7.69 7.69 7.68 7.67 7.63 7.62 7.62 7.61 7.59
O O F
O N S F
S F
3p
8.04 8.04 8.03 8.02 8.02 8.01 8.01 7.71 7.70 7.69 7.69 7.68 7.67 7.63 7.62 7.62 7.61 7.59
4.00 2.01 4.06
8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)
4.00 2.01 4.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

O
O
F
O
N
S
F
S
F

3p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0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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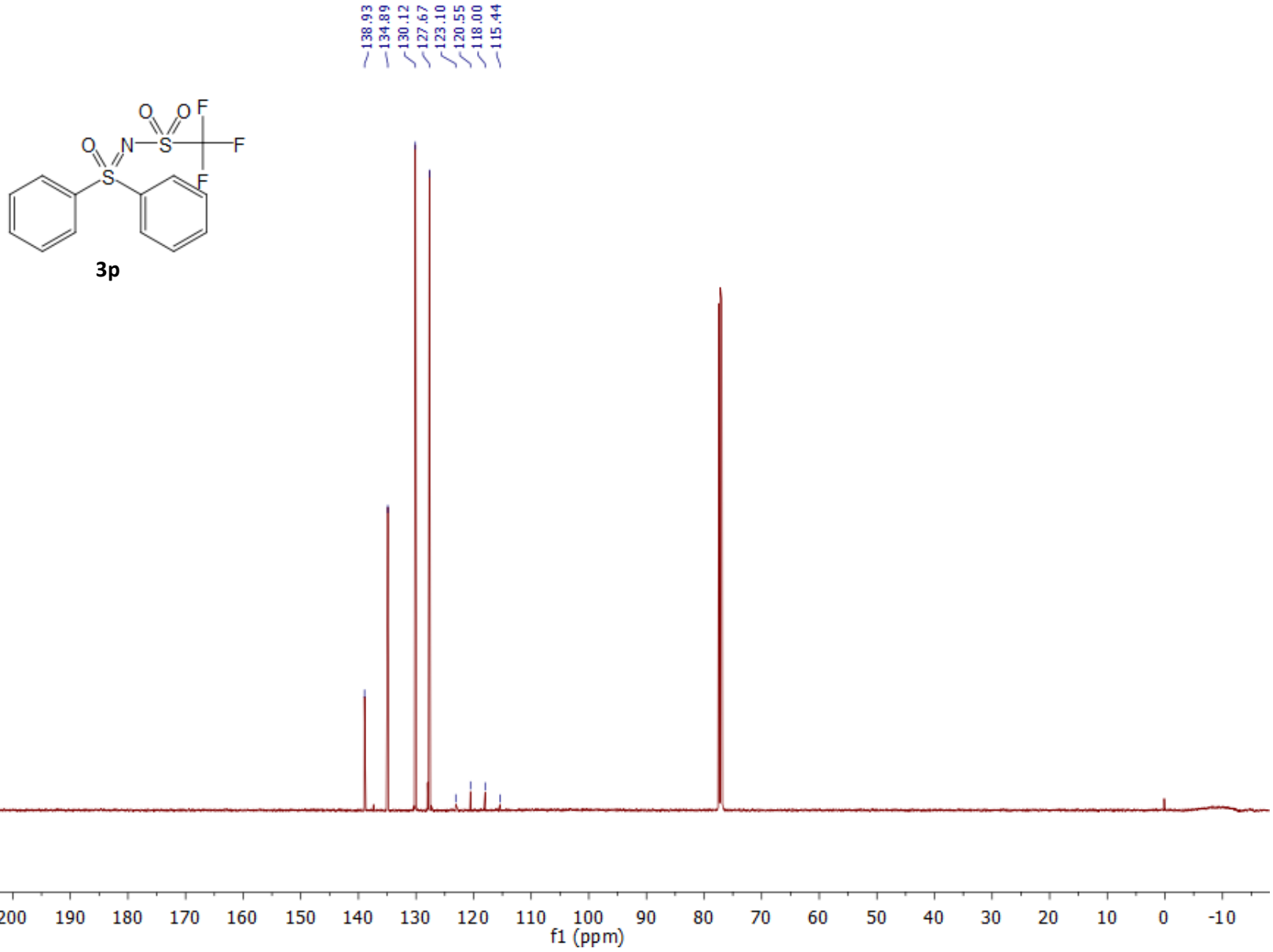
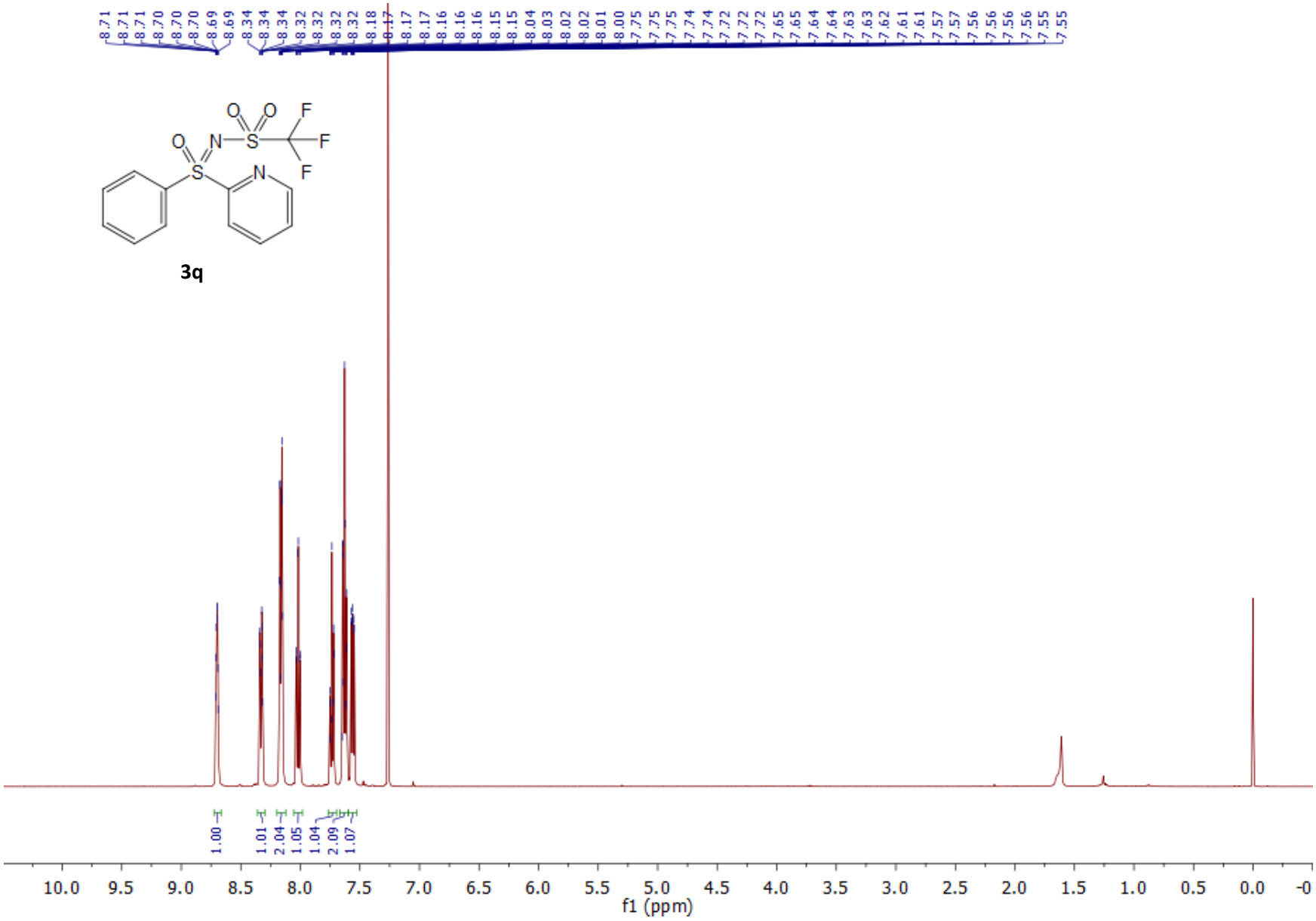
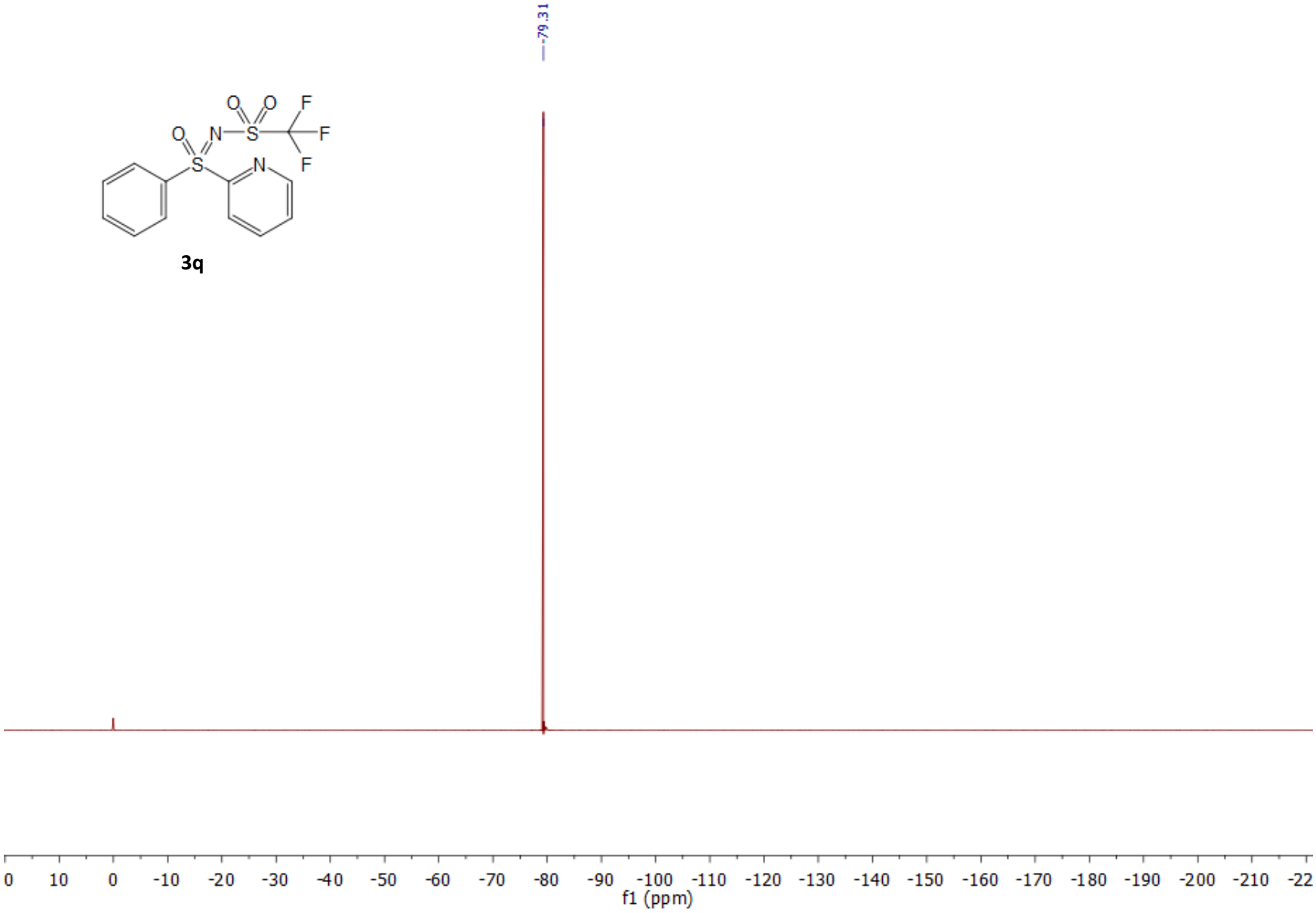
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

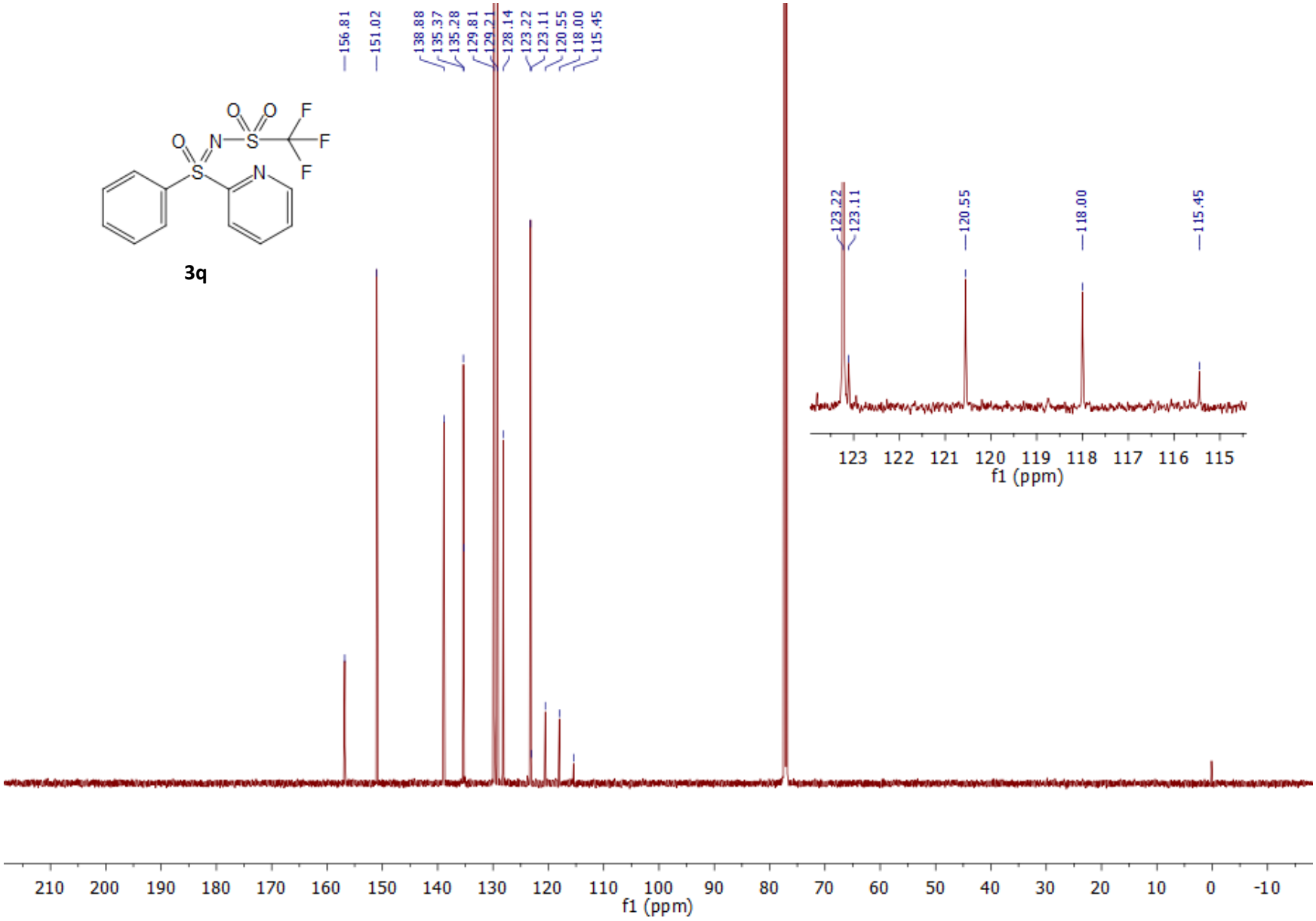

138.93
134.89
130.12
127.67
123.10
120.55
118.00
115.44
O
O
F
O
N
S
S
F
F
3p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

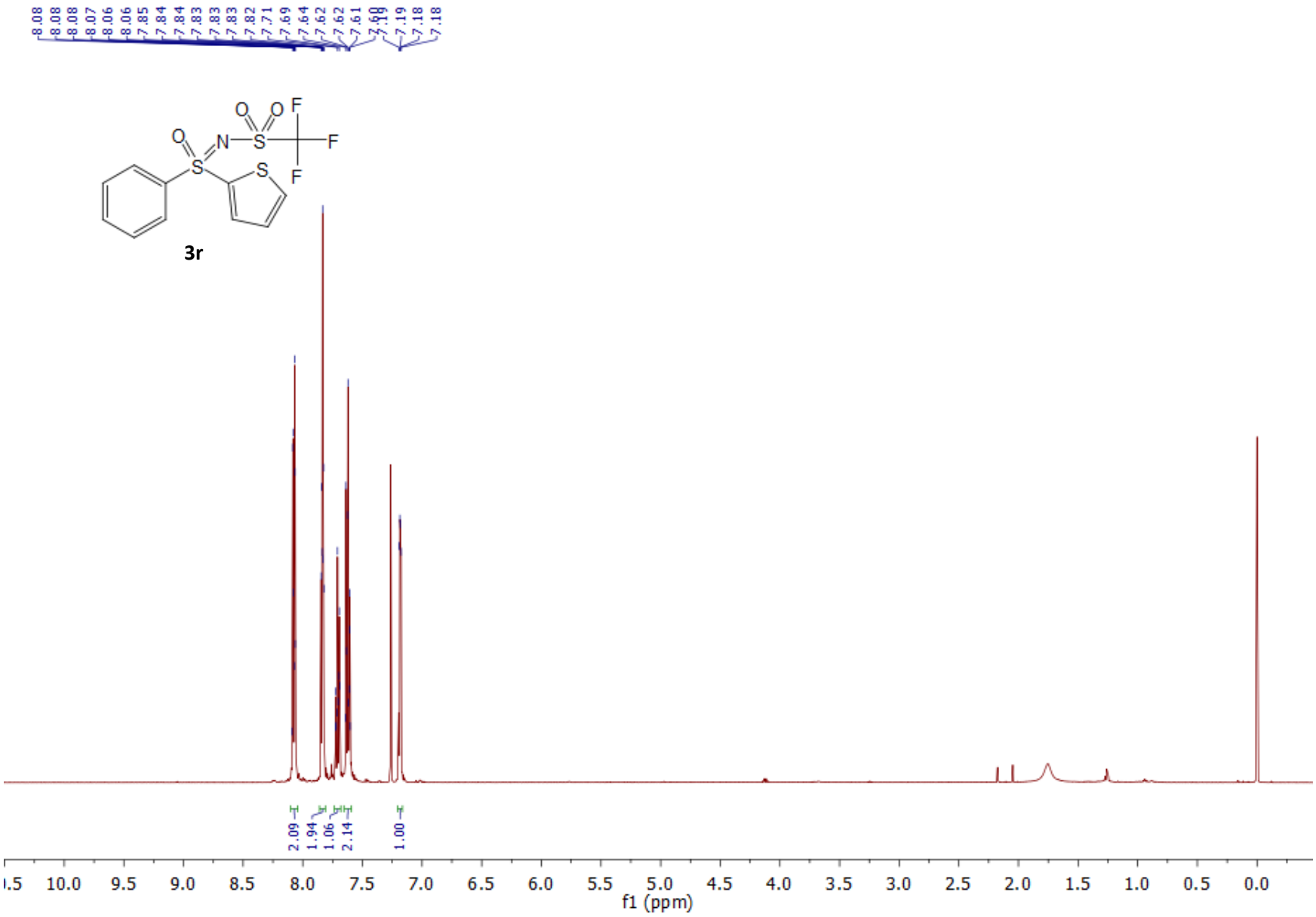

8.71 8.71 8.71 8.70 8.70 8.70 8.69 8.69 8.34 8.34 8.34 8.32 8.32 8.32 8.18 8.17 8.17 8.17 8.16 8.16 8.16 8.15 8.15 8.04 8.03 8.02 8.02 8.01 8.00 7.75 7.75 7.75 7.74 7.74 7.72 7.72 7.72 7.65 7.65 7.64 7.64 7.63 7.63 7.62 7.61 7.61 7.57 7.57 7.56 7.56 7.56 7.55 7.55
O O F
O N S F
F
S N
3q
1.00 1.01 2.04 1.05 1.04 2.09 1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

O
O
F
O
N
S
F
S
N
F

3q


-79.31
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

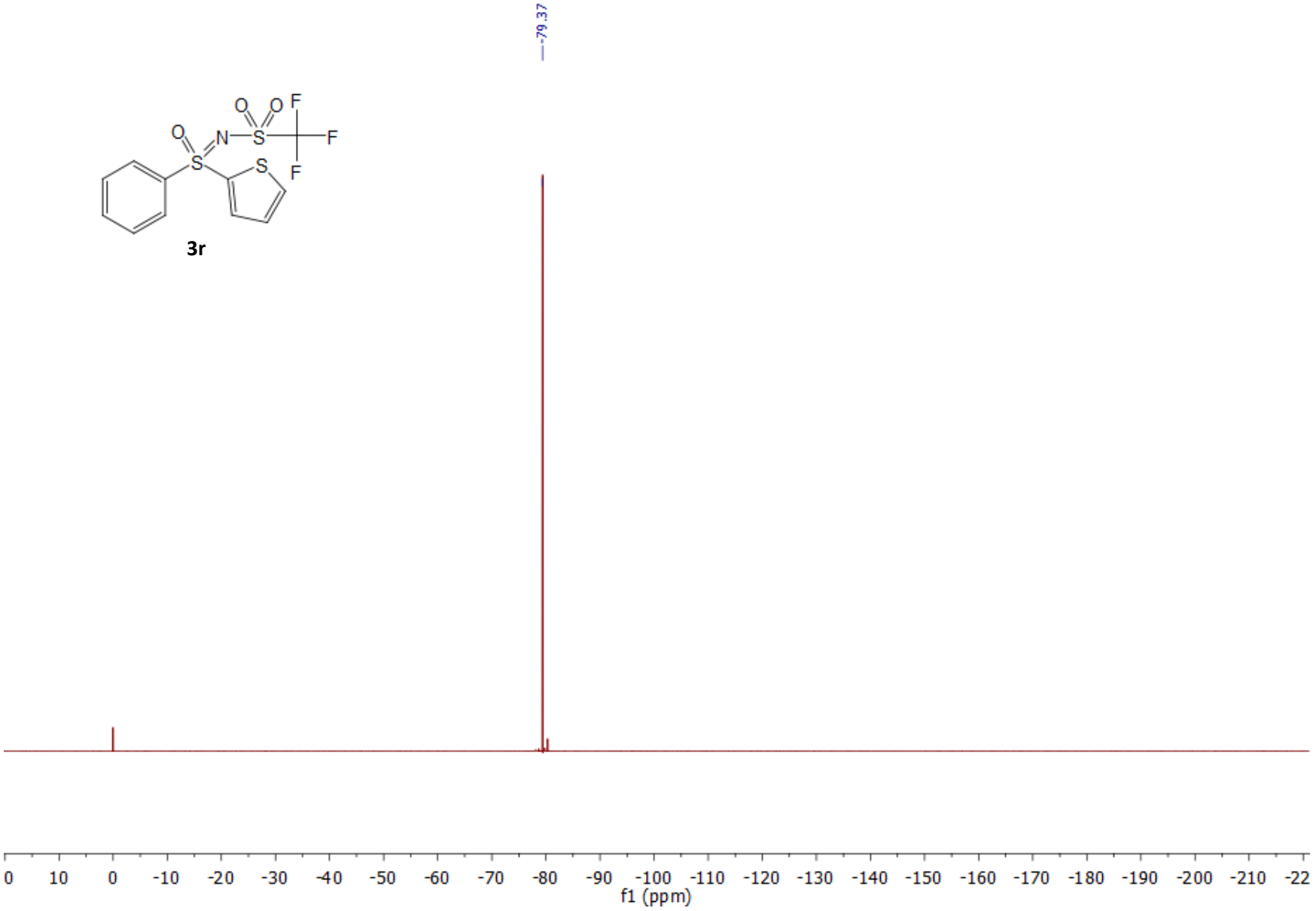

156.81
151.02
138.88
135.37
135.28
129.81
129.21
128.14
123.22
123.11
120.55
118.00
115.45
O
O
F
O
N
S
F
S
N
F
3q
123.22
123.11
120.55
118.00
115.45
123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

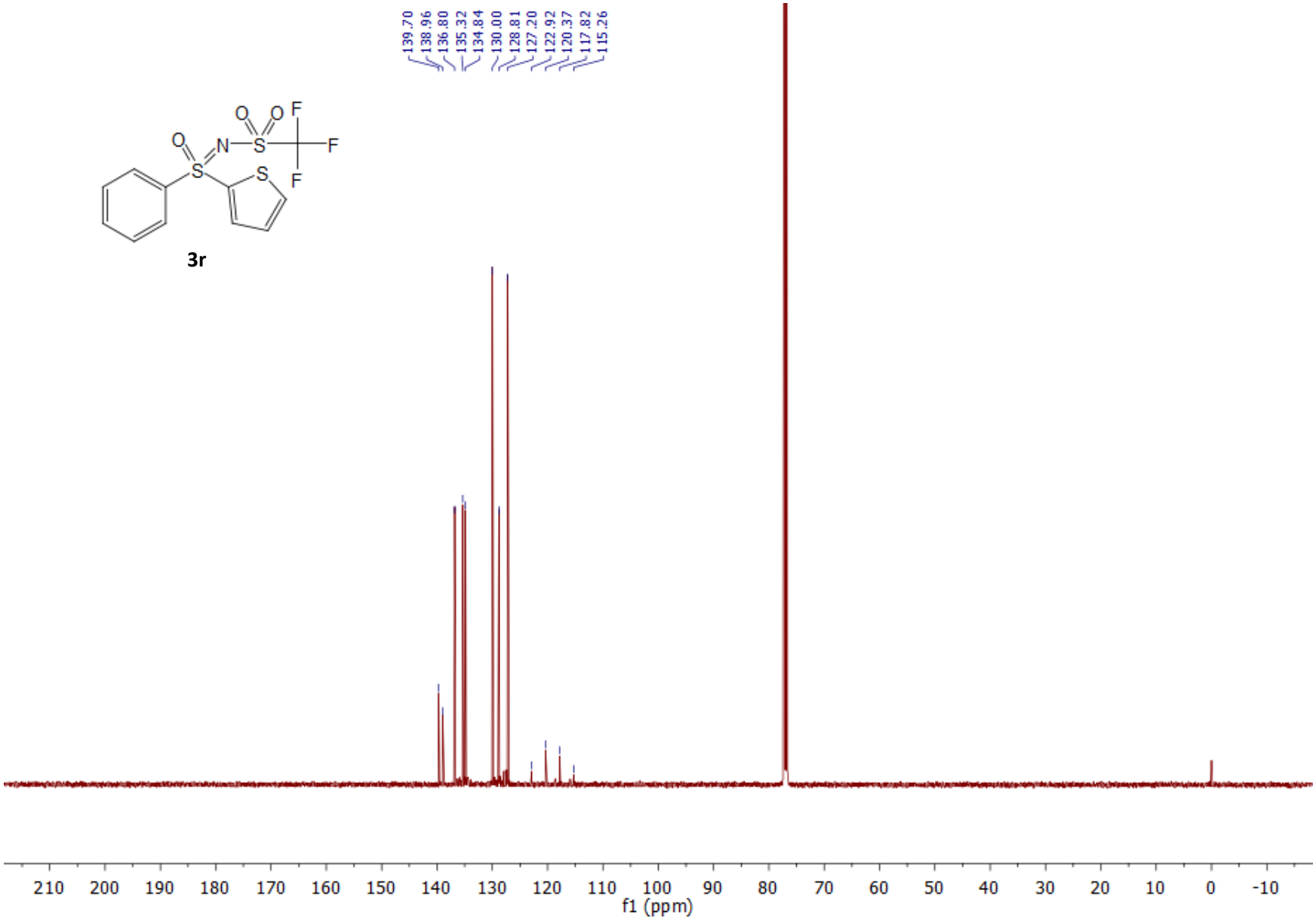

8.08
8.08
8.08
8.07
8.06
8.06
7.85
7.84
7.84
7.83
7.83
7.83
7.82
7.71
7.69
7.64
7.62
7.62
7.61
7.60
7.19
7.18
7.18
O
O
F
O
N
S
S
F
S
F
2.09
1.94
1.06
2.14
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

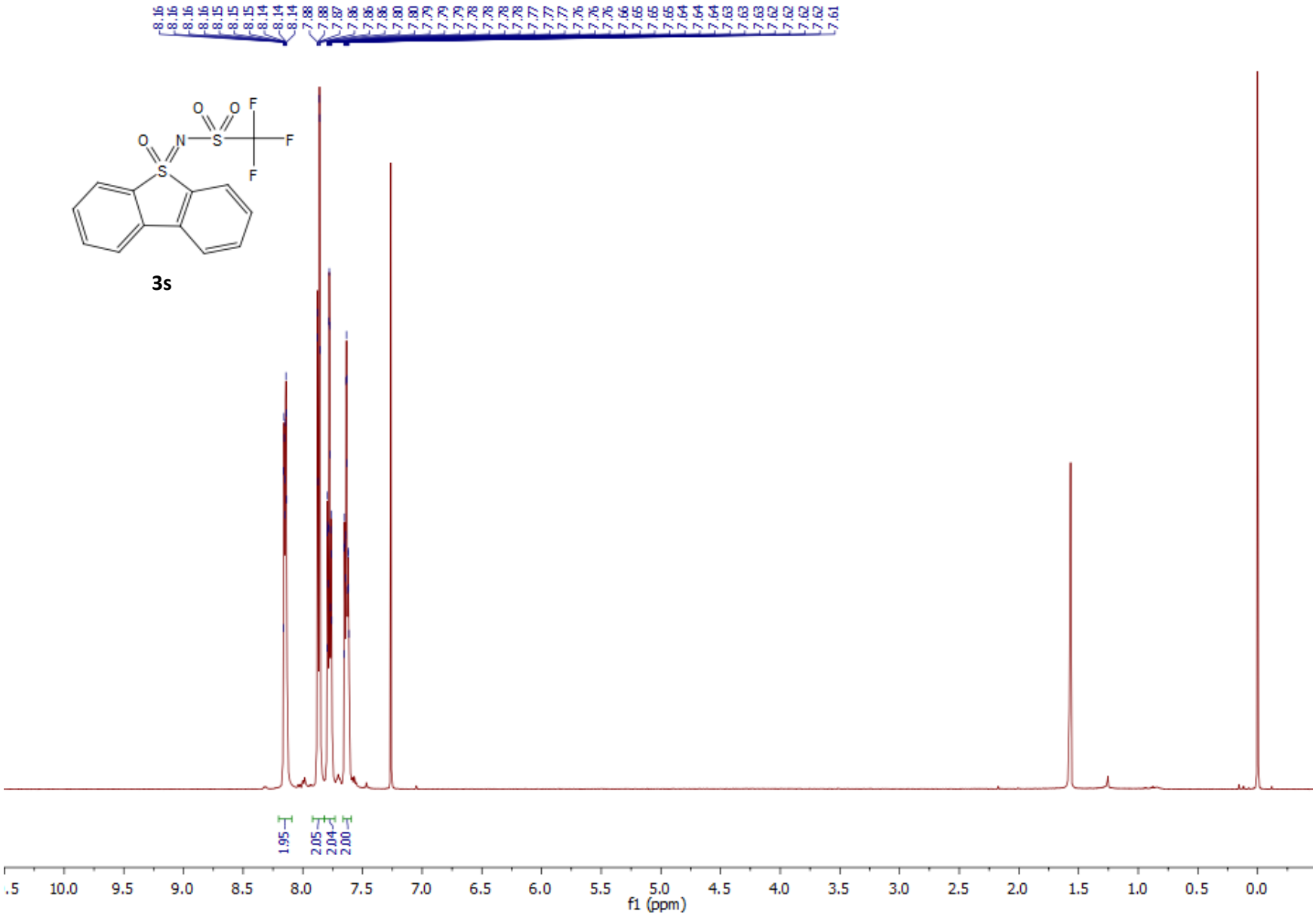
3r

O
O
F
O
N
S
F
S
S
F

3r


-79.37
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

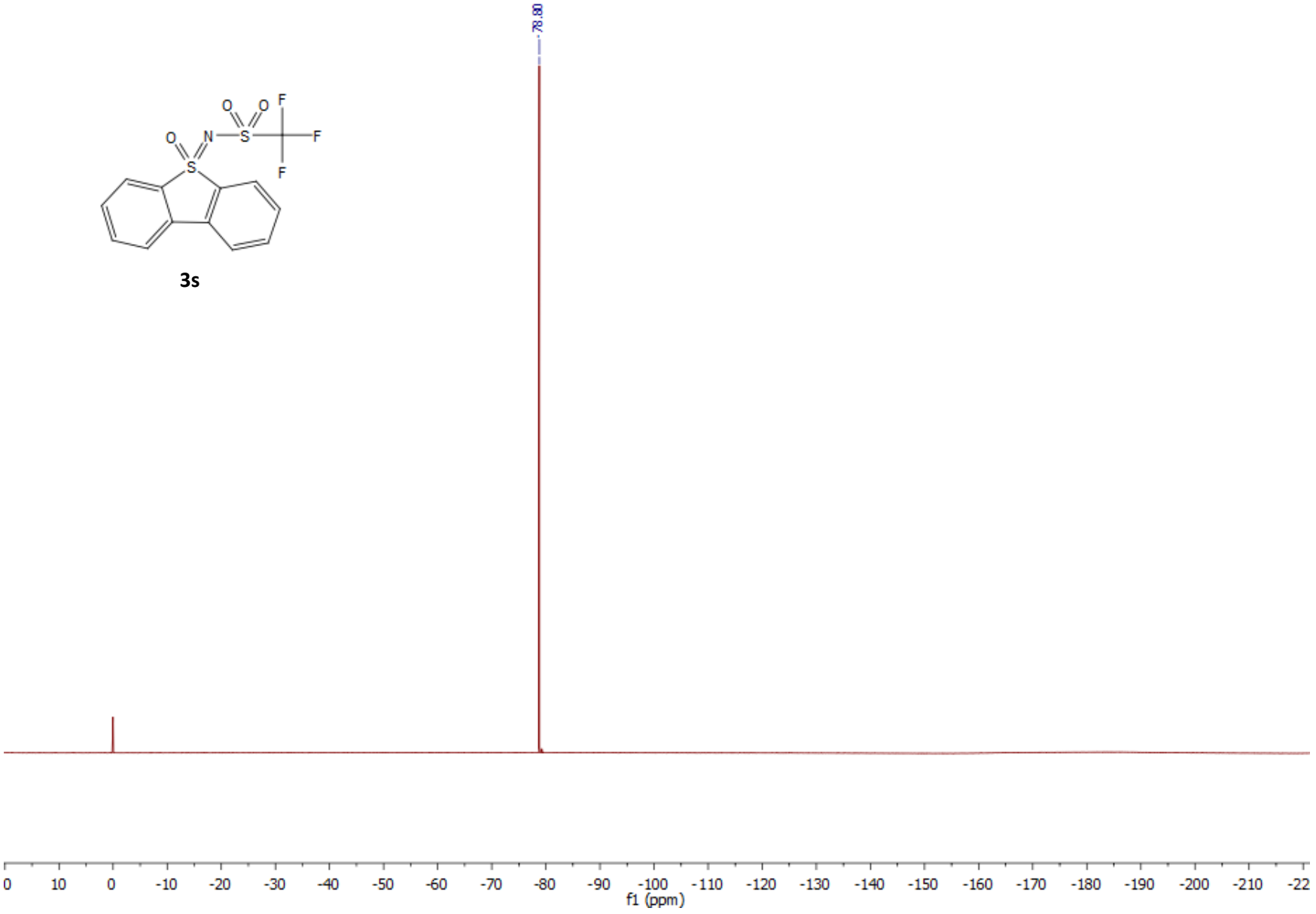

139.70
138.96
136.80
135.32
134.84
130.00
128.81
127.20
122.92
120.37
117.82
115.26
O
O
F
O
N
S
F
S
S
F
3r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

