Direct Transfer Strategy of Trifluoromethylsulfinyl Group by a General Reagent *N*-Trifluoromethylsulfinylphthalimide under Catalytic or Stoichiometric Lewis Acid or Lewis Base

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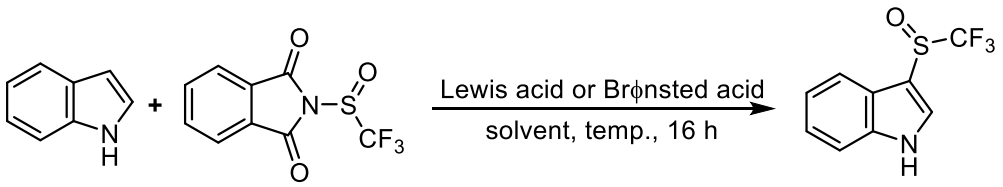
1. General information.

All reactions were carried out under an argon atmosphere using standard Schlenk-Lines. ^{1}H, ^{13}C and ^{19}F NMR spectra were acquired on 400 MHz, 100 MHz, 376 MHz on JOEL-ZETA 400 MHz or Bruker-AVANCE III-400 MHz spectrometer (400 MHz for ^{1}H; 100 MHz for ^{13}C; 376 MHz for ^{19}F). ^{1}H NMR and ^{13}C NMR chemical shifts were determined relative to internal standard TMS at δ 0.0 ppm and ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ as inter standard. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. All reactions were monitored by TLC with 0.25 mm coated commercial silica gel plates (TLC Silica Gel 60 F_{254}). Flash column chromatograph was carried out using 300-400 mesh silica gel at medium pressure. Infrared (IR) data were recorded as films on potassium bromide plates on a Bruker Tensor 27 FT-IR spectrometer. Absorbance frequencies are reported in reciprocal cetimeters (cm^{-1}). Mass spectra were acquired on a Bruker Daltonics MicroTof-Q II mass spectrometer or Agilent 7890B-5977A mass spectrometer.

Materials. All reagents were received from commercial sources unless otherwise noted. Solvents were freshly dried and degassed according to the purification handbook *Purification of Laboratory Chemicals* before using.

2. Reaction optimization

2.1. Optimization of reaction conditions for *N*-trifluoromethylsulfinylphthalimide with electron-rich heteroarenes. [a,b]

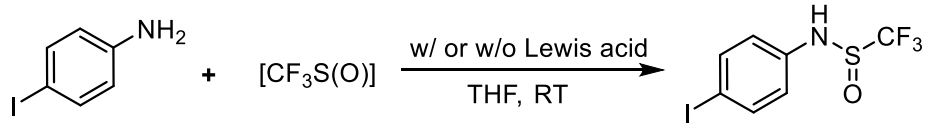


7aa **6** **8aa**

entry[a]	Lewis acid or Brϕnsted acid	solvent	temp. (°C)	yield (**8aa**, %)[b]
1	CF_3SO_3H (1.5 equiv)	$CHCl_3$	50	0
2	PTSA (1.5 equiv)	$CHCl_3$	50	0
3	BF_3 Et_2O (1.5 equiv)	$CHCl_3$	50	0
4	$AlCl_3$ (1.5 equiv)	$CHCl_3$	50	0
5	$ZnCl_2$ (1.5 equiv)	$CHCl_3$	50	0
6	$MgCl_2$ (1.5 equiv)	$CHCl_3$	50	trace
7	LiCl (1.5 equiv)	$CHCl_3$	50	trace
8	Me_3SiBr (1.5 equiv)	$CHCl_3$	50	0
9	**Me_3SiCl (1.5 equiv)**	**$CHCl_3$**	**50**	**99**
10	Me_3SiCl (1.5 equiv)	$ClCH_2CH_2Cl$	50	72
11	Me_3SiCl (1.5 equiv)	CH_2Cl_2	50	88
12	Me_3SiCl (1.5 equiv)	toluene	50	63
13	Me_3SiCl (1.5 equiv)	THF	50	0
14[c]	Me_3SiCl (1.5 equiv)	$CHCl_3$	RT	90

[a] Reaction conditions: indole (0.1 mmol), reagent **6** (0.12 mmol), Lewis acid or Brønsted acid (0.15 mmol) in solvent (1.0 mL) at 50 °C for 16 h; [b] Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard. PTSA = *p*-toluenesulfonic acid. [c] Room temperature was used.

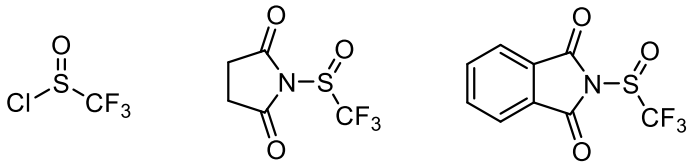
2.2. Optimization of reaction conditions for *N*-trifluoromethylsulfinylphthalimide with amines. [a,b]



9ba **1, 4-6** **10ba**

entry[a]	[$CF_3S(O)$]	Lewis acid	yield (**10ba**, %)[b]
1	**1**	$POCl_3$ (1.0 equiv)	70
2	**4**	–	5
3	**5**	–	0
4	**5**	$Ph_2P(O)Cl$ (1.5 equiv)	75
5	**6**	–	0
6	**6**	Me_3SiCl (1.5 equiv)	28
7	**6**	Ph_2PCl (1.5 equiv)	0
8	**6**	$P(O)Cl_3$ (1.5 equiv)	43
9	**6**	**$Ph_2P(O)Cl$ (1.5 equiv)**	85

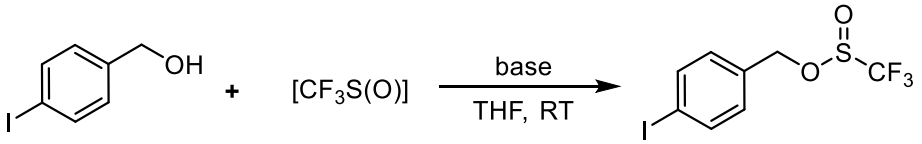
[$CF_3S(O)$] = CF_3SO_2Na



1 **4** **5** **6**

[a] Reaction conditions: reagent (**1,** 0.2 mmol), $POCl_3$ (0.1 mmol) in THF (1.0 mL) at RT for 0.5 h, then 4-iodoaniline (**9ba**, 0.10 mmol) was added to the reaction at RT for another 3 h; reagent (**4**, 0.15 mmol) and 4-iodoaniline (**9ba**, 0.10 mmol) in THF (1.0 mL) at RT for 3 h; reagent (**5** or **6** 0.15 mmol), w/ or w/o Lewis acid (0.15 mmol) in THF (1.0 mL) at RT for 10 h, then 4-iodoaniline (**9ba**, 0.10 mmol) was added to the reaction at RT for another 3 h; [b] Yields were determined by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard.

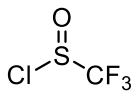
2.3. Optimization of reaction conditions for *N*-trifluoromethylsulfinylphthalimide with alcohols.[a,b]



11ab **4-6** **12ab**

entry[a]	[$CF_3S(O)$]	base	yield (**12ab**, %)[b]
1	**4**	–	20
2	**5**	–	0
3	**6**	–	0
4	**6**	DABCO (1.0 equiv)	trace
5	**6**	DBU (1.0 equiv)	0
6	**6**	NaH (1.0 equiv)	72
7	**6**	KOH (1.0 equiv)	41
8	**6**	K_2CO_3 (1.0 equiv)	48
9	**6**	Et_3N (1.0 equiv)	92
10	**6**	Et_3N (0.1 equiv)	93
11	**5**	Et_3N (0.1 equiv)	65

[$CF_3S(O)$] =



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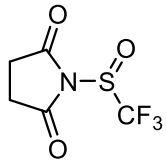

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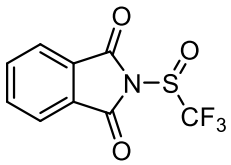
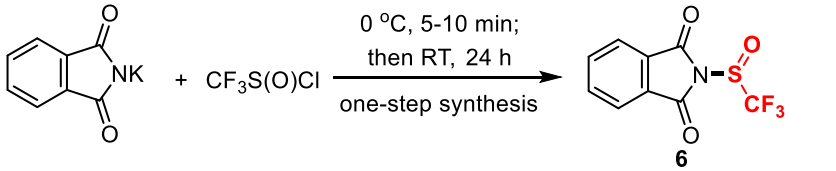


6

[a] Reaction conditions: 4-iodobenzyl alcohol (**11ab**, 0.1 mmol), reagent **4-6** (0.12 mmol), base (0.1 mmol) in THF (1.0 mL) at RT for 3 h; [b] Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard.

3. Experimental procedures

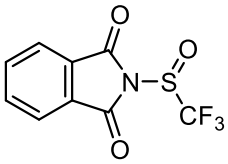
3.1 Large scale preparation of *N*-trifluoromethylsulfinylphthalimide



10.6 g, 78% (52 mmol scale)

A 1000 mL dry round bottom flask charged with potassium phthalimide (52 mmol, 9.63 g) in 600 mL dry toluene under argon atmosphere was added trifluoromethanesulfinyl chloride (57.2 mmol, 1.1 equiv, 8.72 g) slowly at 0 °C for 5-10 min, then the reaction mixture was stirred at RT for 24 h. After the reaction, the resulting precipitate was filtered and washed with toluene in twice. The combined organic phases were removed under vacuum, and the residue was purified by continuous recrystallization from toluene to afford *N*-trifluoromethylsulfinylphthalimide **6** (10.6g, 78%).

***N*-Trifluoromethylsulfinylphthalimide 6**

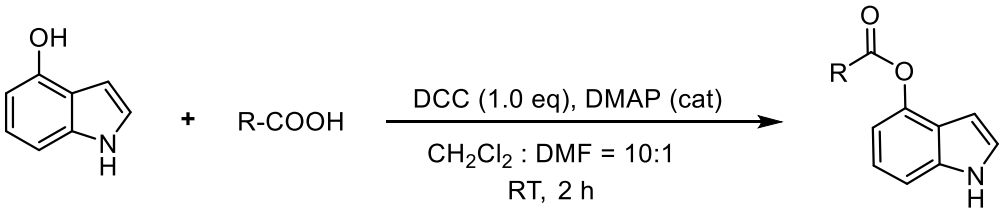


White solid. Mp: 120-121 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.50). **^{1}H NMR** (400 MHz, DMSO-d6) δ 8.03 (s, 4 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -68.8 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 164.8, 136.6, 131.8, 125.0, 124.6 (q, J = 343.4 Hz) ppm. **IR (KBr):** ν = 3196, 2916, 1748, 1604, 1468, 1376, 1306, 1259, 1187, 1099, 1053, 865, 712, 647, 534, 454 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_4F_3NO_3S$ $[M+Na]^+$ calcd 285.9762, found 285.9758 ppm.

3.2 Preparation of substrates

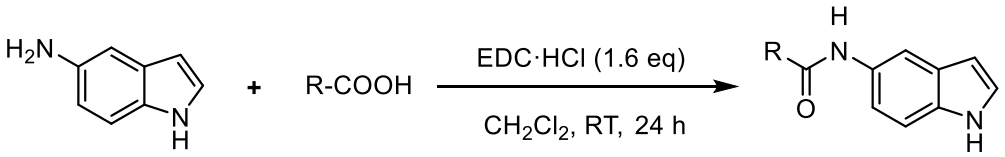
Substrates **7ae**,[1] **7ah**,[2] **7ao**,[3] **7ap**,[4] **7aq-7as**,[5] **7az-7ba**,[6] **7be**[7] and **7bf**[8] were prepared according to literature methods.

General procedure A:



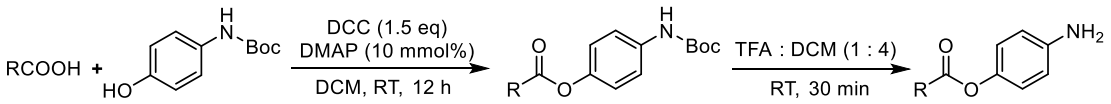
The substrates were prepared following literature procedures[9]**:** To a solution of 4-hydroxyindole (5 mmol, 1.0 eq) in a mixture of CH_2Cl_2 and DMF (20:2 mL), complex carboxylic acid (5.5 mmol, 1.1 eq), DCC (5 mmol, 1.0 eq) and DMAP (1.25 mmol, 25 mmol%) were added. The reaction mixture was stirred at RT for 2 h, and then concentrated under reduced pressure. The solid residue was suspended in ethyl acetate, filtered and the filtrate was washed with brine. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under reduced pressure. The solid residue was purified by silica gel chromatography to give the desired products.

General procedure B:



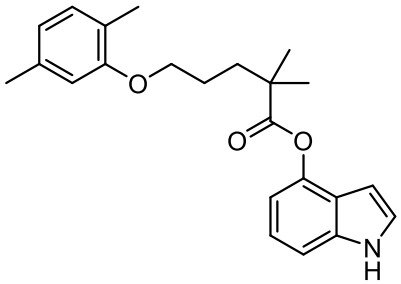
The substrates were prepared following literature procedures[10]**:** To a solution of 1*H*-indol-5-amine (5 mmol, 1.0 eq) in dry CH_2Cl_2 (75 ml) was added complex carboxylic acid (5.5 mmol, 1.1 eq) and EDC·HCl (8 mmol, 1.6 eq). The reaction mixture was stirred at RT for 24 h and then further diluted with CH_2Cl_2 (40 ml). The mixture was washed with water (80 ml×3), saturated potassium bisulfate solution, sodium bicarbonate solution and then brine. The organic solvent was dried over anhydrous Na_2SO_4 and evaporated in vacuo. The solid residue was purified by silica gel chromatography to give the desired products.

General procedure C:



The substrates were prepared following literature procedures[11]: Complex carboxylic acid (5.0 mmol, 1.0 equiv), *tert*-butyl (4-hydroxyphenyl)carbamate (5.0 mmol, 1.0 equiv), DCC (7.5 mmol, 1.5 equiv) and DMAP (0.5 mmol, 10 mmol%) in DCM (30 mL) were stirred in 100mL round bottom flask at RT for 12 h. After the reaction, the mixture was filtered and the filtrate was concentrated by reduced vacuum. Then crude compound was sub*J*ected to 20% of TFA in DCM (v/v, 20 mL) at RT for 30 min. After the concentration under reduced vacuum, the mixture was dissolved in water and treated with saturated $NaHCO_3$ to adjust the pH to 8, subsequently extracted with EtOAc for three times. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified on a silicagel column chromatograph to afford the corresponding complex aniline substrates.

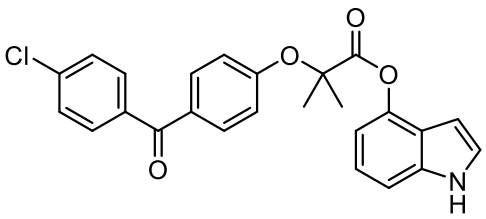
1*H*-Indol-4-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate 13aa



Compound **13aa** was synthesized by following general procedure A.

White solid (0.93 g, 51%). Mp: 85-86 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.62). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.30 (s, 1 H), 7.19 (d, *J* = 8.0 Hz, 1 H), 7.15 (t, *J* = 7.8 Hz, 1 H), 7.05 (d, *J* = 2.7 Hz, 1 H), 7.03 (s, 1H), 6.84 (d, *J* = 7.3 Hz, 1 H), 6.70 (d, *J* = 7.2 Hz, 1 H), 6.68 (s, 1 H), 6.40 (s, 1 H), 4.04 (s, 2 H), 2.34 (s, 3 H), 2.23 (s, 3 H), 2.00 (s, 4 H), 1.49 (s, 6 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.5, 157.1, 144.0, 137.8, 136.6, 130.5, 124.7, 123.8, 122.1, 121.3, 120.9, 112.1, 111.9, 109.2, 99.1, 68.1, 42.8, 37.4, 25.5, 21.5, 16.0 ppm. **IR (KBr):** ν = 2924, 2358, 1735, 1459, 1129, 404 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{23}H_{27}NO_3$ $[M+Na]^+$ calcd 388.1889, found 388.1874 ppm.

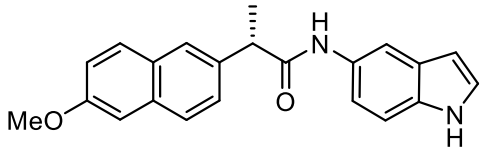
1*H*-Indol-4-yl 2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoate 13ab



Compound **13ab** was synthesized by following general procedure A.

Green solid (1.21 g, 56%). Mp: 158-159 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.54). **^{1}H NMR** (400 MHz, DMSO-d6) δ 11.34 (s, 1 H), 7.78 (d, *J* = 8.4 Hz, 2 H), 7.70 (d, *J* = 8.3 Hz, 2 H), 7.59 (d, *J* = 8.2 Hz, 2 H), 7.31 (d, *J* = 15.0 Hz, 2 H), 7.08 (t, *J* = 8.9 Hz, 3 H), 6.71 (d, *J* = 7.9 Hz, 1 H), 6.10 (s, 1 H), 1.84 (s, 6 H); **^{13}C NMR** (100 MHz, DMSO-d6) δ 193.8, 172.1, 159.7, 143.2, 138.4, 137.7, 136.8, 132.6, 131.8, 130.4, 129.2, 126.6, 121.6, 121.2, 117.7, 111.3, 110.4, 97.9, 79.9, 25.8 ppm. **IR (KBr):** ν = 3389, 2924, 1752, 1651, 1598, 1503, 1351, 1275, 1170, 1128, 928, 852, 746 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{25}H_{20}ClNO_4$ $[M+Na]^+$ calcd 456.0979, found 456.0972 ppm.

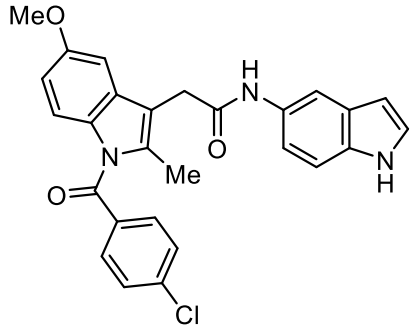
(S)-*N*-(1*H*-Indol-5-yl)-2-(6-methoxynaphthalen-2-yl)propanamide 13ac



Compound **13ac** was synthesized by following general procedure B.

White solid (1.65 g, 96%). Mp: 170-171 °C. Eluent: petroleum ether/ethyl acetate (1:1, R_f = 0.51). **^{1}H NMR** (400 MHz, DMSO-d6) δ 10.96 (s, 1 H), 9.89 (s, 1 H), 7.86 (s, 1 H), 7.81 – 7.72 (m, 3 H), 7.53 (d, *J* = 8.5 Hz, 1 H), 7.29 – 7.22 (m, 3 H), 7.17 (d, *J* = 10.5 Hz, 1 H), 7.12 (d, *J* = 9.1 Hz, 1 H), 6.32 (s, 1 H), 3.94 (q, *J* = 7.0 Hz, 1 H), 3.82 (s, 3 H), 1.48 (d, *J* = 7.0 Hz, 3 H); **^{13}C NMR** (100 MHz, DMSO-d6) δ 172.2, 157.5, 138.0, 133.7, 133.2, 131.7, 129.7, 128.9, 127.9, 127.3, 127.0, 126.4, 125.9, 119.2, 115.4, 111.6, 111.3, 106.2, 101.6, 55.7, 46.3, 19.3 ppm. **IR (KBr):** ν = 2923, 1656, 1605, 1464, 1266, 1208, 853 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{22}H_{20}N_2O_2$ $[M+Na]^+$ calcd 367.1422, found 367.1415 ppm.

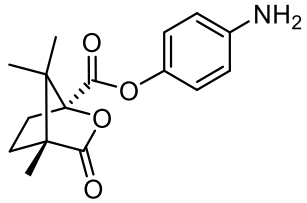
2-(1-(4-Chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(1*H*-indol-5-yl)acetamide 13ad



Compound **13ad** was synthesized by following general procedure B.

Yellow solid (1.01 g, 43%). Mp: 230-231 °C. Eluent: petroleum ether/ethyl acetate (1:1, R_f = 0.50). **^{1}H NMR** (400 MHz, DMSO-d6) δ 10.98 (s, 1 H), 10.01 (s, 1 H), 7.83 (s, 1 H), 7.66 (d, *J* = 8.4 Hz, 2 H), 7.61 (d, *J* = 8.3 Hz, 2 H), 7.33 – 7.24 (m, 2 H), 7.25 – 7.13 (m, 2 H), 6.91 (d, *J* = 9.0 Hz, 1 H), 6.68 (d, *J* = 9.1 Hz, 1 H), 6.32 (s, 1 H), 3.72 (s, 3 H), 3.71 (s, 2 H), 2.28 (s, 3 H); **^{13}C NMR** (100 MHz, DMSO-d6) δ 168.4, 156.1, 138.1, 135.8, 134.8, 133.3, 131.7, 131.6, 131.5, 130.8, 129.6, 128.0, 126.4, 115.5, 115.1, 115.1, 111.7, 111.5, 102.6, 101.6, 56.0, 32.6, 14.0 ppm. **IR (KBr):** ν = 2923, 1661, 1477, 1361, 1324, 1226, 1085, 1014, 851 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{27}H_{22}ClN_3O_3$ $[M+Na]^+$ calcd 494.1247, found 494.1238 ppm.

4-Aminophenyl (1S,4R)-4,7,7-trimethyl-3-oxo-2-oxabicyclo[*2.2.1*]heptane-1-carboxylate 13ag

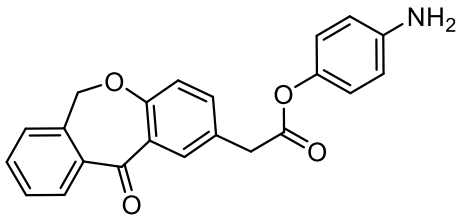


Compound **13ag** was synthesized by following general procedure C.

Yellow solid (0.99 g, 69%). Mp: 140-141 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.44). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.87 (d, *J* = 8.2 Hz, 2 H), 6.64 (d, *J* = 8.4 Hz, 2 H), 3.69 (s, 2 H), 2.59 – 2.46 (m, 1 H), 2.20 – 2.09 (m, 1 H), 2.01 – 1.91 (m, 1 H), 1.77 – 1.68 (m, 1 H), 1.12 (d, *J* = 8.2 Hz, 6 H), 1.06 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.1, 166.7, 144.9, 142.1, 122.0, 115.7, 91.1, 55.0, 54.7, 30.8, 29.1, 17.0, 9.8 ppm. **IR (KBr):** ν = 3376, 2969, 1778, 1624, 1507, 1312, 1260, 1188, 1096, 909,

858, 808, 727, 512 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{16}H_{19}NO_4$ $[M+Na]^+$ calcd 312.1212, found 312.1202 ppm.

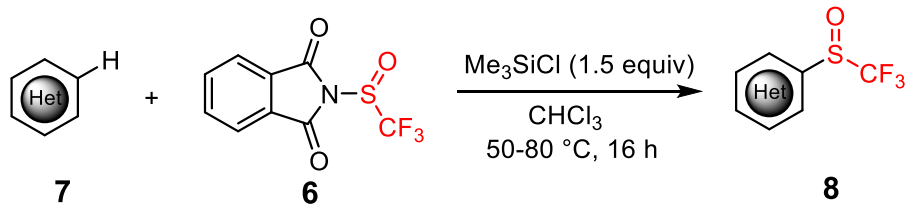
4-Aminophenyl 2-(11-oxo-6,11-dihydrodibenzo[*b,e*]oxepin-2-yl)acetate 13ah



Compound **13ah** was synthesized by following general procedure C.

Yellow solid (1.35 g, 75%). Mp: 125-126 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.42). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 2.4 Hz, 1 H), 7.89 (d, *J* = 7.7 Hz, 1 H), 7.55 (t, *J* = 7.4 Hz, 1 H), 7.50 (dd, *J* = 8.5, 2.4 Hz, 1 H), 7.46 (t, *J* = 7.6 Hz, 1 H), 7.35 (d, *J* = 7.4 Hz, 1 H), 7.05 (d, *J* = 8.3 Hz, 1 H), 6.84 (d, *J* = 8.6 Hz, 2 H), 6.61 (d, *J* = 8.6 Hz, 2 H), 5.18 (s, 2 H), 3.83 (s, 2 H), 3.54 (s, 2 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.0, 170.5, 160.7, 144.4, 142.9, 140.5, 136.5, 135.6, 132.9, 132.7, 129.6, 129.4, 127.9, 127.6, 125.3, 122.1, 121.3, 115.6, 73.7, 40.3 ppm. **IR (KBr):** ν = 3369, 1747, 1644, 1611, 1508, 1413, 1300, 1192, 1135, 1013, 907, 826, 761, 730, 642, 516 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{22}H_{17}NO_4$ $[M+H]^+$ calcd 360.1236, found 360.1240 ppm.

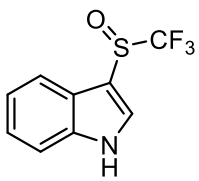
3.3 General procedure for Friedel-Crafts-type trifluoromethylsulfinylation of electron-rich heteroarenes



Method A: A 25 mL Schlenk tube charged with heteroarene (**7**, 0.5 mmol), *N*-trifluoromethylsulfinylphthalimide **6** (0.6 mmol, 1.2 equiv) and Me_3SiCl (0.75 mmol, 1.5 equiv) under argon atmosphere was added freshly distilled $CHCl_3$ (3.0 mL). The mixture was stirred at 50-80 °C for 16 h. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated (hetero)arene **8**.

Method B: A 25 mL Schlenk tube charged with heteroarene (**7**, 0.5 mmol), *N*-trifluoromethylsulfinylphthalimide **6** (0.6 mmol, 1.2 equiv) and NaCl (0.05 mmol, 10 mol%) was added freshly distilled DMF (3.0 mL). The reaction mixture was stirred at 80 °C for 16 h. After the reaction was completed, the mixture was extracted with distilled water (25.0 mL) and ethyl acetate (50.0 mL). The aqueous phase was extracted with ethyl acetate (3×15.0 mL). The combined organic extracts were washed with distilled water (50.0 mL) and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated (hetero)arene **8**.

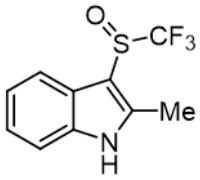
3-((Trifluoromethyl)sulfinyl)-1*H*-indole 8aa



Brown solid (115.3 mg, 99%, Method A, 50 °C). Mp: 118-119 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.34). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.32 (s, 1 H), 7.99 (d, *J* = 7.8 Hz, 1 H), 7.73 (s, 1 H), 7.48 (d, *J* = 8.1 Hz, 1 H), 7.31 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.0, 131.5, 125.6

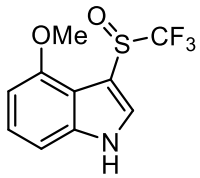
(q, J = 333.3 Hz), 124.5, 124.1, 122.7, 120.1, 112.8, 107.6 ppm. The spectroscopic data were matched with those reported in the literature.[4]

2-Methyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ab



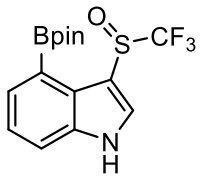
Yellow solid (119.8 mg, 97%, Method A, 80 ºC). Mp: 143-144 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.29). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.32 (s, 1 H), 7.78 (d, J = 7.8 Hz, 1 H), 7.48 (d, J = 8.7 Hz, 1 H), 7.23 (t, J = 8.0 Hz, 1 H), 7.19 (t, J = 8.0 Hz, 1 H), 2.58 (s, 3 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -72.2 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 145.2, 136.3, 126.7 (q, J = 333.3 Hz), 125.5, 123.3, 122.0, 119.7, 112.5, 102.7, 12.2 ppm. The spectroscopic data were matched with those reported in the literature.[4]

4-Methoxy-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ac



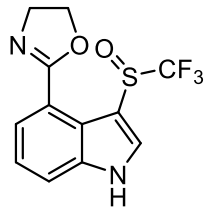
Brown solid (94.7 mg, 72%, Method A, 50 ºC). Mp: 139-140 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.32). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.25 (s, 1 H), 7.81 (s, 1 H), 7.23 (t, J = 8.0 Hz, 1 H), 7.13 (d, J = 7.2 Hz, 1 H), 6.67 (d, J = 7.8 Hz, 1 H), 3.96 (s, 3 H); **^{19}F NMR** (565 MHz, $CDCl_3$) δ -75.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.9, 138.0, 127.7, 125.2 (q, J = 343.4 Hz), 124.9, 115.6, 108.3, 105.6, 102.0, 55.5 ppm. The spectroscopic data were matched with those reported in the literature.[12]

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ad



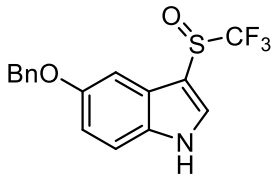
Yellow solid (152.6 mg, 85%, Method A, 80 ºC). Mp: 177-178 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.34). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.57 (s, 1 H), 8.08 (s, 1 H), 7.86 (d, *J* = 7.1 Hz, 1 H), 7.67 (d, *J* = 8.2 Hz, 1 H), 7.33 (t, *J* = 7.7 Hz, 1 H), 1.42 (s, 12 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.1, 131.0, 129.9, 127.7, 125.8 (q, *J* = 333.3 Hz), 123.0, 116.1, 110.9, 84.5, 25.0, 24.6 ppm. The spectroscopic data were matched with those reported in the literature.[4]

2-(3-((Trifluoromethyl)sulfinyl)-1*H*-indol-4-yl)-4,5-dihydrooxazole 8ae



Yellow solid (117.8 mg, 78%, Method A, 80 ºC). Mp: 165-166 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.29). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.54 (s, 1 H), 8.97 (s, 1 H), 7.78 (d, *J* = 8.1 Hz, 1 H), 7.70 (d, *J* = 7.5 Hz, 1 H), 7.37 (t, *J* = 7.8 Hz, 1 H), 3.76 (t, *J* = 6.2 Hz, 2 H), 3.63 (m, 2 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -74.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.0, 143.9, 137.3 (d, *J* = 10.6 Hz), 131.1 (q, *J* = 343.4 Hz), 130.4, 127.4, 126.8, 126.1, 121.8, 114.8, 48.1, 46.7 ppm. **IR (KBr):** ν = 2924, 1639, 1544, 1299, 1188, 1126, 1047 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{12}H_9F_3N_2O_2S$ $[M+H]^+$ calcd 303.0415, found 303.0406.

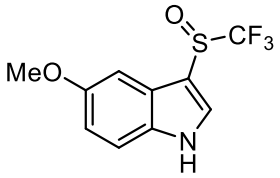
5-(Benzyloxy)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8af



Brown solid (117.0 mg, 69%, Method A, 50 ºC). Mp: 135-136 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.21). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.96 (s, 1 H), 7.61 (s, 1 H), 7.50 (s, 1 H), 7.44 (d, *J* = 6.7 Hz, 2 H), 7.38 (t, *J* = 8.0 Hz, 2 H), 7.33 (d, *J* = 9.1 Hz, 2 H), 7.04 (d, *J* = 8.9 Hz, 1 H), 5.02 (t, *J* = 12.0 Hz, 2 H); **^{19}F NMR** (565 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.2, 136.9, 131.9, 131.4,

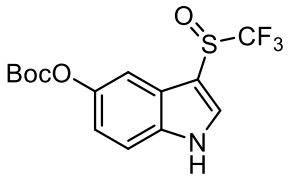
128.6, 128.1, 127.7, 125.7 (q, J = 333.3 Hz), 124.9, 115.7, 113.5, 107.3, 103.1, 70.7 ppm. **IR (KBr):** ν = 2954, 1582, 1484, 1288, 1188, 1130, 1044, 696, 473 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{16}H_{12}F_3NO_2S$ $[M+Na]^+$ calcd 362.0439, found 362.0437.

5-Methoxy-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ag



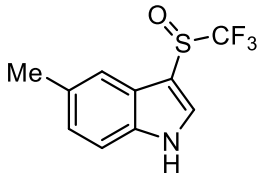
Yellow solid (99.9 mg, 76%, Method A, 50 ºC). Mp: 112-113 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.26). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.21 (s, 1 H), 7.69 (s, 1 H), 7.39 (s, 1 H), 7.35 (d, J = 9.0 Hz, 1 H), 6.96 (d, J = 8.9 Hz, 1 H), 3.78 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.1, 131.8, 131.4, 125.8 (q, J = 333.3 Hz), 124.9, 115.1, 113.5, 107.1, 101.6, 55.7 ppm. The spectroscopic data were matched with those reported in the literature.[4]

***Tert*-butyl (3-((trifluoromethyl)sulfinyl)-1*H*-indol-5-yl) carbonate 8ah**



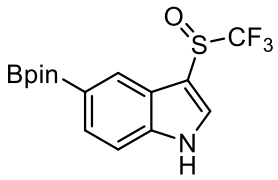
Yellow solid (157.1 mg, 90%, Method B). Mp: 163-164 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.47). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.19 (s, 1 H), 7.73 (s, 1 H), 7.55 (s, 1 H), 7.22 (d, J = 8.5 Hz, 1 H), 7.06 (d, J = 6.6 Hz, 1 H), 1.58 (s, 9 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.7 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.0, 146.5, 134.7, 132.8, 125.5 (q, J = 333.3 Hz), 124.2, 118.5, 113.5, 112.4, 107.5, 84.0, 27.7 ppm. **IR (KBr):** ν = 3271, 1754, 1467, 1416, 1371, 1299, 1253, 1051, 886, 738, 650, 519, 475 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{14}H_{14}F_3NO_4S$ $[M+Na]^+$ calcd 372.0493, found 372.0481.

5-Methyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ai



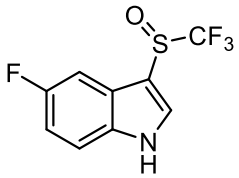
Gray solid (97.6 mg, 79%, Method A, 50 ºC). Mp: 127-128 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.37). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.40 (s, 1 H), 7.78 (s, 1 H), 7.69 (s, 1 H), 7.38 (d, *J* = 8.3 Hz, 1 H), 7.17 (d, *J* = 7.6 Hz, 1 H), 2.44 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.4, 132.4, 131.5, 126.1, 125.7 (q, *J* = 333.3 Hz), 124.3, 119.6, 112.4, 106.8, 21.9 ppm. The spectroscopic data were matched with those reported in the literature.[12]

5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8aj



White solid (141.8 mg, 79%, Method B). Mp: 208-209 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.21). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.57 (s, 1 H), 8.40 (s, 1 H), 8.26 (s, 1 H), 7.62 (q, *J* = 8.3 Hz, 2 H), 1.31 (s, 12 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -72.6 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 139.6, 134.6, 129.8, 127.5,126.3 (q, *J* = 333.3 Hz), 124.1, 113.1, 107.3, 84.1, 25.2, 25.1 ppm. The spectroscopic data were matched with those reported in the literature.[4]

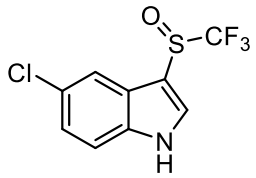
5-Fluoro-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ak



Yellow solid (123.0 mg, 98%, Method A, 50 ºC). Mp: 117-118 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.20). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.32 (s, 1 H), 7.80 (s, 1 H), 7.61 (d, *J* = 9.1 Hz, 1 H), 7.42 (d, *J* = 4.9 Hz, 1 H), 7.08 (t, *J* = 8.9 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.6 (s, 3 F), -119.5 (m, 1 F); **^{13}C NMR** (100 MHz,

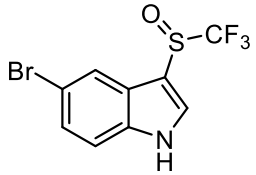
$CDCl_3$) δ 160.3, 158.0, 133.1 (d, *J* = 85.7 Hz), 125.6 (q, *J* = 333.3 Hz), 124.6 (d, *J* = 11.2 Hz), 113.8 (d, *J* = 9.8 Hz), 113.3 (d, *J* = 26.4 Hz), 107.6, 105.5 (d, *J* = 26.4 Hz) ppm. The spectroscopic data were matched with those reported in the literature.[12]

5-Chloro-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8al



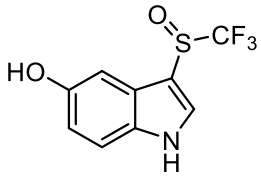
White solid (113.5 mg, 85%, Method A, 50 ºC). Mp: 138-139 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.20). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.12 (s, 1 H), 7.94 (s, 1 H), 7.79 (s, 1 H), 7.41 (d, *J* = 8.8 Hz, 1 H), 7.29 (d, *J* = 8.5 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.3, 132.0, 128.7, 125.5 (q, *J* = 333.3 Hz), 125.1, 125.1, 119.7, 113.8, 107.7 ppm. The spectroscopic data were matched with those reported in the literature.[12]

5-Bromo-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8am



White solid (153.9 mg, 99%, Method B). Mp: 162-163 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.18). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.65 (s, 1 H), 8.41 (s, 1 H), 7.98 (s, 1 H), 7.59 (d, *J* = 8.7 Hz, 1 H), 7.45 (d, *J* = 8.5 Hz, 1 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -72.9 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 136.3, 135.2, 126.8, 126.2 (q, *J* = 343.4 Hz), 126.1, 122.3, 115.7, 114.9, 106.4 ppm. The spectroscopic data were matched with those reported in the literature.[12]

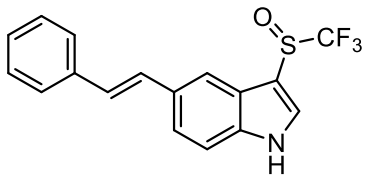
3-((Trifluoromethyl)sulfinyl)-1*H*-indol-5-ol 8an



White solid (104.6 mg, 84%, Method B). Mp: 216-217 °C. Eluent: petroleum

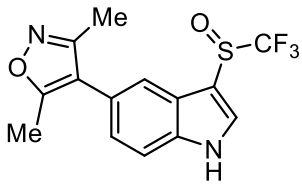
ether/ethyl acetate (2:1, R_f = 0.44). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.19 (s, 1 H), 9.21 (s, 1 H), 8.21 (d, *J* = 3.2 Hz, 1 H), 7.39 (d, *J* = 8.7 Hz, 1 H), 7.20 (s, 1 H), 6.82 (dd, *J* = 8.8, 2.4 Hz, 1 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -72.3 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 153.3, 134.1, 131.6, 126.4 (q, *J* = 343.4 Hz), 125.3, 114.4, 114.1, 105.6, 104.3 ppm. **IR (KBr):** ν = 3235, 2920, 1459, 1187, 1128, 1035, 740 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_6F_3NO_2S$ [M+Na]$^+$ calcd 271.9969, found 271.9962.

(E)-5-Styryl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ao



Yellow solid (117.3 mg, 70%, Method A, 50 ºC). Mp: 190-191 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.21). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.87 (s, 1 H), 8.06 (s, 1 H), 7.72 (d, *J* = 3.0 Hz, 1 H), 7.57 (d, *J* = 10.2 Hz, 1 H), 7.54 – 7.44 (m, 3 H), 7.38 (t, *J* = 7.5 Hz, 2 H), 7.32 – 7.24 (m, 1 H), 7.23 – 7.04 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.3, 136.4, 132.6, 131.3, 128.7, 128.7, 128.3, 127.6, 126.5, 125.6 (q, *J* = 333.3 Hz), 124.7, 123.1, 118.5, 112.9, 108.4 ppm. **IR (KBr):** ν = 3223, 1498, 1415, 1175, 1131, 1048, 960, 804, 742, 691, 630, 490 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{17}H_{12}F_3NOS$ [M+Na]$^+$ calcd 358.0489, found 358.0477.

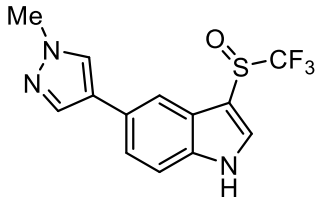
3,5-Dimethyl-4-(3-((trifluoromethyl)sulfinyl)-1*H*-indol-5-yl)isoxazole 8ap



Gray solid (162.4 mg, 99%, Method A, 50 ºC). Mp: 176-177 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.46). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 11.31 (s, 1 H), 7.94 (s, 2 H), 7.65 (d, *J* = 8.5 Hz, 1 H), 7.25 (d, *J* = 8.5 Hz, 1 H), 2.42 (s, 3 H), 2.32 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.5, 159.0, 136.7, 132.4, 125.8 (q, *J* = 333.3 Hz), 125.5, 124.7, 124.4, 121.0, 117.1, 113.3, 107.7, 11.4, 10.7 ppm. The spectroscopic data were matched with those reported in the

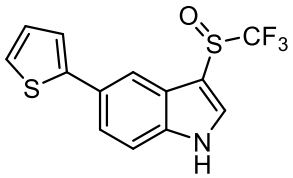
literature.[4]

5-(1-Methyl-1H-pyrazol-4-yl)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8aq



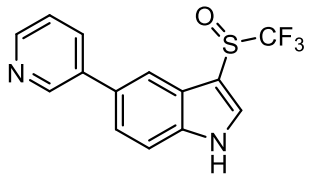
Yellow solid (150.2 mg, 96%, Method B). Mp: 242-243 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.15). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.46 (s, 1 H), 8.34 (d, *J* = 3.1 Hz, 1 H), 8.12 (s, 1 H), 7.97 (s, 1 H), 7.83 (s, 1 H), 7.58 (q, *J* = 10.0 Hz, 2 H), 3.88 (s, 3 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -72.6 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 136.3, 136.2, 134.3, 128.0, 127.3, 126.3 (q, *J* = 333.3 Hz), 125.1, 122.8, 122.4, 115.8, 114.0, 106.7, 39.0 ppm. **IR (KBr):** ν = 2923, 1724, 1174, 1133, 1068, 800, 614 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{13}H_{10}F_3N_3OS$ $[M+Na]^+$ calcd 336.0394, found 336.0382.

5-(Thiophen-2-yl)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ar



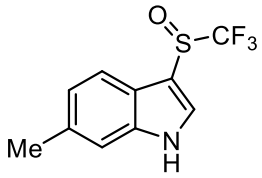
Gray solid (141.8 mg, 90%, Method A, 50 ºC). Mp: 188-189 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.23). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.29 (s, 1 H), 8.18 (s, 1 H), 7.74 (d, *J* = 3.0 Hz, 1 H), 7.56 (dd, *J* = 8.5, 1.8 Hz, 1 H), 7.46 (d, *J* = 8.6 Hz, 1 H), 7.29 – 7.23 (m, 2 H), 7.07 (dd, *J* = 5.1, 3.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.5, 136.5, 132.0, 129.6, 128.1, 125.6 (q, *J* = 333.3 Hz), 124.7, 124.7, 123.5, 123.2, 117.2 (d, *J* = 2.2 Hz), 113.2, 107.9 ppm. **IR (KBr):** ν = 3222, 1471, 1416, 1298, 1174, 1131, 1048, 806, 696, 596, 518, 473cm^{-1}. **HRMS (ESI):** *m/z* for $C_{13}H_8F_3NOS_2$ $[M+Na]^+$ calcd 337.9897, found 337.9890.

5-(Pyridin-3-yl)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8as



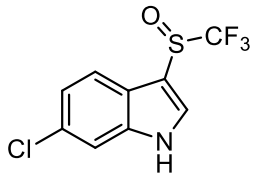
Yellow solid (66.7 mg, 43%, Method B). Mp: 167-168 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.12). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.62 (s, 1 H), 8.88 (s, 1 H), 8.57 (d, *J* = 6.3 Hz, 1 H), 8.44 (s, 1 H), 8.10 (s, 1 H), 8.04 (d, *J* = 8.1 Hz, 1 H), 7.74 (d, *J* = 8.5 Hz, 1 H), 7.67 (d, *J* = 8.6 Hz, 1 H), 7.49 (dd, *J* = 7.9, 4.7 Hz, 1 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -72.7 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 148.6, 148.2, 137.4, 136.7, 134.9, 134.8, 131.8, 126.3 (q, *J* = 343.4 Hz), 125.2, 124.4, 123.5, 118.3, 114.4, 107.3 ppm. **IR (KBr):** ν = 2922, 1624, 1478, 170, 1132, 1046, 952, 737 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{14}H_9F_3N_2OS$ [M+Na]$^+$ calcd 333.0285, found 333.0283.

6-Methyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8at



Yellow solid (86.5 mg, 70%, Method A, 50 ºC). Mp: 176-177 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.28). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.29 (s, 1 H), 7.85 (d, *J* = 8.1 Hz, 1 H), 7.69 (s, 1 H), 7.27 (d, *J* = 7.8 Hz, 1 H), 7.14 (d, *J* = 8.3 Hz, 1 H), 2.48 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.2, 134.8, 129.9, 125.6 (q, *J* = 333.3 Hz), 124.5, 121.9, 119.9, 112.2, 108.9, 21.6 ppm. **IR (KBr):** ν = 2924, 1177, 1133, 1051, 806 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_8F_3NOS$ [M+Na]$^+$ calcd 270.0176, found 270.0171.

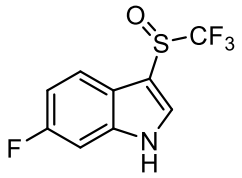
6-Chloro-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8au



Gray solid (97.5 mg, 73%, Method A, 50 ºC). Mp: 124-125 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.30). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.11 (d, *J* = 21.5

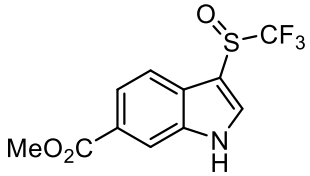
Hz, 1 H), 7.87 (d, J = 8.7 Hz, 1 H), 7.77 (s, 1 H), 7.43 (s, 1 H), 7.25 (d, J = 8.7 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.4, 131.7, 130.6, 125.5 (q, J = 343.4 Hz), 123.6, 122.5, 121.1, 112.7, 108.2 ppm. The spectroscopic data were matched with those reported in the literature.[12]

6-Fluoro-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8av



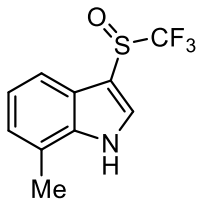
Purple solid (105.4 mg, 84%, Method A, 50 ºC). Mp: 104-105 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.32). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.04 (s, 1 H), 7.89 (dd, J = 8.9, 5.1 Hz, 1 H), 7.76 (d, J = 3.0 Hz, 1 H), 7.15 (dd, J = 9.0, 2.3 Hz, 1 H), 7.05 (td, J = 9.1, 2.3 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.6 (s, 3 F), -116.6 (m, 1 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.8(d, J = 242.5 Hz), 137.2 (d, J = 12.4 Hz), 131.6, 125.5 (q, J = 343.4 Hz), 121.3 (d, J = 9.9 Hz), 120.4, 111.8 (d, J = 24.8 Hz), 108.4, 99.1 (d, J = 26.5 Hz) ppm. The spectroscopic data were matched with those reported in the literature.[12]

Methyl 3-((trifluoromethyl)sulfinyl)-1*H*-indole-6-carboxylate 8aw



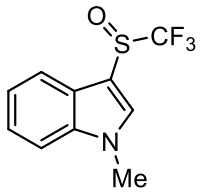
White solid (120.8 mg, 83%, Method B). Mp: 145-146 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.20). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.81 (s, 1 H), 8.25 (s, 1 H), 7.96 (s, 3 H), 3.95 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.5, 136.4, 133.5, 127.8, 126.1, 125.5 (q, J = 343.4 Hz), 123.4, 119.9, 115.0, 108.6, 52.3 ppm. **IR (KBr):** ν = 2923, 1713, 1437, 1351, 1175, 1133, 1052, 767, 603 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_8F_3NO_3S$ $[M+H]^+$ calcd 292.0255, found 292.0246.

7-Methyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ax



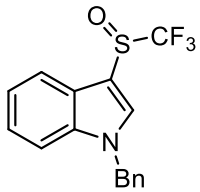
Yellow solid (107.4 mg, 87%, Method A, 50 ºC). Mp: 138-139 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.34). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.35 (s, 1 H), 7.83 (d, *J* = 8.1 Hz, 1 H), 7.75 (s, 1 H), 7.22 (t, *J* = 8.0 Hz, 1 H), 7.16 (d, *J* = 7.3 Hz, 1 H), 2.54 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.7, 131.3, 125.6 (q, *J* = 333.3 Hz), 125.0, 123.8, 122.9, 122.5, 117.7, 107.8, 16.5 ppm. The spectroscopic data were matched with those reported in the literature.[12]

1-Methyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ay



White solid (122.3 mg, 99%, Method A, 50 ºC). Mp: 129-130 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.41). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 1 H), 7.68 (s, 1 H), 7.42 - 7.38 (m, 2 H), 7.34 (d, *J* = 8.4 Hz, 1 H), 3.87 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.8, 134.0, 125.6 (q, *J* = 333.3 Hz), 125.1, 124.1, 122.5, 120.5, 110.6, 107.2, 33.7 ppm. The spectroscopic data were matched with those reported in the literature.[12]

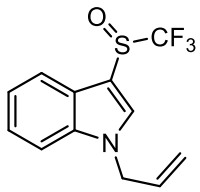
1-Benzyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8az



White solid (129.2 mg, 80%, Method A, 80 ºC). Mp: 119-120 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.62). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1 H), 7.74 (s, 1 H), 7.46 – 7.40 (m, 1 H), 7.40 – 7.38 (m, 1 H), 7.37 (s, 2 H), 7.36 – 7.34 (m, 1 H), 7.34 – 7.31 (m, 1 H), 7.19 (d, *J* = 2.6 Hz, 1 H), 7.18 (s, 1 H), 5.39 (s, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.4,

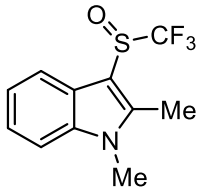
135.0, 133.3, 129.2, 128.5, 127.2, 125.6 (q, J = 333.3 Hz), 125.3, 124.3, 122.7, 120.7, 111.1, 108.1, 51.1 ppm. **IR (KBr):** ν = 2923, 1510, 1480, 1456, 1390, 1172, 1130, 1061, 982, 730, 696, 607, 469 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{16}H_{12}F_3NOS$ $[M+Na]^+$ calcd 346.0489, found 346.0479.

1-Allyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8ba



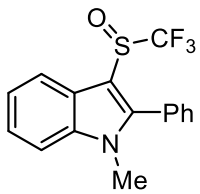
Gray solid (129.7 mg, 95%, Method A, 50 ºC). Mp: 75-76 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.55). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.9 Hz, 1 H), 7.74 (s, 1 H), 7.45 (d, J = 8.4 Hz, 1 H), 7.38 (t, J = 6.0 Hz, 1 H), 7.33 (t, J = 7.5 Hz, 1 H), 6.08 – 5.98 (m, 1 H), 5.35 (d, J = 11.4 Hz, 1 H), 5.20 (d, J = 17.0 Hz, 1 H), 4.82 (d, J = 2.3 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.2, 132.9, 131.5, 125.6 (q, J = 333.3 Hz), 125.3, 124.1, 122.6, 120.7, 119.3, 110.9, 107.8, 49.7 ppm. The spectroscopic data were matched with those reported in the literature.[4]

1,2-Dimethyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8bb



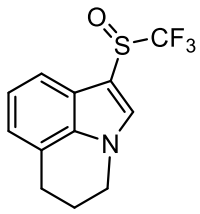
Purple solid (129.2 mg, 99%, Method A, 50 ºC). Mp: 152-153 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.31). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.5 Hz, 1 H), 7.30 (d, J = 3.7 Hz, 2 H), 7.28 – 7.22 (m, 1 H), 3.62 (s, 3 H), 2.50 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.0, 137.3, 126.2 (q, J = 333.3 Hz), 124.9, 123.2, 122.2, 120.1, 109.9, 103.4, 29.8, 10.9 ppm. The spectroscopic data were matched with those reported in the literature.[4]

1-Methyl-2-phenyl-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8bc



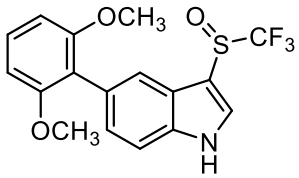
Purple solid (158.3 mg, 98%, Method A, 50 ºC). Mp: 145-146 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.57). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.9 Hz, 1 H), 7.61 – 7.54 (m, 3 H), 7.48 (d, *J* = 7.9 Hz, 1 H), 7.46 – 7.40 (m, 3 H), 7.40 – 7.34 (m, 1 H), 3.68 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -70.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.5, 137.8, 130.6, 130.3, 128.8, 127.9, 126.5 (q, *J* = 343.4 Hz), 124.6, 124.3, 122.8, 121.4 (d, *J* = 2.6 Hz), 110.6, 106.4, 31.3 ppm. The spectroscopic data were matched with those reported in the literature.[4]

1-((Trifluoromethyl)sulfinyl)-5,6-dihydro-4*H*-pyrrolo[3,2,1-*iJ*]quinoline 8bd



Yellow solid (135.1 mg, 99%, Method A, 50 ºC). Mp: 86-87 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.38). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.1 Hz, 1 H), 7.69 (s, 1 H), 7.23 (t, *J* = 8.0 Hz, 1 H), 7.09 (d, *J* = 7.1 Hz, 1 H), 4.24 (t, *J* = 5.8 Hz, 2 H), 3.03 (t, *J* = 6.1 Hz, 2 H), 2.32 – 2.24 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.1, 131.4, 125.7 (q, *J* = 343.4 Hz), 123.1, 123.1, 123.0, 121.2, 118.0 (d, *J* = 1.8 Hz), 107.2, 45.2, 24.3, 22.5 ppm. The spectroscopic data were matched with those reported in the literature.[4]

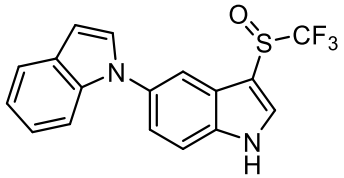
5-(2,6-Dimethoxyphenyl)-3-((trifluoromethyl)sulfinyl)-1*H*-indole 8be



Yellow solid (83.0 mg, 45%, Method A, 50 ºC). Mp: 216-217 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.44). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.47 (s, 1 H), 8.36 (s, 1 H), 7.70 (s, 1 H), 7.59 (d, *J* = 8.5 Hz, 1 H), 7.31 (t, *J* = 8.4 Hz, 1 H), 7.19 (d,

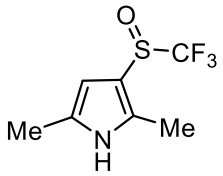
J = 8.4 Hz, 1 H), 6.75 (d, *J* = 8.4 Hz, 2 H), 3.66 (s, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 157.8, 136.4, 134.2, 129.3, 128.1, 127.4,126.3 (q, *J* = 343.4 Hz), 124.1, 122.4, 119.5, 112.5, 106.8, 105.0, 56.1 ppm. **IR (KBr):** ν = 3230, 1588, 1471, 1246, 1173, 1108, 1046, 731, 600, 472 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{17}H_{14}F_3NO_3S$ $[M+Na]^+$ calcd 392.0544, found 392.0540.

3'-((Trifluoromethyl)sulfinyl)-1'*H*-1,5'-biindole 8bf



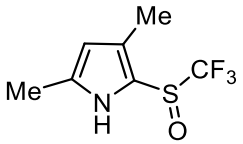
White oil (92.3 mg, 53%, Method B). Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.19). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.70 (s, 1 H), 8.48 (s, 1 H), 7.94 (s, 1 H), 7.79 (s, 1 H), 7.61 (s, 2 H), 7.49 (s, 2 H), 7.14 (d, *J* = 19.5 Hz, 2 H), 6.68 (s, 1 H); **^{19}F NMR** (376 MHz, DMSO-d6) δ -73.1 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 136.2, 136.1, 135.7, 134.2, 129.5, 129.4, 126.4 (q, *J* = 333.3 Hz), 125.0, 122.8, 121.5, 121.4, 120.7, 115.5, 115.0, 110.4, 107.1, 103.7 ppm. **IR (KBr):** ν = 2922, 2853, 1585, 1491, 1222, 1173, 1042, 1017, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{17}H_{11}F_3N_2OS$ $[M+Na]^+$ calcd 371.0442, found 371.0434.

2,5-Dimethyl-3-((trifluoromethyl)sulfinyl)-1*H*-pyrrole 8bg



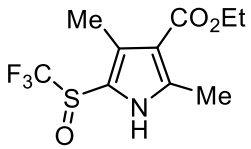
Gray solid (101.3 mg, 96%, Method A, 50 ºC). Mp: 122-123 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.67). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.63 (s, 1 H), 6.16 (s, 1 H), 2.37 (s, 3 H), 2.20 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.7, 130.1, 125.2 (q, *J* = 333.3 Hz), 111.0, 104.0, 12.5, 11.0 ppm. The spectroscopic data were matched with those reported in the literature.[13]

3,5-Dimethyl-2-((trifluoromethyl)sulfinyl)-1*H*-pyrrole 8bh



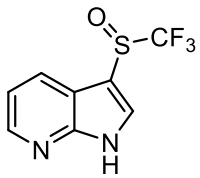
Yellow solid (97.1 mg, 92%, Method A, 50 ºC). Mp: 91-92 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.59). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.21 (s, 1 H), 5.86 (d, *J* = 2.6 Hz, 1 H), 2.27 (s, 3 H), 2.19 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.8, 132.6, 124.9 (q, *J* = 333.3 Hz), 113.6, 110.9, 13.1, 11.0 ppm. The spectroscopic data were matched with those reported in the literature.[4]

Ethyl 2,4-dimethyl-5-((trifluoromethyl)sulfinyl)-1*H*-pyrrole-3-carboxylate 8bi



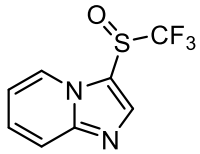
White solid (111.8 mg, 79%, Method A, 50 ºC). Mp: 136-137 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.19). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.91 (s, 1 H), 4.30 (d, *J* = 7.5 Hz, 2 H), 2.56 (s, 3 H), 2.41 (s, 3 H), 1.35 (t, *J* = 7.0 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.6, 144.7, 134.1, 124.7 (q, *J* = 343.4 Hz), 114.8, 113.6, 59.8, 14.3, 13.9, 11.3 ppm. The spectroscopic data were matched with those reported in the literature.[12]

3-((Trifluoromethyl)sulfinyl)-1*H*-pyrrolo[2,3-*b*]pyridine 8bj



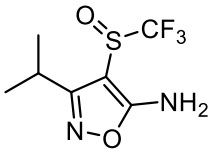
White solid (115.8 mg, 99%, Method B). Mp: 180-181 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.33). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.46 (s, 1 H), 8.53 (s, 1 H), 8.43 (d, *J* = 7.9 Hz, 1 H), 8.09 (s, 1 H), 7.35 (s, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.0, 144.5, 131.5, 130.5, 125.5 (q, *J* = 333.3 Hz), 118.5, 117.9, 108.1 ppm. The spectroscopic data were matched with those reported in the literature.[13]

3-((Trifluoromethyl)sulfinyl)imidazo[1,2-*a*]pyridine 8bk



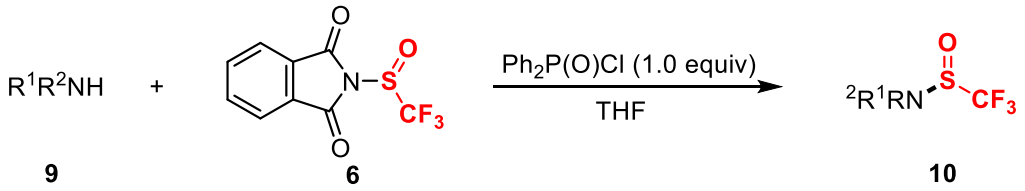
Gray solid (84.2 mg, 72%, Method B). Mp: 63-64 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.22). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 6.8 Hz, 1 H), 8.17 (s, 1 H), 7.82 (d, *J* = 9.1 Hz, 1 H), 7.53 (t, *J* = 7.4 Hz, 1 H), 7.09 (t, *J* = 6.9 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -70.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.3, 142.2, 129.2, 127.8, 125.7 (q, *J* = 333.3 Hz), 118.6, 114.9, 113.1 ppm. **IR (KBr):** ν = 2924, 1635, 1496, 1448, 1320, 1301, 1264, 1173, 1129, 1069, 763, 743 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5F_3N_2OS$ $[M+H]^+$ calcd 235.0153, found 235.0146.

3-Isopropyl-4-((trifluoromethyl)sulfinyl)isoxazol-5-amine 8bl



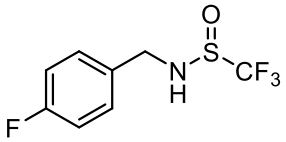
White solid (110.1 mg, 91%, Method B). Mp: 65-66 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.54). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.12 (s, 2 H), 2.97 - 2.87 (m, 1 H), 1.32 (dd, *J* = 7.0, 3.5 Hz, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.3, 167.1, 125.9 (q, *J* = 333.3 Hz), 81.4, 26.7, 21.2, 20.7 ppm. **IR (KBr):** ν = 3245, 2975, 1640, 1567, 1521, 1185, 1134, 1063 cm^{-1}. **HRMS (ESI):** *m/z* for $C_7H_9F_3N_2O_2S$ $[M+Na]^+$ calcd 265.0235, found 265.0228.

3.4 General procedure for trifluoromethylsulfinylation of aryl or alkyl amines



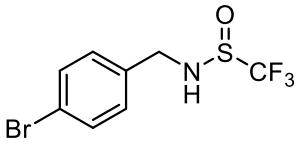
A 25 mL Schlenk tube charged with *N*-trifluoromethylsulfinylphthalimide **6** (0.75 mmol) and $Ph_2P(O)Cl$ (0.75 mmol) was added freshly distilled THF (3.0 mL). The mixture was stirred at RT for 10 h, then amine (**9**, 0.5 mmol) was added to the mixture. The reaction was stirred at RT for another 3 h. After the reaction was completed, the mixture was extracted with distilled water and ethyl acetate. Then the organic phase was combinated and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated amine **10**.

1,1,1-Trifluoro-*N*-(4-fluorobenzyl)methanesulfinamide 10aa



White solid (51.8 mg, 43%). Mp: 45-46 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.61). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.22 (m, 2 H), 7.07 – 6.98 (m, 2 H), 4.95 (s, 1 H), 4.40 (dd, *J* = 14.2, 5.6 Hz, 1 H), 4.26 (dd, *J* = 14.2, 5.4 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.7 (s, 3 F), -113.58 (m, 1 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 247.1 Hz), 132.5, 130.0 (d, *J* = 8.2 Hz), 123.7 (q, *J* = 333.3 Hz), 115.9 (d, *J* = 21.7 Hz), 45.7 ppm. **IR (KBr):** ν = 3223, 2924, 1604, 1511, 1178, 1152, 1094, 1042, 826, 760 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_7F_4NOS$ $[M+Na]^+$ calcd 264.0082, found 264.0074.

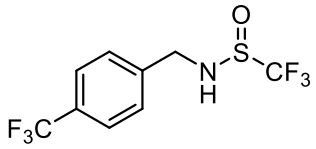
***N*-(4-bromobenzyl)-1,1,1-trifluoromethanesulfinamide 10ab**



White solid (57.2 mg, 38%). Mp: 56-57 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.60). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.6 Hz, 2 H), 7.20 (d, *J* = 8.0 Hz,

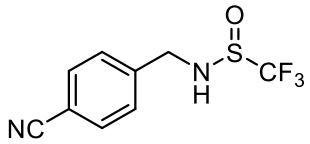
2 H), 4.76 (s, 1 H), 4.41 (dd, J = 14.0, 6.1 Hz, 1 H), 4.27 (dd, J = 14.2, 5.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.7 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.7, 132.2, 129.9, 123.6 (q, J = 343.4 Hz), 122.5, 45.9 ppm. **IR (KBr):** ν = 3220, 2924, 1489, 1184, 1154, 1095, 1072, 1012, 811 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_7BrF_3NOS$ $[M+Na]^+$ calcd 323.9282, found 323.9274.

1,1,1-Trifluoro-*N*-(4-(trifluoromethyl)benzyl)methanesulfinamide 10ac



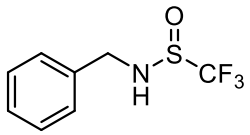
White solid (72.8 mg, 50%). Mp: 68-69 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.58). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.0 Hz, 2 H), 7.44 (d, J = 7.9 Hz, 2 H), 5.05 (s, 1 H), 4.49 (dd, J = 14.7, 6.3 Hz, 1 H), 4.38 (dd, J = 14.7, 5.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.6 (s, 3 F), -76.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.7, 130.6 (q, J = 32.7 Hz), 128.3, 126.0 (q, J = 3.7 Hz), 123.9 (q, J = 272.7 Hz), 123.7 (q, J = 333.3 Hz), 45.9 ppm. **IR (KBr):** ν = 3246, 2922, 1332, 1168, 1121, 1068, 1019, 825, 633, 466 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_7F_6NOS$ $[M+Na]^+$ calcd 314.0050, found 314.0045.

***N*-(4-Cyanobenzyl)-1,1,1-trifluoromethanesulfinamide 10ad**



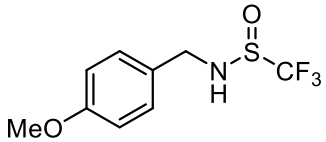
White solid (98.0 mg, 79%). Mp: 58-59 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.31). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (d, J = 8.0 Hz, 2 H), 7.41 (d, J = 7.9 Hz, 2 H), 5.63 (s, 1H), 4.45 (dd, J = 15.3, 6.5 Hz, 1 H), 4.36 (dd, J = 15.4, 5.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.6, 132.6, 128.6, 123.7 (q, J = 333.3 Hz), 118.6, 111.6, 45.3 ppm. **IR (KBr):** ν = 3235, 2231, 1417, 1175, 1153, 1098, 1020, 822, 549 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_7F_3N_2OS$ $[M+Na]^+$ calcd 271.0129, found 271.0119.

***N*-Benzyl-1,1,1-trifluoromethanesulfinamide 10ae**



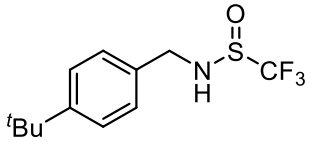
Colourless oil (60.2 mg, 54%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.62). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.35 (m, 1 H), 7.34 (s, 1 H), 7.32 (d, *J* = 2.0 Hz, 2 H), 7.31 (d, *J* = 3.5 Hz, 1 H), 4.91 (s, 1 H), 4.43 (dd, *J* = 14.1, 6.2 Hz, 1 H), 4.27 (dd, *J* = 14.1, 5.4 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.6 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.7, 129.0, 128.4, 128.2, 123.8 (q, *J* = 333.3 Hz), 46.4 ppm. The spectroscopic data were matched with those reported in the literature.[14]

1,1,1-Trifluoro-*N*-(4-methoxybenzyl)methanesulfinamide 10af



White solid (64.5 mg, 51%). Mp: 40-41 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.49). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.6 Hz, 2 H), 6.87 (d, *J* = 8.7 Hz, 2 H), 4.76 (s, 1 H), 4.39 (dd, *J* = 13.7, 6.0 Hz, 1 H), 4.21 (dd, *J* = 13.4, 6.0 Hz, 1 H), 3.78 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.6 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.7, 129.7, 128.7, 123.8 (q, *J* = 333.3 Hz), 114.4, 55.4, 46.0 ppm. **IR (KBr):** ν = 3227, 2926, 1613, 1514, 1252, 1175, 1096, 1032, 825 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_{10}F_3NO_2S$ $[M+Na]^+$ calcd 276.0282, found 276.0278.

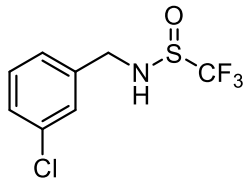
***N*-(4-(*tert*-butyl)benzyl)-1,1,1-trifluoromethanesulfinamide 10ag**



Yellow oil (72.6 mg, 52%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.60). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.1 Hz, 2 H), 7.26 (d, *J* = 8.3 Hz, 2 H), 4.79 (s, 1 H), 4.43 (dd, *J* = 14.0, 6.2 Hz, 1 H), 4.26 (dd, *J* = 13.9, 5.4 Hz, 1 H), 1.31 (s, 9 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.6 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.6, 133.7, 128.1, 126.0, 123.8 (q, *J* = 333.3 Hz), 46.2, 34.7, 31.4 ppm. **IR (KBr):** ν = 3230, 2963, 1516, 1269, 1181, 1154, 1096, 826, 749 cm^{-1}. **HRMS (ESI):** *m/z* for

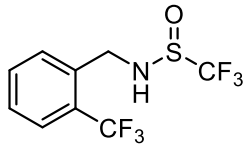
$C_{12}H_{16}F_3NOS$ $[M+Na]^+$ calcd 302.0802, found 302.0800.

***N*-(3-Chlorobenzyl)-1,1,1-trifluoromethanesulfinamide 10ah**



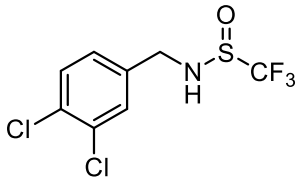
Colourless oil (77.1 mg, 60%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.57). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 3 H), 7.22 – 7.18 (m, 1 H), 5.01 (s, 1 H), 4.41 (dd, *J* = 14.5, 5.5 Hz, 1 H), 4.27 (dd, *J* = 14.5, 5.5 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.6 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.8, 134.8, 130.3, 128.5, 128.2, 126.2, 123.7 (q, *J* = 333.3 Hz), 45.7 ppm. **IR (KBr):** ν = 3228, 2924, 1275, 1183, 1097, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_7ClF_3NOS$ $[M+Na]^+$ calcd 279.9787, found 279.9770.