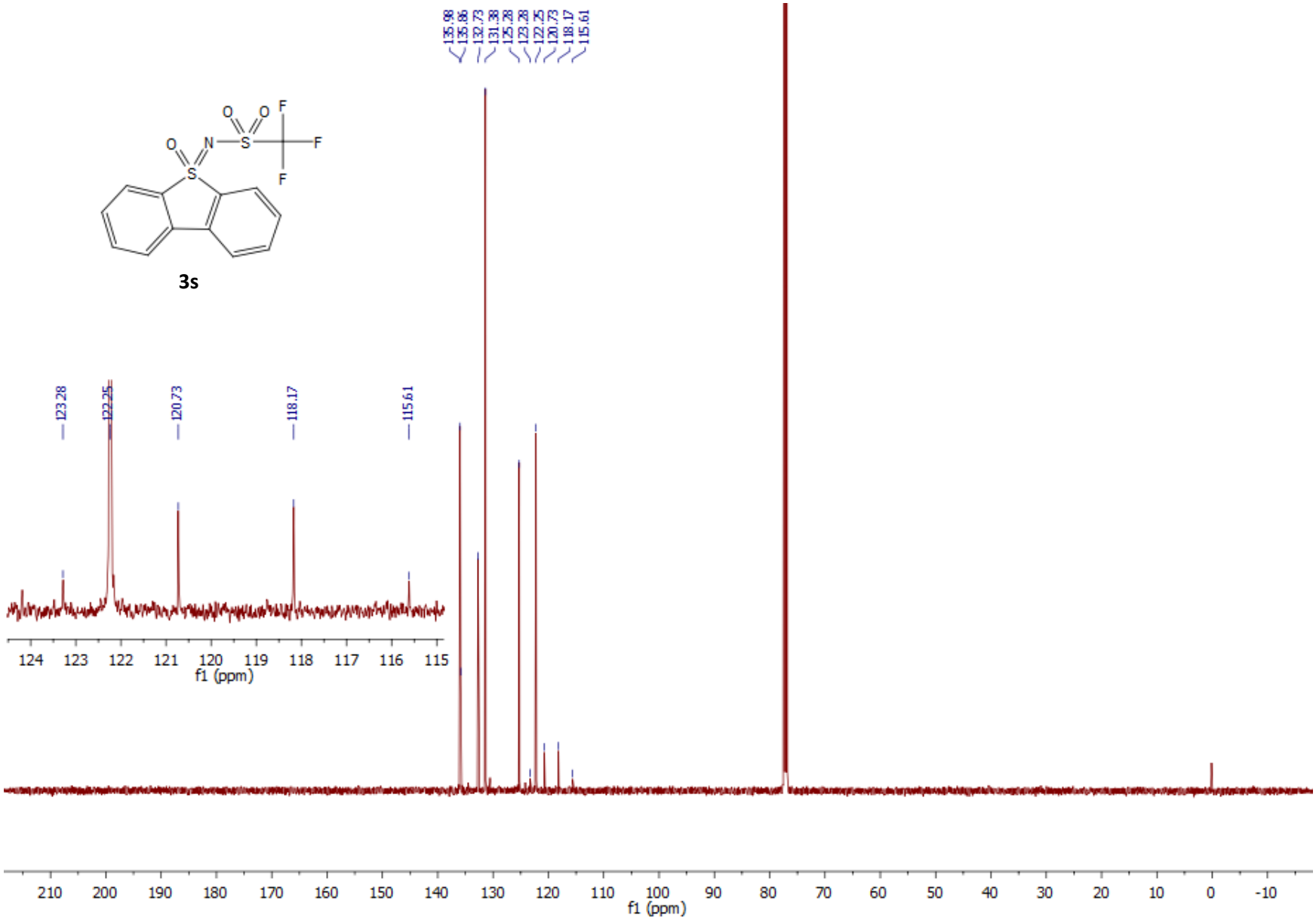

8.16 8.16 8.16 8.15 8.15 8.15 8.14 8.14 8.14 7.88 7.87 7.86 7.86 7.80 7.80 7.79 7.79 7.78 7.78 7.78 7.77 7.77 7.77 7.76 7.76 7.76 7.66 7.65 7.65 7.64 7.64 7.64 7.63 7.63 7.63 7.62 7.62 7.62 7.62 7.61
O O F
O N S F
S F
1.95 2.05 2.04 2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

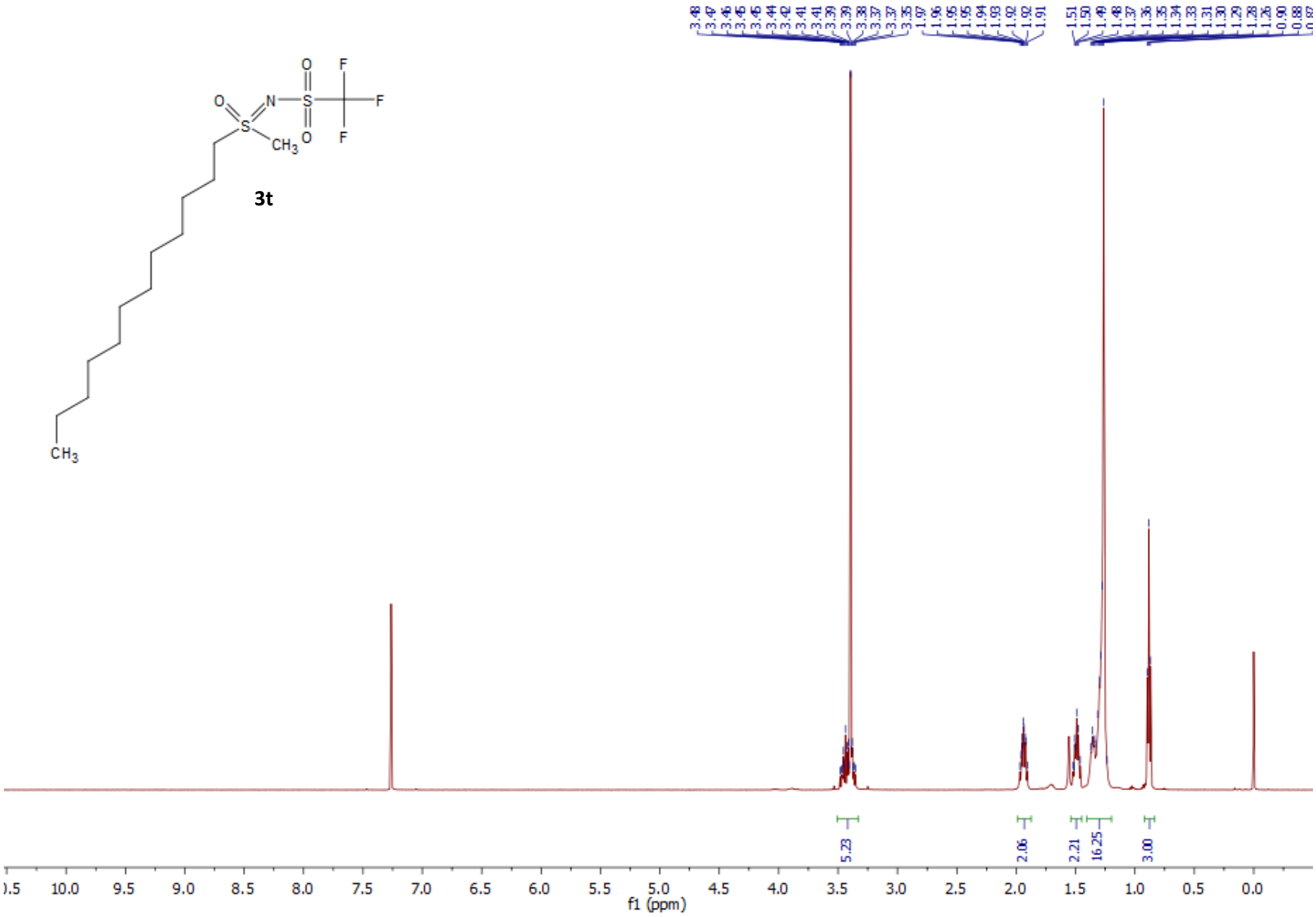
3s

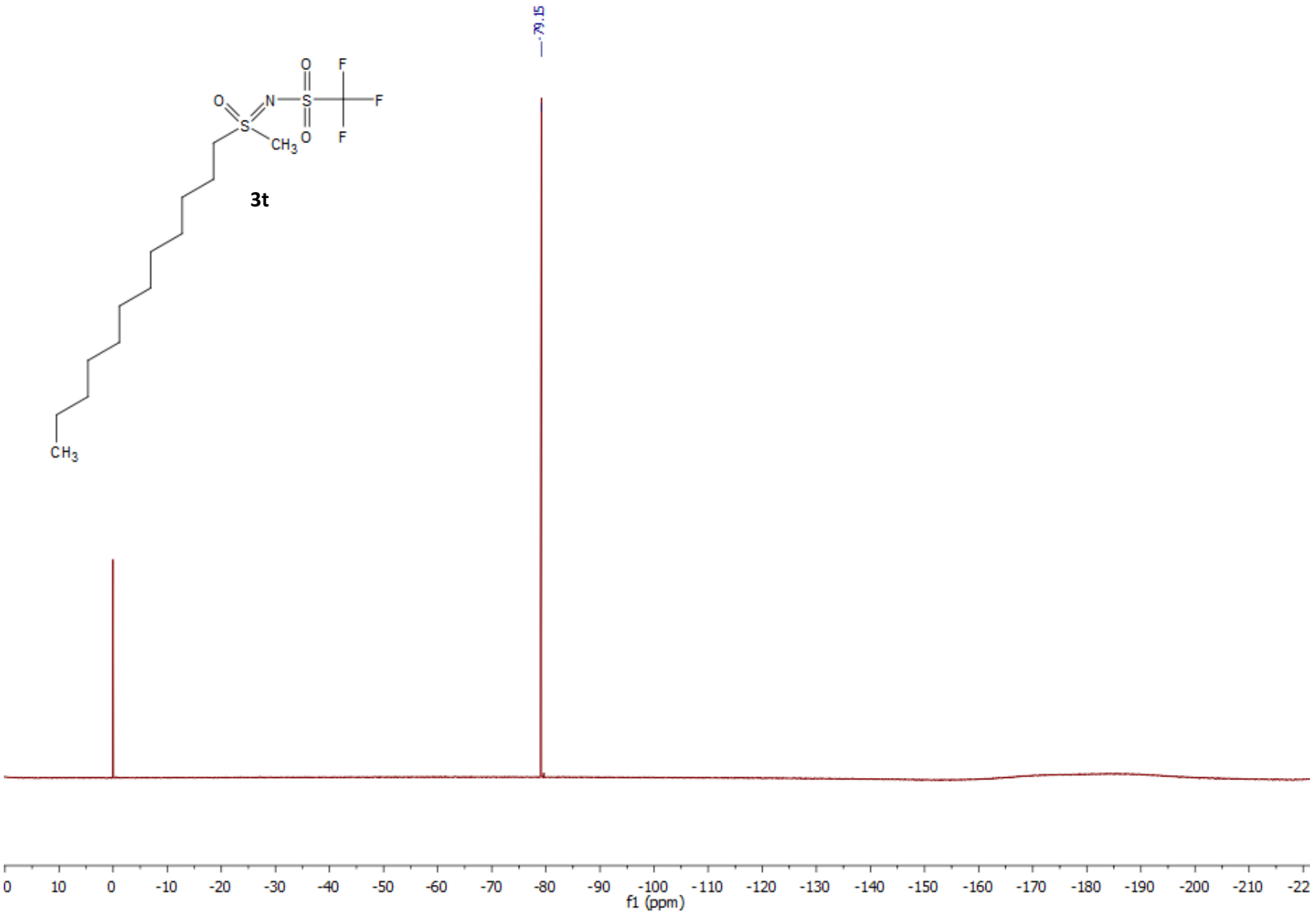
O
O
F
O
N
S
F
S
F

3s

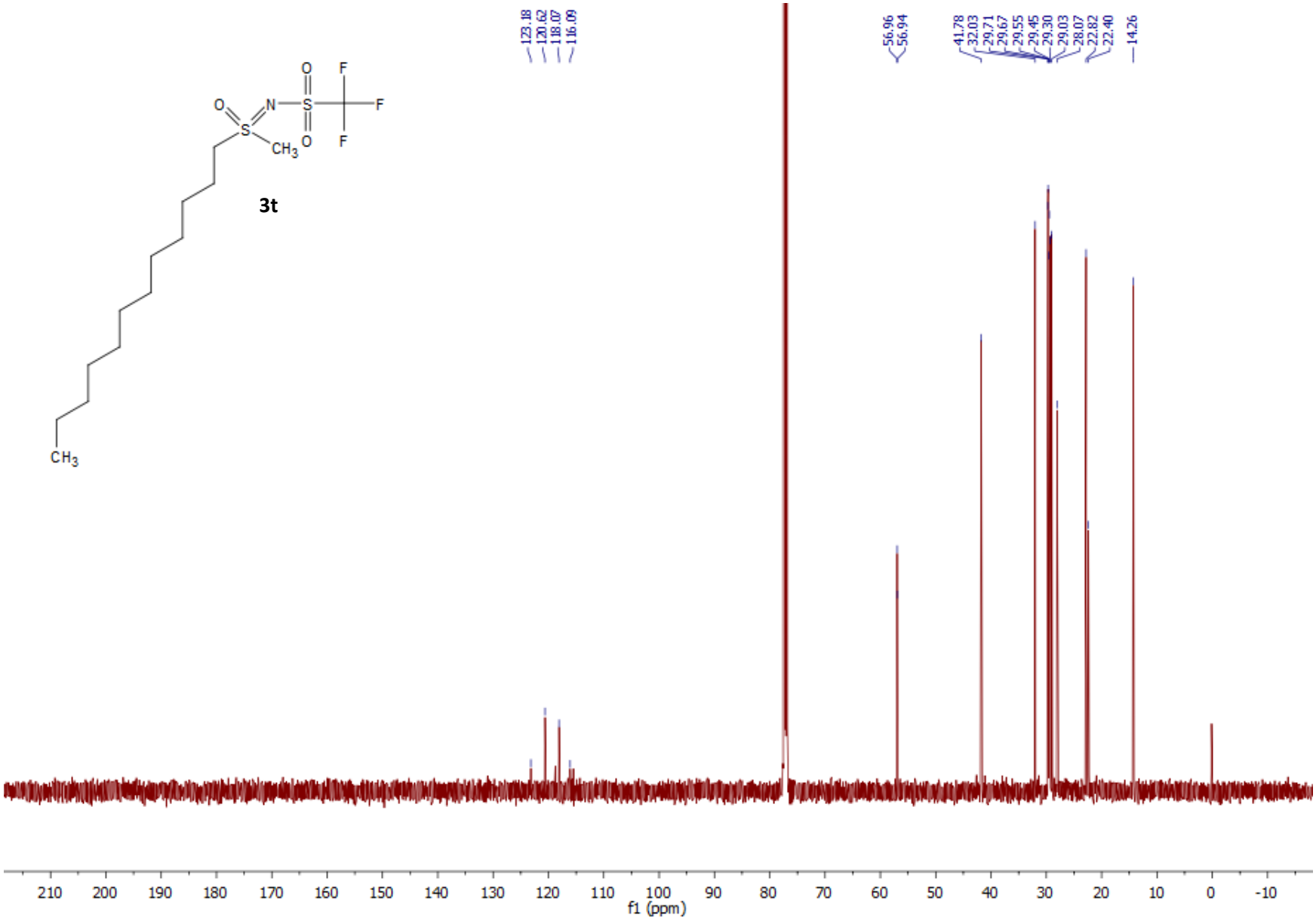

-78.80
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

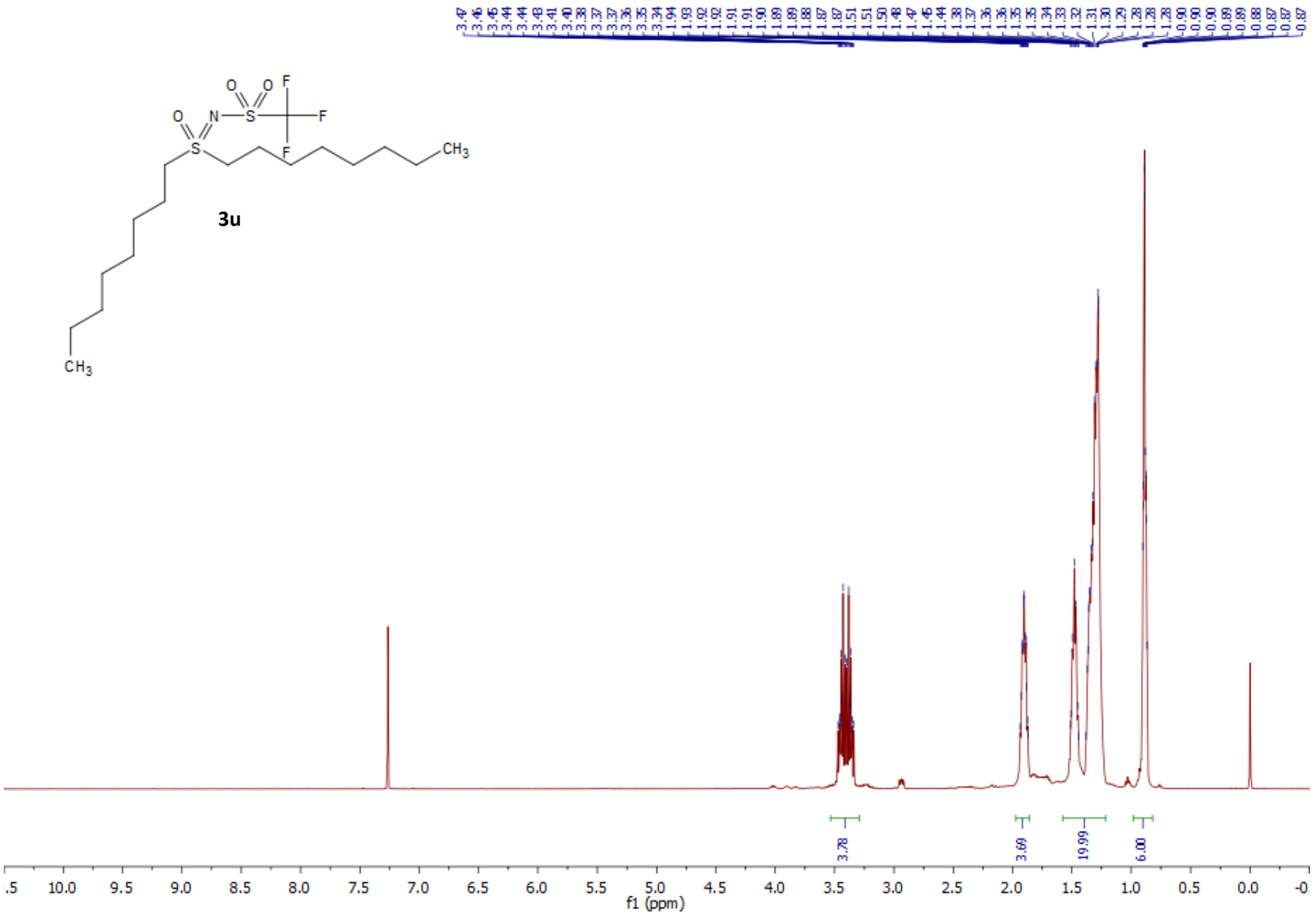

135.98
135.86
132.73
131.38
125.28
123.28
122.25
120.73
118.17
115.61
O
O
F
O
N
S
F
S
F
3s
123.28
122.25
120.73
118.17
115.61
124 123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

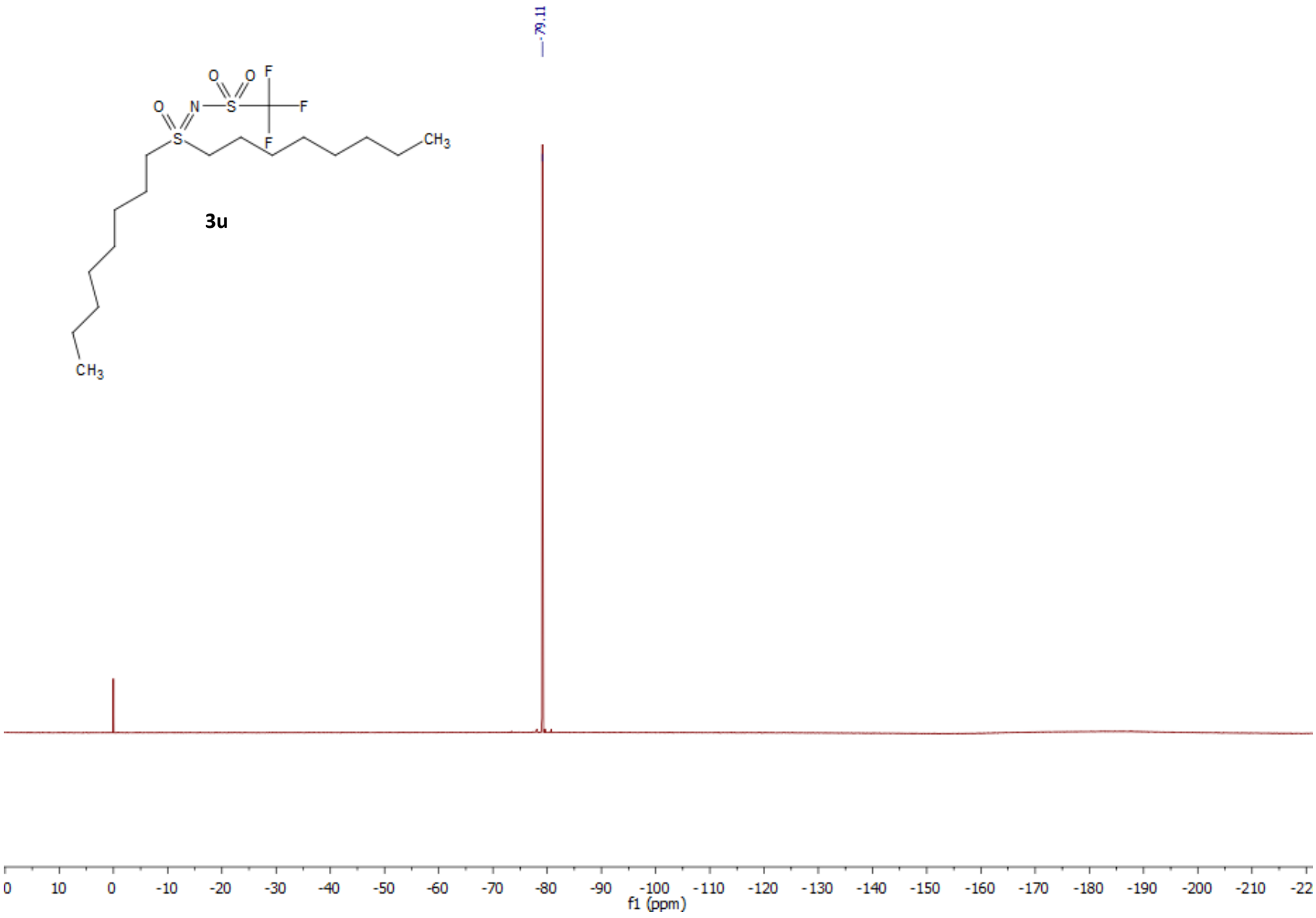

3t
f1 (ppm)

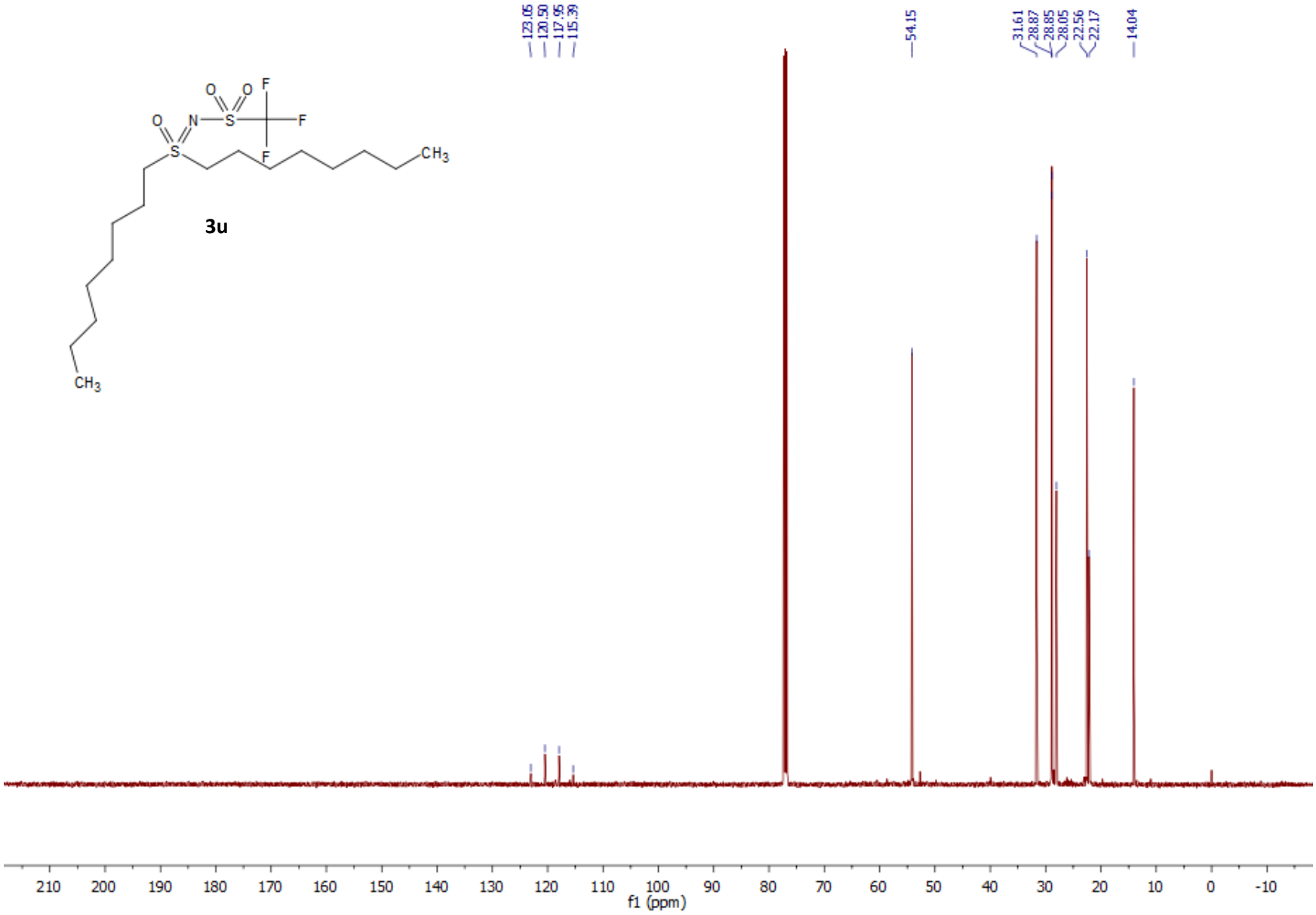

-79.15
O
F
O
N
S
F
O
S
F
CH3
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

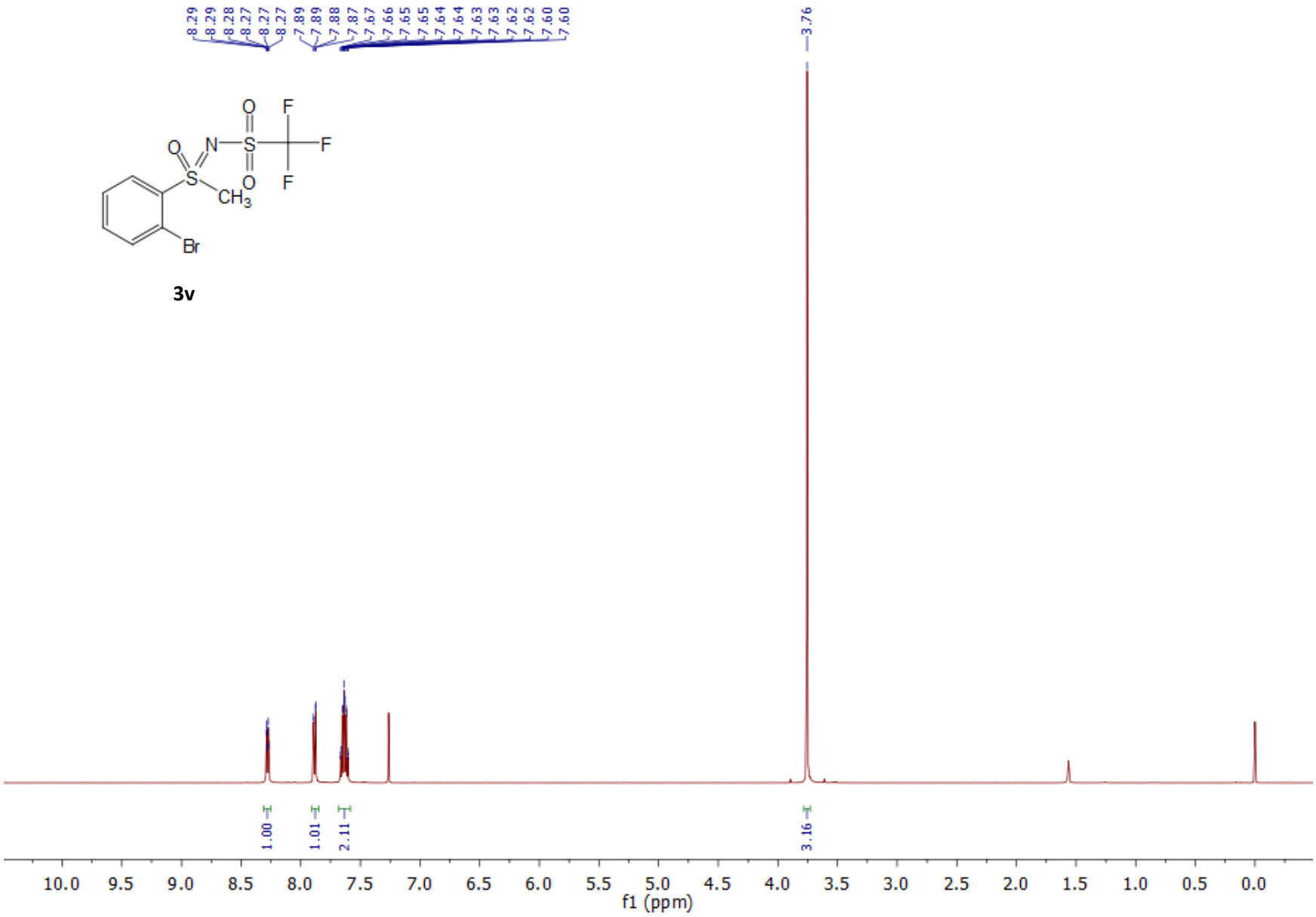
3t


123.18
120.62
118.07
116.09
56.96
56.94
41.78
32.03
29.71
29.67
29.55
29.45
29.30
29.03
28.07
22.82
22.40
14.26
O
N
S
F
F
F
O
O
CH3
CH3
3t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


3u
3.78
3.69
19.99
6.00
f1 (ppm)


-79.11
O
O
F
O
N
S
F
S
F
CH3
CH3
3u
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

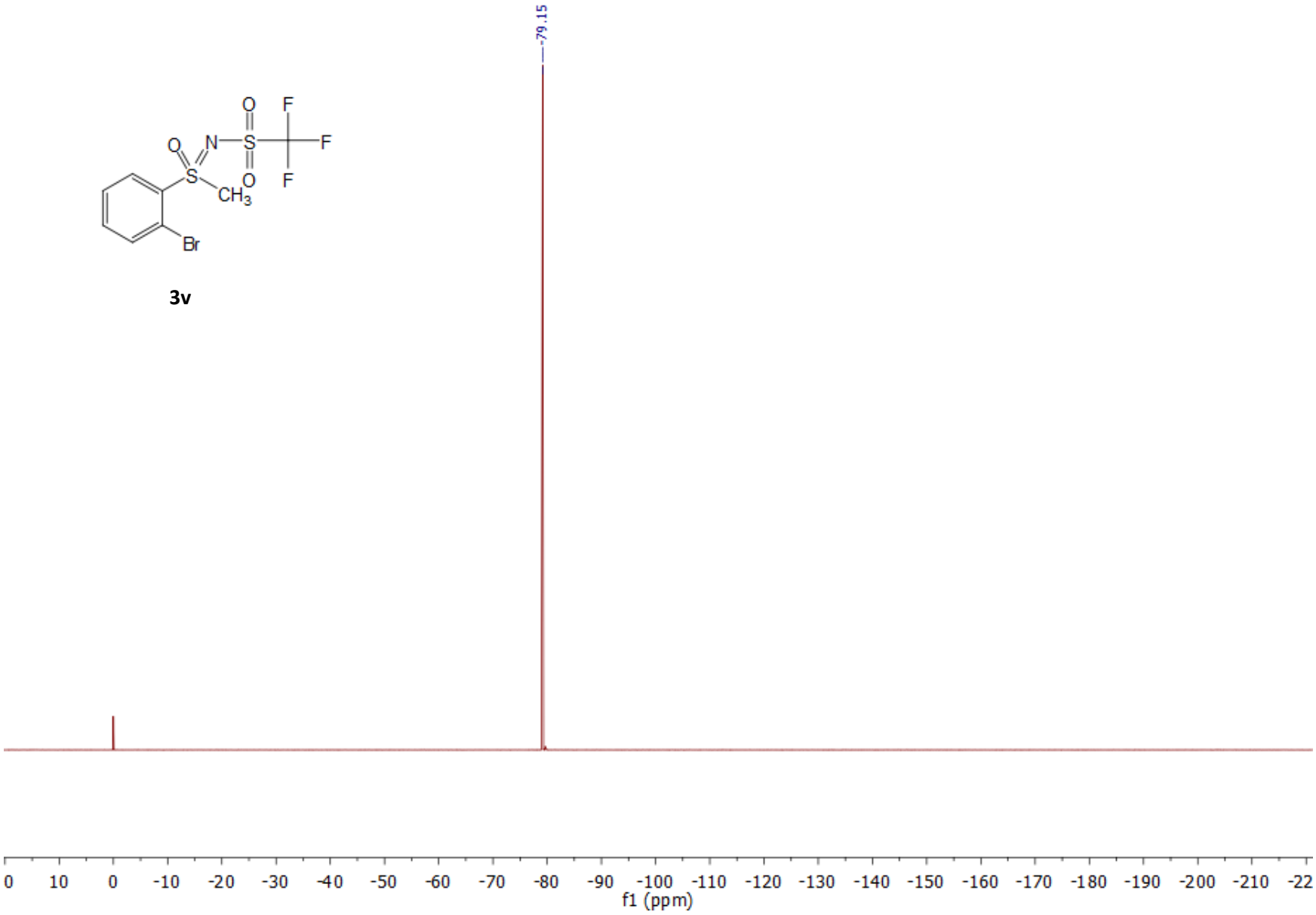

123.05
120.50
117.95
115.39
54.15
31.61
28.87
28.85
28.05
22.56
22.17
14.04
O
O
F
O
N
S
F
S
F
CH3
CH3
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