1,1,1-Trifluoro-*N*-(2-(trifluoromethyl)benzyl)methanesulfinamide 10ai



White solid (75.7 mg, 52%). Mp: 41-42 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.72). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.8 Hz, 1 H), 7.57 (d, *J* = 4.8 Hz, 2 H), 7.45 – 7.40 (m, 1 H), 5.04 (s, 1 H), 4.63 – 4.48 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -59.4 (s, 3 F), -77.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.2, 132.7, 130.6, 128.4, 126.4 (d, *J* = 5.7 Hz), 126.3 (d, *J* = 5.3 Hz), 124.2 (q, *J* = 272.7 Hz), 123.7 (q, *J* = 333.3 Hz), 43.2 ppm. **IR (KBr):** ν = 1316, 1275, 1156, 1119, 1038, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_7F_6NOS$ $[M+Na]^+$ calcd 314.0050, found 314.0041.

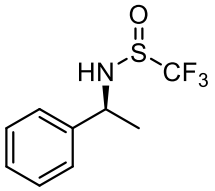
***N*-(3,4-Dichlorobenzyl)-1,1,1-trifluoromethanesulfinamide 10aj**



White solid (72.8 mg, 50%). Mp: 40-41 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.70). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (s, 1 H), 7.37 (s, 1 H), 7.13 (d, *J* = 7.7

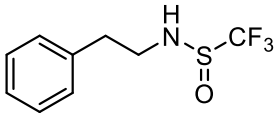
Hz, 1 H), 5.27 (s, 1 H), 4.35 (dd, J = 14.7, 6.5 Hz, 1 H), 4.23 (dd, J = 14.7, 5.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.53 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.1, 133.0, 132.4, 130.9, 129.9, 127.3, 123.7 (q, J = 333.3 Hz), 45.1 ppm. **IR (KBr):** ν = 3205, 1677, 1589, 1464, 1358, 1283, 1152, 1096, 912, 790, 686, 587, 465 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_6Cl_2F_3NOS$ $[M+Na]^+$ calcd 313.9397, found 313.9389.

1,1,1-Trifluoro-*N*-((S)-1-phenylethyl)methanesulfinamide 10ak



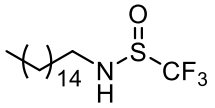
Colourless oil (80.6 mg, 68%, dr = 1:1). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.45). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 7.42 – 7.27 (m, 5 H), 4.92 (s, 0.5 H), 4.84 (s, 0.5 H), 4.70 (t, J = 7.3 Hz, 1 H), 1.59 (t, J = 8.4 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.8 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.9 (d, J = 49.9 Hz), 129.0 (d, J = 2.5 Hz), 128.3, 126.6 (d, J = 36.8 Hz), 123.7 (q, J = 333.3 Hz), 54.4 (d, J = 36.6 Hz), 24.1 (d, J = 32.0 Hz) ppm. The spectroscopic data were matched with those reported in the literature.[15]

1,1,1-Trifluoro-*N*-phenethylmethanesulfinamide 10al



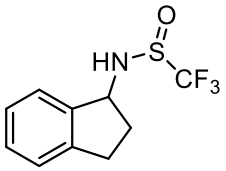
Colourless oil (86.5 mg, 73%). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.23). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 (t, J = 7.4 Hz, 2 H), 7.26 (d, J = 7.4 Hz, 1 H), 7.20 (d, J = 7.6 Hz, 2 H), 4.54 (s, 1 H), 3.60 – 3.42 (m, 2 H), 2.90 (t, J = 7.0 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.4, 129.0, 127.1, 123.7 (q, J = 333.3 Hz), 44.0, 37.3 ppm. **IR (KBr):** ν = 3232, 1176, 1154, 1057, 1062, 749, 699 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_{10}F_3NOS$ $[M+Na]^+$ calcd 260.0333, found 260.0326.

1,1,1-Trifluoro-*N*-propylmethanesulfinamide 10am



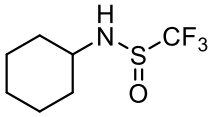
White solid (108.9 mg, 61%). Mp: 37-38 °C. Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.51). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.60 (t, *J* = 6.1 Hz, 1 H), 3.30 – 3.12 (m, 2 H), 1.61 – 1.52 (m, 2 H), 1.23 (s, 26 H), 0.85 (t, *J* = 6.8 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 123.7 (q, *J* = 333.3 Hz), 43.3, 32.0, 31.0, 29.8 - 29.7 (m, 6 C), 29.6, 29.5, 29.4, 29.2, 26.5, 22.8, 14.2 ppm. **IR (KBr):** ν = 2923, 2853, 1466, 1275, 1260, 1185, 1155, 1095, 764, 750 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{17}H_{34}F_3NOS$ $[M+Na]^+$ calcd 198.0176, found 198.0178.

***N*-(2,3-Dihydro-1*H*-inden-1-yl)-1,1,1-trifluoromethanesulfinamide 10an**



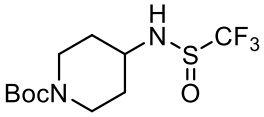
Colourless oil (79.7 mg, 64%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.63). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.0 Hz, 1 H), 7.33 (d, *J* = 7.1 Hz, 1 H), 7.25 (s, 2 H), 5.10 – 4.96 (m, 1 H), 4.85 (d, *J* = 9.5 Hz, 1 H), 3.08 – 2.96 (m, 1 H), 2.91 – 2.79 (m, 1 H), 2.68 – 2.53 (m, 1 H), 2.05 – 1.90 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.2 (d, *J* = 11.7 Hz), 141.9 (d, *J* = 29.6 Hz), 128.7, 127.2 (d, *J* = 5.6 Hz), 125.1 (d, *J* = 7.0 Hz), 124.6 (d, *J* = 5.8 Hz), 123.7 (qd, *J* = 333.3, 3.6 Hz), 60.3 (d, *J* = 100.6 Hz), 35.7 (d, *J* = 56.3 Hz), 30.1 (d, *J* = 7.7 Hz) ppm. **IR (KBr):** ν = 3217, 2926, 1180, 1155, 1095, 765, 748 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_{10}F_3NOS$ $[M+Na]^+$ calcd 272.0333, found 272.0324.

***N*-Cyclohexyl-1,1,1-trifluoromethanesulfinamide 10ao**



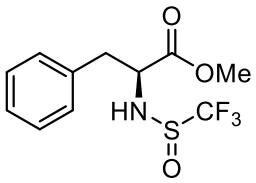
Colourless oil (66.7 mg, 62%). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.48). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.56 (s, 1 H), 3.31 (s, 1 H), 1.96 (s, 2 H), 1.73 (d, *J* = 11.1 Hz, 2 H), 1.58 (d, *J* = 13.7 Hz, 1 H), 1.39 – 1.23 (m, 4 H), 1.20 – 1.10 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 123.6 (q, *J* = 333.3 Hz), 54.4, 35.0 (d, *J* = 16.4 Hz), 25.1, 24.8 (d, *J* = 9.8 Hz) ppm. The spectroscopic data were matched with those reported in the literature.[16]

***Tert*-butyl 4-(((trifluoromethyl)sulfinyl)amino)piperidine-1-carboxylate 10ap**



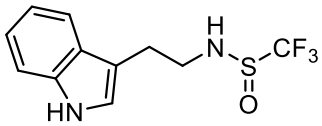
Colourless oil (77.4 mg, 49%). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.62). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.92 (s, 1 H), 4.01 (s, 2 H), 3.49 (s, 1 H), 2.81 (t, *J* = 8.1 Hz, 2 H), 1.92 (d, *J* = 13.0 Hz, 2 H), 1.47 (d, *J* = 10.9 Hz, 2 H), 1.41 (s, 9 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.7, 123.6 (q, *J* = 333.3 Hz), 80.1, 52.1, 42.4, 33.9, 28.4 ppm. **IR (KBr):** ν = 3207, 2928, 1670, 1428, 1367, 1311, 1276, 1240, 1174, 1069, 868, 766 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{19}F_3N_2O_3S$ $[M+Na]^+$ calcd 339.0966, found 339.0964.

Methyl ((trifluoromethyl)sulfinyl)-*L*-phenylalaninate 10aq



Colourless oil (64.9 mg, 44%, dr = 3:2). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.37). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 7.33 – 7.23 (m, 3 H), 7.13 (t, *J* = 2.0 Hz, 1 H), 7.12 – 7.10 (m, 1 H), 5.22 (dd, *J* = 37.5, 9.2 Hz, 1 H), 4.58 – 4.50 (m, 0.4 H), 4.42 – 4.36 (m, 0.6 H), 3.74 (d, *J* = 12.7 Hz, 3 H), 3.20 – 3.00 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8 (d, *J* = 61.2 Hz), 134.9 (d, *J* = 12.8 Hz), 129.6 (d, *J* = 3.9 Hz), 128.8 (d, *J* = 4.3 Hz), 127.6, 123.6 (dq, *J* = 333.3, 20.9 Hz), 55.7 (d, *J* = 382.7 Hz), 53.0 (d, *J* = 8.3 Hz), 39.9 (d, *J* = 127.6 Hz) ppm. **IR (KBr):** ν = 2923, 1742, 1455, 1275, 1187, 1156, 1101, 749, 701 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{12}F_3NO_3S$ $[M+Na]^+$ calcd 318.0388, found 318.0381.

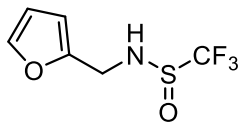
***N*-(2-(1*H*-Indol-3-yl)ethyl)-1,1,1-trifluoromethanesulfinamide 10ar**



Colourless oil (73.1 mg, 53%). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.50). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22 (s, 1 H), 7.58 (d, *J* = 7.6 Hz, 1 H), 7.37 (d, *J* = 8.0

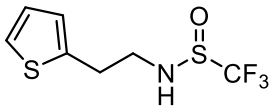
Hz, 1 H), 7.23 (t, J = 8.0 Hz, 1 H), 7.15 (t, J = 7.5 Hz, 1 H), 7.05 (s, 1 H), 4.51 (s, 1 H), 3.65 – 3.46 (m, 2 H), 3.05 (t, J = 6.7 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.13 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.6, 127.1, 123.7 (d, J = 333.3 Hz), 122.9, 122.5, 119.8, 118.6, 111.6, 111.3, 43.0, 27.0 ppm. **IR (KBr):** ν = 3314, 1457, 1422, 1338, 1173, 1151, 1091, 743, 585, 462, 424 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{11}F_3N_2OS$ $[M+Na]^+$ calcd 299.0442, found 299.0437.

1,1,1-Trifluoro-*N*-(furan-2-ylmethyl)methanesulfinamide 10as



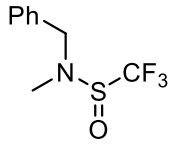
Colourless oil (70.3 mg, 66%). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.30). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (d, J = 2.0 Hz, 1 H), 6.32 (dd, J = 3.3, 1.8 Hz, 1 H), 6.29 (d, J = 3.3 Hz, 1 H), 4.97 (s, 1 H), 4.42 (dd, J = 15.1, 5.6 Hz, 1 H), 4.30 (dd, J = 15.1, 6.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.0, 143.2, 123.7 (q, J = 333.3 Hz), 110.7, 108.9, 39.1 ppm. **IR (KBr):** ν = 3223, 1179, 1153, 1196, 1014, 921, 742, 598, 459 cm^{-1}. **HRMS (ESI):** *m/z* for $C_6H_6F_3NO_2S$ $[M+Na]^+$ calcd 235.9969, found 235.9953.

1,1,1-Trifluoro-*N*-(2-(thiophen-2-yl)ethyl)methanesulfinamide 10at



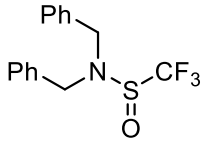
Colourless oil (64.4 mg, 53%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.56). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.19 (d, J = 5.3 Hz, 1 H), 6.96 (t, J = 4.4 Hz, 1 H), 6.87 (d, J = 3.3 Hz, 1 H), 4.67 (s, 1 H), 3.60 – 3.43 (m, 2 H), 3.12 (t, J = 6.9 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 139.6, 127.4, 126.2, 124.7, 123.6 (q, J = 333.3 Hz), 44.1, 31.5 ppm. **IR (KBr):** ν = 3234, 2925, 1179, 1097, 749, 699 cm^{-1}. **HRMS (ESI):** *m/z* for $C_7H_8F_3NOS_2$ $[M+Na]^+$ calcd 265.9897, found 265.9888.

***N*-Benzyl-1,1,1-trifluoro-*N*-methylmethanesulfinamide 10au**



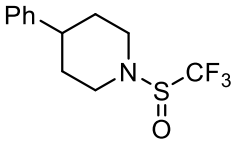
Yellow oil (52.1 mg, 44%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.78). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 2 H), 7.34 – 7.31 (m, 1 H), 7.29 (d, *J* = 1.9 Hz, 1 H), 7.28 (s, 1 H), 4.44 (d, *J* = 14.6 Hz, 1 H), 4.26 (d, *J* = 14.6 Hz, 1 H), 2.73 (q, *J* = 1.5 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.1, 129.0, 128.4, 128.3, 124.4 (q, *J* = 343.4 Hz), 54.3, 31.5 ppm. **IR (KBr):** ν = 1455, 1166, 1106, 981, 931, 902, 761, 711, 602, 468 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_{10}F_3NOS$ $[M+Na]^+$ calcd 260.0333, found 260.0327.

***N,N*-Dibenzyl-1,1,1-trifluoromethanesulfinamide 10av**



Yellow solid (109.6 mg, 70%). Mp: 44-45 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.83). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 3 H), 7.35 (s, 2 H), 7.33 (d, *J* = 4.6 Hz, 1 H), 7.23 (d, *J* = 2.1 Hz, 2 H), 7.22 (s, 2 H), 4.42 (d, *J* = 14.9 Hz, 2 H), 4.18 (d, *J* = 14.9 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 134.7, 129.0, 128.9, 128.3, 124.4 (q, *J* = 333.3 Hz), 50.1 ppm. **IR (KBr):** ν = 2955, 1456, 1177, 1150, 1108, 1050, 891, 749, 698, 469 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{15}H_{14}F_3NOS$ $[M+Na]^+$ calcd 336.0646, found 336.0636.

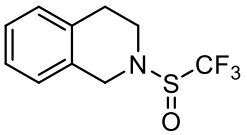
4-Phenyl-1-((trifluoromethyl)sulfinyl)piperidine 10aw



Colourless oil (81.7 mg, 59%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.70). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 (t, *J* = 7.5 Hz, 2 H), 7.28 – 7.18 (m, 3 H), 3.93 (d, *J* = 12.7 Hz, 1 H), 3.77 (d, *J* = 14.3 Hz, 1 H), 3.08 (t, *J* = 12.5 Hz, 1 H), 3.00 (t, *J* = 12.4 Hz, 1 H), 2.72 (t, *J* = 12.2 Hz, 1 H), 1.94 (s, 2 H), 1.85 – 1.68 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.9, 128.8, 126.8,

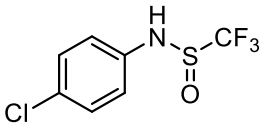
124.5 (q, J = 343.4 Hz), 46.7, 44.1, 42.2, 33.5 (d, J = 10.0 Hz) ppm. **IR (KBr):** ν = 2943, 1494, 1451, 1376, 1248, 1141, 1103, 1045, 931, 757, 699, 585 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{12}H_{14}F_3NOS$ $[M+Na]^+$ calcd 300.0646, found 300.0645.

2-((Trifluoromethyl)sulfinyl)-1,2,3,4-tetrahydroisoquinoline 10ax



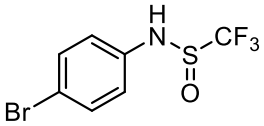
Yellow oil (61.0 mg, 49%). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.90). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23 – 7.17 (m, 2 H), 7.17 – 7.10 (m, 1 H), 7.08 (t, J = 4.6 Hz, 1 H), 4.61 (d, J = 15.8 Hz, 1 H), 4.40 (d, J = 15.8 Hz, 1 H), 3.74 – 3.63 (m, 1 H), 3.63 – 3.52 (m, 1 H), 3.03 – 2.88 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 133.3, 131.6, 129.3, 127.1, 126.7, 126.3, 124.4 (q, J = 343.3 Hz), 45.3, 43.4, 29.3 ppm. **IR (KBr):** ν = 2944, 1452, 1377, 1167, 1105, 1046, 933, 758, 699, 586, 450 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_{10}F_3NOS$ $[M+Na]^+$ calcd 272.0333, found 272.0323.

***N*-(4-Chlorophenyl)-1,1,1-trifluoromethanesulfinamide 10ay**



Yellow solid (89.9 mg, 74%). Mp: 86-87 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.68). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (s, 1 H), 7.26 (d, J = 8.8 Hz, 2 H), 7.00 (d, J = 8.8 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.9, 130.9, 129.9, 123.6 (q, J = 333.3 Hz), 121.5 ppm. The spectroscopic data were matched with those reported in the literature.[14]

***N*-(4-Bromophenyl)-1,1,1-trifluoromethanesulfinamide 10az**



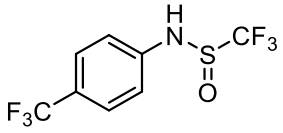
Yellow solid (111.9 mg, 78%). Mp: 90-91 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.67). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.5 Hz, 2 H), 7.36 (s, 1 H), 6.94

(d, J = 8.4 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.5, 132.8, 123.6 (q, J = 333.3 Hz), 121.7, 118.3 ppm. The spectroscopic data were matched with those reported in the literature.[14]

1,1,1-Trifluoro-*N*-(4-iodophenyl)methanesulfinamide 10ba

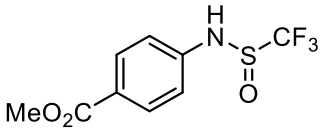
Yellow solid (135.7 mg, 81%). Mp: 87-88 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.81). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 (d, J = 8.7 Hz, 2 H), 7.35 (s, 1 H), 6.82 (d, J = 8.8 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.8, 138.3, 123.6 (q, J = 333.3 Hz), 121.8, 88.8 ppm. The spectroscopic data were matched with those reported in the literature.[14]

1,1,1-Trifluoro-*N*-(4-(trifluoromethyl)phenyl)methanesulfinamide 10bb



White solid (116.3 mg, 84%). Mp: 87-88 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.76). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (s, 1 H), 7.56 (d, J = 8.3 Hz, 2 H), 7.15 (d, J = 8.3 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.3 (s, 3 F), -77.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.8, 127.2, 127.1, 124.0 (q, J = 272.7 Hz), 123.6 (q, J = 333.3 Hz), 118.7 ppm. **IR (KBr):** ν = 3218, 2923, 1618, 1335, 1220, 1194, 1157, 1117, 1090, 1071, 842 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5F_6NOS$ $[M+Na]^+$ calcd 299.9894, found 299.9884.

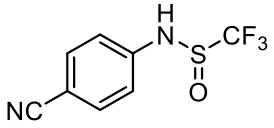
Methyl 4-(((trifluoromethyl)sulfinyl)amino)benzoate 10bc



White solid (117.5 mg, 88%). Mp: 68-69 °C. Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.38). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, J = 8.9 Hz, 2 H), 7.73 (s, 1 H), 7.10 (d, J = 8.8 Hz, 2 H), 3.88 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (s, 3 F); **^{13}C**

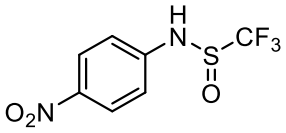
NMR (100 MHz, $CDCl_3$) δ 166.6, 143.1, 131.6, 126.2, 123.7 (q, *J* = 333.3 Hz), 118.0, 52.3 ppm. **IR (KBr):** ν = 3201, 2923, 1720, 1700, 1606, 1511, 1436, 1280, 1178, 1152, 1108, 892, 766 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_8F_3NO_3S$ $[M+Na]^+$ calcd 290.0075, found 290.0067.

***N*-(4-Cyanophenyl)-1,1,1-trifluoromethanesulfinamide 10bd**



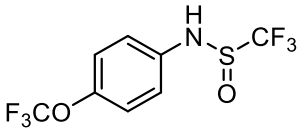
Yellow oil (115.8 mg, 99%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.42). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (s, 1 H), 7.61 (d, *J* = 8.3 Hz, 2 H), 7.17 (d, *J* = 6.9 Hz, 2 H);**^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.1, 134.1, 123.7 (q, *J* = 333.3 Hz), 118.6, 118.4, 107.7 ppm. **IR (KBr):** ν = 3192, 2922, 1606, 1509, 1189, 1154, 1110, 892, 832 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5F_3N_2OS$ $[M+Na]^+$ calcd 256.9972, found 256.9963.

1,1,1-Trifluoro-*N*-(4-nitrophenyl)methanesulfinamide 10be



White solid (104.1 mg, 82%). Mp: 102-103 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.58). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.7 Hz, 2 H), 7.65 (s, 1 H), 7.19 (d, *J* = 8.7 Hz, 2 H);**^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.7, 144.2, 126.0, 123.6 (q, *J* = 333.3 Hz), 118.0 ppm. The spectroscopic data were matched with those reported in the literature.[14]

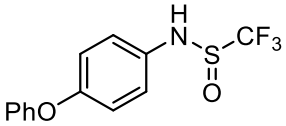
1,1,1-Trifluoro-*N*-(4-(trifluoromethoxy)phenyl)methanesulfinamide 10bf



Yellow solid (139.2 mg, 95%). Mp: 58-59 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.77). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (s, 1 H), 7.16 (d, *J* = 8.7 Hz, 2 H), 7.11 (d, *J* = 8.7 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.3 (s, 3 F), -77.4 (s, 3 F); **^{13}C**

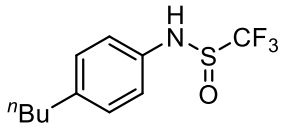
NMR (100 MHz, $CDCl_3$) δ 146.4, 137.1, 123.6 (q, *J* = 333.3 Hz), 122.5, 121.4, 120.5 (q, *J* = 262.6 Hz) ppm. **IR (KBr):** ν = 2955,1508, 1264, 1201, 1154, 1096 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5F_6NO_2S$ $[M+Na]^+$ calcd 315.9843, found 315.9831.

1,1,1-Trifluoro-*N*-(4-phenoxyphenyl)methanesulfinamide 10bg



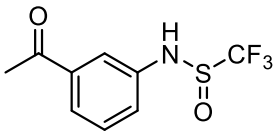
Gray solid (91.8 mg, 61%). Mp: 88-89 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.69). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.8 Hz, 2 H), 7.13 (d, *J* = 7.6 Hz, 1 H), 7.10 (d, *J* = 8.5 Hz, 3 H), 6.99 (t, *J* = 8.1 Hz, 4 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.1, 155.3, 133.2, 130.0, 123.8 (q, *J* = 333.3 Hz), 123.7, 123.2, 120.1, 118.9 ppm. **IR (KBr):** ν = 1504,1246, 1213, 1194,1153, 1094, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{13}H_{10}F_3NO_2S$ $[M+Na]^+$ calcd 324.0282, found 324.0272.

***N*-(4-Butylphenyl)-1,1,1-trifluoromethanesulfinamide 10bh**



Gray solid (106.0 mg, 80%). Mp: 34-35 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.79). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.13 (d, *J* = 8.4 Hz, 2 H), 7.08 (s, 1 H), 7.02 (d, *J* = 8.2 Hz, 2 H), 2.58 (t, *J* = 7.8 Hz, 2 H), 1.62 – 1.52 (m, 2 H), 1.35 (q, *J* = 7.4 Hz, 2 H), 0.93 (t, *J* = 7.3 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.6 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.4, 135.8, 129.7, 123.7 (q, *J* = 333.3 Hz), 120.9, 35.0, 33.7, 22.3, 14.0 ppm. **IR (KBr):** ν = 2928, 1512, 1188, 1153, 1095, 910 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{14}F_3NOS$ $[M+Na]^+$ calcd 288.0646, found 288.0637.

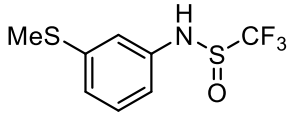
***N*-(3-Acetylphenyl)-1,1,1-trifluoromethanesulfinamide 10bi**



White solid (123.0 mg, 98%). Mp: 92-93 °C. Eluent: petroleum ether/ethyl acetate (5:1,

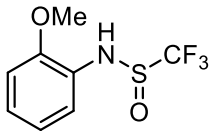
R_f = 0.61). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (s, 1 H), 7.74 (s, 1 H), 7.67 (d, *J* = 7.7 Hz, 1 H), 7.39 (t, *J* = 7.9 Hz, 1 H), 7.32 (d, *J* = 8.1 Hz, 1 H), 2.56 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.2, 139.5, 138.4, 130.2, 125.0, 123.9, 123.8 (q, *J* = 333.3 Hz), 119.1, 26.7 ppm. **IR (KBr):** ν = 1606, 1345, 1191, 1154, 1109, 783 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_8F_3NO_2S$ $[M+Na]^+$ calcd 274.0126, found 274.0122.

1,1,1-Trifluoro-*N*-(3-(methylthio)phenyl)methanesulfinamide 10bj



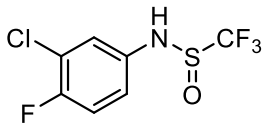
Yellow solid (126.2 mg, 99%). Mp: 70-71 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.54). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44 (s, 1 H), 7.18 (t, *J* = 7.9 Hz, 1 H), 6.99 (d, *J* = 9.9 Hz, 1 H), 6.93 (t, *J* = 2.1 Hz, 1 H), 6.82 (d, *J* = 8.0 Hz, 1 H), 2.41 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.0, 139.0, 130.0, 123.8 (q, *J* = 333.3 Hz), 122.8, 117.2, 116.2, 15.3 ppm. **IR (KBr):** ν = 3194, 2923, 1591, 1482, 1376, 1274, 1182, 1152, 1094, 923, 684, 469 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_8F_3NOS_2$ $[M+Na]^+$ calcd 277.9897, found 277.9888.

1,1,1-Trifluoro-*N*-(2-methoxyphenyl)methanesulfinamide 10bk



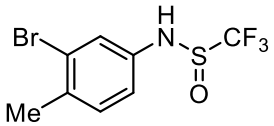
Purple solid (62.1 mg, 52%). Mp: 32-33 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.74). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.16 (d, *J* = 7.8 Hz, 1 H), 7.10 (t, *J* = 7.9 Hz, 1 H), 6.94 (d, *J* = 7.7 Hz, 1 H), 6.90 (d, *J* = 8.1 Hz, 1 H), 6.81 (s, 1 H), 3.85 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.7, 127.8, 125.4, 123.8 (q, *J* = 333.3 Hz), 121.3, 118.6, 111.3, 55.9 ppm. **IR (KBr):** ν = 2926, 1599, 1502, 1466, 1256, 1183, 1153, 1113, 1026, 897, 747, 463 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_8F_3NO_2S$ $[M+Na]^+$ calcd 262.0126, found 262.0117.

***N*-(3-Chloro-4-fluorophenyl)-1,1,1-trifluoromethanesulfinamide 10bl**



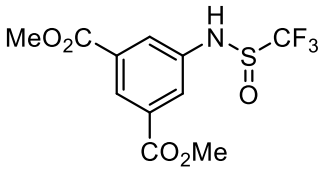
Yellow oil (108.3 mg, 83%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.53). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (s, 1 H), 7.16 (dd, *J* = 6.3, 2.7 Hz, 1 H), 7.10 (d, *J* = 8.6 Hz, 1 H), 7.02 – 6.93 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.1 (s, 3 F), -119.0 (m, 1 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.1 (d, *J* = 248.0 Hz), 134.7 (d, *J* = 3.6 Hz), 123.6 (q, *J* = 333.3 Hz), 123.2, 122.2 (d, *J* = 19.2 Hz), 120.7 (d, *J* = 7.1 Hz), 117.6 (d, *J* = 22.6 Hz). **IR (KBr):** ν = 3202, 1499, 1367, 1264, 1187, 1154, 1096, 929, 787, 573 cm^{-1}. **HRMS (ESI):** *m/z* for $C_7H_4ClF_4NOS$ $[M+Na]^+$ calcd 283.9536, found 283.9531.

***N*-(3-Bromo-4-methylphenyl)-1,1,1-trifluoromethanesulfinamide 10bm**



Yellow solid (120.4 mg, 80%). Mp: 74-75 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.78). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (s, 1 H), 7.27 (d, *J* = 2.5 Hz, 1 H), 7.13 (d, *J* = 8.0 Hz, 1 H), 6.93 (dd, *J* = 8.2, 2.5 Hz, 1 H), 2.32 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.1, 135.0, 131.5, 125.5, 124.1, 123.7 (q, *J* = 333.3 Hz), 119.3, 22.2 ppm. **IR (KBr):** ν = 3216, 2362, 1492, 1184, 1163, 1092, 873, 816 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_7BrF_3NOS$ $[M+Na]^+$ calcd 323.9282, found 323.9274.

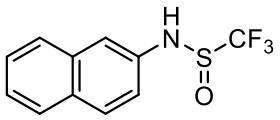
Dimethyl 5-(((trifluoromethyl)sulfinyl)amino)isophthalate 10bn



White solid (141.4 mg, 87%). Mp: 112-113 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.24). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.35 (s, 1 H), 8.06 (s, 1 H), 7.98 (s, 2 H), 3.91 (s, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.7, 139.8, 132.1, 126.5, 124.1, 123.7 (q, *J* = 333.3 Hz), 52.8 ppm. **IR (KBr):** ν = 3224, 2956, 1728, 1603, 1437, 1337, 1250, 1192, 1158, 1113,1012, 756 cm^{-}

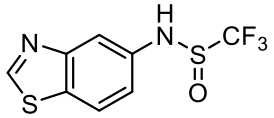
[1]. **HRMS (ESI):** *m/z* for $C_{11}H_{10}F_3NO_5S$ $[M+Na]^+$ calcd 348.0129, found 348.0119.

1,1,1-Trifluoro-*N*-(naphthalen-2-yl)methanesulfinamide 10bo



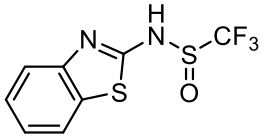
White solid (73.8 mg, 57%). Mp: 129-130 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.51). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (s, 2 H), 7.72 (d, *J* = 8.1 Hz, 1 H), 7.53 – 7.40 (m, 3 H), 7.22 (d, *J* = 8.9 Hz, 1 H), 6.94 (s, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.7, 133.8, 131.2, 130.2, 127.9, 127.3, 127.3, 125.8, 123.8 (q, *J* = 343.4 Hz), 120.0, 117.1 ppm. **IR (KBr):** ν = 3189, 2921, 1192, 1087, 854, 815, 749, 476 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_8F_3NOS$ $[M+Na]^+$ calcd 282.0176, found 282.0176.

***N*-(Benzo[*d*]thiazol-5-yl)-1,1,1-trifluoromethanesulfinamide 10bp**



Gray oil (81.1 mg, 61%). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.41). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.03 (s, 1 H), 8.18 (d, *J* = 14.4 Hz, 1 H), 7.85 (d, *J* = 2.4 Hz, 1 H), 7.82 (d, *J* = 8.5 Hz, 1 H), 7.22 (dd, *J* = 8.9, 2.4 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.5, 153.9, 137.6, 130.3, 123.8 (d, *J* = 333.3 Hz), 123.0, 119.0, 114.5 ppm. **IR (KBr):** ν = 2924, 1605, 1433, 1275, 1185, 1158, 1139, 1104, 963, 867, 807, 630, 571, 466 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5F_3N_2OS_2$ $[M+Na]^+$ calcd 288.9693, found 288.9687.

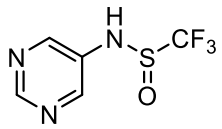
***N*-(Benzo[*d*]thiazol-2-yl)-1,1,1-trifluoromethanesulfinamide 10bq**



White solid (50.6 mg, 38%). Mp: 174-175 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.53). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.39 (s, 1 H), 7.73 (d, *J* = 7.7 Hz, 1 H), 7.51 (d, *J* = 7.9 Hz, 1 H), 7.40 (t, *J* = 7.2 Hz, 1 H), 7.25 (t, *J* = 8.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.9, 136.7,

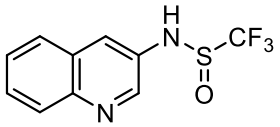
128.1, 124.7, 124.4 (q, J = 333.3 Hz), 123.6, 122.0, 114.3 ppm. **IR (KBr):** ν = 2923, 1557, 1466, 1187, 1145, 816 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5F_3N_2OS_2$ $[M+Na]^+$ calcd 288.9693, found 288.9679.

1,1,1-Trifluoro-*N*-(pyrimidin-5-yl)methanesulfinamide 10br



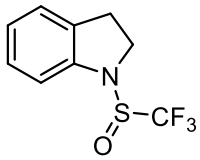
White solid (44.3 mg, 42%). Mp: 92-93 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.21). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.02 (s, 1 H), 8.63 (s, 2 H), 8.49 (s, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.9, 148.5, 134.6, 123.6 (q, J = 333.3 Hz) ppm. **IR (KBr):** ν = 2919, 1570, 1421, 1268, 1187, 1157, 1108, 893, 719, 628, 468 cm^{-1}. **HRMS (ESI):** *m/z* for $C_5H_4F_3N_3OS$ $[M+Na]^+$ calcd 233.9925, found 233.9927.

1,1,1-Trifluoro-*N*-(quinolin-3-yl)methanesulfinamide 10bs



Yellow solid (124.8 mg, 96%). Mp: 127-128 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.40). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.77 (d, J = 2.7 Hz, 1 H), 8.05 (d, J = 8.5 Hz, 1 H), 7.92 (d, J = 2.6 Hz, 1 H), 7.73 (d, J = 8.3 Hz, 1 H), 7.65 (t, J = 7.0 Hz, 1 H), 7.54 (t, J = 7.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.6, 144.7, 132.5, 129.4, 128.9, 128.1, 127.4, 125.0, 123.9 (q, J = 333.3 Hz). **IR (KBr):** ν = 2915, 1606, 1345, 1191, 1154, 1109, 783 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_7F_3N_2OS$ $[M+Na]^+$ calcd 283.0129, found 283.0120.

1-((Trifluoromethyl)sulfinyl)indoline 10bt



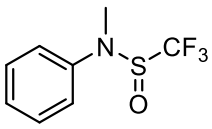
Colourless oil (104.6 mg, 89%). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.85). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (q, J = 7.6, 7.0 Hz, 2 H), 7.04 (d, J = 7.5 Hz, 1 H),

7.00 (d, J = 7.9 Hz, 1 H), 4.42 (td, J = 10.5, 6.2 Hz, 1 H), 3.75 – 3.62 (m, 1 H), 3.32 – 3.21 (m, 1 H), 3.21 – 3.10 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.8, 131.2, 127.9, 125.7, 124.2, 124.1 (q, J = 333.3 Hz), 112.2, 42.9, 29.2 ppm. **IR (KBr):** ν = 2922, 1481, 1247, 1188, 1155, 1113, 1097, 1016, 750, 557, 479, 421 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_8F_3NOS$ $[M+Na]^+$ calcd 258.0176, found 258.0168.

1-((Trifluoromethyl)sulfinyl)-1,2,3,4-tetrahydroquinoline 10bu

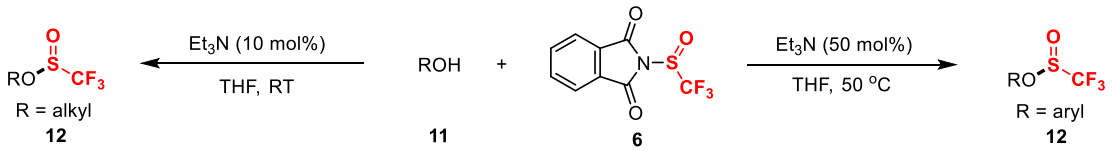
White solid (105.8 mg, 85%). Mp: 48-49 °C. Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.86). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 – 7.10 (m, 2 H), 7.04 (t, J = 7.4 Hz, 1 H), 6.98 (d, J = 8.0 Hz, 1 H), 4.22 (dt, J = 12.9, 4.5 Hz, 1 H), 3.28 (t, J = 11.6 Hz, 1 H), 2.85 (dd, J = 8.3, 5.1 Hz, 2 H), 2.17 – 2.00 (m, 1 H), 1.98 – 1.84 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.8, 130.2, 127.6, 127.2, 124.4 (q, J = 343.4 Hz), 124.0, 118.6, 39.4, 26.5, 22.9 ppm. **IR (KBr):** ν = 2923, 1490, 1456, 1304, 1178, 1113, 1111, 1016, 976, 840, 752, cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_{10}F_3NOS$ $[M+Na]^+$ calcd 272.0333, found 272.0319.

1,1,1-Trifluoro-*N*-methyl-*N*-phenylmethanesulfinamide 10bv



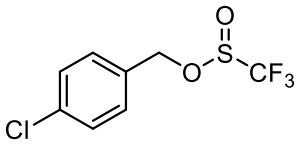
Yellow oil (49.1 mg, 44%). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.84). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (t, J = 8.0 Hz, 2 H), 7.25 – 7.15 (m, 3 H), 3.24 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.1, 129.8, 126.1, 124.4 (q, J = 343.4 Hz), 122.1, 31.1 ppm. The spectroscopic data were matched with those reported in the literature.[15]

3.5 General procedure for trifluoromethylsulfinylation of alkyl alcohols or phenols



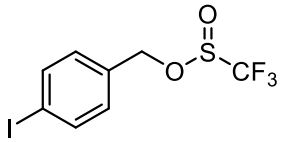
A 25 mL Schlenk tube charged with alcohol or phenol (**11**, 0.5 mmol) and *N*-trifluoromethylsulfinylphthalimide **6** (0.6 mmol, 1.2 equiv) was added freshly distilled THF (3.0 mL) and Et_3N (0.05 mmol for alcohol; 0.25 mmol for phenol). The mixture was stirred at corresponding temperature for 3 h. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated alcohol or phenol **12**.

4-Chlorobenzyl trifluoromethanesulfinate 12aa



Colourless oil (89.0 mg, 69%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.81). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.5 Hz, 2 H), 7.30 (d, *J* = 8.5 Hz, 2 H), 5.33 (d, *J* = 11.6 Hz, 1 H), 5.04 (d, *J* = 11.5 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.6, 132.3, 130.3, 129.3, 123.1 (q, *J* = 343.4 Hz), 68.8 ppm. **IR (KBr):** ν = 1563, 1419, 1359, 1180, 1125, 1061, 884, 787, 684, 656 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_6ClF_3O_2S$ $[M+Na]^+$ calcd 280.9627, found 280.9623.

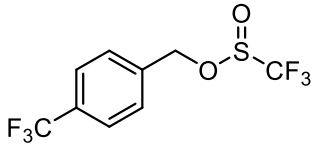
4-Iodobenzyl trifluoromethanesulfinate 12ab



Yellow oil (166.3 mg, 95%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.92). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.3 Hz, 2 H), 7.11 (d, *J* = 8.2 Hz, 2 H), 5.30 (d, *J* = 11.6 Hz, 1 H), 5.01 (d, *J* = 11.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.2, 133.4, 130.6, 123.1 (q, *J* = 333.3 Hz), 95.7, 68.9 ppm. **IR (KBr):** ν = 1486, 1198, 1129, 920, 846, 799, 773 cm^{-1}. **HRMS**

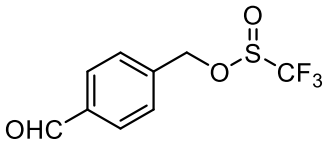
(ESI): *m/z* for $C_8H_6F_3IO_2S$ $[M+Na]^+$ calcd 372.8983, found 372.8976.

4-(Trifluoromethyl)benzyl trifluoromethanesulfinate 12ac



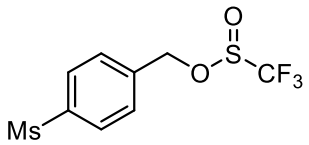
Colourless oil (102.2 mg, 70%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.68). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.8 Hz, 2 H), 7.50 (d, *J* = 7.9 Hz, 2 H), 5.43 (dd, *J* = 12.0, 7.1 Hz, 1 H), 5.14 (dd, *J* = 12.2, 6.9 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.9 (s, 3 F), -78.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.8, 131.5 (q, *J* = 32.6 Hz), 128.8, 125.9 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 272.7 Hz), 123.1 (q, *J* = 333.3 Hz), 68.2 ppm. **IR (KBr):** ν = 2363, 1490, 1453, 1275, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_6F_6O_2S$ $[M+Na]^+$ calcd 314.9890, found 314.9890.

4-Formylbenzyl trifluoromethanesulfinate 12ad



Colourless oil (109.6 mg, 87%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.65). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.00 (s, 1 H), 7.89 (d, *J* = 8.1 Hz, 2 H), 7.53 (d, *J* = 7.9 Hz, 2 H), 5.42 (d, *J* = 12.2 Hz, 1 H), 5.14 (d, *J* = 12.2 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.7, 140.2, 136.9, 130.2, 128.9, 123.0 (q, *J* = 343.4 Hz), 68.4 ppm. **IR (KBr):** ν = 1698, 1611, 1185, 1123, 922, 829, 784, 736, 589, 483, 457 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_7F_3O_3S$ $[M+Na]^+$ calcd 274.9966, found 274.9957.

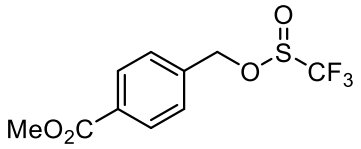
4-(Methylsulfonyl)benzyl trifluoromethanesulfinate 12ae



White solid (149.5 mg, 99%, RT). Mp: 63-64 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.76). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.4 Hz, 2 H), 7.55 (d, *J* = 8.3 Hz, 2 H), 5.42 (d, *J* = 12.3 Hz, 1 H), 5.15 (d, *J* = 12.3 Hz, 1 H), 3.02 (s, 3 H); **^{19}F**

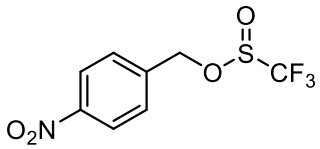
NMR (376 MHz, $CDCl_3$) δ -77.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.3, 139.9, 129.1, 128.1, 123.0 (q, *J* = 343.4 Hz), 68.0, 44.5 ppm. **IR (KBr):** ν = 2854, 1730, 1302, 1191, 1124, 1088, 954, 758, 653, 525 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_9F_3O_4S_2$ $[M+Na]^+$ calcd 324.9792, found 324.9798.

Methyl 4-((((trifluoromethyl)sulfinyl)oxy)methyl)benzoate 12af



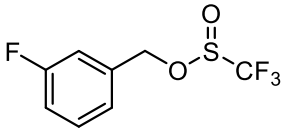
Yellow oil (131.1 mg, 93%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.45). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.3 Hz, 2 H), 7.40 (d, *J* = 8.5 Hz, 2 H), 5.37 (d, *J* = 12.0 Hz, 1 H), 5.09 (d, *J* = 12.0 Hz, 1 H), 3.87 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.4, 138.6, 131.0, 130.2, 128.4, 123.0 (q, *J* = 343.4 Hz), 68.6, 52.3 ppm. **IR (KBr):** ν = 1719, 1436, 1278, 1178, 1125, 900, 864, 747, 694, 589, 454 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_9F_3O_4S$ $[M+Na]^+$ calcd 305.0071, found 305.0066.

4-Nitrobenzyl trifluoromethanesulfinate 12ag



White solid (111.7 mg, 83%, RT). Mp: 49-50 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.47). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 6.8 Hz, 2 H), 7.55 (d, *J* = 6.8 Hz, 2 H), 5.46 (d, *J* = 12.4 Hz, 1 H), 5.17 (d, *J* = 12.4 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.4, 140.9, 129.0, 124.1, 123.0 (q, *J* = 343.4 Hz), 67.5 ppm. The spectroscopic data were matched with those reported in the literature.[17]

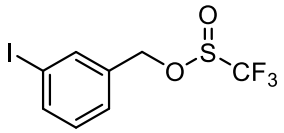
3-Fluorobenzyl trifluoromethanesulfinate 12ah



Colourless oil (76.2 mg, 63%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f =

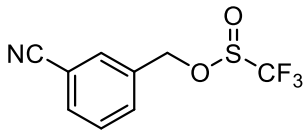
0.82). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42 – 7.32 (m, 1 H), 7.15 (d, *J* = 7.8 Hz, 1 H), 7.09 (d, *J* = 8.6 Hz, 2 H), 5.35 (d, *J* = 12.0 Hz, 1 H), 5.06 (d, *J* = 12.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.0 (s, 3 F), -111.8 (m, 1 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 247.6 Hz), 136.1 (d, *J* = 7.5 Hz), 130.7 (d, *J* = 8.2 Hz), 124.3 (d, *J* = 3.1 Hz), 123.1 (q, *J* = 343.4 Hz), 116.5 (d, *J* = 21.1 Hz), 115.6 (d, *J* = 22.3 Hz), 68.6 ppm. **IR (KBr):** ν = 1593, 1490, 1453, 1262, 1183, 1123, 910, 867, 742, 683, 583, 453 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_6F_4O_2S$ $[M+Na]^+$ calcd 264.9922, found 264.9916.

3-Iodobenzyl trifluoromethanesulfinate 12ai



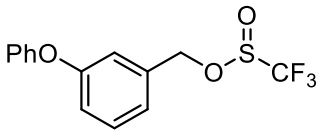
Yellow oil (157.5 mg, 90%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.89). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 – 7.70 (m, 2 H), 7.34 (d, *J* = 7.8 Hz, 1 H), 7.17 – 7.07 (m, 1 H), 5.30 (d, *J* = 11.6 Hz, 1 H), 4.99 (d, *J* = 11.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.5, 137.6, 136.0, 130.7, 128.0, 123.1 (q, *J* = 343.4 Hz), 94.6, 68.3 ppm. **IR (KBr):** ν = 1568, 1424, 1366, 1185, 1125, 1064, 883, 787, 684, 657, 579, 454 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_6F_3IO_2S$ $[M+Na]^+$ calcd 372.8983, found 372.8977.

3-Cyanobenzyl trifluoromethanesulfinate 12aj



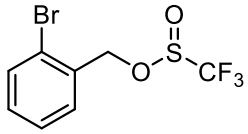
Yellow oil (113.2 mg, 91%, RT). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.71). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 6.6 Hz, 2 H), 7.60 (d, *J* = 7.9 Hz, 1 H), 7.51 (t, *J* = 7.9 Hz, 1 H), 5.38 (d, *J* = 12.0 Hz, 1 H), 5.09 (d, *J* = 12.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.5, 132.9, 132.8, 131.9, 130.0, 123.0 (q, *J* = 343.4 Hz), 118.2, 113.2, 67.8 ppm. **IR (KBr):** ν = 2232, 1190, 1126, 929, 885, 808, 764, 686, 456 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_6F_3NO_2S$ $[M+Na]^+$ calcd 271.9969, found 271.9969.

3-Phenoxybenzyl trifluoromethanesulfinate 12ak



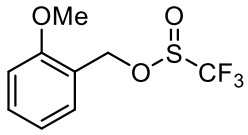
Colourless oil (121.6 mg, 77%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.71). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (t, *J* = 8.0 Hz, 3 H), 7.15 (dd, *J* = 16.7, 7.4 Hz, 2 H), 7.05 (d, *J* = 7.8 Hz, 4 H), 5.34 (d, *J* = 11.6 Hz, 1 H), 5.06 (d, *J* = 11.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.1, 156.7, 135.7, 130.5, 130.1, 124.0, 123.4, 123.1 (q, *J* = 333.3 Hz), 119.6, 119.4, 118.8, 69.4 ppm. **IR (KBr):** ν = 1585, 1487, 1448, 1259, 1198, 1128, 921, 875, 764, 691, 454 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{14}H_{11}F_3O_3S$ $[M+Na]^+$ calcd 339.0279, found 339.0270.

2-Bromobenzyl trifluoromethanesulfinate 12al



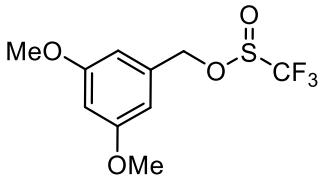
Yellow oil (143.5 mg, 95%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.84). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 1 H), 7.44 (d, *J* = 7.6 Hz, 1 H), 7.35 (t, *J* = 7.5 Hz, 1 H), 7.25 (t, *J* = 7.7 Hz, 1 H), 5.44 (d, *J* = 11.8 Hz, 1 H), 5.22 (d, *J* = 11.9 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 133.4, 133.3, 131.1, 130.9, 128.0, 123.9, 123.0 (q, *J* = 333.3 Hz), 69.5 ppm. The spectroscopic data were matched with those reported in the literature.[18]

2-Methoxybenzyl trifluoromethanesulfinate 12am



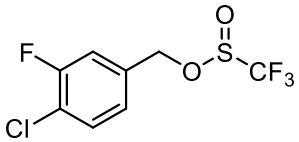
White solid (53.4 mg, 42%, RT). Mp: 41-42 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.64). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 – 7.33 (m, 2 H), 7.10 – 6.93 (m, 2 H), 4.63 (s, 2 H), 3.87 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.3, 132.7, 131.7, 121.1, 120.0 (q, *J* = 333.3 Hz), 112.5, 111.3, 55.8, 50.6 ppm. **IR (KBr):** ν = 1497, 1362, 1256, 1194, 1119 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_9F_3O_3S$ $[M+Na]^+$ calcd 277.0122, found 277.0120.

3,5-Dimethoxybenzyl trifluoromethanesulfinate 12an



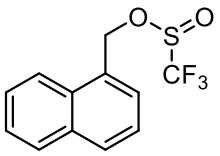
Colourless oil (140.6 mg, 99%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.80). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.50 (d, *J* = 2.3 Hz, 2 H), 6.46 (t, *J* = 2.3 Hz, 1 H), 5.28 (d, *J* = 11.4 Hz, 1 H), 5.01 (d, *J* = 11.5 Hz, 1 H), 3.78 (s, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.3, 135.8, 123.1 (q, *J* = 343.4 Hz), 106.6, 101.3, 70.0, 55.4 ppm. **IR (KBr):** ν = 1596, 1459, 1325, 1152, 1067, 904, 833, 776, 687, 593, 489, 454 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_{11}F_3O_4S$ $[M+Na]^+$ calcd 307.0228, found 307.0218.

4-Chloro-3-fluorobenzyl trifluoromethanesulfinate 12ao



Colourless oil (103.5 mg, 75%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.66). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (t, *J* = 7.8 Hz, 1 H), 7.16 (dd, *J* = 9.3, 2.0 Hz, 1 H), 7.10 (d, *J* = 8.3 Hz, 1 H), 5.32 (d, *J* = 11.8 Hz, 1 H), 5.02 (d, *J* = 11.9 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.0 (s, 3 F), -113.8 (m, 1 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.2 (d, *J* = 250.4 Hz), 134.6 (d, *J* = 6.6 Hz), 131.3, 125.0 (d, *J* = 4.0 Hz), 123.0 (q, *J* = 343.4 Hz), 122.3 (d, *J* = 17.6 Hz), 116.8 (d, *J* = 22.0 Hz), 67.8 ppm. **IR (KBr):** ν = 1585, 1492, 1428, 1282, 1183, 1123, 1064, 918, 869, 821, 775, 739, 668, 598, 453 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_5ClF_4O_2S$ $[M+Na]^+$ calcd 298.9533, found 298.9528.

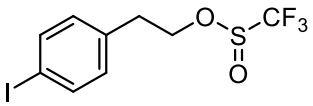
Naphthalen-1-ylmethyl trifluoromethanesulfinate 12ap



White solid (59.0 mg, 43%, RT). Mp: 108-109 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.82). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 1 H), 7.97 – 7.90

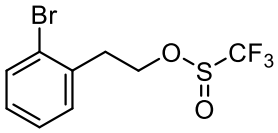
(m, 2 H), 7.64 (t, J = 7.5 Hz, 1 H), 7.60 – 7.53 (m, 2 H), 7.48 (t, J = 7.8 Hz, 1 H), 5.81 (d, J = 11.5 Hz, 1 H), 5.54 (d, J = 11.6 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 134.1, 132.4, 131.7, 131.2, 129.1, 127.6, 126.7, 125.4, 123.5, 120.1 (q, J = 333.3 Hz), 119.3, 53.0 ppm. **IR (KBr):** ν = 1355, 1198, 1121, 804, 775, 659, 486 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{12}H_9F_3O_2S$ $[M+Na]^+$ calcd 297.0173, found 297.0166.

4-Iodophenethyl trifluoromethanesulfinate 12aq



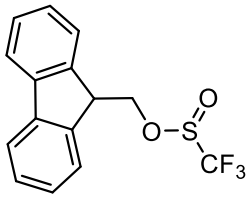
Yellow oil (165.6 mg, 91%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.51). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.1 Hz, 2 H), 6.96 (d, J = 8.2 Hz, 2 H), 4.54 – 4.45 (m, 1 H), 4.34 – 4.22 (m, 1 H), 2.99 (t, J = 6.7 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.9, 135.9, 131.1, 122.9 (q, J = 333.3 Hz), 92.7, 68.4, 35.8 ppm. **IR (KBr):** ν = 1486, 1194, 1129, 1007, 956, 880, 810, 741, 458 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_8F_3IO_2S$ $[M+Na]^+$ calcd 386.9139, found 386.9138.

2-Bromophenethyl trifluoromethanesulfinate 12ar



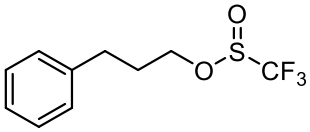
Colourless oil (153.2 mg, 97%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.76). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (d, J = 7.5 Hz, 1 H), 7.29 – 7.24 (m, 2 H), 7.16 – 7.10 (m, 1 H), 4.60 – 4.52 (m, 1 H), 4.40 – 4.32 (m, 1 H), 3.21 (td, J = 7.0, 2.9 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.4, 133.2, 131.6, 129.1, 127.8, 124.6, 123.0 (q, J = 333.3 Hz), 67.5, 36.6 ppm. **IR (KBr):** ν = 1473, 1195, 1129, 957, 881, 752 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_8BR_{f3}O_2S$ $[M+Na]^+$ calcd 338.9278, found 338.9270.

(9*H*-Fluoren-9-yl)methyl trifluoromethanesulfinate 12as



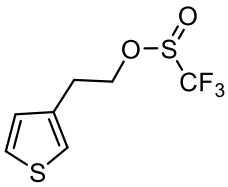
Colourless oil (70.2 mg, 45%, RT). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.81). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 7.4 Hz, 2 H), 7.63 (t, *J* = 7.5 Hz, 2 H), 7.47 (q, *J* = 7.6 Hz, 2 H), 7.37 (q, *J* = 7.6 Hz, 2 H), 4.63 (dd, *J* = 16.5, 7.5 Hz, 1 H), 4.42 (dd, *J* = 16.5, 7.5 Hz, 1 H), 4.29 (q, *J* = 7.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.4, 141.5, 128.4, 127.5, 125.2, 122.9 (q, *J* = 343.4 Hz), 120.4, 70.1, 47.6 ppm. **IR (KBr):** ν = 1275, 909, 830, 751, 417 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{15}H_{11}F_3O_2S$ $[M+Na]^+$ calcd 335.0330, found 335.0326.

3-Phenylpropyl trifluoromethanesulfinate 12at



Colourless oil (113.4 mg, 90%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.72). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.5 Hz, 2 H), 7.26 (d, *J* = 7.3 Hz, 1 H), 7.22 (d, *J* = 6.8 Hz, 2 H), 4.41 – 4.34 (m, 1 H), 4.20 – 4.13 (m, 1 H), 2.77 (t, *J* = 7.6 Hz, 2 H), 2.18 – 2.03 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.4, 128.7, 128.6, 126.5, 123.0 (q, *J* = 333.3 Hz), 68.4, 31.5, 31.4 ppm. The spectroscopic data were matched with those reported in the literature.[17]

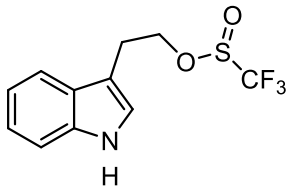
2-(Thiophen-3-yl)ethyl trifluoromethanesulfinate 12au



Colourless oil (98.8 mg, 81%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.78). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 1 H), 7.08 (s, 1 H), 6.99 – 6.95 (m, 1 H), 4.58 – 4.49 (m, 1 H), 4.37 – 4.27 (m, 1 H), 3.10 (td, *J* = 6.8, 2.5 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.3, 128.1, 126.2, 123.0 (q, *J* = 343.4 Hz), 122.5, 68.5, 30.8 ppm. **IR (KBr):** ν = 1197, 1129, 952,

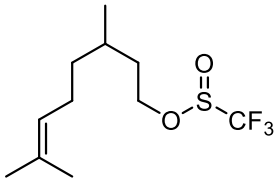
882, 778 cm^{-1}. **HRMS (ESI):** *m/z* for $C_7H_7F_3O_2S_2$ $[M+Na]^+$ calcd 266.9737, found 266.9731.

2-(1*H*-Indol-3-yl)ethyl trifluoromethanesulfinate 12av



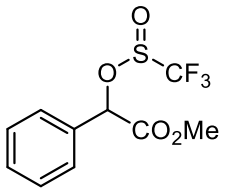
Yellow oil (108.0 mg, 80%, RT). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.71). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12 (s, 1 H), 7.62 (d, *J* = 7.9 Hz, 1 H), 7.38 (d, *J* = 8.2 Hz, 1 H), 7.30 – 7.24 (m, 1 H), 7.23 – 7.17 (m, 1 H), 7.05 (d, *J* = 2.4 Hz, 1 H), 4.61 (dt, *J* = 10.0, 7.1 Hz, 1 H), 4.42 (dt, *J* = 10.1, 7.0 Hz, 1 H), 3.25 (t, *J* = 7.1 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.5 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.3, 127.2, 123.1 (q, *J* = 333.3 Hz), 123.0, 122.4, 119.8, 118.5, 111.6, 110.0, 69.2, 26.3 ppm. **IR (KBr):** ν = 2361, 1275, 1167, 1065, 763, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{10}F_3NO_2S$ $[M+Na]^+$ calcd 300.0282, found 300.0272.

3,7-Dimethyloct-6-en-1-yl trifluoromethanesulfinate 12aw



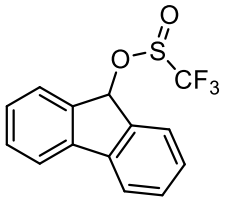
Colourless oil (99.3 mg, 73%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.89). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.17 – 4.94 (m, 1 H), 4.44 – 4.32 (m, 1 H), 4.21 – 4.08 (m, 1 H), 2.04 – 1.87 (m, 2 H), 1.84 – 1.71 (m, 1 H), 1.65 (s, 3 H), 1.58 (s, 4 H), 1.39 – 1.28 (m, 1 H), 1.25 – 1.14 (m, 2 H), 0.90 (d, *J* = 6.1 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.6 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 131.6, 124.3, 123.0 (q, *J* = 333.3 Hz), 67.5, 36.8 (d, *J* = 8.9 Hz), 36.6 (d, *J* = 4.0 Hz), 28.9, 25.7, 25.3, 19.1 (d, *J* = 6.4 Hz), 17.6 ppm. The spectroscopic data were matched with those reported in the literature.[15]

Methyl 2-phenyl-2-(((trifluoromethyl)sulfinyl)oxy)acetate 12ax



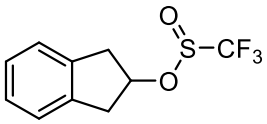
Colourless oil (63.5 mg, 45%, RT). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.70). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.42 (m, 2 H), 7.41 – 7.40 (m, 3 H), 5.87 (d, *J* = 8.7 Hz, 1 H), 3.76 (d, *J* = 7.4 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.7 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.3 (d, *J* = 57.0 Hz), 132.8 (d, *J* = 14.3 Hz), 130.4, 129.3, 128.1, 123.0 (dq, *J* = 333.3, 9.1 Hz), 77.6 (d, *J* = 45.9 Hz), 53.3 ppm. **IR (KBr):** ν = 2958, 1752, 1457, 1439, 1271, 1195, 1127, 1017, 951, 801, 696 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_9F_3O_4S$ $[M+Na]^+$ calcd 305.0071, found 305.0070.

9*H*-Fluoren-9-yl trifluoromethanesulfinate 12ay



White solid (82.0 mg, 55%, RT). Mp: 142-143 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.80). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93 (t, *J* = 8.1 Hz, 2 H), 7.78 (t, *J* = 8.0 Hz, 2 H), 7.54 (q, *J* = 7.9 Hz, 2 H), 7.42 (q, *J* = 7.9 Hz, 2 H), 5.49 (d, *J* = 7.7 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.0, 132.3, 130.6, 128.3, 127.2, 120.7, 120.0 (q, *J* = 333.3 Hz), 68.8 ppm. **IR (KBr):** ν = 2924, 1454, 1352, 1236, 1209, 1112, 757, 586, 535, 514 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{14}H_9F_3O_2S$ $[M+Na]^+$ calcd 321.0173, found 321.0173.

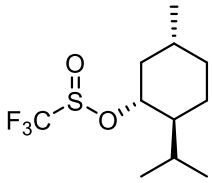
2,3-Dihydro-1*H*-inden-2-yl trifluoromethanesulfinate 12az



Colourless oil (116.3 mg, 93%, RT). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.81). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 4 H), 5.51 – 5.45 (m, 1 H), 3.44 – 3.32 (m, 2 H), 3.31 – 3.19 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.2 (s, 3 F);

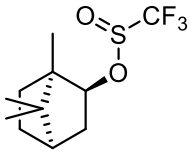
^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1 (d, *J* = 16.9 Hz), 127.4 (d, *J* = 2.6 Hz), 124.8 (d, *J* = 4.5 Hz), 122.9 (q, *J* = 333.3 Hz), 82.6, 40.6 (d, *J* = 46.6 Hz) ppm. **IR (KBr):** ν = 1194, 1129, 996, 862, 739, 752 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_9F_3O_2S$ $[M+Na]^+$ calcd 273.0173, found 273.0173.

(1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl trifluoromethanesulfinate 12ba



Yellow oil (114.3 mg, 84%, RT, dr = 5:3). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.93). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 4.22 (qd, *J* = 10.5, 4.6 Hz, 1 H), 2.21 – 1.95 (m, 2 H), 1.77 – 1.63 (m, 2 H), 1.53 – 1.40 (m, 2 H), 1.40 – 1.15 (m, 1 H), 1.11 – 0.96 (m, 1 H), 0.95 – 0.86 (m, 7 H), 0.78 (d, *J* = 7.0 Hz, 1.9 H), 0.75 (d, *J* = 7.0 Hz, 1.1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.2 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.7 (dq, *J* = 333.3, 7.0 Hz), 85.0 (d, *J* = 89.0 Hz), 47.9 (d, *J* = 18.5 Hz), 42.5 (d, *J* = 70.2 Hz), 33.7, 31.9 (d, *J* = 10.9 Hz), 25.4 (d, *J* = 16.7 Hz), 23.1 (d, *J* = 19.6 Hz), 21.8 (d, *J* = 3.8 Hz), 20.7 (d, *J* = 5.8 Hz), 15.5 (d, *J* = 18.0 Hz) ppm. The spectroscopic data were matched with those reported in the literature.[17]

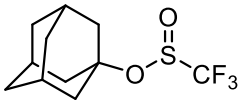
(1R,2S,4R)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl trifluoromethanesulfinate 12bb



Colourless oil (103.5 mg, 77%, RT, dr = 3:2). Eluent: petroleum ether/ethyl acetate (20:1, R_f = 0.79). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 4.75 (d, *J* = 10.3 Hz, 0.4 H), 4.66 (d, *J* = 9.9 Hz, 0.6 H), 2.42 – 2.28 (m, 1 H), 1.97 – 1.83 (m, 1 H), 1.75 (dd, *J* = 14.8, 3.8 Hz, 2 H), 1.43 – 1.20 (m, 3 H), 0.91 (s, 3 H), 0.88 – 0.85 (m, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.5 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.9 (dq, *J* = 333.3, 7.0 Hz), 89.1 (d, *J* = 147.1 Hz), 50.2 (d, *J* = 4.1 Hz), 48.2 (d, *J* = 15.6 Hz), 44.9 (d, *J* = 4.7 Hz), 36.7 (d, *J* = 52.7 Hz), 27.9 (d, *J* = 9.0 Hz), 26.4 (d, *J* = 9.0 Hz),

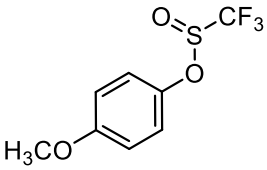
19.3 (d, J = 106.6 Hz), 13.0 ppm. The spectroscopic data were matched with those reported in the literature.[19]

(3s,5s,7s)-Adamantan-1-yl trifluoromethanesulfinate 12bc



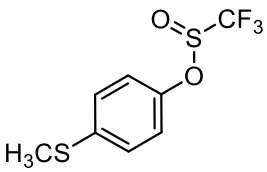
Yellow oil (113.9 mg, 85%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.91). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.24 (s, 3 H), 2.02 (s, 6 H), 1.64 (q, J = 11.9 Hz, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.7 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.9 (q, J = 333.3 Hz), 86.5, 43.4, 35.4, 31.3 ppm. The spectroscopic data were matched with those reported in the literature.[17]

4-Methoxyphenyl trifluoromethanesulfinate 12bd



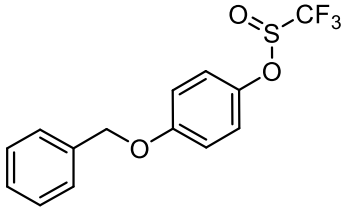
Colourless oil (87.6 mg, 73%, 50 °C). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.90). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.17 – 7.08 (m, 2 H), 6.93 – 6.84 (m, 2 H), 3.80 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.5, 145.3, 122.8 (q, J = 343.4 Hz), 122.3, 115.3, 55.7 ppm. The spectroscopic data were matched with those reported in the literature.[20]

4-(Methylthio)phenyl trifluoromethanesulfinate 12be



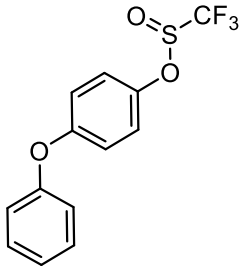
Yellow oil (67.9 mg, 53%, 50 °C). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.83). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.23 (m, 2 H), 7.18 – 7.09 (m, 2 H), 2.48 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.4, 138.1, 128.2, 122.8 (q, J = 333.3 Hz), 121.6, 16.1 ppm. **IR (KBr):** ν = 2924, 1487, 1439, 1194, 1127, 1095, 969, 840, 742, 651 cm^{-1}. **HRMS (ESI):** *m/z* for $C_8H_7F_3O_2S_2$ $[M+Na]^+$ calcd 278.9737, found 278.9745.

4-(Benzyloxy)phenyl trifluoromethanesulfinate 12bf



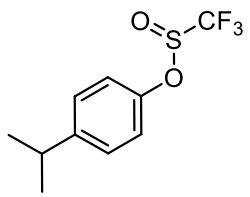
White solid (134.3 mg, 85%, 50 ºC). Mp: 56-57 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.82). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 (q, *J* = 7.4 Hz, 4 H), 7.37 (d, *J* = 6.8 Hz, 1 H), 7.15 (d, *J* = 8.9 Hz, 2 H), 6.99 (d, *J* = 8.8 Hz, 2 H), 5.07 (s, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.0 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.7, 145.5, 136.5, 128.8, 128.3, 127.6, 122.8 (q, *J* = 333.3 Hz), 122.4, 116.3, 70.6 ppm. **IR (KBr):** ν = 2929, 1593, 1500, 1455, 1247, 1192, 1169, 1154, 1128, 1105, 1008, 833, 795, 738, 697 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{14}H_{11}F_3O_3S$ $[M+Na]^+$ calcd 339.0279, found 339.0280.

4-Phenoxyphenyl trifluoromethanesulfinate 12bg



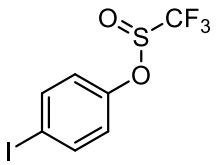
Colourless oil (104.2 mg, 69%, 50 ºC). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.84). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 (t, *J* = 8.1 Hz, 2 H), 7.21 – 7.11 (m, 3 H), 7.02 (d, *J* = 1.5 Hz, 2 H), 7.00 (d, *J* = 1.0 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.7, 156.4, 147.0, 130.1, 124.1, 122.8 (q, *J* = 343.4 Hz), 122.5, 120.1, 119.3 ppm. **IR (KBr):** ν = 1588, 1488, 1244, 1198, 1164, 1129, 1072, 831, 791, 752, 692 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{13}H_9F_3O_3S$ $[M+Na]^+$ calcd 325.0122, found 325.0112.

4-Isopropylphenyl trifluoromethanesulfinate 12bh



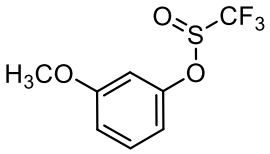
Colourless oil (102.0 mg, 81%, 50 °C). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.90). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 – 7.21 (m, 2 H), 7.16 – 7.08 (m, 2 H), 2.98 – 2.87 (m, 1 H), 1.25 (s, 3 H), 1.23 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.9, 148.1, 128.2, 122.7 (q, *J* = 333.3 Hz), 120.7, 33.7, 23.9 ppm. **IR (KBr):** ν = 2965, 1504, 1196, 1155, 1131, 843, 755 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_{11}F_3O_2S$ $[M+Na]^+$ calcd 275.0330, found 275.0322.

4-Iodophenyl trifluoromethanesulfinate 12bi



Yellow oil (85.7 mg, 51%, 100 °C). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.85). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.4 Hz, 2 H), 6.94 (d, *J* = 8.4 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.8, 139.5, 123.0, 122.7 (q, *J* = 333.3 Hz), 91.6 ppm. **IR (KBr):** ν = 1511, 1193, 1154, 1129, 852, 739, 752 cm^{-1}. **HRMS (ESI):** *m/z* for $C_7H_4F_3O_2S$ $[M+Na]^+$ calcd 358.8826, found 358.8821.