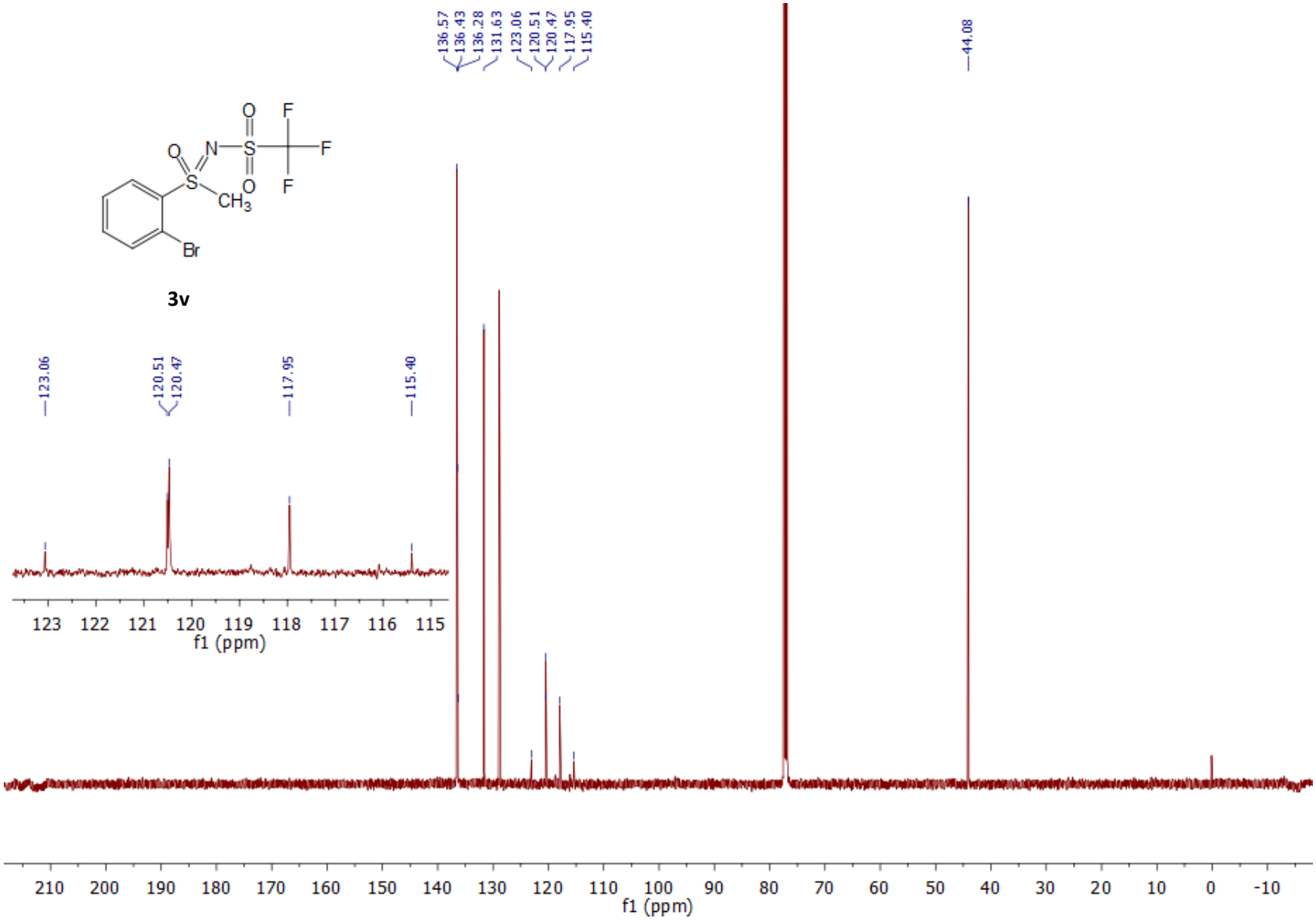

8.29
8.29
8.28
8.27
8.27
8.27
7.89
7.89
7.88
7.87
7.67
7.66
7.65
7.65
7.64
7.64
7.63
7.63
7.62
7.62
7.60
7.60
3.76
O
F
O
N
S
F
S
O
F
CH3
Br
1.00
1.01
2.11
3.16
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

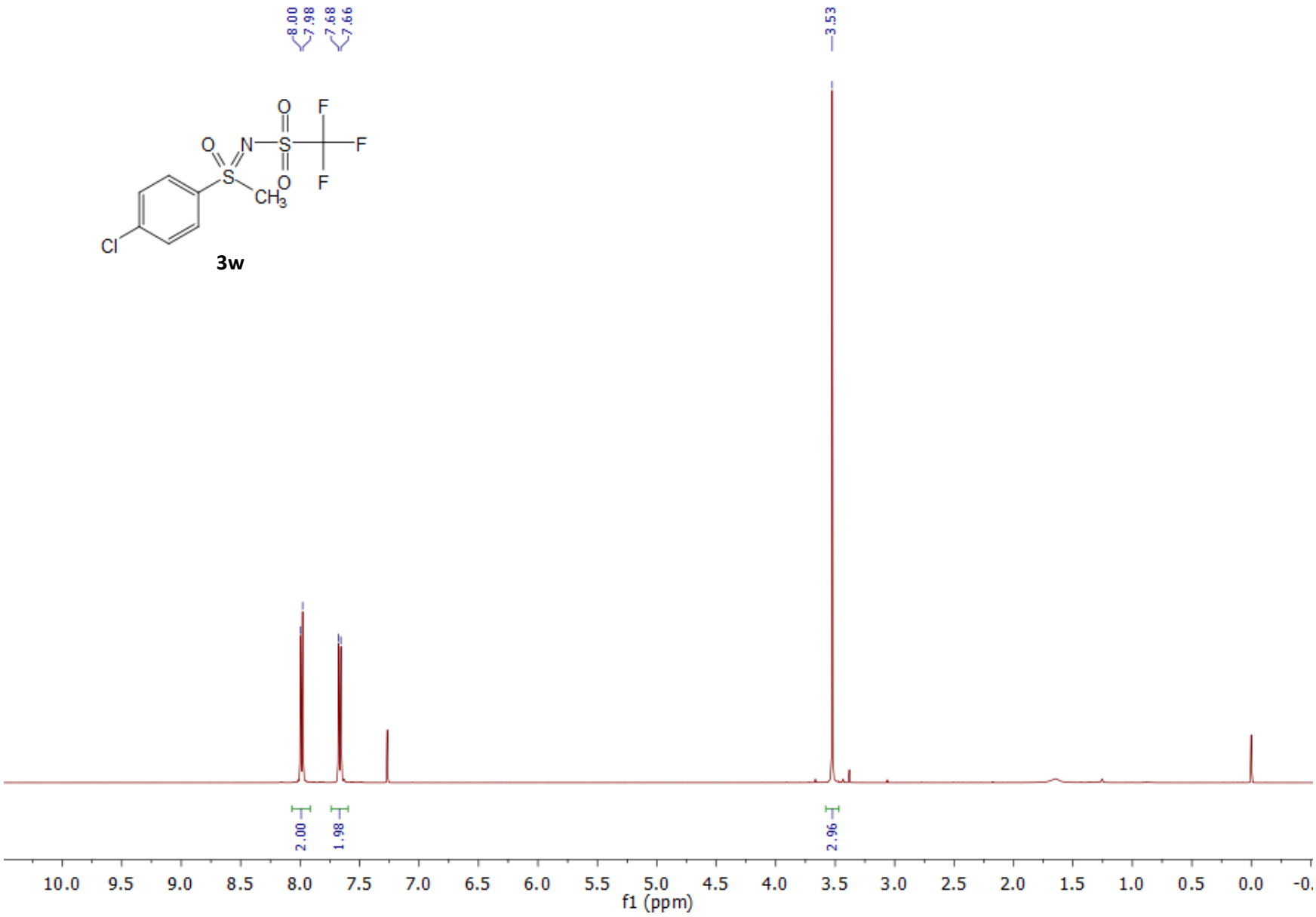
3v

O
F
O
N
S
F
S
O
F
CH3
Br

3v


-79.15
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

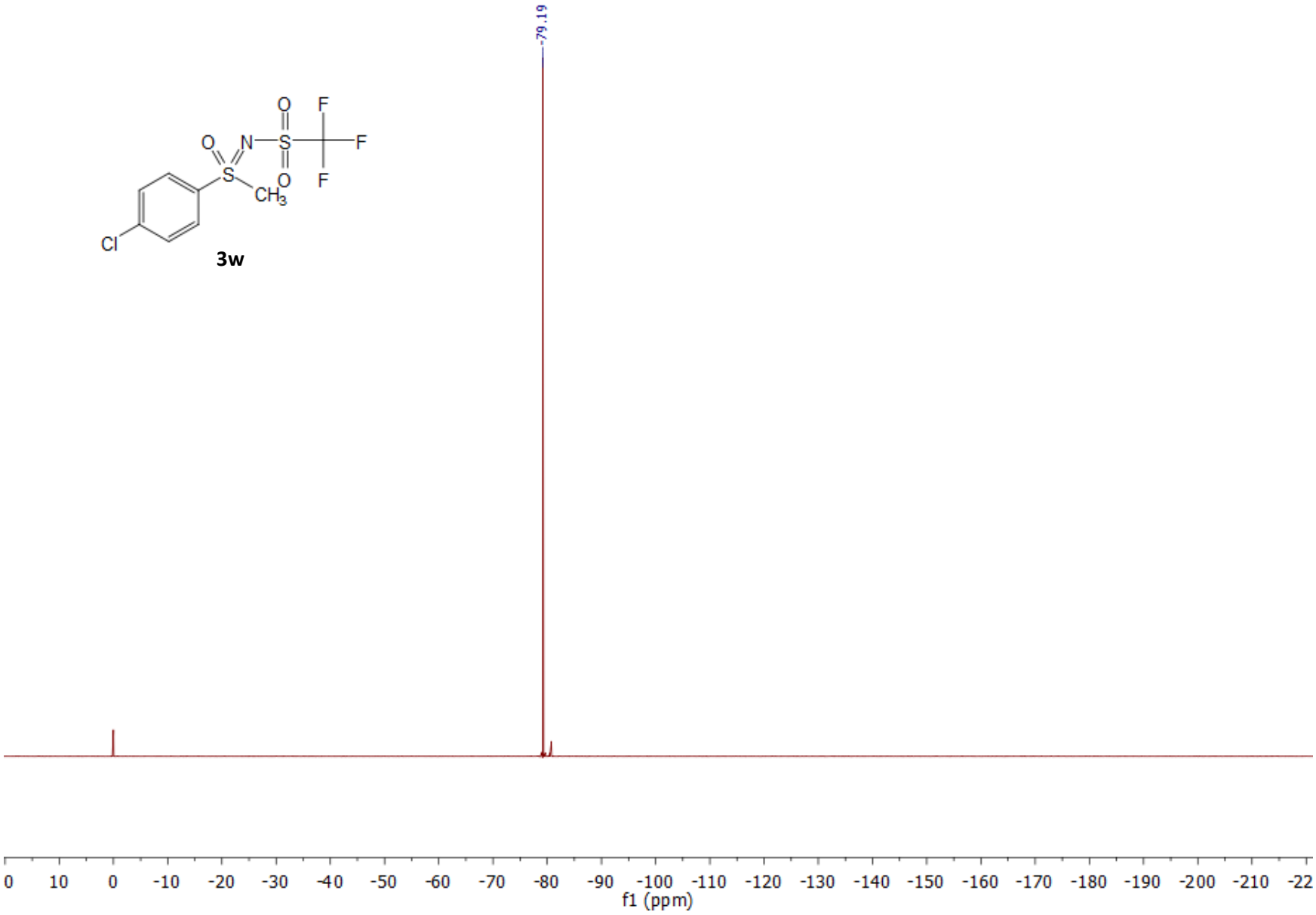

136.57
136.43
136.28
131.63
123.06
120.51
120.47
117.95
115.40
44.08
O
F
O
N
S
F
O
S
F
CH3
Br
3v
123.06
120.51
120.47
117.95
115.40
123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

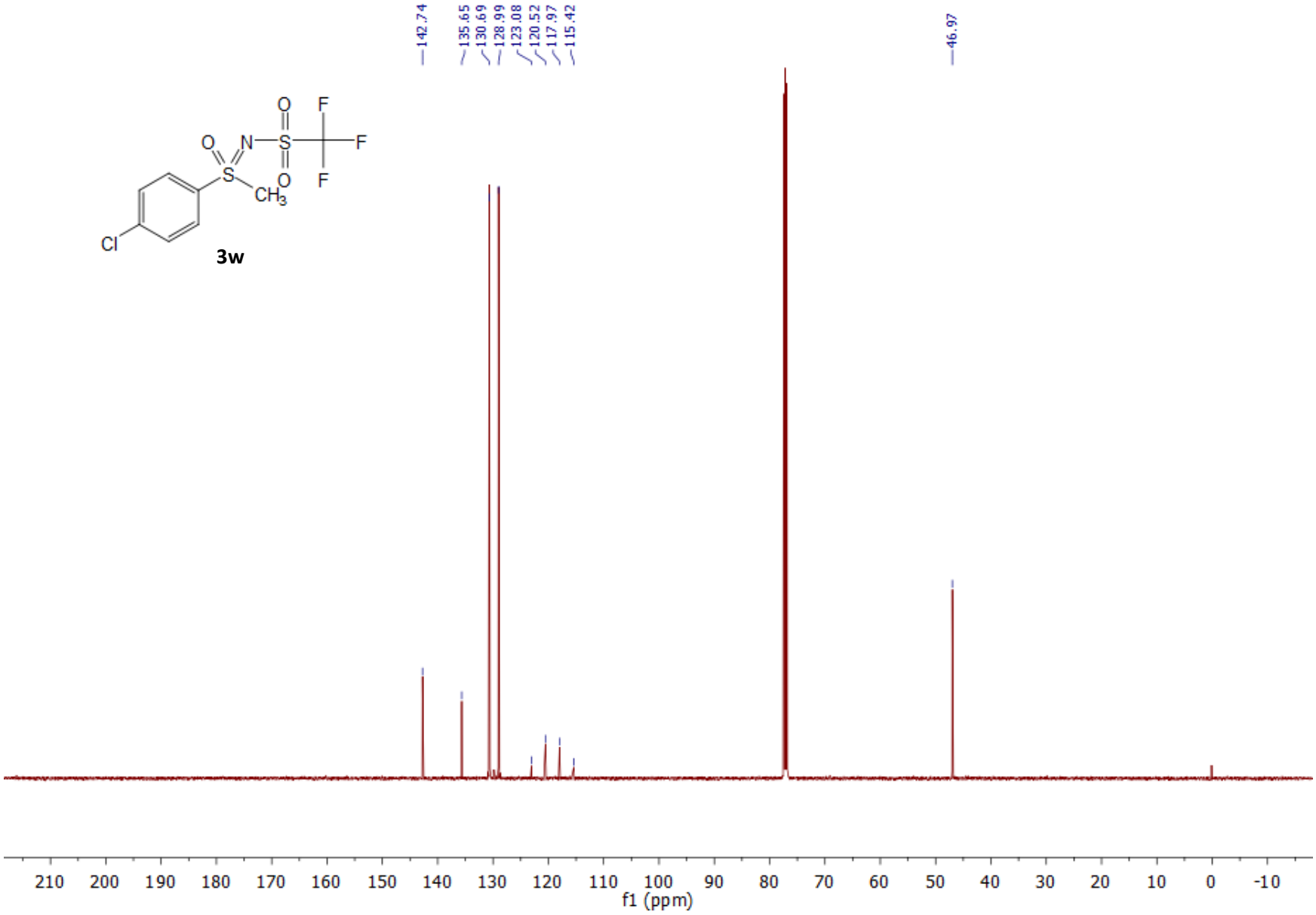

8.00
7.98
7.68
7.66
3.53
O
F
O
N
S
F
O
S
F
CH3
Cl
2.00
1.98
2.96
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

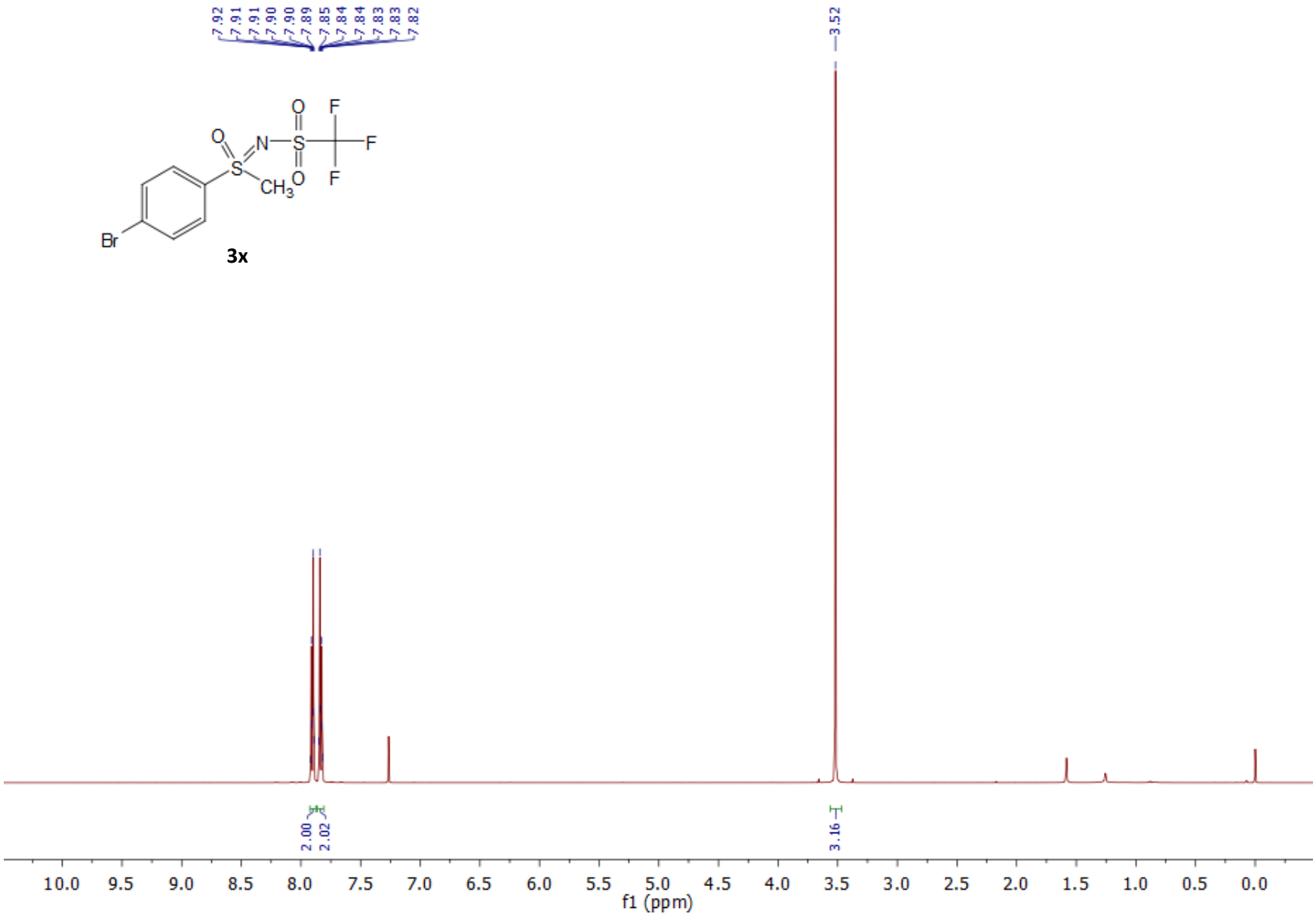
3w

O
F
O
N
S
F
S
O
F
CH3
Cl

3w


-79.19
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

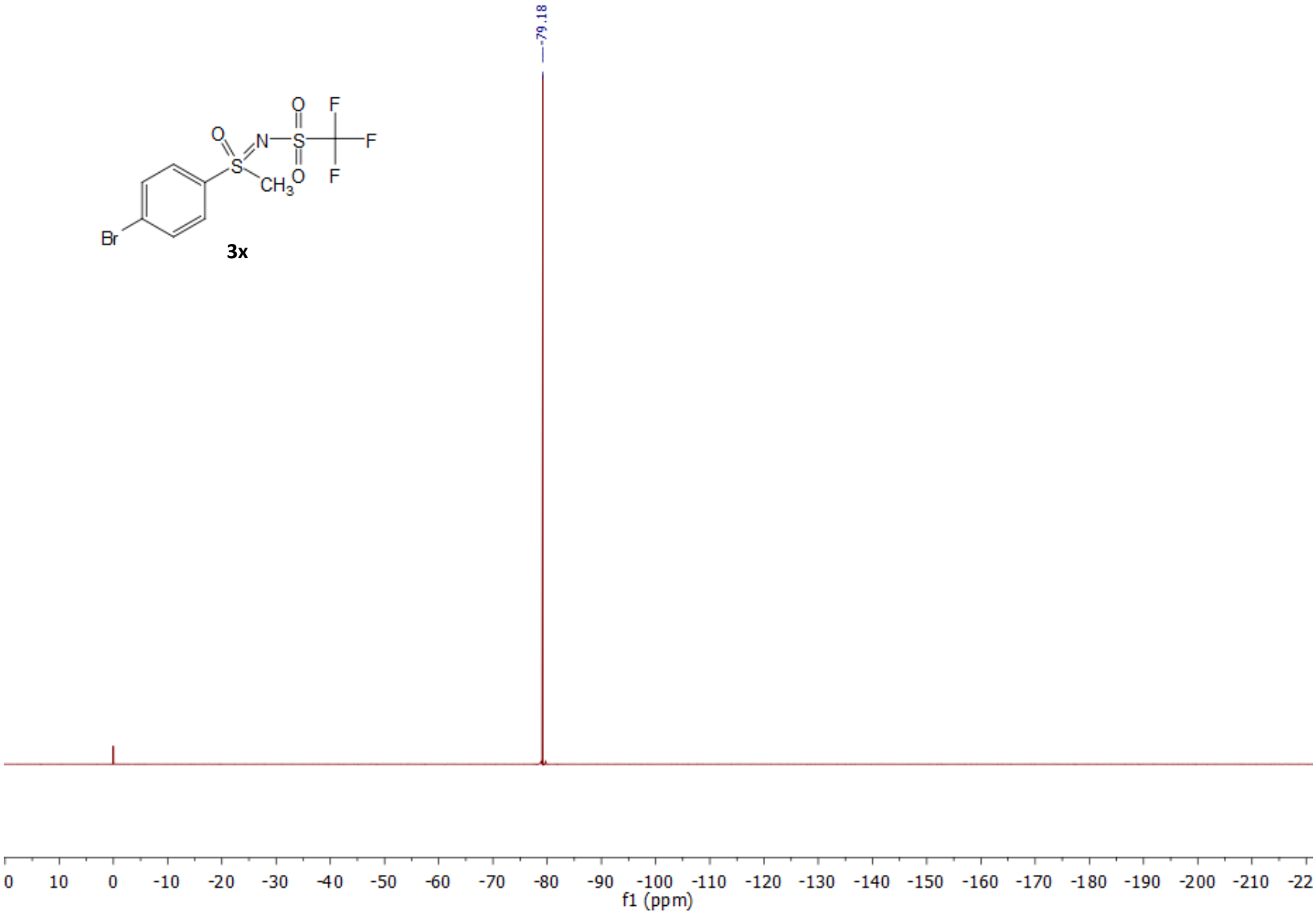

142.74
135.65
130.69
128.99
123.08
120.52
117.97
115.42
46.97
O
F
O
N
S
F
S
F
O
CH3
Cl
3w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.92
7.91
7.91
7.90
7.90
7.89
7.85
7.84
7.84
7.83
7.83
7.82
3.52
O
F
O
N
S
F
S
CH3
O
F
Br
2.00
2.02
3.16
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3x

O
F
O
N
S
F
S
CH3
O
F
Br

3x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-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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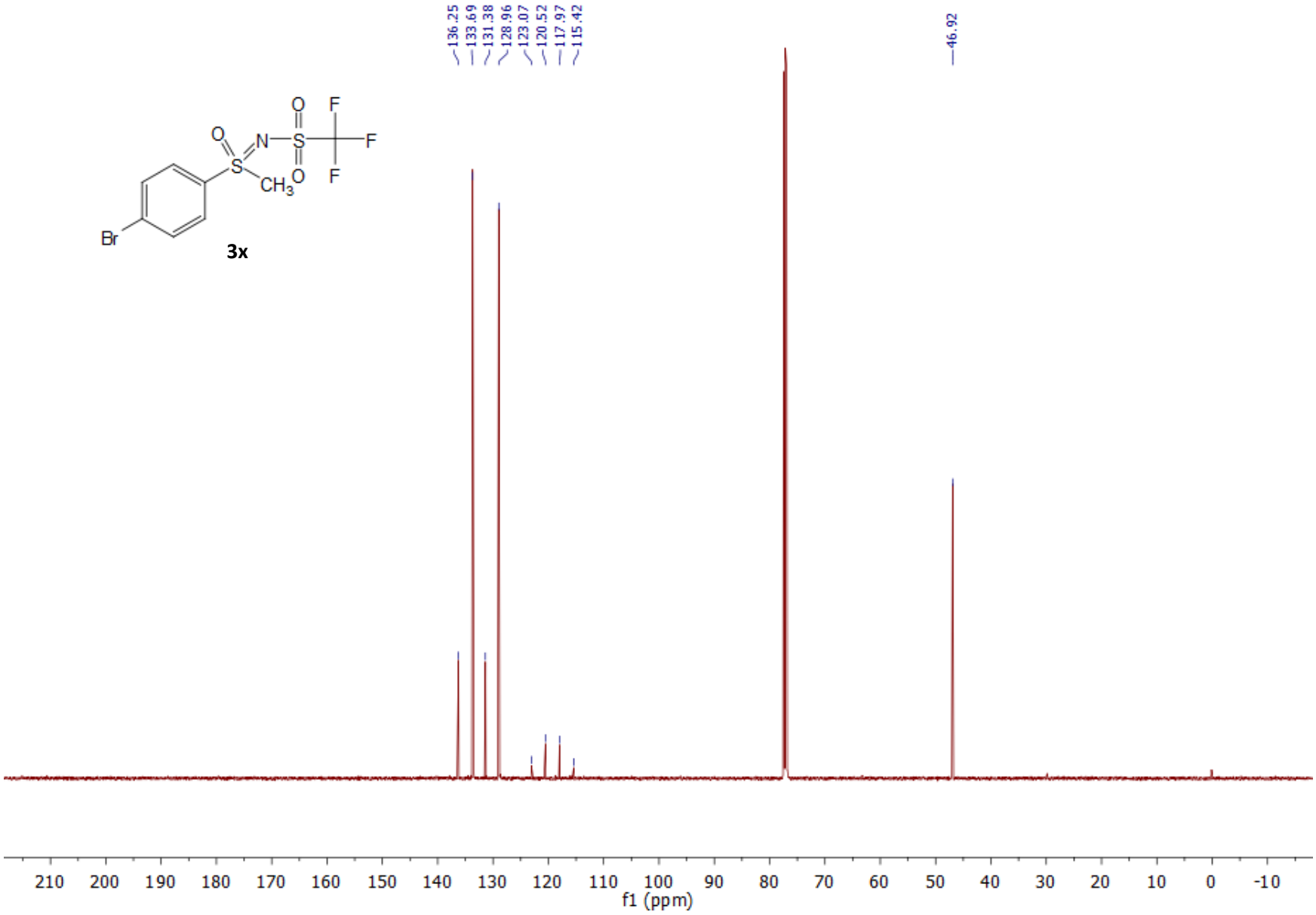
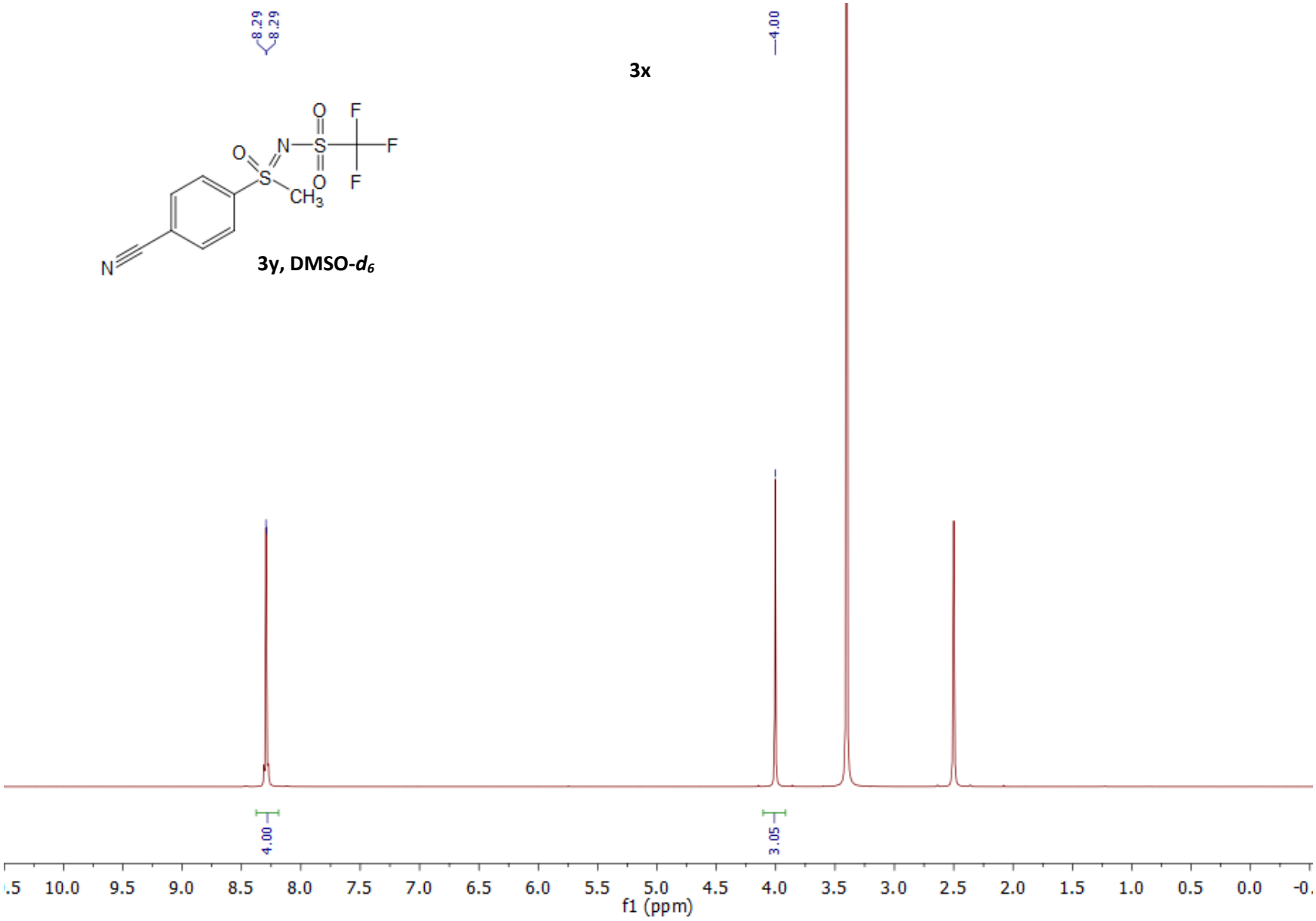
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

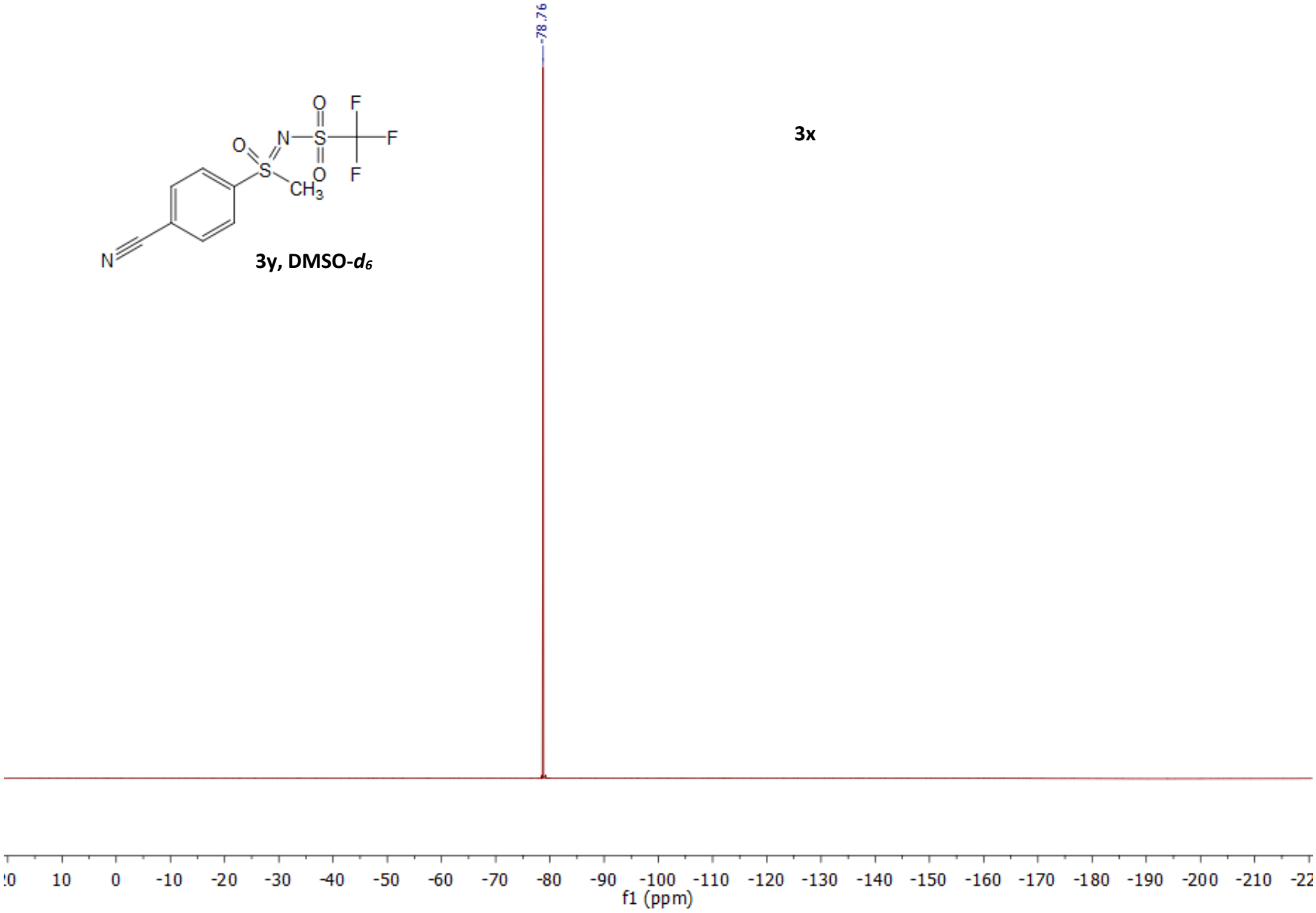

136.25
133.69
131.38
128.96
123.07
120.52
117.97
115.42
46.92
O
F
O
N
S
F
S
F
O
CH3
Br
3x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.29
8.29
4.00
3x
O
F
N
S
F
O
S
F
O
CH3
N
3y, DMSO-d6
4.00
3.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