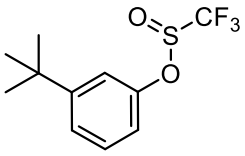
3-Methoxyphenyl trifluoromethanesulfinate 12bj



Colourless oil (75.6 mg, 63%, 50 °C). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.72). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 8.3 Hz, 1 H), 6.84 (dd, *J* = 8.9, 1.9 Hz, 1 H), 6.79 (dd, *J* = 8.1, 1.3 Hz, 1 H), 6.73 (t, *J* = 2.3 Hz, 1 H), 3.81 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.1 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.2, 153.0, 130.9, 122.8 (q, *J* = 343.4 Hz), 113.2, 112.5, 106.7, 55.7 ppm. **IR (KBr):** ν = 2920, 1609, 1586, 1491, 1450, 1288, 1200, 1121, 1042, 936, 844, 777 cm^{-1}. **HRMS (ESI):** *m/z* for

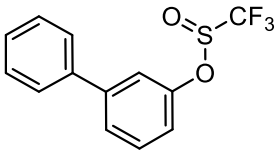
$C_8H_7F_3O_3S$ $[M+Na]^+$ calcd 262.9966, found 262.9962.

3-(Tert-butyl)phenyl trifluoromethanesulfinate 12bk



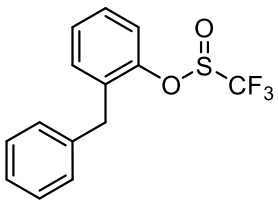
Colourless oil (111.7 mg, 84%, 50 °C). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.92). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (s, 2 H), 7.25 (s, 1 H), 7.06 (s, 1 H), 1.37 (s, 9 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.6, 152.0, 129.9, 124.3, 122.8 (q, *J* = 343.4 Hz), 117.9, 117.5, 35.0, 31.1 ppm. **IR (KBr):** ν = 2967, 1608, 1487, 1268, 1201, 1161, 1131, 910, 822, 792, 741, 697 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{13}F_3O_2S$ $[M+Na]^+$ calcd 289.0486, found 289.0480.

[1,1'-Biphenyl]-3-yl trifluoromethanesulfinate 12bl



Colourless oil (98.6 mg, 69%, 50 °C). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.85). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 – 7.56 (m, 2 H), 7.56 – 7.52 (m, 1 H), 7.50 – 7.47 (m, 1 H), 7.47 – 7.43 (m, 2 H), 7.43 – 7.36 (m, 2 H), 7.19 (d, *J* = 8.0 Hz, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.5, 144.1, 139.4, 130.8, 129.1, 128.3, 127.3, 126.0, 122.8 (q, *J* = 333.3 Hz), 119.5, 119.4 ppm. **IR (KBr):** ν = 1604, 1572, 1420, 1199, 1127, 881, 796, 761, 744, 695 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{13}H_9F_3O_2S$ $[M+Na]^+$ calcd 309.0173, found 309.0163.

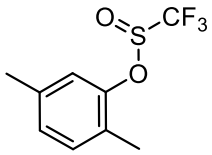
2-Benzylphenyl trifluoromethanesulfinate 12bm



Colourless oil (130.5 mg, 87%, 50 °C). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.86). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.29 (m, 2 H), 7.29 – 7.26 (m, 1 H), 7.26 – 7.22 (m, 3 H), 7.22 – 7.06 (m, 3 H), 4.08 (q, *J* = 8.0 Hz, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.4, 139.3, 133.7, 131.9,

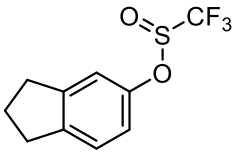
129.1, 128.7, 128.4, 127.4, 126.6, 122.9 (q, J = 343.4 Hz), 120.9, 35.8 ppm. **IR (KBr):** ν = 3029, 2923, 1601, 1581, 1486, 1451, 1193, 1155, 1123, 1088, 855, 796, 768, 732, 696, 608, 456 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{14}H_{11}F_3O_2S$ $[M+Na]^+$ calcd 323.0330, found 323.0324.

2,5-Dimethylphenyl trifluoromethanesulfinate 12bn



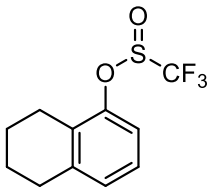
Colourless oil (98.7 mg, 83%, 50 ºC). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.92). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.17 (d, J = 7.7 Hz, 1 H), 7.08 – 7.00 (m, 2 H), 2.37 (s, 3 H), 2.30 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.6, 137.9, 131.6, 127.8, 127.1, 122.8 (q, J = 333.3 Hz), 121.3, 20.8, 15.7 ppm. **IR (KBr):** ν = 2928, 1509, 1197, 1130, 1095, 995, 930, 814, 776, 696, 622 cm^{-1}. **HRMS (ESI):** *m/z* for $C_9H_9F_3O_2S$ $[M+Na]^+$ calcd 261.0173, found 261.0164.

2,3-Dihydro-1*H*-inden-5-yl trifluoromethanesulfinate 12bo



Colourless oil (113.8 mg, 91%, 50 ºC). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.79). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (d, J = 8.1 Hz, 1 H), 7.06 (s, 1 H), 6.95 (dd, J = 8.1, 2.4 Hz, 1 H), 2.90 (q, J = 7.8 Hz, 4 H), 2.16 – 2.06 (m, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.7, 147.1, 143.5, 125.7, 122.8 (q, J = 333.3 Hz), 118.6, 117.1, 33.0, 32.3, 25.8 ppm. **IR (KBr):** ν = 2956, 1609, 1480, 1439, 1198, 1085, 929, 867, 818, 791, 719, 563 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{10}H_9F_3O_2S$ $[M+Na]^+$ calcd 273.0173, found 273.0166.

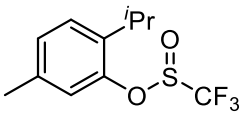
5,6,7,8-Tetrahydronaphthalen-1-yl trifluoromethanesulfinate 12bp



Colourless oil (96.3 mg, 73%, 50 ºC). Eluent: petroleum ether/ethyl acetate (5:1, R_f =

0.89). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.12 (t, *J* = 7.8 Hz, 1 H), 7.02 (dd, *J* = 15.5, 7.8 Hz, 2 H), 2.79 (t, *J* = 6.5 Hz, 3 H), 2.74 – 2.63 (m, 1 H), 1.85 – 1.76 (m, 4 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.7, 140.5, 129.8, 128.1, 126.5, 123.0 (q, *J* = 333.3 Hz), 117.6, 29.5, 23.5, 22.5, 22.4 ppm. **IR (KBr):** ν = 2936, 2862, 1575, 1455, 1194, 1126, 1066, 1012, 966, 895, 864, 780, 742, 464 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{11}F_3O_2S$ $[M+Na]^+$ calcd 287.0330, found 287.0318.

2-Isopropyl-5-methylphenyl trifluoromethanesulfinate 12bq



Colourless oil (95.8 mg, 72%, 50 ºC). Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.88). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 7.9 Hz, 1 H), 7.10 (d, *J* = 7.9 Hz, 1 H), 7.01 (s, 1 H), 3.31 – 3.21 (m, 1 H), 2.34 (s, 3 H), 1.24 (d, *J* = 5.5 Hz, 3 H), 1.22 (d, *J* = 5.6 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.3 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.6, 137.8, 137.6, 128.2, 127.3, 123.0 (q, *J* = 333.3 Hz), 121.1, 26.6, 23.0 (d, *J* = 8.9 Hz), 20.8 ppm. **IR (KBr):** ν = 2966, 1620, 1506, 1460, 1194, 1126, 1078, 1056, 938, 873, 820, 772, 711, 619, 457 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{11}H_{13}F_3O_2S$ $[M+Na]^+$ calcd 289.0486, found 289.0478.

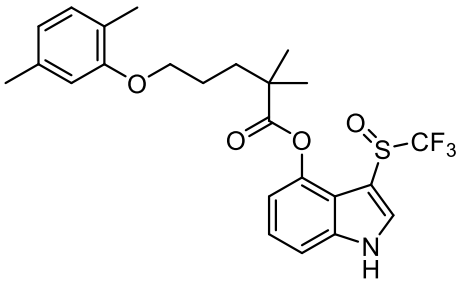
3.6 Late-stage trifluoromethylsulfinylation of bioactive molecules or natural products

General procedure I: trifluoromethylsulfinylation of bioactive electron-rich heteroarenes

Method A: A 25 mL Schlenk tube charged with heteroarene (0.5 mmol), *N*-trifluoromethylsulfinylphthalimide **6** (0.6 mmol, 1.2 equiv) and Me_3SiCl (0.75 mmol, 1.5 equiv) under argon atmosphere was added freshly distilled $CHCl_3$ (3.0 mL). The mixture was stirred at 80 °C for 16 h. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated heteroarene.

Method B: A 25 mL Schlenk tube charged with heteroarene (0.5 mmol), *N*-trifluoromethylsulfinylphthalimide **6** (0.6 mmol, 1.2 equiv) and NaCl (0.05 mmol, 10 mol%) was added freshly distilled DMF (3.0 mL). The reaction mixture was stirred at 80 °C for 16 h. After the reaction was completed, the mixture was extracted with distilled water (25.0 mL) and ethyl acetate (50.0 mL). The aqueous phase was extracted with ethyl acetate (3×15.0 mL). The combined organic extracts were washed with distilled water (50.0 mL) and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated heteroarene.

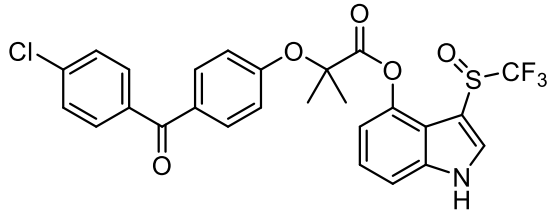
3-((Trifluoromethyl)sulfinyl)-1*H*-indol-4-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate 14aa



Yellow oil (137.1 mg, 57% on 0.5 mmol scale; 1.39 g, 58% on 5 mmol scale, Method B). Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.40).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.20 (s, 1 H), 7.64 (s, 1 H), 7.24 (s, 2 H), 7.08 (d, *J* = 7.3 Hz, 1 H), 6.96 (s, 1 H), 6.75 (d, *J* = 10.3 Hz, 2 H), 4.09 (s, 2 H), 2.39 (s, 3 H), 2.27 (s, 3 H), 2.04 (s, 4 H), 1.55

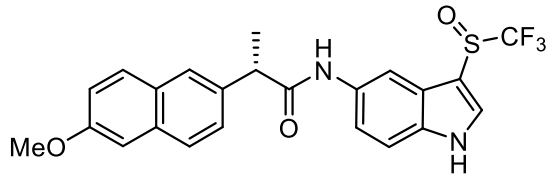
(s, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 177.5, 157.0, 143.2, 138.6, 136.6, 130.5, 130.3, 125.1 (q, *J* = 333.3 Hz), 124.2, 123.7, 121.0, 118.4, 115.1, 112.2, 110.7, 106.6, 67.9, 42.7, 37.4, 25.2, 25.0, 24.9, 21.4, 15.8 ppm. **IR (KBr):** ν = 3198, 1750, 1387, 1307, 1184, 1139, 1054, 713 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{24}H_{26}F_3NO_4S$ $[M+Na]^+$ calcd 504.1432, found 504.1418.

3-((Trifluoromethyl)sulfinyl)-1*H*-indol-4-yl 2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoate 14ab



Yellow solid (118.0 mg, 43% on 0.5 mmol scale; 1.15 g, 42% on 5 mmol scale, Method B). Mp: 52-53 °C. Eluent: petroleum ether/ethyl acetate (2:1, R_f = 0.37). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.82 (s, 1 H), 7.80 (d, *J* = 8.5 Hz, 2 H), 7.77 (d, *J* = 3.1 Hz, 1 H), 7.69 (d, *J* = 8.2 Hz, 2 H), 7.40 (d, *J* = 8.2 Hz, 2 H), 7.25 (t, *J* = 4.2 Hz, 1 H), 7.18 (t, *J* = 8.0 Hz, 1 H), 7.11 (d, *J* = 8.6 Hz, 2 H), 7.00 (d, *J* = 7.7 Hz, 1 H), 1.91 (s, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.1, 172.7, 159.7, 142.8, 138.9 (d, *J* = 12.8 Hz), 136.2, 132.3 (d, *J* = 24.6 Hz), 131.4 (d, *J* = 9.2 Hz), 130.9, 130.8 (d, *J* = 9.9 Hz), 128.7 (d, *J* = 21.8 Hz), 125.1 (q, *J* = 333.3 Hz), 124.2 (d, *J* = 30.9 Hz), 118.4 (d, *J* = 35.6 Hz), 117.9, 114.5 (d, *J* = 25.5 Hz), 111.2 (d, *J* = 31.6 Hz), 106.6, 80.1, 26.02 (d, *J* = 16.8 Hz), 25.76, 25.55 (d, *J* = 6.9 Hz), 25.35, 25.09 (d, *J* = 16.7 Hz) ppm. **IR (KBr):** ν = 2924, 1759, 1654, 1598, 1254, 1172, 1113, 928, 764 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{24}H_{26}F_3NO_4S$ $[M+Na]^+$ calcd 572.0522, found 572.0504.

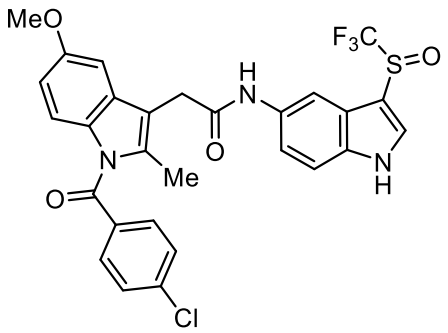
(2S)-2-(6-Methoxynaphthalen-2-yl)-*N*-(3-((trifluoromethyl)sulfinyl)-1*H*-indol-5-yl)propenamide 14ac



Yellow solid (193.2 mg, 84% on 0.5 mmol scale; 1.88 g, 82% on 5 mmol scale, Method

A). Mp: 130-131 °C. Eluent: petroleum ether/ethyl acetate (1:1, R_f = 0.19). **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.39 (s, 1 H), 10.20 (s, 1 H), 8.28 (s, 1 H), 8.22 (d, *J* = 15.2 Hz, 1 H), 7.83 – 7.73 (m, 3 H), 7.60 (t, *J* = 10.2 Hz, 1 H), 7.54 (d, *J* = 8.7 Hz, 1 H), 7.49 (d, *J* = 8.8 Hz, 1 H), 7.24 (s, 1 H), 7.12 (d, *J* = 8.1 Hz, 1 H), 3.98 (d, *J* = 6.9 Hz, 1 H), 3.81 (s, 3 H), 1.50 (d, *J* = 7.0 Hz, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.6 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 172.7, 157.6, 137.7 (d, *J* = 4.8 Hz), 134.8, 134.7, 134.0, 133.8, 129.7, 128.9, 127.3, 126.9, 126.4 (q, *J* = 333.3 Hz), 126.0, 124.4, 119.2, 117.5, 113.5, 110.4, 106.6, 106.2, 55.6, 46.4, 19.3 (d, *J* = 9.4 Hz) ppm. **IR (KBr):** ν = 2924, 1662, 1605, 1555, 1482, 1417, 1264, 1175, 1133, 1051, 853, 809, 749, 475 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{23}H_{19}F_3N_2O_3S$ $[M+Na]^+$ calcd 483.0966, found 483.0947.

2-(1-(4-Chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(3-((trifluoromethyl)sulfinyl)-1*H*-indol-5-yl)acetamide 14ad

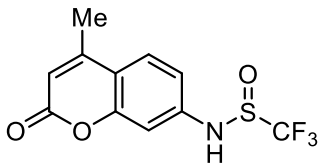


Yellow solid (228.9 mg, 78% on 0.5 mmol scale; 1.23 g, 70% on 3 mmol scale, Method A). Mp: 127-128 °C. Eluent: petroleum ether/ethyl acetate (1:1, R_f = 0.14). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.86 (s, 1 H), 8.70 (s, 1 H), 7.97 (s, 1 H), 7.44 (d, *J* = 8.1 Hz, 2 H), 7.32 (d, *J* = 7.6 Hz, 3 H), 7.23 (s, 1 H), 7.02 (s, 1 H), 6.98 (d, *J* = 10.5 Hz, 1 H), 6.84 (d, *J* = 8.9 Hz, 1 H), 6.64 (d, *J* = 9.1 Hz, 1 H), 3.76 (s, 2 H), 3.70 (s, 3 H), 2.29 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -72.4 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 168.4, 156.3, 139.3, 136.5, 134.5, 133.6, 132.7, 132.3, 131.0, 130.7, 129.1, 125.6 (q, *J* = 333.3 Hz), 124.1, 119.1, 113.0, 112.7, 111.8, 106.7, 101.4, 55.6, 32.6, 13.3 ppm. **IR (KBr):** ν = 2923, 1668, 1590, 1556, 1478, 1358, 1321, 1223, 1178, 1132, 1066, 807, 737, 477 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{28}H_{21}ClF_3N_3O_4S$ $[M+Na]^+$ calcd 610.0791, found 610.0778.

General procedure II: trifluoromethylsulfinylation of bioactive amines

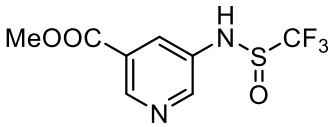
A 25 mL Schlenk tube charged with *N*-trifluoromethylsulfinylphthalimide **6** (0.75 mmol) and $Ph_2P(O)Cl$ (0.75 mmol) was added freshly distilled THF (3.0 mL). The mixture was stirred at RT for 10 h, then bioactive amine (0.5 mmol) was added to the mixture. The reaction was stirred at RT for another 3 h. After the reaction was completed, the mixture was extracted with distilled water and ethyl acetate. Then the organic phase was combinated and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated amine.

1,1,1-Trifluoro-*N*-(4-methyl-2-oxo-2*H*-chromen-7-yl)methanesulfinamide 14ae



Yellow solid (69.9 mg, 48%). Mp: 164-165 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.30).**^{1}H NMR** (400 MHz, DMSO-d6) δ 7.66 (d, *J* = 8.6 Hz, 1 H), 7.11 (d, *J* = 8.5 Hz, 1 H), 7.07 (s, 1 H), 6.20 (s, 1 H), 3.46 (s, 1 H), 2.34 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 160.4, 154.6, 153.7, 145.3, 127.3, 124.6 (q, *J* = 333.3 Hz), 115.3, 114.9, 112.5, 105.2, 18.5 ppm. **IR (KBr):** ν = 2922, 1716, 1616, 1463, 1391, 1261, 1190, 1145, 1111, 855, 763 cm^{-1}. **HRMS (ESI):** m/z for $C_{11}H_8F_3NO_3S$ $[M+Na]^+$ calcd 314.0075, found 314.0076.

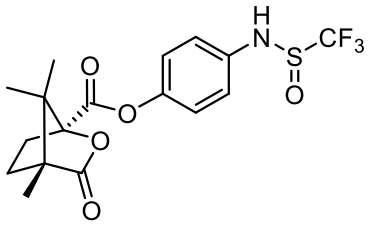
Methyl 5-(((trifluoromethyl)sulfinyl)amino)nicotinate 14af



White solid (63.0 mg, 47%). Mp: 115-116 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.25). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.96 (s, 1 H), 8.75 (s, 1 H), 8.61 (s, 1 H), 8.09 (s, 1 H), 3.95 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.0 (s, 3 F); **^{13}C NMR** (100 MHz, DMSO-d6) δ 165.1, 145.3, 144.6, 136.8, 126.8, 126.6, 124.4 (q, *J* = 333.3 Hz), 53.1 ppm. **IR (KBr):** ν = 2925, 1730, 1597, 1441, 1300, 1186, 1154,1110, 1000,

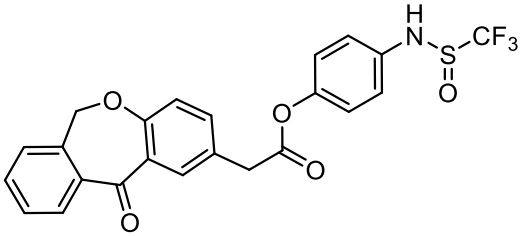
767, 699, 466 cm^{-1}. **HRMS (ESI):** m/z for $C_8H_7F_3N_2O_3S$ $[M+Na]^+$ calcd 291.0027, found 291.0027.

4-(((Trifluoromethyl)sulfinyl)amino)phenyl (1S,4R)-4,7,7-trimethyl-3-*oxo*-2-oxabicyclo[2.2.1]heptane-1-carboxylate 14ag



White solid (155.9 mg, 77%). Mp: 87-88 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.33). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 (s, 1 H), 7.12 (d, *J* = 8.5 Hz, 2 H), 7.06 (d, *J* = 8.9 Hz, 2 H), 2.59 – 2.47 (m, 1 H), 2.20 – 2.12 (m, 1 H), 2.08 – 1.92 (m, 1 H), 1.78 – 1.69 (m, 1 H), 1.14 (s, 3 H), 1.11 (s, 3 H), 1.05 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.2, 166.3, 147.1, 136.6, 123.7 (q, *J* = 333.3 Hz), 122.7, 121.7, 91.0, 55.0, 54.9, 30.8, 29.0, 16.9, 9.8 ppm. **IR (KBr):** ν = 3218, 2966, 1772, 1505, 1263, 1194, 1103, 1047, 899, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{17}H_{18}F_3NO_5S$ $[M+Na]^+$ calcd 428.0755, found 428.0739.

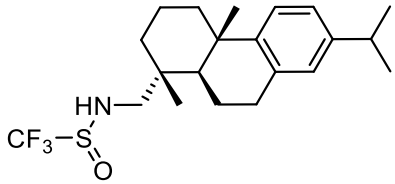
4-(((Trifluoromethyl)sulfinyl)amino)phenyl 2-(11-oxo-6,11-dihydrodibenzo[*b,e*]oxepin-2-yl)acetate 14ah



White solid (192.4 mg, 81%). Mp: 123-124 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.45). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.20 (s, 1 H), 7.87 (d, *J* = 7.7 Hz, 1 H), 7.54 (t, *J* = 7.4 Hz, 1 H), 7.46 (q, *J* = 8.2, 7.4 Hz, 2 H), 7.34 (d, *J* = 7.3 Hz, 1 H), 7.19 (s, 1 H), 7.06 (s, 1 H), 7.04 – 7.01 (m, 3 H), 7.00 (s, 1 H), 5.17 (s, 2 H), 3.86 (s, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.1, 170.2, 160.8, 148.0, 140.4, 136.5, 136.0, 135.6, 133.0, 132.7, 129.6, 129.4, 128.0, 127.1, 125.3, 123.7 (q, *J* = 333.3 Hz), 122.9, 121.7, 121.4, 73.7, 40.2 ppm. **IR (KBr):** ν =

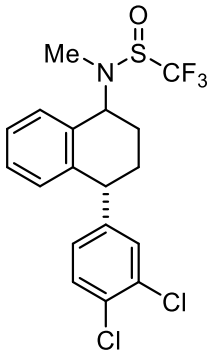
2922, 1754, 1646, 1611, 1505, 1456, 1414, 1378, 1301, 1194, 1153, 1118, 1015, 906, 830, 762, 641 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{23}H_{16}F_3NO_5S$ $[M+Na]^+$ calcd 498.0599, found 498.0593.

(S)-1,1,1-trifluoro-*N*-(((1R,4aS,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)methanesulfinamide 14ai



Colourless oil (152.4 mg, 76%, dr = 3:2). Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.95). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 7.21 (dd, *J* = 8.2, 2.0 Hz, 1 H), 7.04 (d, *J* = 8.2 Hz, 1 H), 6.94 (s, 1 H), 4.92 (s, 1 H), 3.22 – 3.13 (m, 1 H), 3.09 – 3.04 (m, 1 H), 2.98 – 2.91 (m, 2 H), 2.90 – 2.84 (m, 1 H), 2.35 (d, *J* = 13.9 Hz, 1 H), 1.85 – 1.73 (m, 5 H), 1.58 – 1.50 (m, 2 H), 1.48 – 1.42 (m, 3 H), 1.28 (d, *J* = 6.7 Hz, 6 H), 1.00 (d, *J* = 6.8 Hz, 3 H), 0.94 – 0.90 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.10 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.0 (d, *J* = 7.5 Hz), 145.8 (d, *J* = 4.0 Hz), 134.6 (d, *J* = 6.3 Hz), 127.0, 124.3 (d, *J* = 6.1 Hz), 124.1 (d, *J* = 6.5 Hz), 123.8 (q, *J* = 333.3 Hz), 54.9 (d, *J* = 91.2 Hz), 45.2 (d, *J* = 63.1 Hz), 38.3 (d, *J* = 5.2 Hz), 37.6 (d, *J* = 2.9 Hz), 37.4 (d, *J* = 5.6 Hz), 35.6 (d, *J* = 41.2 Hz), 33.6, 30.0 (d, *J* = 11.4 Hz), 25.4 (d, *J* = 7.9 Hz), 24.1 (d, *J* = 2.8 Hz), 18.9 (d, *J* = 11.6 Hz), 18.6, 18.6 (d, *J* = 3.3 Hz), 18.2 ppm. **IR (KBr):** ν = 3232, 2958, 1459, 1186, 1154, 1096, 1059, 882, 749 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{21}H_{30}F_3NOS$ $[M+Na]^+$ calcd 424.1898, found 424.1885.

(S)-*N*-((4R)-4-(3,4-Dichlorophenyl)-1,2,3,4-tetrahydronaphthalen-1-yl)-1,1,1-trifluoro-*N*-methylmethanesulfinamide 14aj

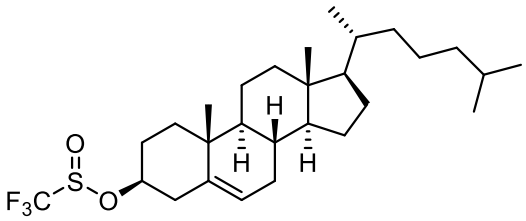


White solid (88.4 mg, 42%, dr = 9:1). Mp: 111-112 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.59). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 7.44 (d, *J* = 7.8 Hz, 1 H), 7.34 (d, *J* = 8.4 Hz, 1 H), 7.32 (dt, *J* = 7.7, 1.4 Hz, 1 H), 7.23 (t, *J* = 7.6 Hz, 1 H), 7.08 (d, *J* = 2.1 Hz, 1 H), 6.95 (d, *J* = 7.1 Hz, 1 H), 6.81 (dd, *J* = 8.3, 2.2 Hz, 1 H), 4.86 (dd, *J* = 9.4, 6.1 Hz, 1 H), 4.15 (t, *J* = 5.0 Hz, 1 H), 2.77 (d, *J* = 1.3 Hz, 3 H), 2.28 – 2.18 (m, 1 H), 2.04 – 1.91 (m, 2 H), 1.91 – 1.82 (m, 1 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.0 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.5, 139.0, 134.2, 132.5, 130.9, 130.7, 130.5, 130.4, 128.5, 128.3, 128.0, 128.0, 124.3 (q, *J* = 333.3 Hz), 43.3, 43.1, 29.6, 29.1, 23.3 ppm. **IR (KBr):** ν = 2924, 1487, 1466, 1275, 1260, 1185, 1155, 1095, 764, 750 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{18}H_{16}C_{l2}F_3NOS$ $[M+Na]^+$ calcd 444.0179, found 444.0159.

General procedure III: trifluoromethylsulfinylation of bioactive alcohols or phenols

A 25 mL Schlenk tube charged with bioactive alcohol or phenol (0.5 mmol) and *N*-trifluoromethylsulfinylphthalimide **6** (0.6 mmol, 1.2 equiv) was added freshly distilled THF (3.0 mL) and Et_3N (0.05 mmol for alcohol; 0.25 mmol for phenol). The mixture was stirred at RT-50 °C for 3 h. The solvent was removed under vacuum and the residue was purified by flask column chromatography to give trifluoromethylsulfinylated alcohol or phenol.

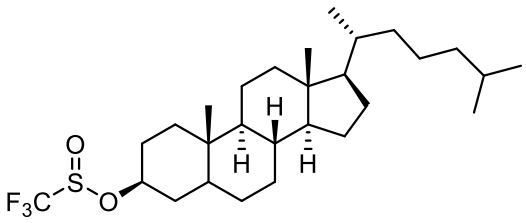
(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-yl trifluoromethanesulfinate 14ak



White solid (200.7 mg, 80%, RT, dr = 3:2). Mp: 144-145 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.15). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 5.40 (t, *J* = 5.0 Hz, 1 H), 4.41 – 4.29 (m, 1 H), 2.63 – 2.35 (m, 2 H), 2.09 – 1.74 (m, 6 H),

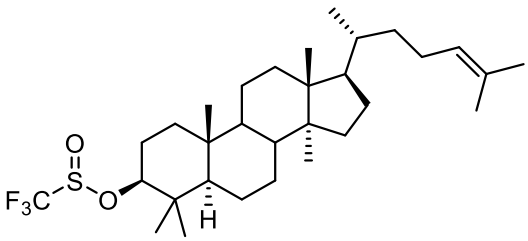
1.62 – 1.41 (m, 6 H), 1.38 – 1.22 (m, 4 H), 1.19 – 0.95 (m, 12 H), 0.90 (d, J = 6.6 Hz, 4 H), 0.85 (dd, J = 6.7, 1.9 Hz, 6 H), 0.66 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.9 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.6, 122.8 (q, J = 343.4 Hz), 124.0, 83.1, 56.5 (d, J = 49.0 Hz), 50.0, 42.4, 39.9, 39.7 (d, J = 13.4 Hz), 37.1 (d, J = 8.7 Hz), 36.4 (d, J = 22.1 Hz), 35.9, 31.9 (d, J = 10.0 Hz), 29.6 (d, J = 12.0 Hz), 28.2 (d, J = 20.8 Hz), 24.1 (d, J = 41.2 Hz), 22.8 (d, J = 26.0 Hz), 21.1, 19.0 (d, J = 48.8 Hz), 11.9 ppm. The spectroscopic data were matched with those reported in the literature.[17]

(3S,8R,9S,10S,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl trifluoromethanesulfinate 14al



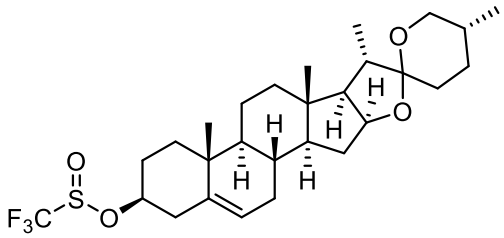
Colourless oil (229.4 mg, 91%, RT, dr = 1:1). Eluent: petroleum ether/ethyl acetate (20:1, R_f = 0.77). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 4.48 – 4.37 (m, 1 H), 1.95 (dt, J = 12.7, 3.4 Hz, 2 H), 1.82 – 1.63 (m, 4 H), 1.60 – 1.41 (m, 4 H), 1.38 – 1.19 (m, 9 H), 1.18 – 0.93 (m, 11 H), 0.88 (d, J = 6.5 Hz, 4 H), 0.84 (dd, J = 6.6, 1.8 Hz, 6 H), 0.82 (s, 3 H), 0.63 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.1 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 122.8 (q, J = 333.3 Hz), 83.0 (d, J = 9.8 Hz), 56.4 (d, J = 3.6 Hz), 54.2, 45.0 (d, J = 9.4 Hz), 42.6, 39.8 (d, J = 40.4 Hz), 36.9 (d, J = 8.7 Hz), 36.1 (d, J = 37.3 Hz), 35.7 (d, J = 12.7 Hz), 35.4 (d, J = 11.8 Hz), 32.0, 29.3 (d, J = 15.7 Hz), 28.4 (d, J = 23.2 Hz), 28.1, 24.1 (d, J = 26.0 Hz), 22.7 (d, J = 24.9 Hz), 21.3, 18.7, 12.2 (d, J = 11.9 Hz) ppm. **IR (KBr):** ν = 2931, 1467, 1374, 1193, 1128, 926, 810, 735, 613, 468 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{28}H_{47}F_3O_2S$ $[M+Na]^+$ calcd 527.3147, found 527.3136.

(3S,5R,10R,13R,14S,17R)-4,4,10,13,14-Pentamethyl-17-((R)-6-methylhept-5-en-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl trifluoromethanesulfinate 14am



White solid (182.2 mg, 67%, RT, dr = 4:3). Mp: 107-108 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.91). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 5.08 (t, *J* = 7.0 Hz, 1 H), 3.21 (dd, *J* = 11.5, 4.6 Hz, 1 H), 2.08 – 1.94 (m, 6 H), 1.74 – 1.39 (m, 19 H), 0.98 (s, 4 H), 0.96 (s, 3 H), 0.91 – 0.83 (m, 11 H), 0.79 (s, 3 H), 0.67 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.0 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.0 (d, *J* = 10.1 Hz), 133.8 (d, *J* = 10.7 Hz), 130.8, 125.3, 122.8 (dq, *J* = 333.3, 11.1 Hz), 92.2 (d, *J* = 84.9 Hz), 50.8 (d, *J* = 12.8 Hz), 50.5 (d, *J* = 14.3 Hz), 49.8, 44.5, 39.6, 39.0 (d, *J* = 19.3 Hz), 36.8, 36.6 (d, *J* = 4.6 Hz), 36.4 (d, *J* = 8.6 Hz), 35.4 (d, *J* = 9.6 Hz), 30.9 (d, *J* = 12.6 Hz), 28.2 (d, *J* = 20.3 Hz), 27.7 (d, *J* = 22.6 Hz), 26.6 (d, *J* = 40.8 Hz), 25.9 (d, *J* = 27.9 Hz), 25.0, 24.3 (d, *J* = 4.6 Hz), 22.7 (d, *J* = 28.0 Hz), 21.1, 19.1, 18.7 (d, *J* = 8.1 Hz), 18.3 (d, *J* = 6.1 Hz), 17.6, 15.9 (d, *J* = 9.4 Hz), 15.8 ppm. **IR (KBr):** ν = 2946, 1454, 1371, 1193, 1129, 955, 918, 865, 816, 739, 599, 460 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{31}H_{51}F_3O_2S$ $[M+Na]^+$ calcd 567.3460, found 567.3453.

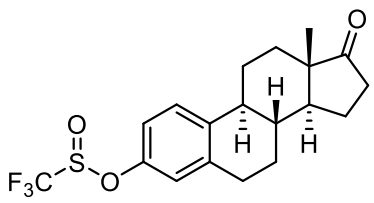
(4S,5'R,6aR,6bS,8aS,8bR,9S,11aS,12aS,12bS)-5',6a,8a,9-Tetramethyl-1,3,3',4,4',5,5',6,6a,6b,6',7,8,8a,8b,9,11a,12,12a,12b-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-*b*]furan-10,2'-pyran]-4-yl trifluoromethanesulfinate 14an



White solid (225.2 mg, 85%, RT, dr = 1:1). Mp: 136-137 °C. Eluent: petroleum ether/ethyl acetate (3:1, R_f = 0.92). **^{1}H NMR** (400 MHz, $CDCl_3$) of two isomers δ 5.35 (s, 1 H), 4.32 (q, *J* = 9.1, 7.9 Hz, 2 H), 3.38 (d, *J* = 11.2 Hz, 1 H), 3.28 (t, *J* = 9.1 Hz, 1 H), 2.70 – 2.21 (m, 2 H), 1.99 – 1.65 (m, 8 H), 1.61 – 1.34 (m, 9 H), 1.26 – 1.01 (m, 4

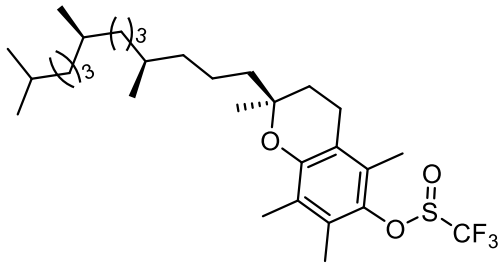
H), 0.97 (d, J = 3.6 Hz, 3 H), 0.89 (dd, J = 7.1, 3.6 Hz, 4 H), 0.71 (d, J = 4.0 Hz, 6 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.0 (d, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.6 (d, J = 3.8 Hz), 123.6, 122.7 (q, J = 333.3 Hz), 109.2, 82.8 (d, J = 6.5 Hz), 80.7, 66.8, 62.2, 56.4, 49.9, 41.6, 40.2, 39.8, 39.7, 37.0 (d, J = 8.6 Hz), 36.6, 31.9 (d, J = 19.0 Hz), 31.4 (d, J = 4.5 Hz), 30.3, 29.5 (d, J = 10.5 Hz), 28.8, 20.8, 19.2, 17.1, 16.3, 14.6 ppm. **IR (KBr):** ν = 2948, 1454, 1377, 1196, 1131, 1052, 980, 899, 800, 746 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{28}H_{41}F_3O_4S$ $[M+Na]^+$ calcd 553.2575, found 553.2570.

(8R,9S,13S,14S)-13-Methyl-17-*oxo*-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl trifluoromethanesulfinate 14ao



White solid (133.4 mg, 69%, 50 ºC). Mp: 120-121 °C. Eluent: petroleum ether/ethyl acetate (5:1, R_f = 0.52). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, J = 8.6 Hz, 1 H), 6.93 (d, J = 8.4 Hz, 1 H), 6.90 (s, 1 H), 2.88 (dd, J = 9.1, 4.3 Hz, 2 H), 2.46 (dd, J = 18.5, 8.7 Hz, 1 H), 2.36 (d, J = 12.6 Hz, 1 H), 2.28 – 2.19 (m, 1 H), 2.11 (q, J = 9.8, 9.3 Hz, 1 H), 2.06 – 1.96 (m, 2 H), 1.93 (d, J = 9.4 Hz, 1 H), 1.63 – 1.53 (m, 2 H), 1.53 – 1.37 (m, 4 H), 0.87 (s, 3 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -79.2 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 220.5, 149.9, 139.4, 139.1, 127.4, 122.8 (q, J = 343.4 Hz), 120.8, 117.9, 50.4, 47.9, 44.1, 37.9, 35.8, 31.6, 29.4, 26.2, 25.8, 21.6, 13.8 ppm. **IR (KBr):** ν = 2931, 1735, 1490, 1264, 1194, 1125, 1052, 928, 912, 880, 853, 796, 734, 473 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{19}H_{21}F_3O_3S$ $[M+Na]^+$ calcd 409.1061, found 409.1048.

(S)-2,5,7,8-Tetramethyl-2-((4R,6R)-4,6,8-trimethylnonyl)chroman-6-ol 14ap



Yellow oil (161.3 mg, 59%, RT). Eluent: petroleum ether/ethyl acetate (10:1, R_f = 0.92).

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.61 (t, *J* = 7.0 Hz, 2 H), 2.21 (s, 3 H), 2.18 (s, 3 H), 2.13 (s, 3 H), 1.89 – 1.74 (m, 2 H), 1.61 – 1.49 (m, 3 H), 1.46 – 1.35 (m, 4 H), 1.34 – 1.22 (m, 12 H), 1.20 – 1.04 (m, 7 H), 0.89 (d, *J* = 6.6 Hz, 11 H), 0.86 (s, 2 H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.7 (s, 3 F); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.5, 141.3, 128.4, 127.0, 124.1, 123.2 (q, *J* = 333.3 Hz), 118.3, 75.5, 40.0 (dd, *J* = 17.9, 8.0 Hz), 39.5, 37.6, 37.5, 37.4 (d, *J* = 3.6 Hz), 32.9 (d, *J* = 2.3 Hz), 32.8, 31.1 (d, *J* = 5.8 Hz), 28.1, 24.8 (d, *J* = 38.8 Hz), 23.9 (d, *J* = 12.9 Hz), 22.8 (d, *J* = 9.7 Hz), 21.0 (d, *J* = 29.7 Hz), 19.8 (d, *J* = 6.8 Hz), 19.7, 19.7 (d, *J* = 2.5 Hz), 13.8, 12.9, 12.0 ppm. **IR (KBr):** ν = 2925, 2867, 1460, 1407, 1378, 1244, 1196, 1130, 1107, 1053, 912, 855, 756, 726, 651, 452 cm^{-1}. **HRMS (ESI):** *m/z* for $C_{30}H_{49}F_3O_3S$ $[M+Na]^+$ calcd 569.3252, found 569.3236.

4. References

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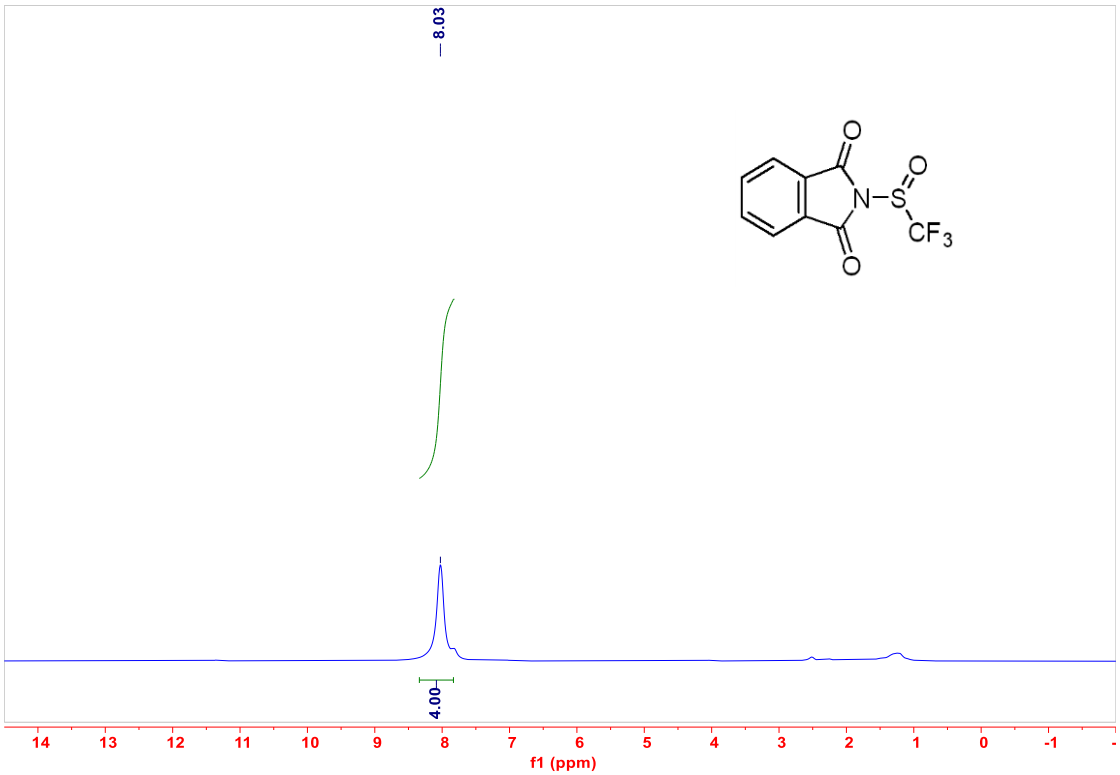
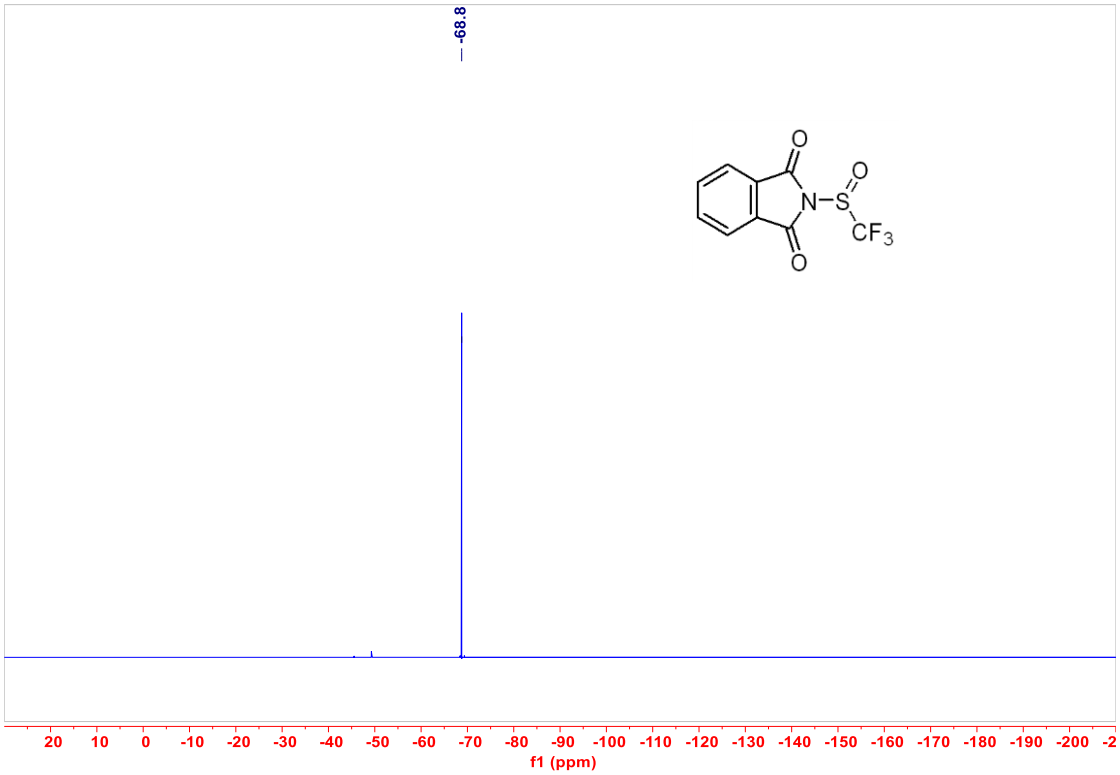
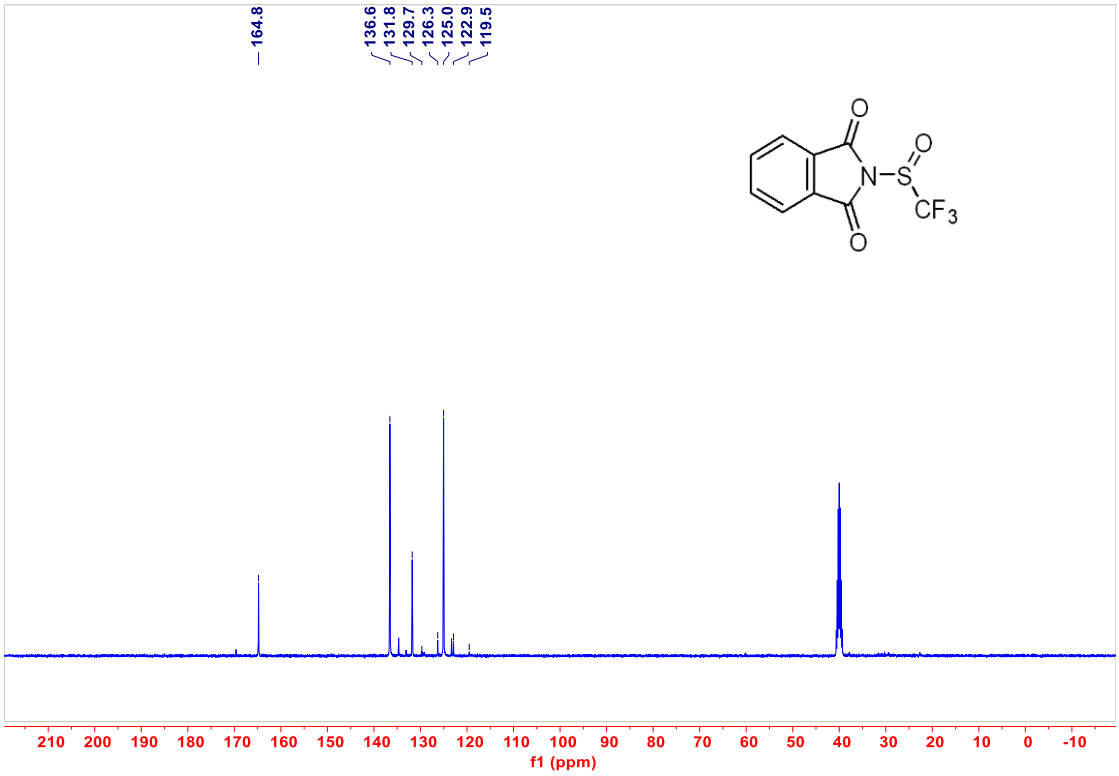
5. NMR spectra



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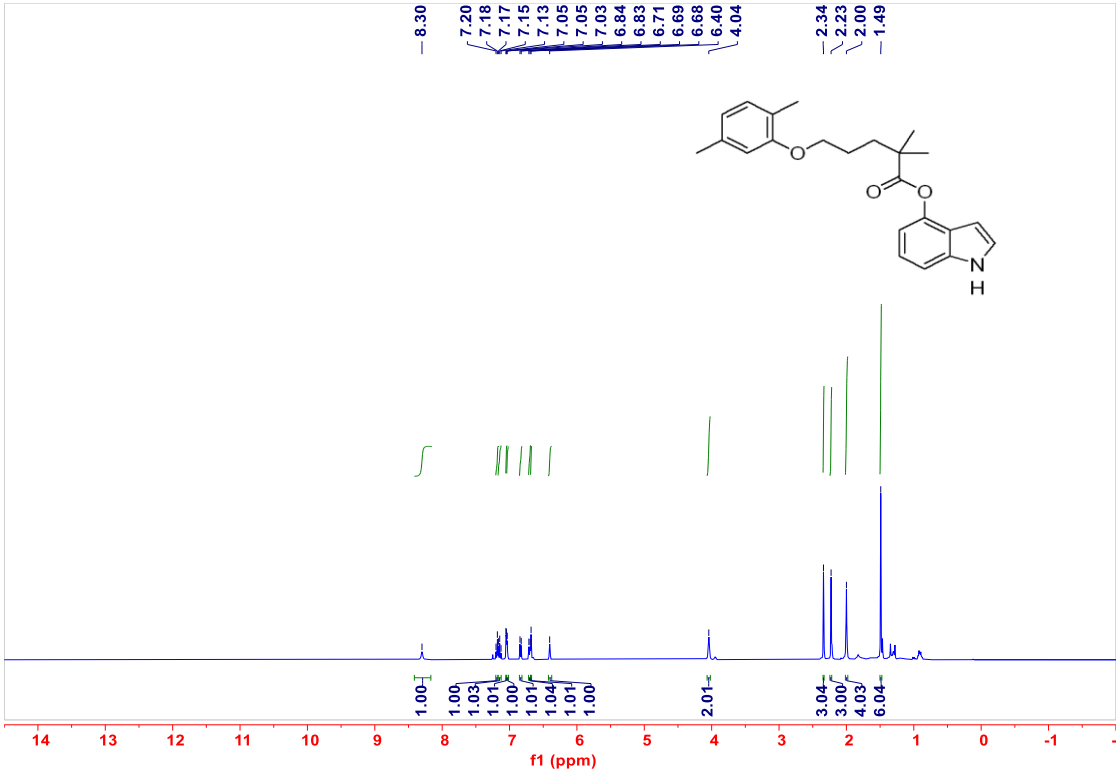
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6.69
6.68
6.40
4.04
2.34
2.23
2.00
1.49
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O
O
N
H
1.00
1.00
1.03
1.01
1.00
1.01
1.04
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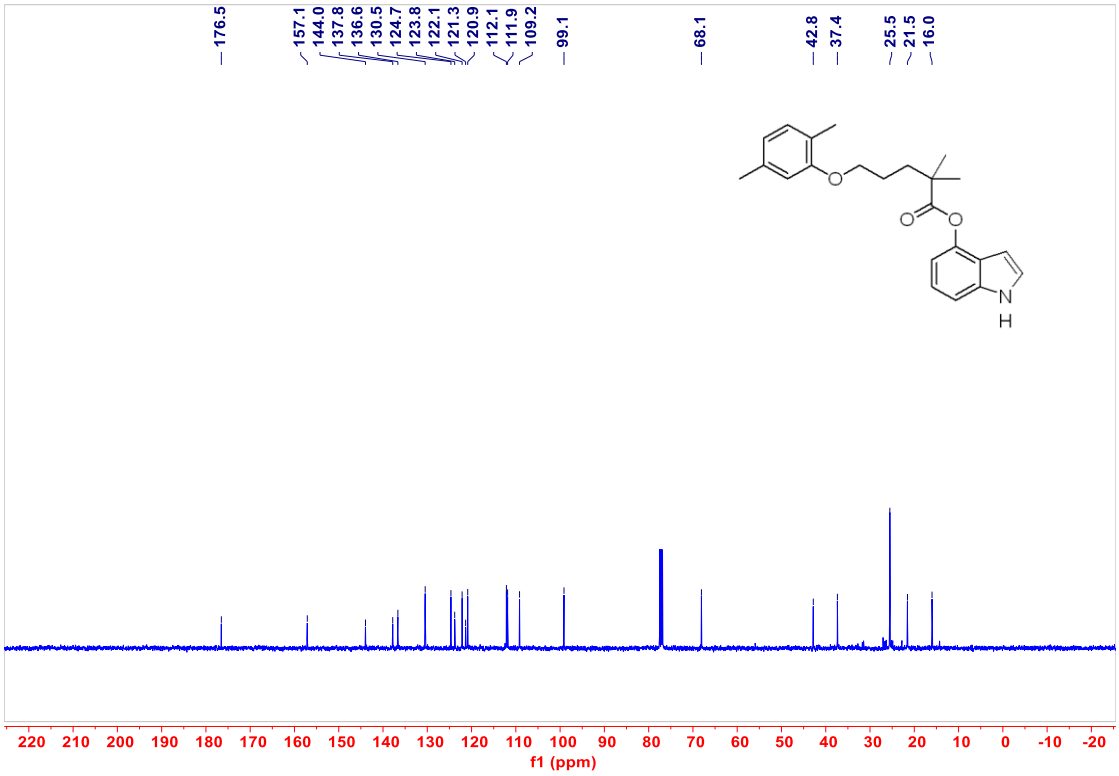
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37.4
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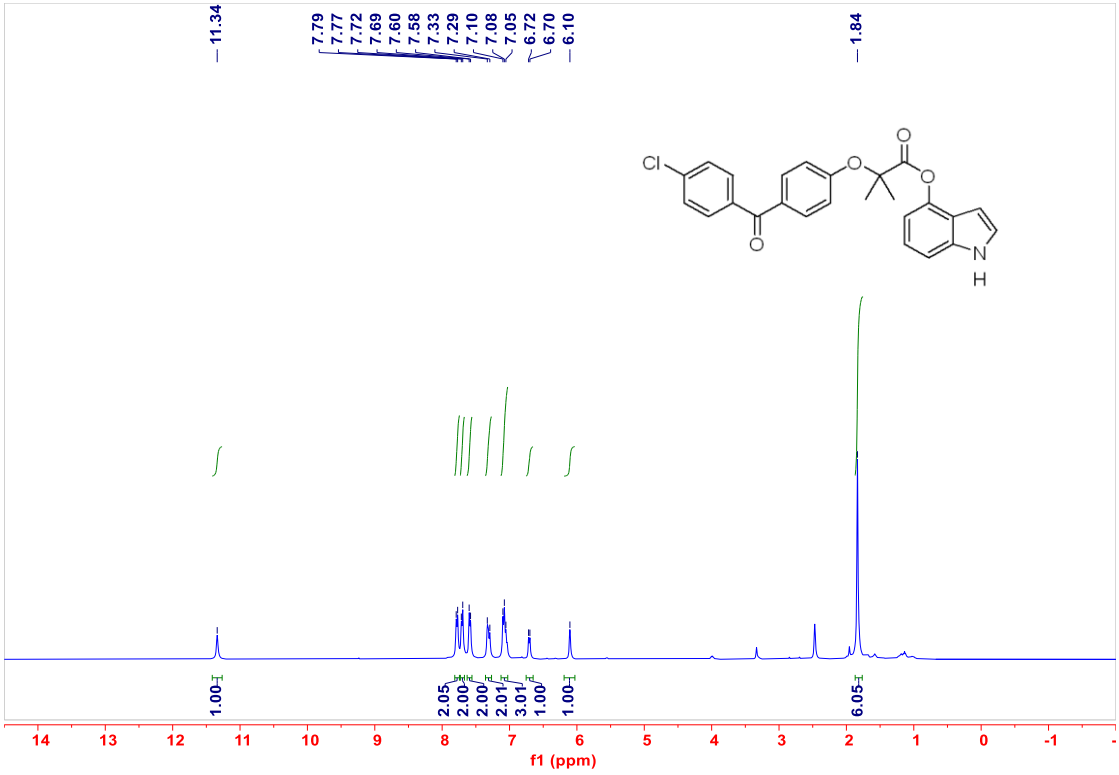
f1 (ppm)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6.10
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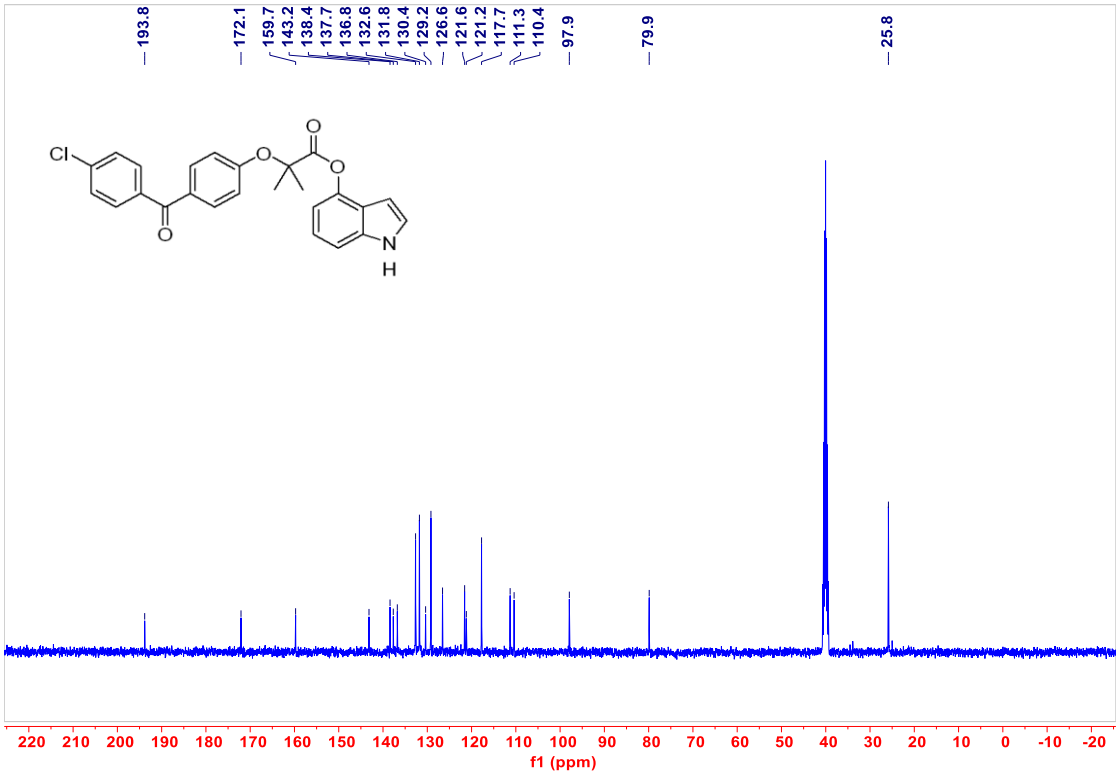
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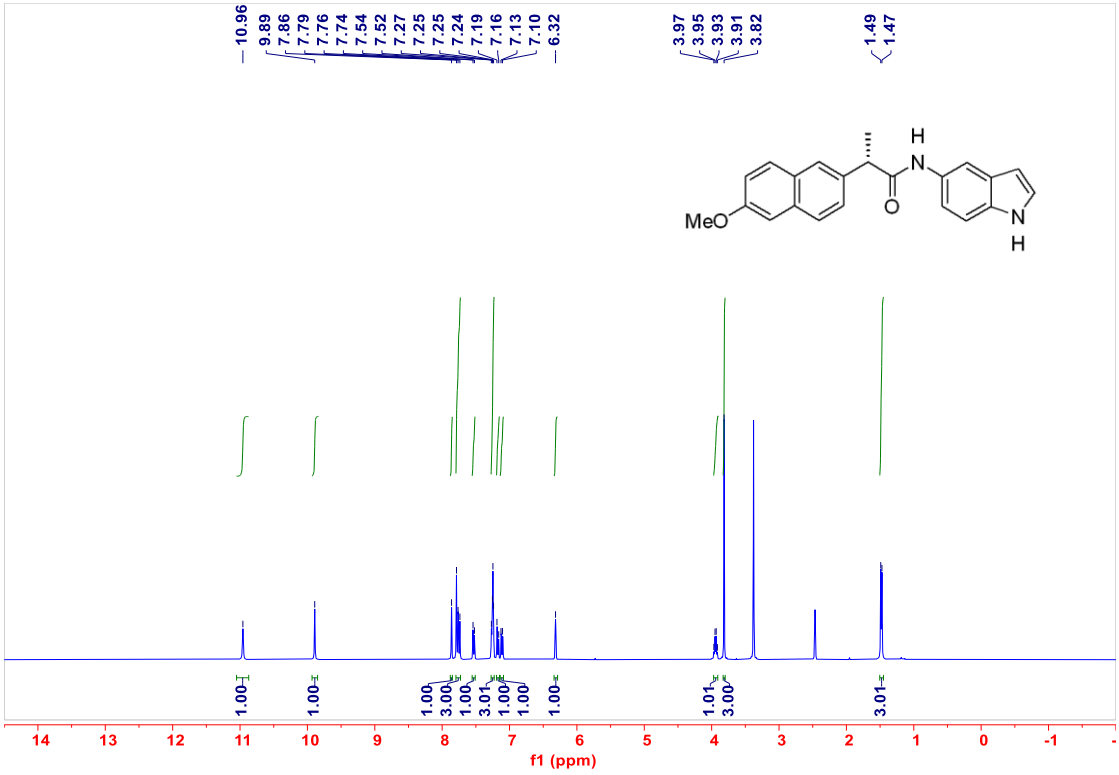
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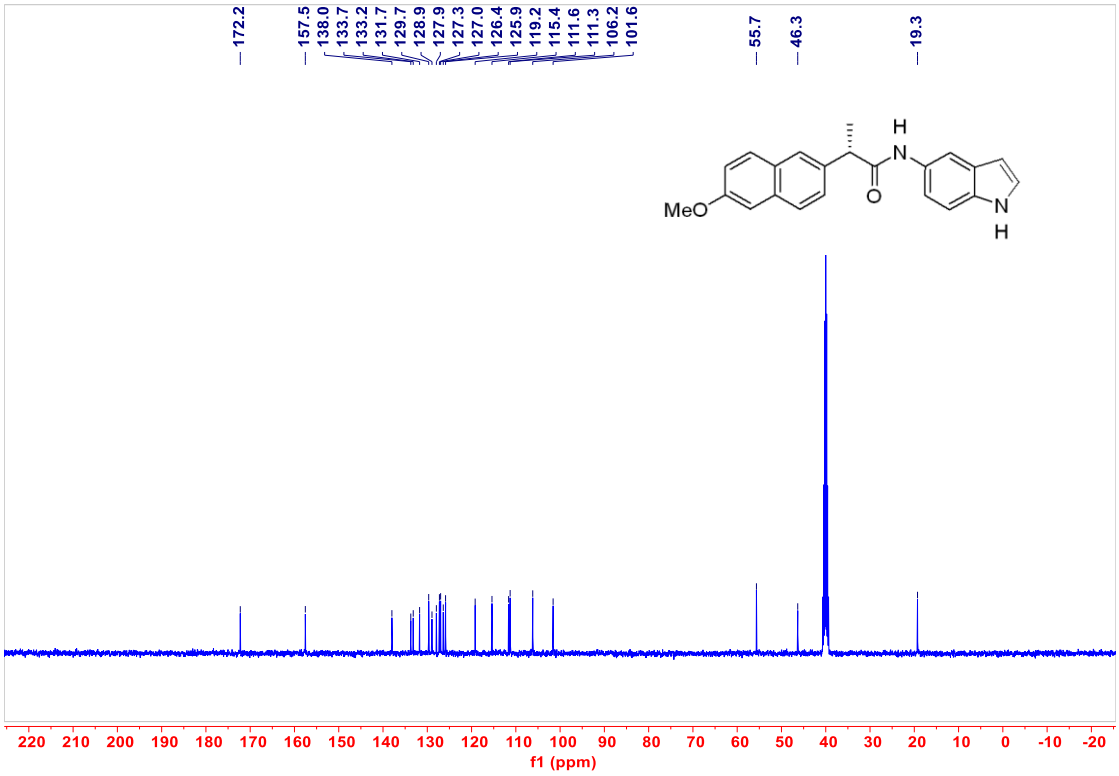
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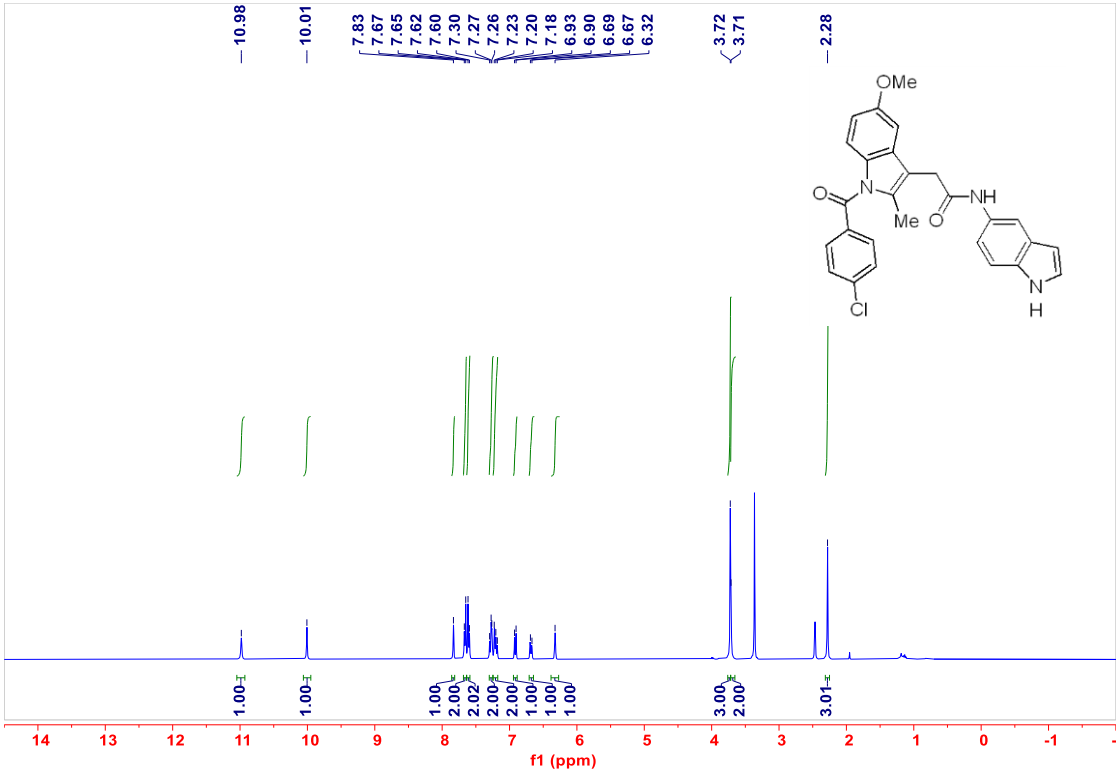
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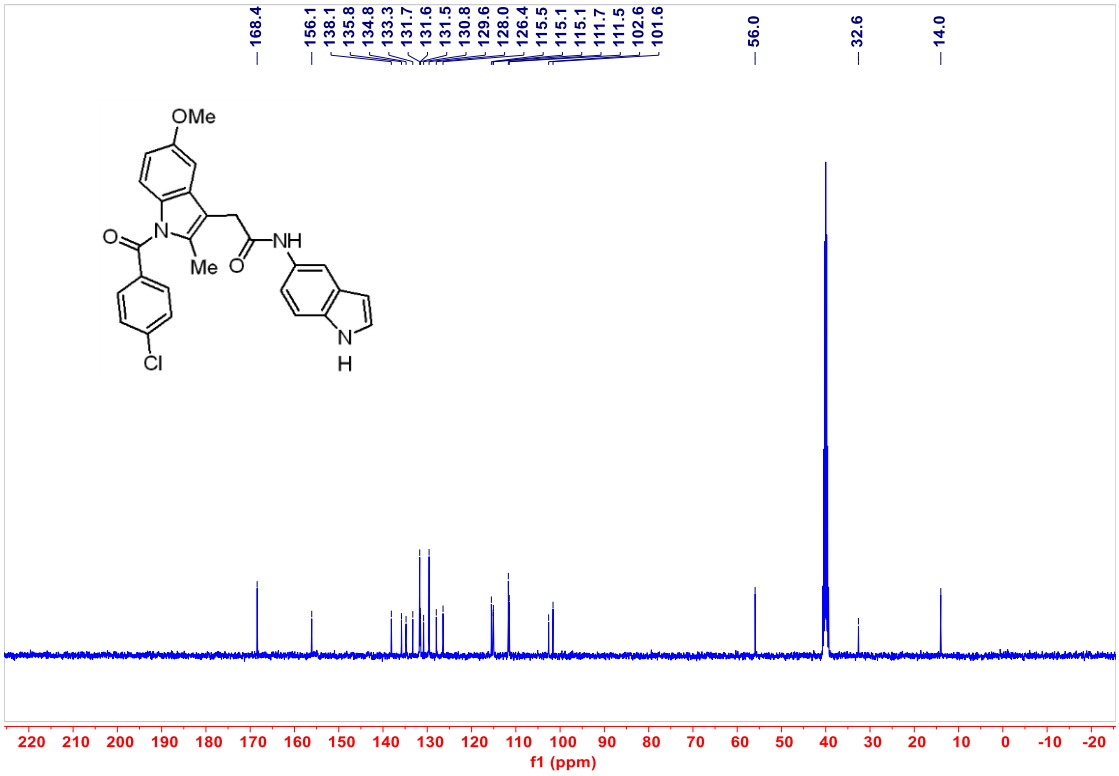
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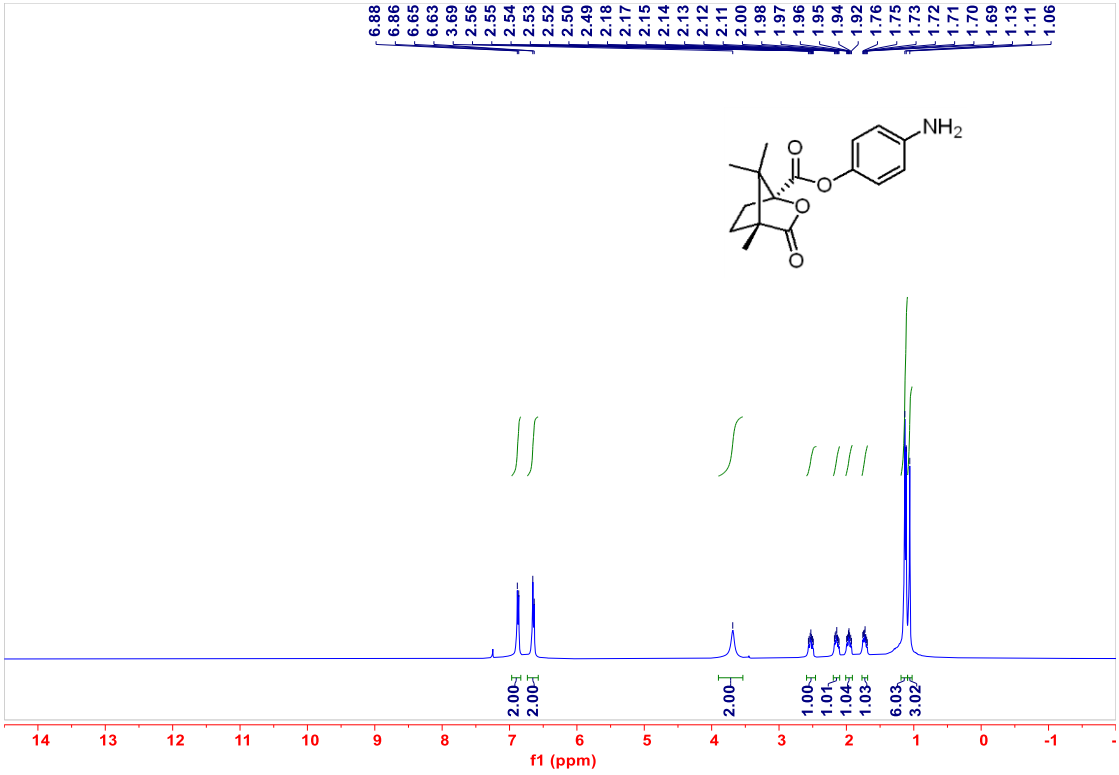
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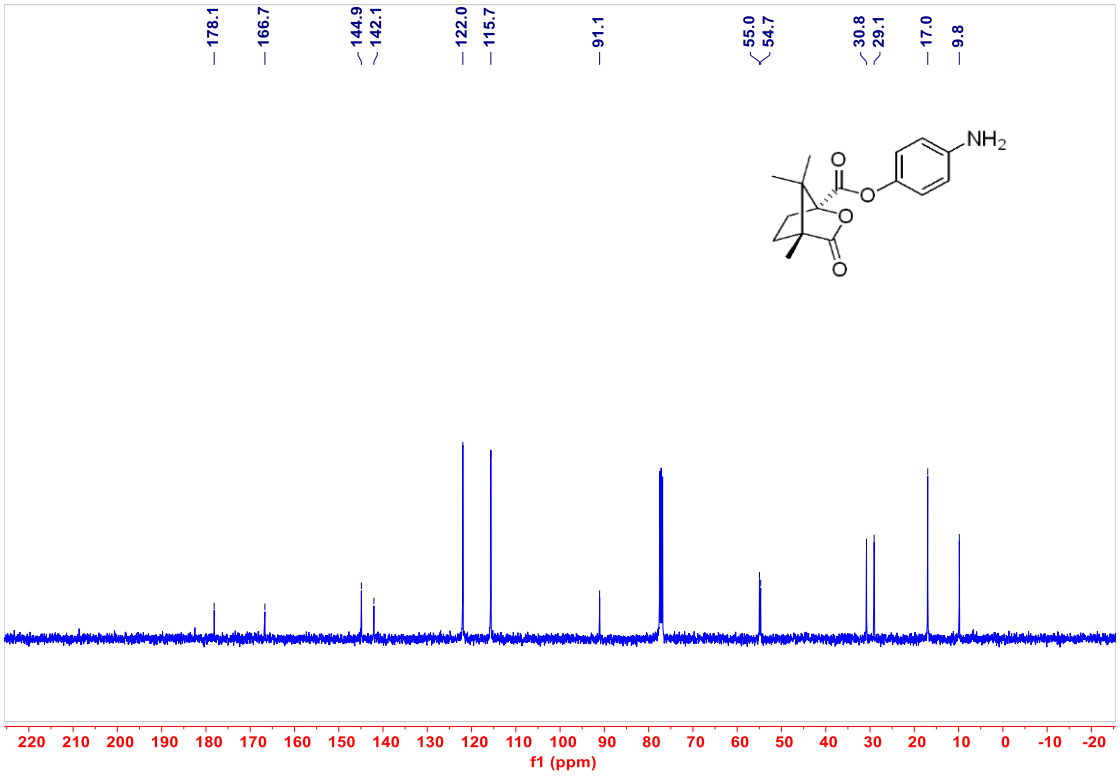
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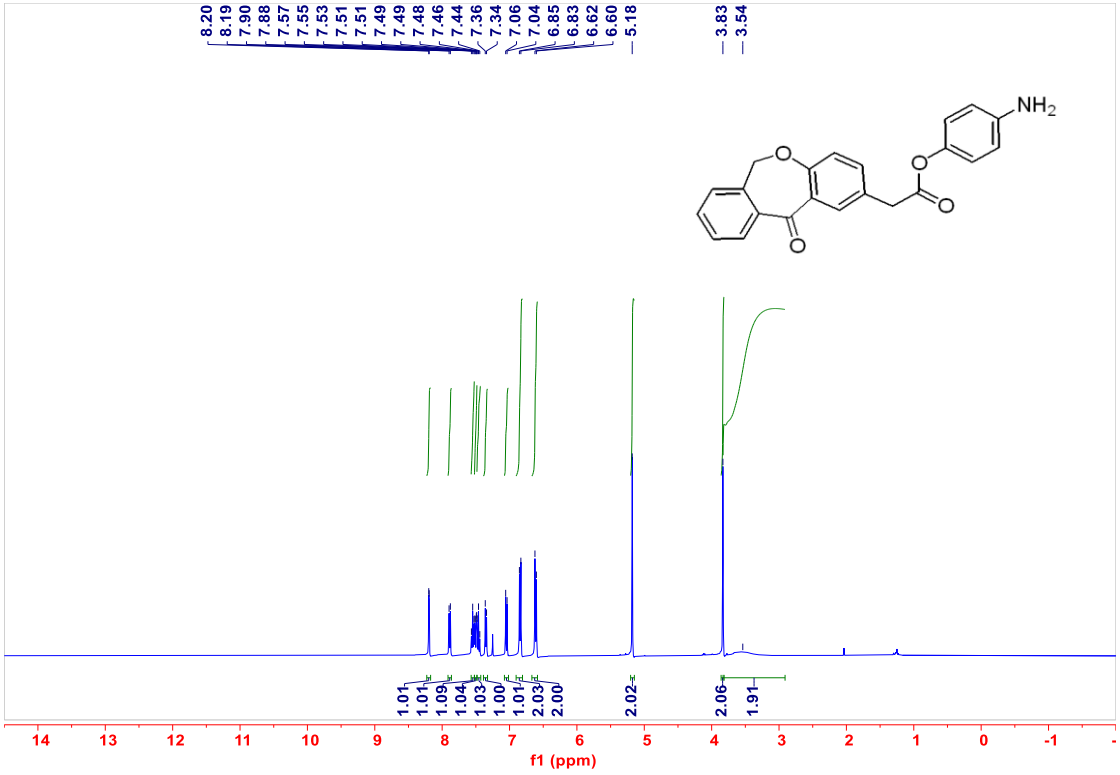
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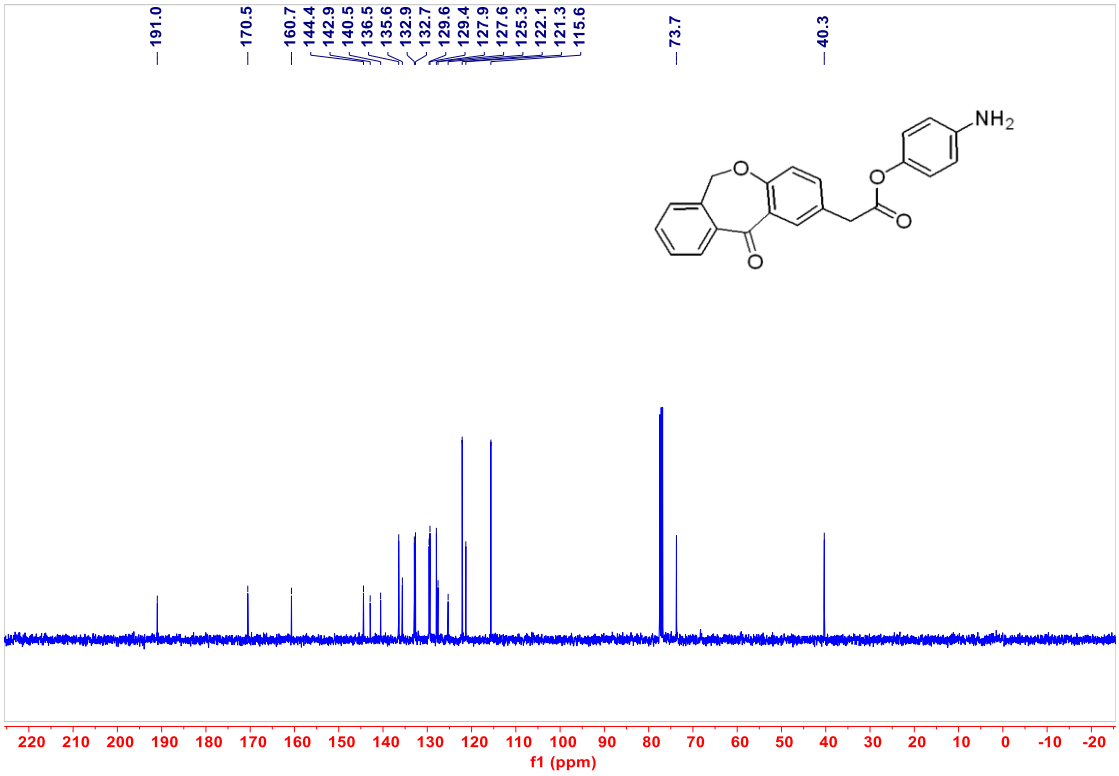
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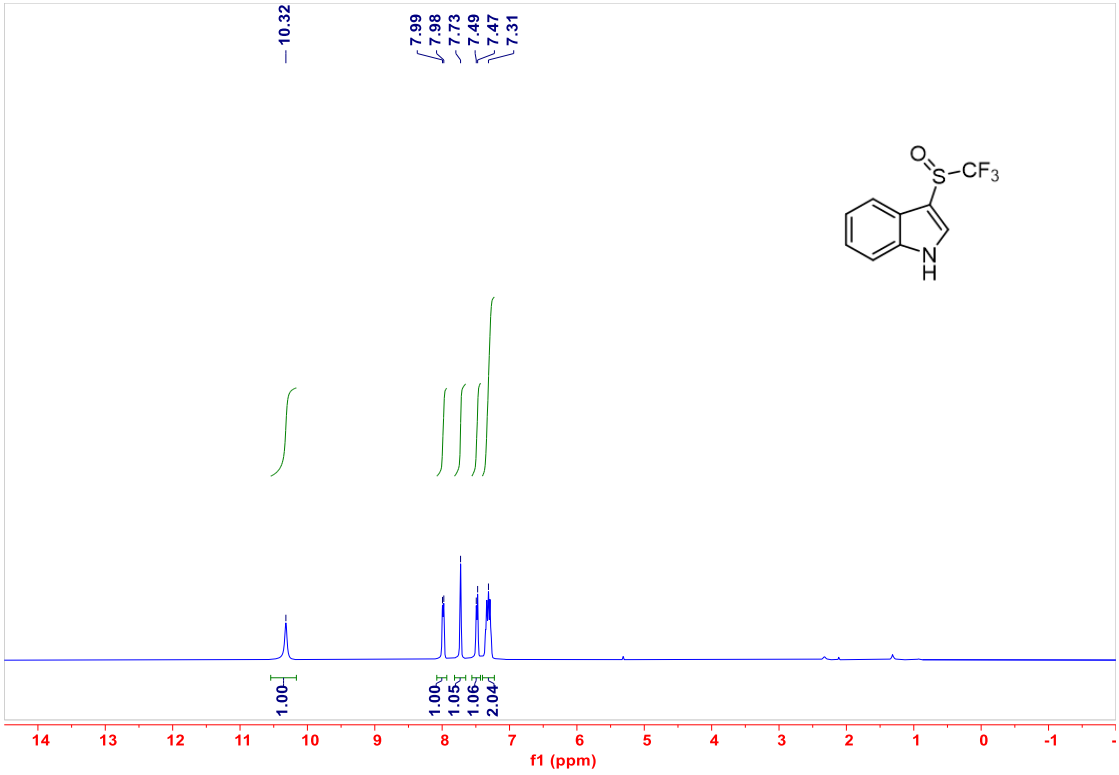
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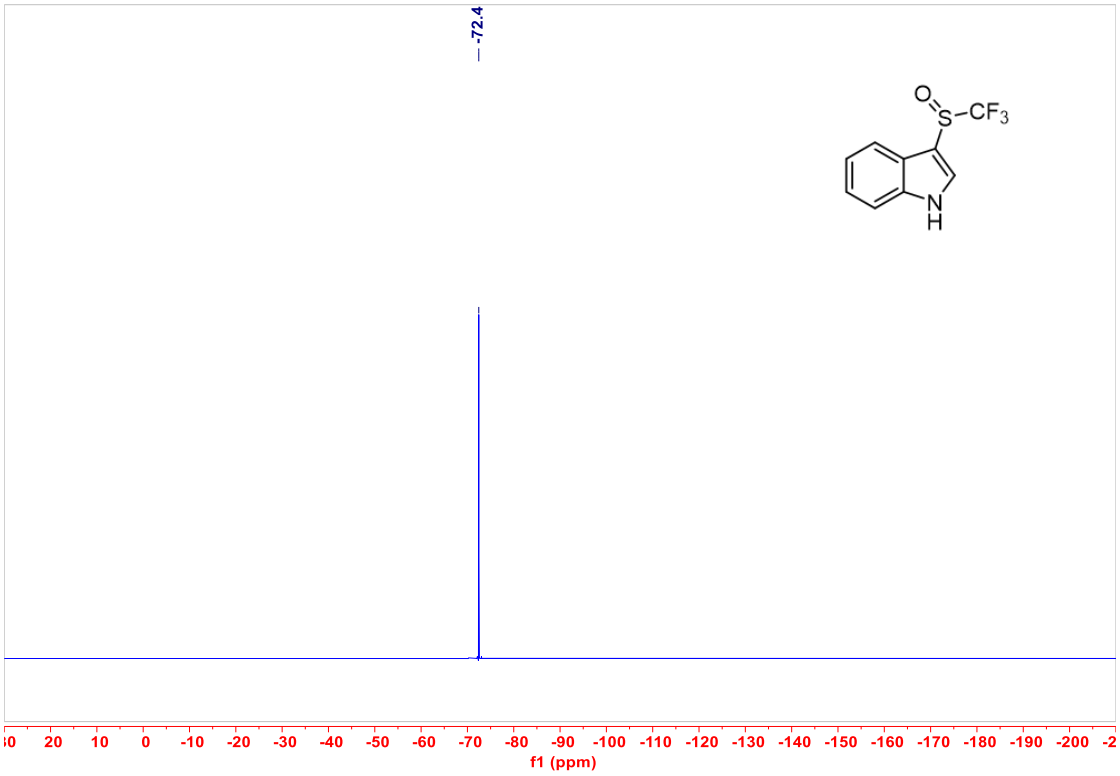
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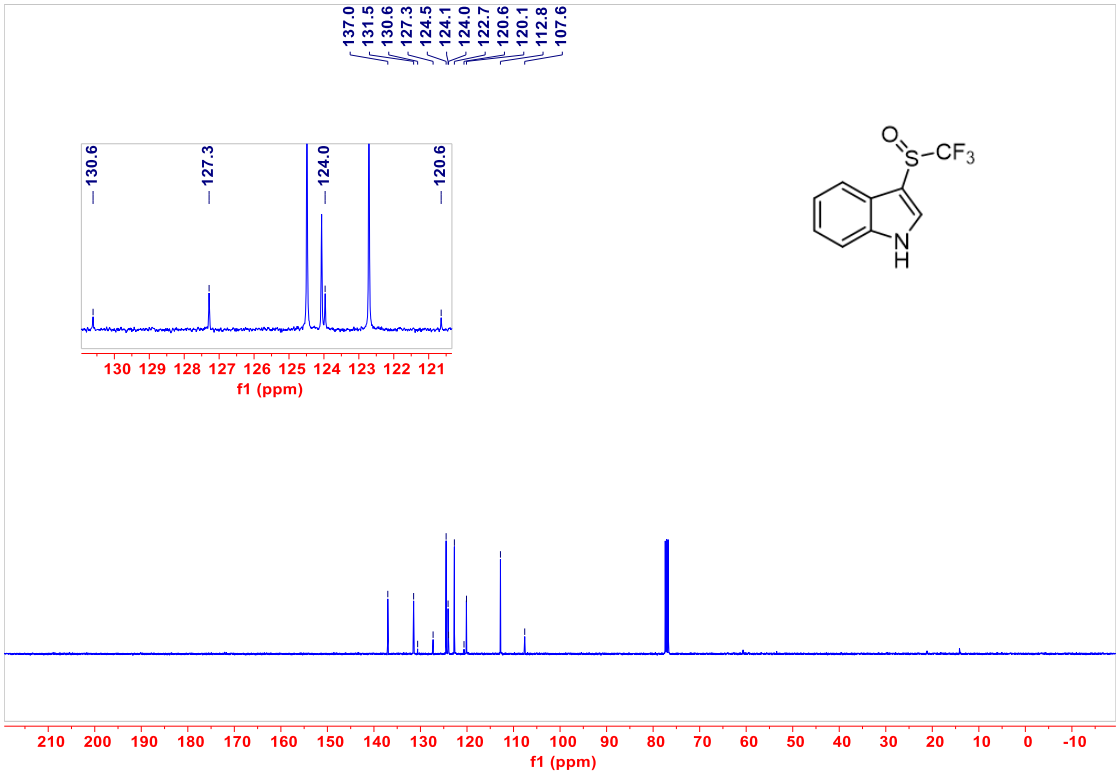
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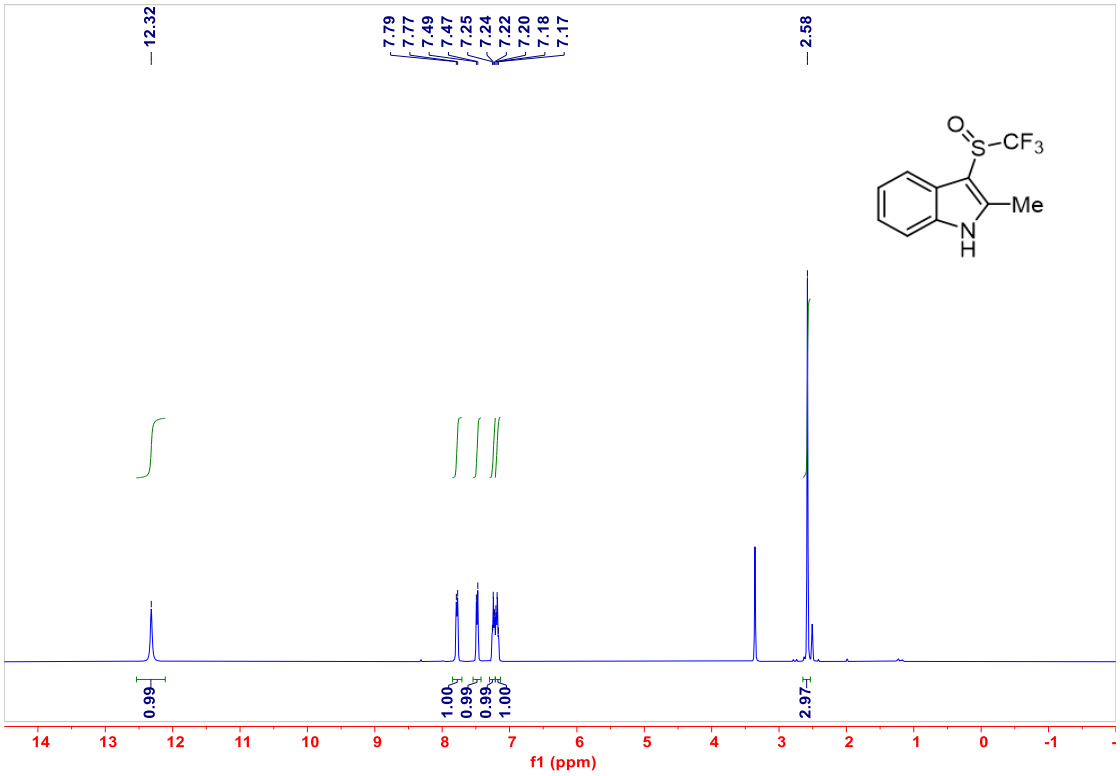
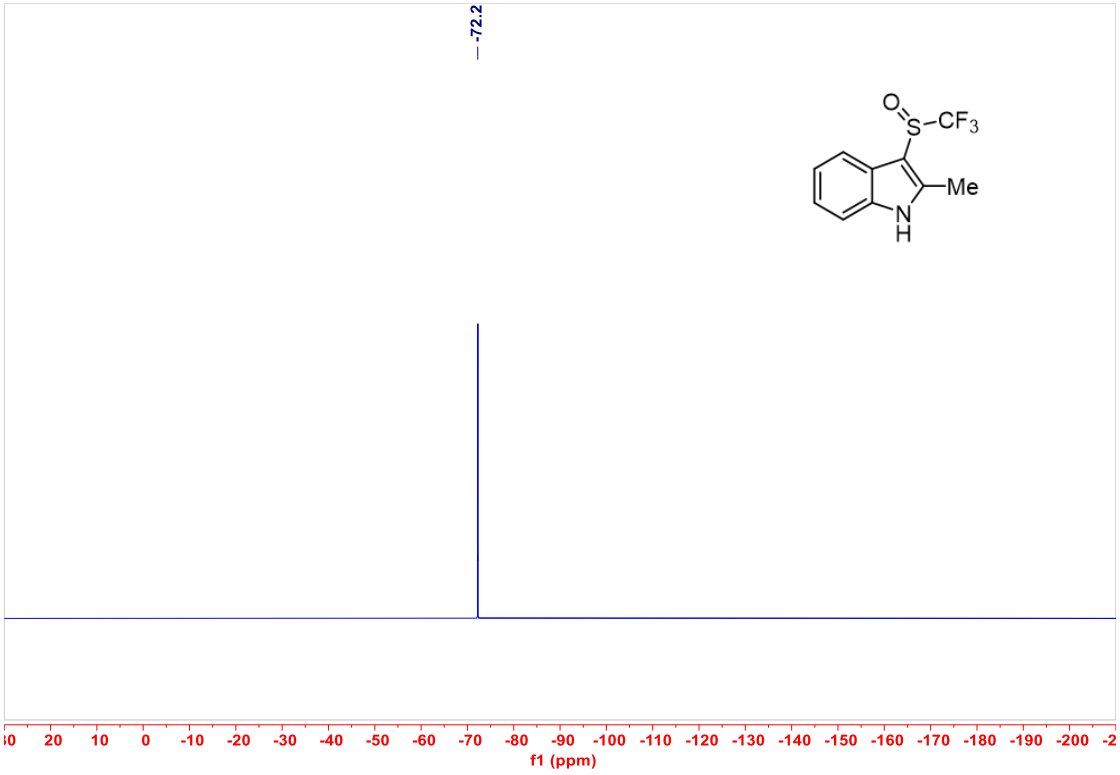
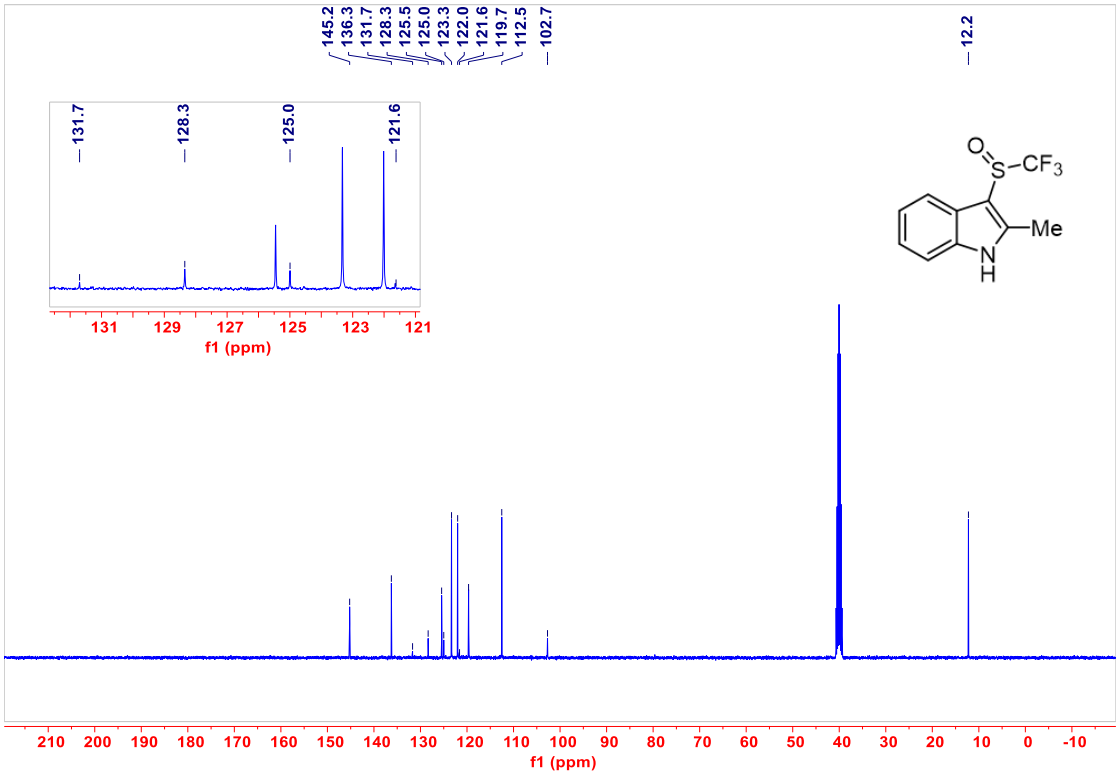
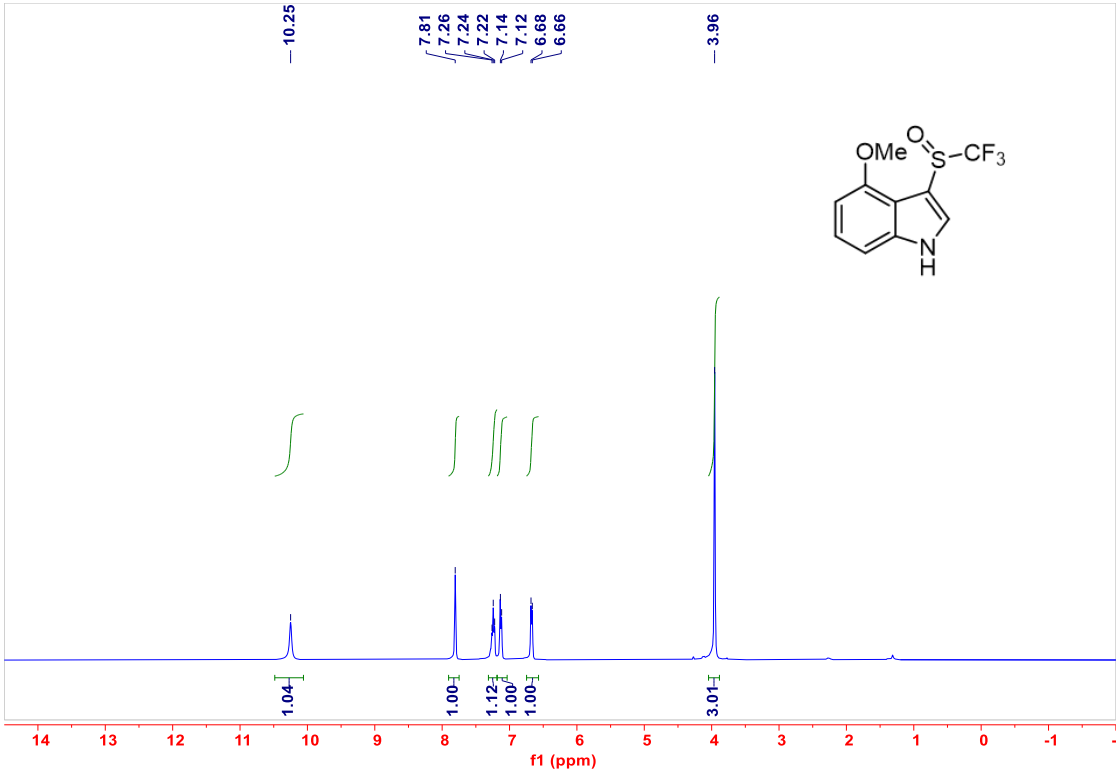
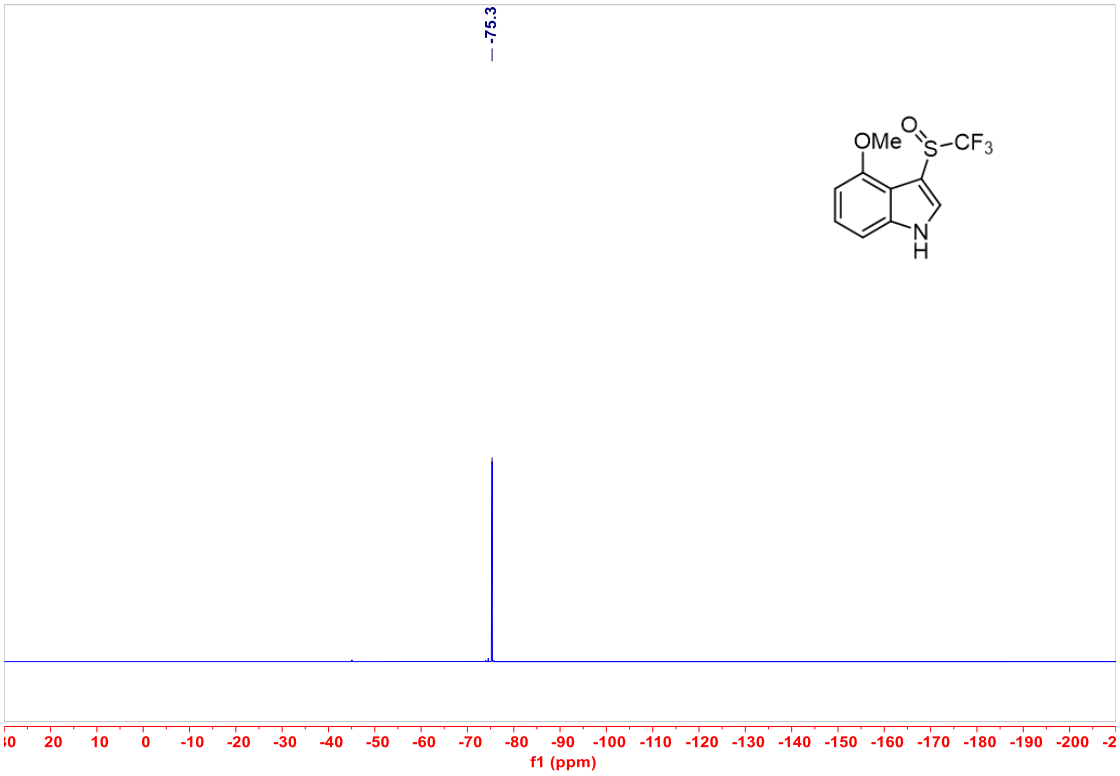
H
f1 (ppm)


12.32
7.79
7.77
7.49
7.47
7.25
7.24
7.22
7.20
7.18
7.17
2.58
0.99
1.00
0.99
0.99
1.00
2.97
f1 (ppm)


-72.2
f1 (ppm)


145.2
136.3
131.7
128.3
125.5
125.0
123.3
122.0
121.6
119.7
112.5
102.7
12.2
131.7
128.3
125.0
121.6
131 129 127 125 123 121
f1 (ppm)
O
S
CF3
Me
N
H
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)


10.25
7.81
7.26
7.24
7.22
7.14
7.12
6.68
6.66
3.96
OMe
O
S
CF3
N
H
1.04
1.00
1.12
1.00
1.00
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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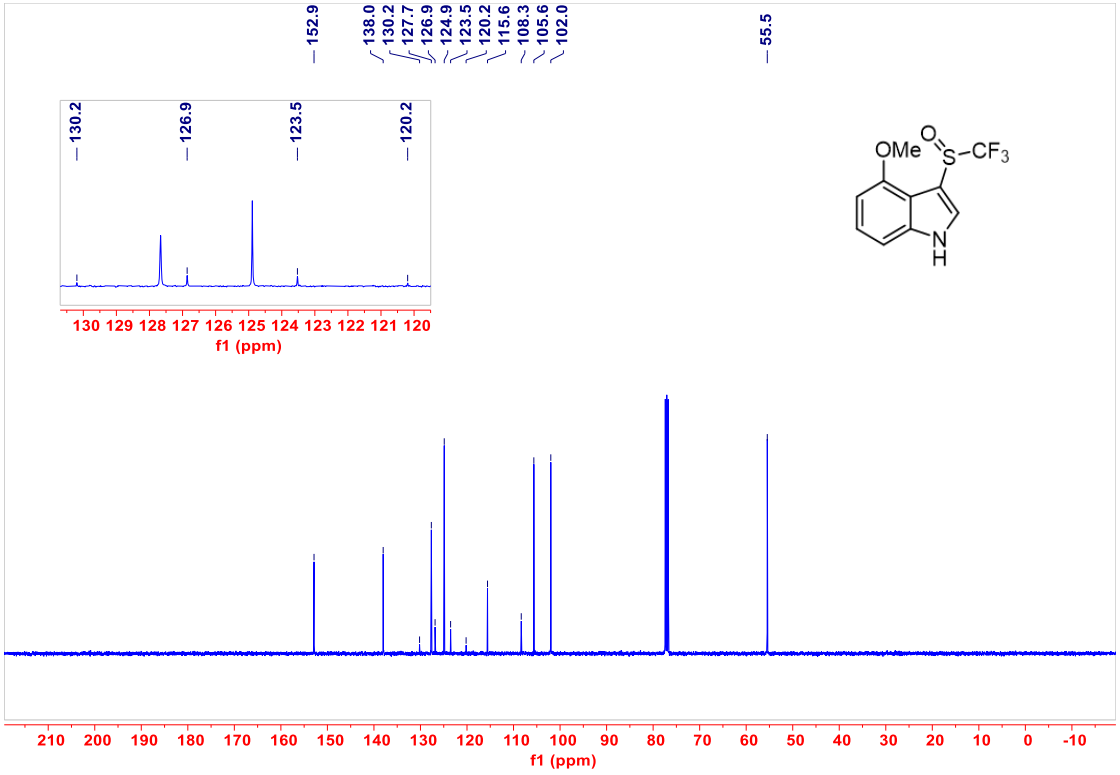
OMe
O
S
CF3
N
H
f1 (ppm)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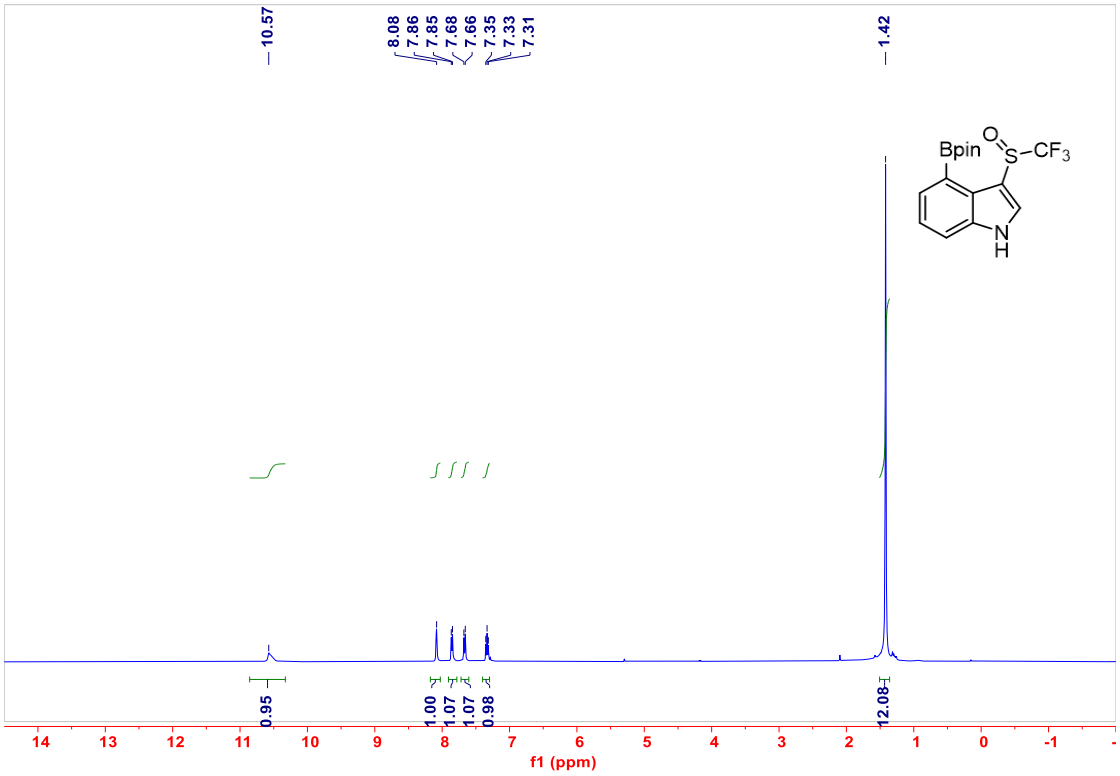
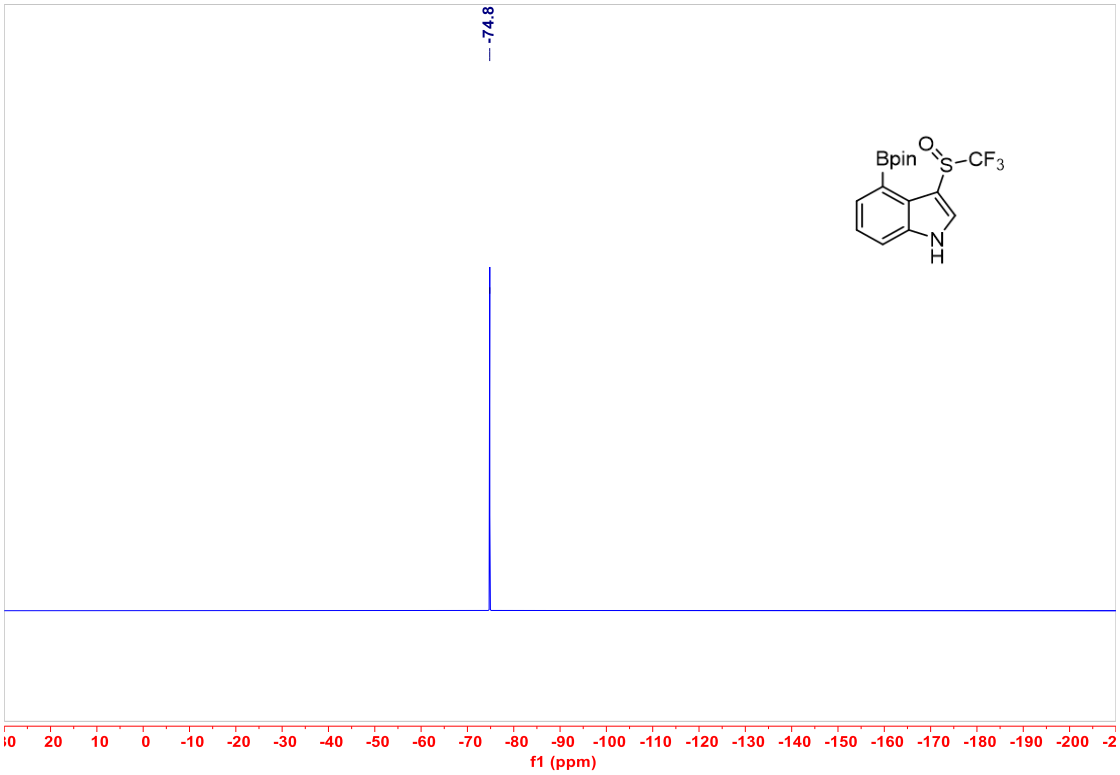
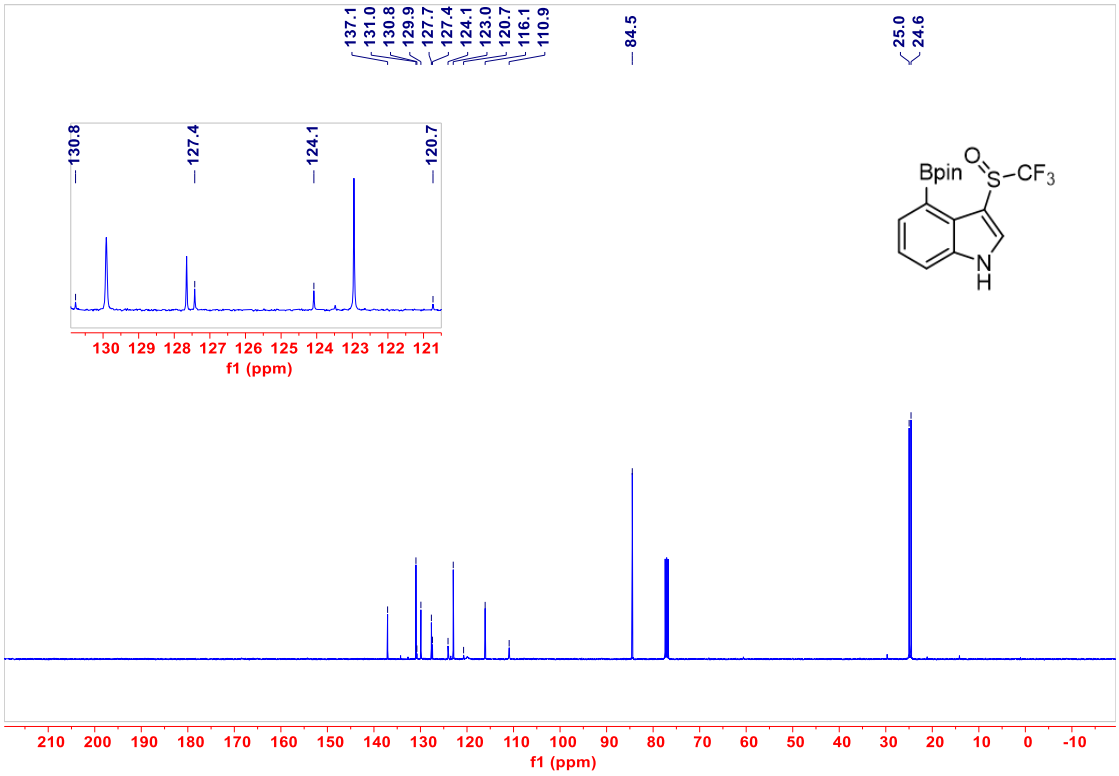
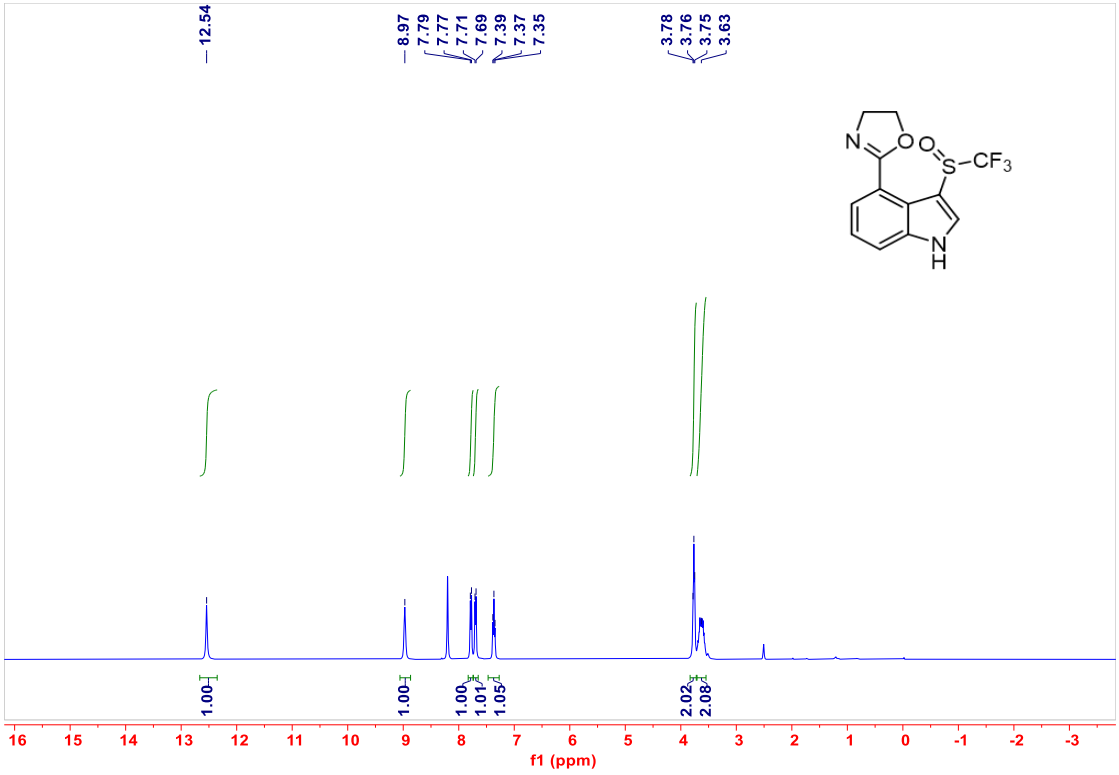
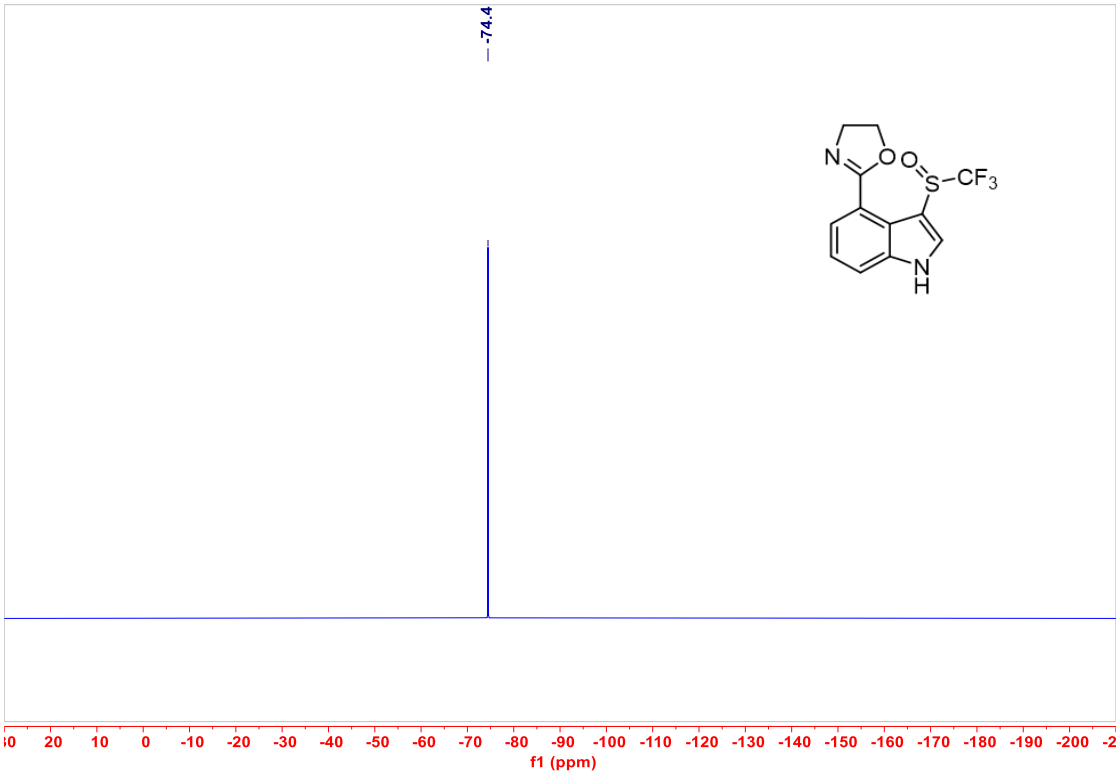
138.0
130.2
127.7
126.9
124.9
123.5
120.2
115.6
108.3
105.6
102.0
55.5
130.2
126.9
123.5
120.2
OMe
O
S
CF3
N
H
f1 (ppm)

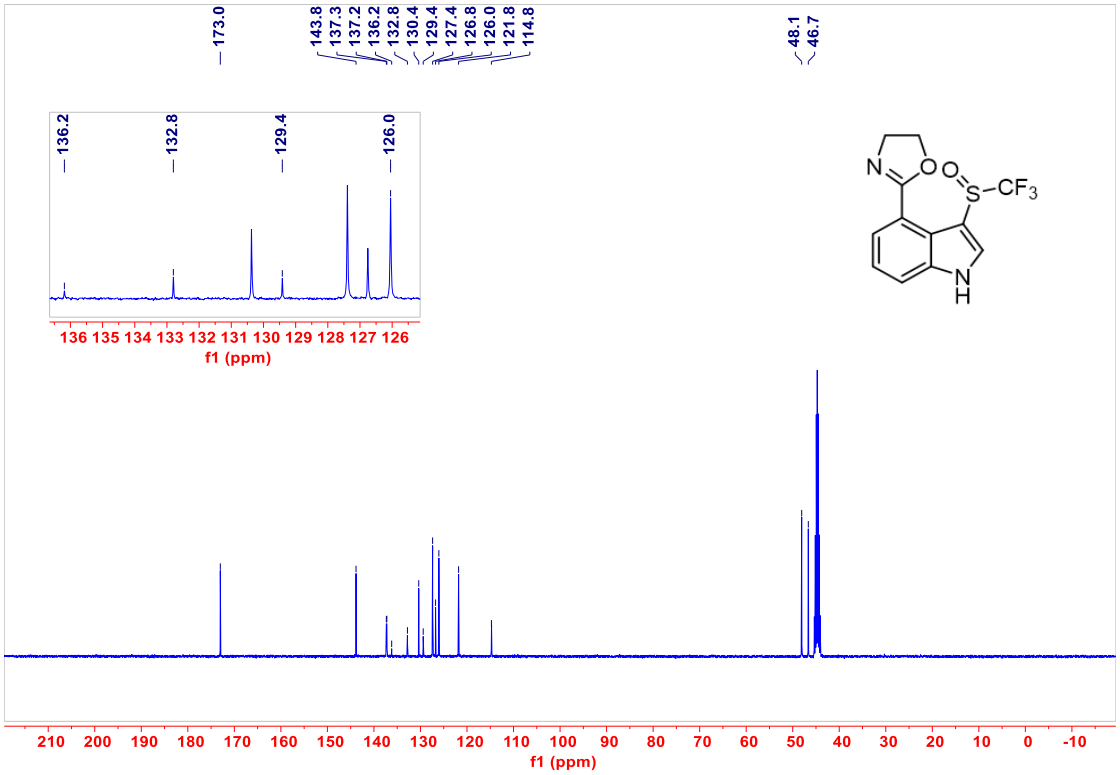

10.57
8.08
7.86
7.85
7.68
7.66
7.35
7.33
7.31
1.42
Bpin
O
S
CF3
N
H
0.95
1.00
1.07
1.07
0.98
12.08
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

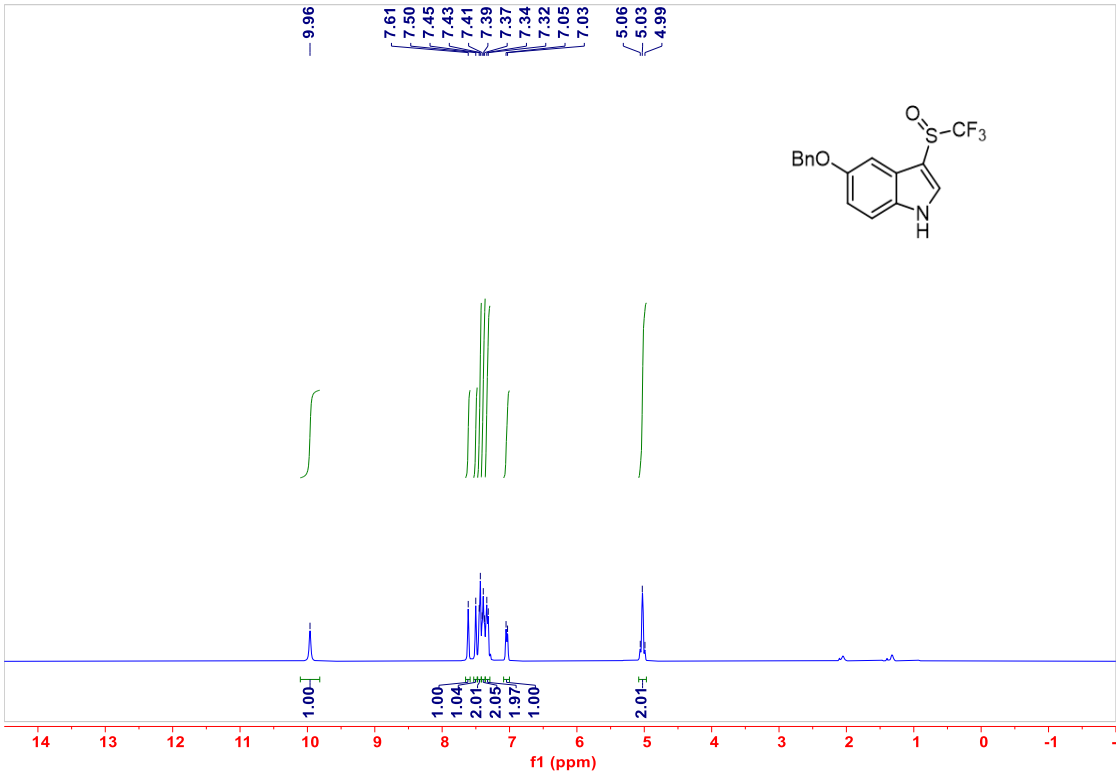

-74.8
Bpin
O
S
CF3
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

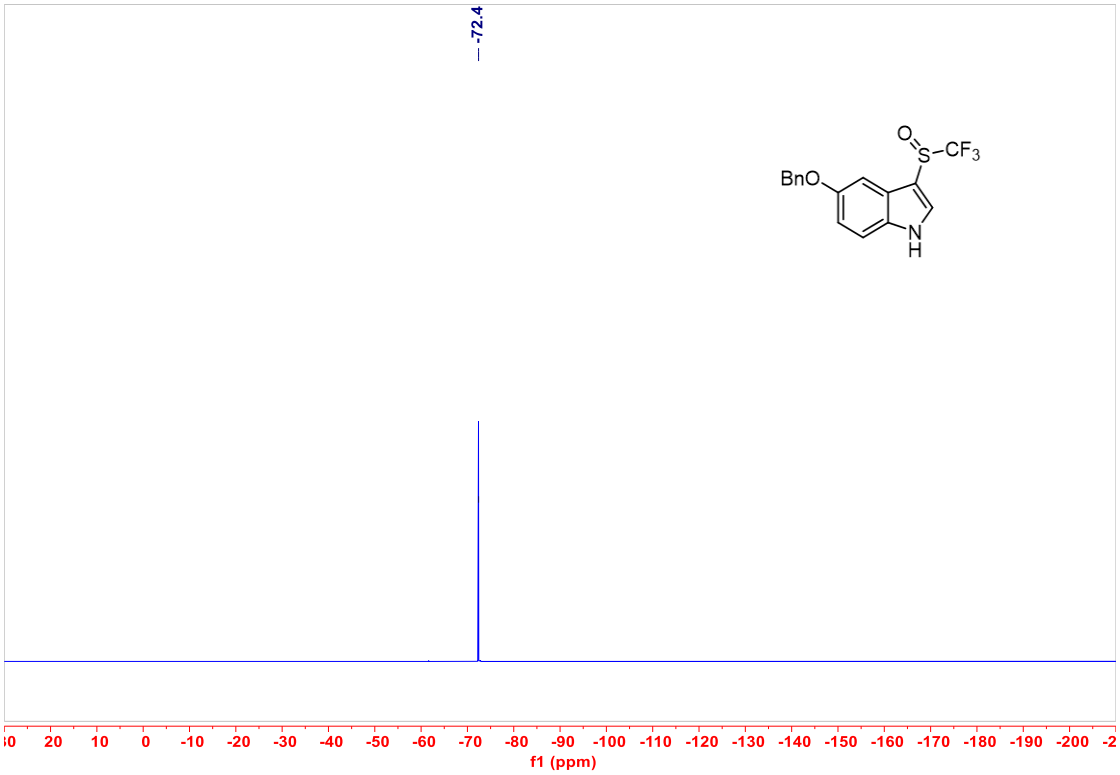

137.1
131.0
130.8
129.9
127.7
127.4
124.1
123.0
120.7
116.1
110.9
84.5
25.0
24.6
130.8
127.4
124.1
120.7
130 129 128 127 126 125 124 123 122 121
f1 (ppm)
Bpin
O
S
CF3
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

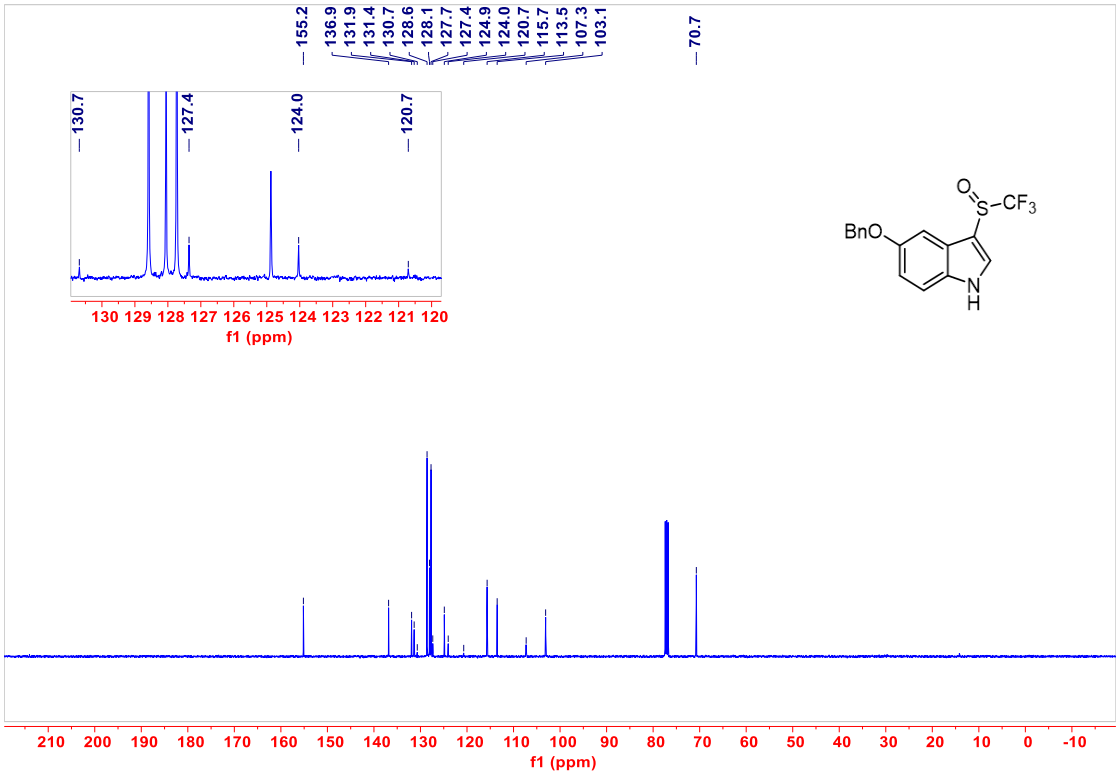

12.54
8.97
7.79
7.77
7.71
7.69
7.39
7.37
7.35
3.78
3.76
3.75
3.63
N
O
O
S
CF3
N
H
1.00
1.00
1.00
1.01
1.05
2.02
2.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

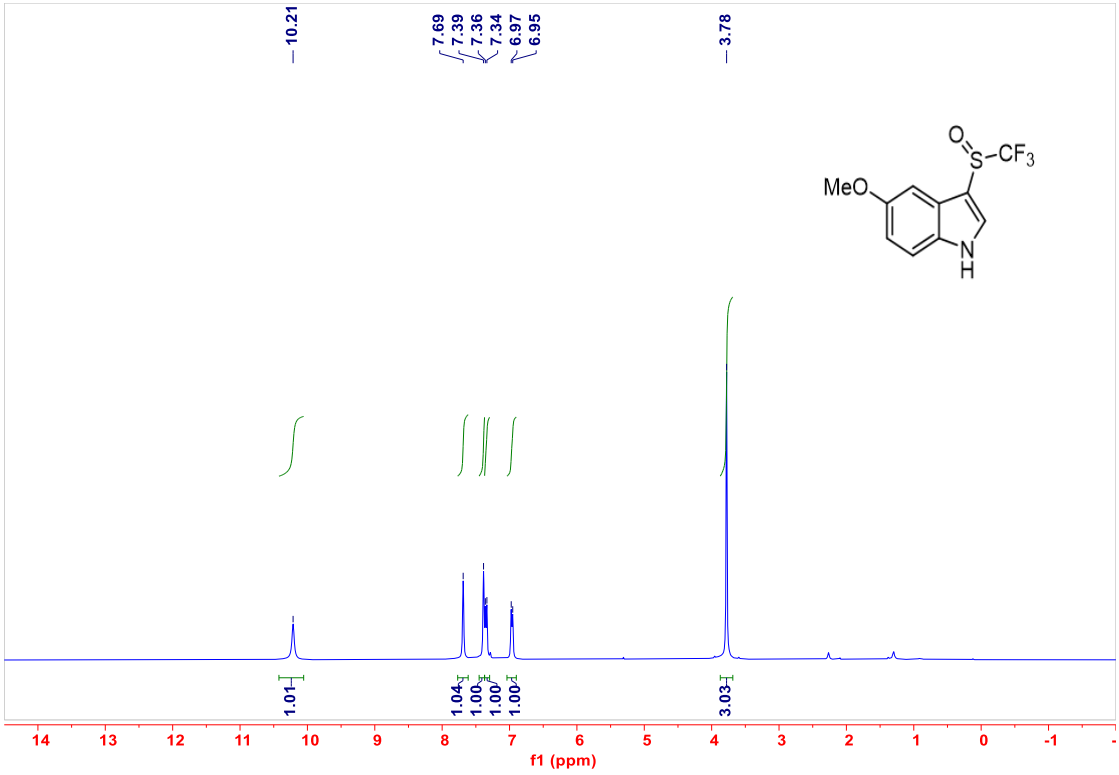

-74.4
N
O
O
S
CF3
N
H
f1 (ppm)

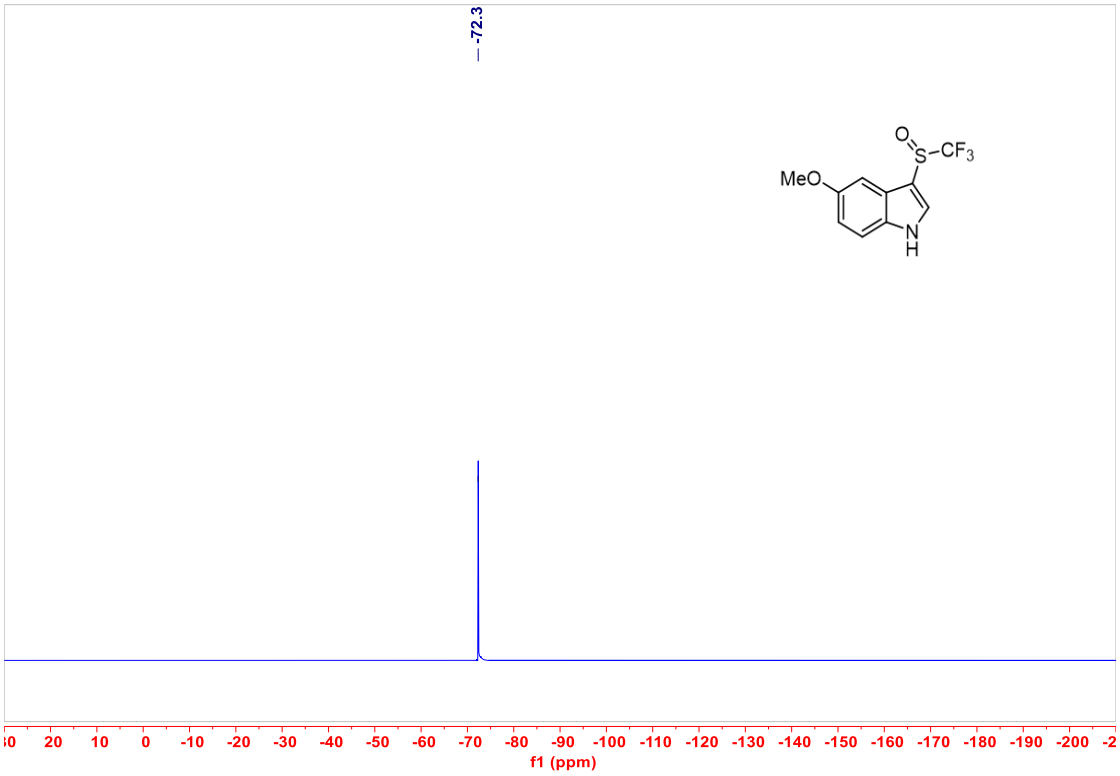

173.0
143.8
137.3
137.2
136.2
132.8
130.4
129.4
127.4
126.8
126.0
121.8
114.8
48.1
46.7
136.2
132.8
129.4
126.0
f1 (ppm)
N
O
O
S
CF3
N
H
f1 (ppm)

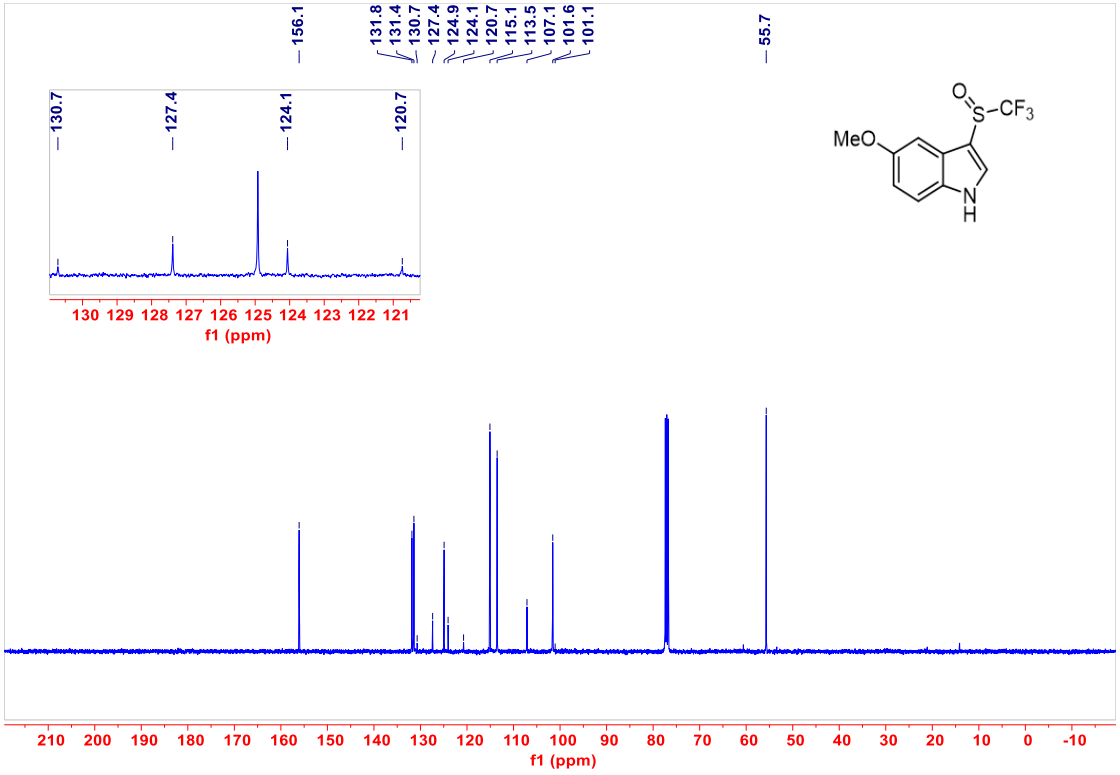

9.96
7.61
7.50
7.45
7.43
7.41
7.39
7.37
7.34
7.32
7.05
7.03
5.06
5.03
4.99
BnO
S
CF3
O
N
H
1.00
1.00
1.04
2.01
2.05
1.97
1.00
2.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