O
F
N
S
F
O
S
O
F
CH3
N

3y, DMSO-*d*$_6$

3x


-78.76
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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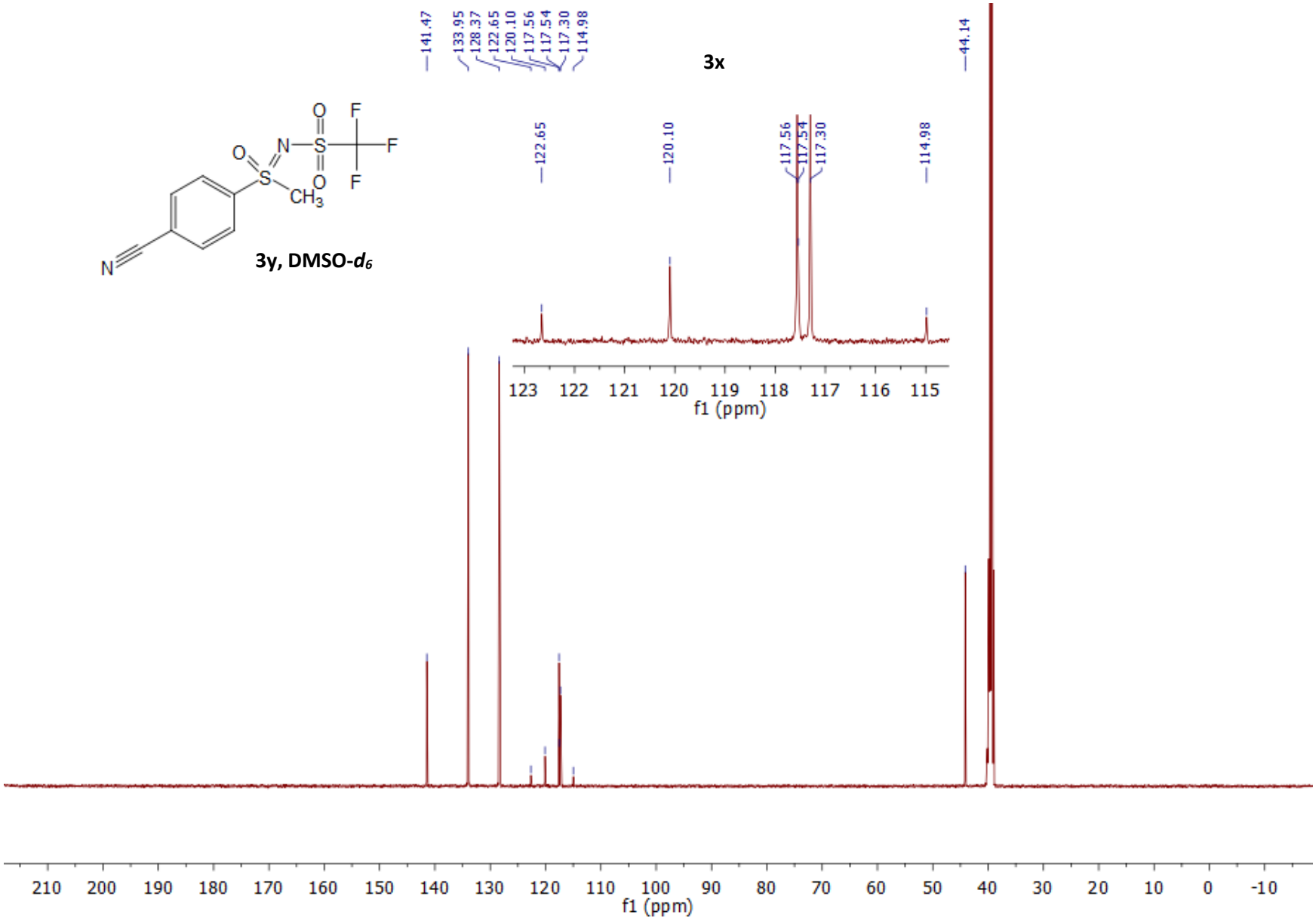
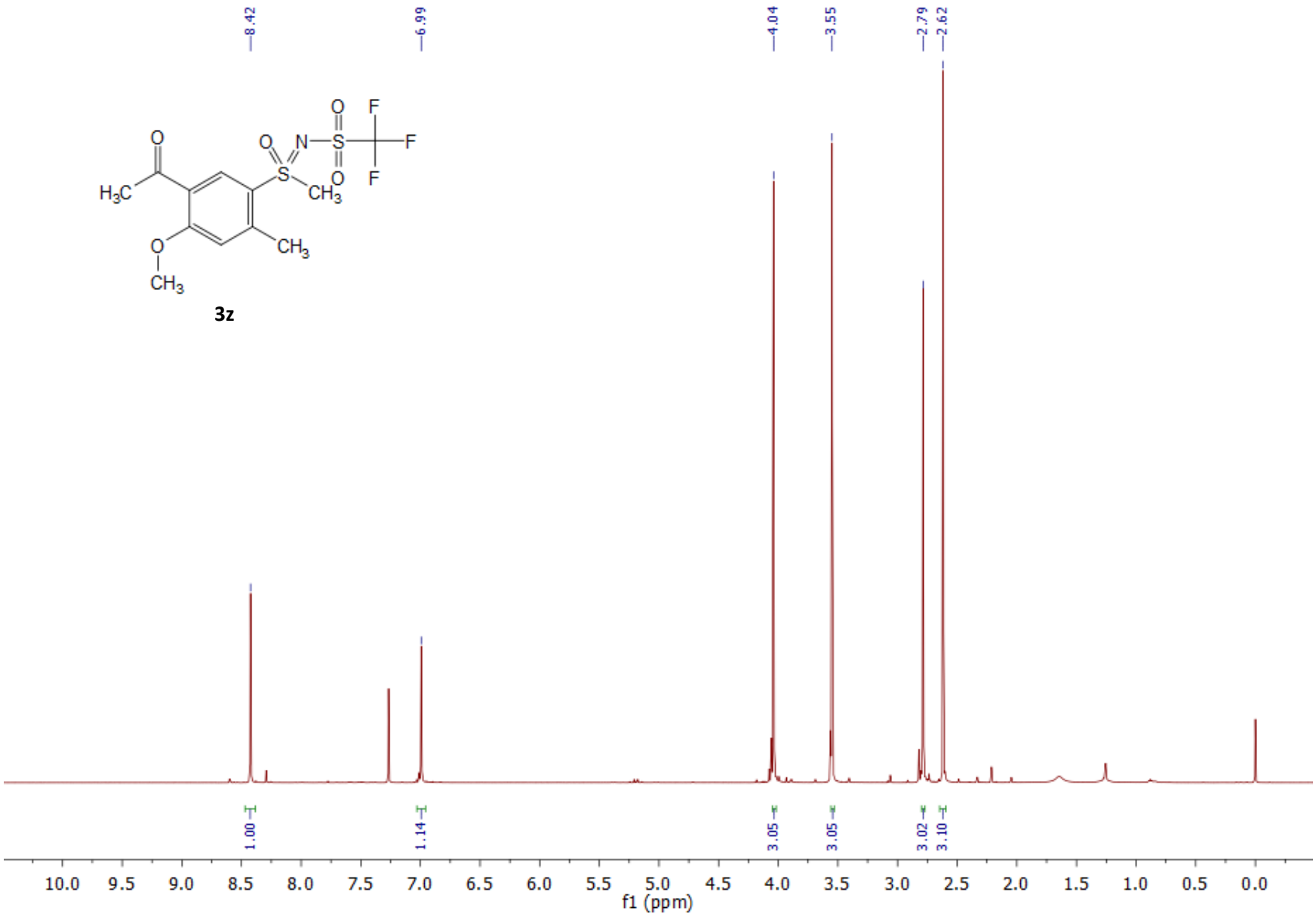
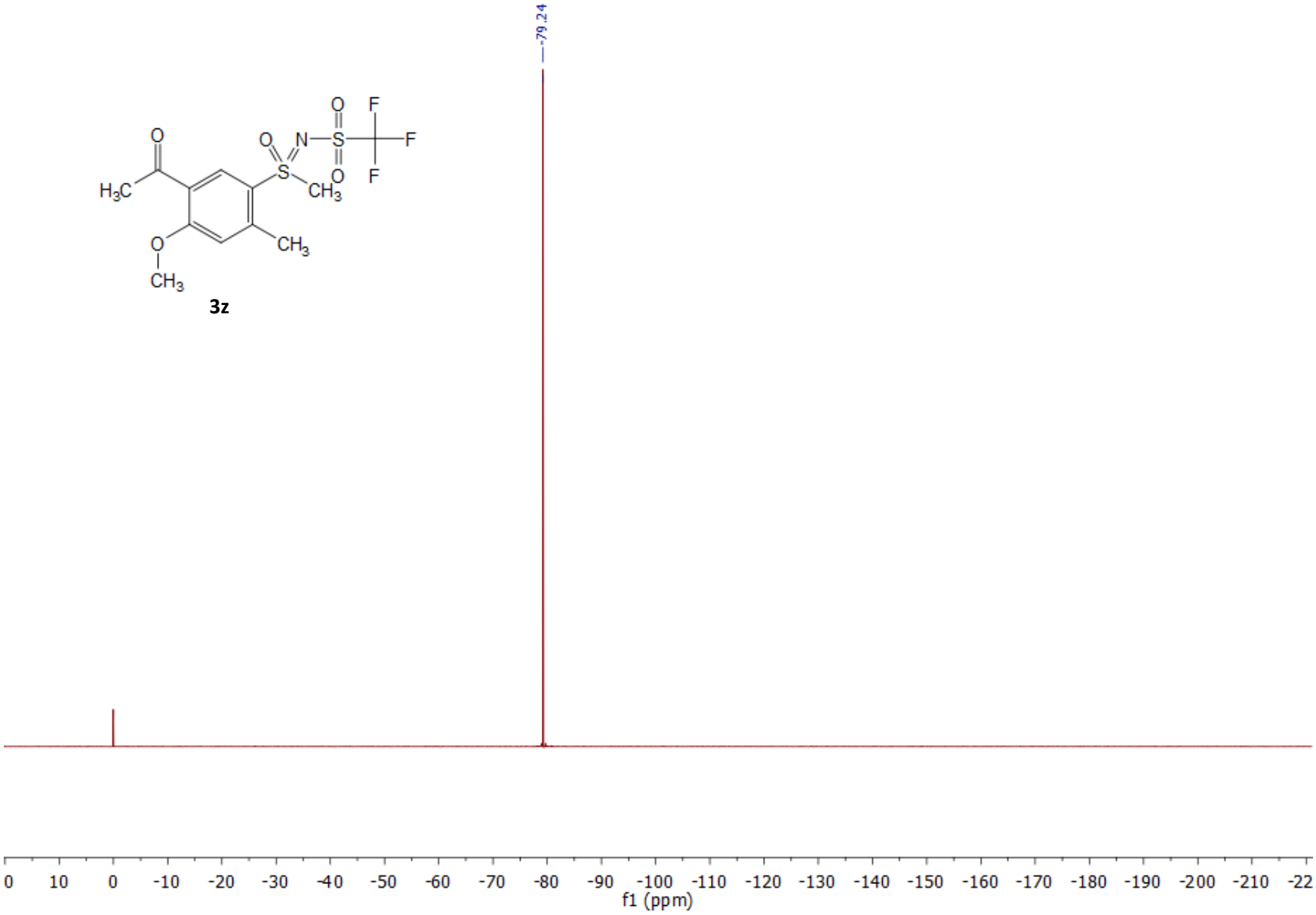
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

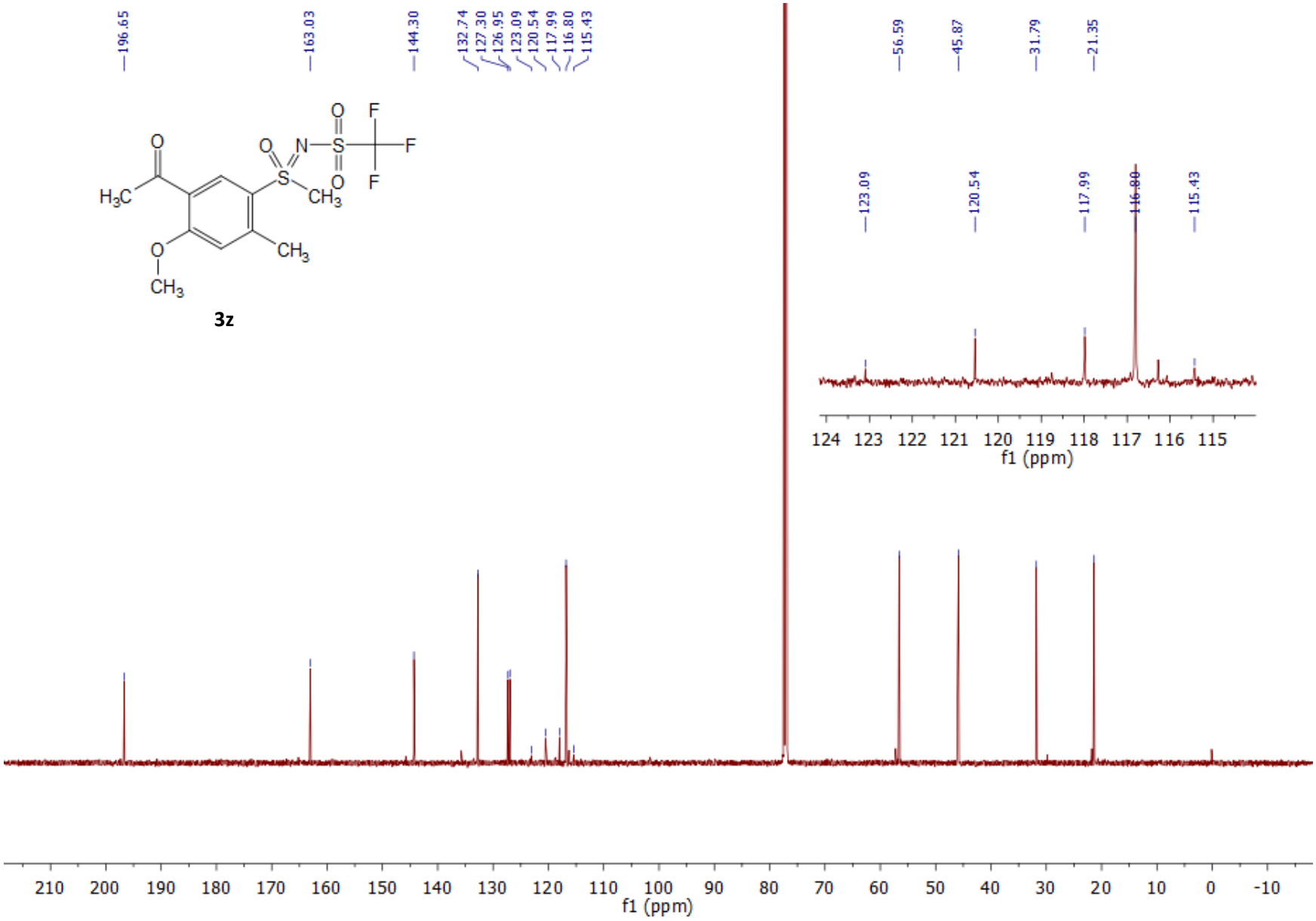

141.47
133.95
128.37
122.65
120.10
117.56
117.54
117.30
114.98
44.14
3x
3y, DMSO-d_6
f1 (ppm)
f1 (ppm)


8.42
6.99
4.04
3.55
2.79
2.62
1.00
1.14
3.05
3.05
3.02
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

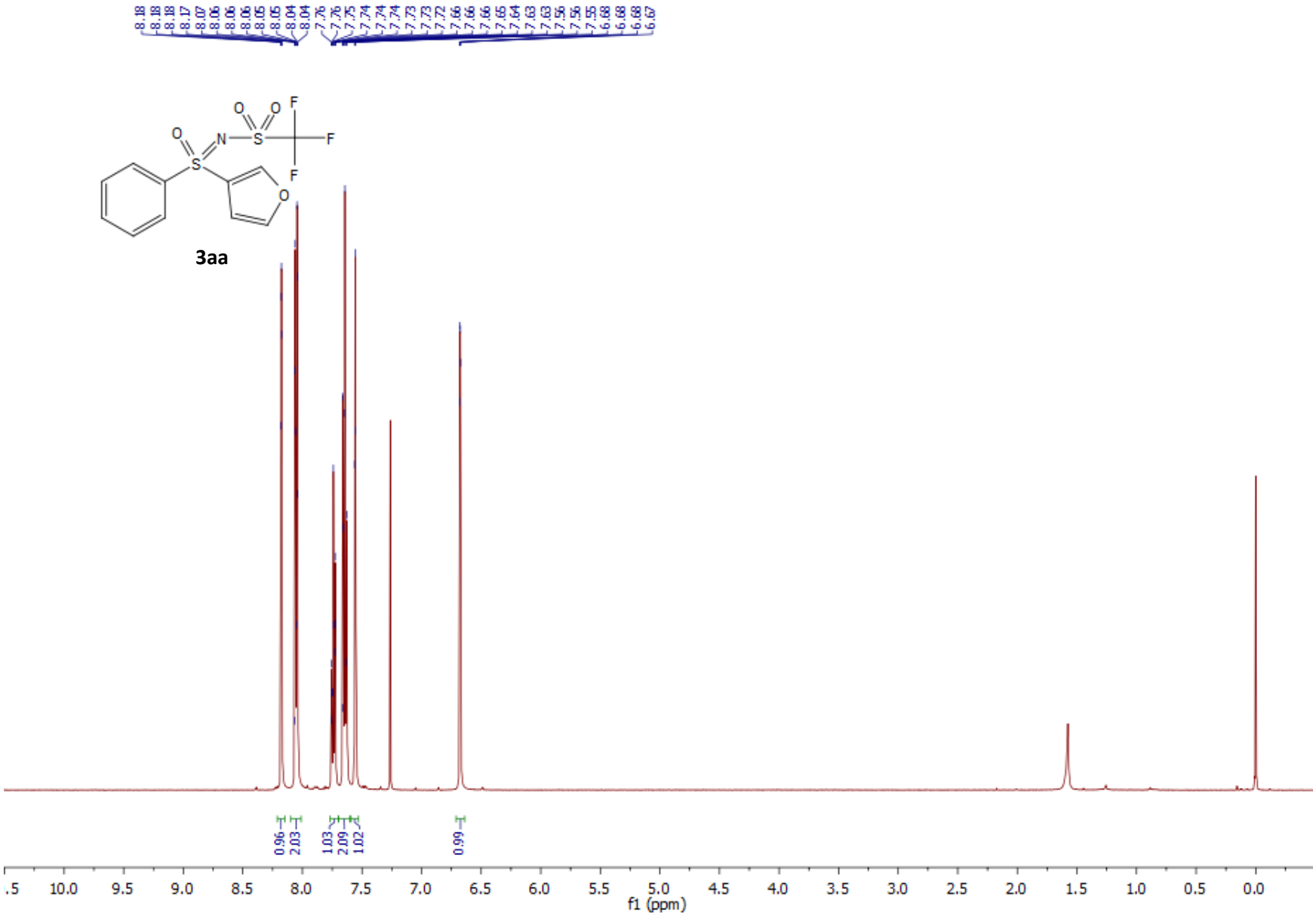
3z

3z


-79.24
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

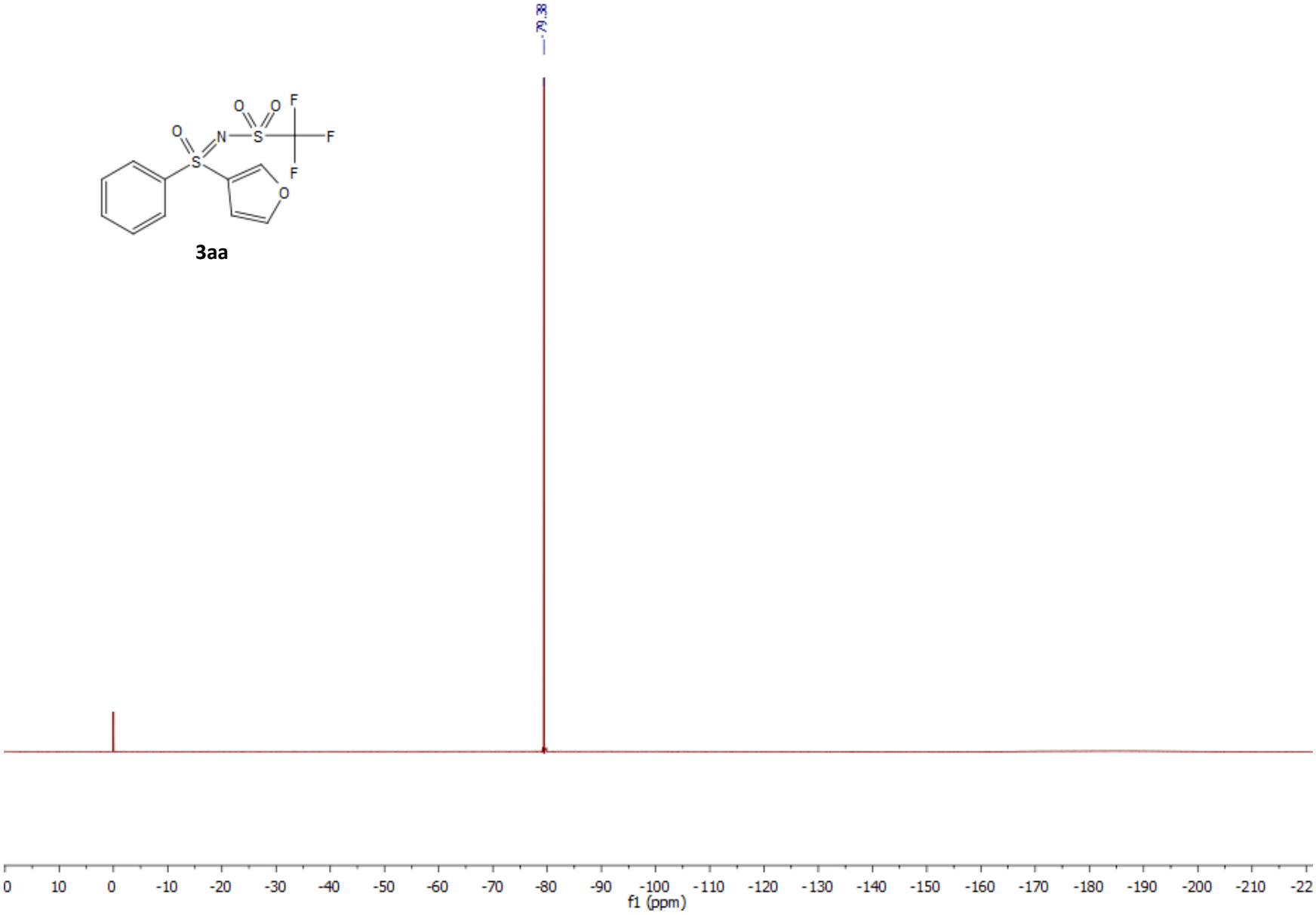

196.65
163.03
144.30
132.74
127.30
126.95
123.09
120.54
117.99
116.80
115.43
56.59
45.87
31.79
21.35
123.09
120.54
117.99
116.80
115.43
124 123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

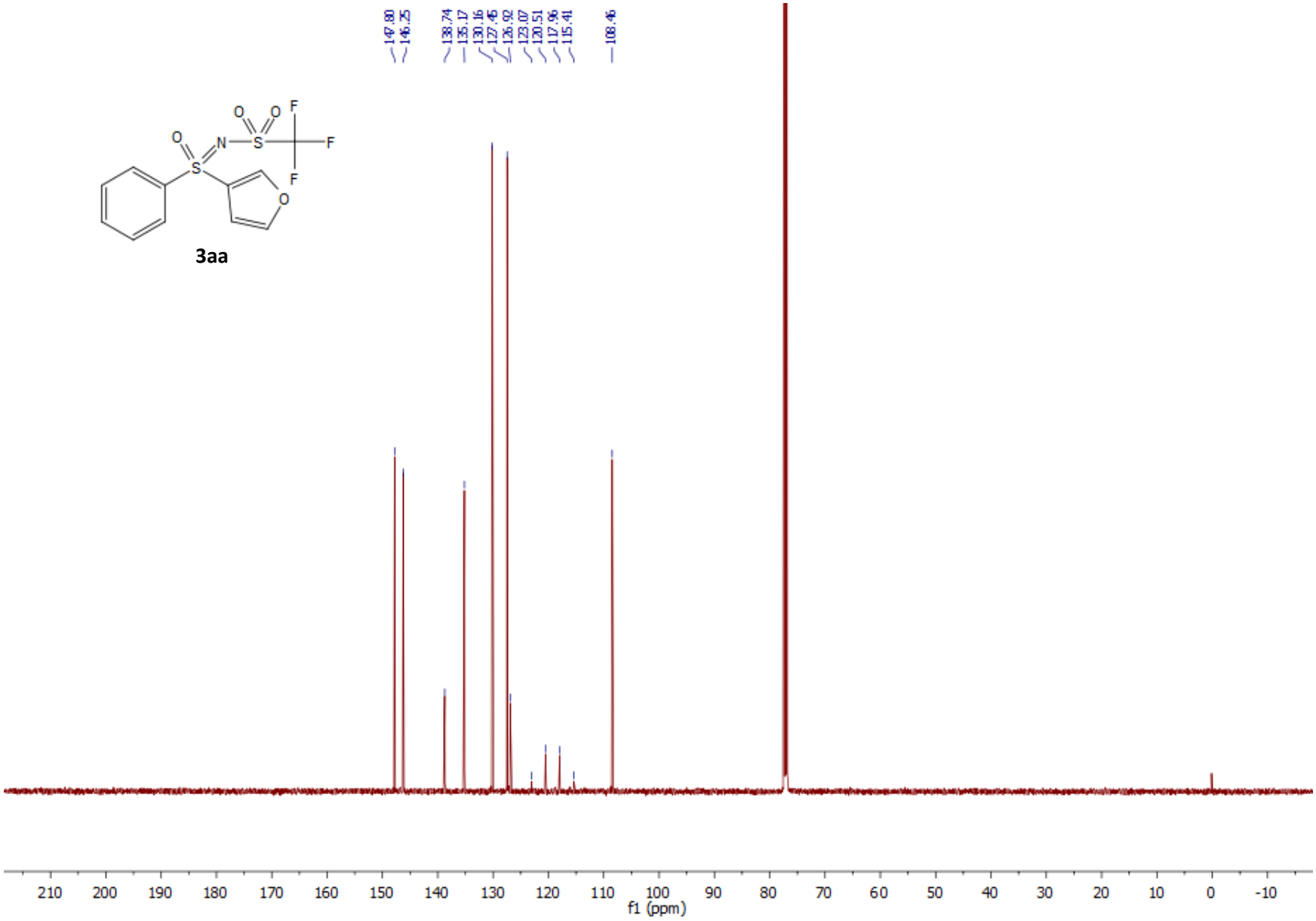
3z

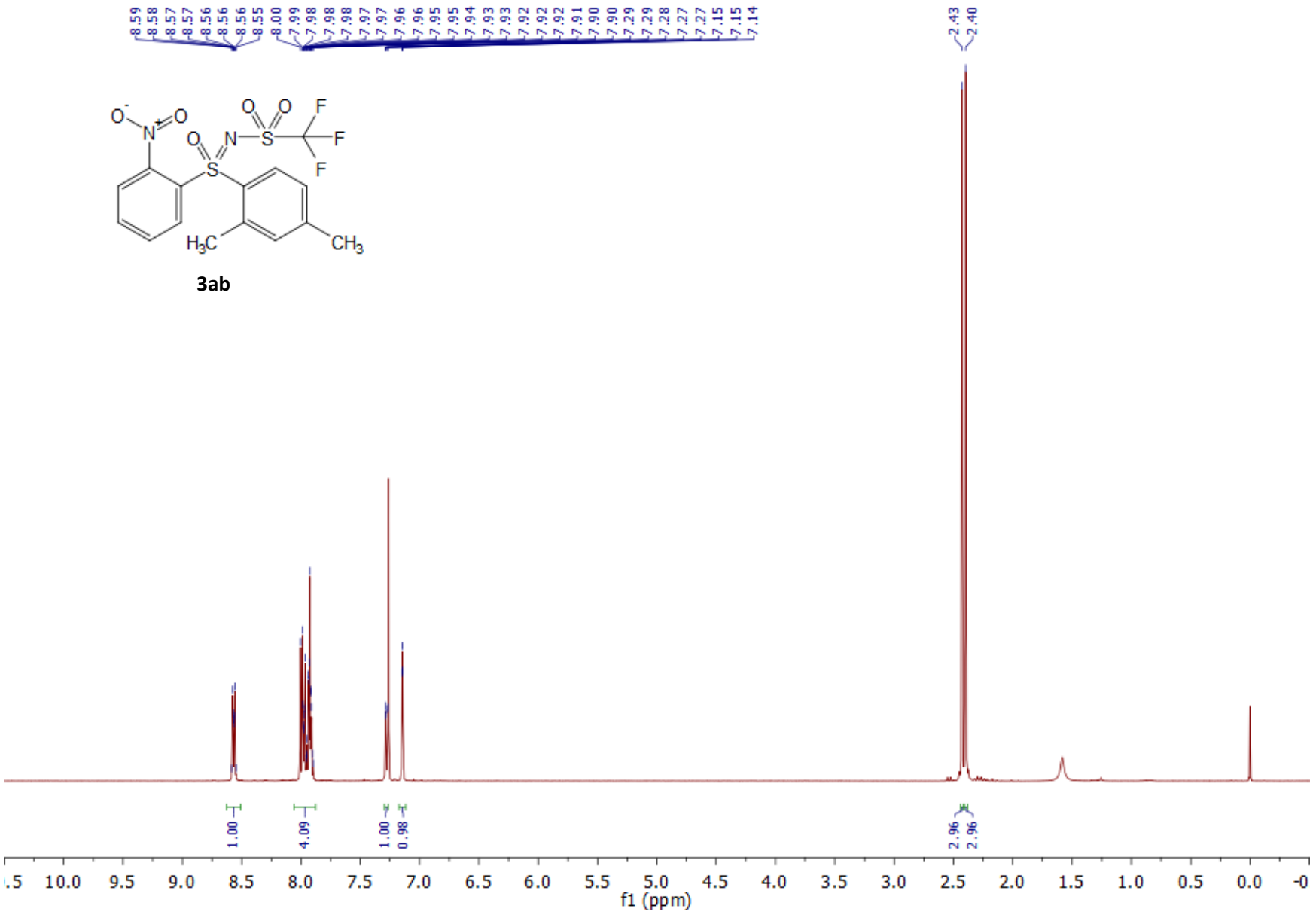

8.18
8.18
8.18
8.17
8.07
8.06
8.06
8.06
8.05
8.05
8.04
8.04
7.76
7.76
7.75
7.74
7.74
7.74
7.73
7.73
7.72
7.66
7.66
7.65
7.64
7.63
7.63
7.56
7.56
7.55
6.68
6.68
6.67
O
O
F
O
N
S
F
S
F
O
3aa
0.96
2.03
1.03
2.09
1.02
0.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