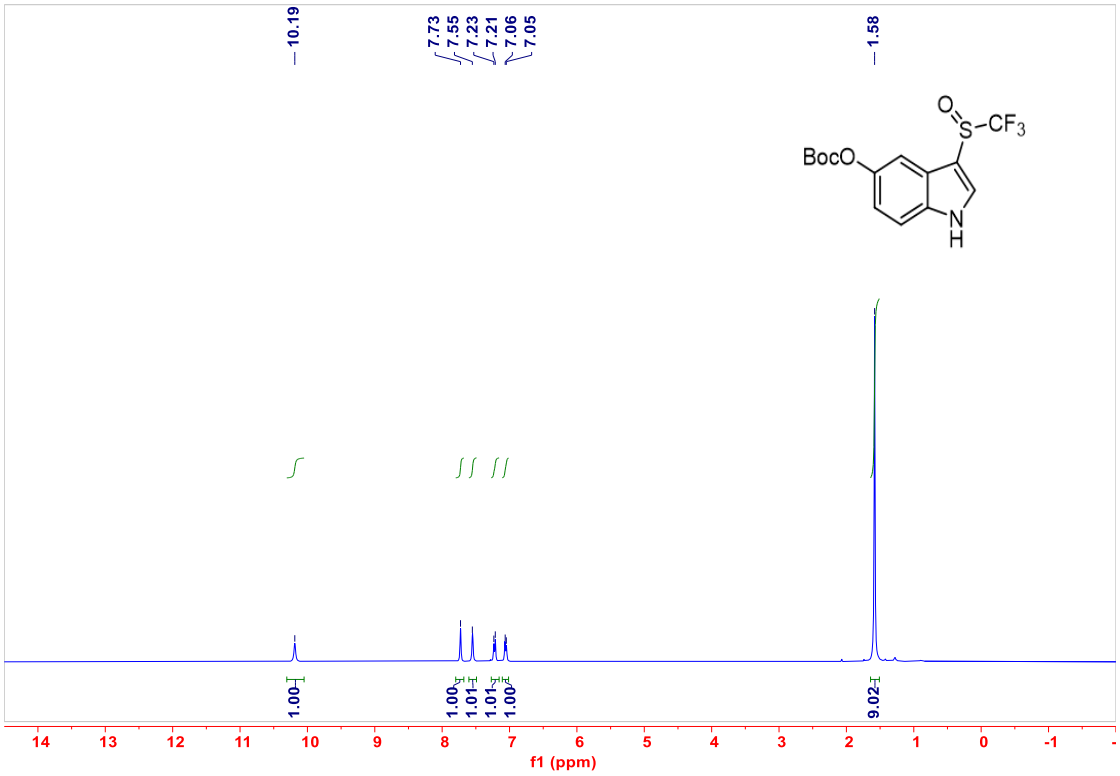

-72.4
BnO
S
CF3
O
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

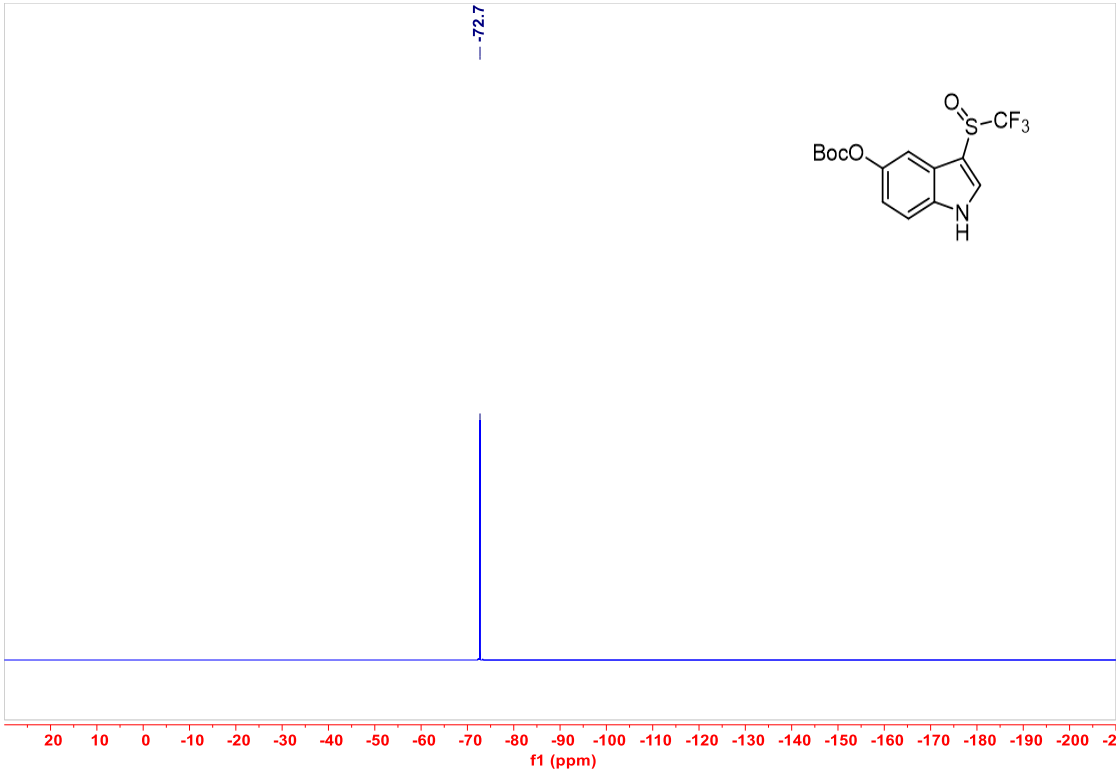

155.2
136.9
131.9
131.4
130.7
128.6
128.1
127.7
127.4
124.9
124.0
120.7
115.7
113.5
107.3
103.1
70.7
130.7
127.4
124.0
120.7
130 129 128 127 126 125 124 123 122 121 120
f1 (ppm)
BnO
S
CF3
O
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

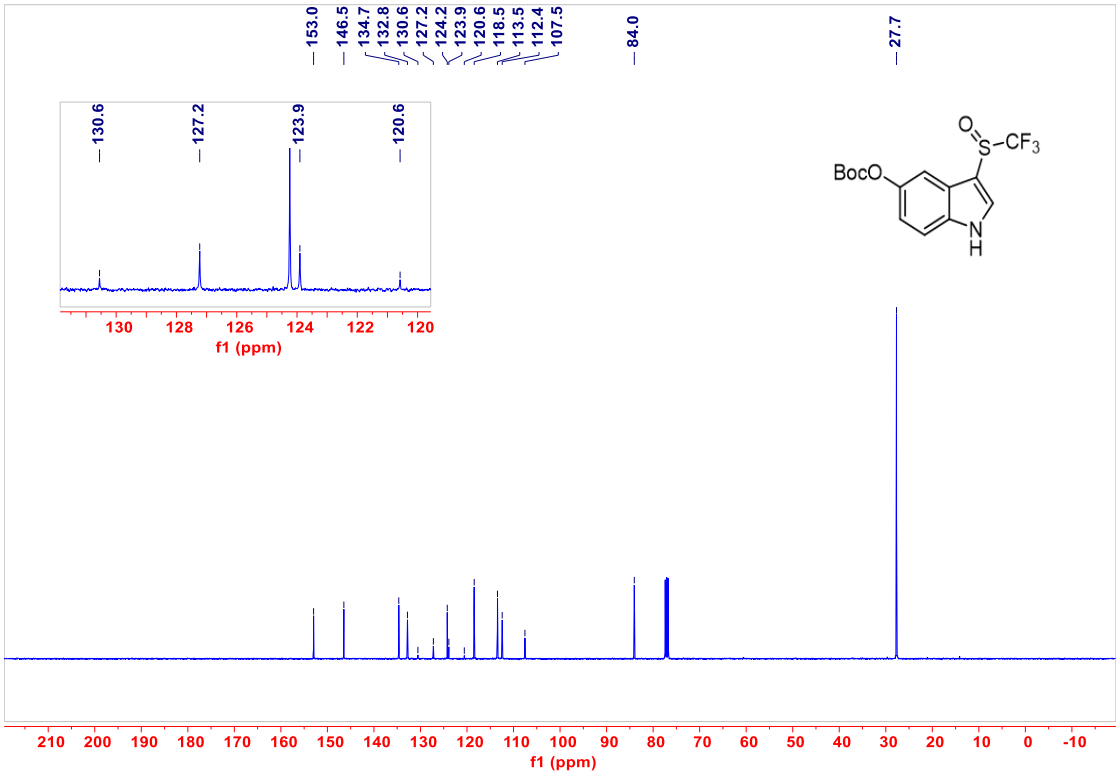

10.21
7.69
7.39
7.36
7.34
6.97
6.95
3.78
MeO
S
CF3
O
N
H
1.01
1.04
1.00
1.00
1.00
3.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

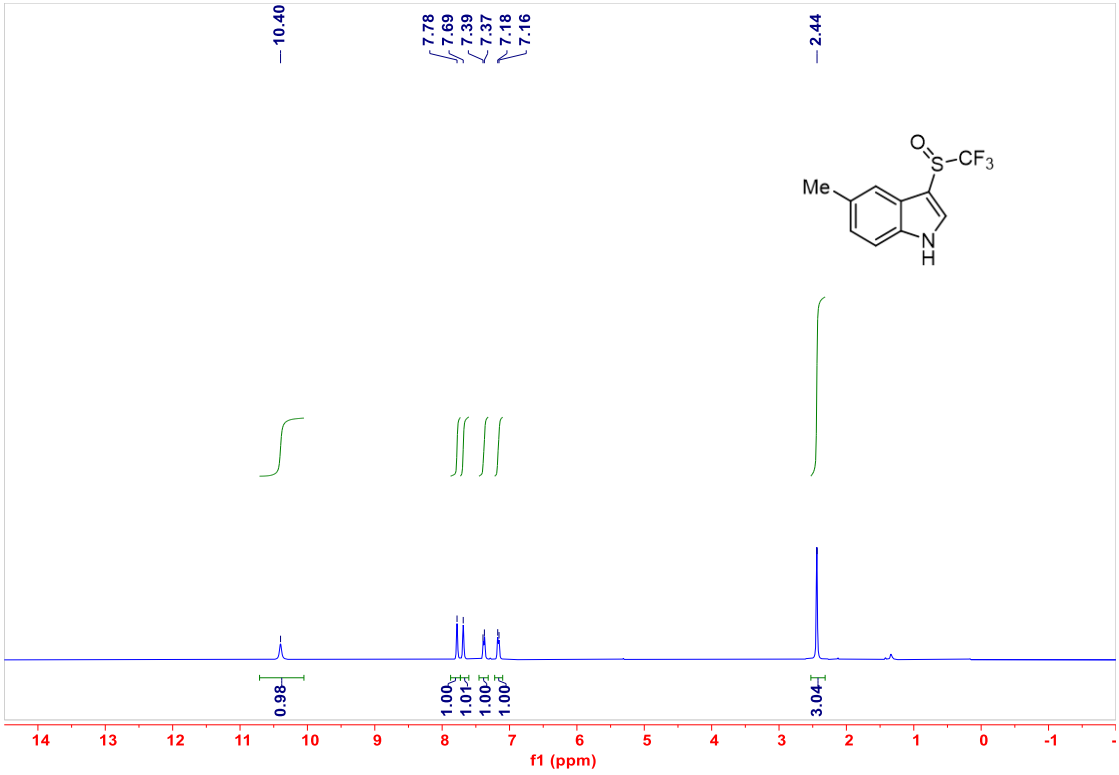

-72.3
MeO
S
CF3
N
H
f1 (ppm)

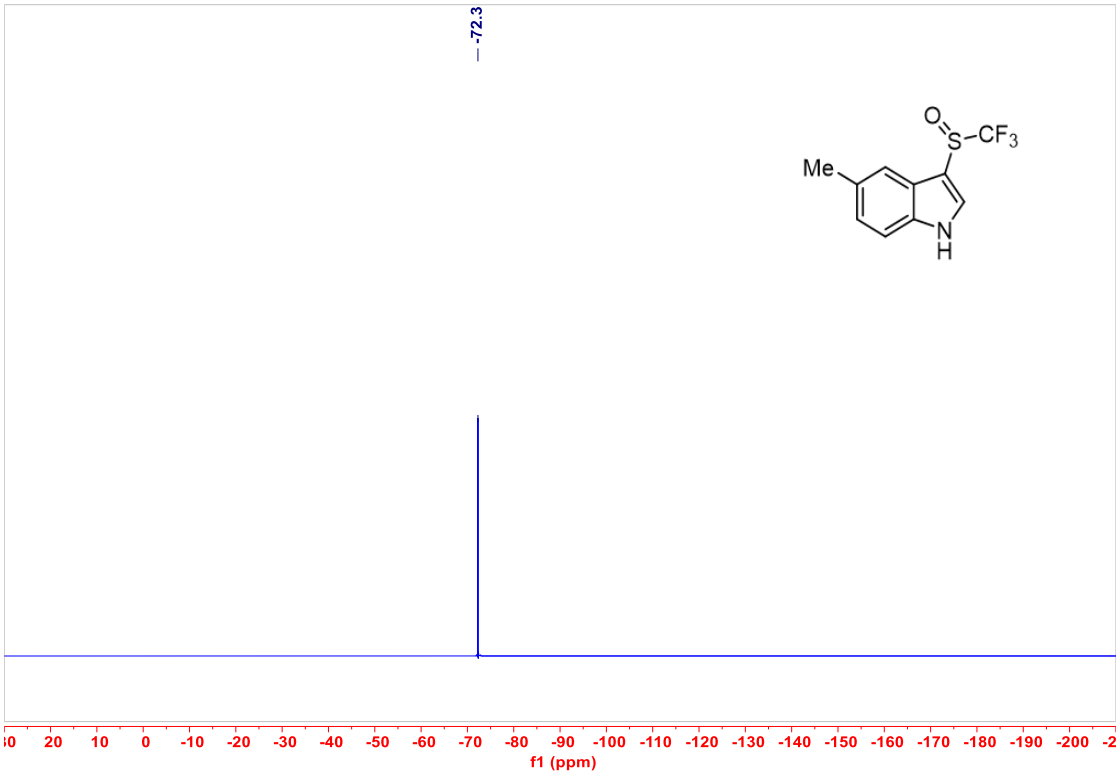

156.1
131.8
131.4
130.7
127.4
124.9
124.1
120.7
115.1
113.5
107.1
101.6
101.1
55.7
130.7
127.4
124.1
120.7
f1 (ppm)
MeO
S
CF3
N
H
f1 (ppm)


10.19
7.73
7.55
7.23
7.21
7.06
7.05
1.58
BocO
S
CF3
O
N
H
1.00
1.00
1.01
1.01
1.00
9.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-72.7
BocO
S
CF3
O
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


153.0
146.5
134.7
132.8
130.6
127.2
124.2
123.9
120.6
118.5
113.5
112.4
107.5
84.0
27.7
130.6
127.2
123.9
120.6
130 128 126 124 122 120
f1 (ppm)
BocO
O
S
CF3
N
H
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)


10.40
7.78
7.69
7.39
7.37
7.18
7.16
2.44
O
S
CF3
Me
N
H
0.98
1.00
1.01
1.00
1.00
3.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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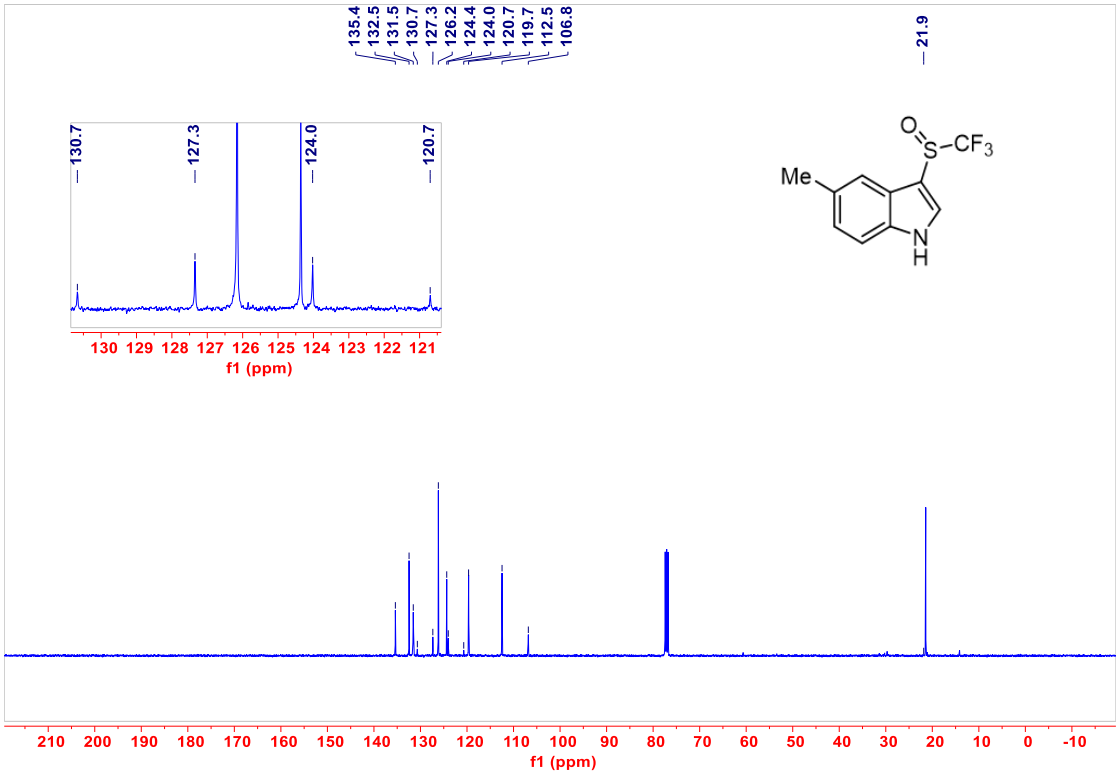
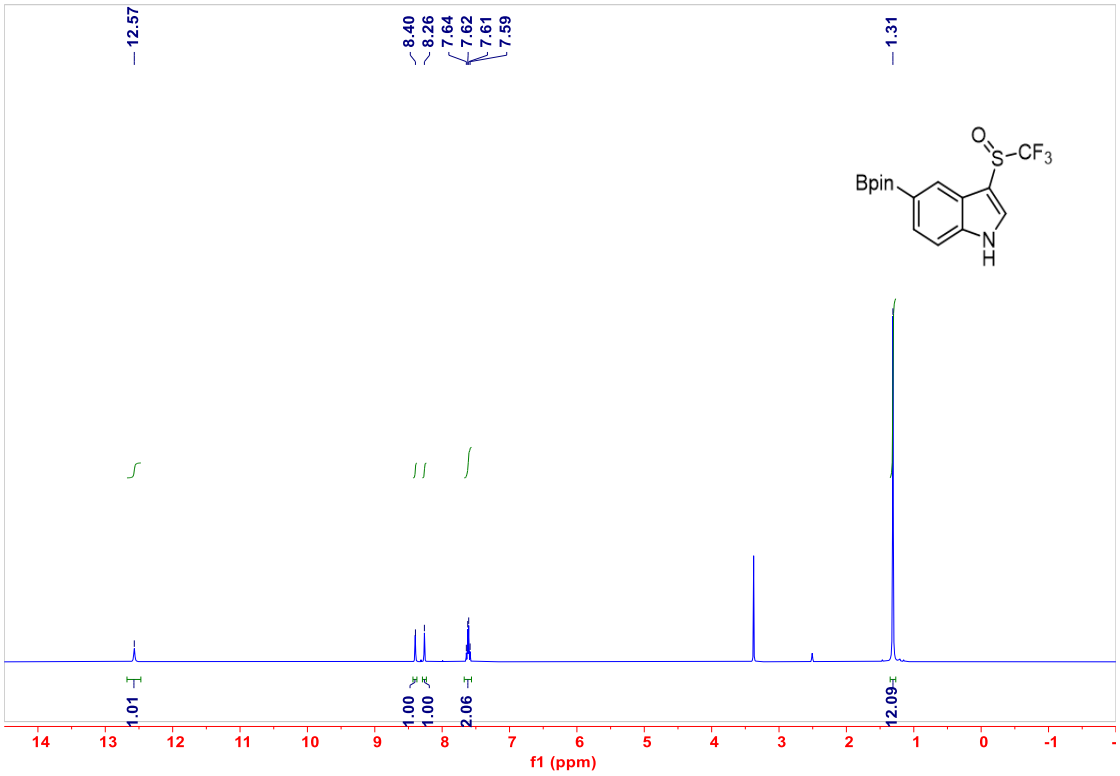
Me
O
S
CF3
N
H
f1 (ppm)


135.4
132.5
131.5
130.7
127.3
126.2
124.4
124.0
120.7
119.7
112.5
106.8
21.9
130.7
127.3
124.0
120.7
Me
O
S
CF3
N
H
f1 (ppm)


12.57
8.40
8.26
7.64
7.62
7.61
7.59
1.31
Bpin
S
CF3
N
H
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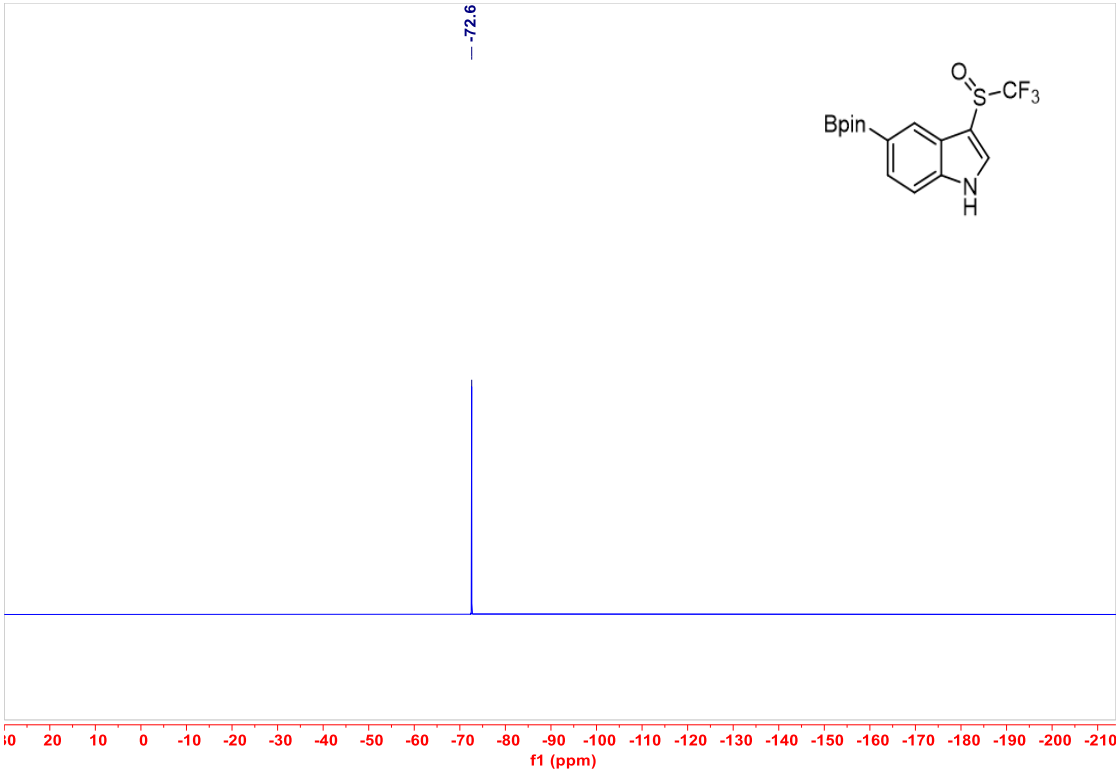
1.00
1.00
2.06
12.09
f1 (ppm)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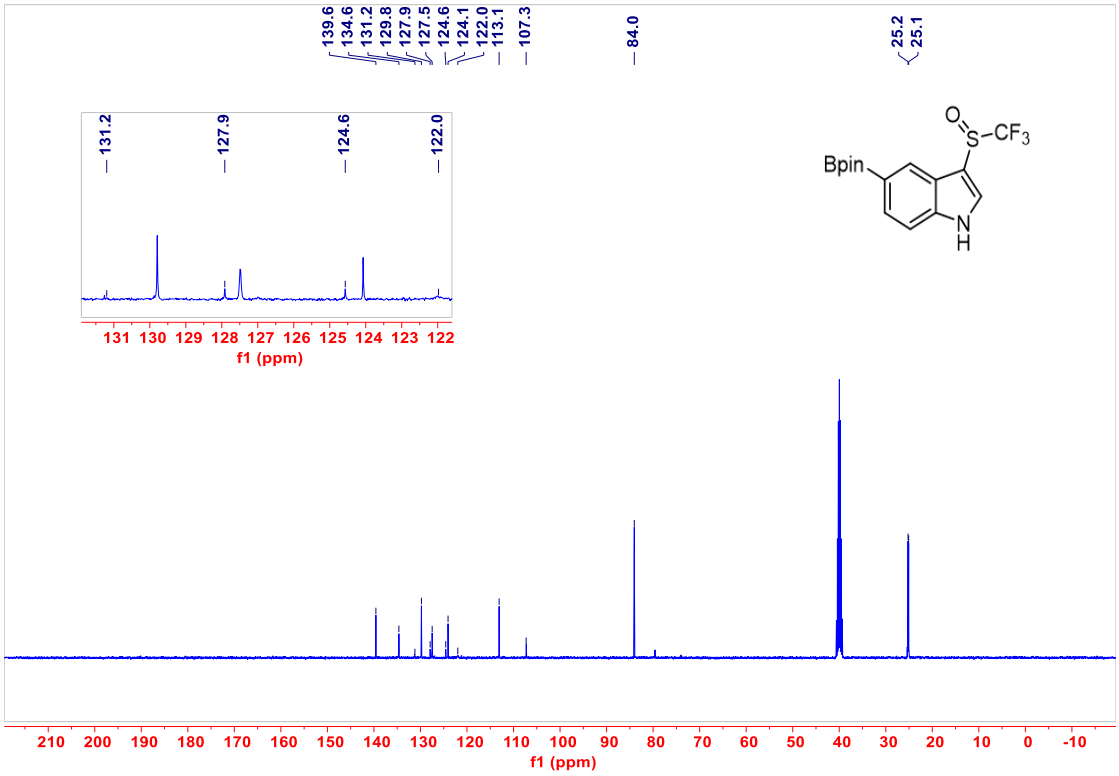
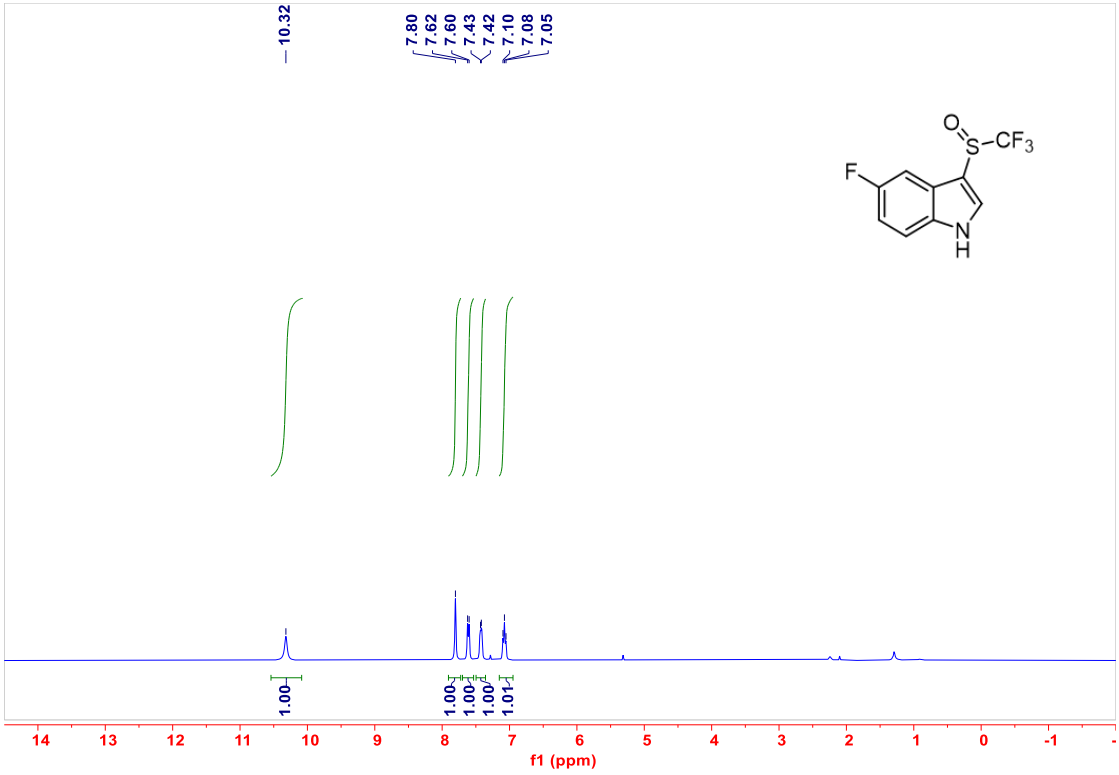
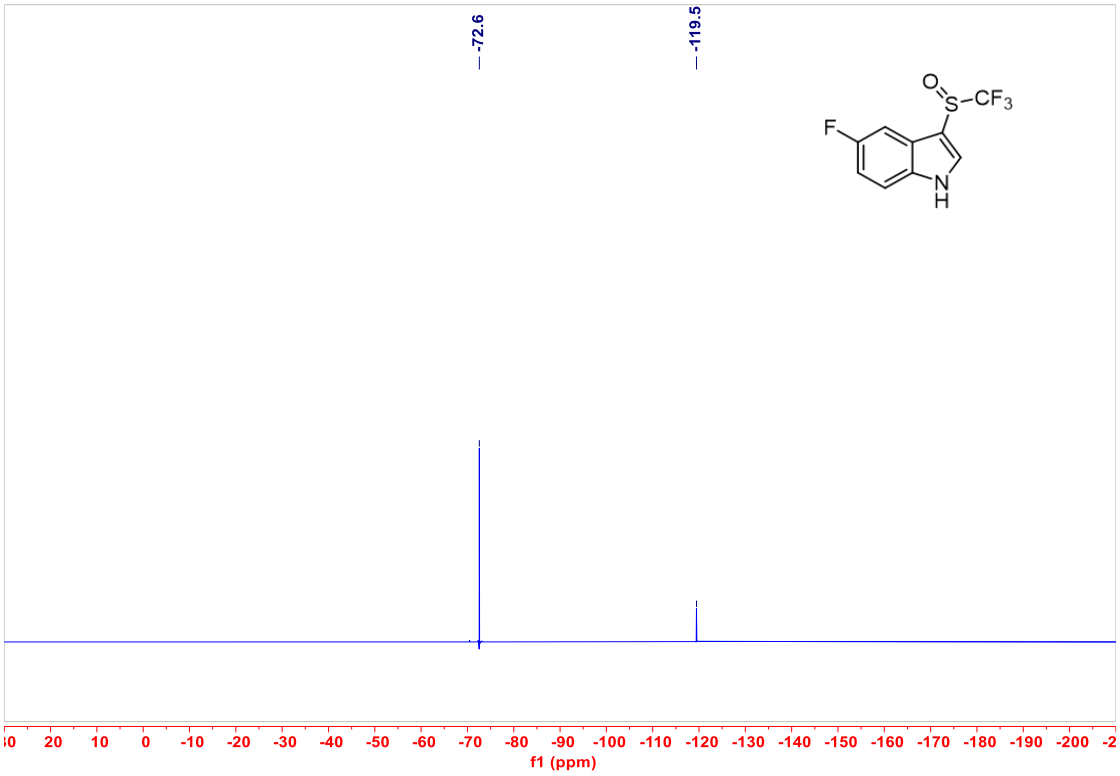
Bpin
S
CF3
N
H
f1 (ppm)


139.6
134.6
131.2
129.8
127.9
127.5
124.6
124.1
122.0
113.1
107.3
84.0
25.2
25.1
131.2
127.9
124.6
122.0
131 130 129 128 127 126 125 124 123 122
f1 (ppm)
Bpin
O
S
CF3
N
H
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)


10.32
7.80
7.62
7.60
7.43
7.42
7.10
7.08
7.05
F
O
S
CF3
N
H
1.00
1.00
1.00
1.00
1.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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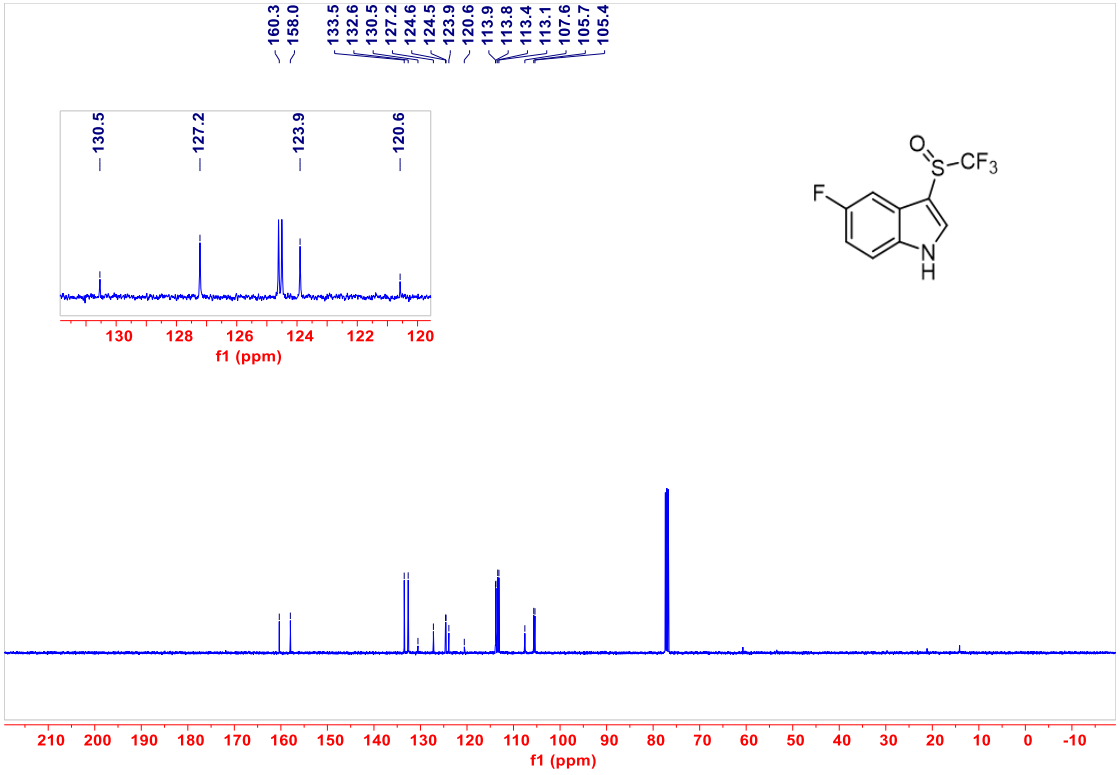
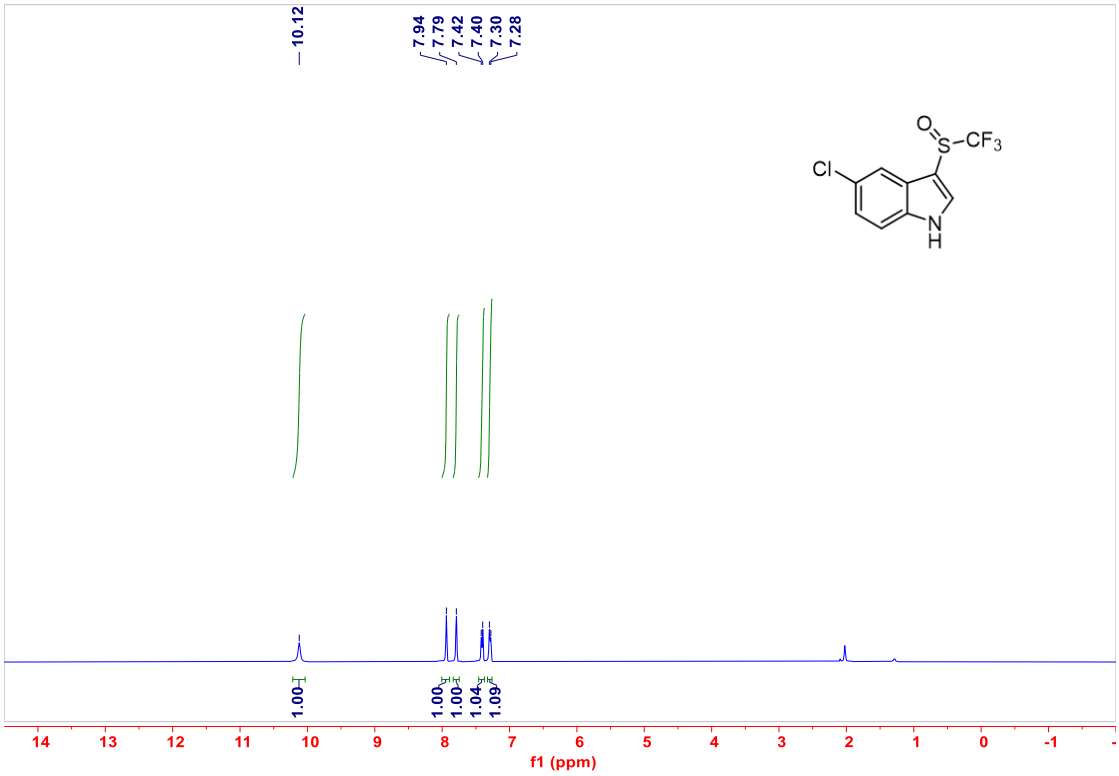
-119.5
O
S
CF3
F
N
H
f1 (ppm)


160.3
158.0
133.5
132.6
130.5
127.2
124.6
124.5
123.9
120.6
113.9
113.8
113.4
113.1
107.6
105.7
105.4
130.5
127.2
123.9
120.6
f1 (ppm)
O
S
CF3
F
N
H
f1 (ppm)


10.12
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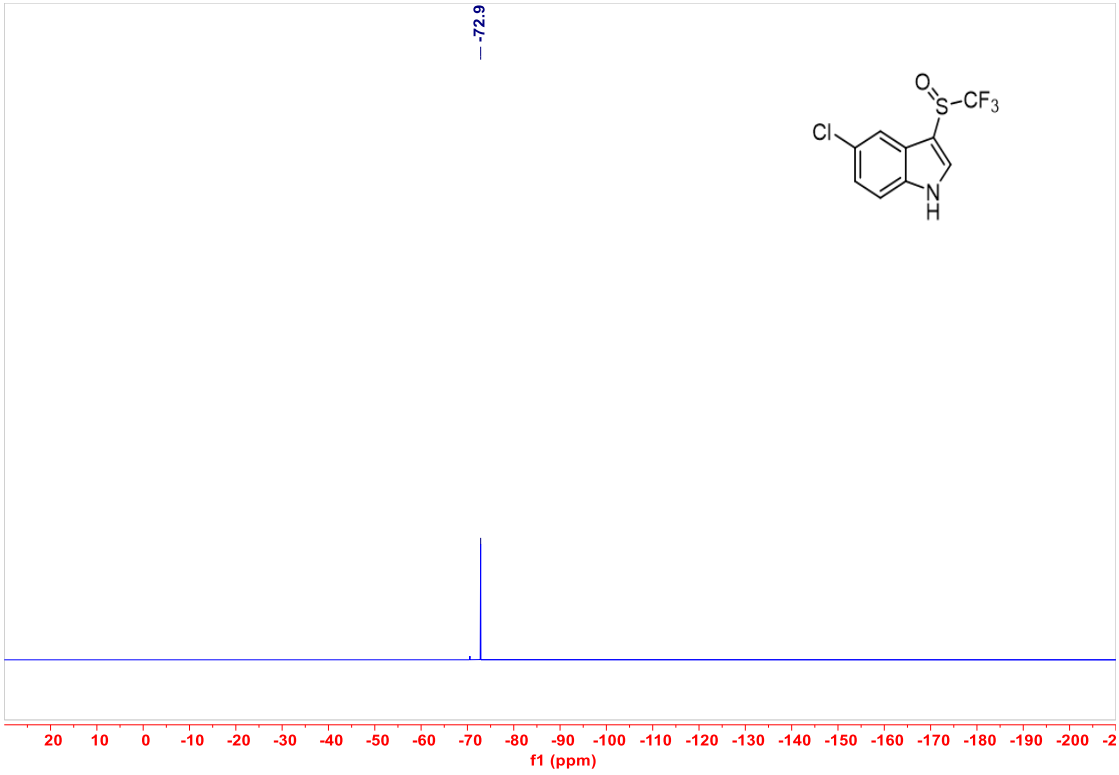
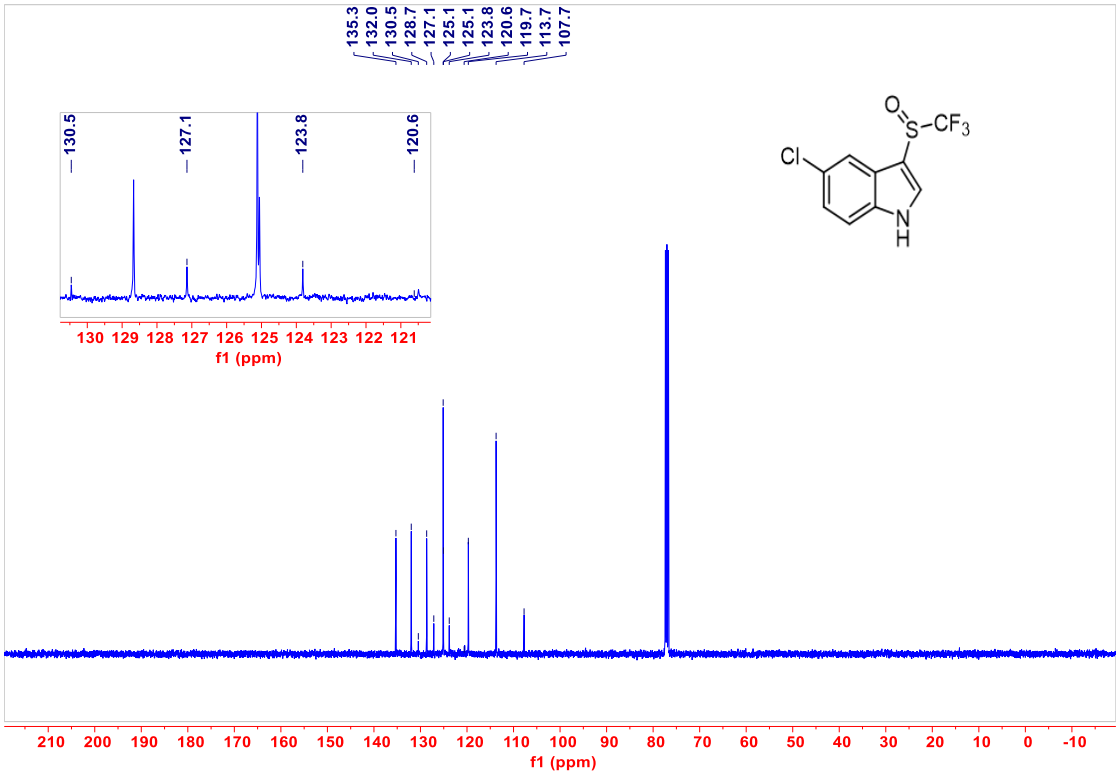
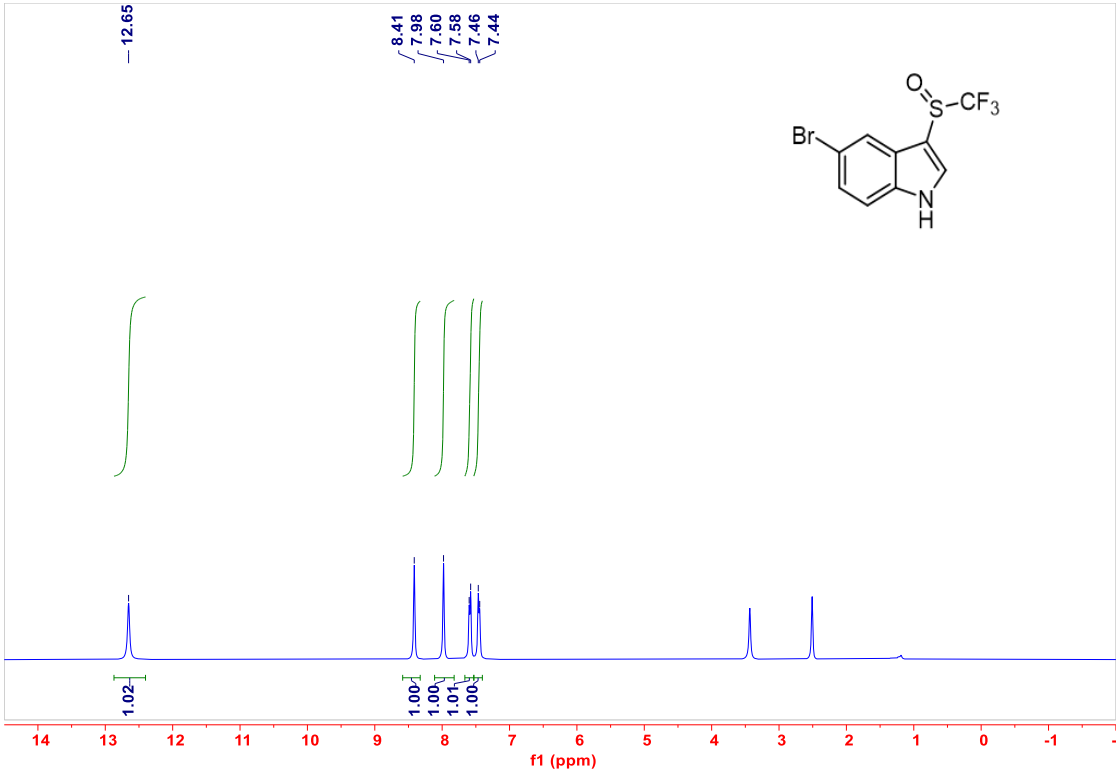
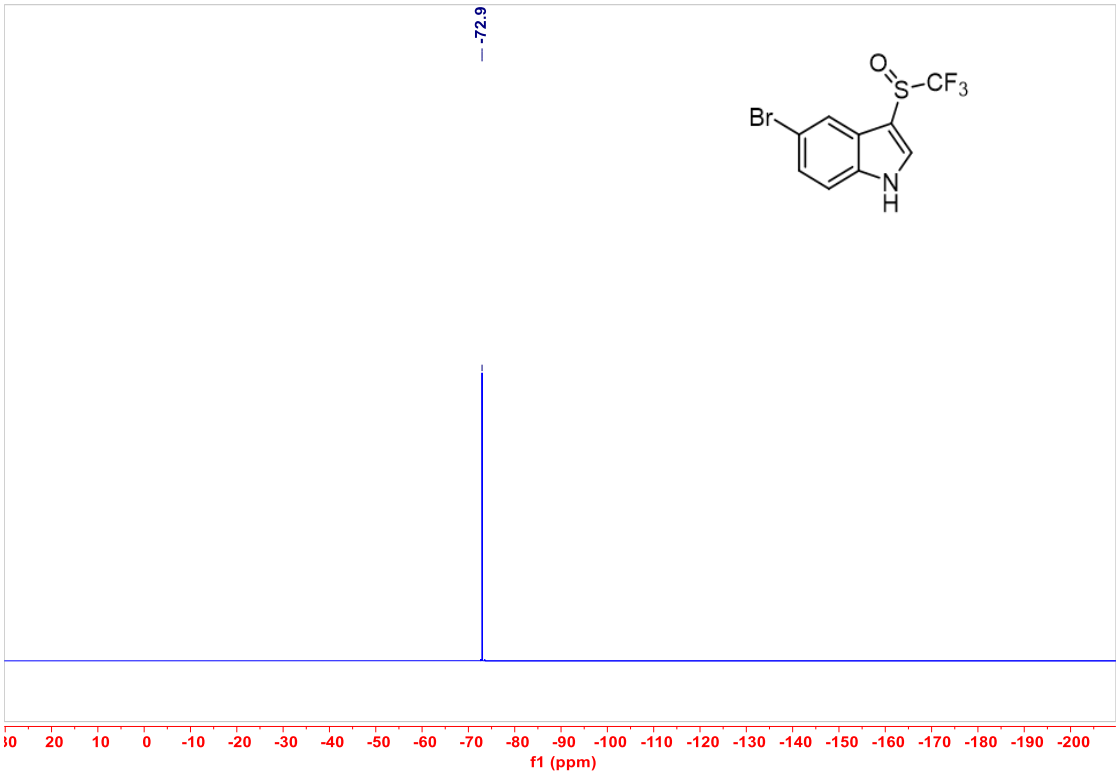
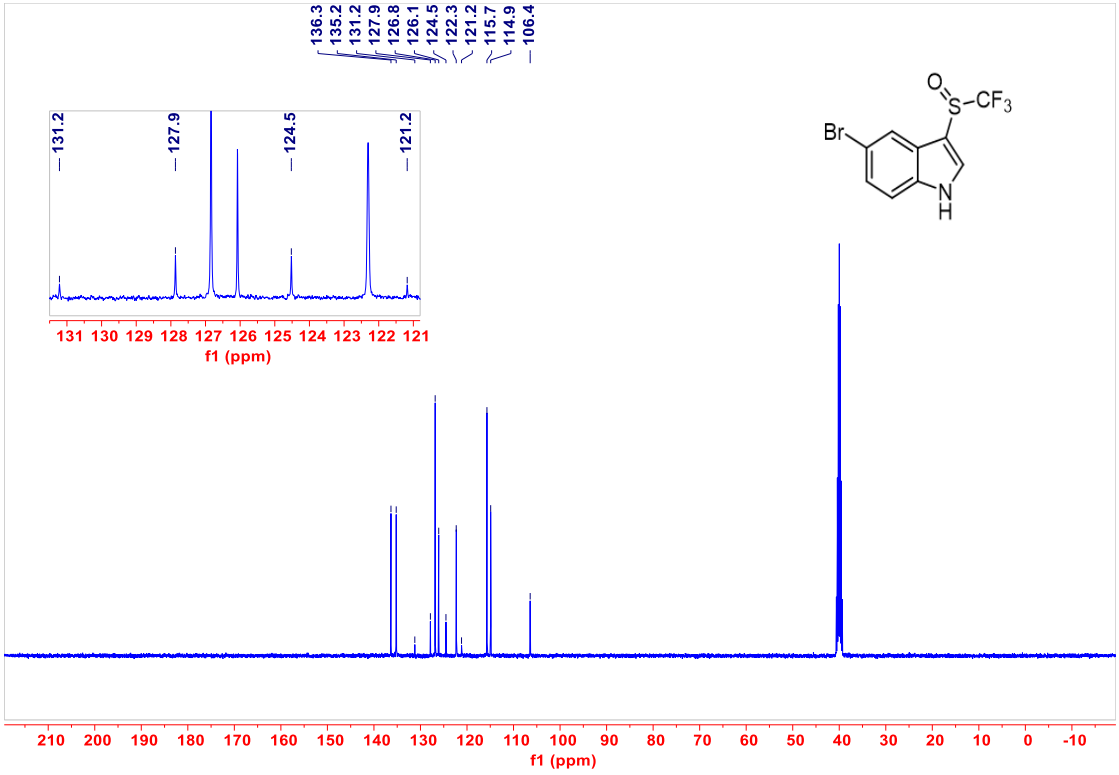
7.40
7.30
7.28
1.00
1.00
1.00
1.04
1.09
f1 (ppm)

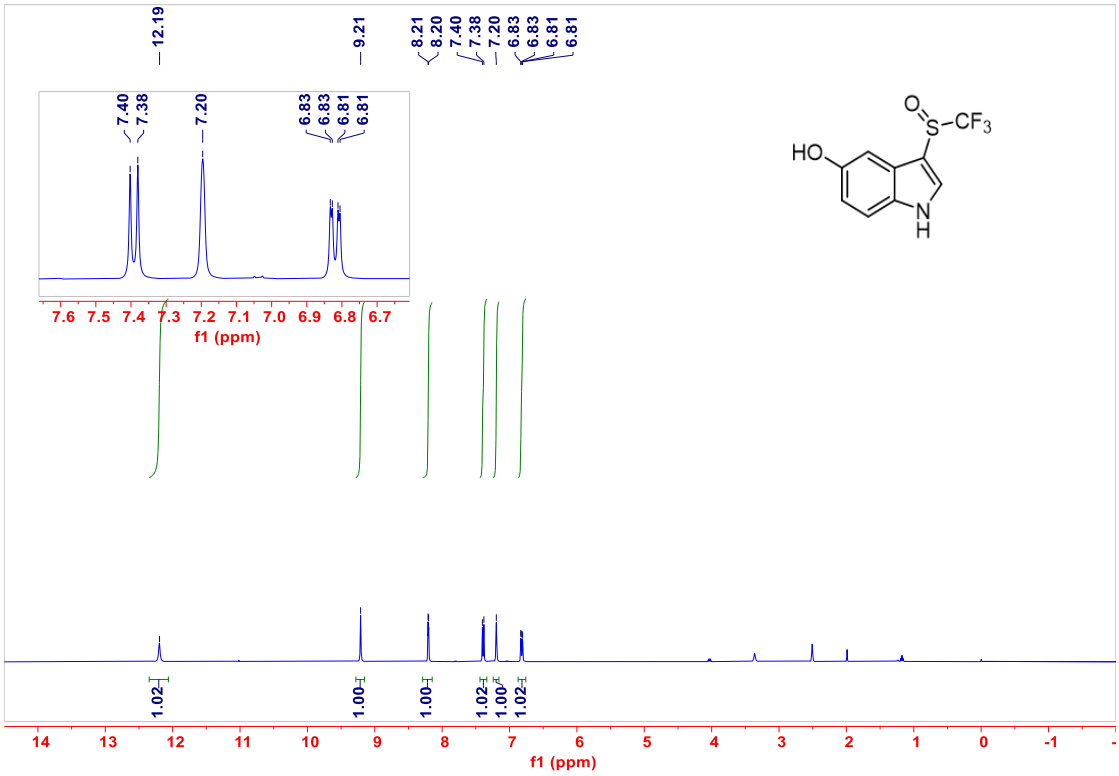

-72.9
f1 (ppm)

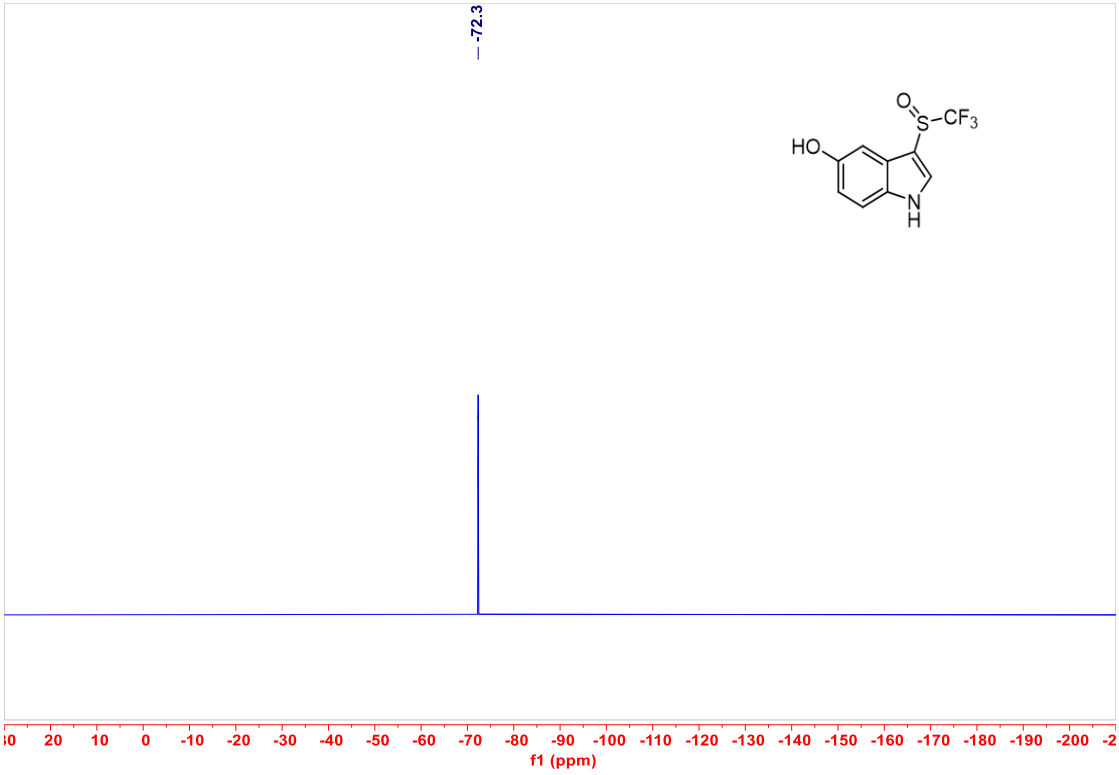

135.3
132.0
130.5
128.7
127.1
125.1
125.1
123.8
120.6
119.7
113.7
107.7
130.5
127.1
123.8
120.6
130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
Cl
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

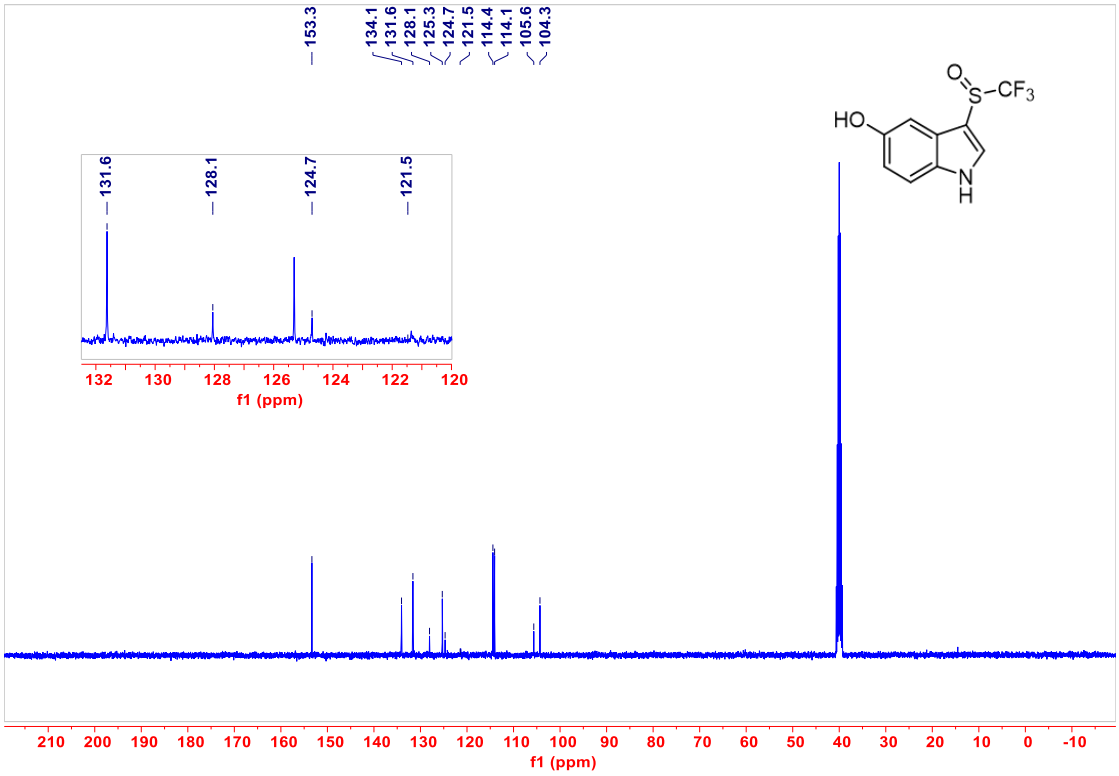

12.65
8.41
7.98
7.60
7.58
7.46
7.44
O
S
CF3
Br
N
H
1.02
1.00
1.00
1.01
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

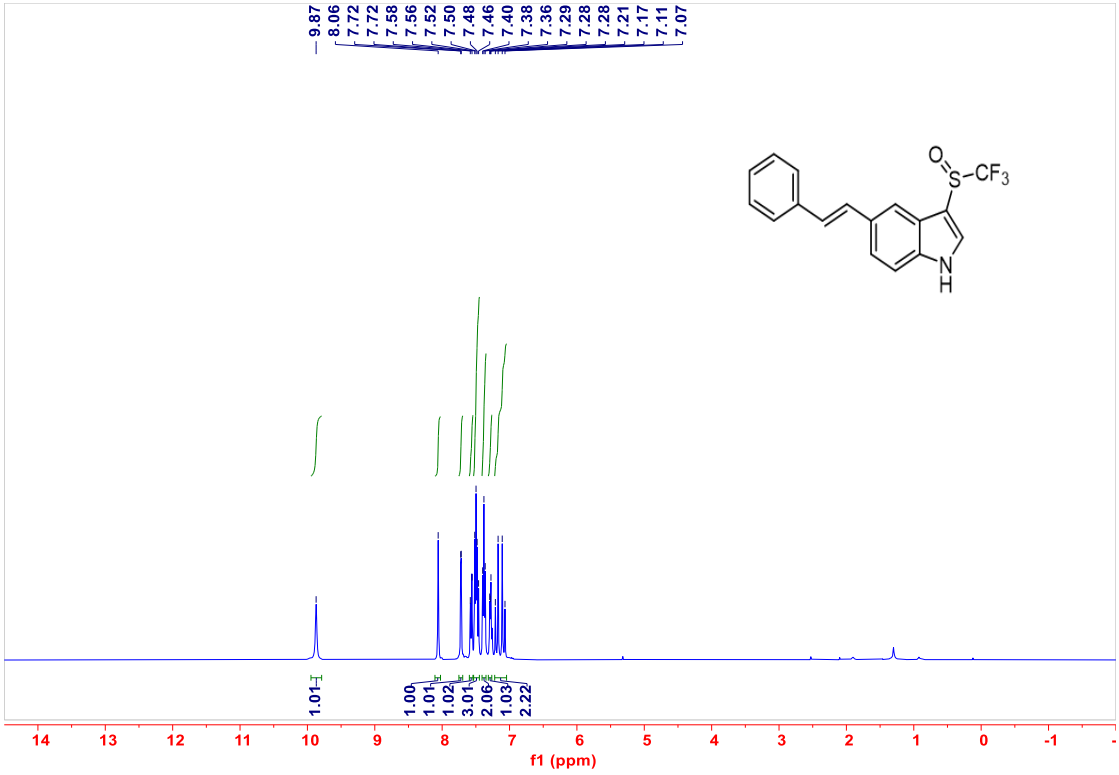

-72.9
Br
O
S
CF3
N
H
f1 (ppm)

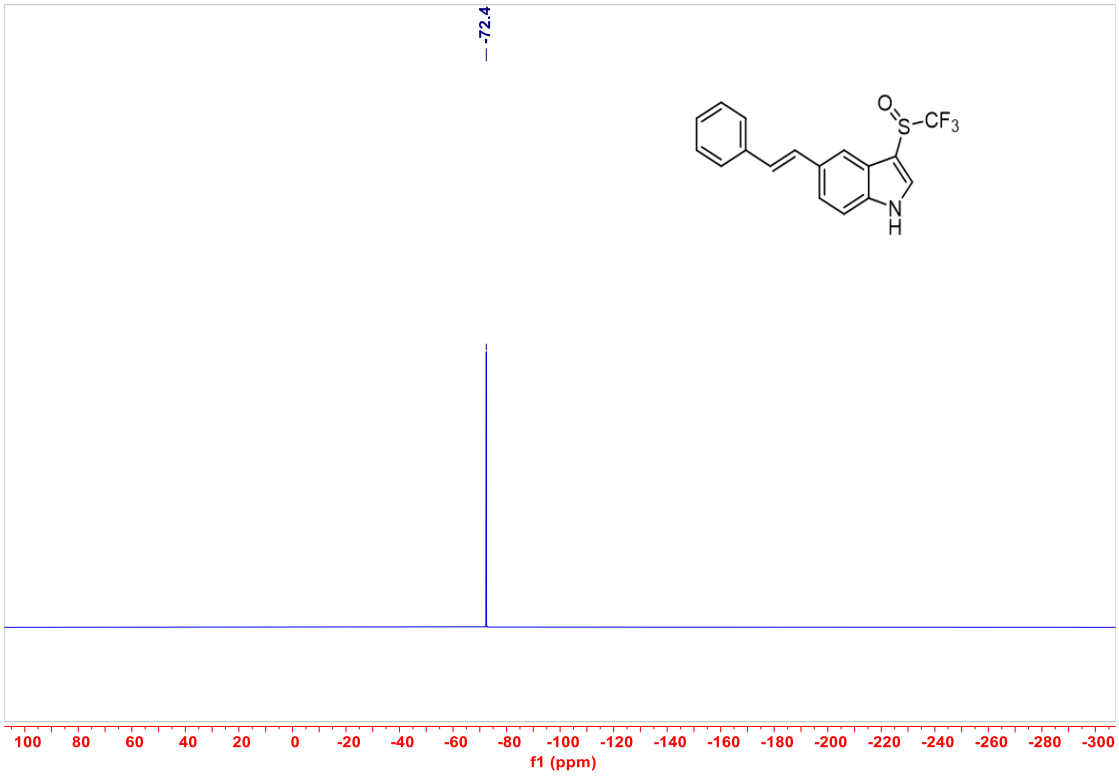

136.3
135.2
131.2
127.9
126.8
126.1
124.5
122.3
121.2
115.7
114.9
106.4
131.2
127.9
124.5
121.2
Br
O
S
CF3
N
H
f1 (ppm)

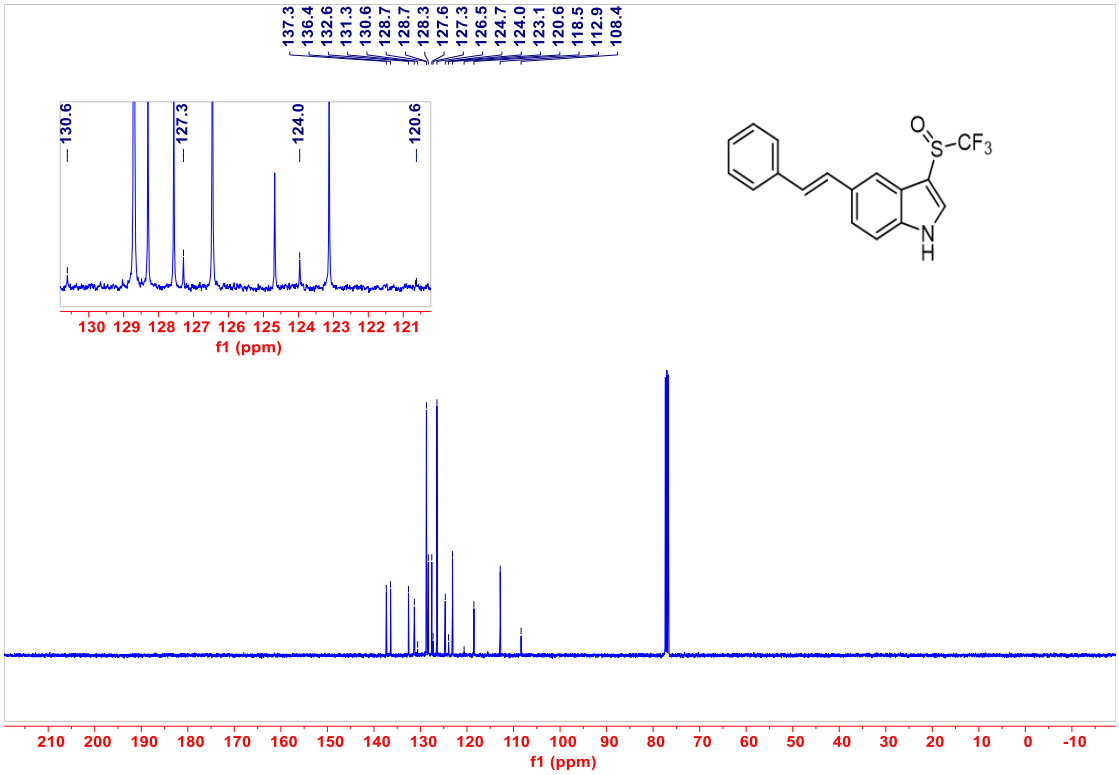

12.19
9.21
8.21
8.20
7.40
7.38
7.20
6.83
6.83
6.81
6.81
7.40
7.38
7.20
6.83
6.83
6.81
6.81
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
1.02
1.00
1.00
1.02
1.00
1.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
HO
S
CF3
O
N
H

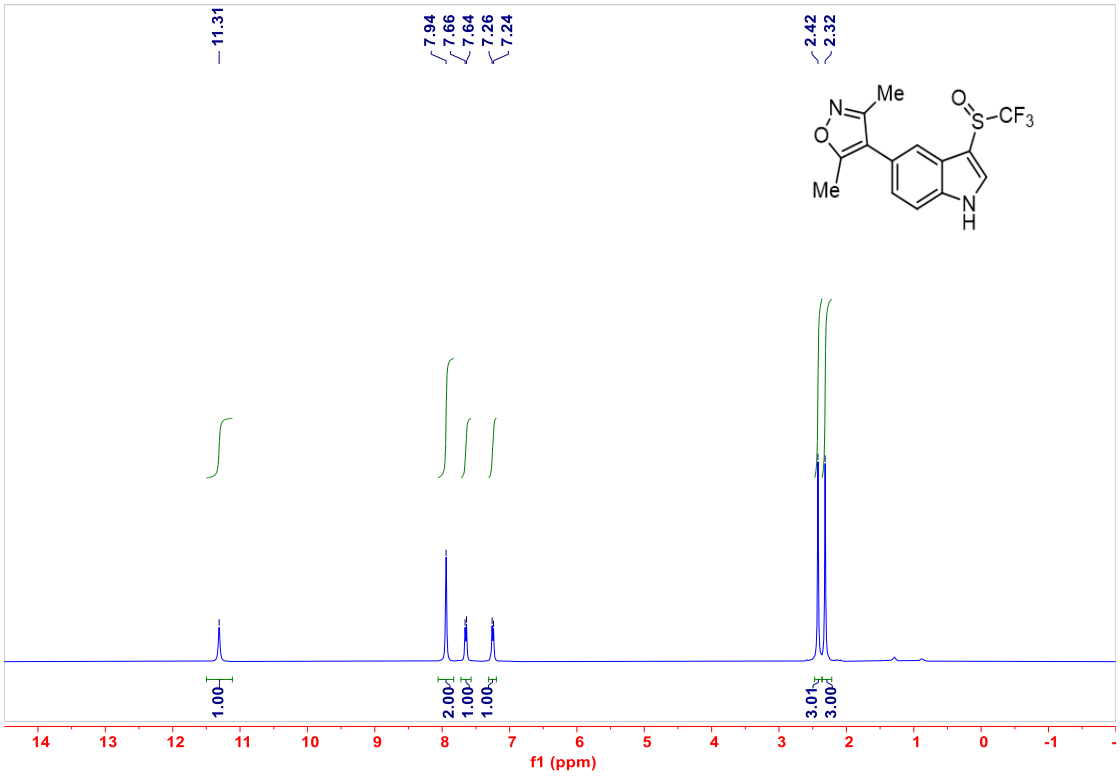

-72.3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)
HO
S
CF3
O
N
H

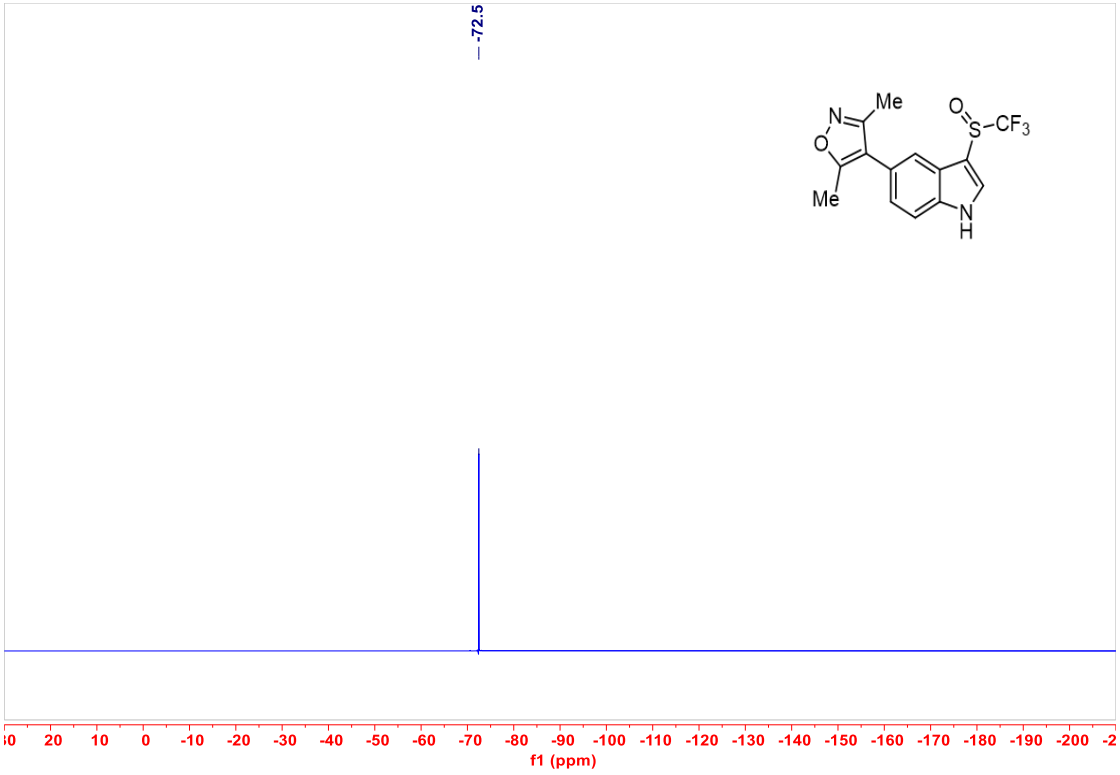

153.3
134.1
131.6
128.1
125.3
124.7
121.5
114.4
114.1
105.6
104.3
131.6
128.1
124.7
121.5
132 130 128 126 124 122 120
f1 (ppm)
HO
S
CF3
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

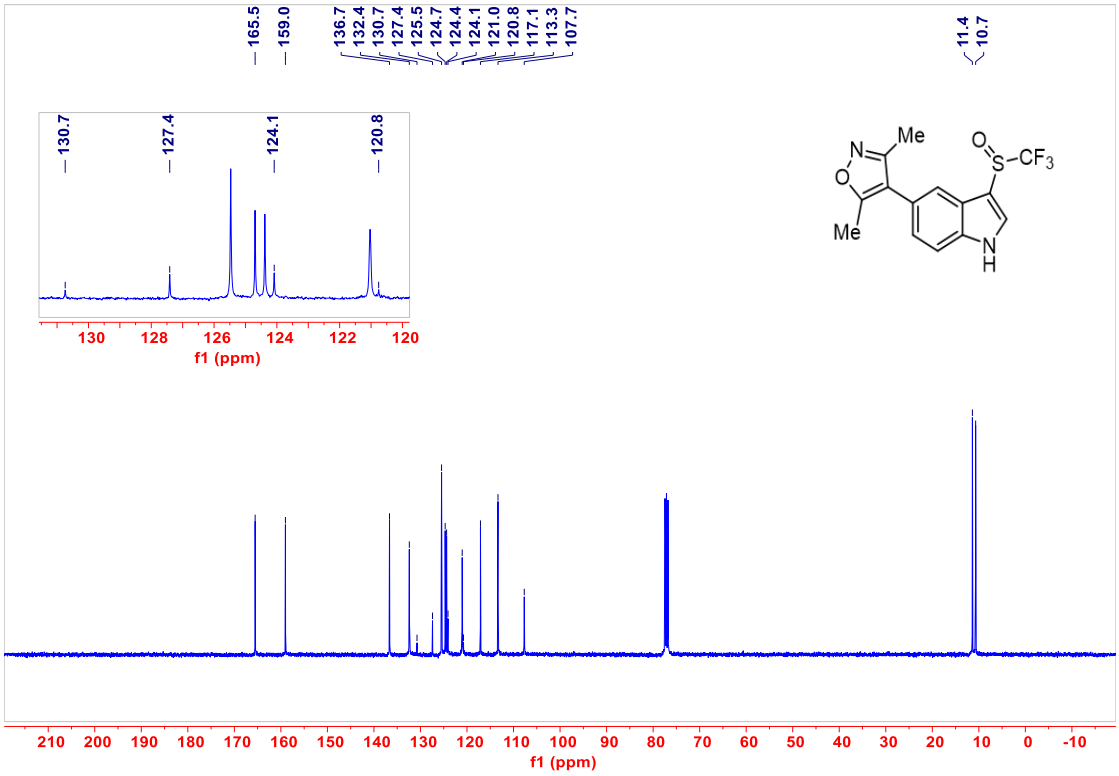

9.87
8.06
7.72
7.72
7.58
7.56
7.52
7.50
7.48
7.46
7.40
7.38
7.36
7.29
7.28
7.28
7.21
7.17
7.11
7.07
S
CF3
N
H
1.01
1.00
1.01
1.02
3.01
2.06
1.03
2.22
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

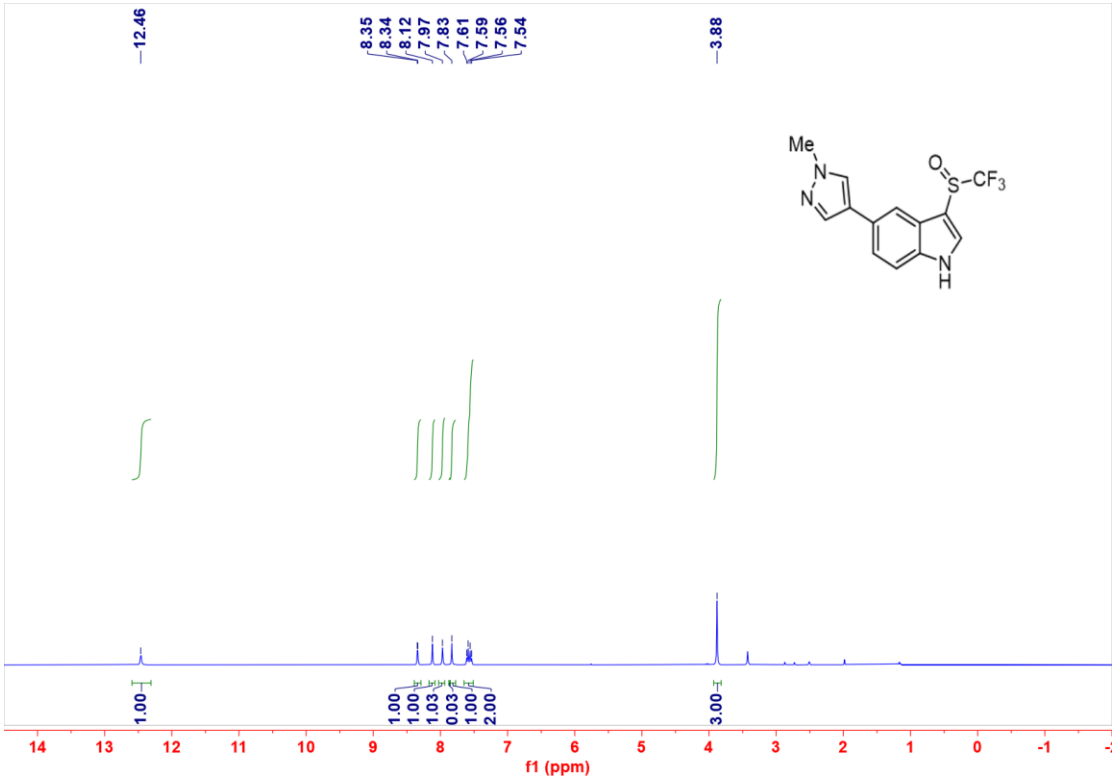

-72.4
O
S
CF3
N
H
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)

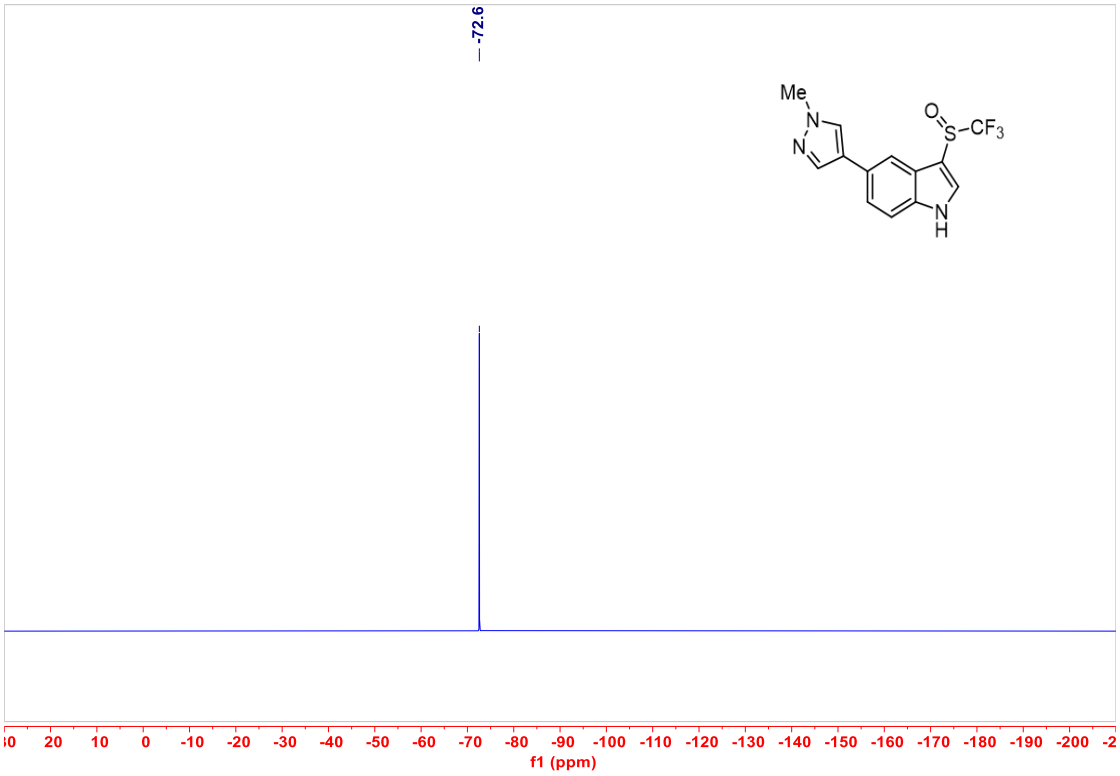

137.3
136.4
132.6
131.3
130.6
128.7
128.7
128.3
127.6
127.3
126.5
124.7
124.0
123.1
120.6
118.5
112.9
108.4
130.6
127.3
124.0
120.6
130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

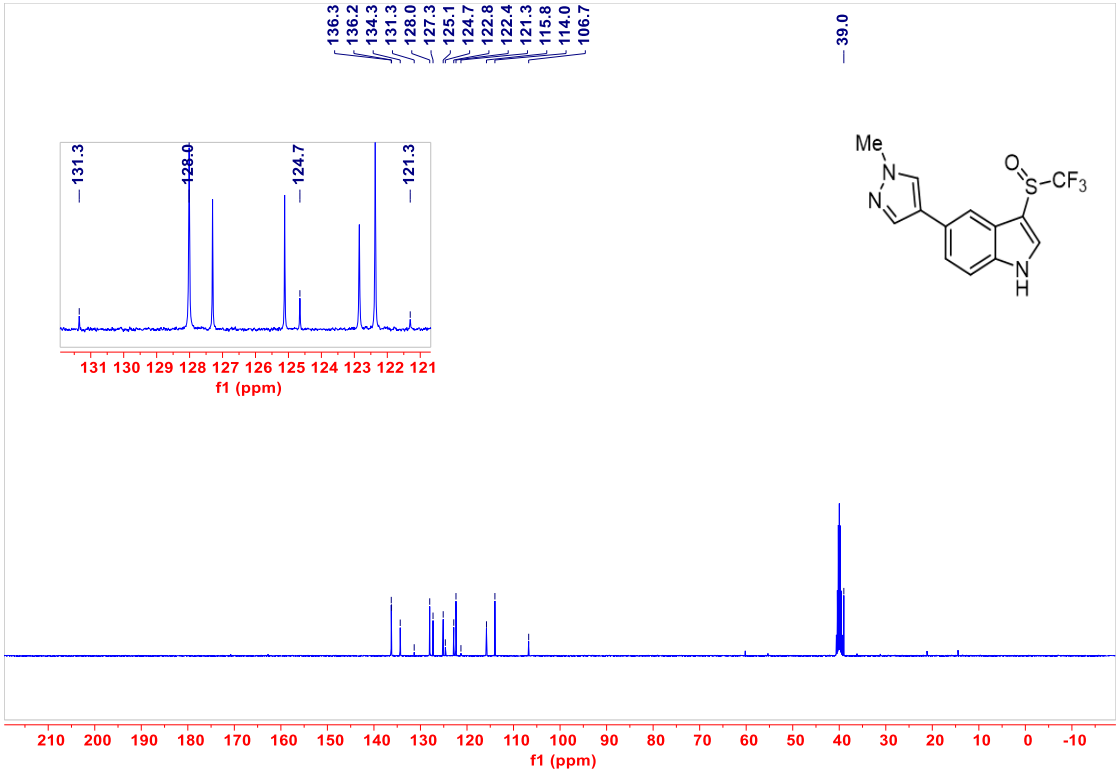

11.31
7.94
7.66
7.64
7.26
7.24
2.42
2.32
Me
N
O
Me
O
S
CF3
N
H
1.00
2.00
1.00
1.00
3.01
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

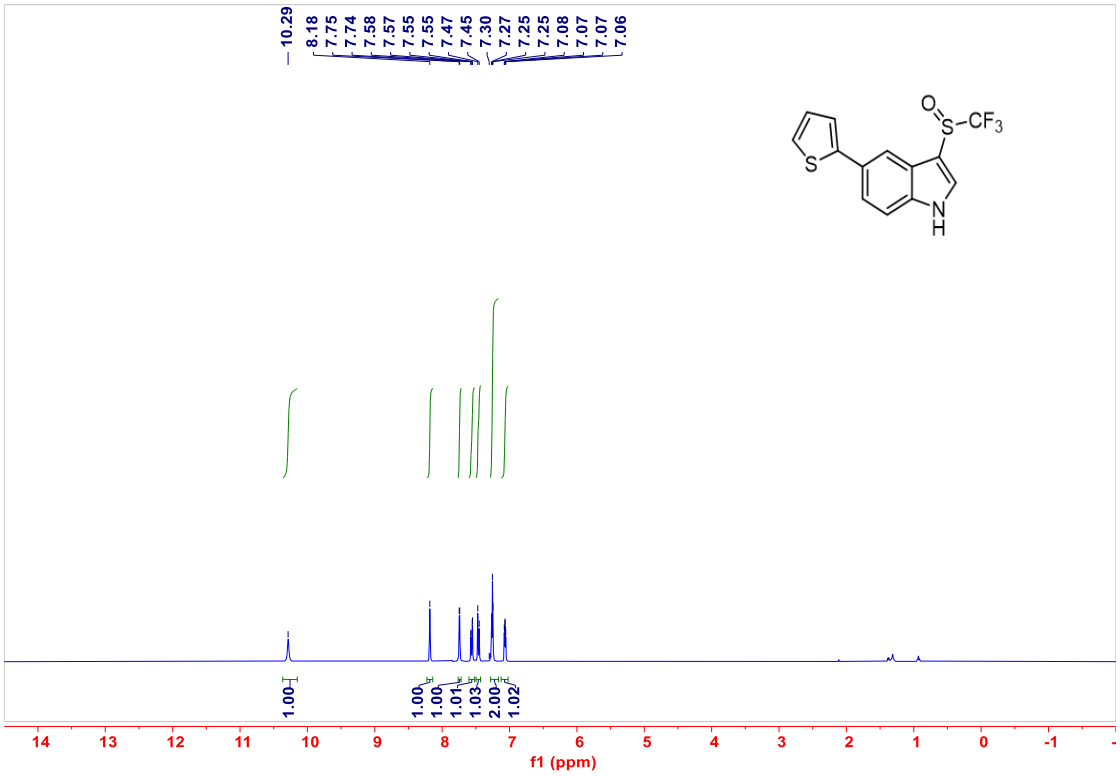

-72.5
Me
N
O
Me
O
S
CF3
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


165.5
159.0
136.7
132.4
130.7
127.4
125.5
124.7
124.4
124.1
121.0
120.8
117.1
113.3
107.7
11.4
10.7
130.7
127.4
124.1
120.8
130 128 126 124 122 120
f1 (ppm)
Me
N
O
Me
S
CF3
N
H
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)


12.46
8.35
8.34
8.12
7.97
7.83
7.61
7.59
7.56
7.54
3.88
Me
N
N
S
CF3
N
H
1.00
1.00
1.00
1.03
0.03
1.00
2.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-72.6
Me
N
N
O
S
CF3
N
H
f1 (ppm)


136.3
136.2
134.3
131.3
128.0
127.3
125.1
124.7
122.8
122.4
121.3
115.8
114.0
106.7
39.0
131.3
128.0
124.7
121.3
f1 (ppm)
Me
N
N
O
S
CF3
N
H
f1 (ppm)


10.29
8.18
7.75
7.74
7.58
7.57
7.55
7.55
7.47
7.45
7.30
7.27
7.25
7.25
7.08
7.07
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7.06
1.00
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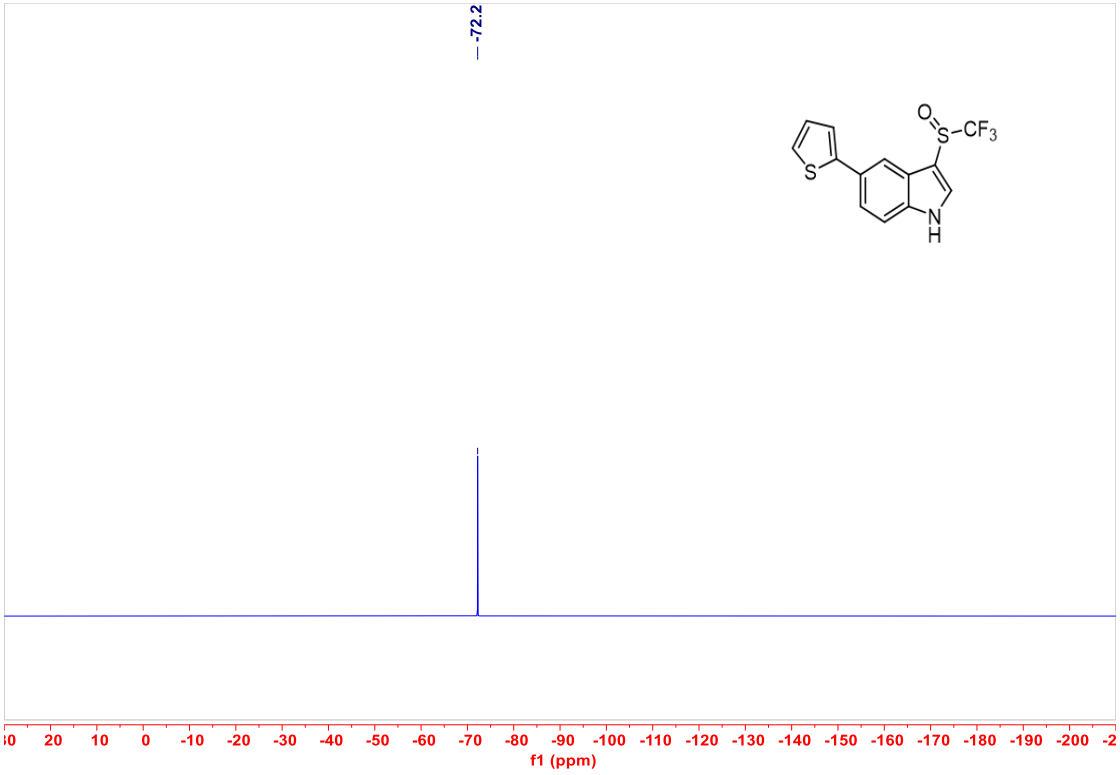
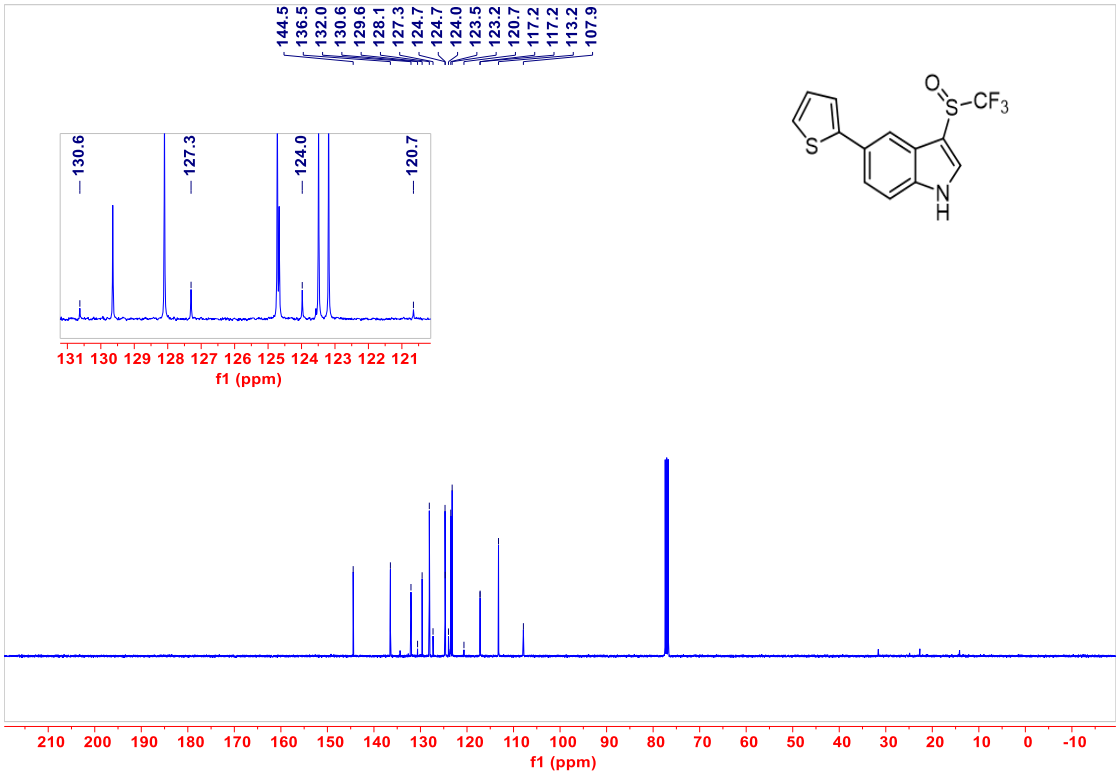
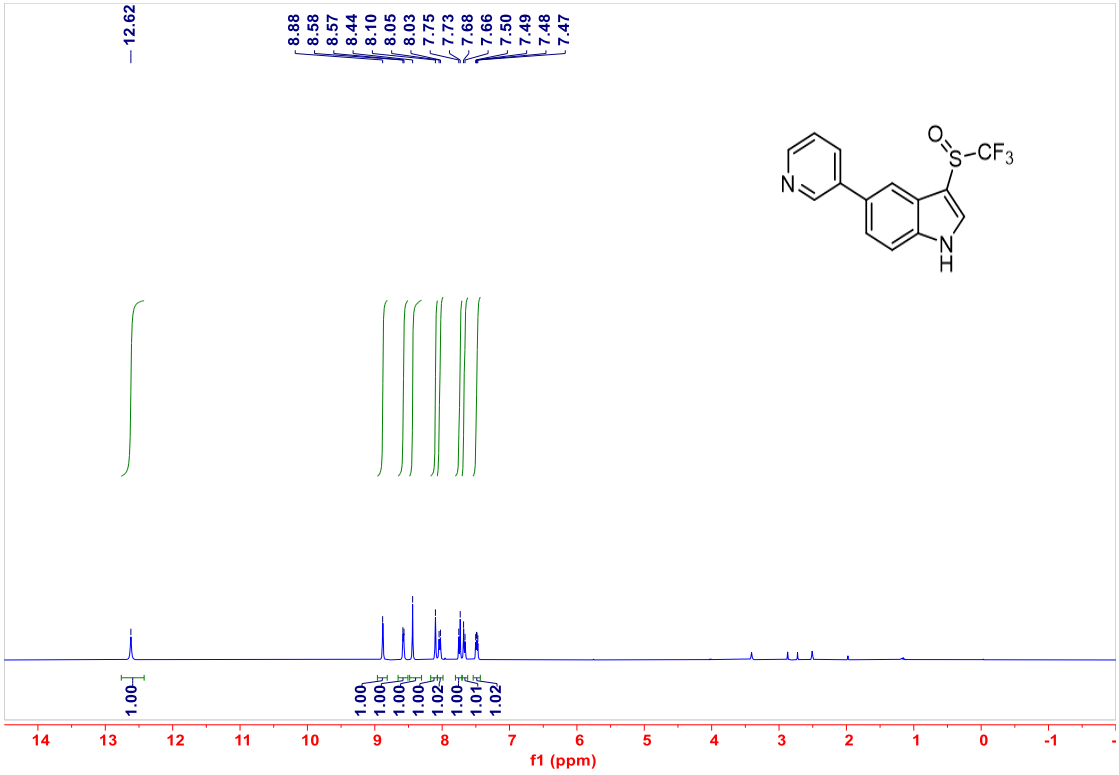
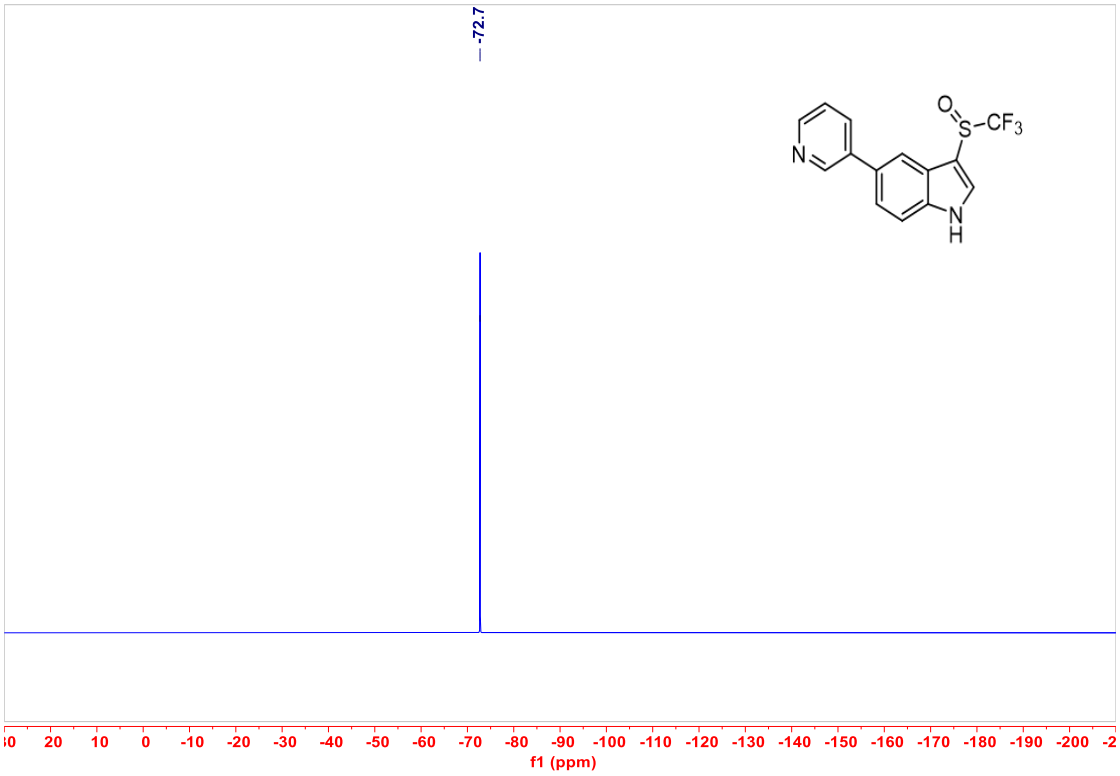
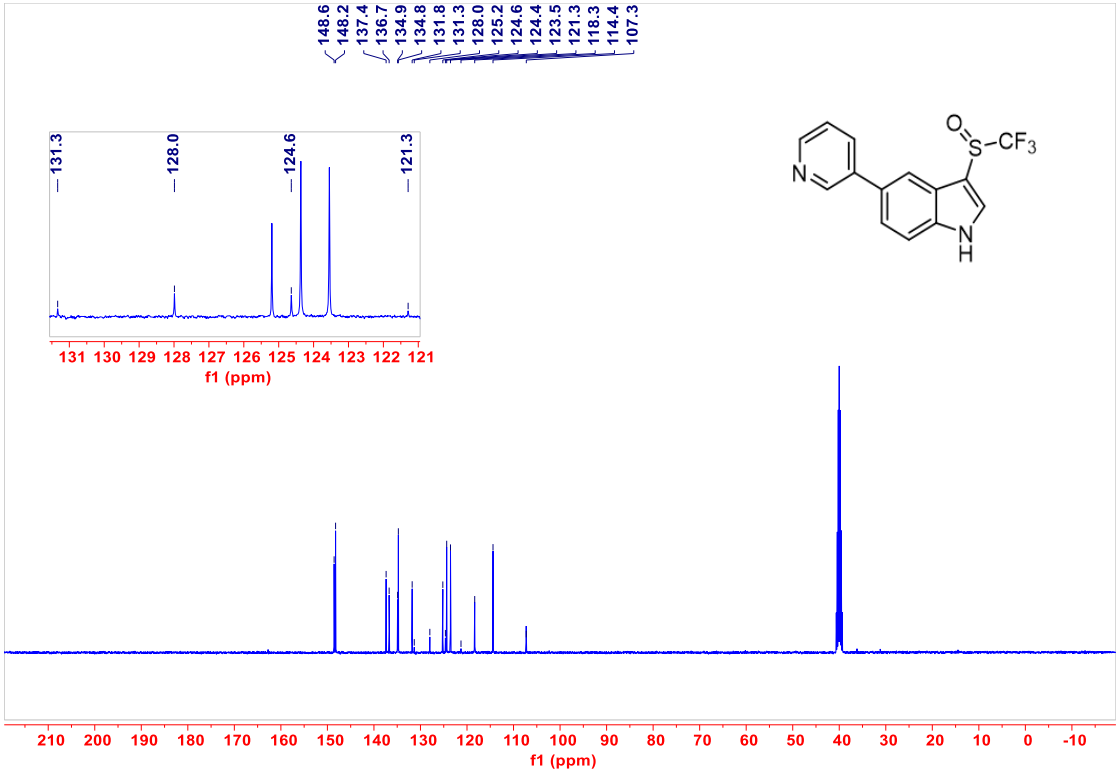
1.00
1.01
1.03
2.00
1.02
f1 (ppm)

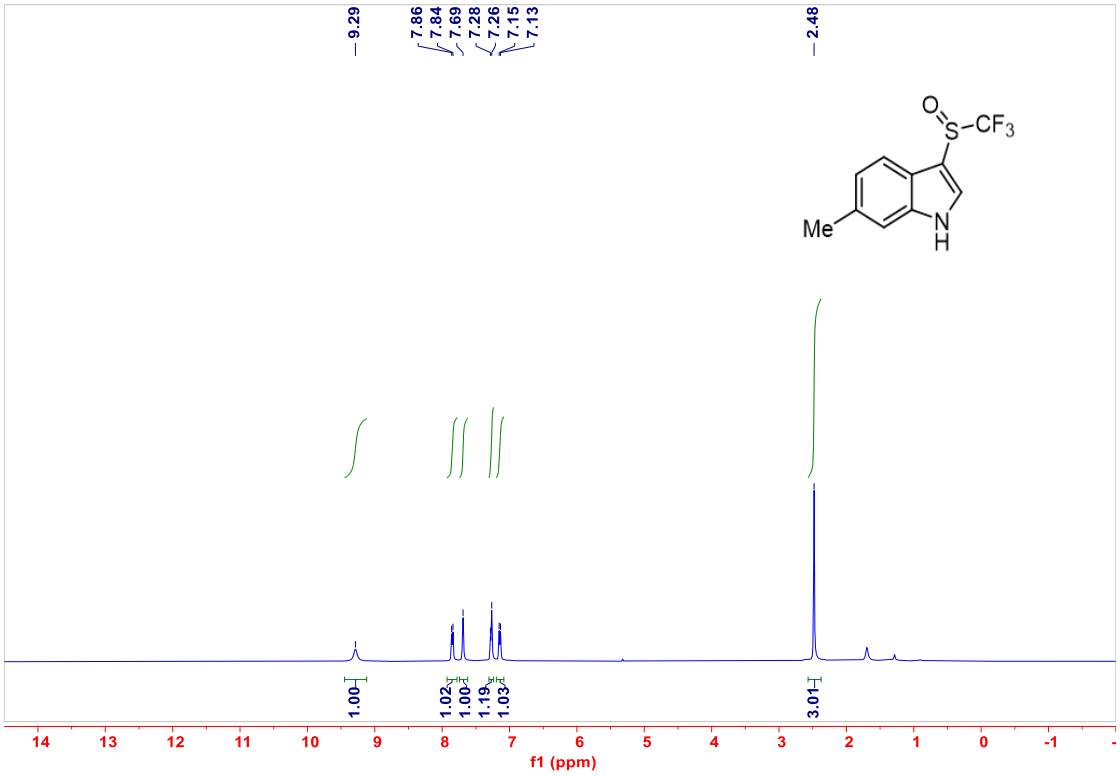

-72.2
f1 (ppm)

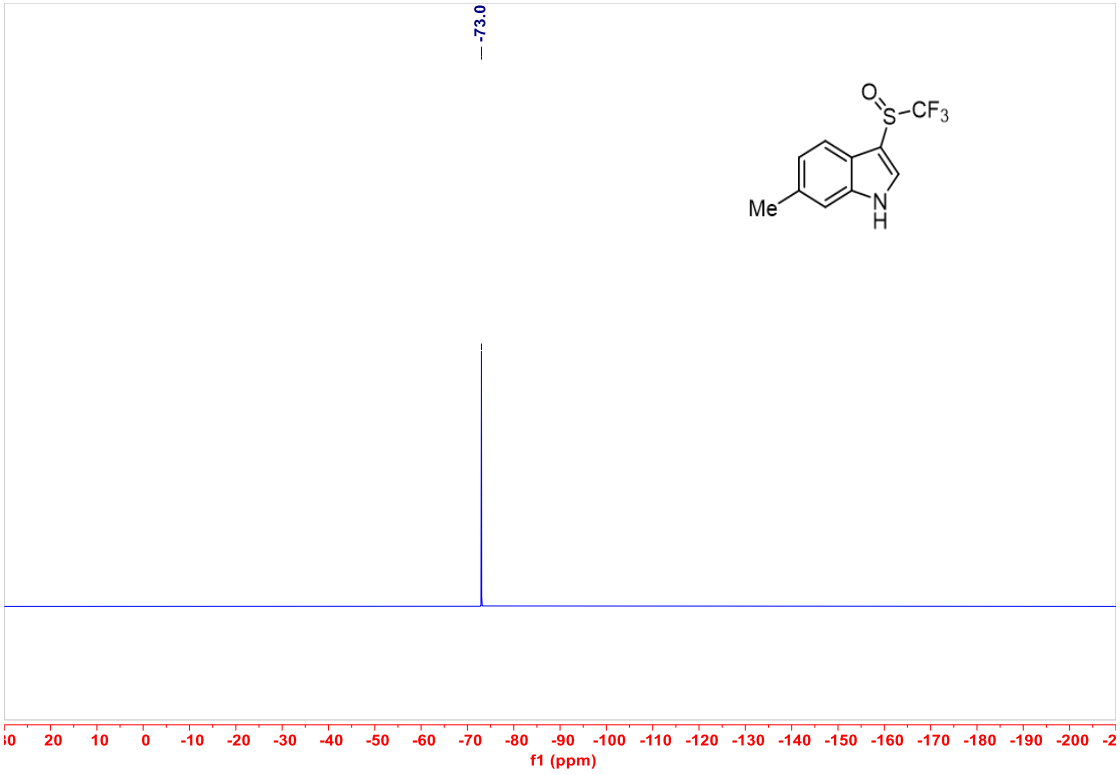

144.5
136.5
132.0
130.6
129.6
128.1
127.3
124.7
124.7
124.0
123.5
123.2
120.7
117.2
117.2
113.2
107.9
130.6
127.3
124.0
120.7
131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
S
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

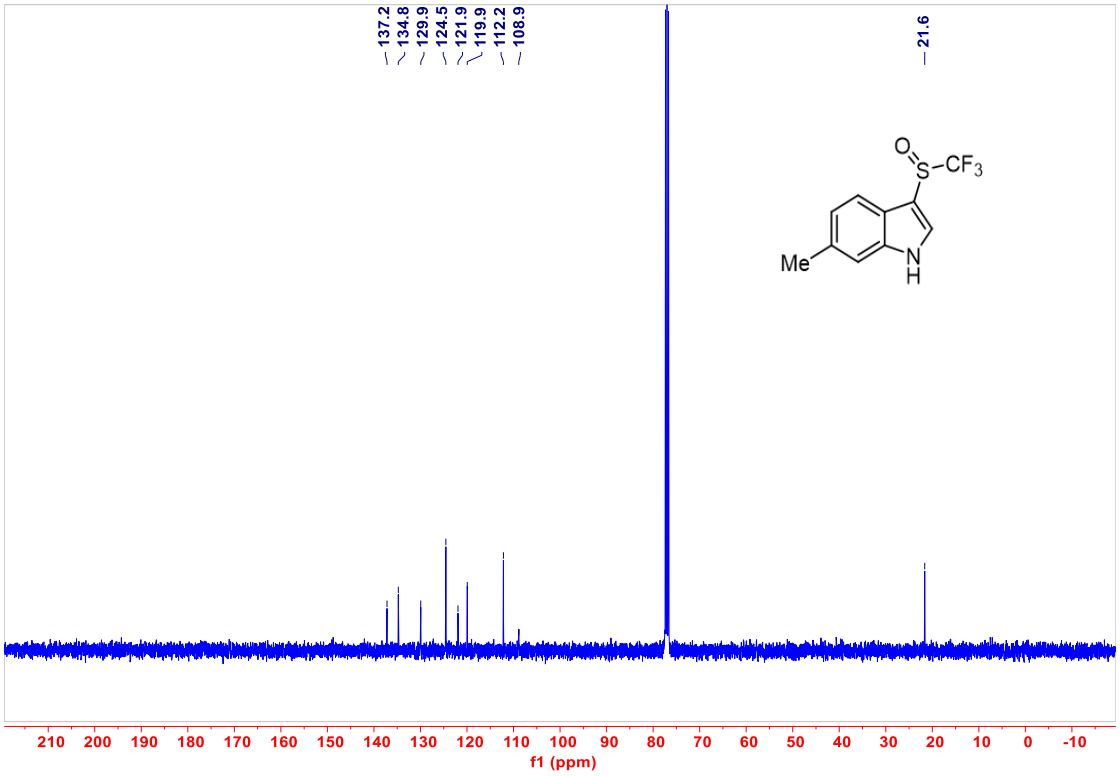

12.62
8.88
8.58
8.57
8.44
8.10
8.05
8.03
7.75
7.73
7.68
7.66
7.50
7.49
7.48
7.47
O
S
CF3
N
N
H
1.00
1.00
1.00
1.00
1.00
1.02
1.00
1.01
1.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

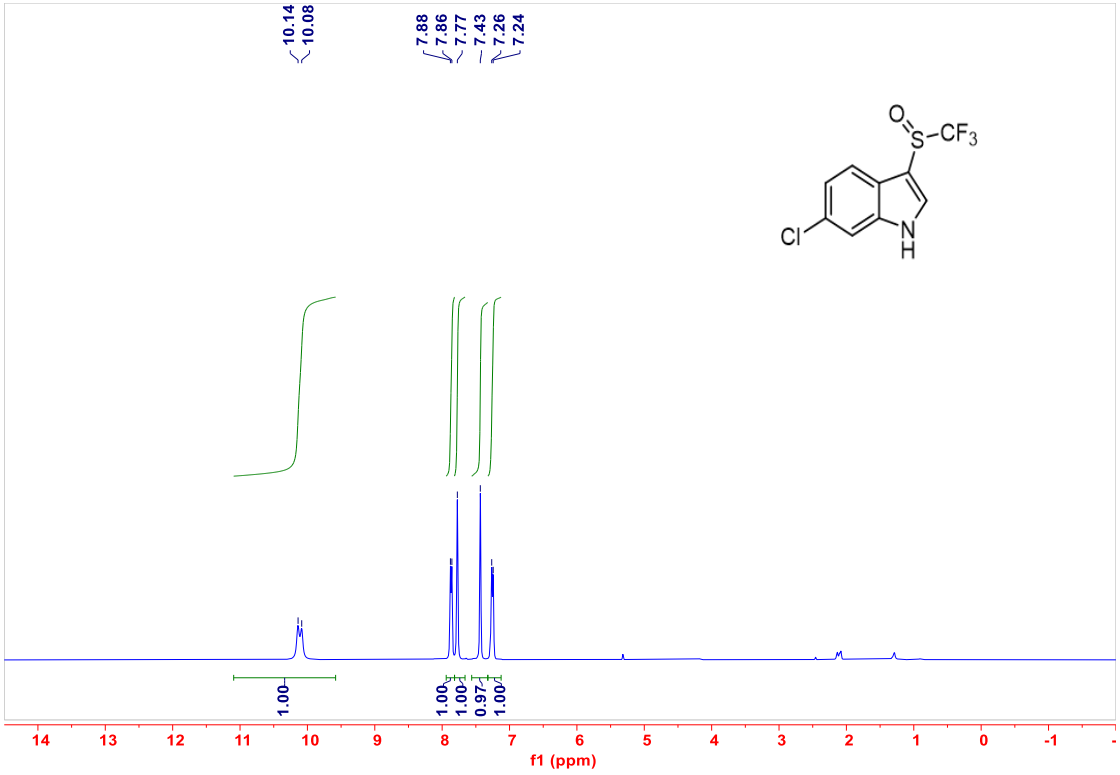

-72.7
O
S
CF3
N
N
H
f1 (ppm)

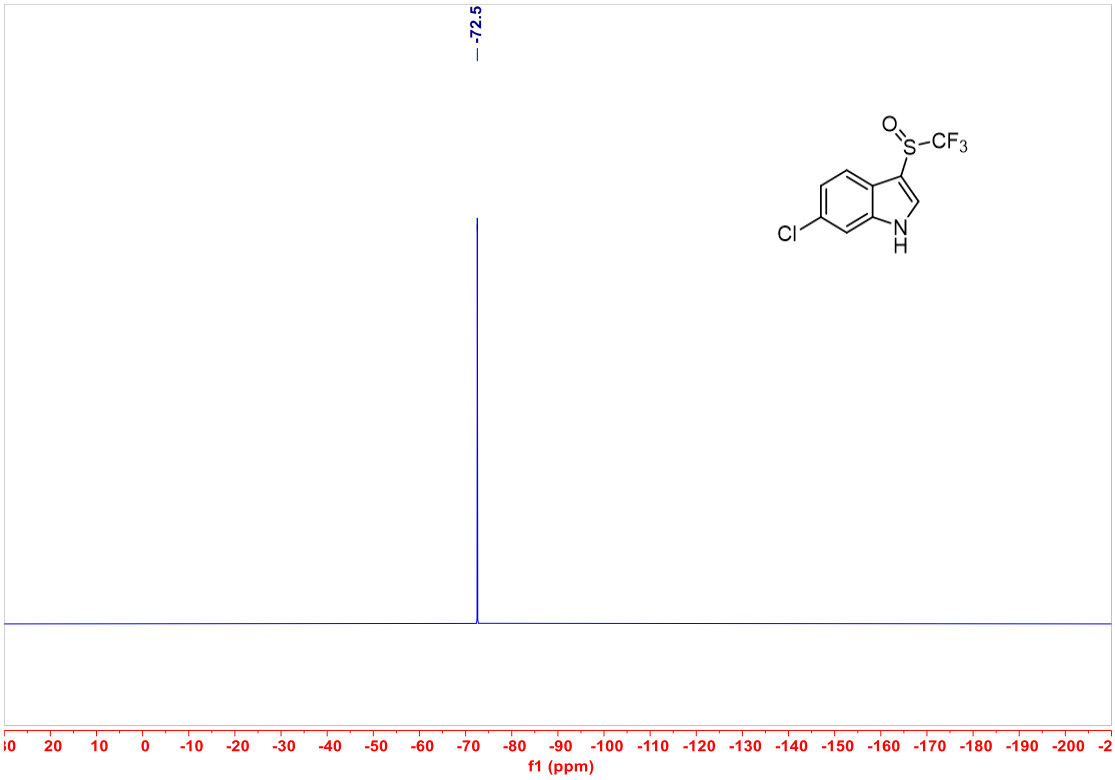

148.6
148.2
137.4
136.7
134.9
134.8
131.8
131.3
128.0
125.2
124.6
124.4
123.5
121.3
118.3
114.4
107.3
131.3
128.0
124.6
121.3
f1 (ppm)
O
S
CF3
N
N
H
f1 (ppm)

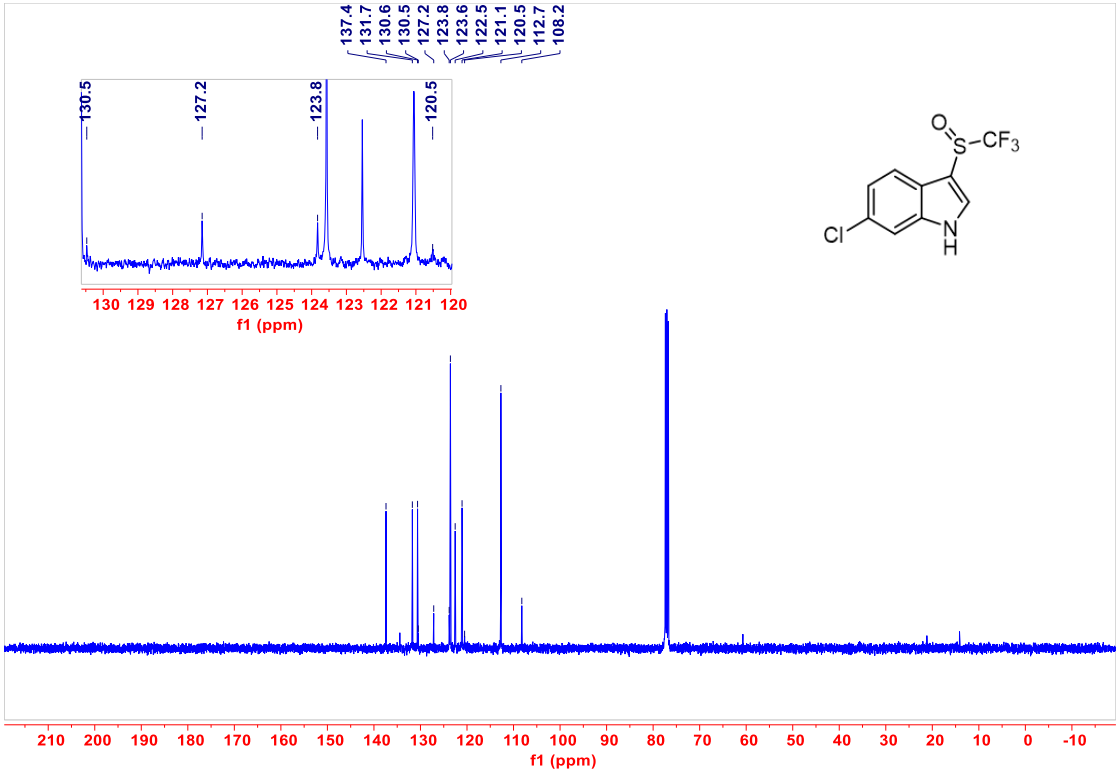

9.29
7.86
7.84
7.69
7.28
7.26
7.15
7.13
2.48
O
S
CF3
Me
N
H
1.00
1.02
1.00
1.19
1.03
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

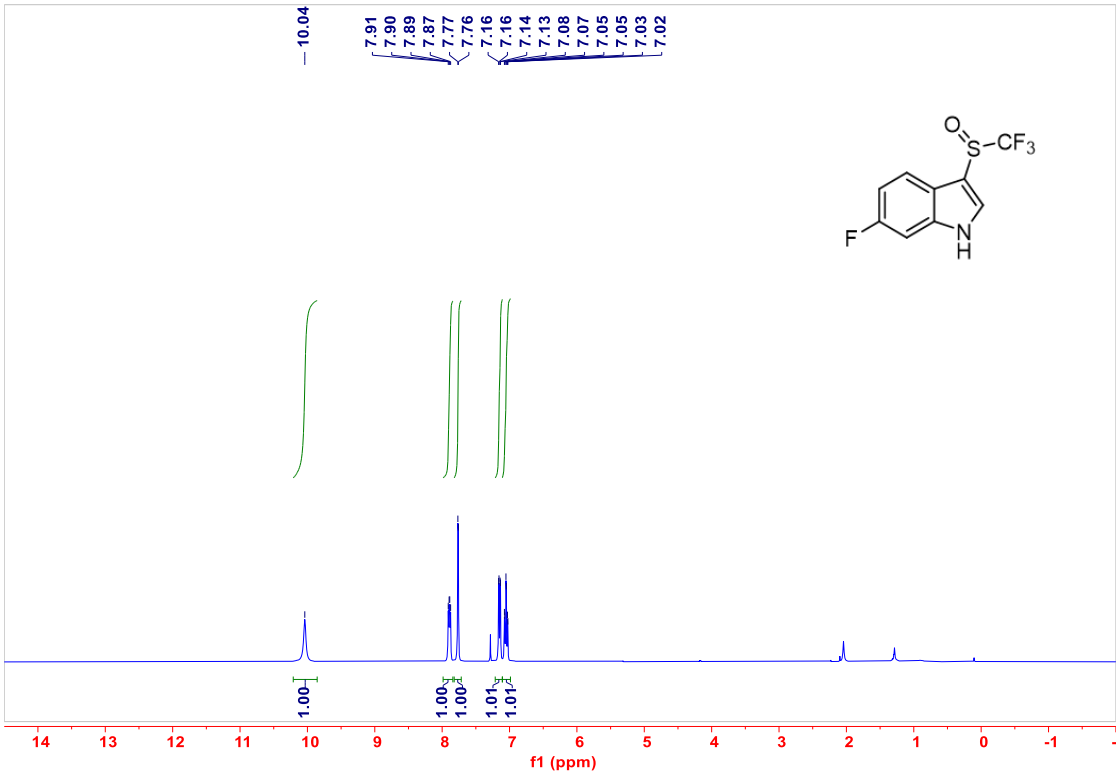

-73.0
O
S
CF3
Me
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

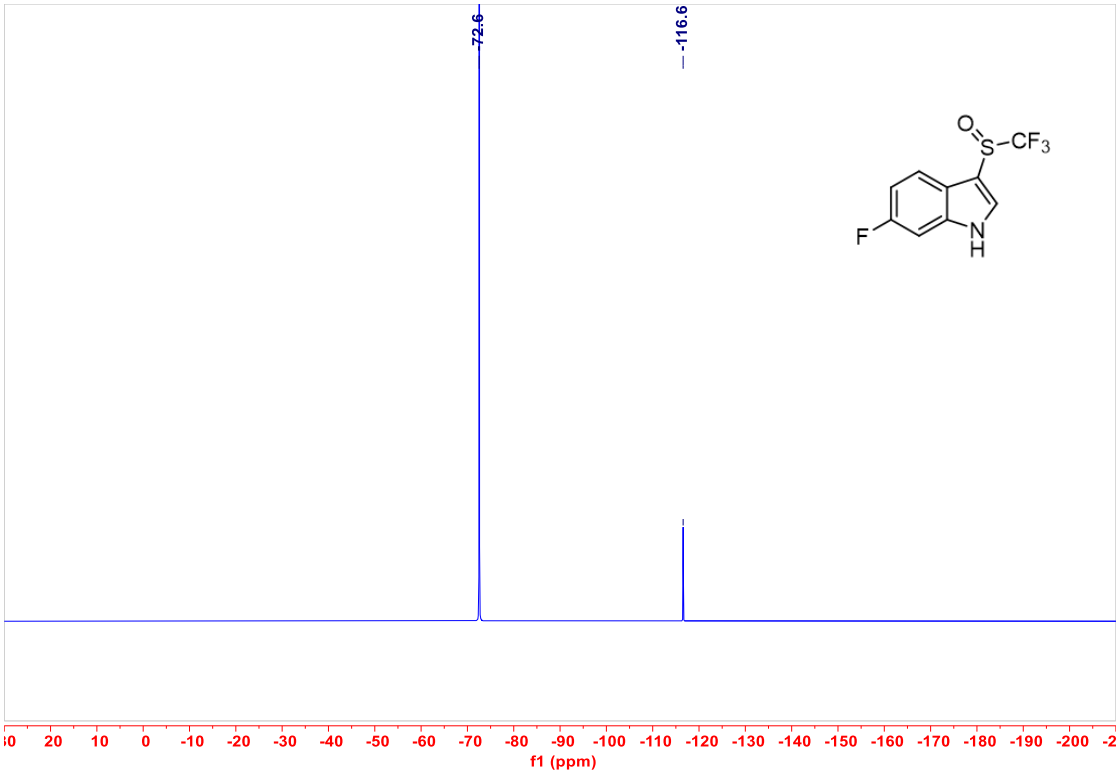

137.2
134.8
129.9
124.5
121.9
119.9
112.2
108.9
21.6
O
S
CF3
Me
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

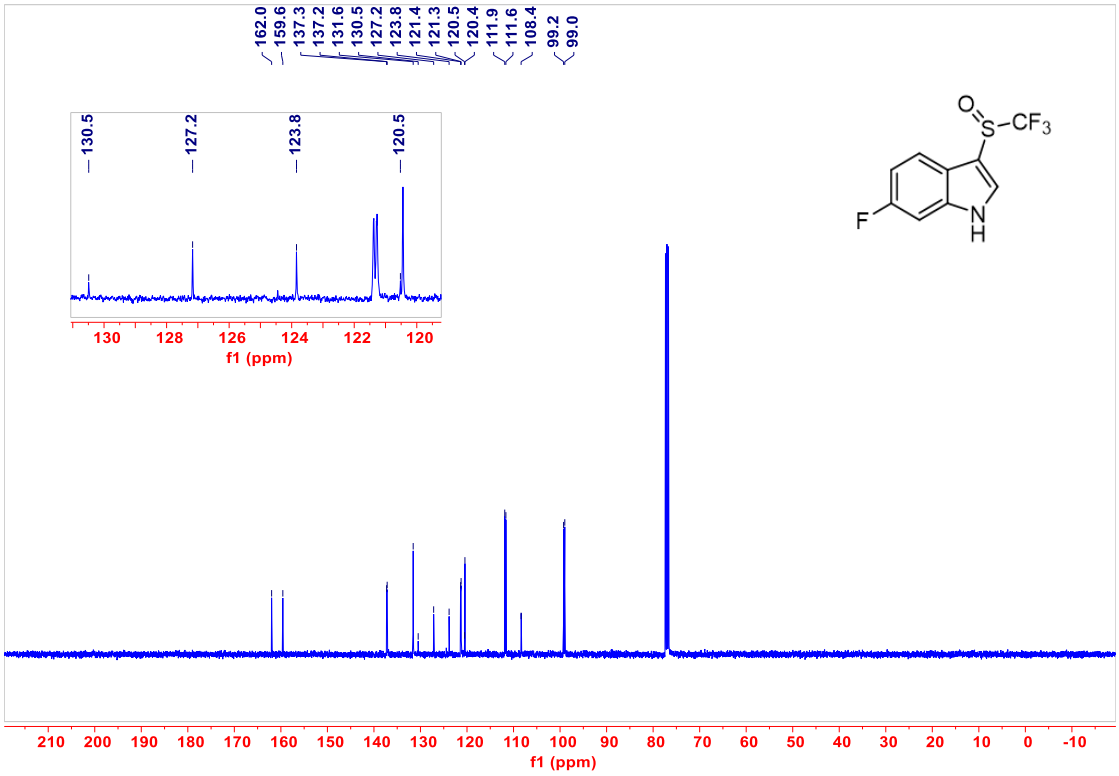

10.14
10.08
7.88
7.86
7.77
7.43
7.26
7.24
O
S
CF3
Cl
N
H
1.00
1.00
1.00
0.97
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

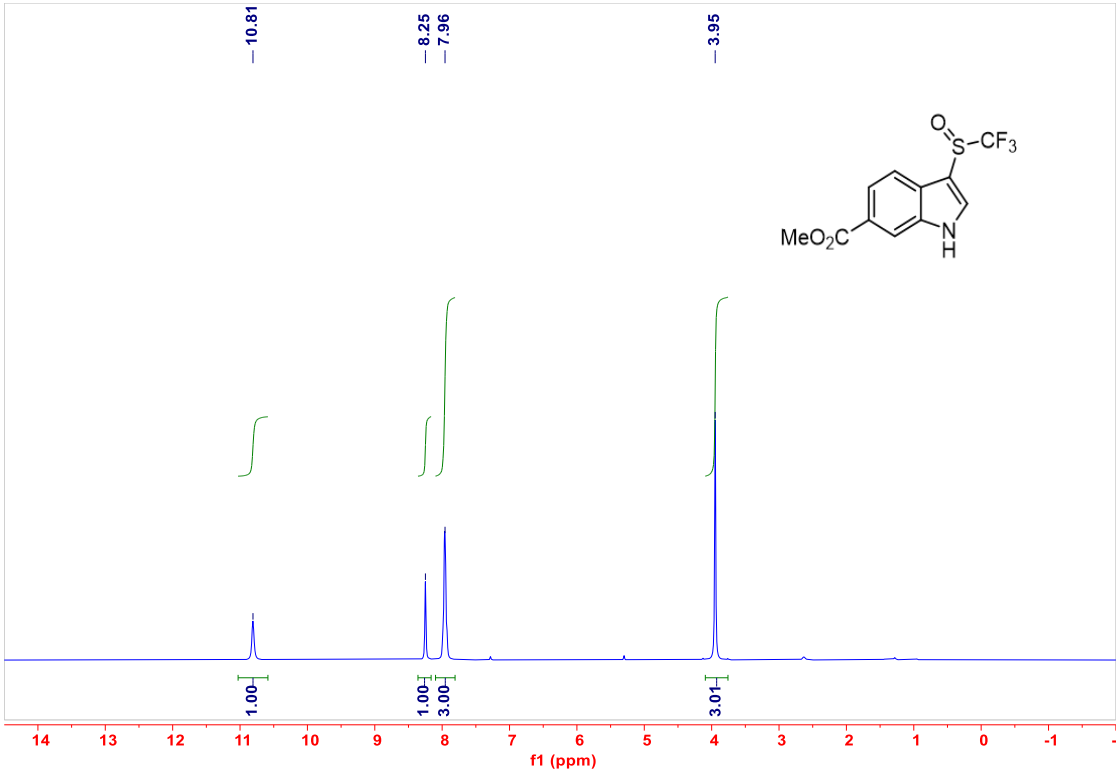

-72.5
O
S
CF3
Cl
N
H
f1 (ppm)

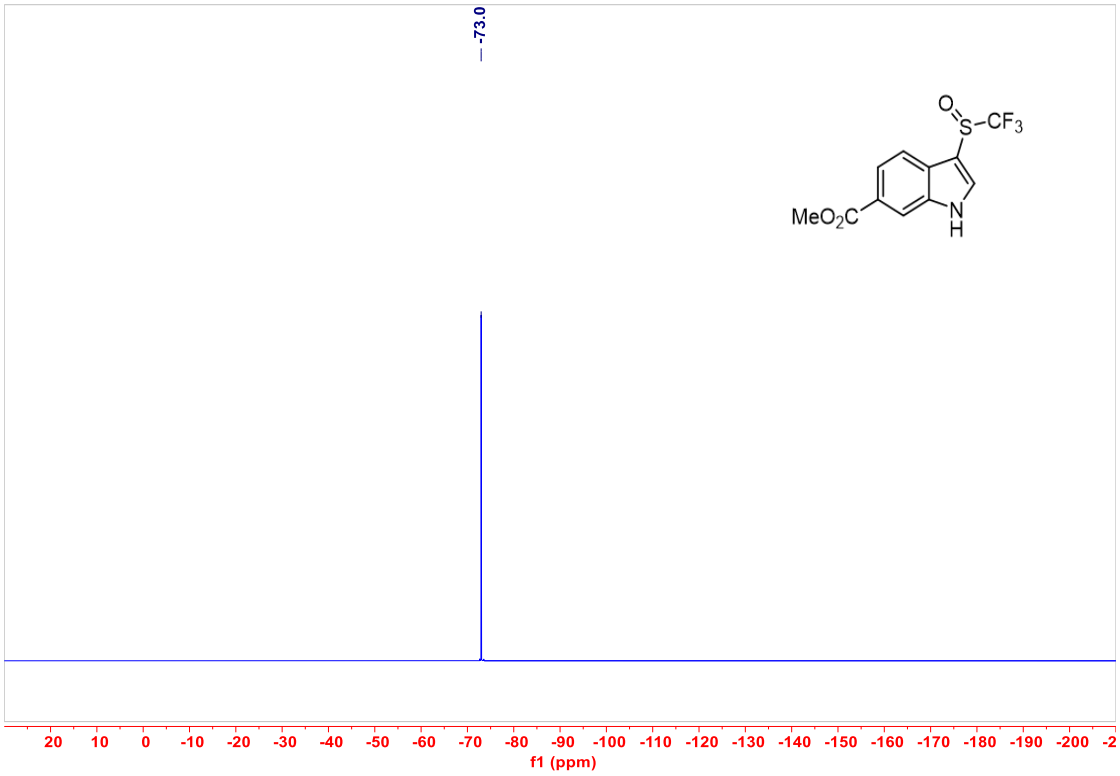

137.4
131.7
130.6
130.5
127.2
123.8
123.6
122.5
121.1
120.5
112.7
108.2
130.5
127.2
123.8
120.5
f1 (ppm)
O
S
CF3
Cl
N
H
f1 (ppm)

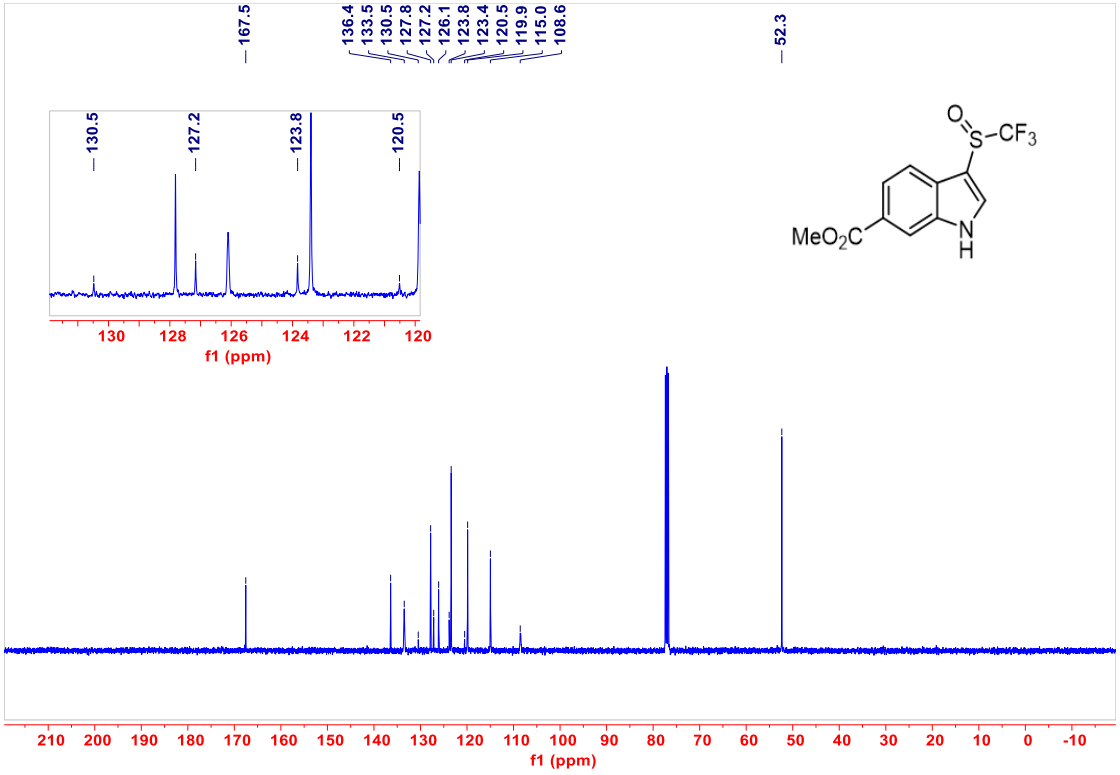

10.04
7.91
7.90
7.89
7.87
7.77
7.76
7.16
7.16
7.14
7.13
7.08
7.07
7.05
7.05
7.03
7.02
O
S
CF3
F
N
H
1.00
1.00
1.00
1.01
1.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