O
O
F
O
N
S
F
S
F
O

3aa

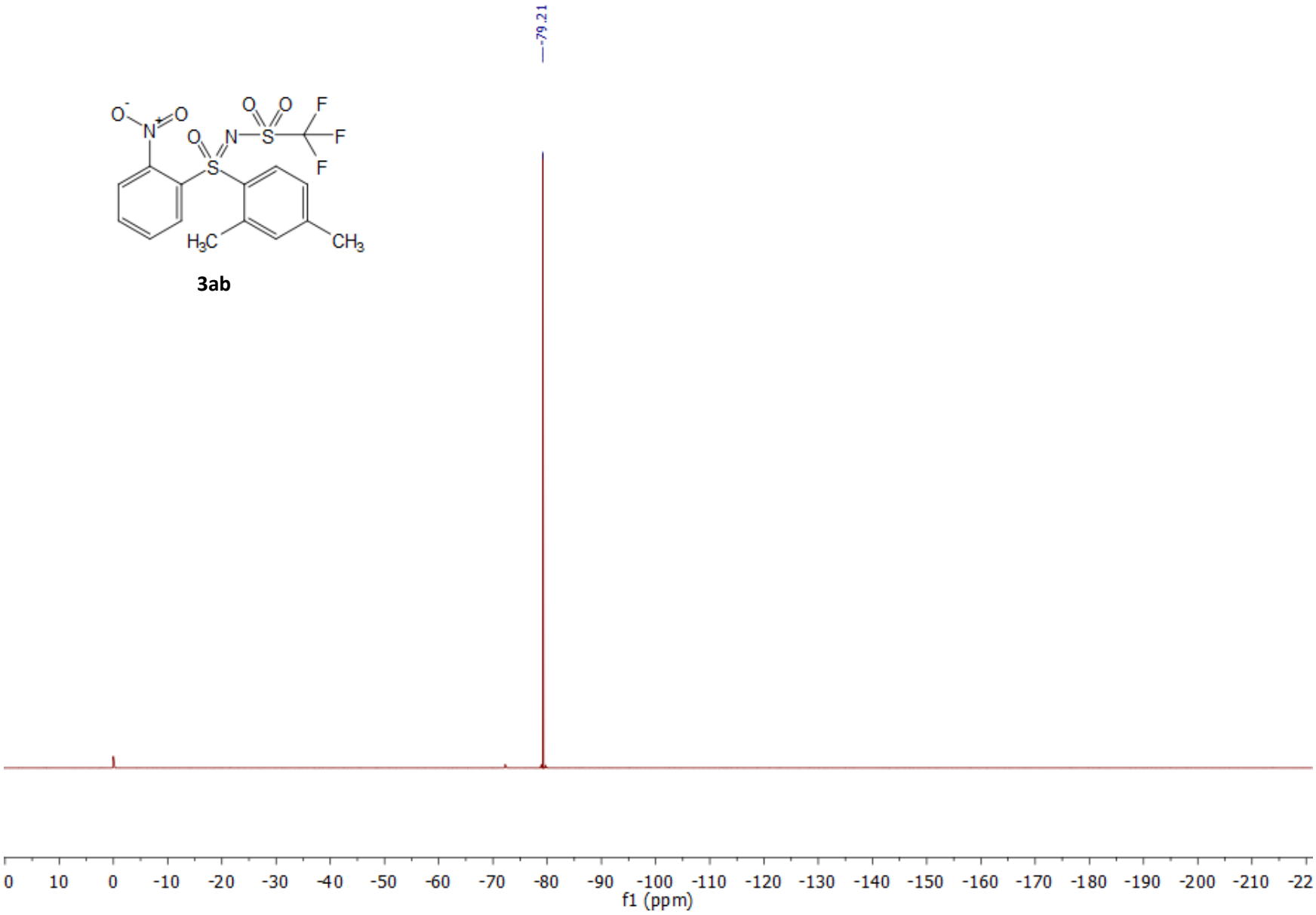

-79.38
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

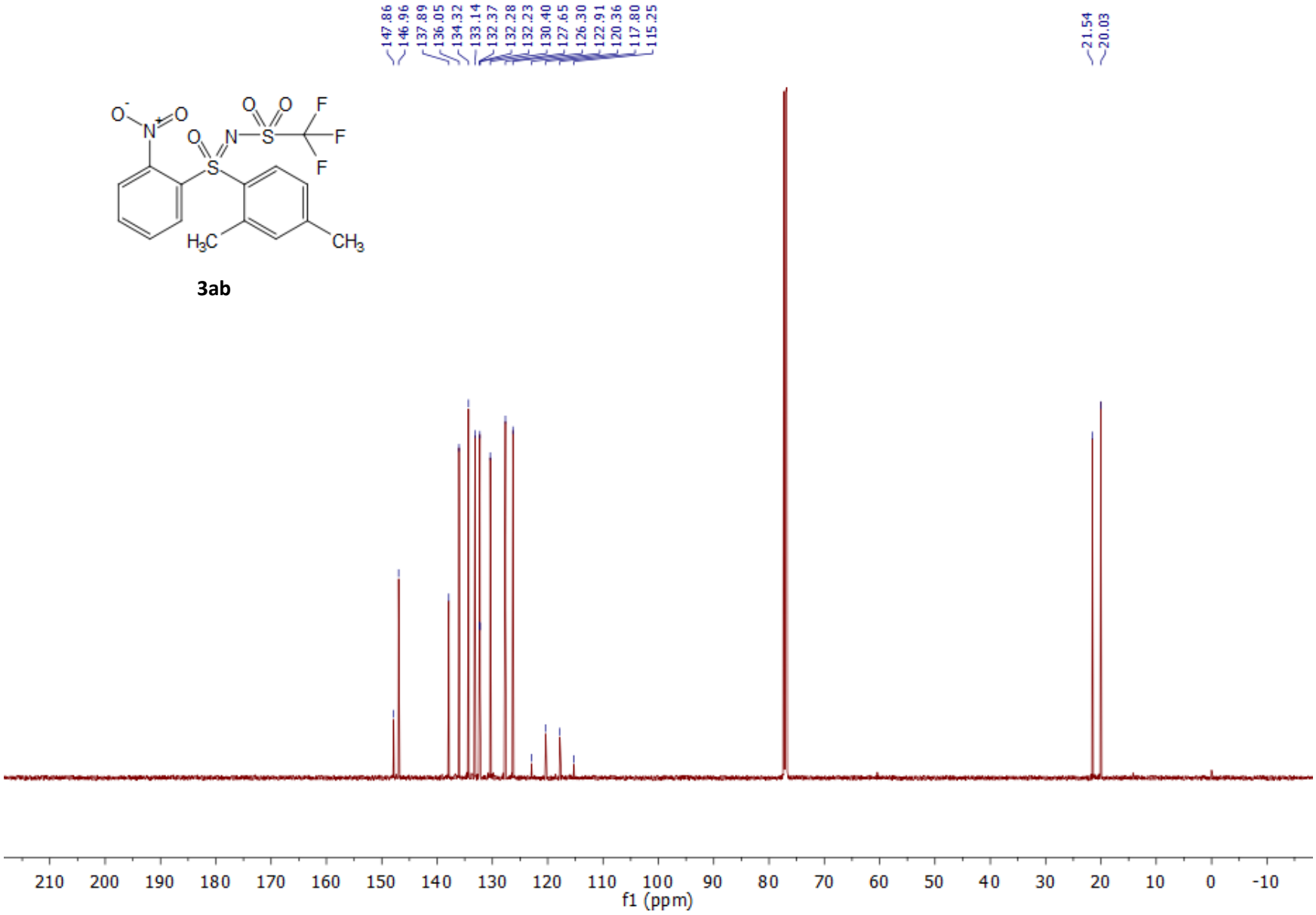

149.80
146.25
138.74
135.17
130.16
127.45
126.92
123.07
120.51
117.96
115.41
108.46
O
O
F
O
N
S
S
F
F
O
3aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.59
8.58
8.57
8.57
8.56
8.56
8.56
8.55
8.00
7.99
7.98
7.98
7.98
7.97
7.97
7.96
7.96
7.95
7.95
7.94
7.93
7.93
7.92
7.92
7.92
7.91
7.90
7.90
7.29
7.29
7.28
7.27
7.27
7.15
7.15
7.14
2.43
2.40
O
N
O
O
N
S
O
O
S
F
F
F
H3C
CH3
1.00
4.09
1.00
0.98
2.96
2.96
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

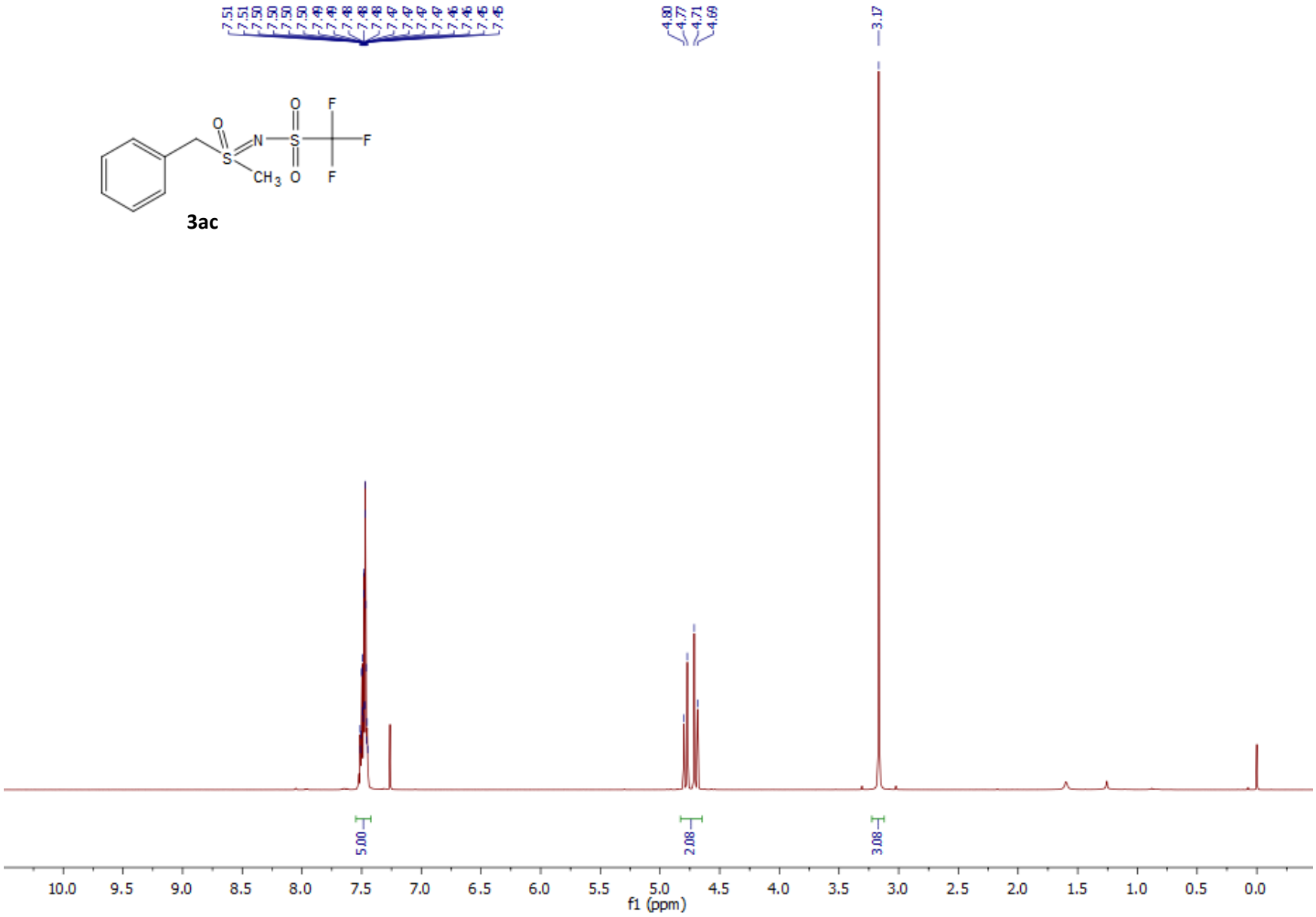
3ab

3ab


-79.21
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

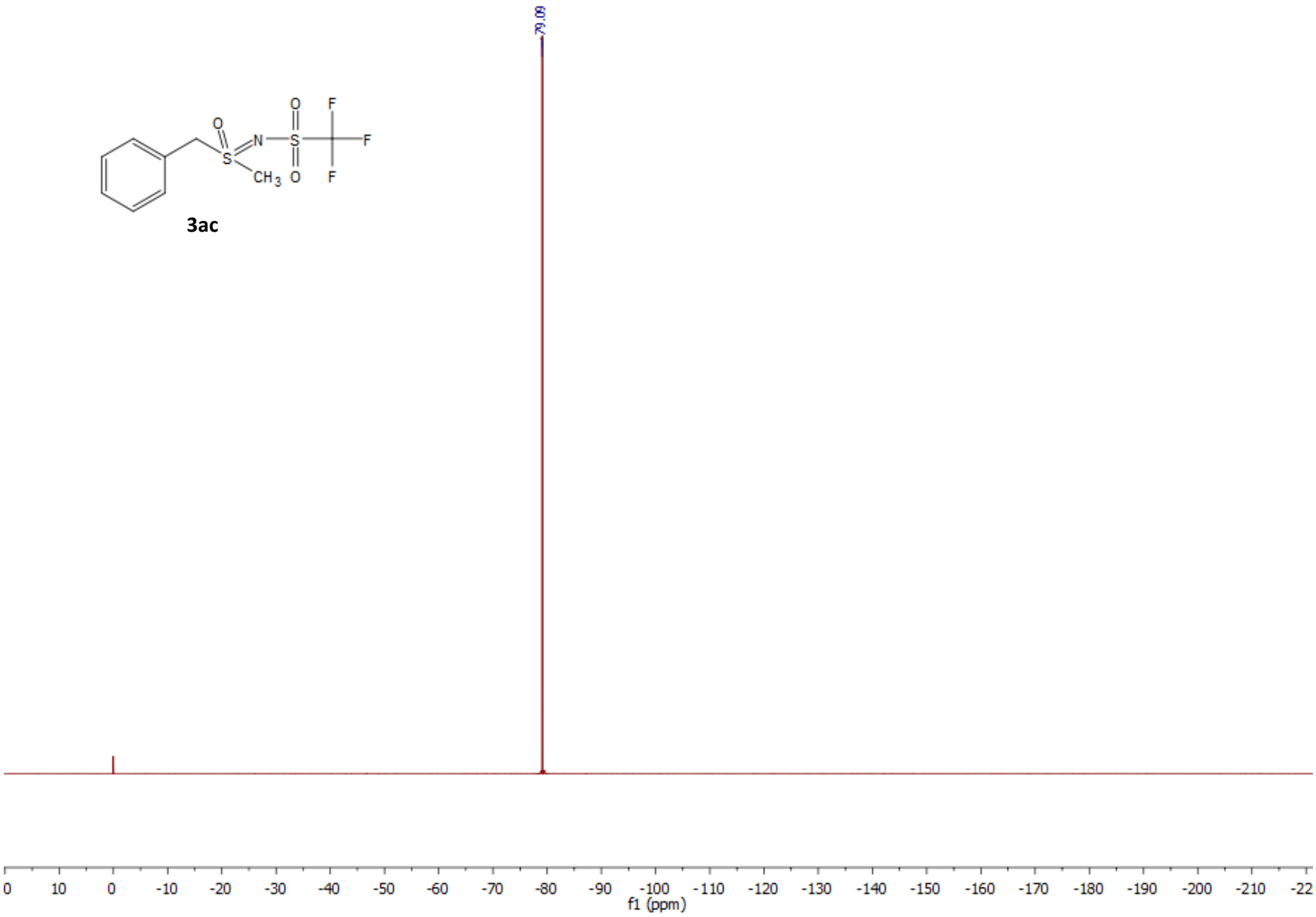

147.86
146.96
137.89
136.05
134.32
133.14
132.37
132.28
132.23
130.40
127.65
126.30
122.91
120.36
117.80
115.25
21.54
20.03
O
N
O
O
S
N
S
O
O
F
F
F
H3C
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ab


7.51
7.51
7.50
7.50
7.50
7.50
7.49
7.49
7.48
7.48
7.48
7.48
7.47
7.47
7.47
7.47
7.46
7.46
7.45
7.45
4.80
4.77
4.71
4.69
3.17
O
F
O
N
S
F
S
CH3
O
F
5.00
2.08
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3ac

3ac


-79.09
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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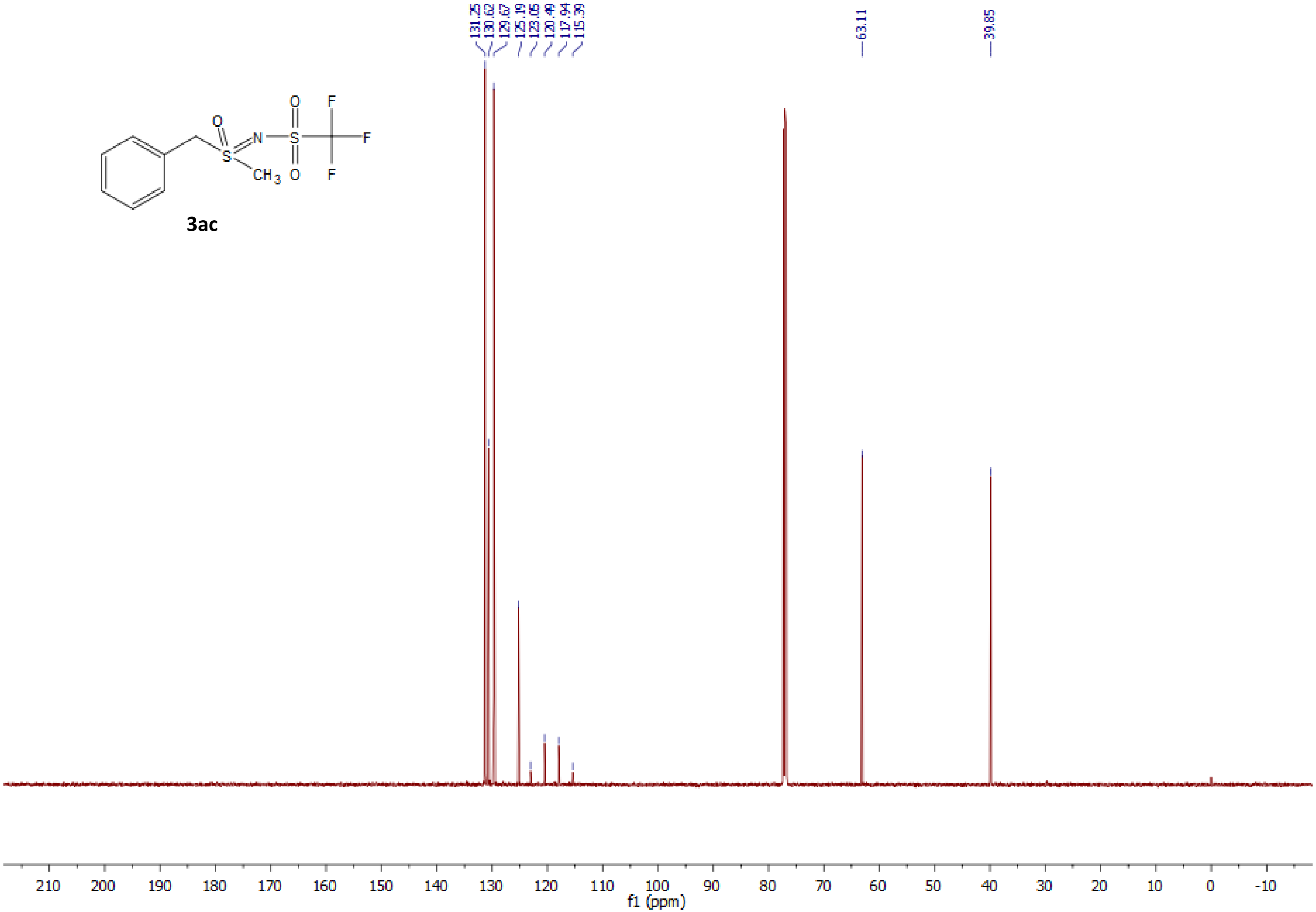
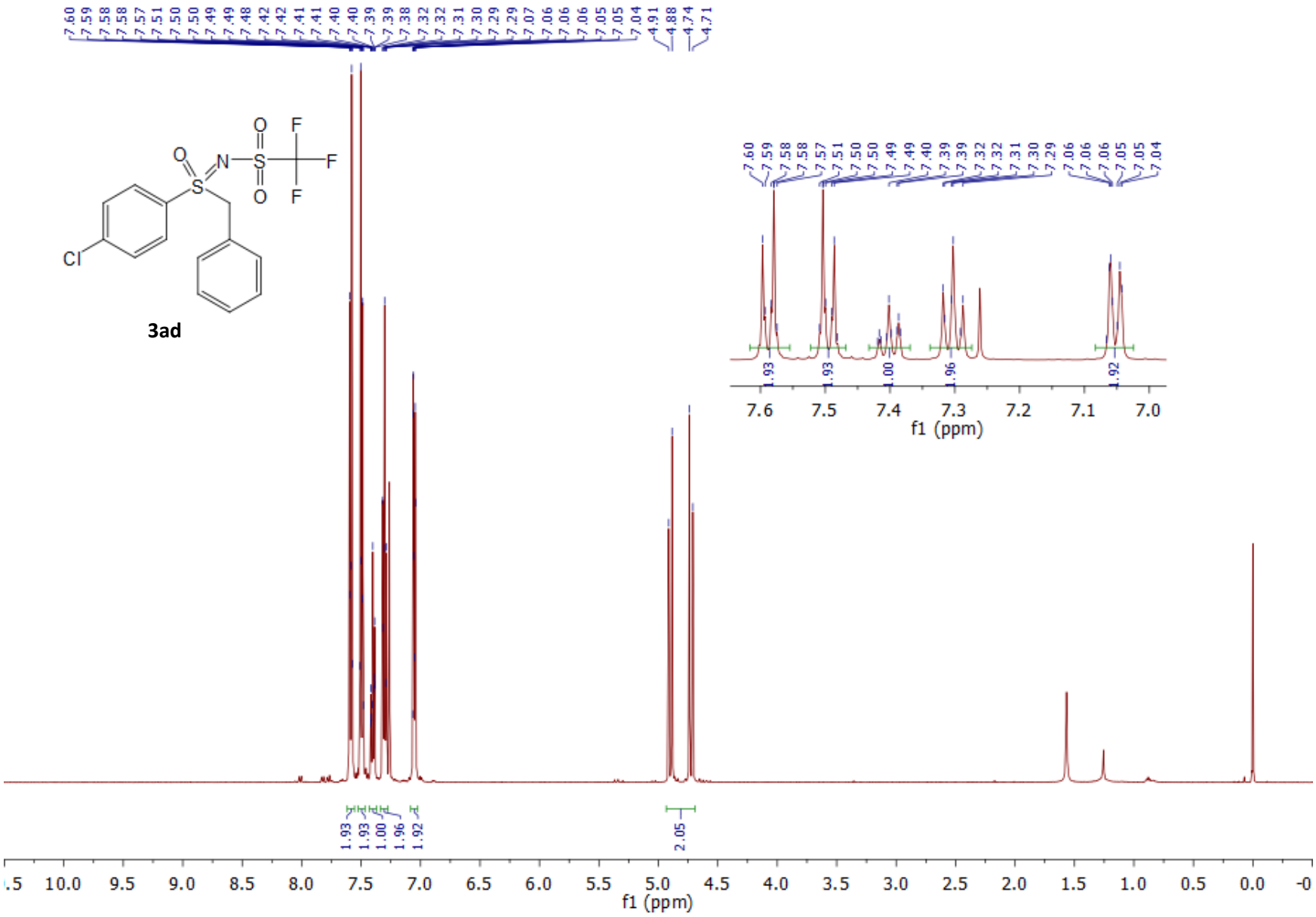
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

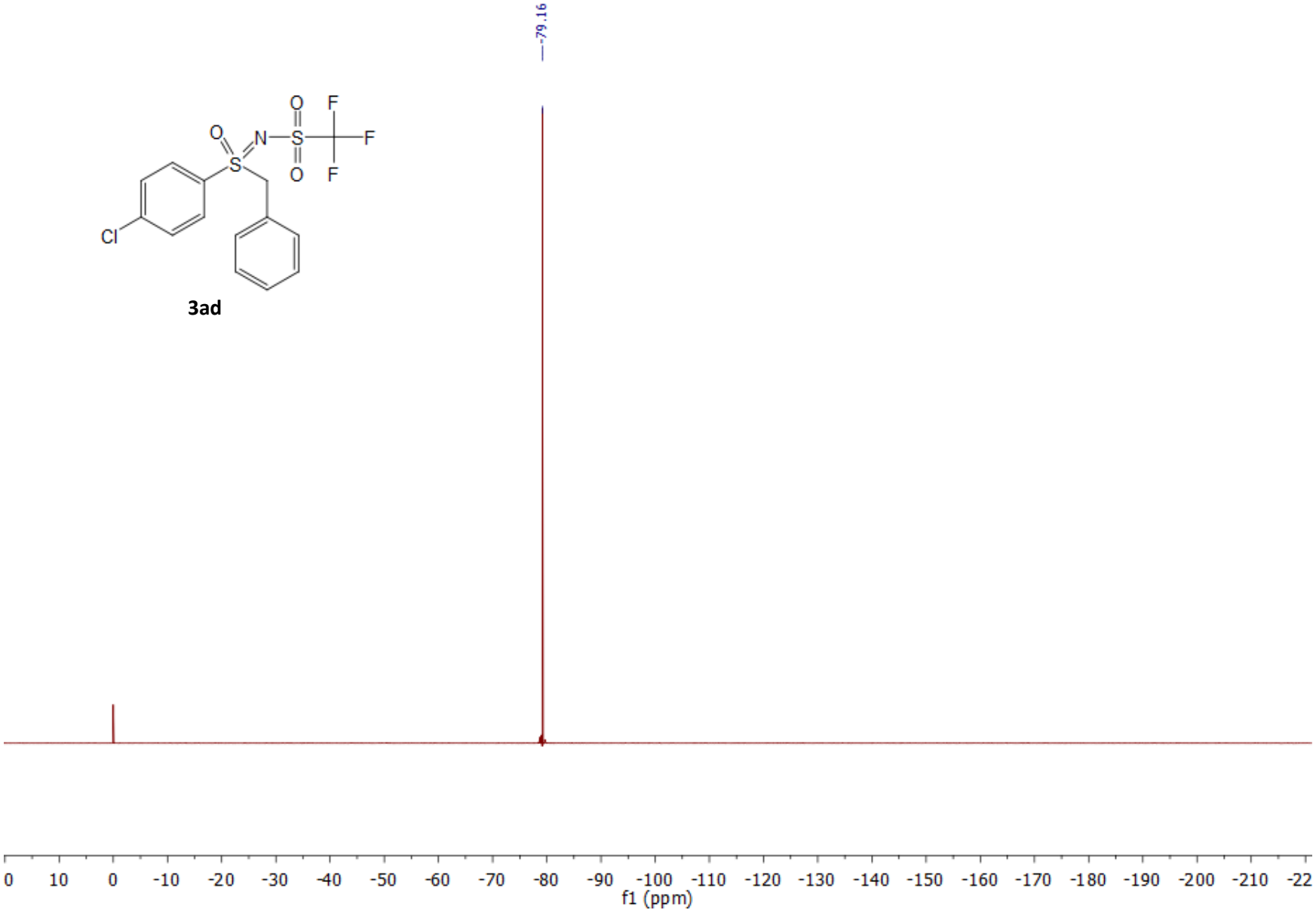

131.25
130.62
129.67
125.19
123.05
120.49
117.94
115.39
63.11
39.85
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

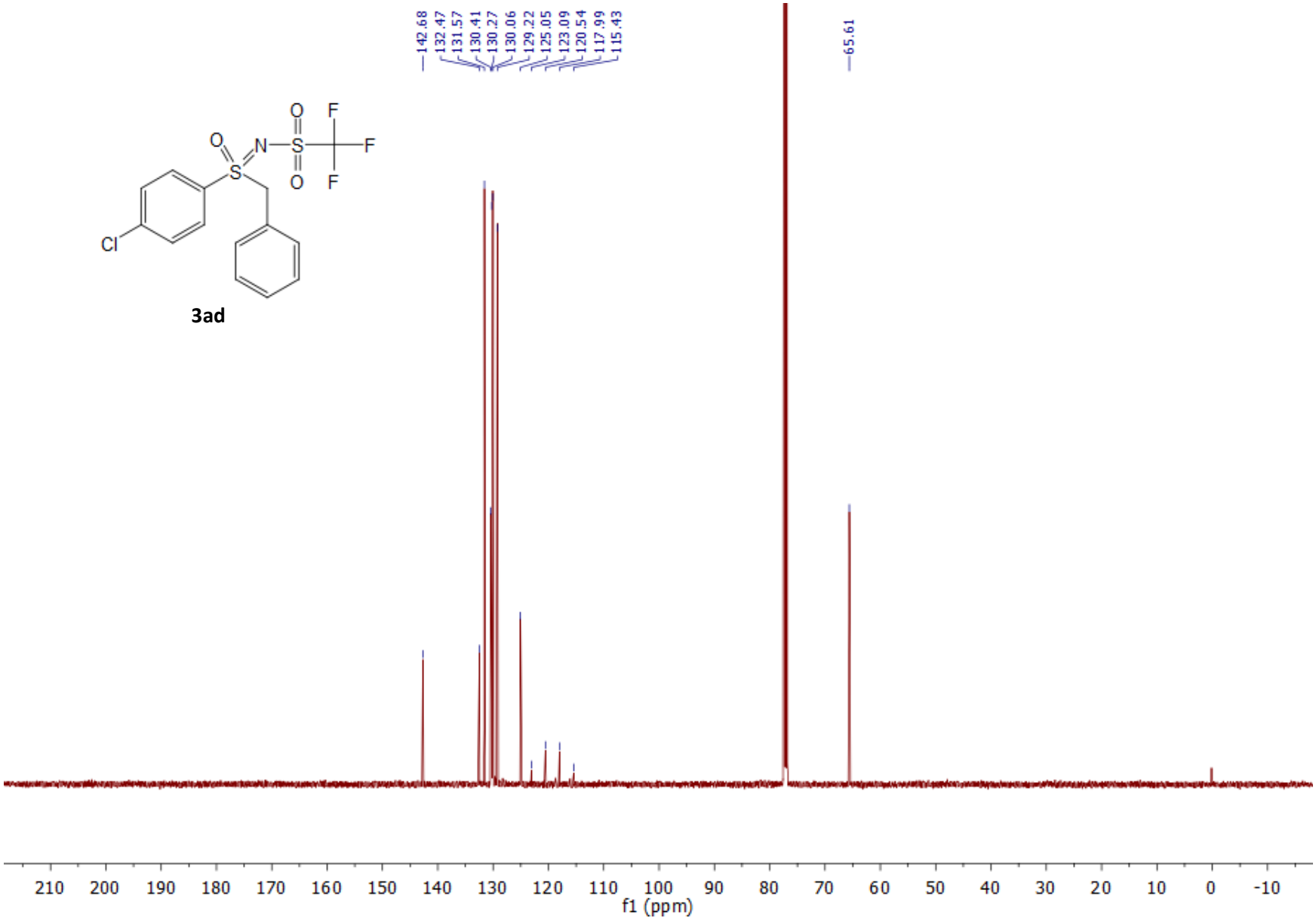
3ac

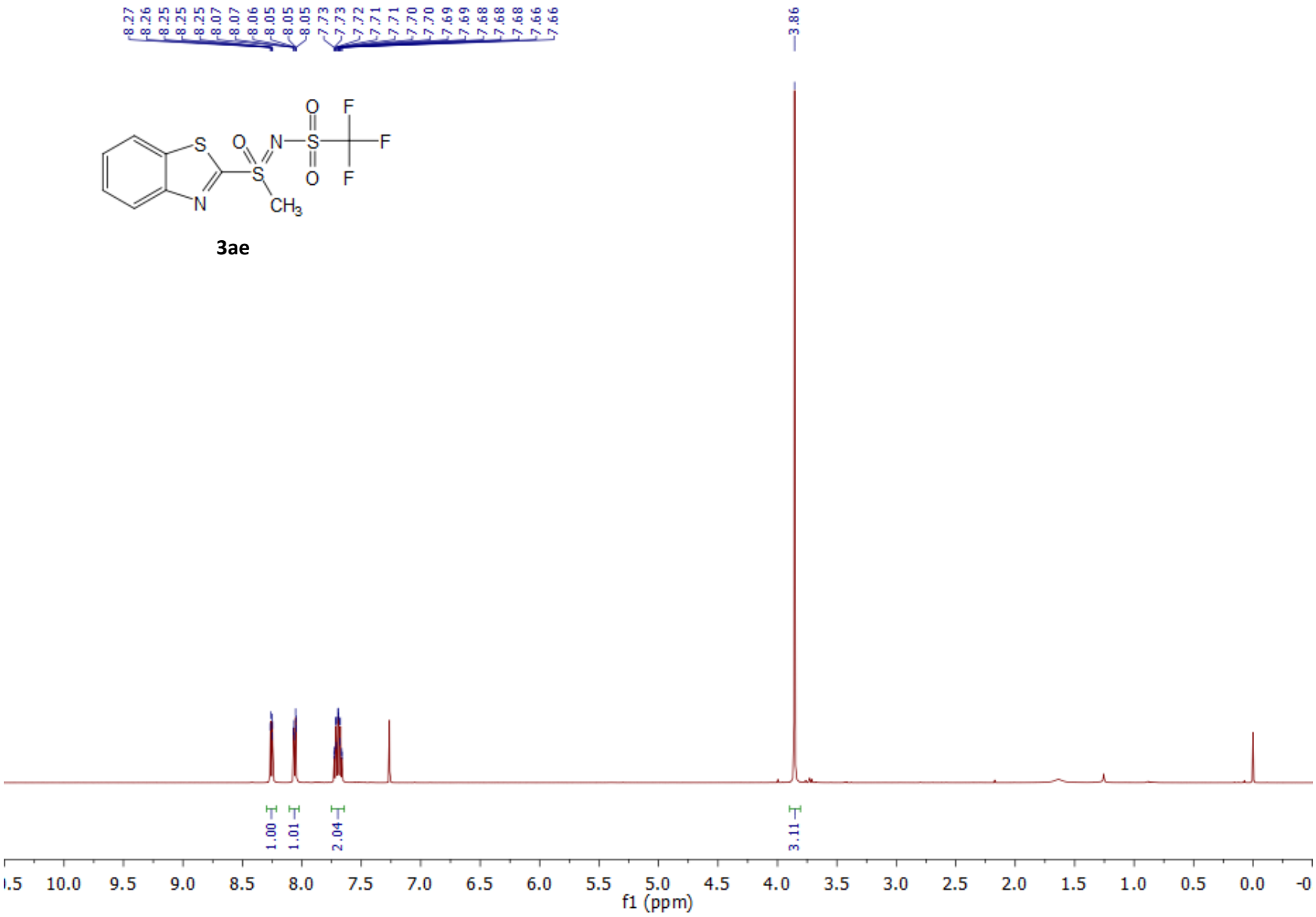

7.60 7.59 7.58 7.58 7.57 7.51 7.50 7.50 7.49 7.49 7.48 7.42 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.32 7.32 7.31 7.30 7.29 7.29 7.07 7.06 7.06 7.06 7.05 7.05 7.04 4.91 4.88 4.74 4.71
O F
O N S F
S
O F F
Cl
3ad
1.93 1.93 1.00 1.96 1.92
2.05
f1 (ppm)
1.93 1.93 1.00 1.96 1.92
7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)

O
F
O
N
S
F
O
S
F
Cl

3ad


-79.16
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

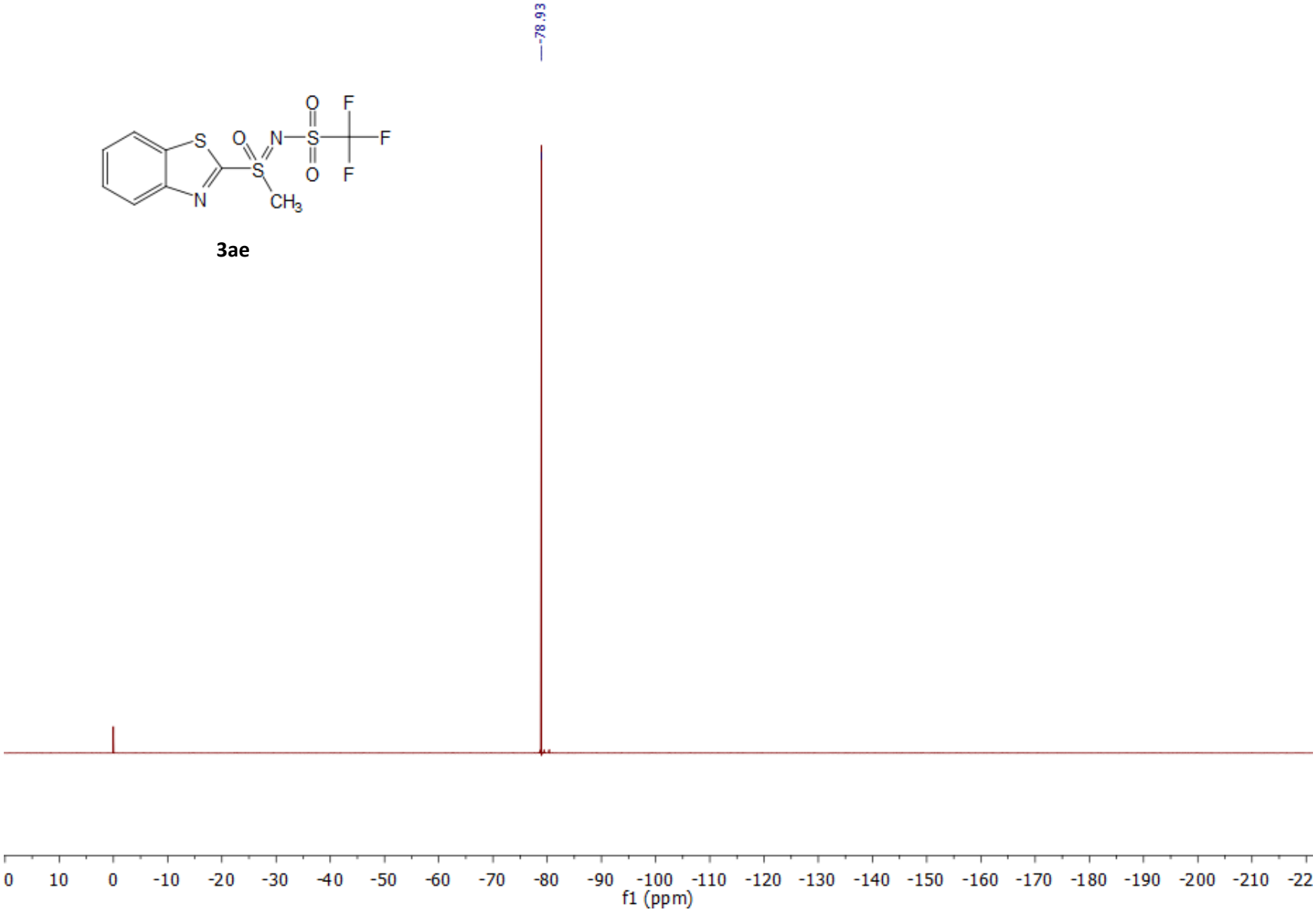

142.68
132.47
131.57
130.41
130.27
130.06
129.22
125.05
123.09
120.54
117.99
115.43
65.61
O
N
S
O
F
F
F
O
S
Cl
3ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.27
8.26
8.25
8.25
8.25
8.07
8.07
8.06
8.05
8.05
8.05
7.73
7.73
7.72
7.71
7.71
7.70
7.70
7.69
7.69
7.68
7.68
7.68
7.66
7.66
3.86
O
F
S
O
N
S
F
S
O
F
N
CH3
1.00
1.01
2.04
3.11
f1 (ppm)

3ae

S
O
N
S
O
F
F
F
S
N
CH3

3ae


-78.93
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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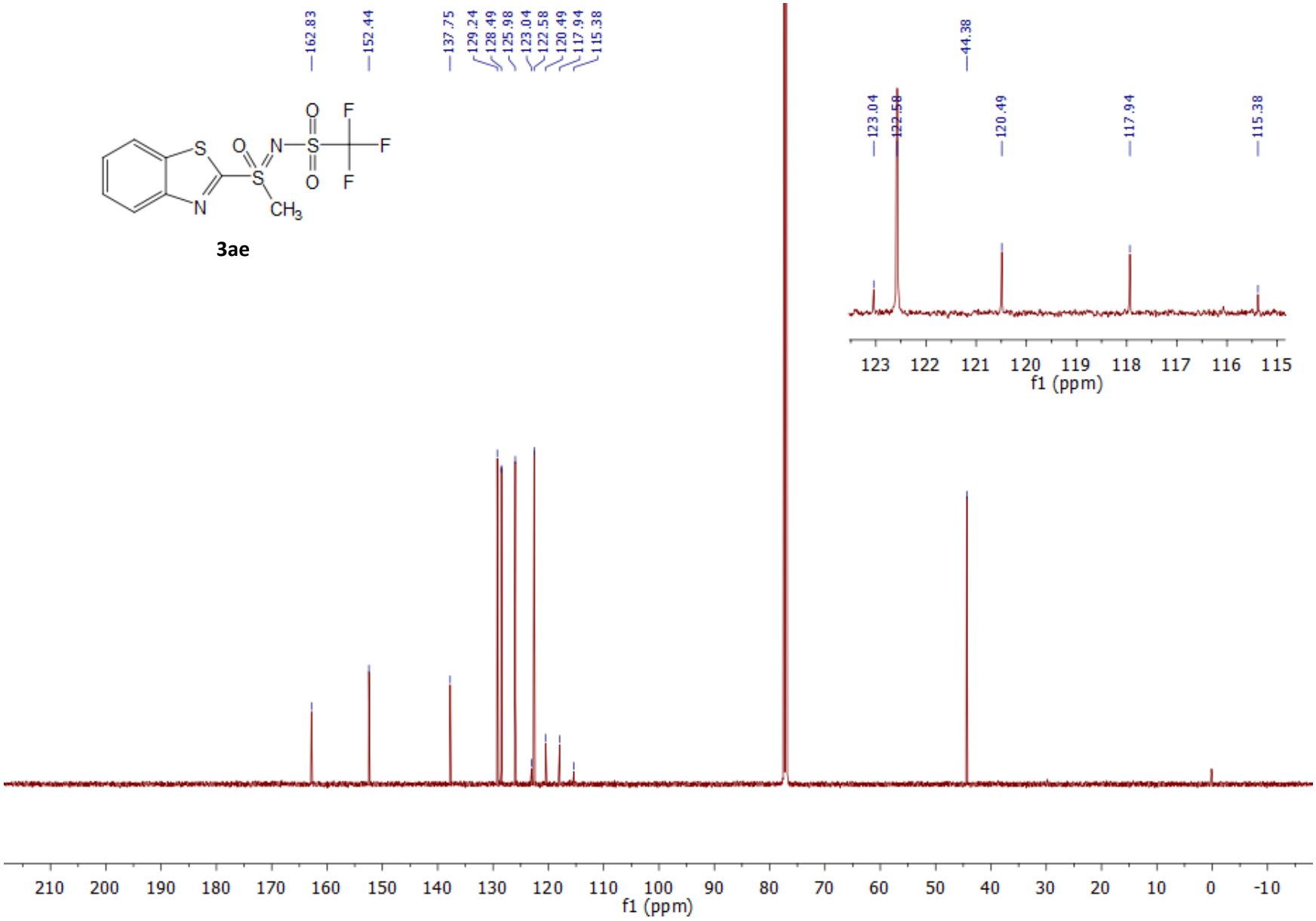
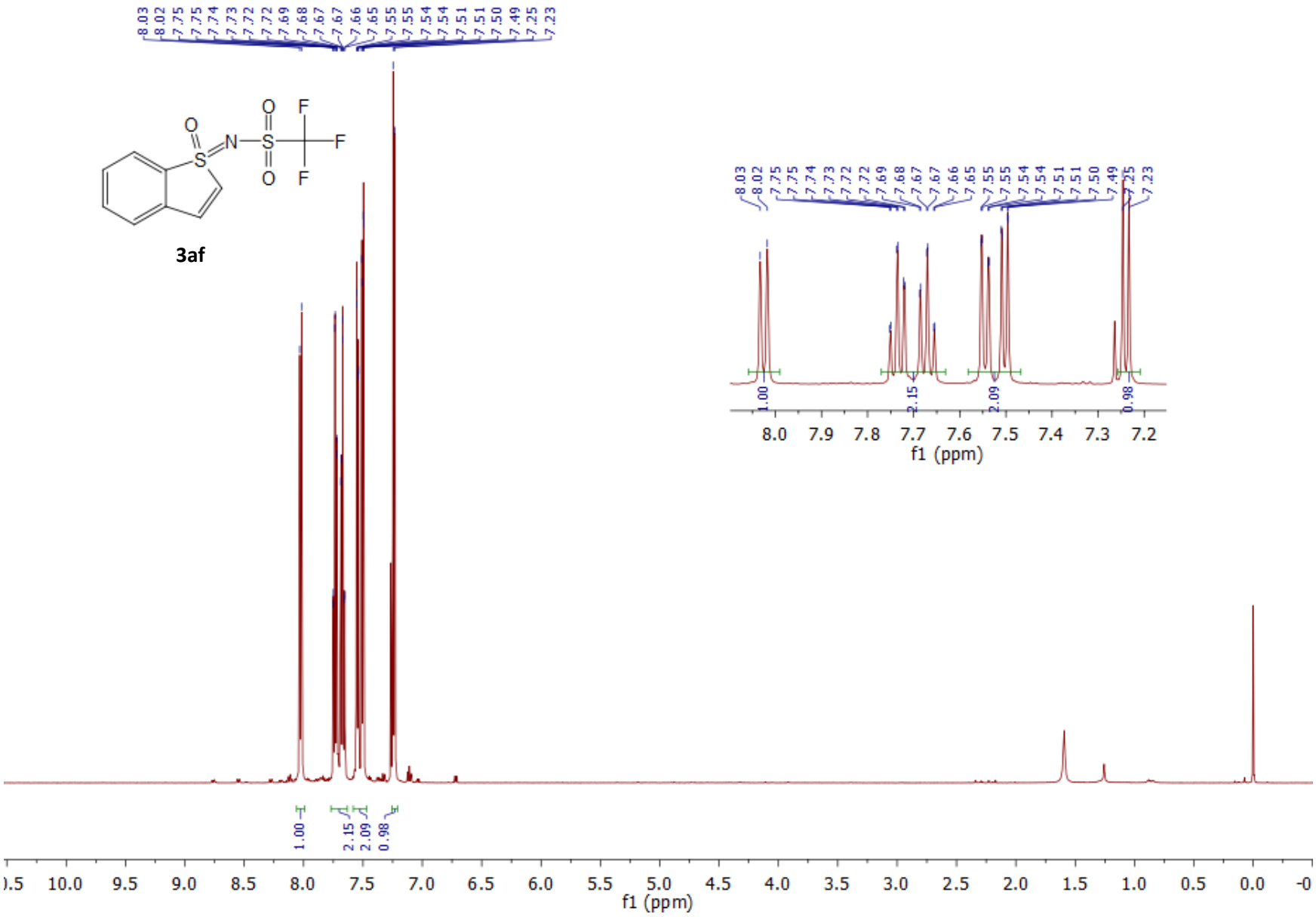
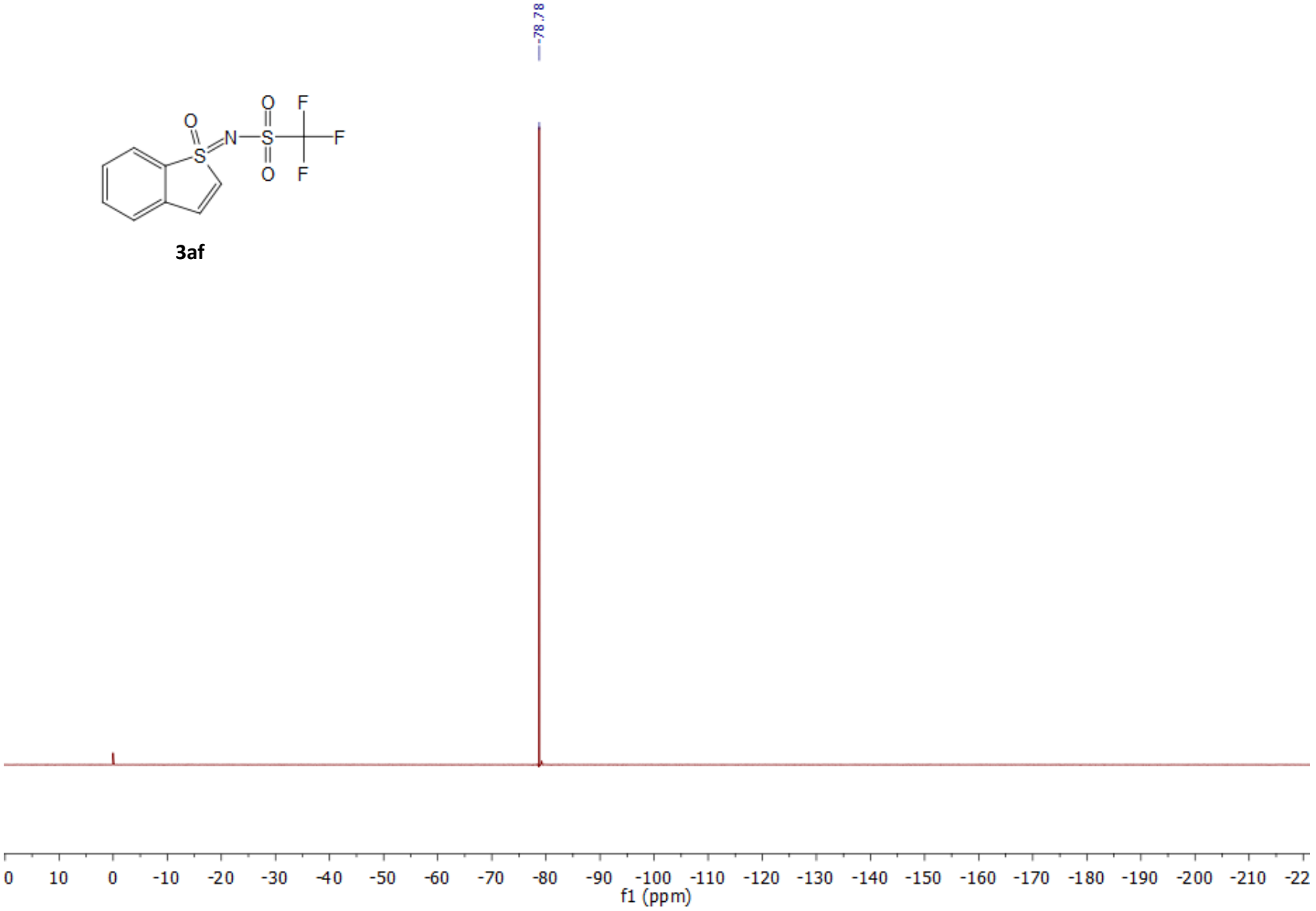
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

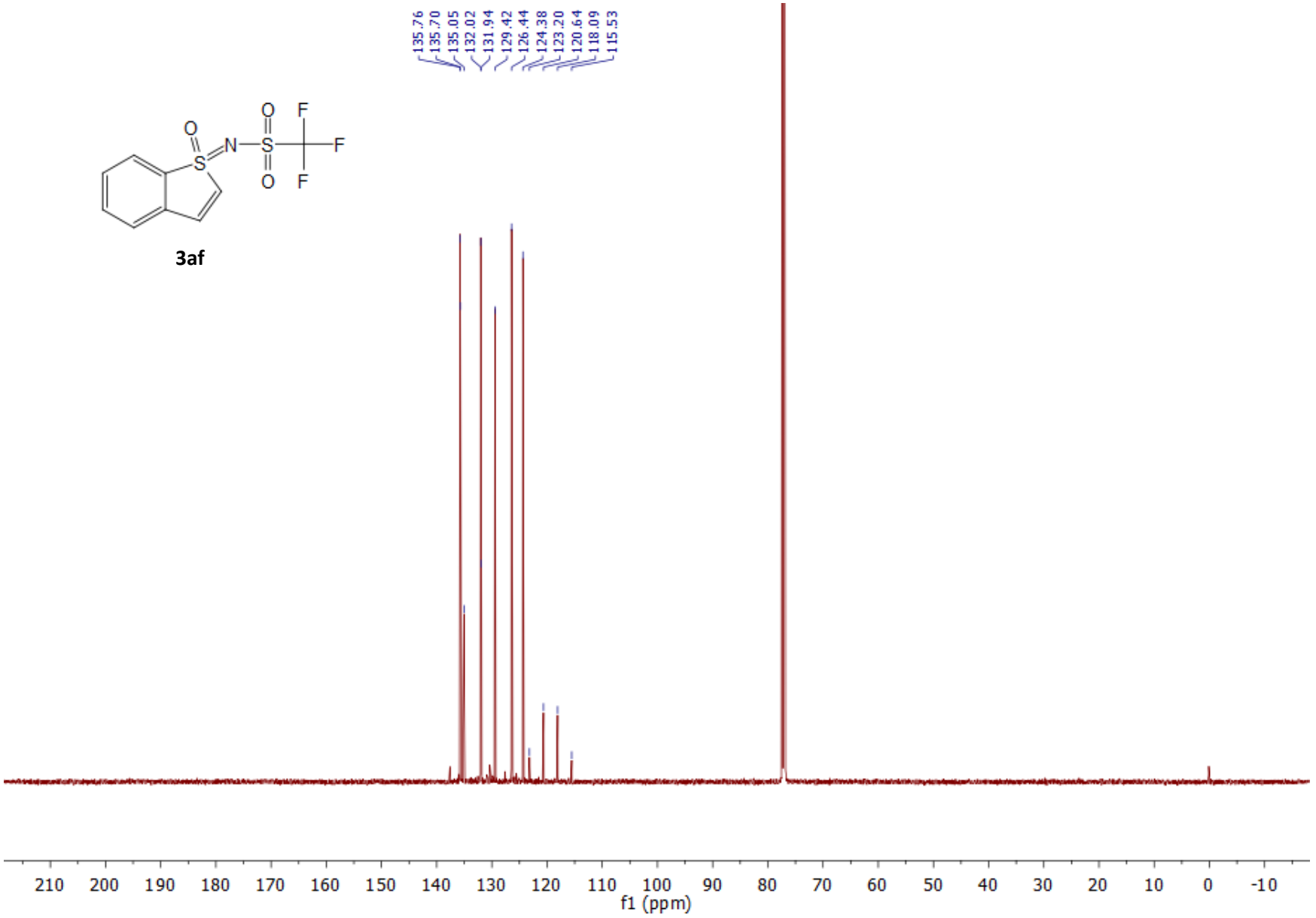

162.83
152.44
137.75
129.24
128.49
125.98
123.04
122.58
120.49
117.94
115.38
44.38
S
O
N
S
O
F
F
F
O
S
N
CH3
3ae
123.04
122.58
120.49
117.94
115.38
123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.03 8.02 7.75 7.75 7.74 7.73 7.72 7.72 7.69 7.68 7.67 7.67 7.66 7.65 7.55 7.55 7.54 7.54 7.51 7.51 7.50 7.49 7.25 7.23
O F
O N S F
S
O F
3af
1.00 2.15 2.09 0.98
f1 (ppm)

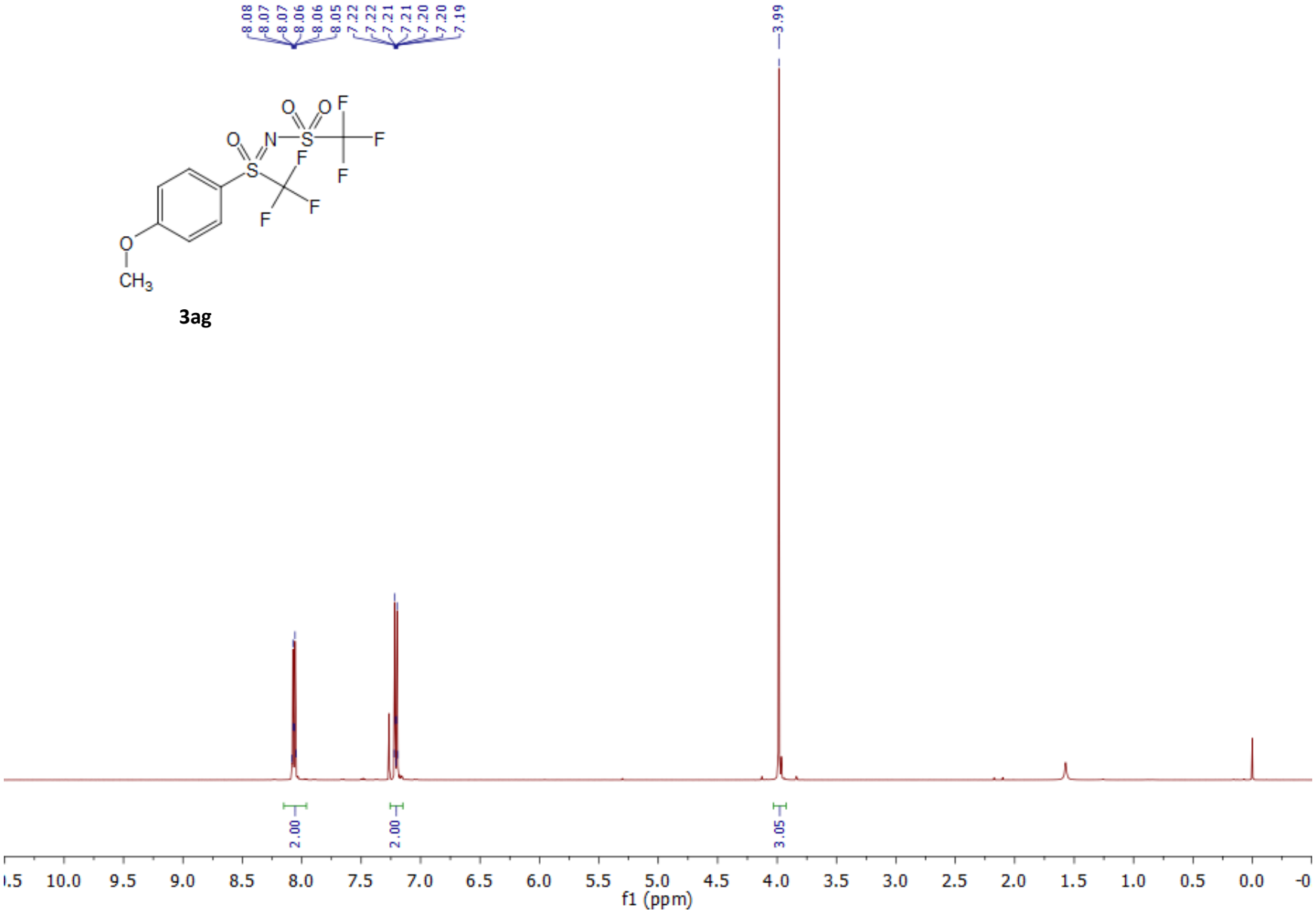
O
N
S
O
F
F
O
F

3af

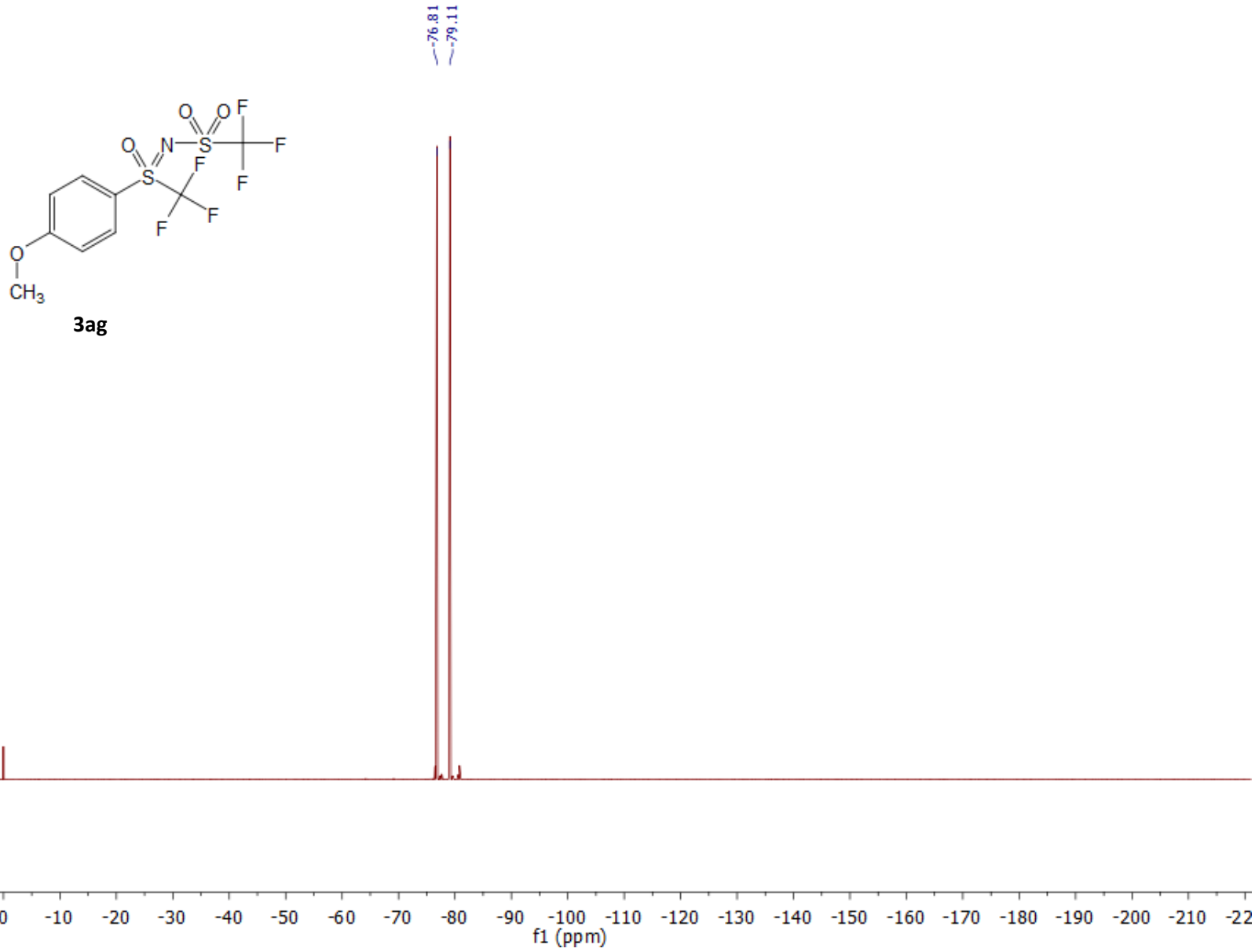

-78.78
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


135.76
135.70
135.05
132.02
131.94
129.42
126.44
124.38
123.20
120.64
118.09
115.53
O
S
N
S
O
O
F
F
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

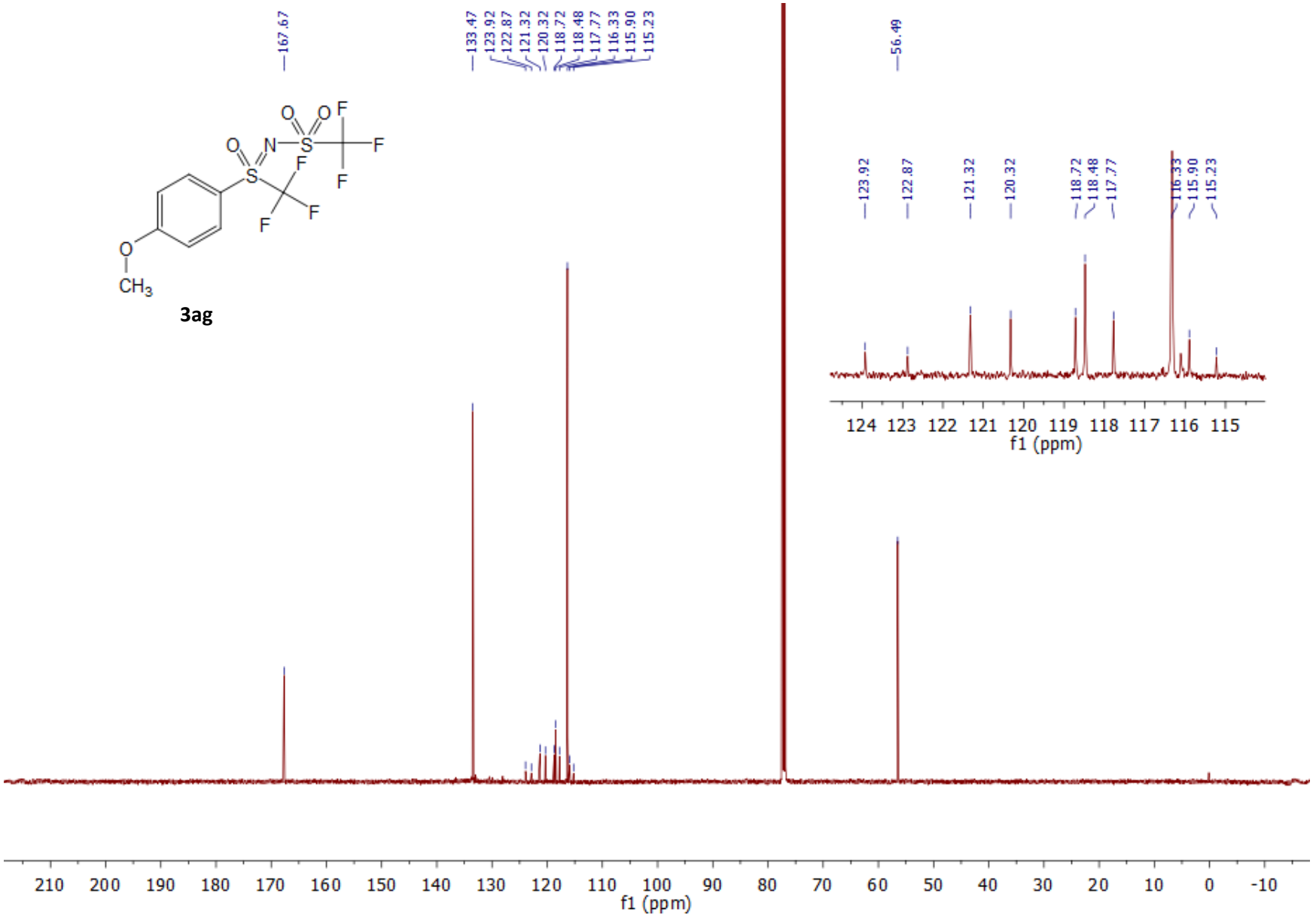
3af

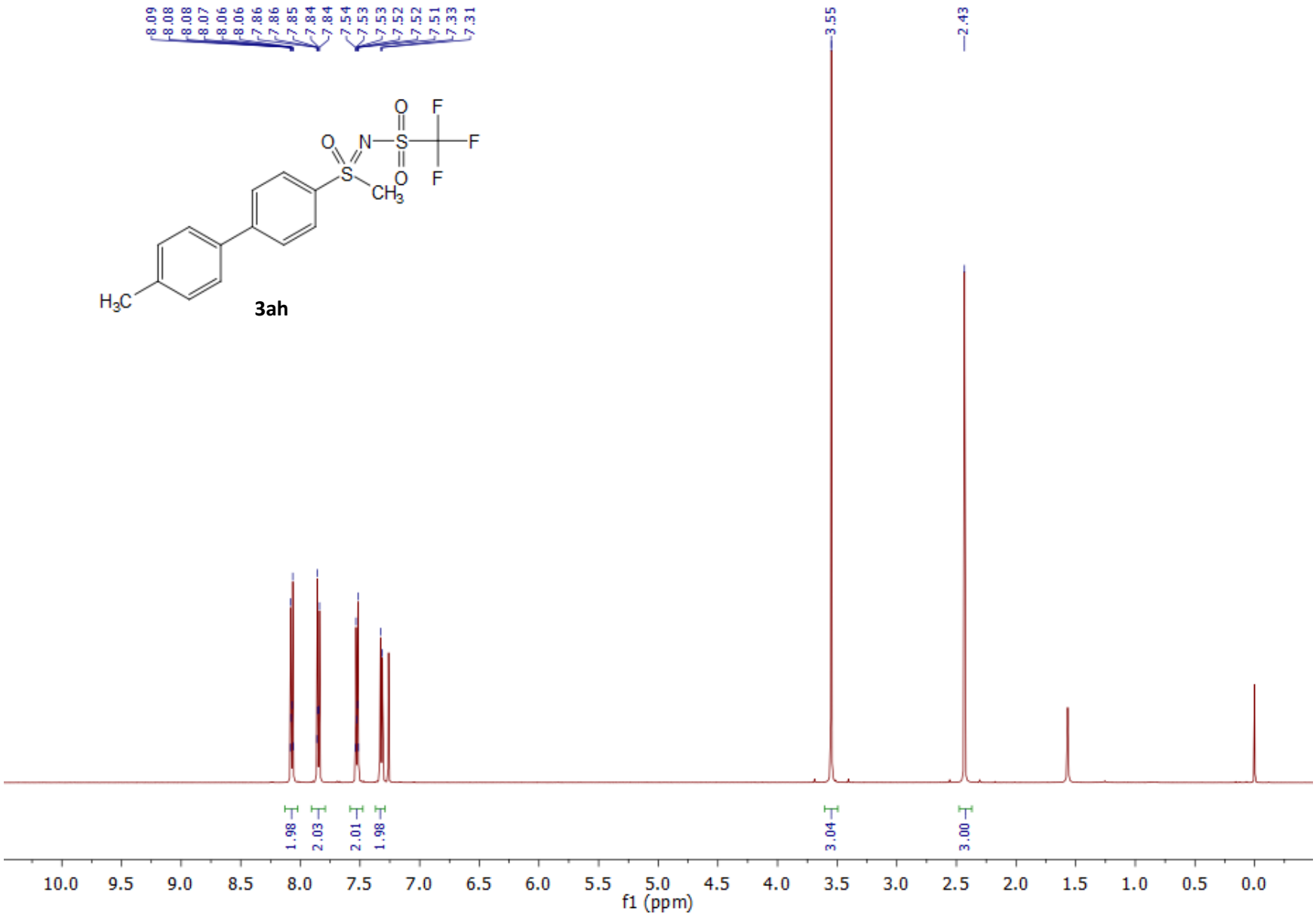

8.08
8.07
8.07
8.06
8.06
8.05
7.22
7.22
7.21
7.21
7.20
7.20
7.19
3.99
O
O
F
O
N
S
F
S
F
F
F
F
O
CH3
2.00
2.00
3.05
f1 (ppm)