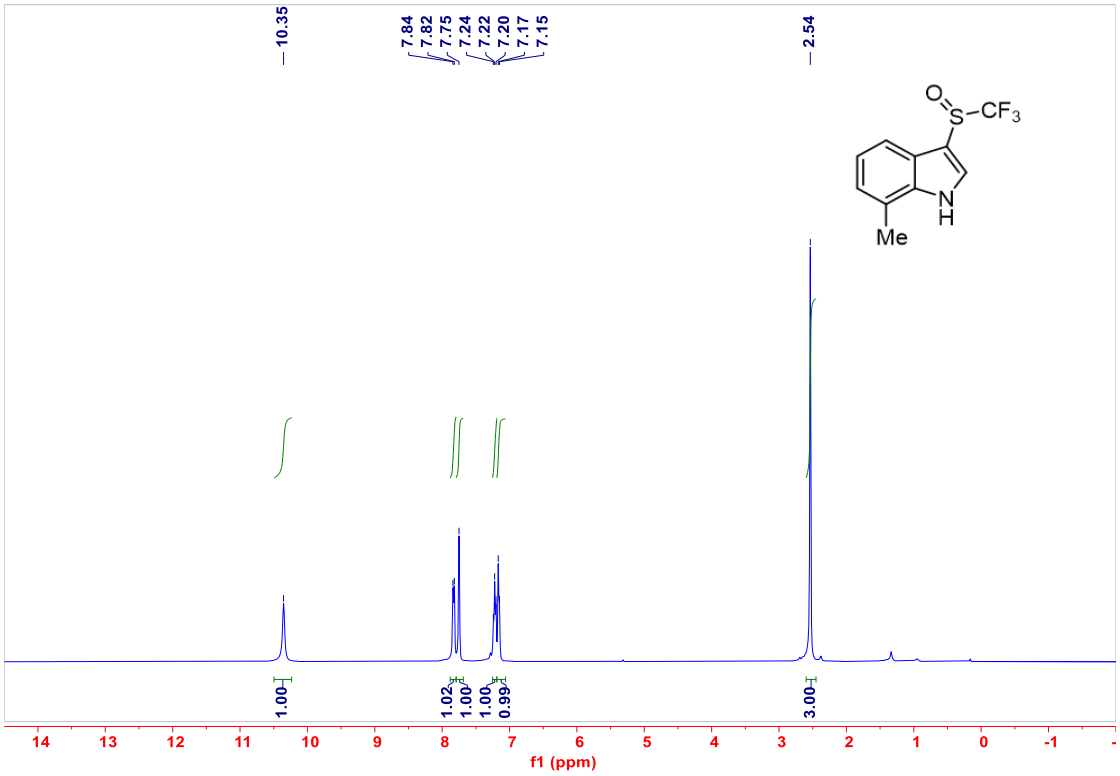

-72.6
-116.6
O
S
CF3
F
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

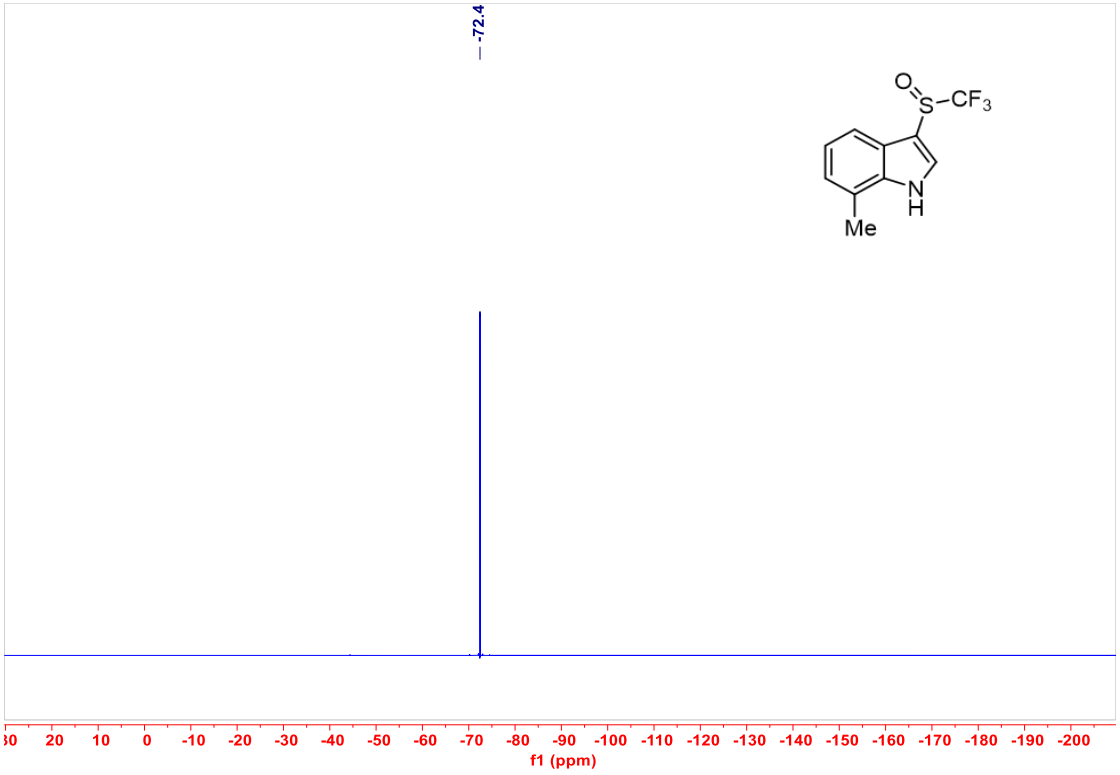

162.0
159.6
137.3
137.2
131.6
130.5
127.2
123.8
121.4
121.3
120.5
120.4
111.9
111.6
108.4
99.2
99.0
130.5
127.2
123.8
120.5
130 128 126 124 122 120
f1 (ppm)
O
S
CF3
F
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

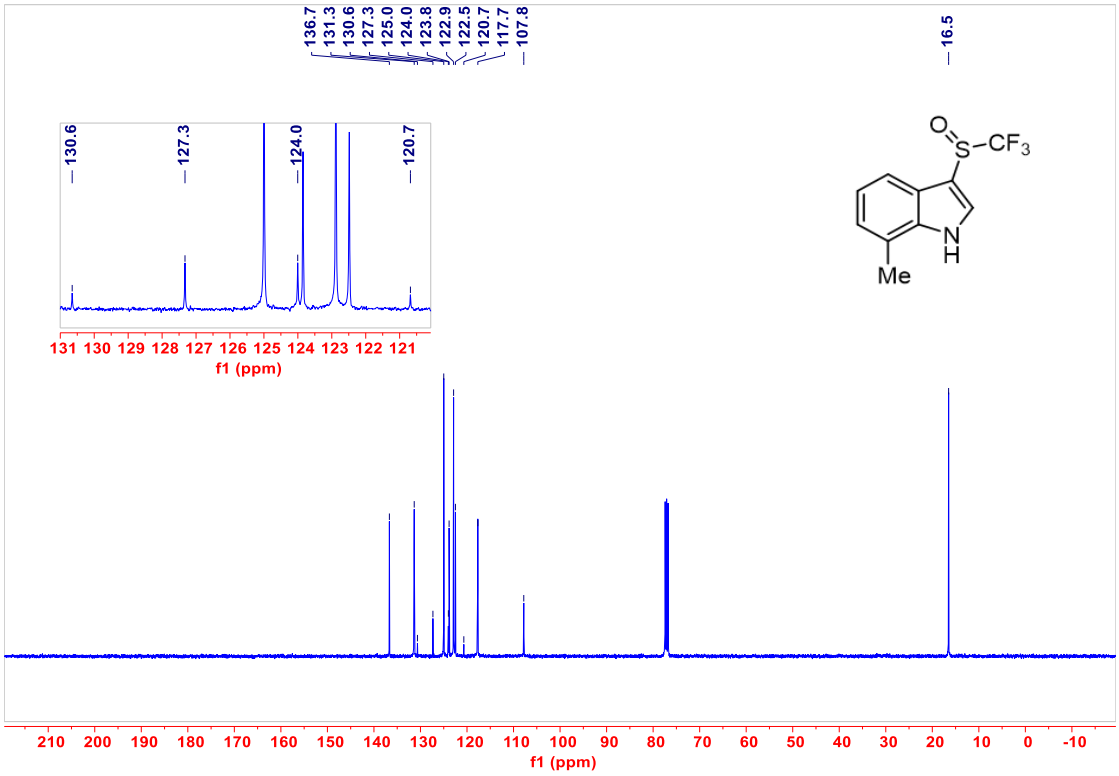

10.81
8.25
7.96
3.95
O
S
CF3
MeO2C
N
H
1.00
1.00
3.00
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

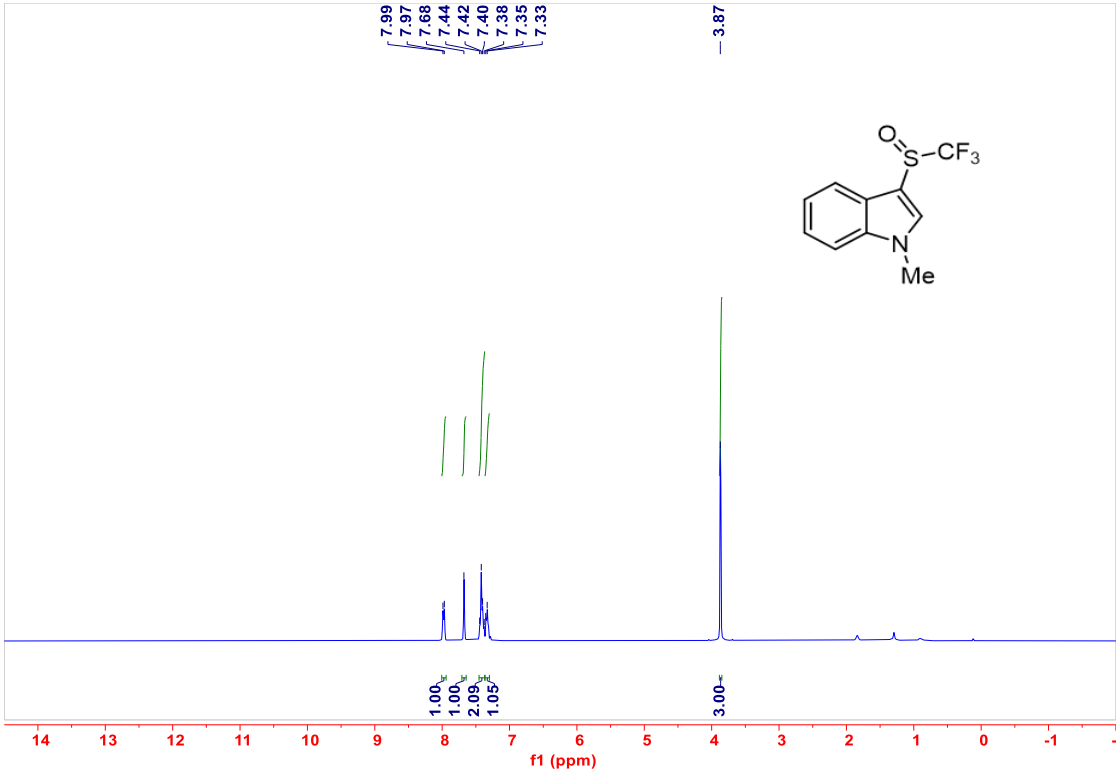

-73.0
MeO2C
S
CF3
O
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

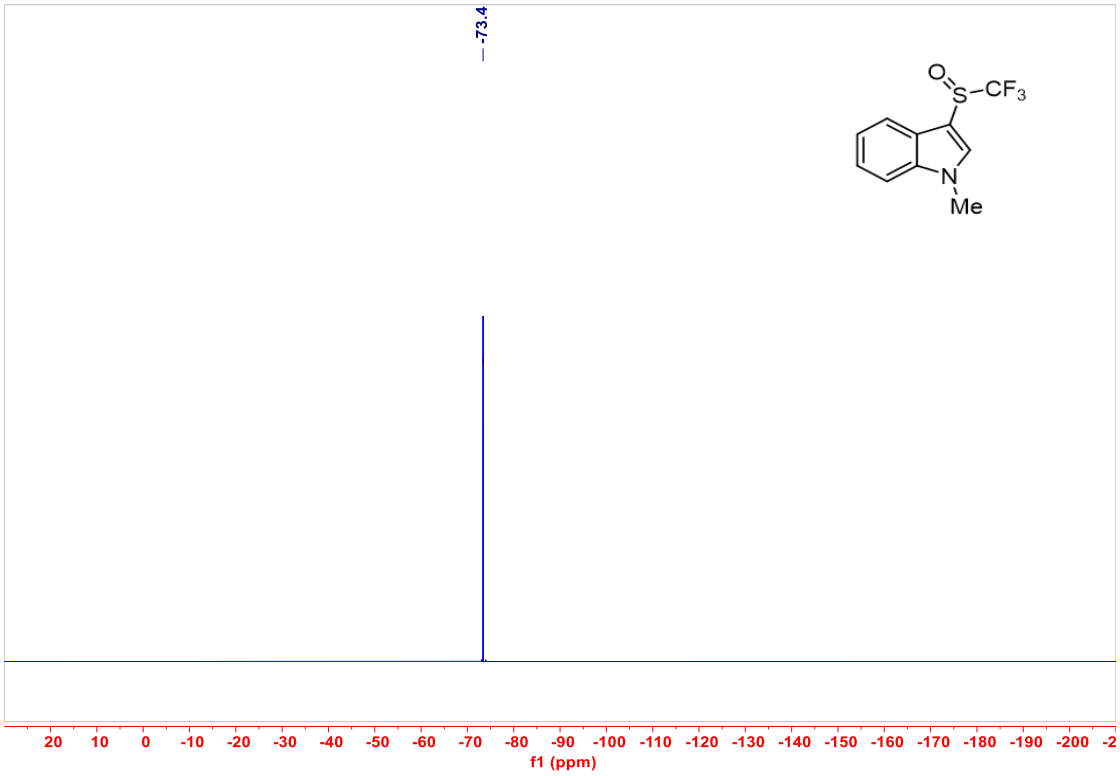

167.5
136.4
133.5
130.5
127.8
127.2
126.1
123.8
123.4
120.5
119.9
115.0
108.6
52.3
130.5
127.2
123.8
120.5
130 128 126 124 122 120
f1 (ppm)
MeO2C
S
CF3
O
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

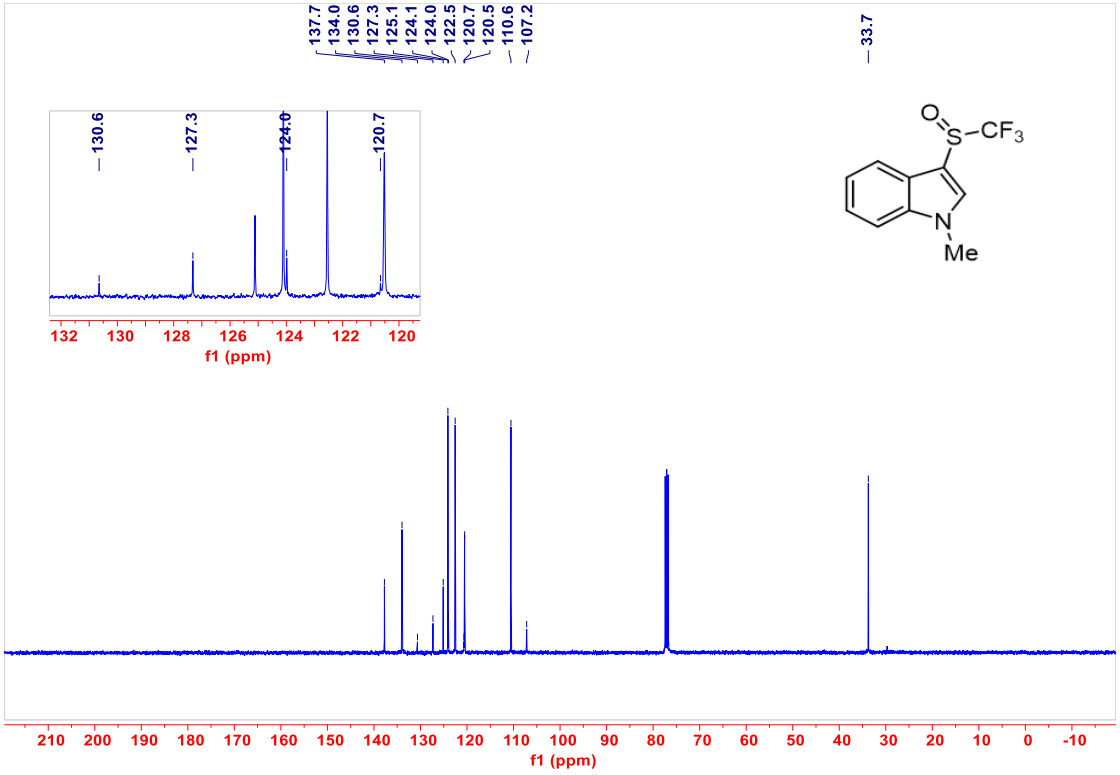

10.35
7.84
7.82
7.75
7.24
7.22
7.20
7.17
7.15
2.54
1.00
1.02
1.00
1.00
0.99
3.00
f1 (ppm)

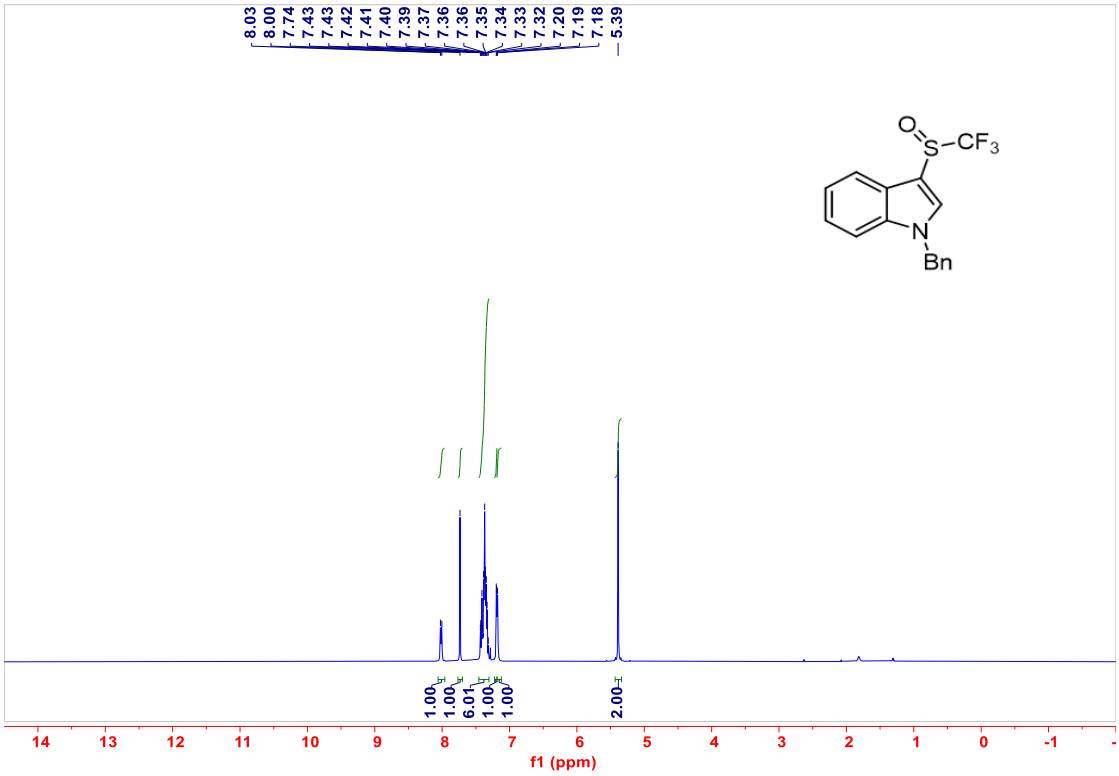

-72.4
f1 (ppm)


136.7
131.3
130.6
127.3
125.0
124.0
123.8
122.9
122.5
120.7
117.7
107.8
16.5
130.6
127.3
124.0
120.7
131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
N
H
Me
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
7.97
7.68
7.44
7.42
7.40
7.38
7.35
7.33
3.87
O
S
CF3
N
Me
1.00
1.00
2.09
1.05
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-73.4
O
S
CF3
N
Me
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


137.7
134.0
130.6
127.3
125.1
124.1
124.0
122.5
120.7
120.5
110.6
107.2
33.7
130.6
127.3
124.0
120.7
132 130 128 126 124 122 120
f1 (ppm)
O
S
CF3
N
Me
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
8.00
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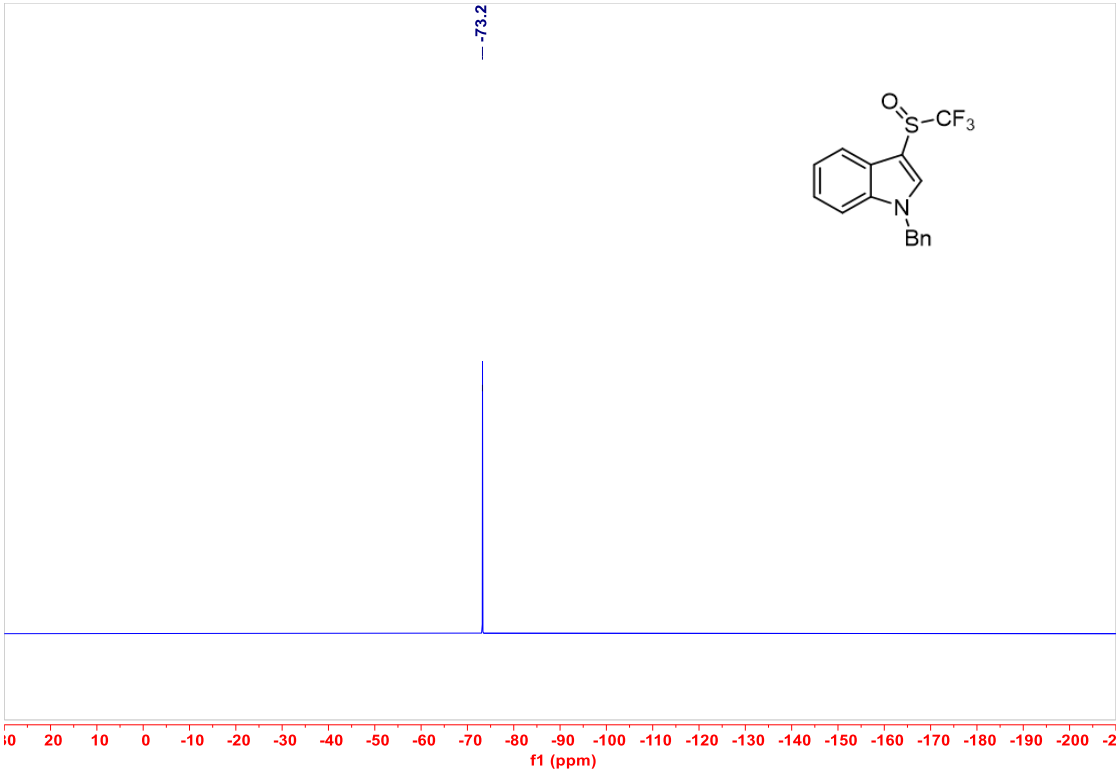
7.43
7.43
7.42
7.41
7.40
7.39
7.37
7.36
7.36
7.35
7.34
7.33
7.32
7.20
7.19
7.18
5.39
O
S
CF3
N
Bn
1.00
1.00
6.01
1.00
1.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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O
S
CF3
N
Bn
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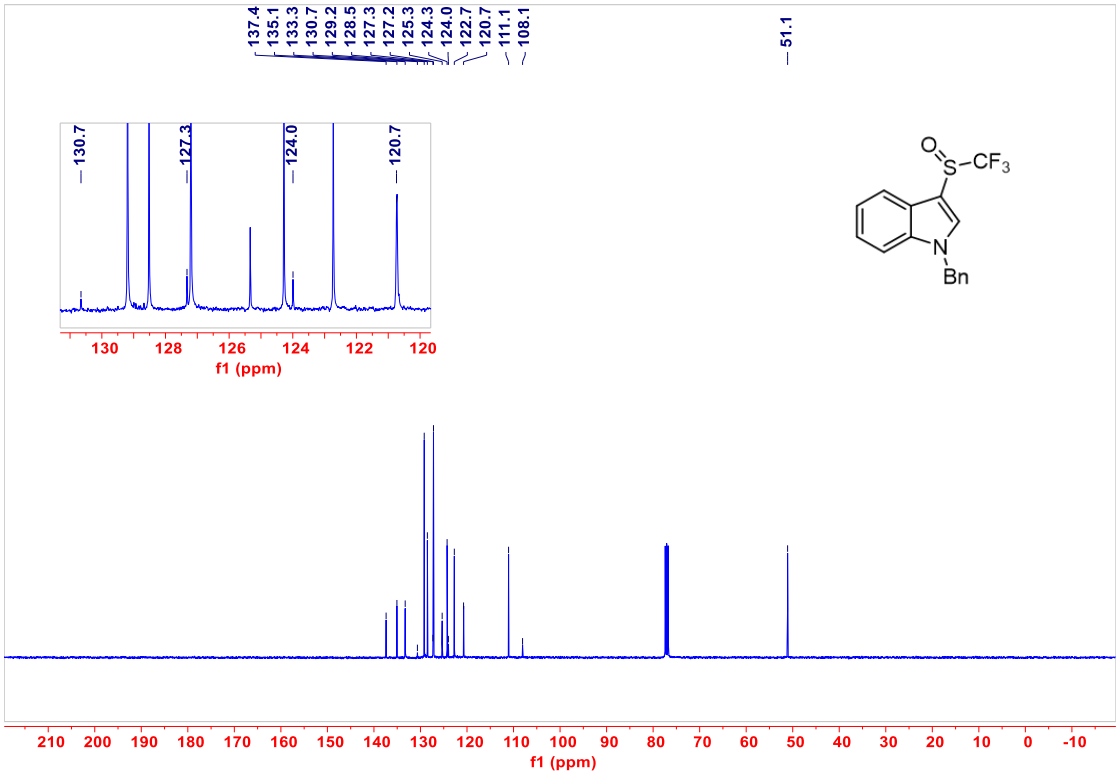
f1 (ppm)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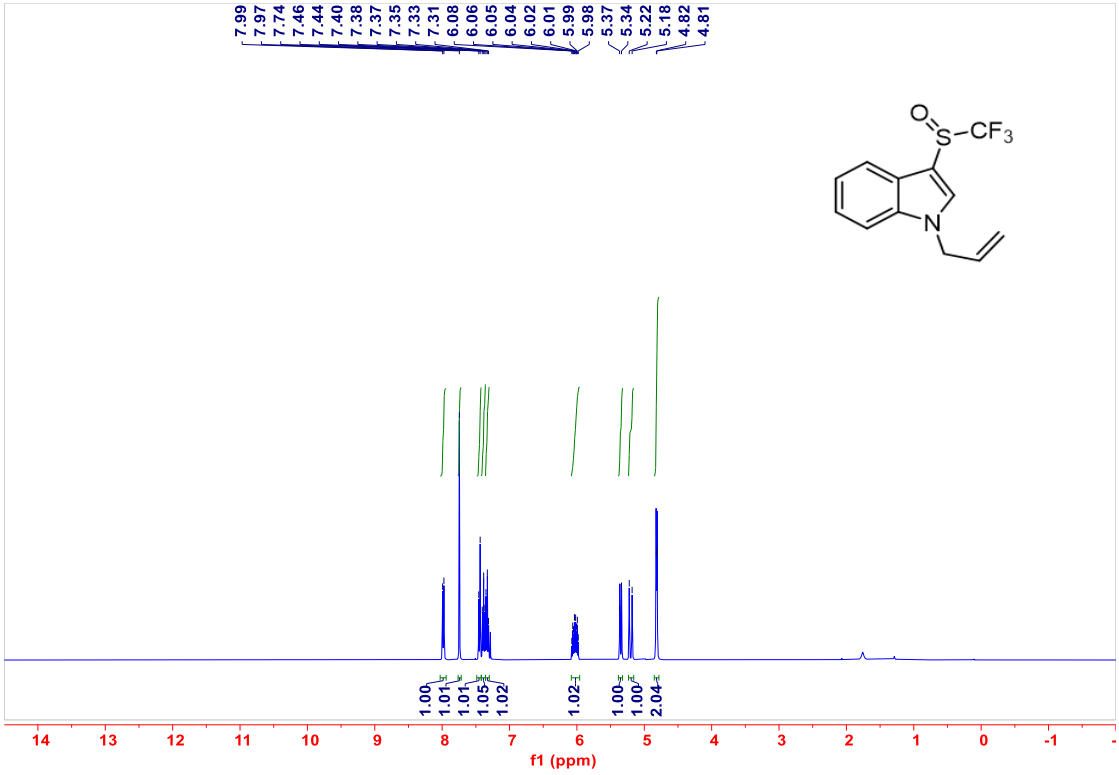
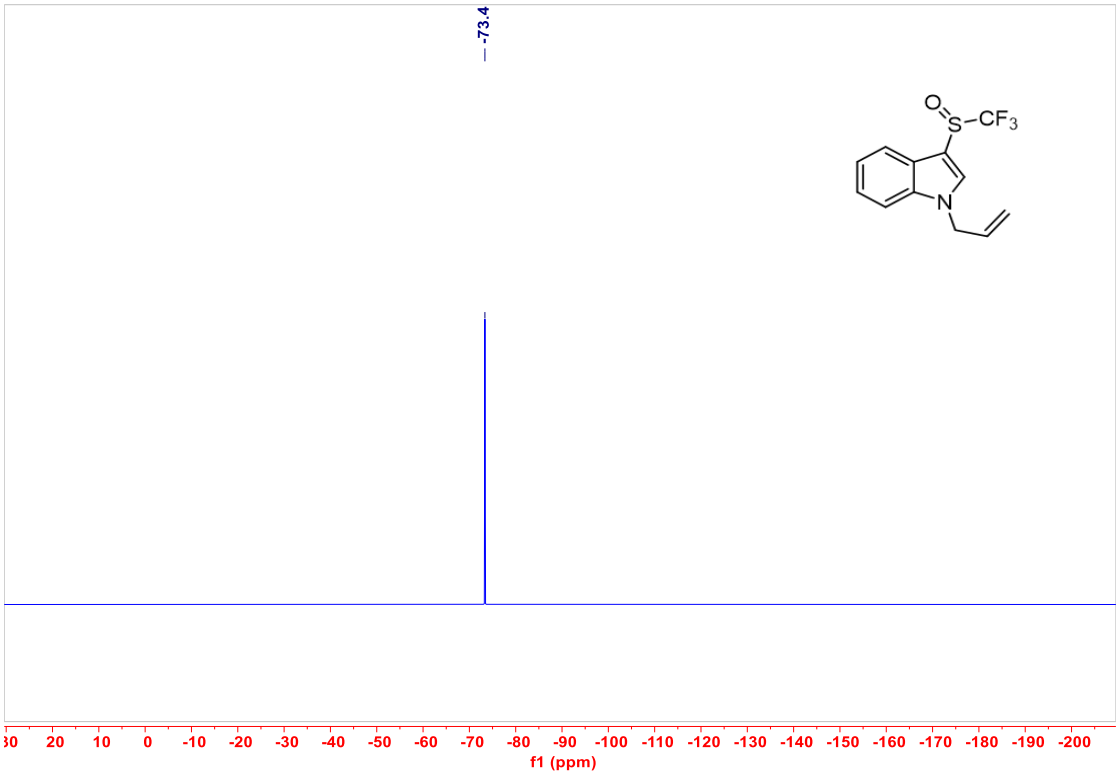
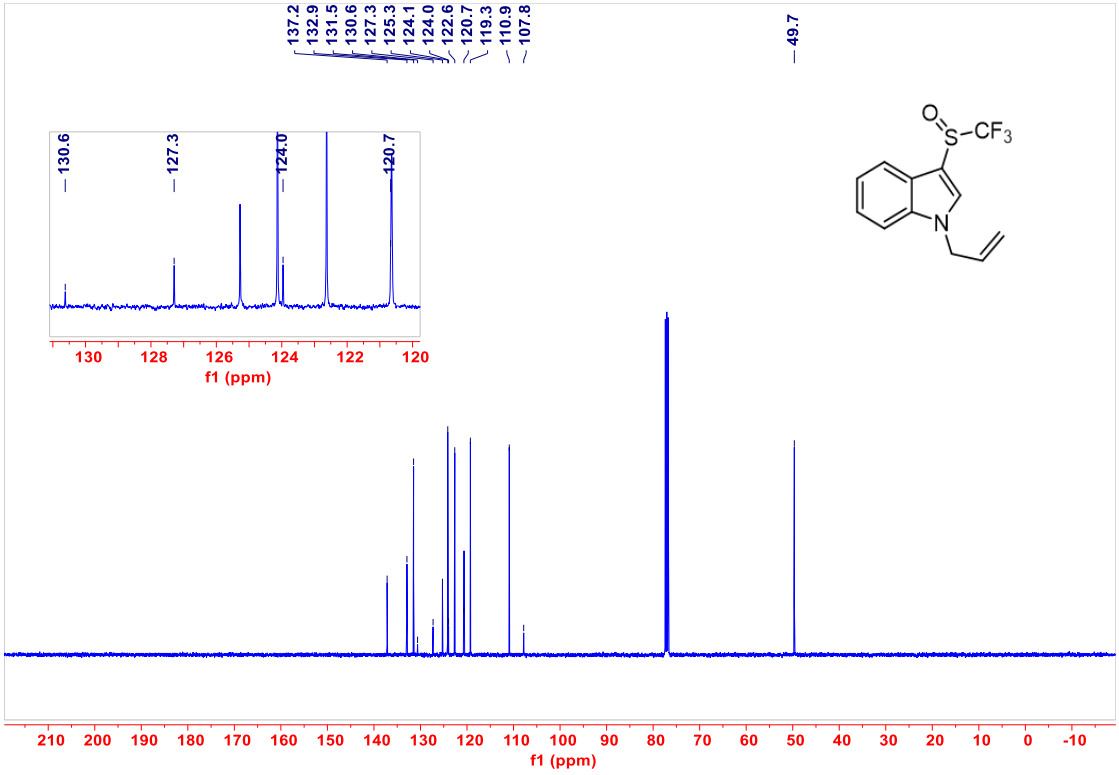
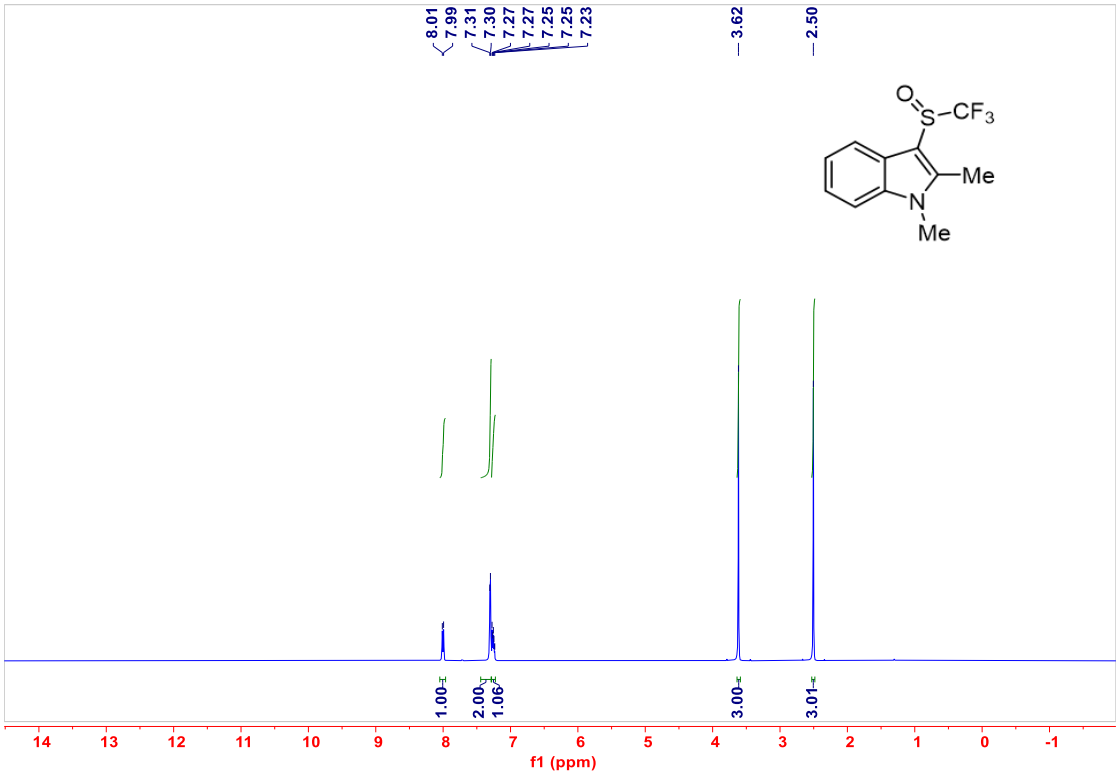
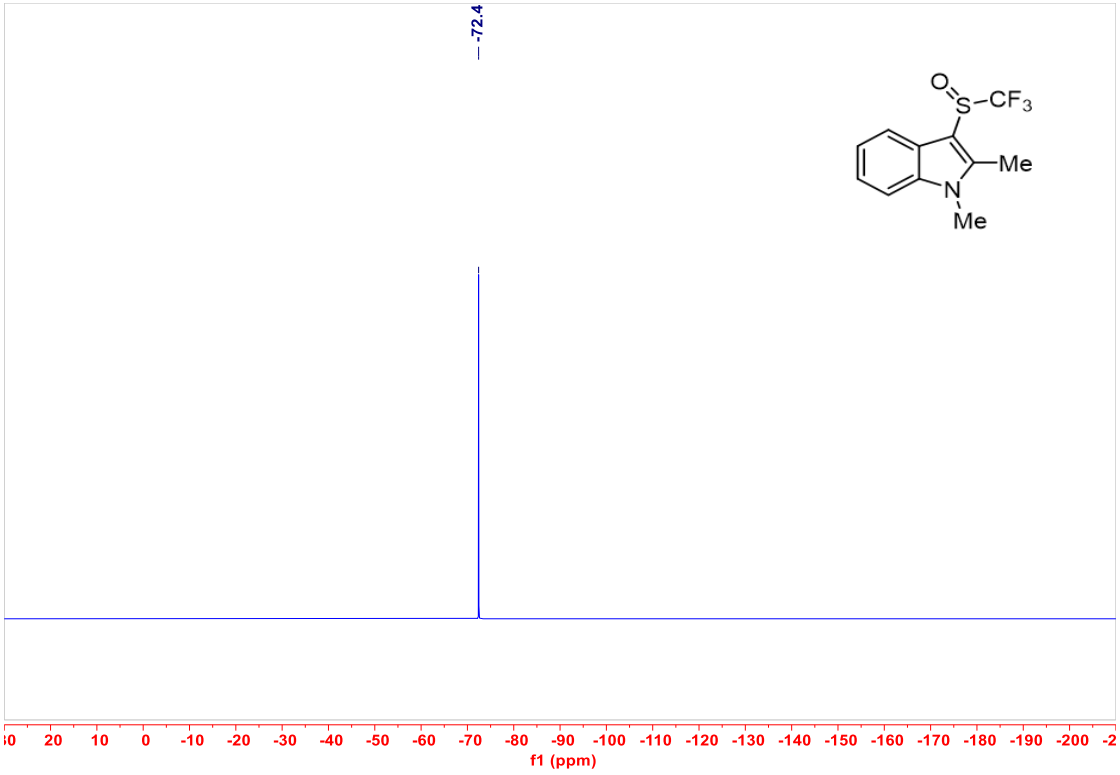
135.1
133.3
130.7
129.2
128.5
127.3
127.2
125.3
124.3
124.0
122.7
120.7
111.1
108.1
51.1
130.7
127.3
124.0
120.7
130 128 126 124 122 120
f1 (ppm)
O
S
CF3
N
Bn
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

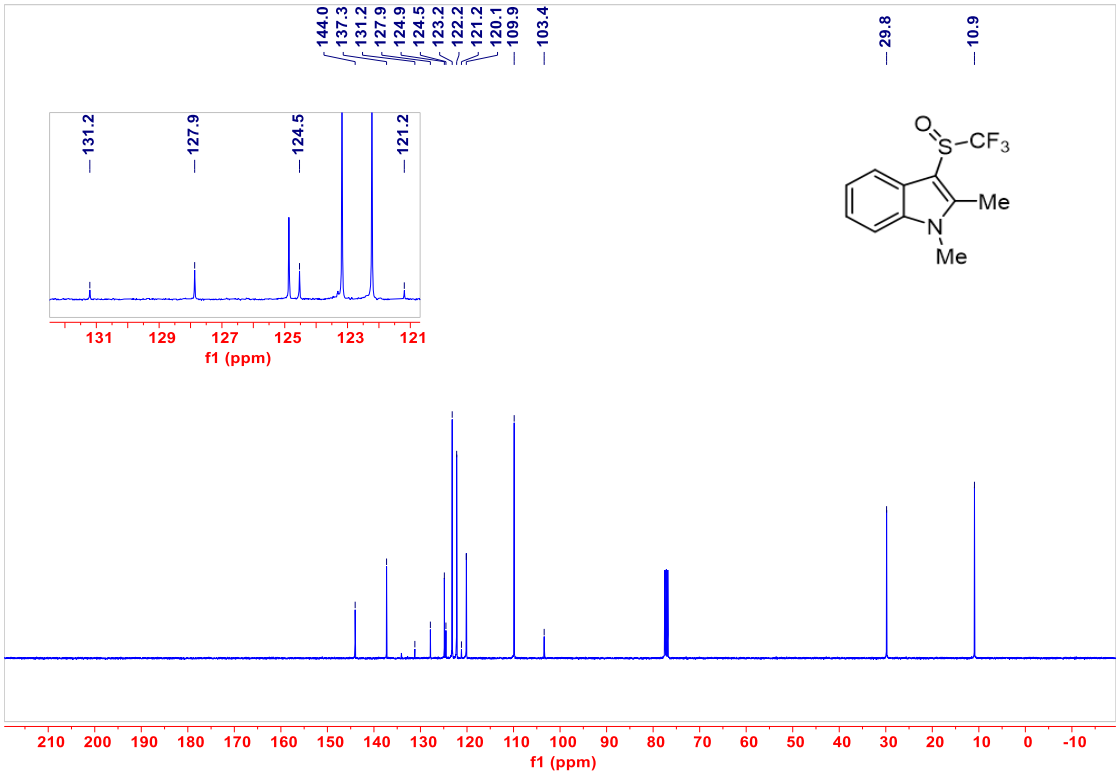

7.99
7.97
7.74
7.46
7.44
7.40
7.38
7.37
7.35
7.33
7.31
6.08
6.06
6.05
6.04
6.02
6.01
5.99
5.98
5.37
5.34
5.22
5.18
4.82
4.81
O
S
CF3
N
1.00
1.01
1.01
1.05
1.02
1.02
1.00
1.00
2.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

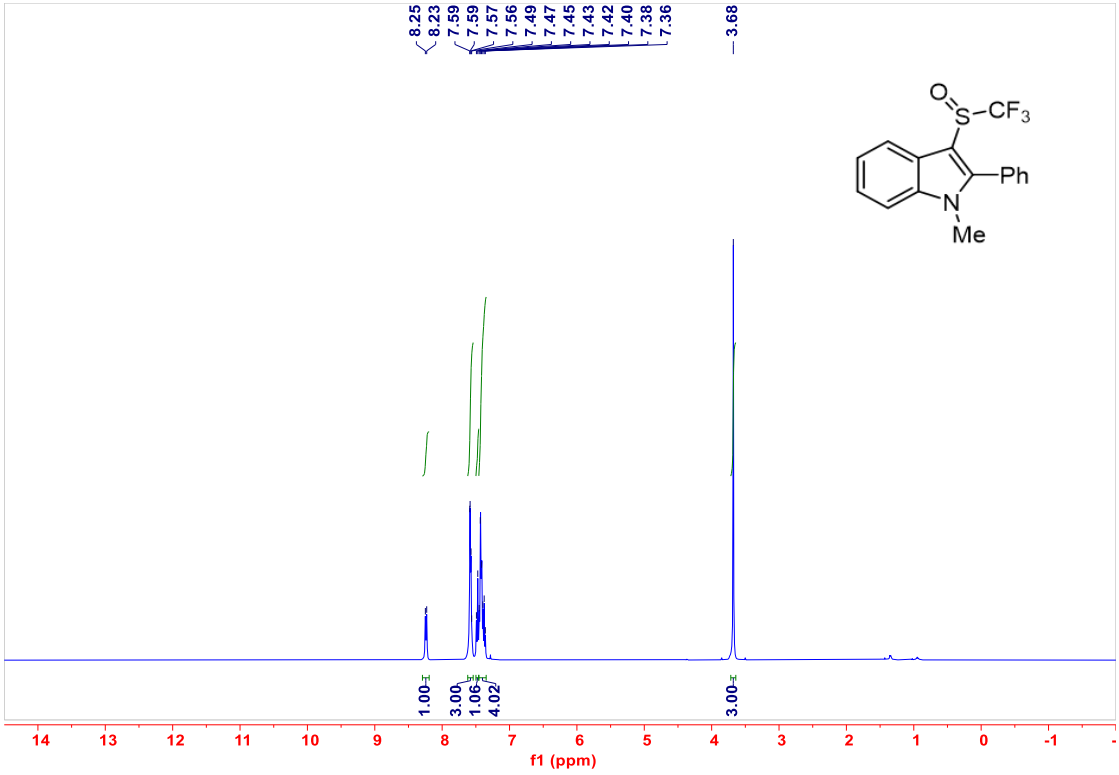

-73.4
O
S
CF3
N
f1 (ppm)

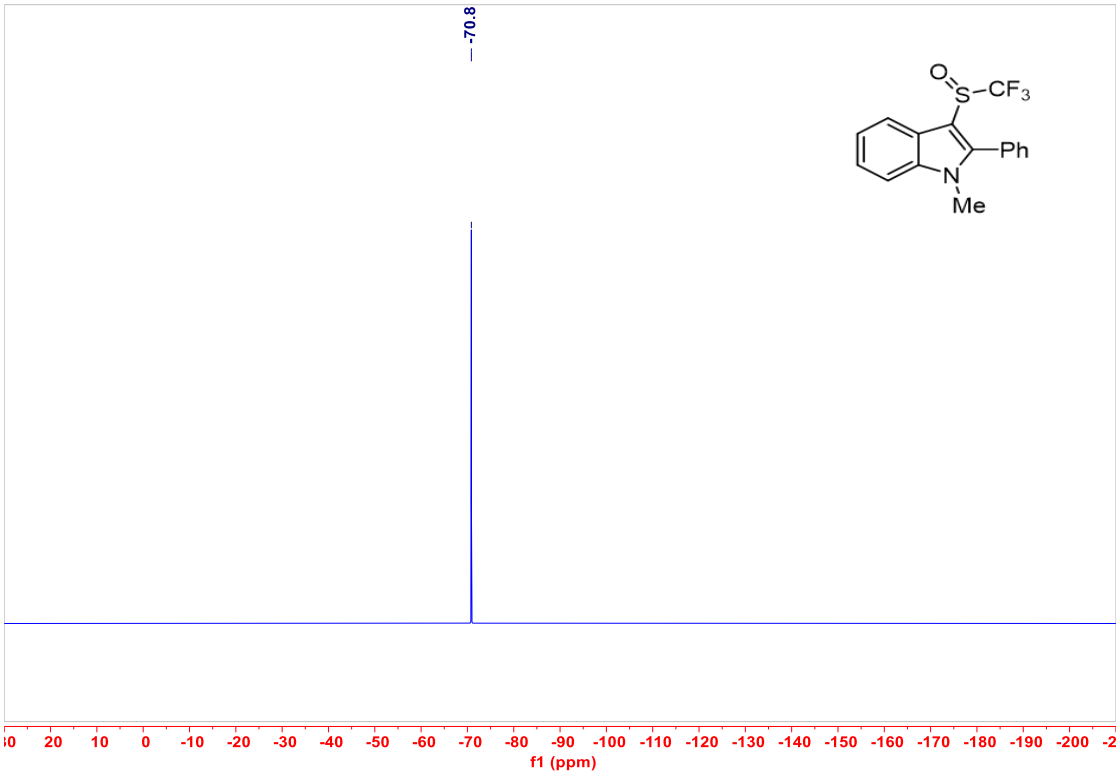

137.2
132.9
131.5
130.6
127.3
125.3
124.1
124.0
122.6
120.7
119.3
110.9
107.8
49.7
130.6
127.3
124.0
120.7
f1 (ppm)
O
S
CF3
N
f1 (ppm)

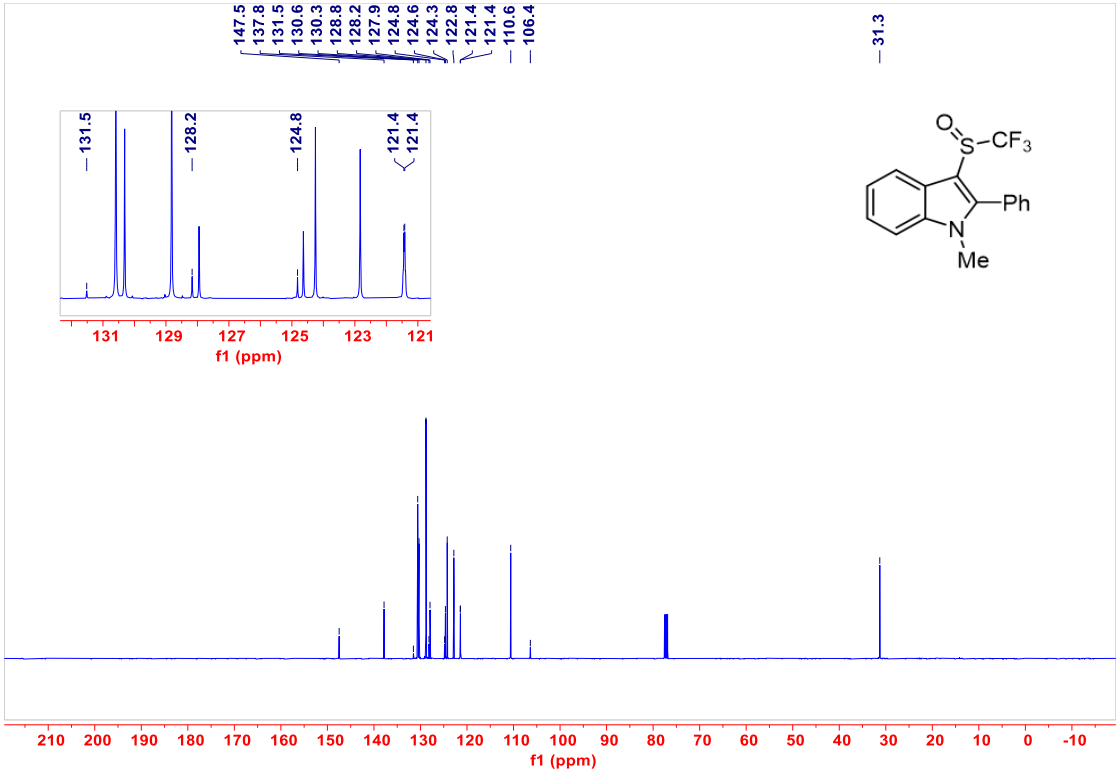

8.01
7.99
7.31
7.30
7.27
7.27
7.25
7.25
7.23
3.62
2.50
O
S
CF3
Me
N
Me
1.00
2.00
1.06
3.00
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

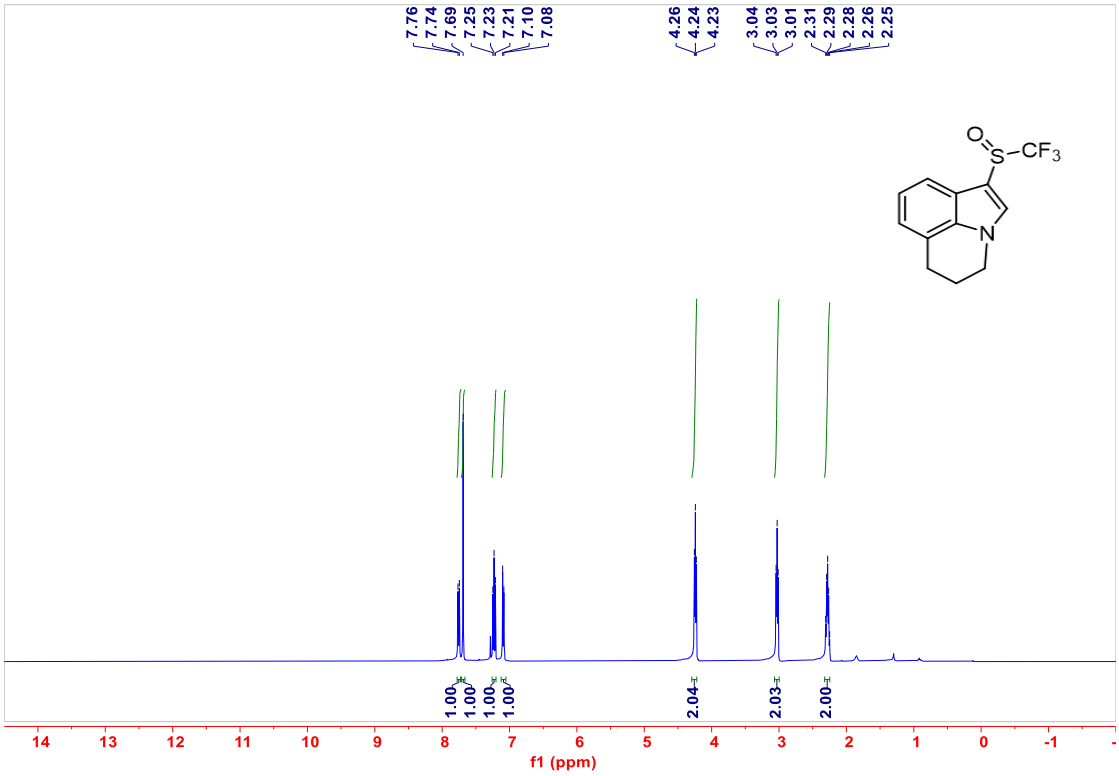

-72.4
O
S
CF3
Me
N
Me
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

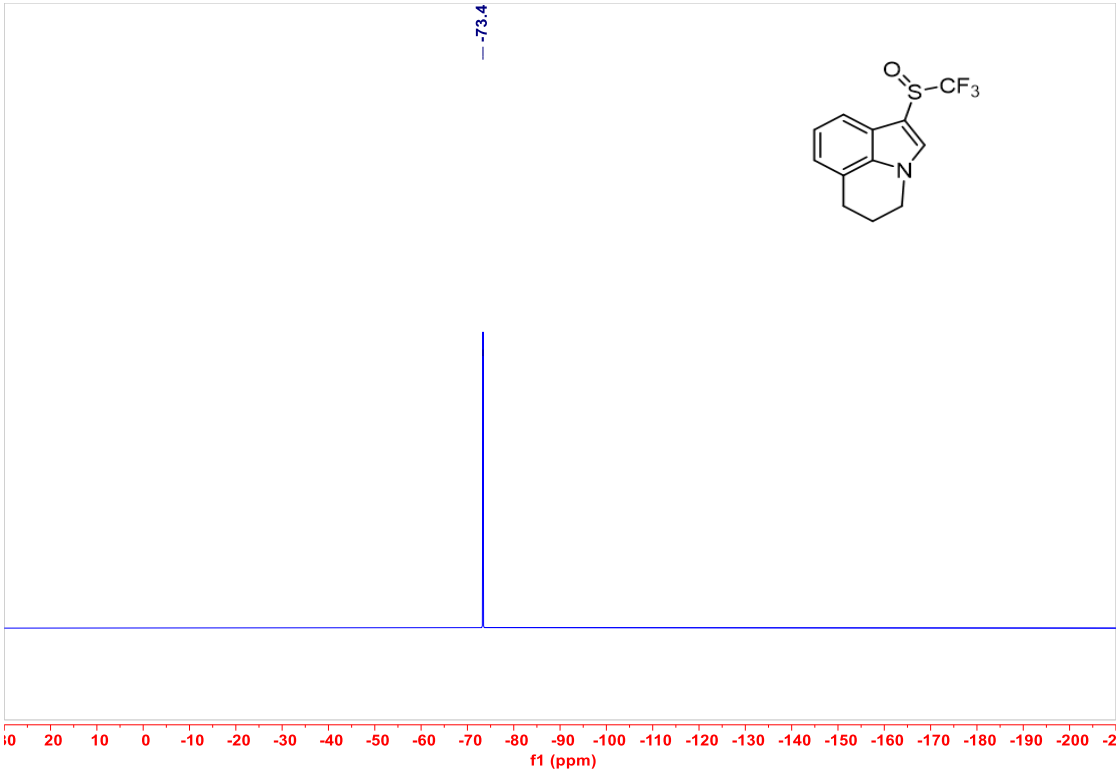

144.0
137.3
131.2
127.9
124.9
124.5
123.2
122.2
121.2
120.1
109.9
103.4
29.8
10.9
131.2
127.9
124.5
121.2
131 129 127 125 123 121
f1 (ppm)
O
S
CF3
Me
N
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

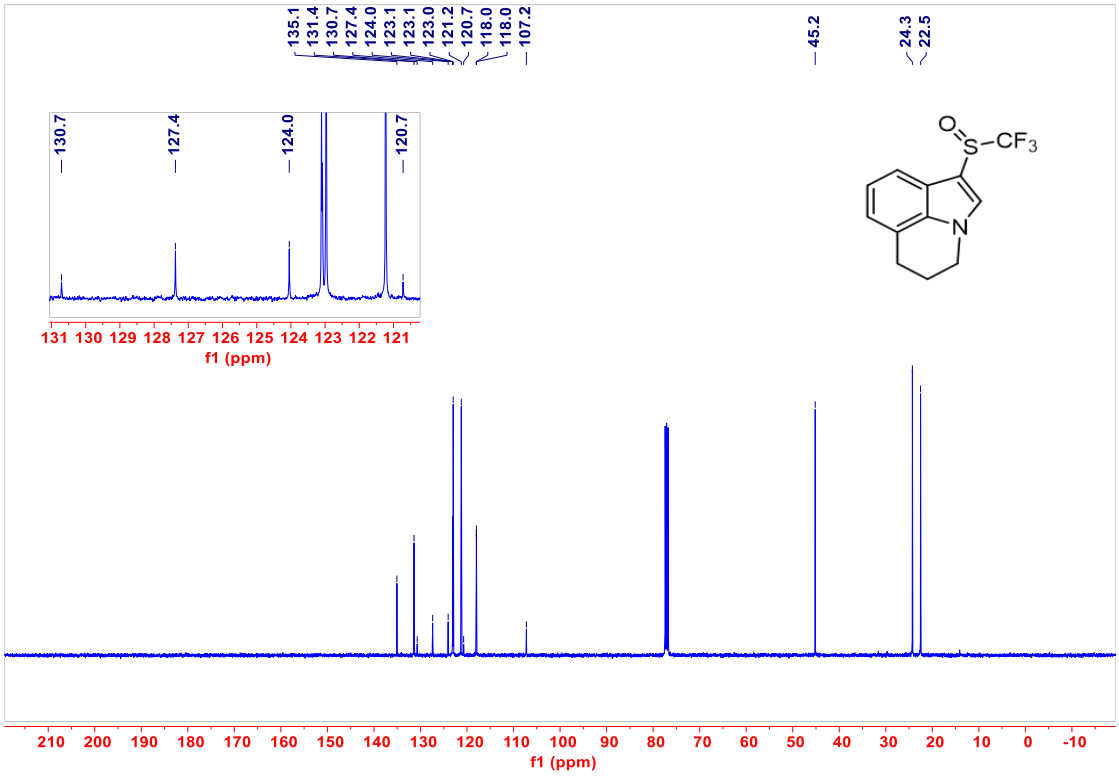

8.25
8.23
7.59
7.59
7.57
7.56
7.49
7.47
7.45
7.43
7.42
7.40
7.38
7.36
3.68
O
S
CF3
Ph
N
Me
1.00
3.00
1.06
4.02
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

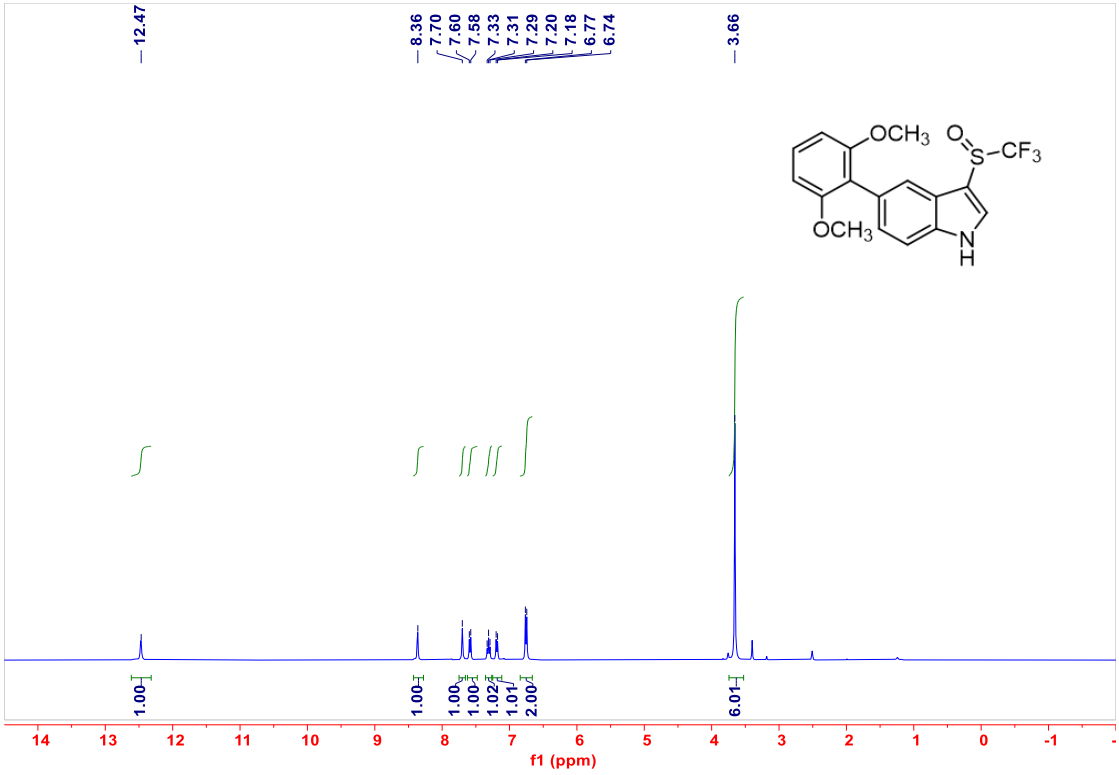

-70.8
O
S
CF3
Ph
N
Me
f1 (ppm)

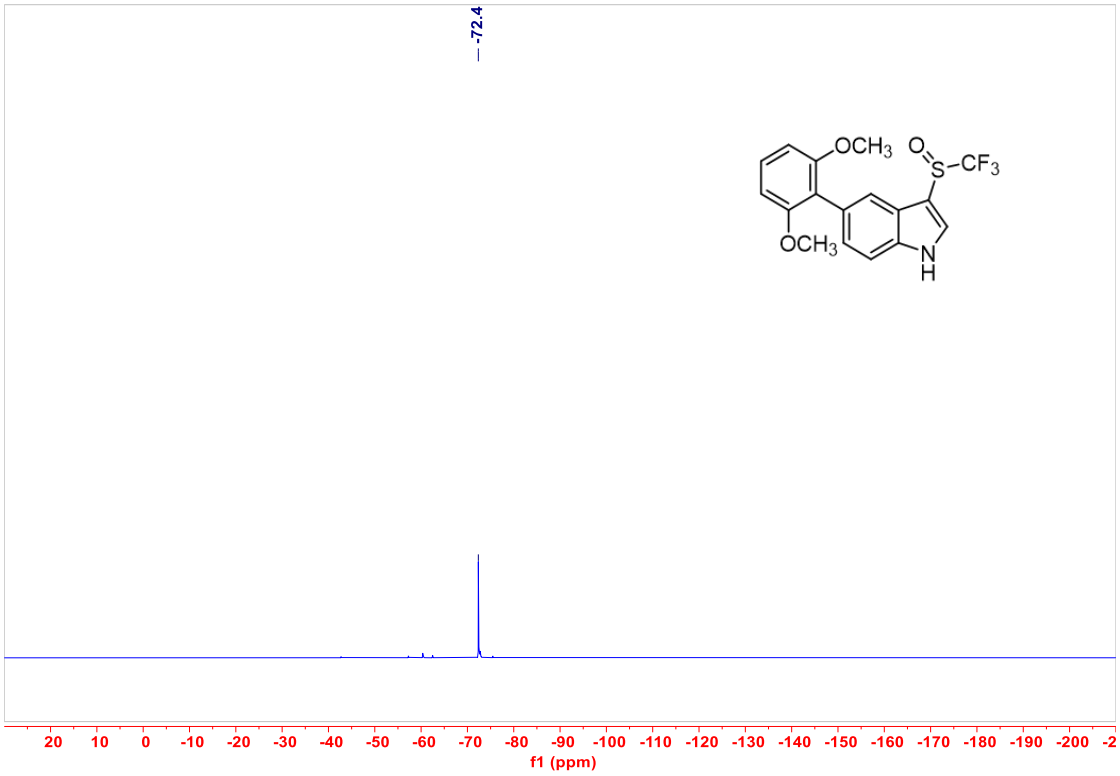

147.5
137.8
131.5
130.6
130.3
128.8
128.2
127.9
124.8
124.6
124.3
122.8
121.4
121.4
110.6
106.4
31.3
131.5
128.2
124.8
121.4
121.4
O
S
CF3
Ph
N
Me
f1 (ppm)

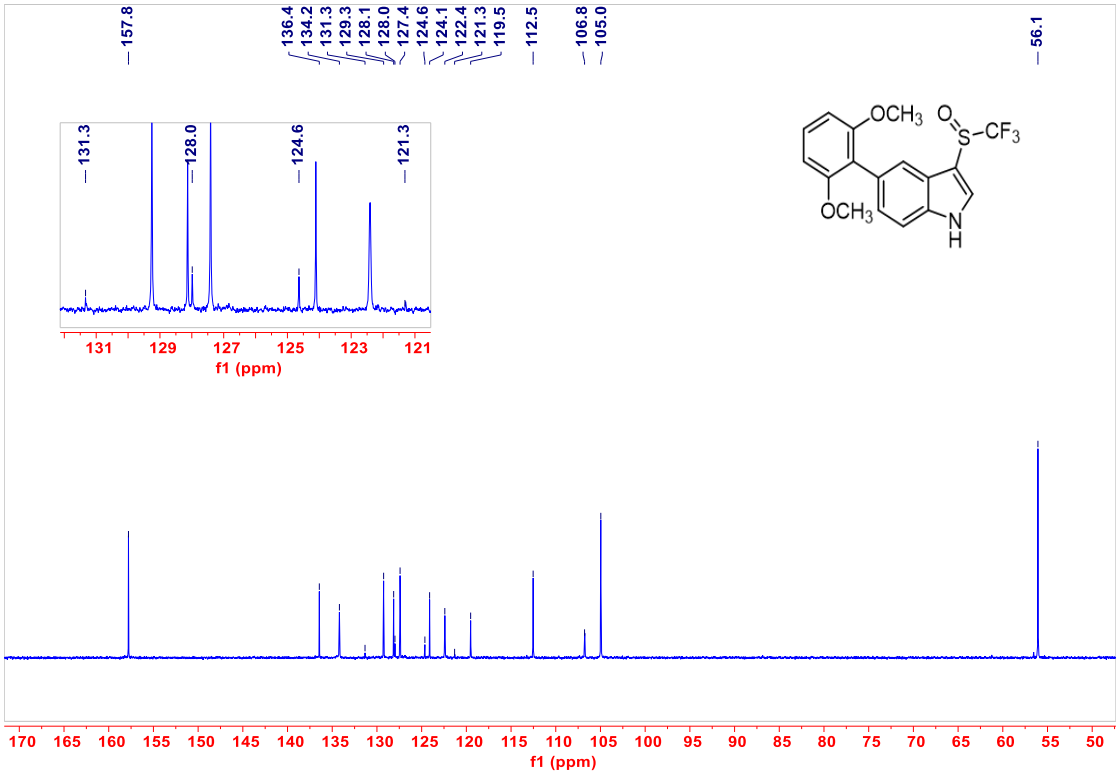

7.76
7.74
7.69
7.25
7.23
7.21
7.10
7.08
4.26
4.24
4.23
3.04
3.03
3.01
2.31
2.29
2.28
2.26
2.25
O
S
CF3
N
1.00
1.00
1.00
1.00
2.04
2.03
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