3ag

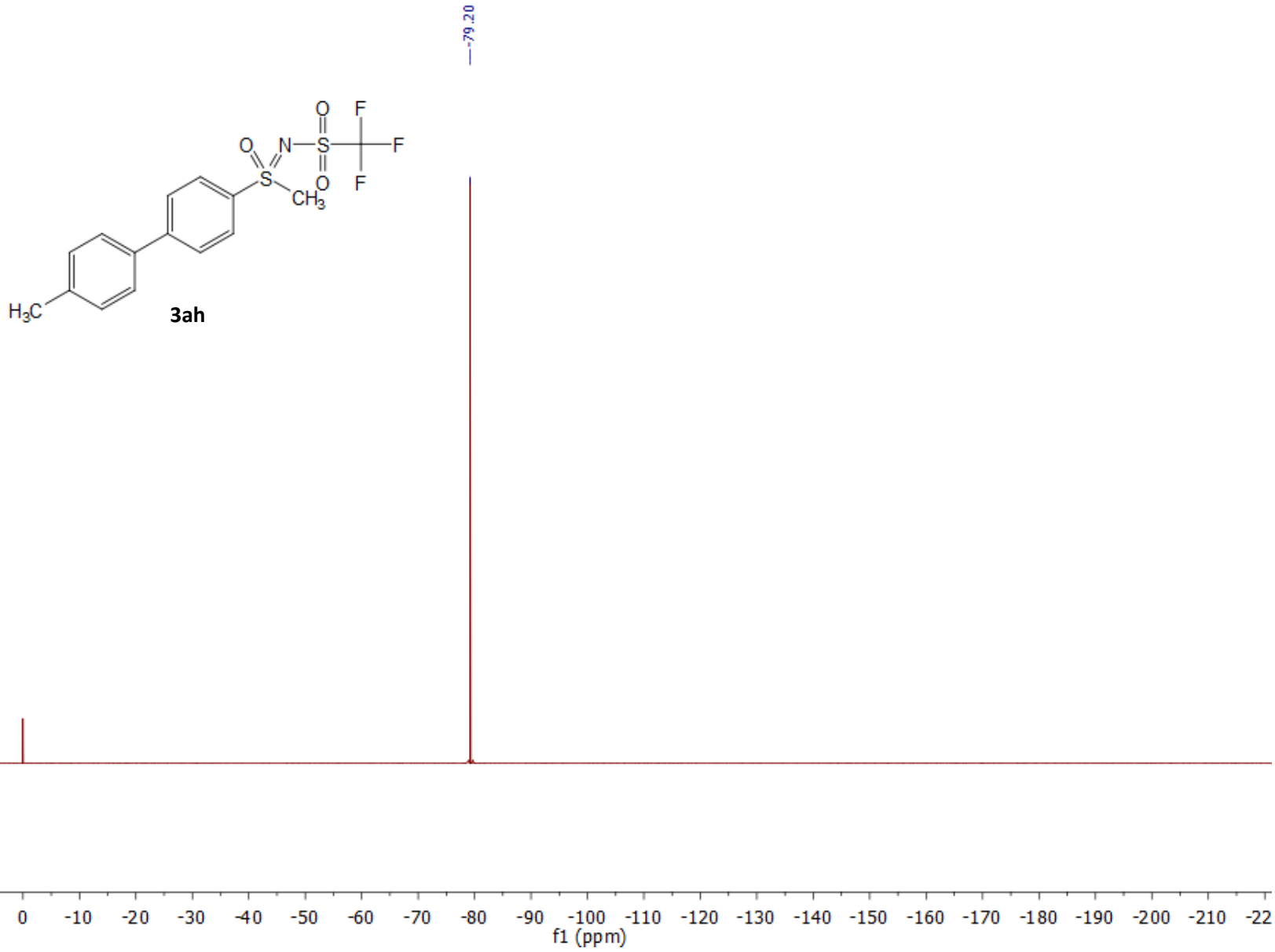

-76.81
-79.11
O
O
F
O
N
S
F
S
F
F
F
F
O
CH3
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

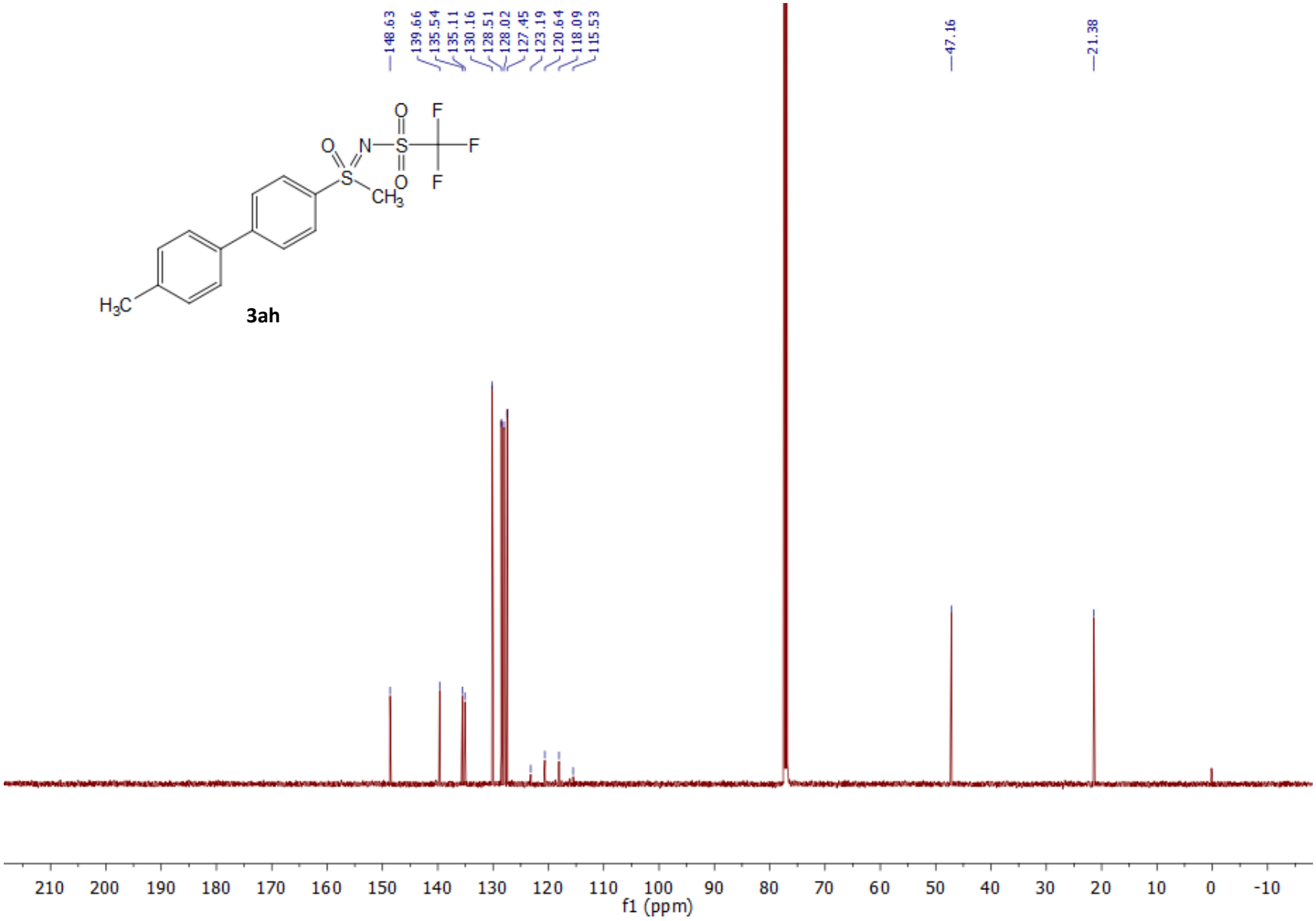
3ag

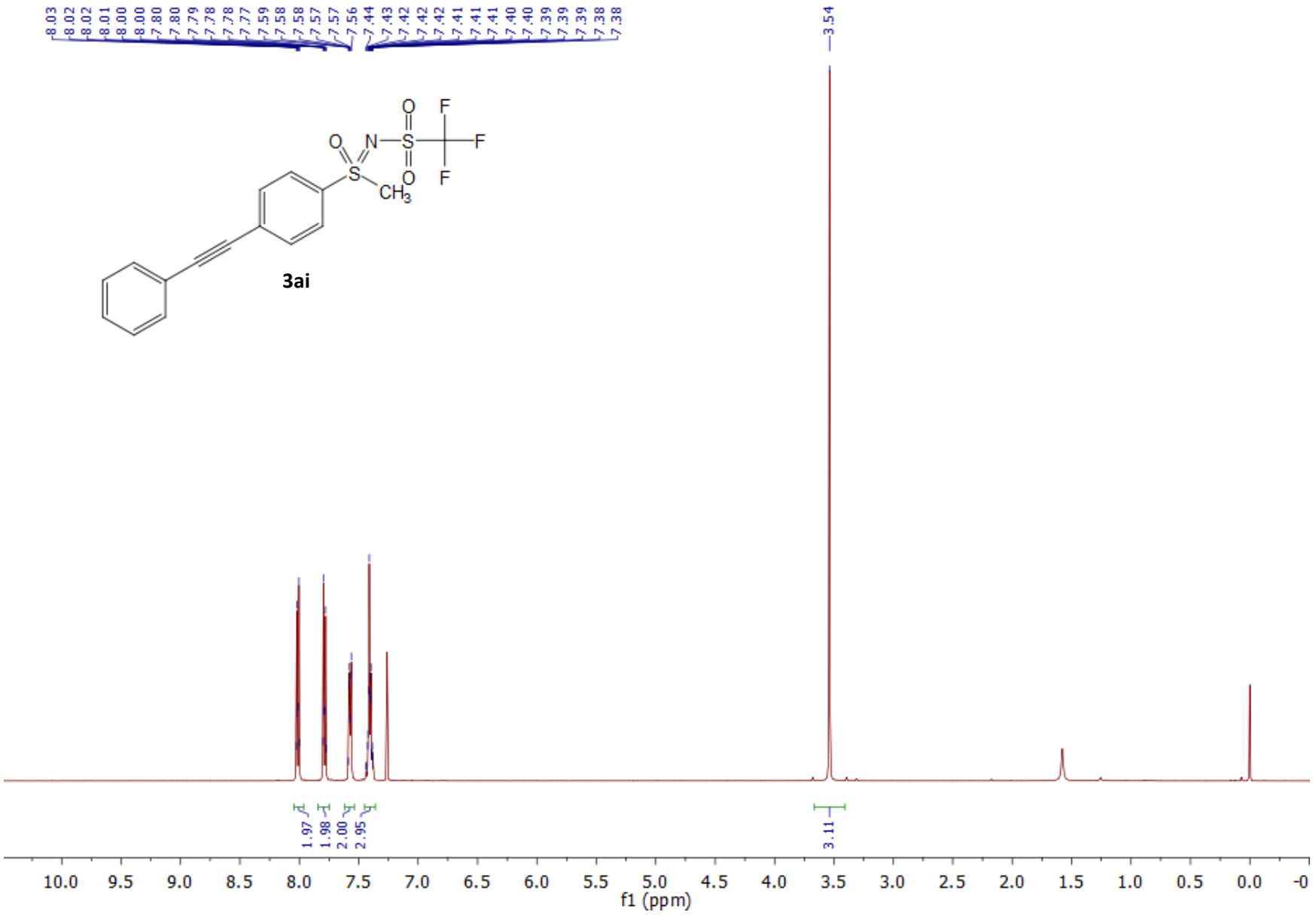

167.67
133.47
123.92
122.87
121.32
120.32
118.72
118.48
117.77
116.33
115.90
115.23
56.49
O
O
F
O
N
S
F
S
F
F
F
F
O
CH3
3ag
123.92
122.87
121.32
120.32
118.72
118.48
117.77
116.33
115.90
115.23
124 123 122 121 120 119 118 117 116 115
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

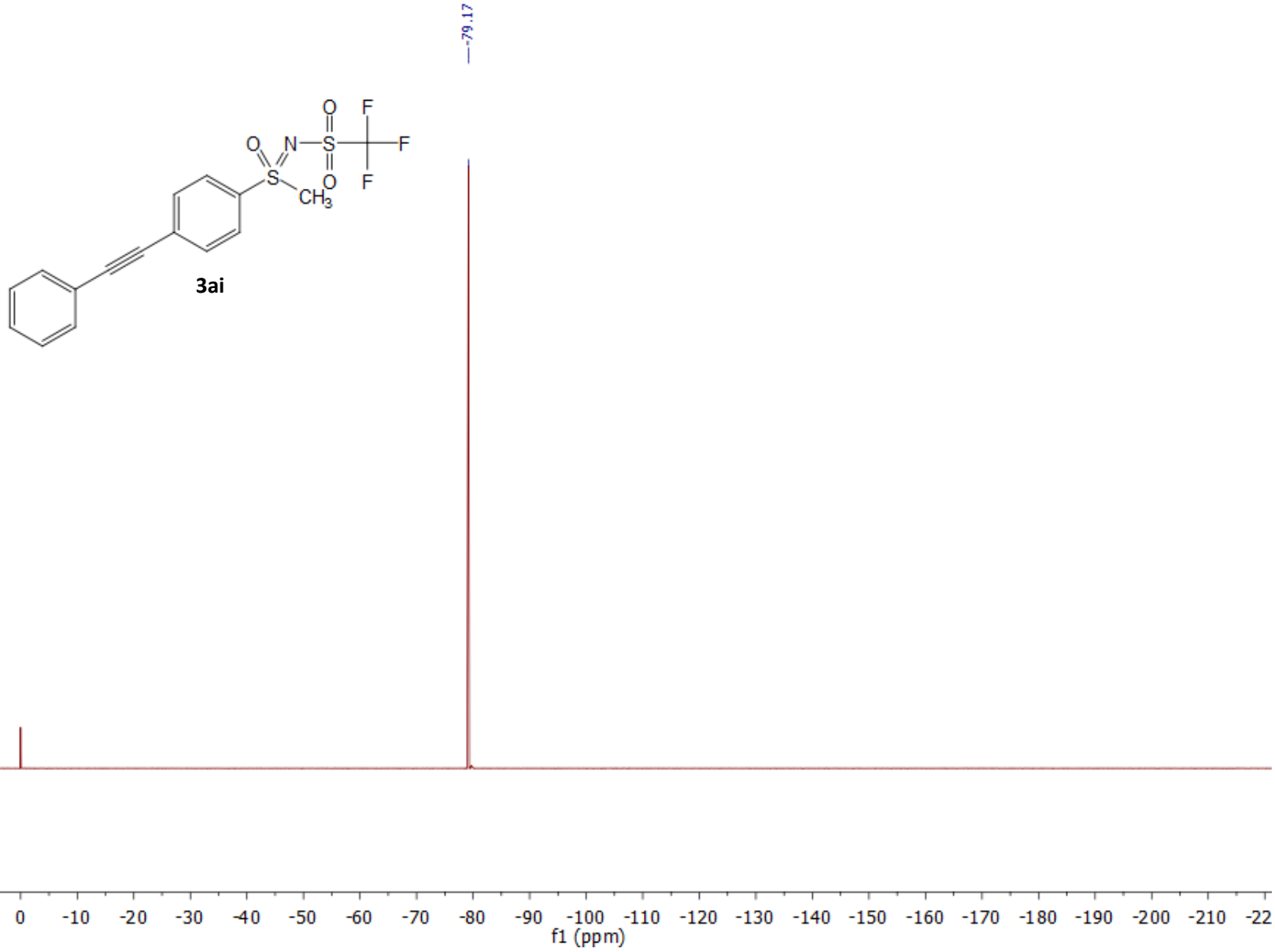

8.09
8.08
8.08
8.07
8.06
8.06
7.86
7.86
7.85
7.84
7.84
7.54
7.53
7.53
7.52
7.52
7.51
7.33
7.31
3.55
2.43
O
F
O
N
S
F
O
S
F
CH3
H3C
1.98
2.03
2.01
1.98
3.04
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

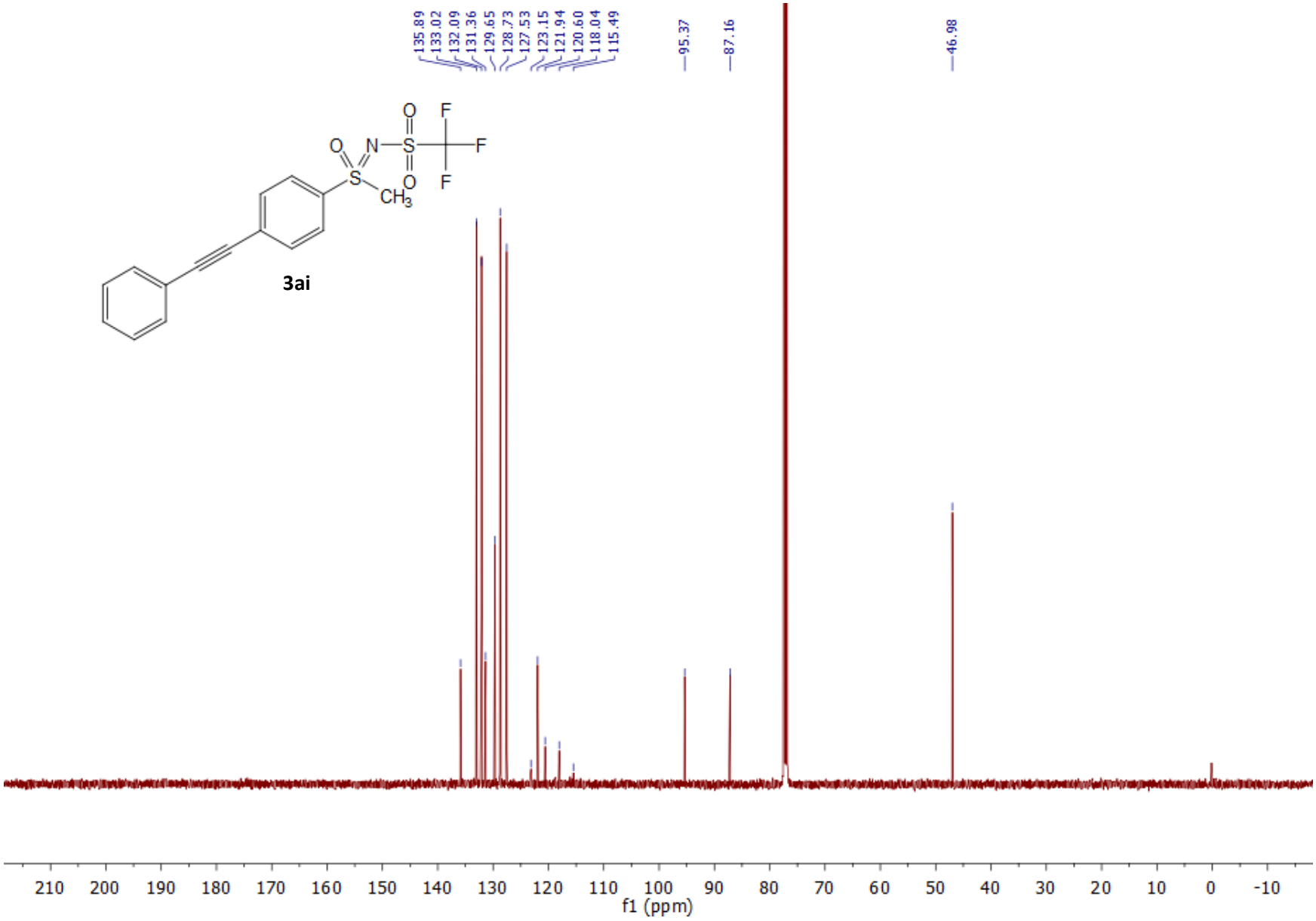
3ah

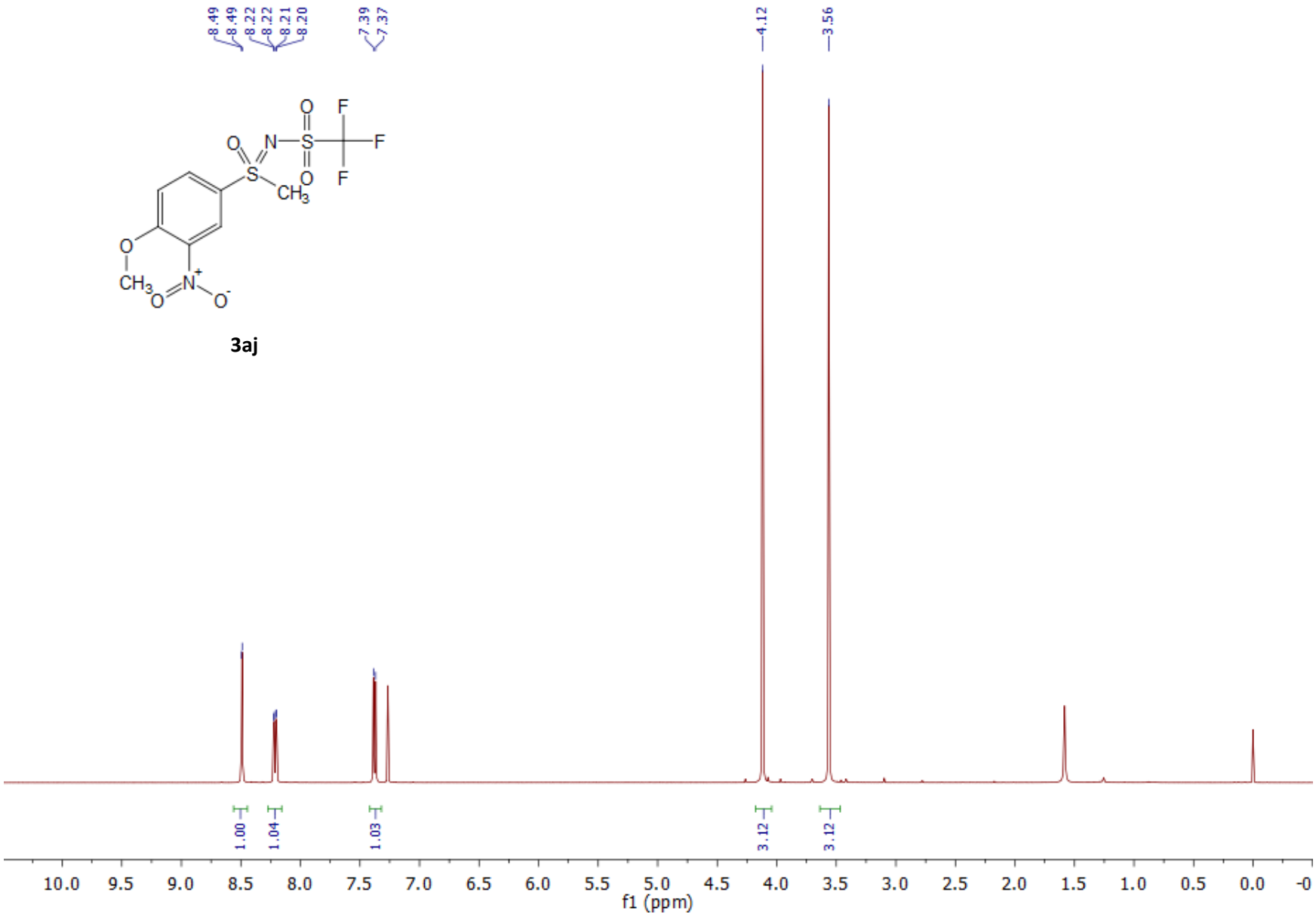

-79.20
O
F
O
N
S
F
S
F
O
CH3
H3C
3ah
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


148.63
139.66
135.54
135.11
130.16
128.51
128.02
127.45
123.19
120.64
118.09
115.53
47.16
21.38
O
N
S
F
F
F
O
O
S
CH3
H3C
3ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.03
8.02
8.02
8.01
8.00
8.00
7.80
7.80
7.79
7.78
7.78
7.77
7.59
7.58
7.58
7.57
7.57
7.56
7.44
7.43
7.42
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.39
7.39
7.38
7.38
3.54
O
N
S
F
F
F
O
O
S
CH3
3ai
1.97
1.98
2.00
2.95
3.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

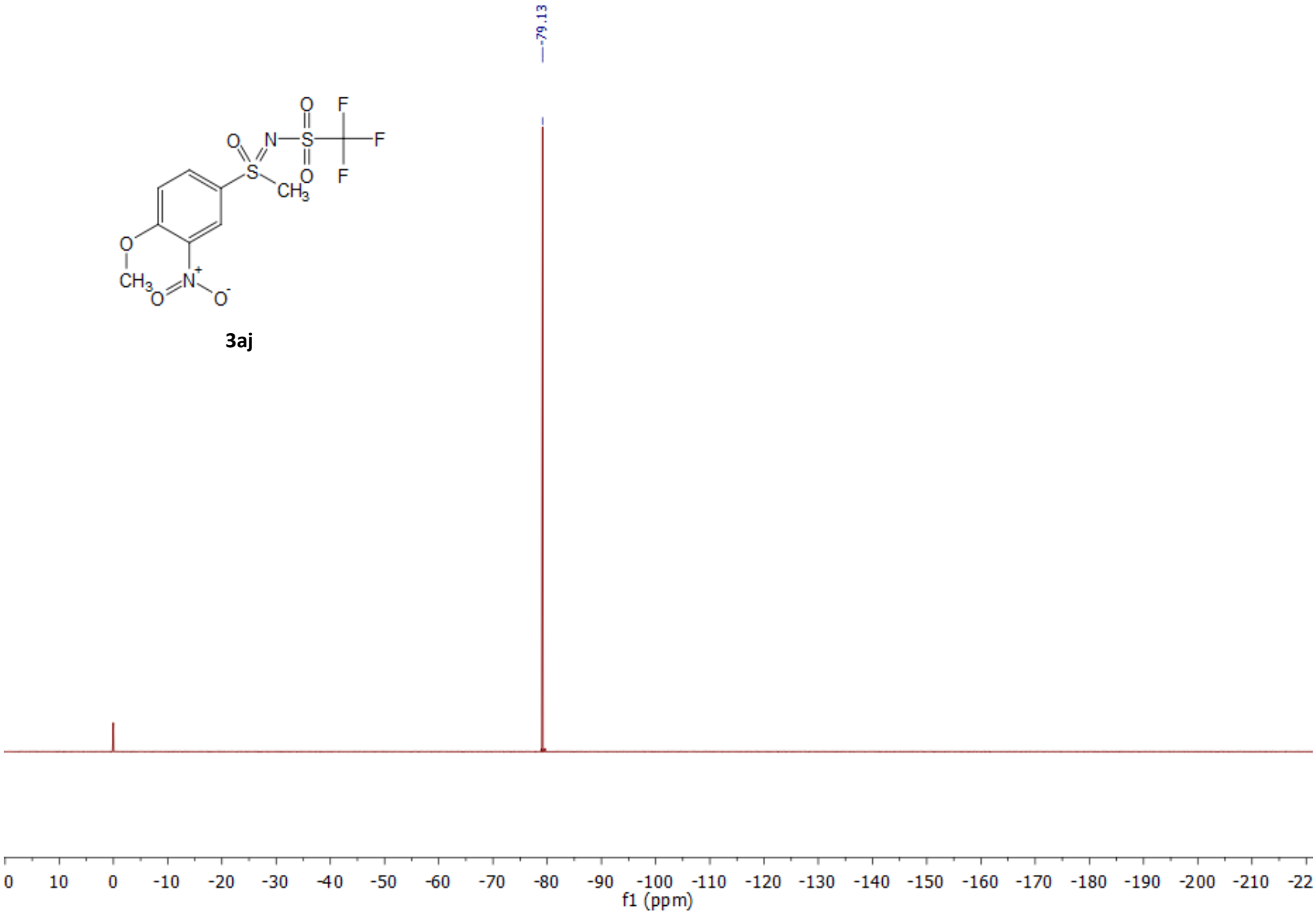

-79.17
O
F
O
N
S
F
S
F
O
CH3
3ai
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

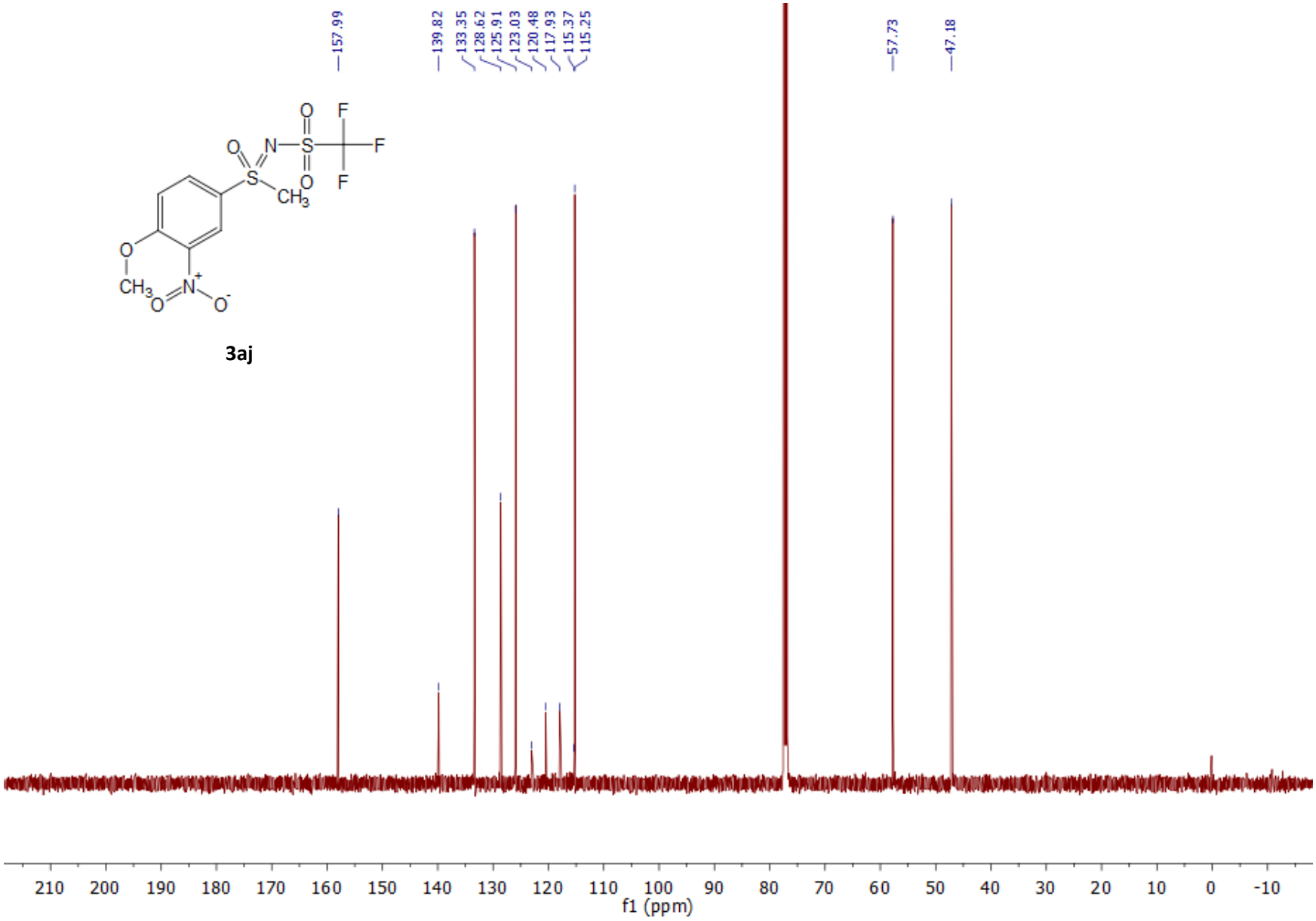

135.89
133.02
132.09
131.36
129.65
128.73
127.53
123.15
121.94
120.60
118.04
115.49
95.37
87.16
46.98
O
N
S
F
F
F
O
O
S
CH3
3ai
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.49
8.49
8.22
8.22
8.21
8.20
7.39
7.37
4.12
3.56
1.00
1.04
1.03
3.12
3.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

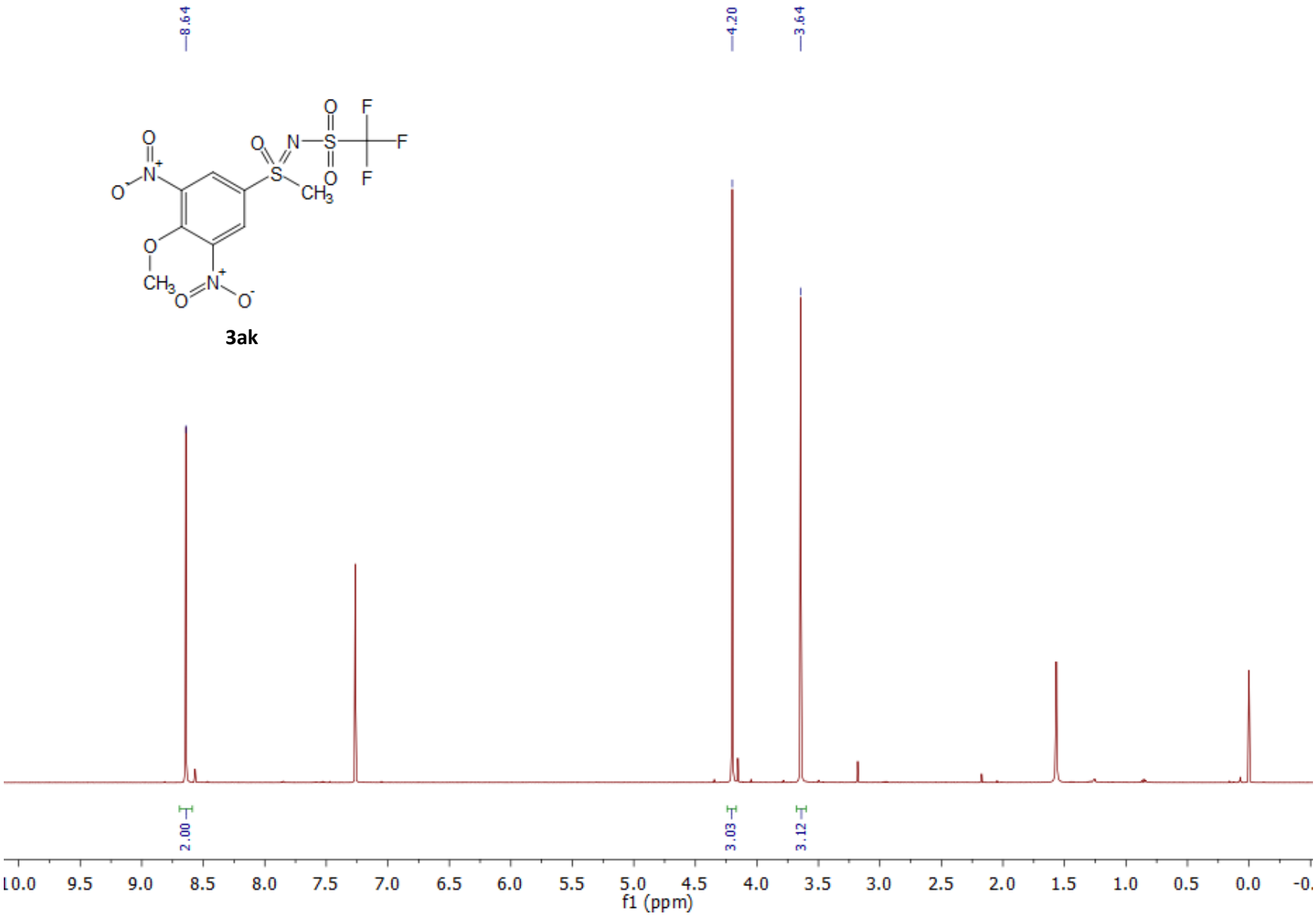
3aj

3aj


-79.13
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

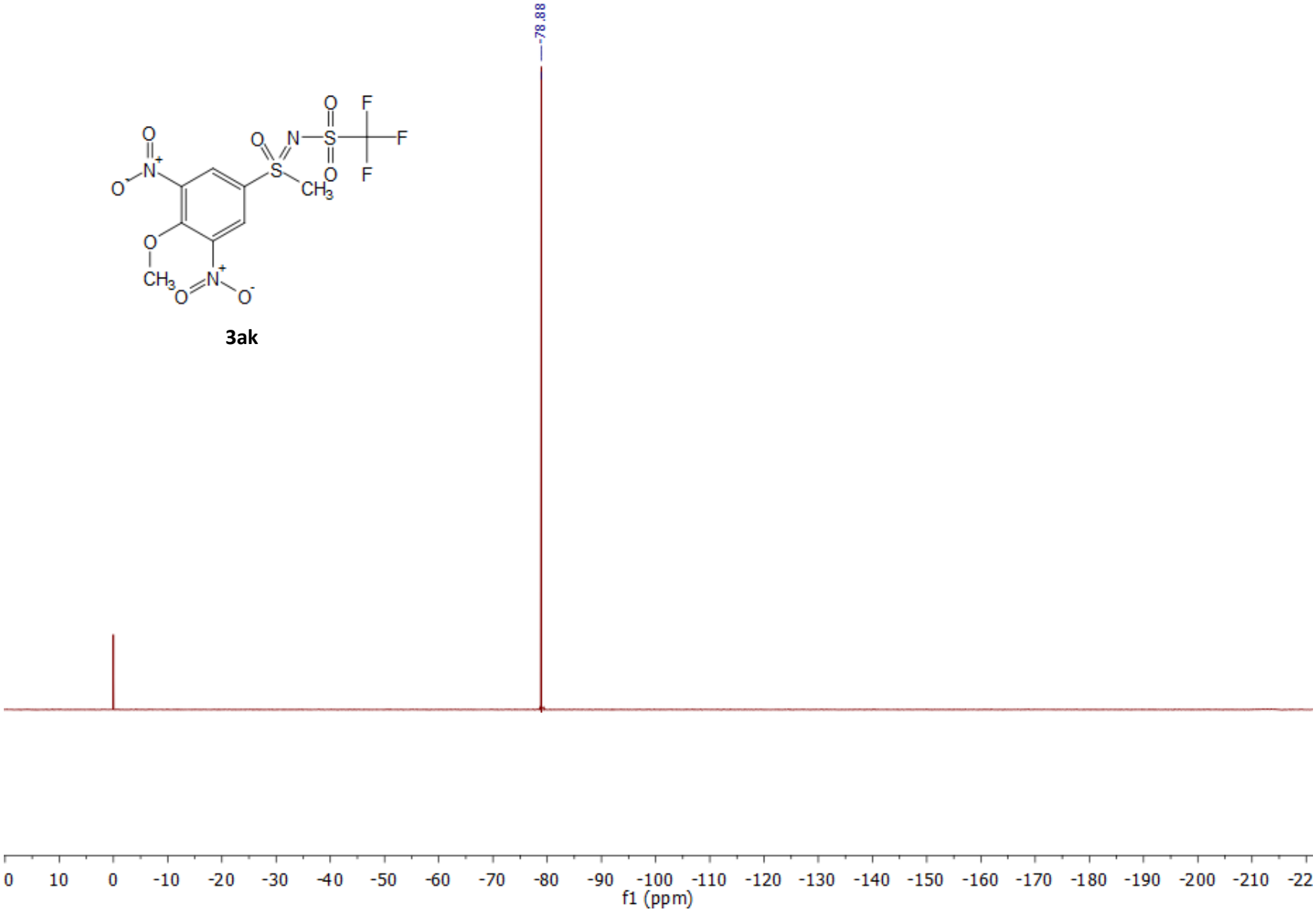

157.99
139.82
133.35
128.62
125.91
123.03
120.48
117.93
115.37
115.25
57.73
47.18
O
F
O
N
S
F
O
F
CH3
O
CH3
N+
O
O-
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

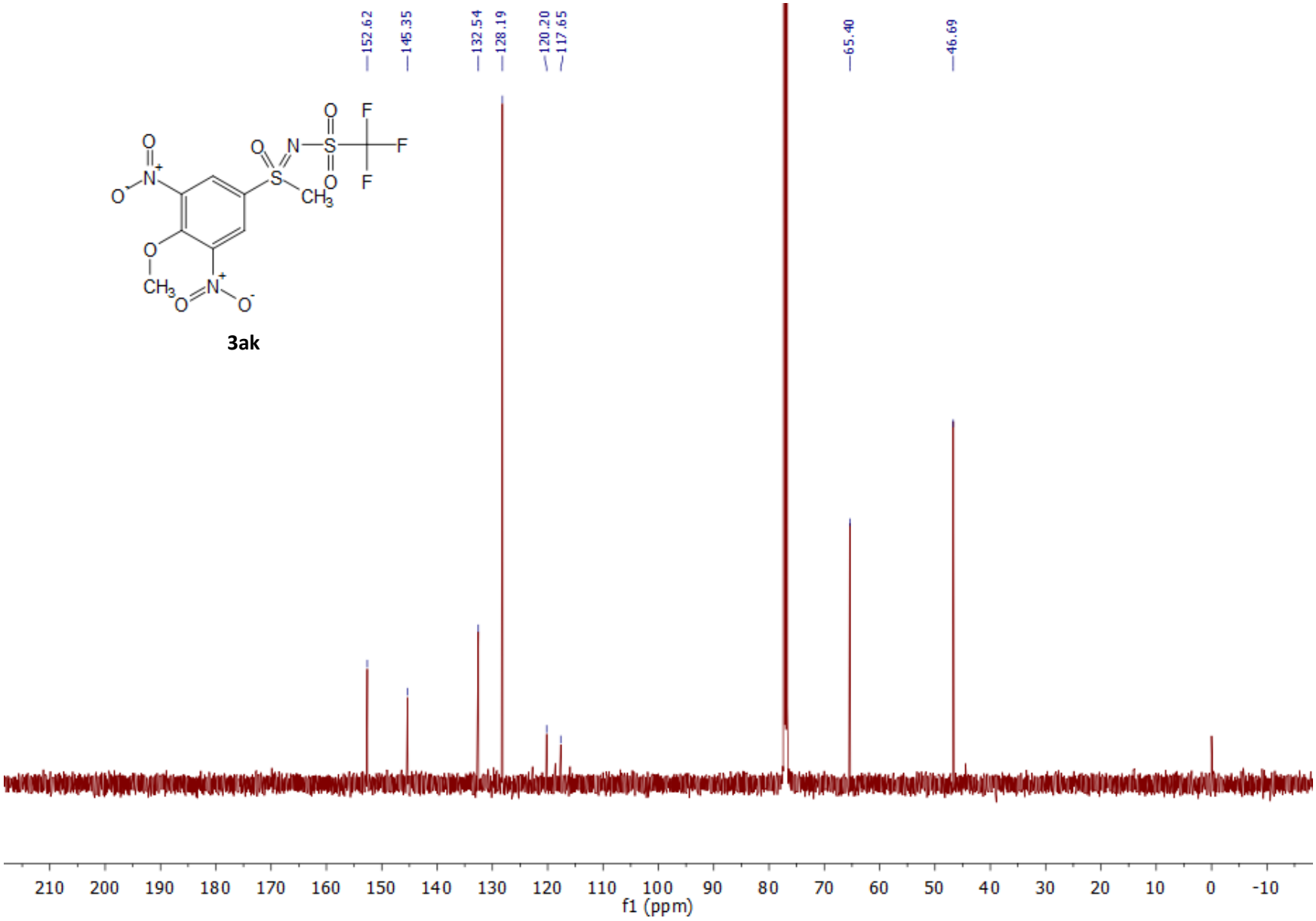
3aj



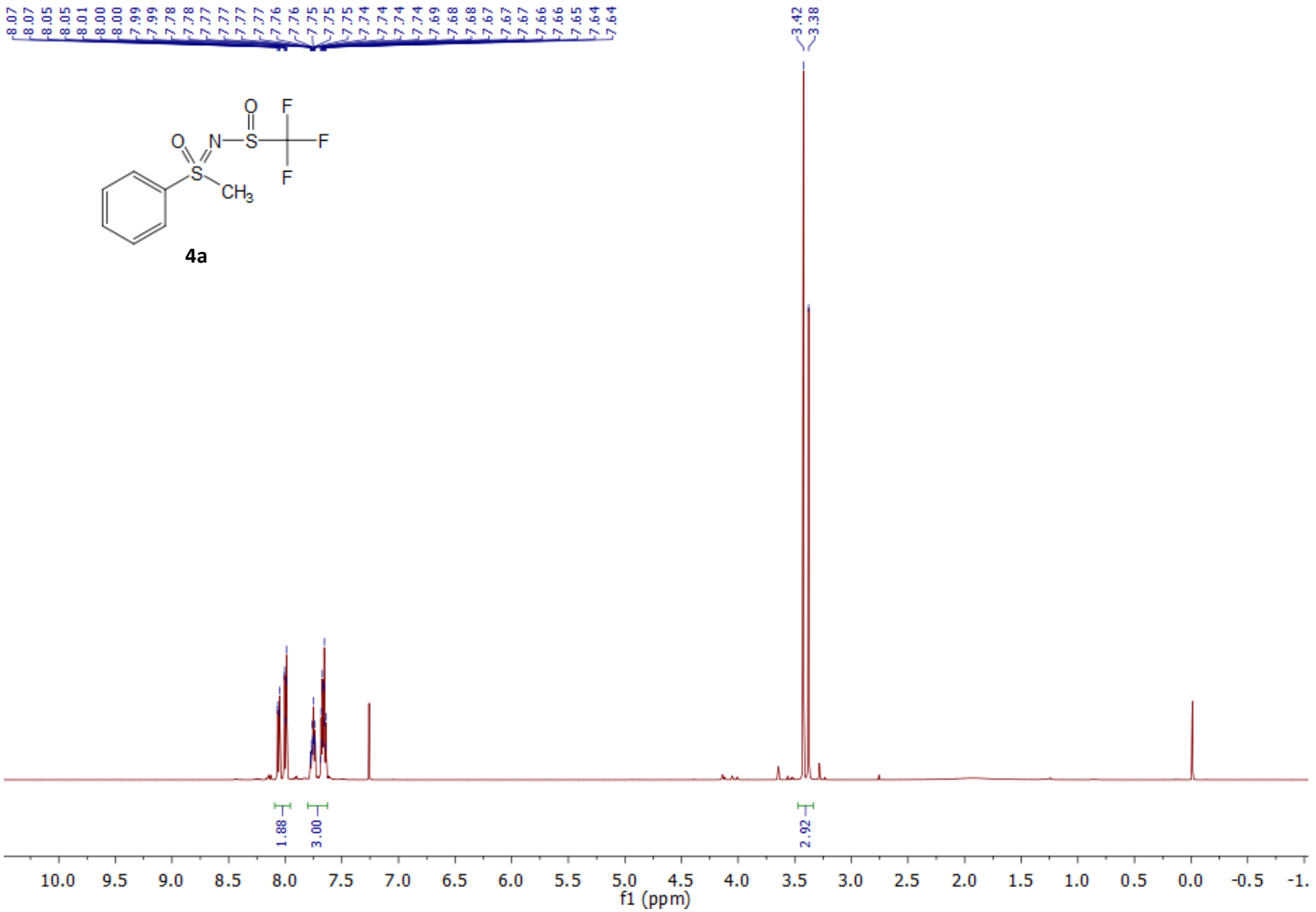
3ak

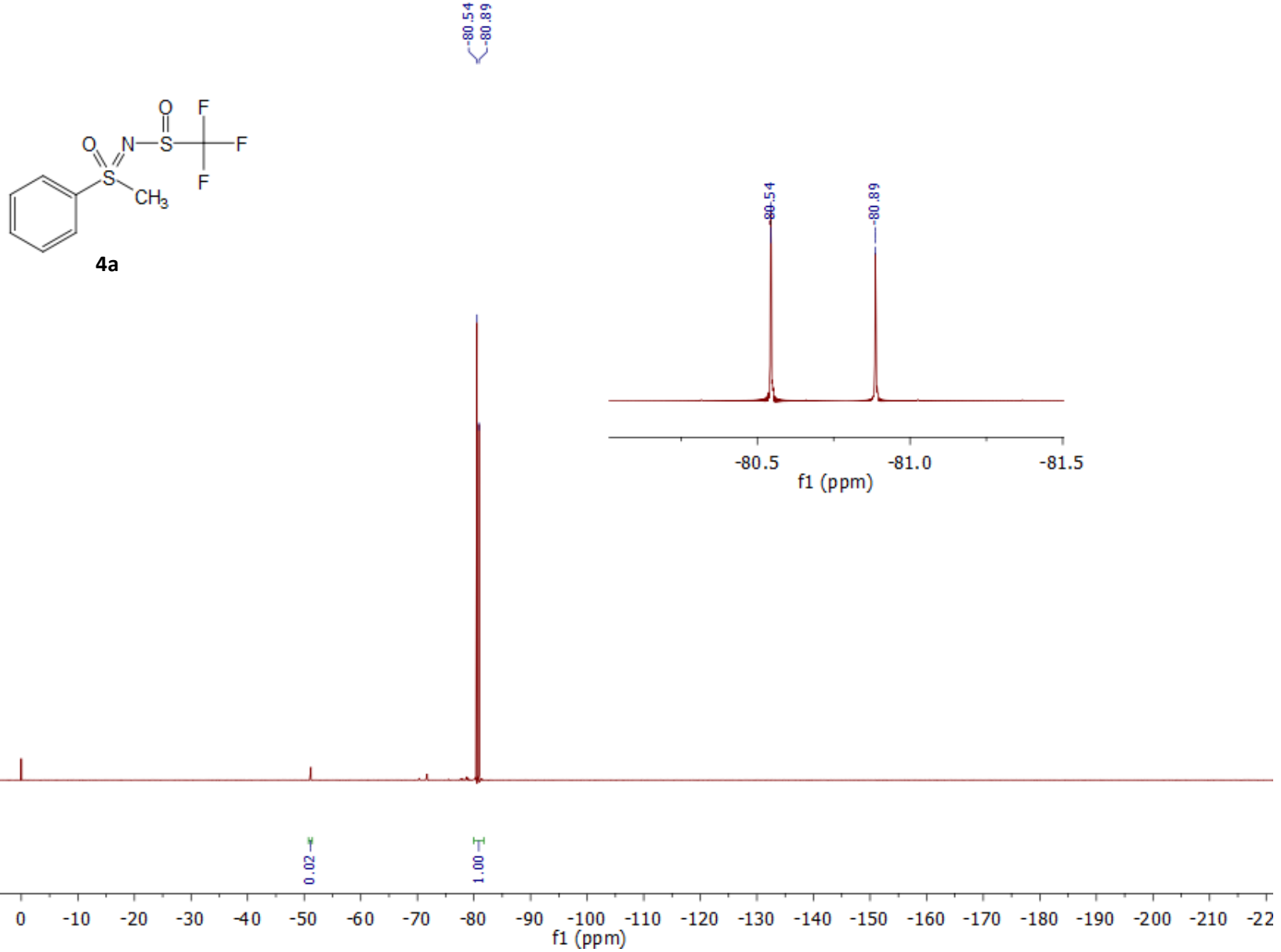
3ak

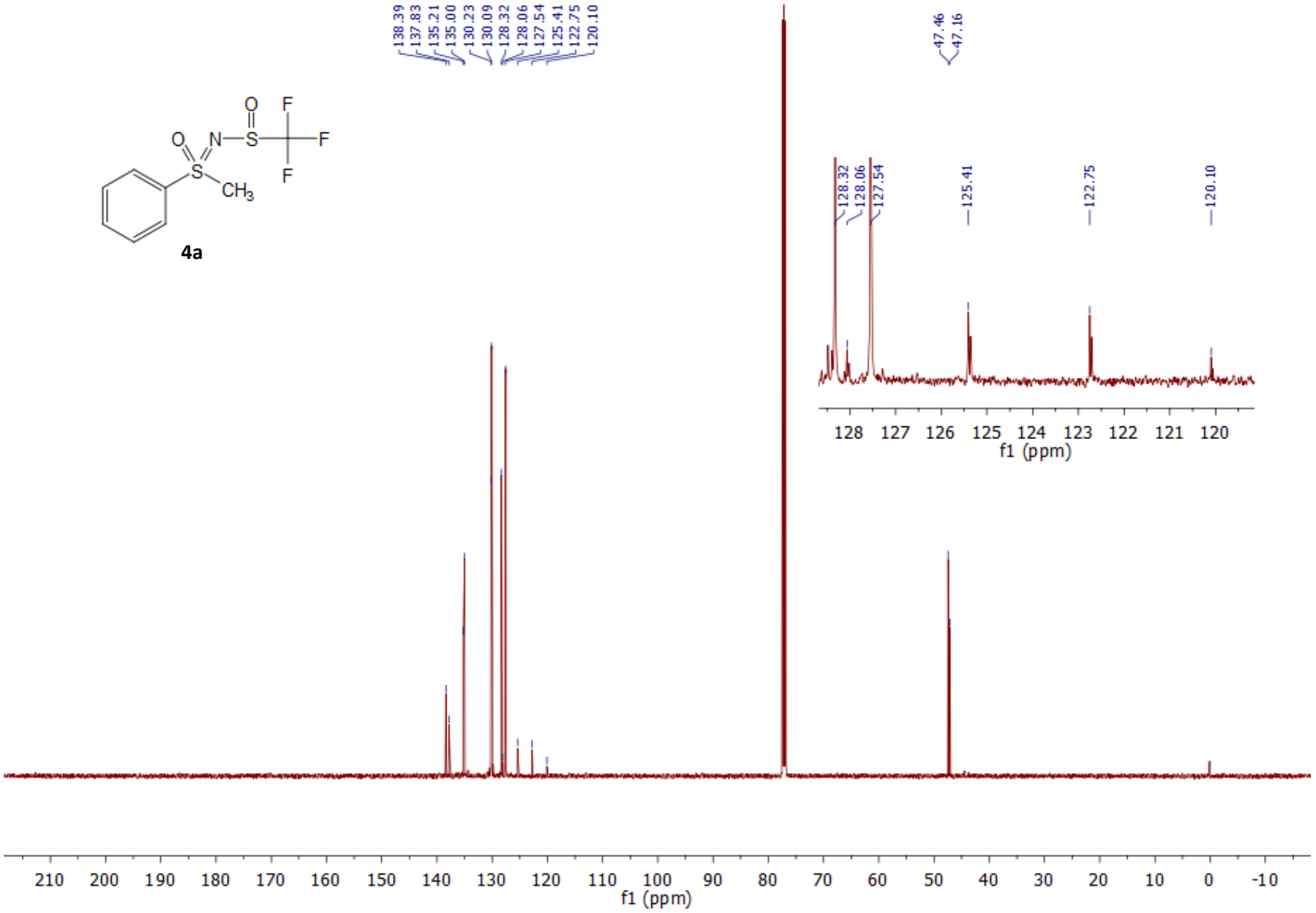

-78.88
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)

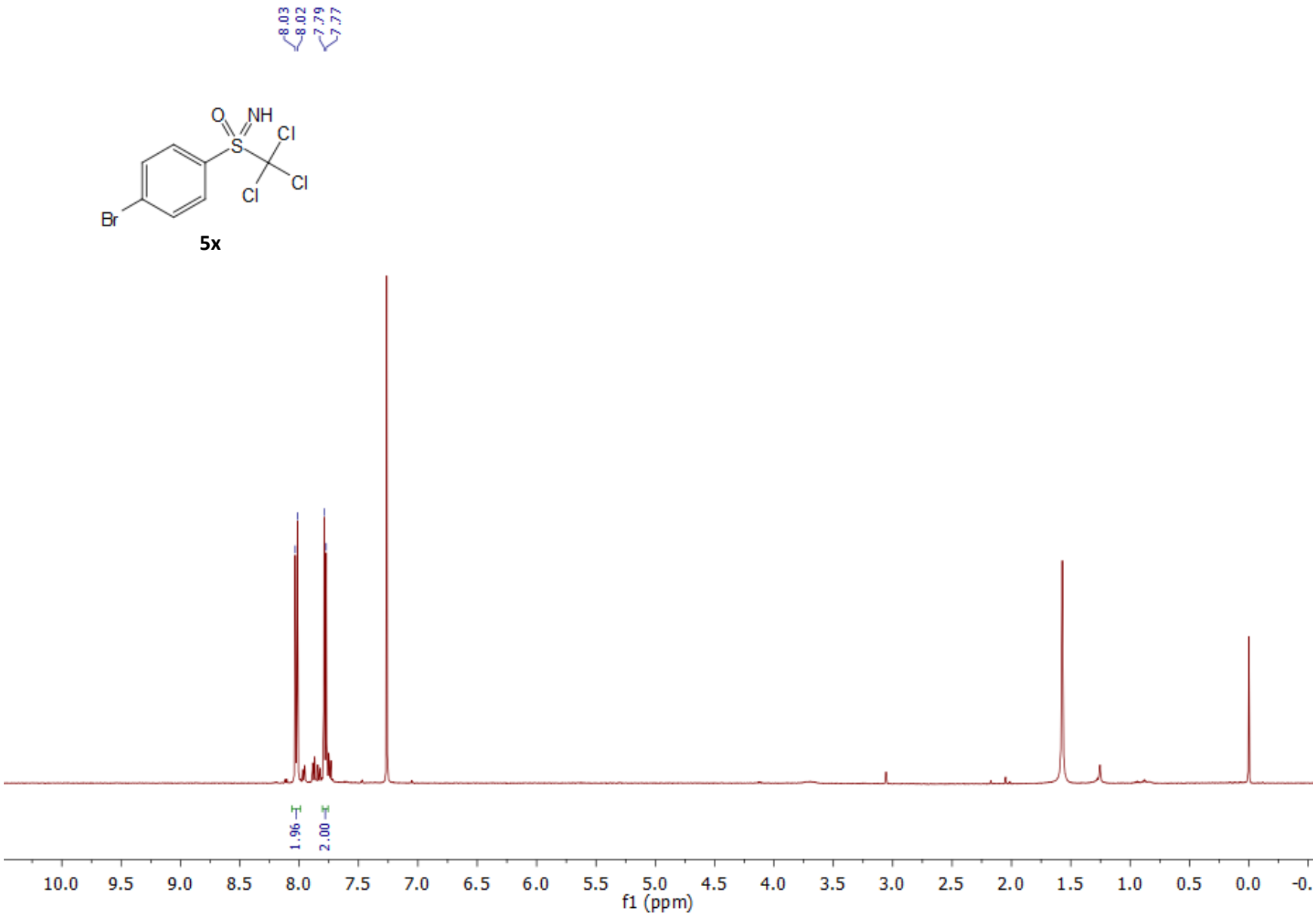

152.62
145.35
132.54
128.19
120.20
117.65
65.40
46.69
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ak

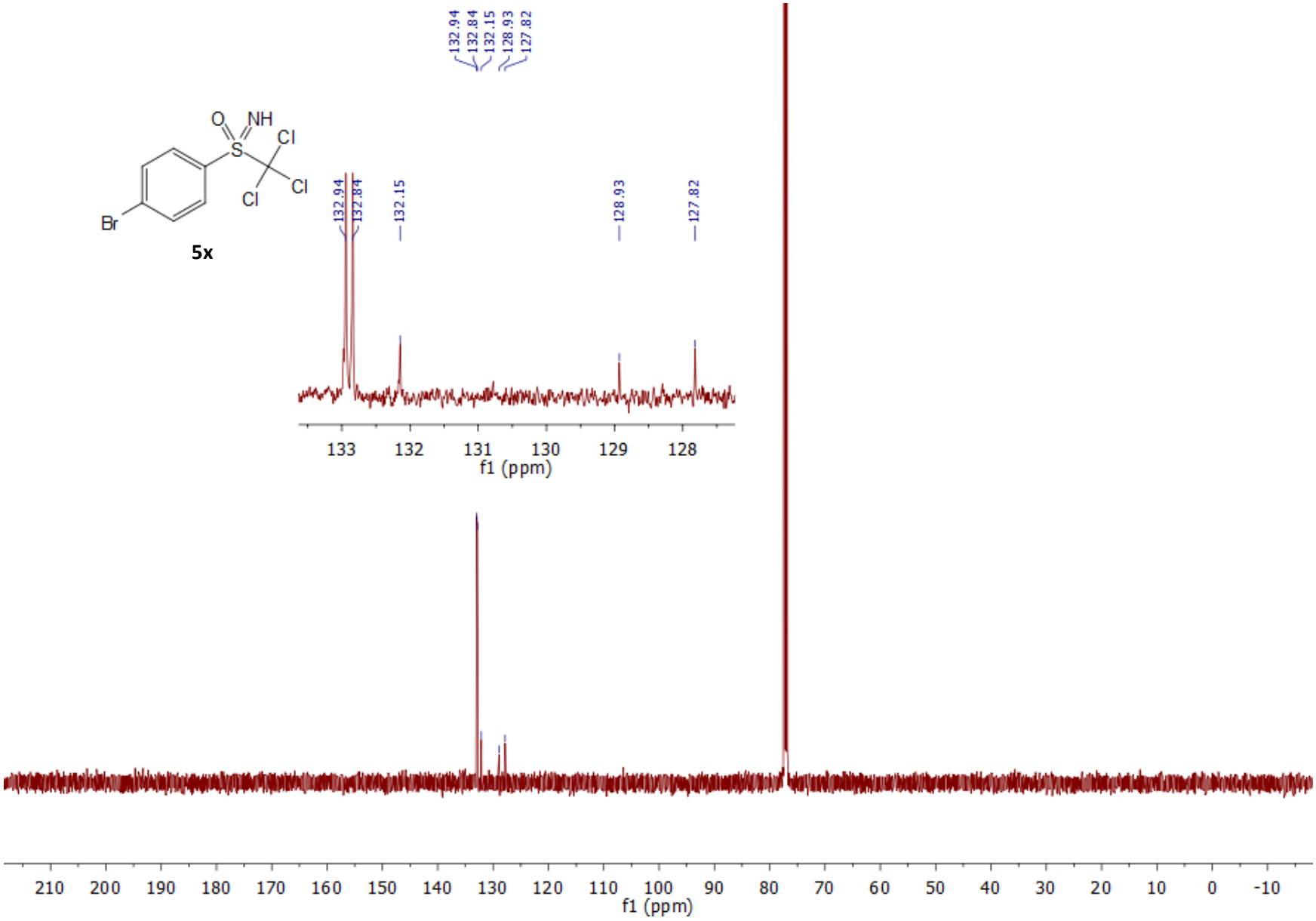

8.07
8.07
8.05
8.05
8.01
8.00
8.00
7.99
7.99
7.78
7.78
7.77
7.77
7.77
7.77
7.76
7.76
7.75
7.75
7.75
7.74
7.74
7.74
7.74
7.69
7.68
7.68
7.67
7.67
7.67
7.66
7.66
7.65
7.64
7.64
3.42
3.38
O
F
O
N
S
F
S
F
CH3
4a
1.88
3.00
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

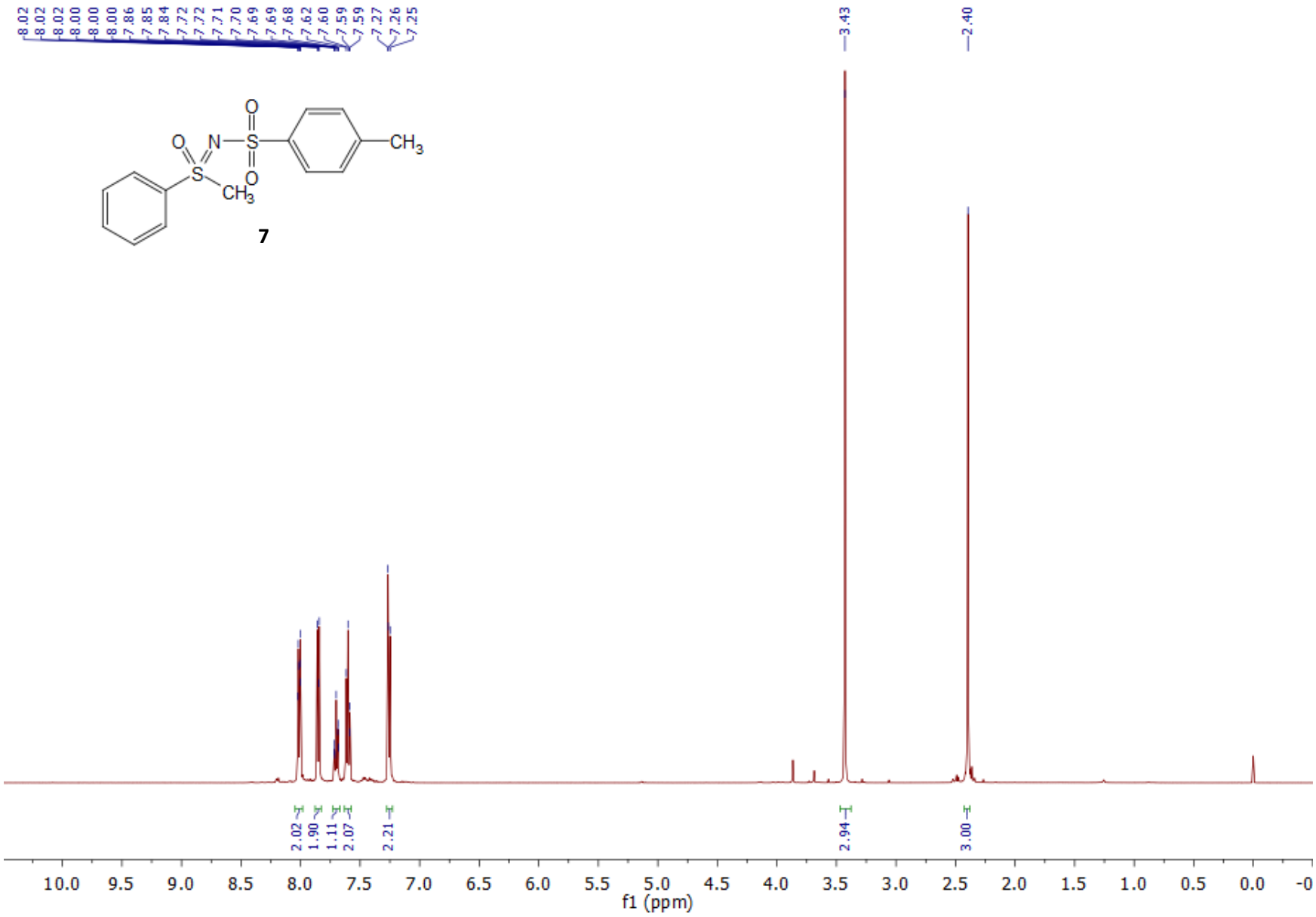

-80.54
-80.89
O
F
O
N
S
F
S
F
CH3
4a
-80.54
-80.89
-80.5
-81.0
-81.5
f1 (ppm)
0.02
1.00
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-22
f1 (ppm)


138.39
137.83
135.21
135.00
130.23
130.09
128.32
128.06
127.54
125.41
122.75
120.10
47.46
47.16
O
F
O
N
S
F
S
F
CH3
4a
128.32
128.06
127.54
125.41
122.75
120.10
128 127 126 125 124 123 122 121 120
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

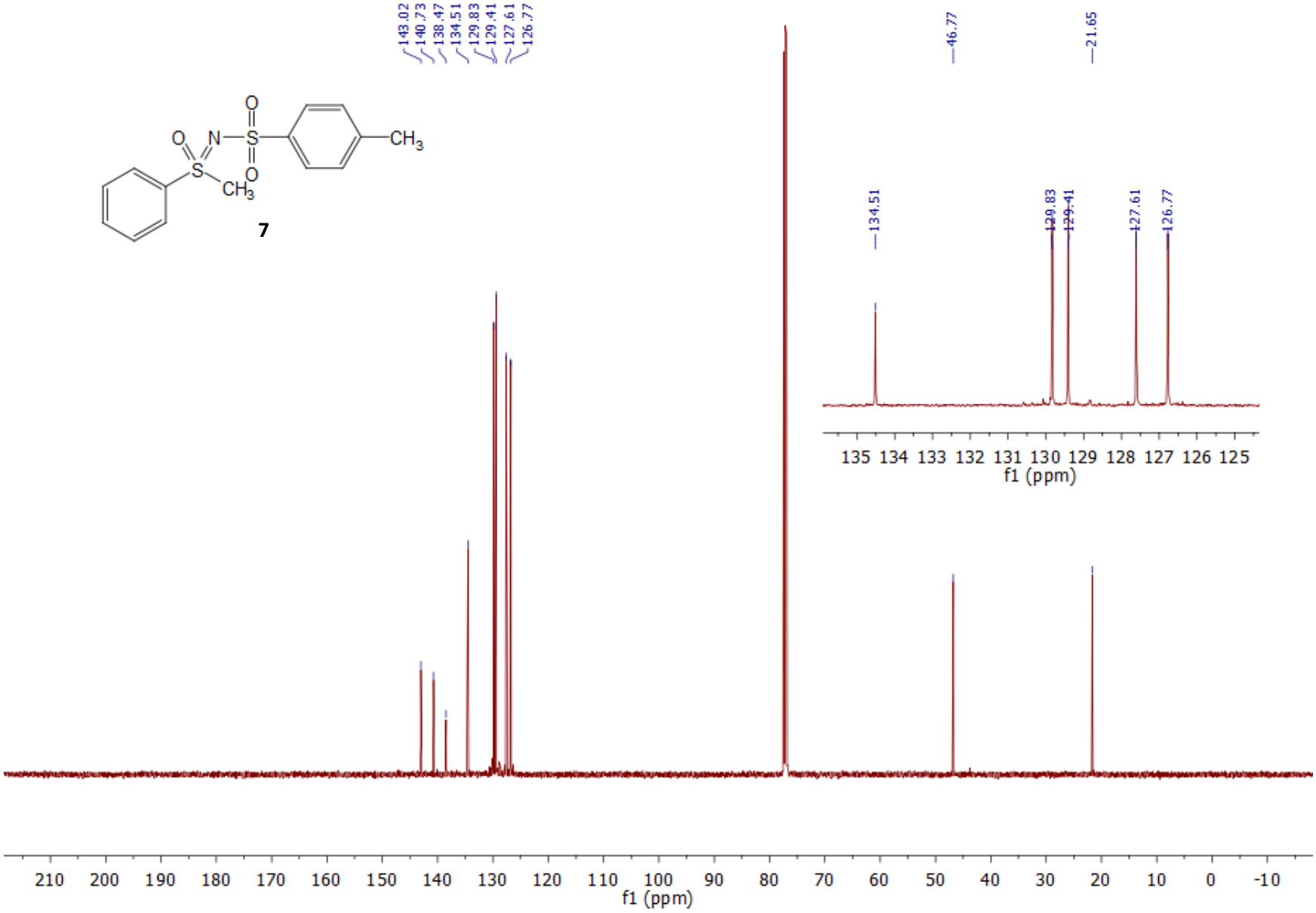

8.03
8.02
7.79
7.77
O
NH
S
Cl
Cl
Cl
Br
1.96
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

5x


132.94
132.84
132.15
128.93
127.82
O
NH
S
Cl
Cl
Cl
Br
5x
132.94
132.84
132.15
128.93
127.82
133
132
131
130
129
128
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.02
8.02
8.02
8.00
8.00
8.00
7.86
7.85
7.84
7.72
7.72
7.71
7.70
7.69
7.69
7.68
7.62
7.60
7.59
7.59
7.27
7.26
7.25
3.43
2.40
O
N
S
O
S
O
CH3
CH3
2.02
1.90
1.11
2.07
2.21
2.94
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

7


143.02
140.73
138.47
134.51
129.83
129.41
127.61
126.77
46.77
21.65
O
N
S
O
O
S
CH3
CH3
7
134.51
129.83
129.41
127.61
126.77
135 134 133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)