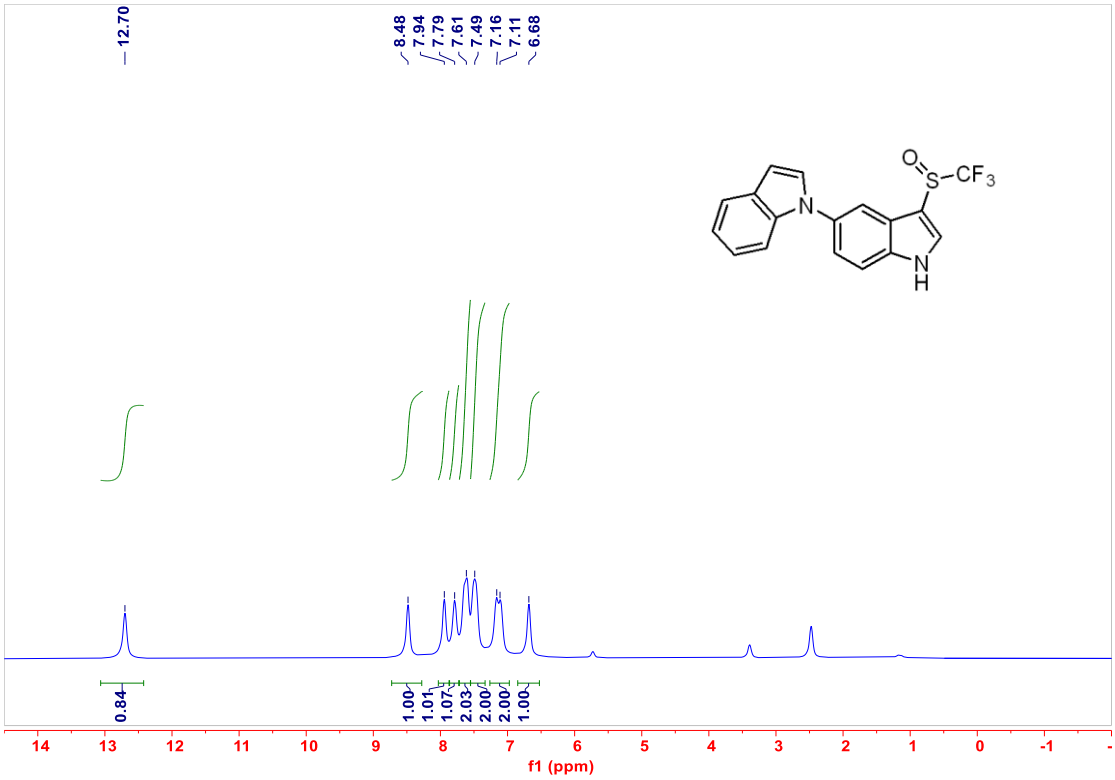

-73.4
O
S
CF3
N
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

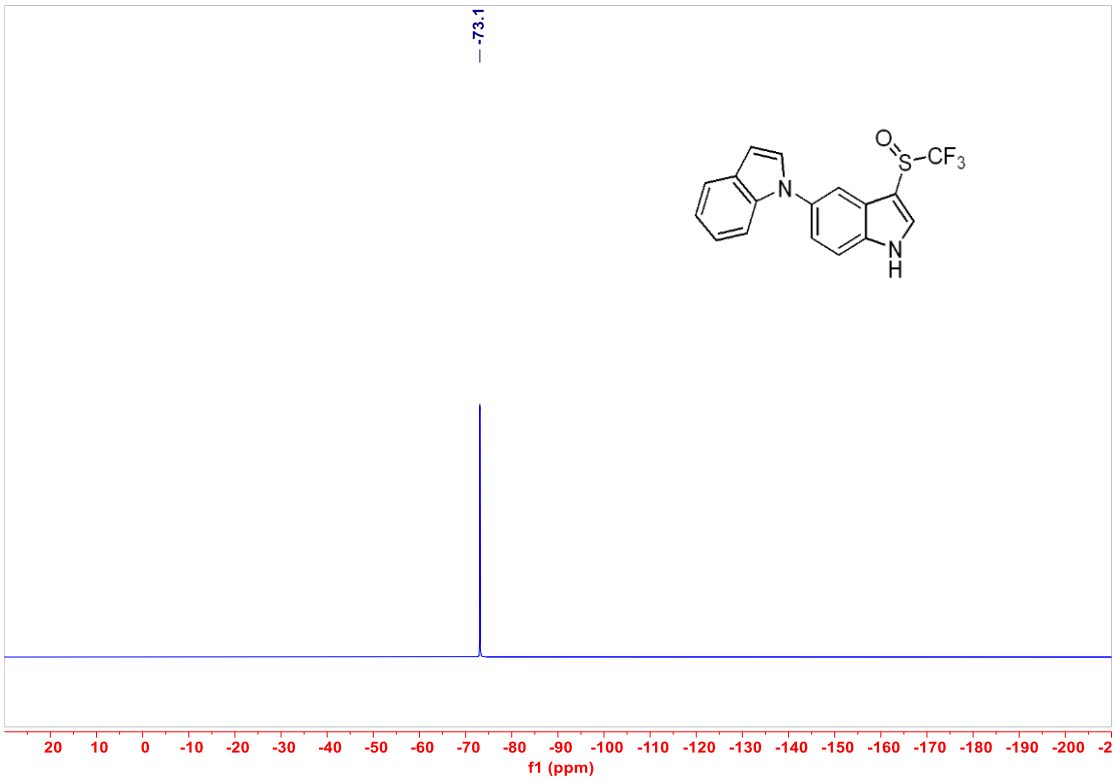

135.1
131.4
130.7
127.4
124.0
123.1
123.1
123.0
121.2
120.7
118.0
118.0
107.2
45.2
24.3
22.5
130.7
127.4
124.0
120.7
131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

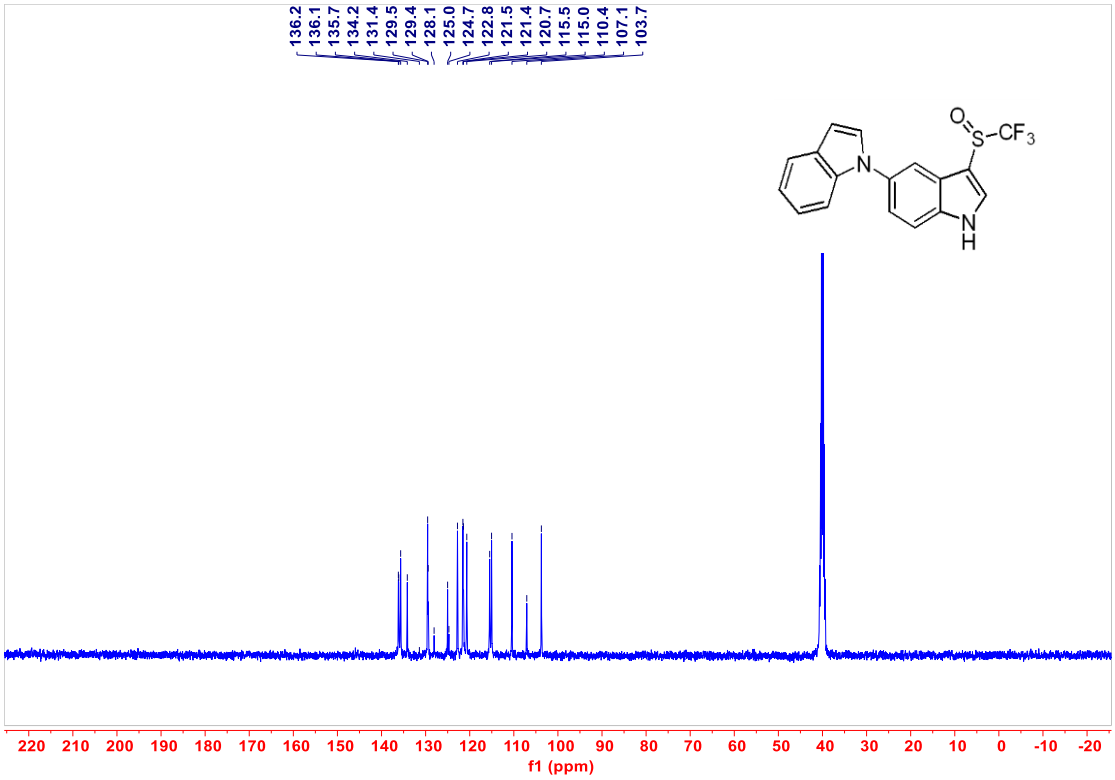

12.47
8.36
7.70
7.60
7.58
7.33
7.31
7.29
7.20
7.18
6.77
6.74
3.66
OCH3
OCH3
O
S
CF3
N
H
1.00
1.00
1.00
1.00
1.02
1.01
2.00
6.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

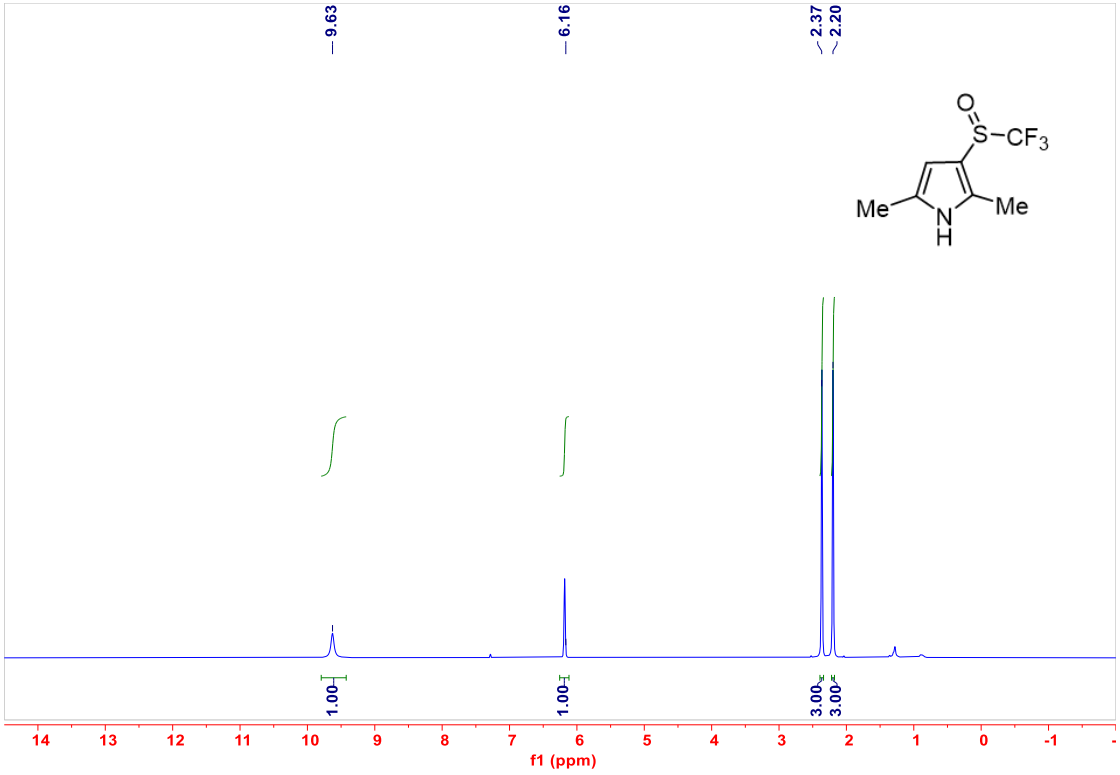

-72.4
OCH3
O
S
CF3
OCH3
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

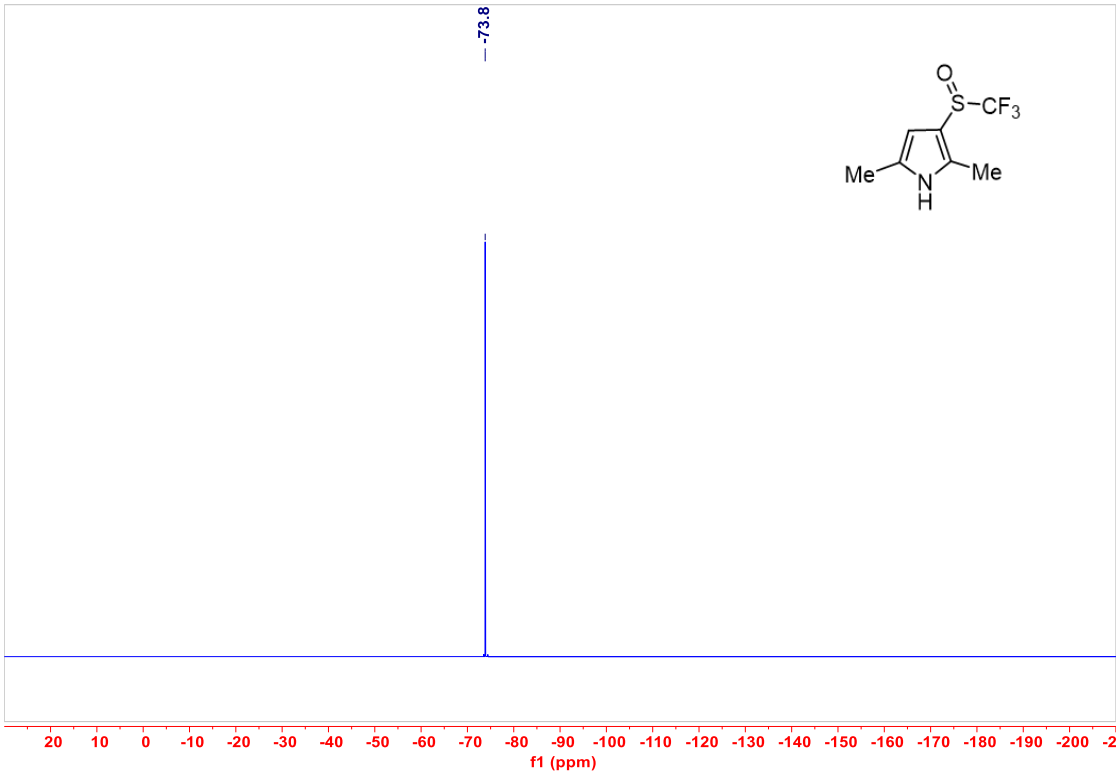

157.8
136.4
134.2
131.3
129.3
128.1
128.0
127.4
124.6
124.1
122.4
121.3
119.5
112.5
106.8
105.0
56.1
131.3
128.0
124.6
121.3
131 129 127 125 123 121
f1 (ppm)
OCH3
O
S
CF3
OCH3
N
H
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

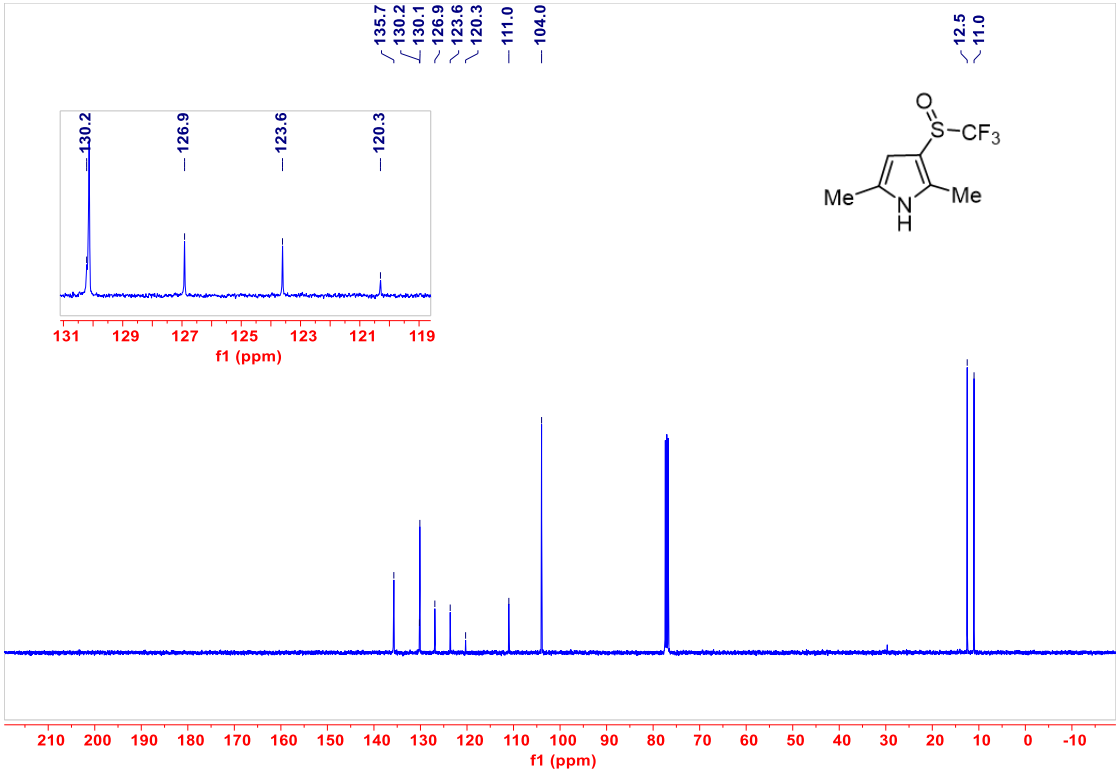

12.70
8.48
7.94
7.79
7.61
7.49
7.16
7.11
6.68
0.84
1.00
1.01
1.07
2.03
2.00
2.00
1.00
f1 (ppm)

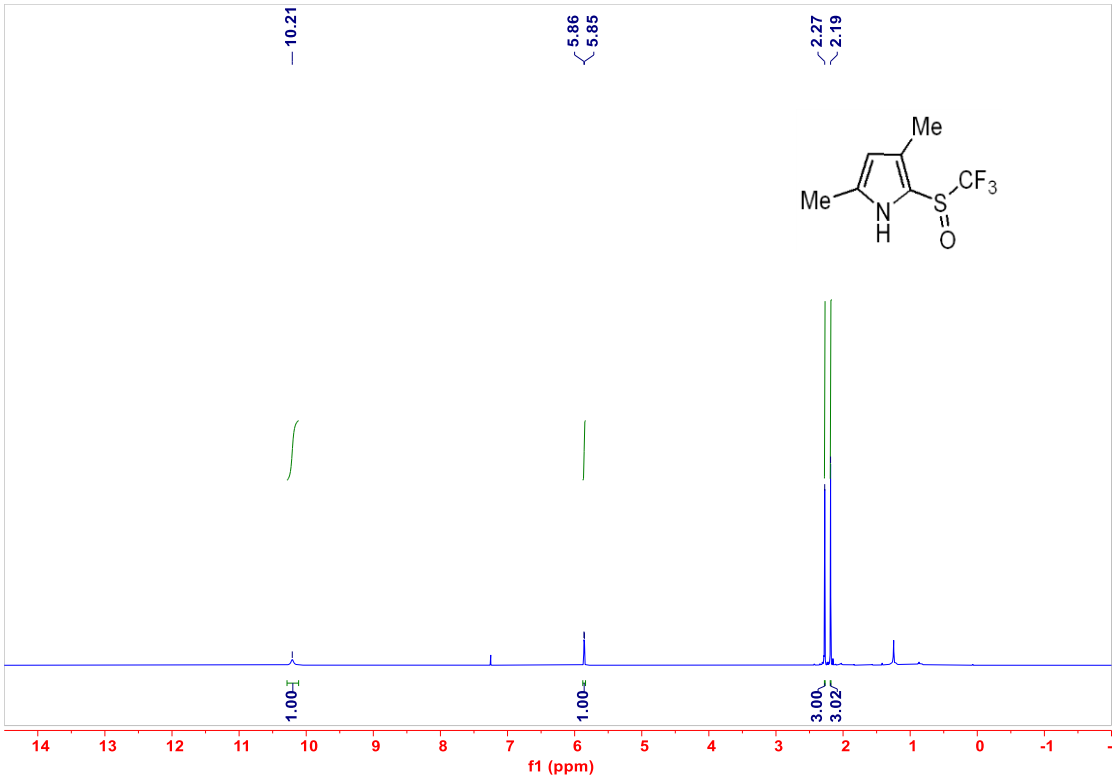

-73.1
f1 (ppm)

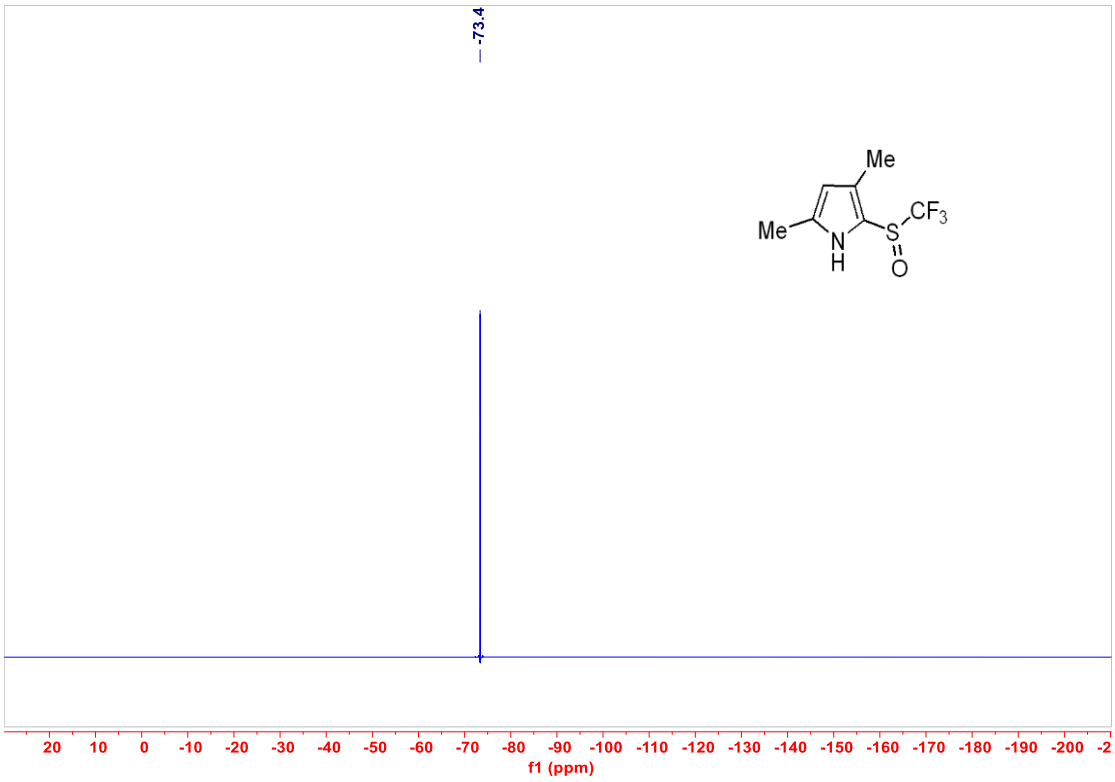

136.2
136.1
135.7
134.2
131.4
129.5
129.4
128.1
125.0
124.7
122.8
121.5
121.4
120.7
115.5
115.0
110.4
107.1
103.7
O
S
CF3
N
N
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

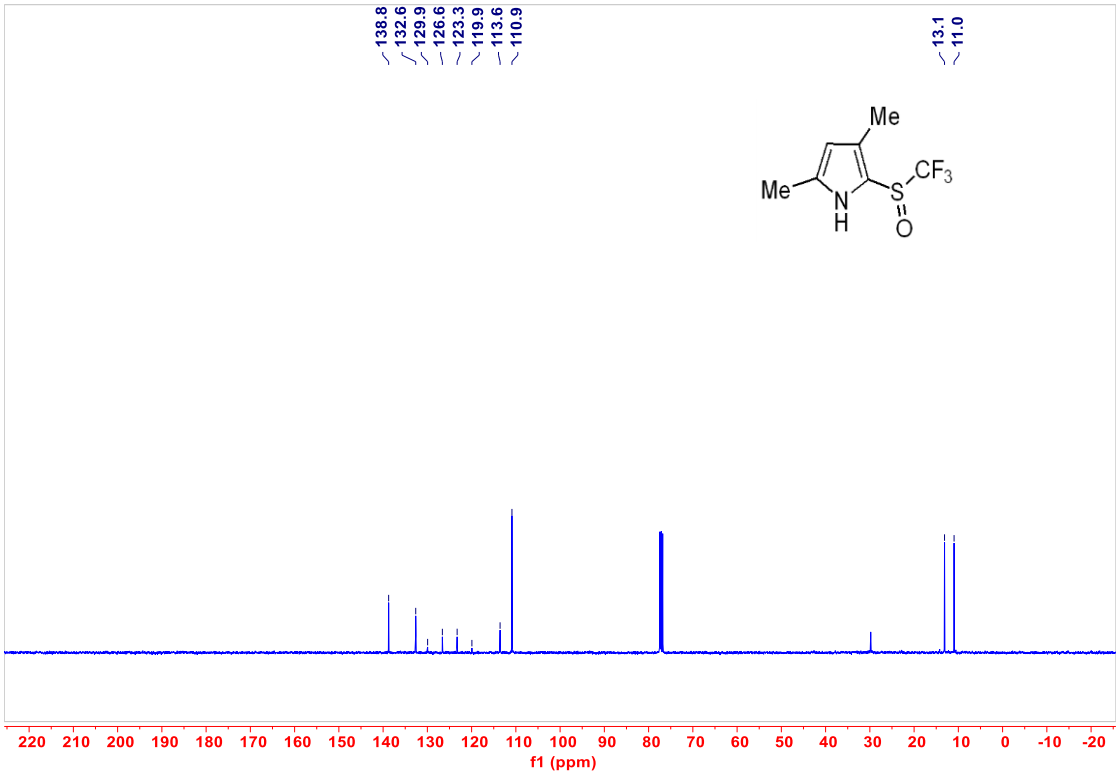

9.63
6.16
2.37
2.20
O
S
CF3
Me
N
H
Me
1.00
1.00
3.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

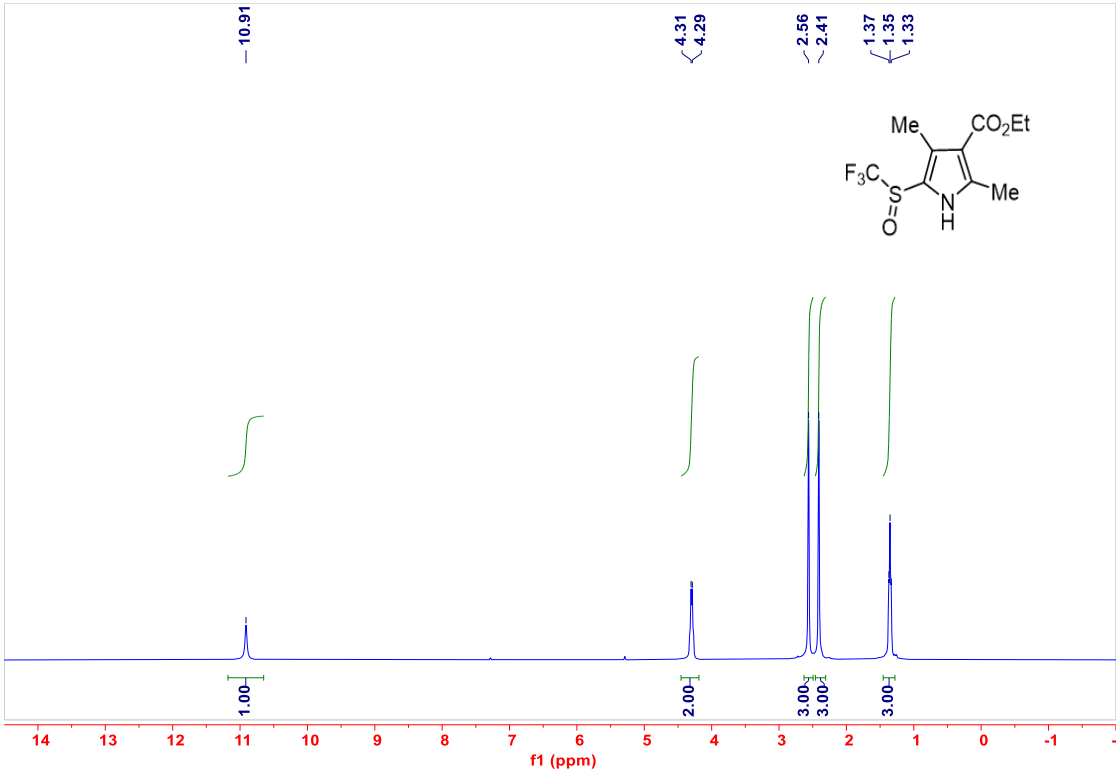

-73.8
O
S–CF3
Me
N
H
Me
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

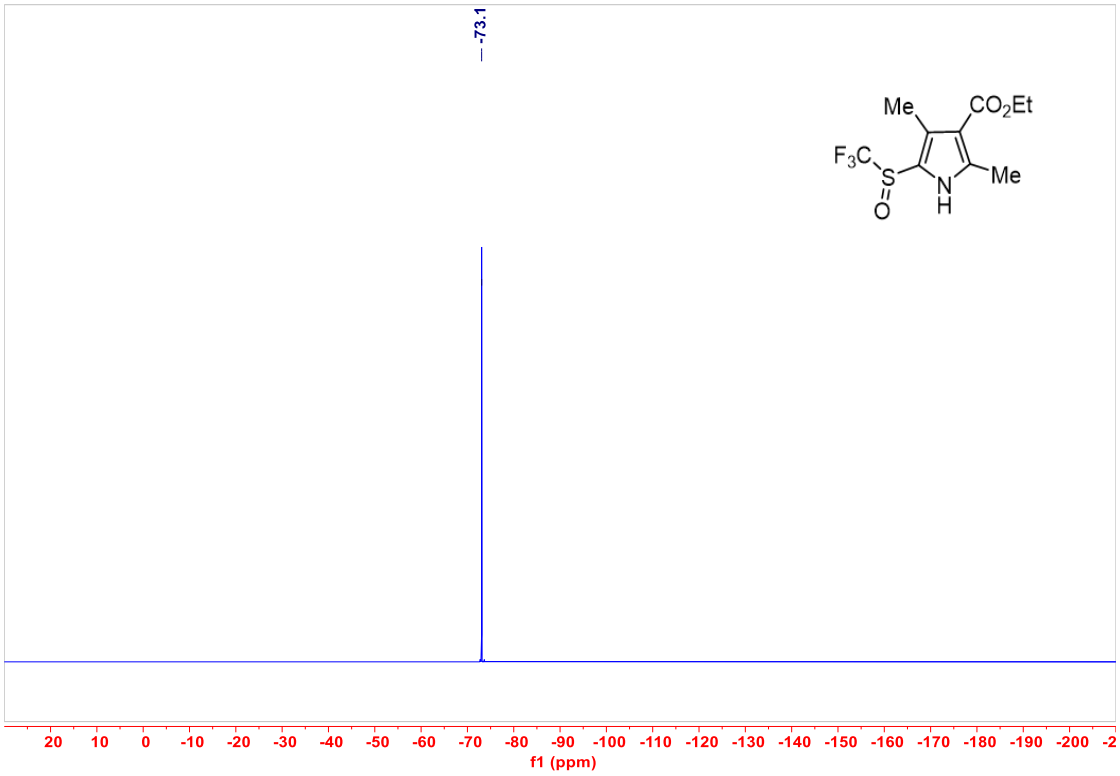

135.7
130.2
130.1
126.9
123.6
120.3
111.0
104.0
12.5
11.0
130.2
126.9
123.6
120.3
131 129 127 125 123 121 119
f1 (ppm)
O
S–CF3
Me
N
H
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

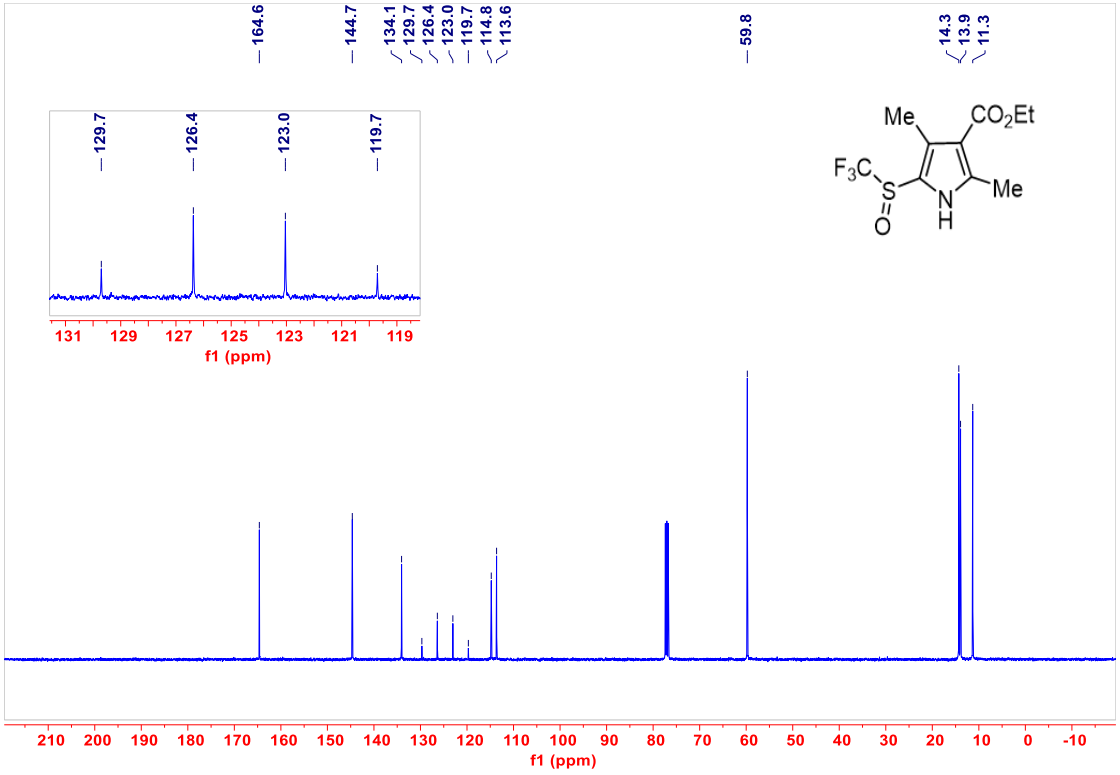

10.21
5.86
5.85
2.27
2.19
Me
Me
N
H
S
CF3
O
1.00
1.00
3.00
3.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

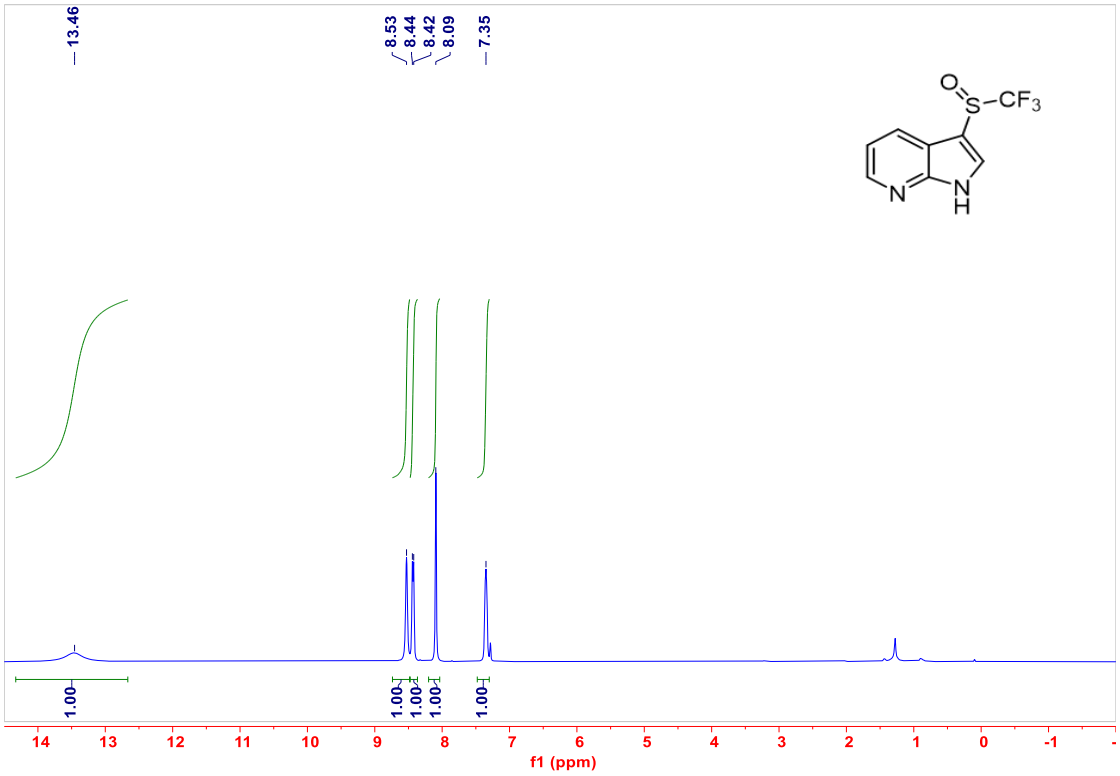

-73.4
Me
Me
N
H
S
CF3
O
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

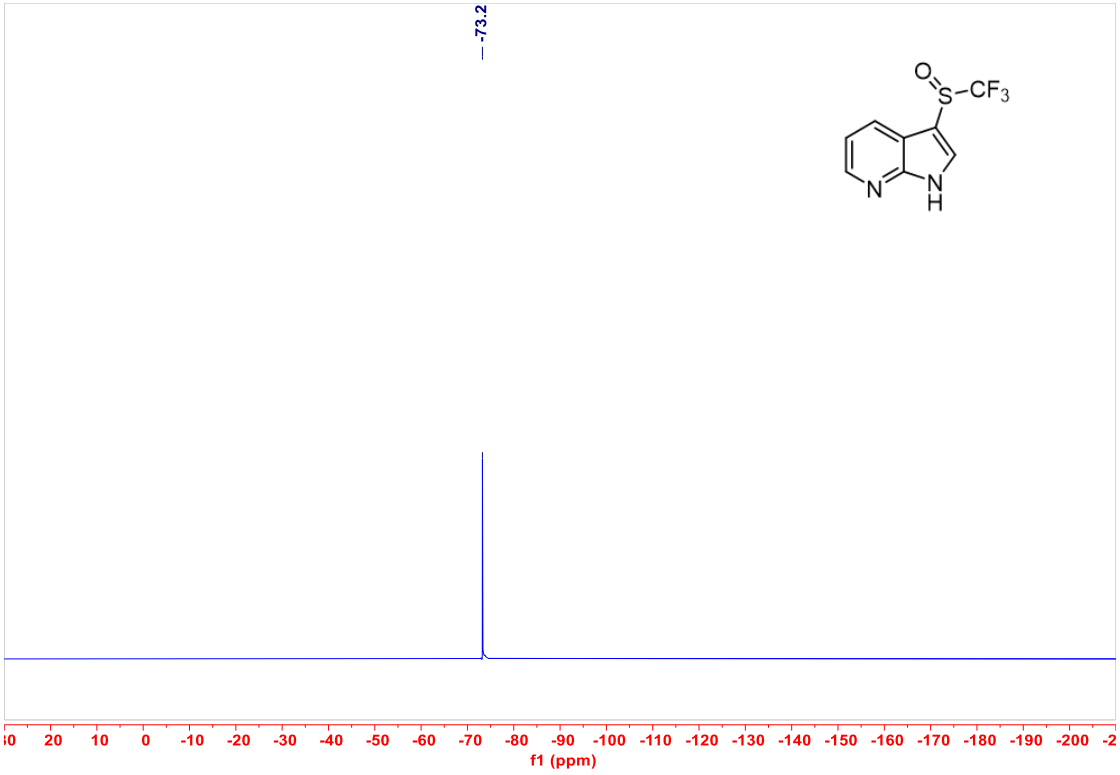

138.8
132.6
129.9
126.6
123.3
119.9
113.6
110.9
13.1
11.0
Me
Me
N
H
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

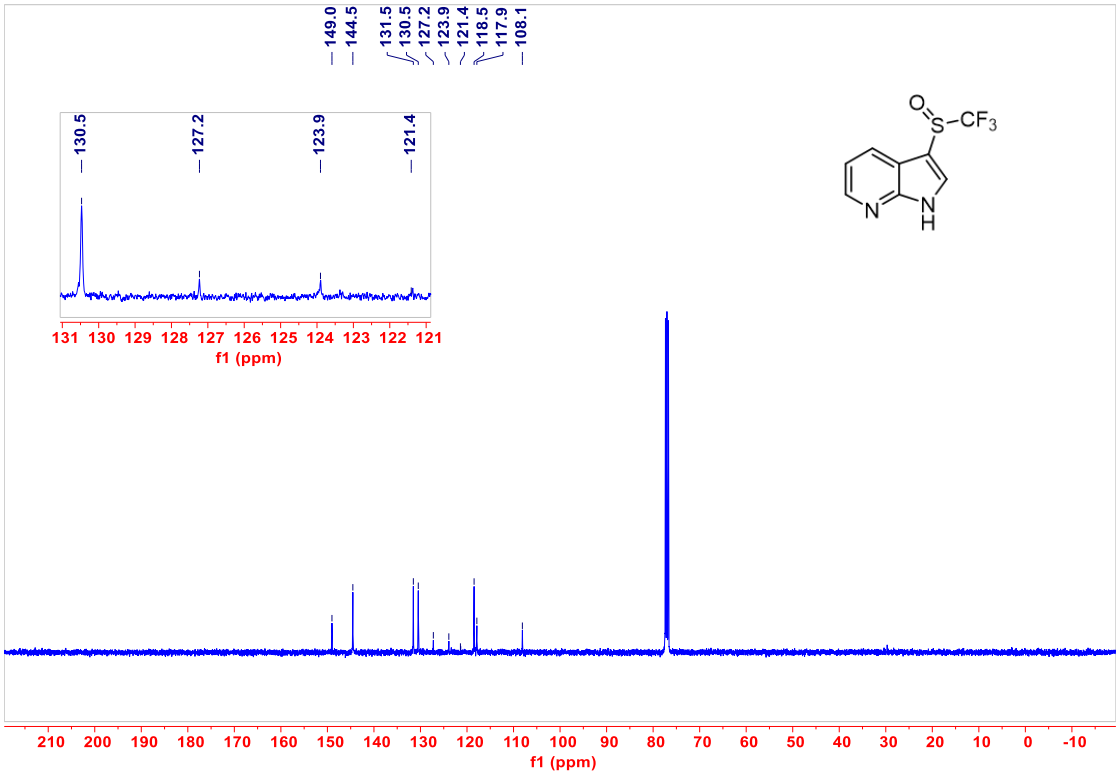

10.91
4.31
4.29
2.56
2.41
1.37
1.35
1.33
Me
CO2Et
F3C
S
O
N
H
Me
1.00
2.00
3.00
3.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

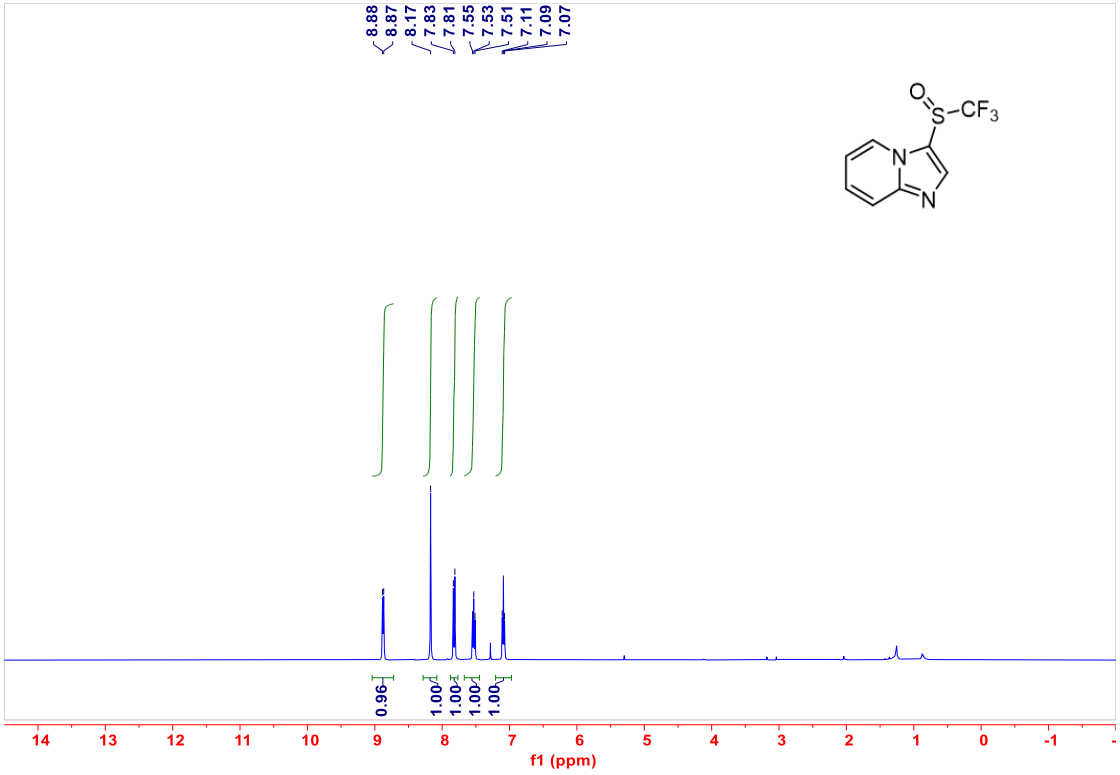

-73.1
Me
CO2Et
F3C
S
O
N
H
Me
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

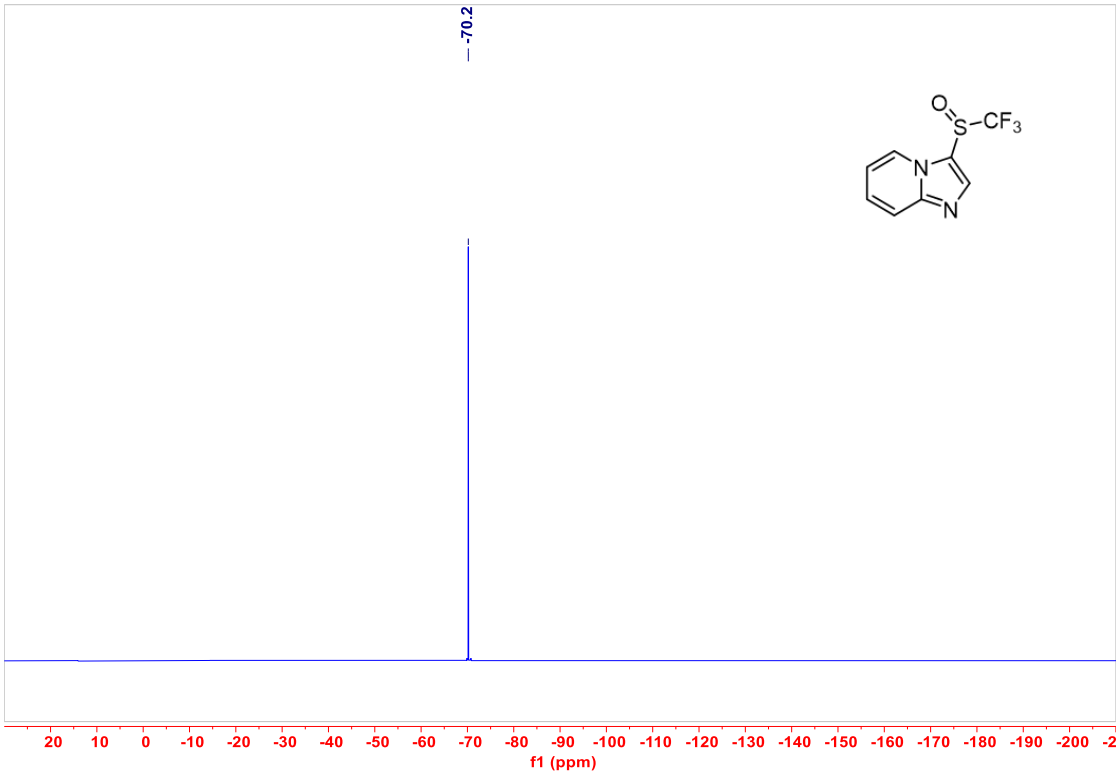

164.6
144.7
134.1
129.7
126.4
123.0
119.7
114.8
113.6
59.8
14.3
13.9
11.3
129.7
126.4
123.0
119.7
131 129 127 125 123 121 119
f1 (ppm)
Me
CO2Et
F3C
S
O
N
H
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


13.46
8.53
8.44
8.42
8.09
7.35
1.00
1.00
1.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-73.2
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


149.0
144.5
131.5
130.5
127.2
123.9
121.4
118.5
117.9
108.1
130.5
127.2
123.9
121.4
131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
N
N
H
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)


8.88
8.87
8.17
7.83
7.81
7.55
7.53
7.51
7.11
7.09
7.07
O
S
CF3
N
N
0.96
1.00
1.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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S
CF3
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N
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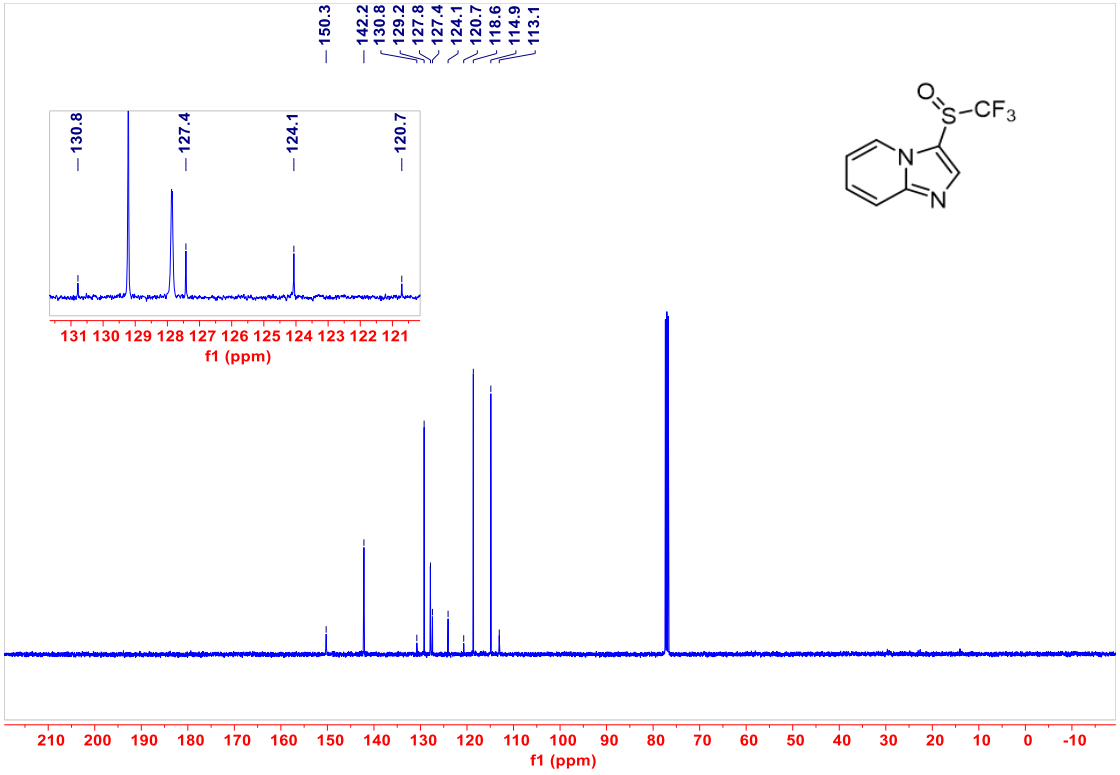
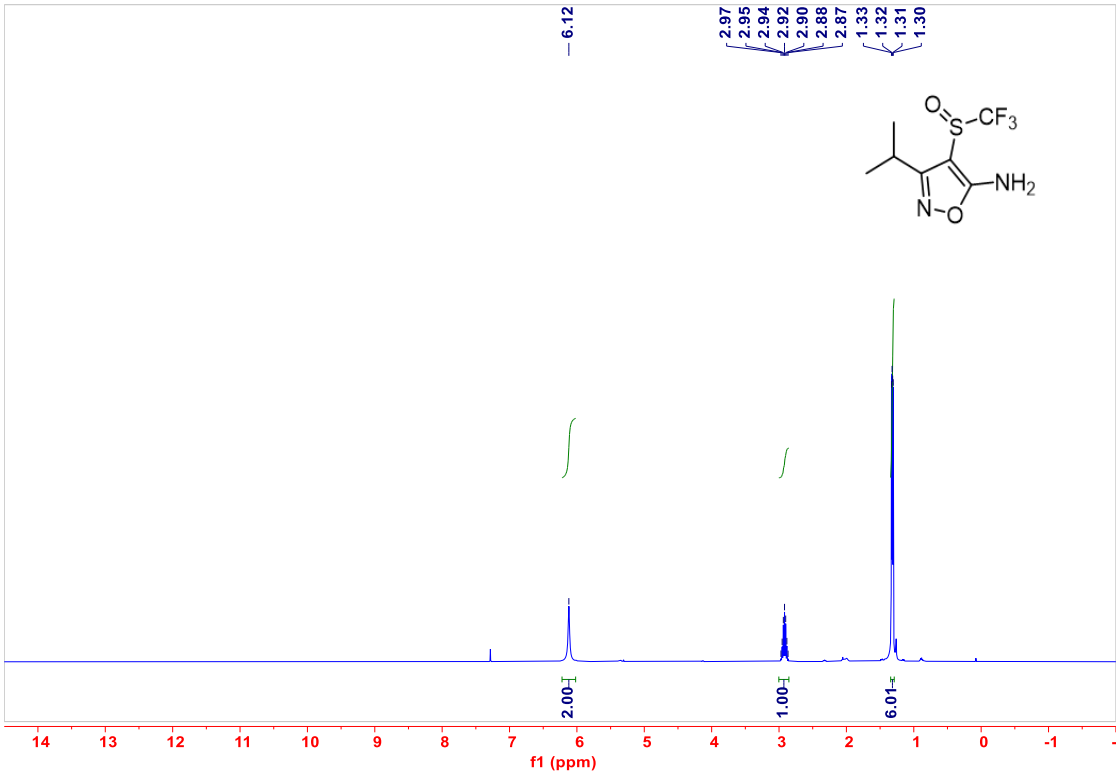
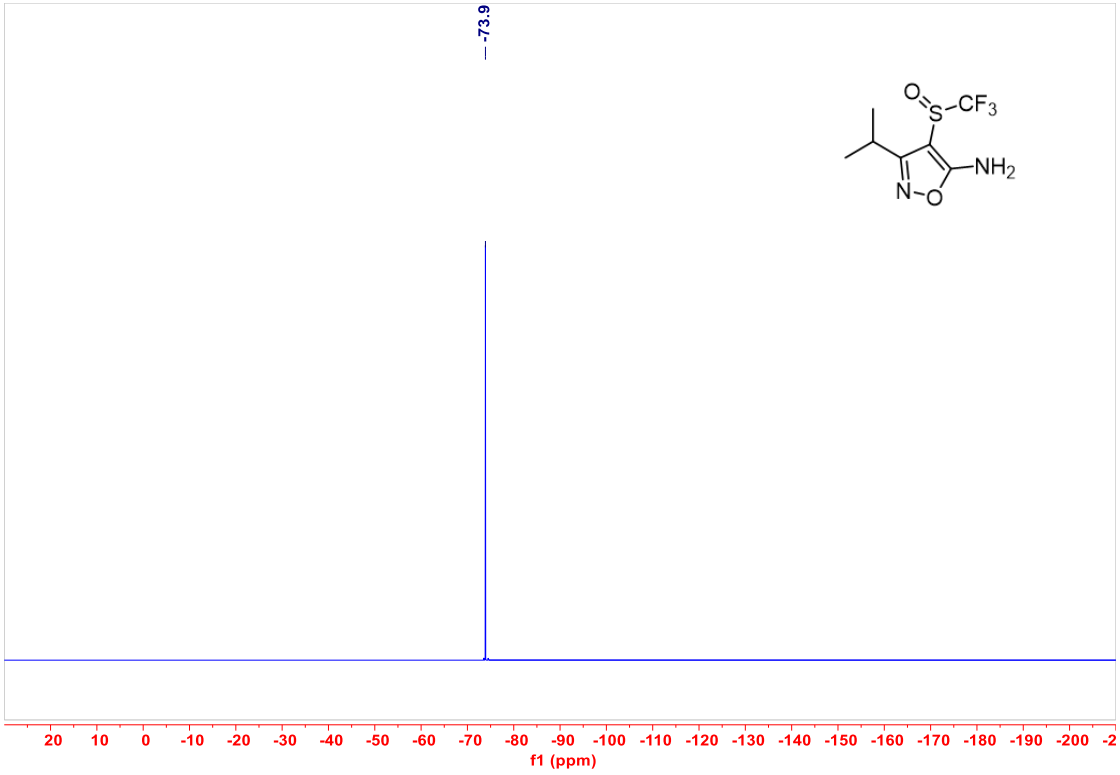
f1 (ppm)


150.3
142.2
130.8
129.2
127.8
127.4
124.1
120.7
118.6
114.9
113.1
130.8
127.4
124.1
120.7
131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
O
S
CF3
N
N
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)


6.12
2.97
2.95
2.94
2.92
2.90
2.88
2.87
1.33
1.32
1.31
1.30
O
S
CF3
NH2
N
O
2.00
1.00
6.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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CF3
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O
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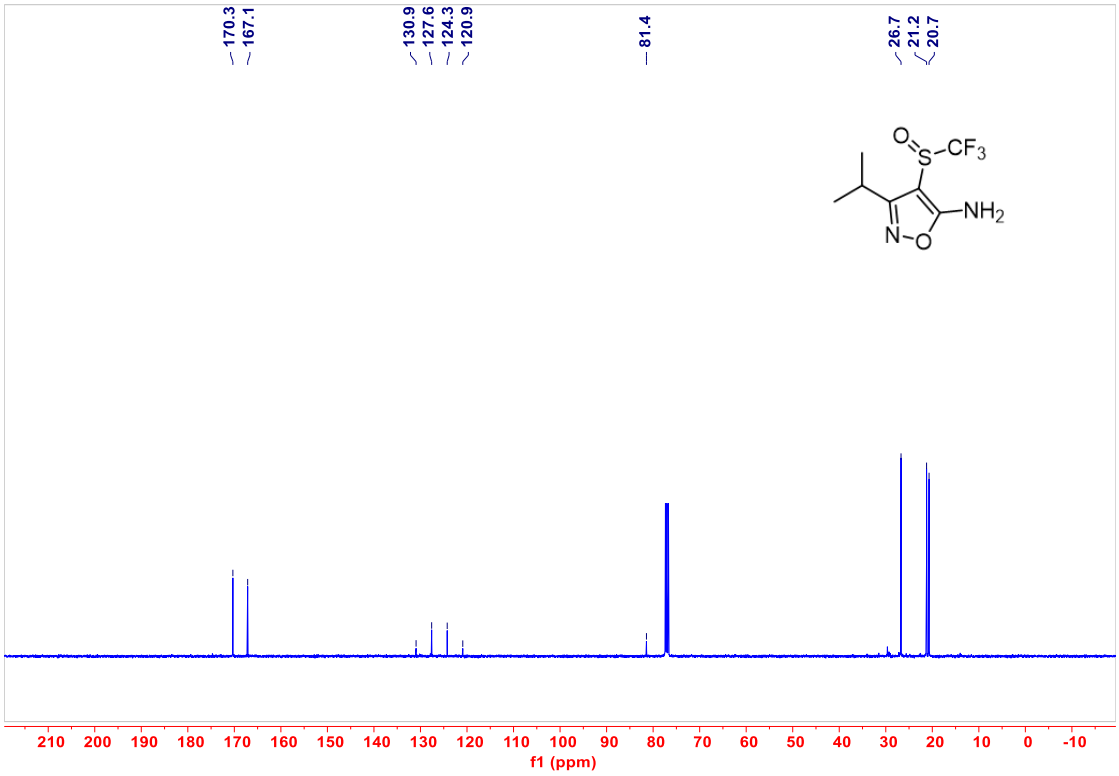
f1 (ppm)


170.3
167.1
130.9
127.6
124.3
120.9
81.4
26.7
21.2
20.7
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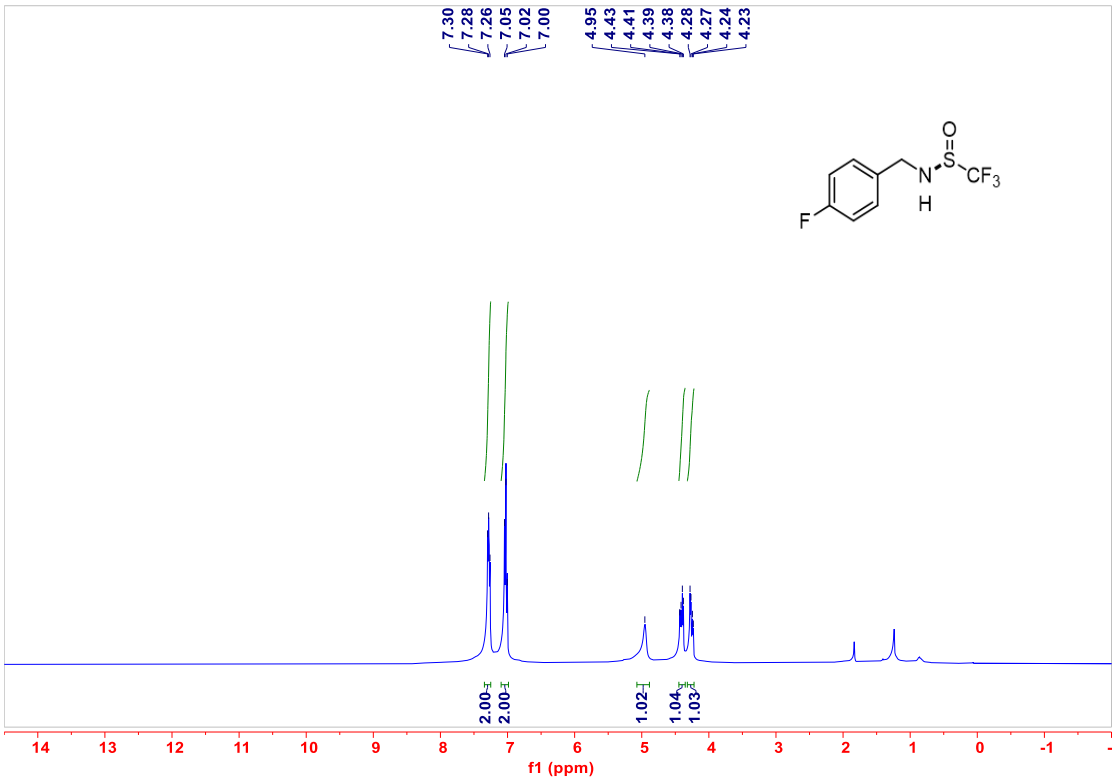
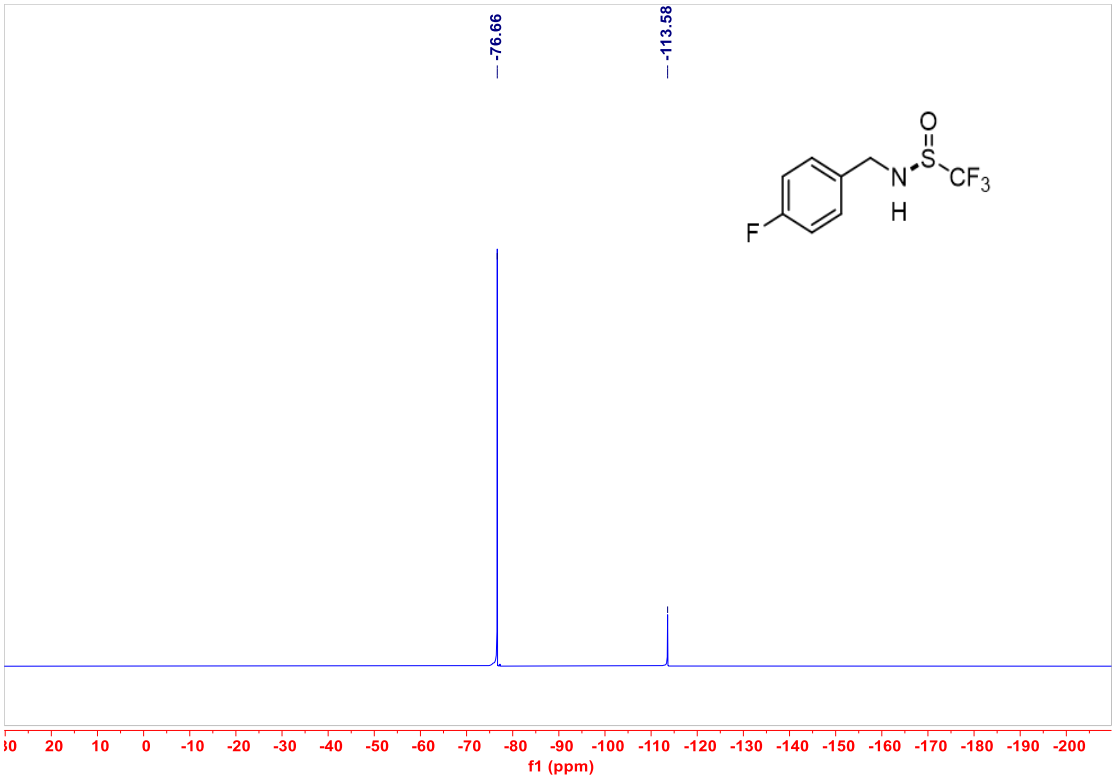
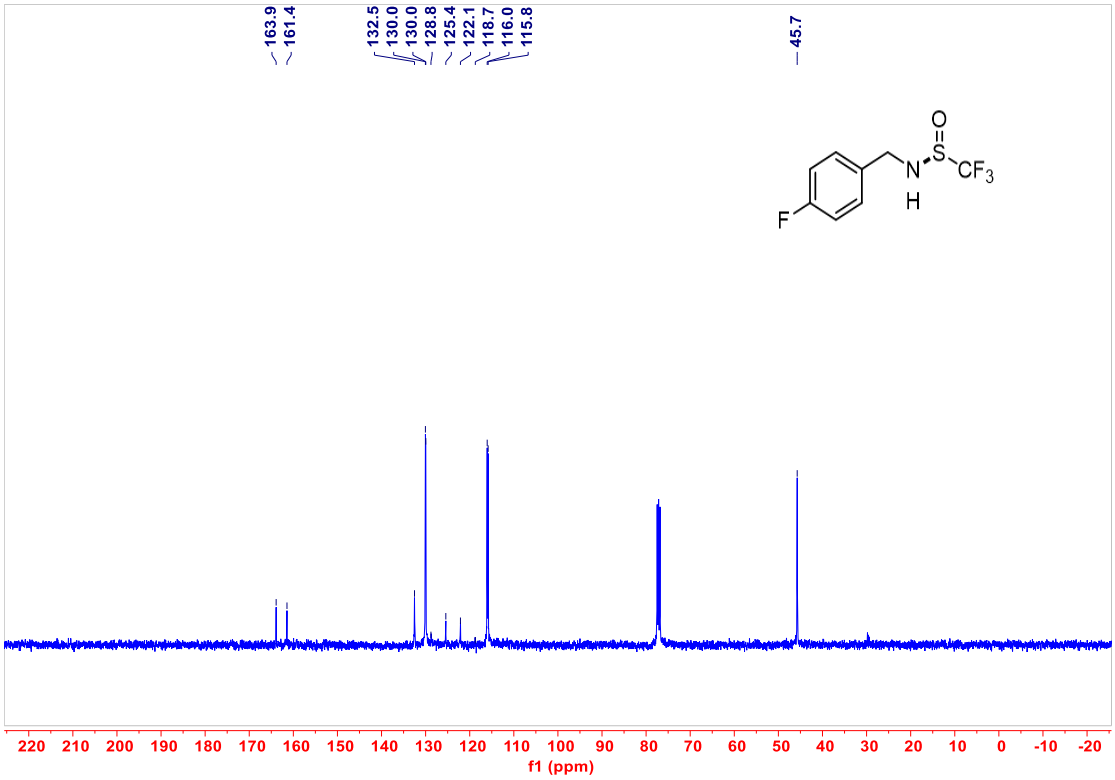
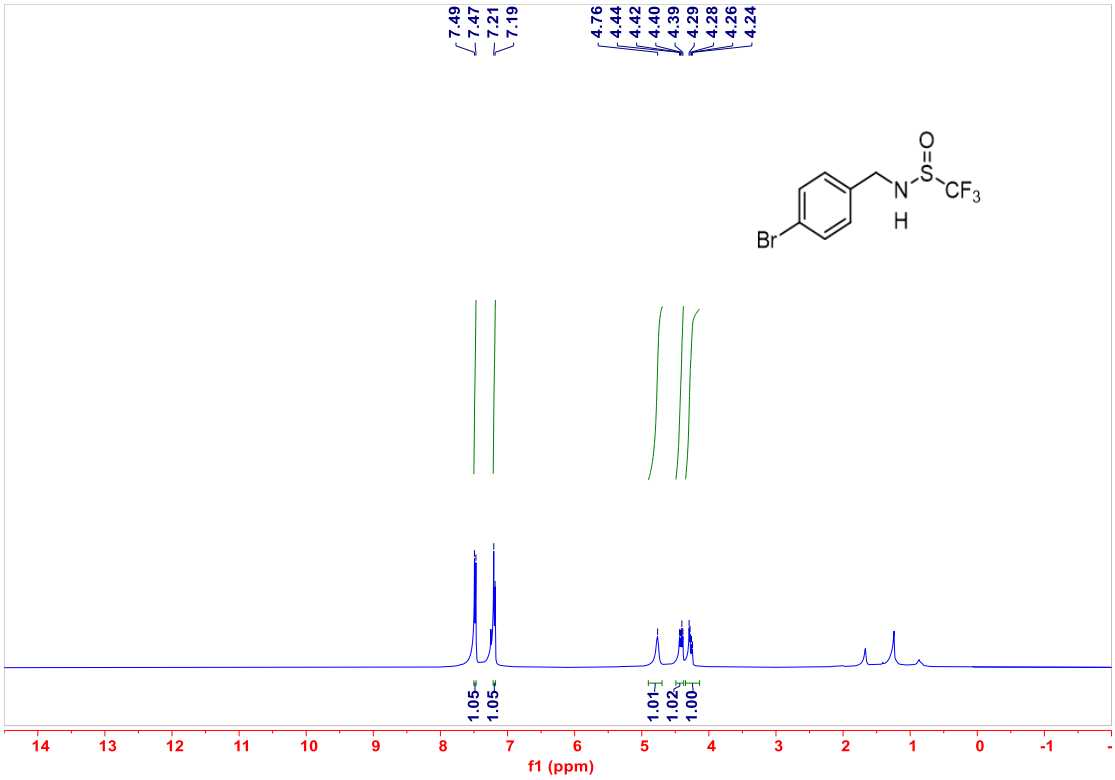
S
CF3
NH2
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.30
7.28
7.26
7.05
7.02
7.00
4.95
4.43
4.41
4.39
4.38
4.28
4.27
4.24
4.23
O
S
N
H
CF3
F
2.00
2.00
1.02
1.04
1.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-76.66
-113.58
O
S
N
H
CF3
F
f1 (ppm)


163.9
161.4
132.5
130.0
130.0
128.8
125.4
122.1
118.7
116.0
115.8
45.7
O
S
N
H
CF3
F
f1 (ppm)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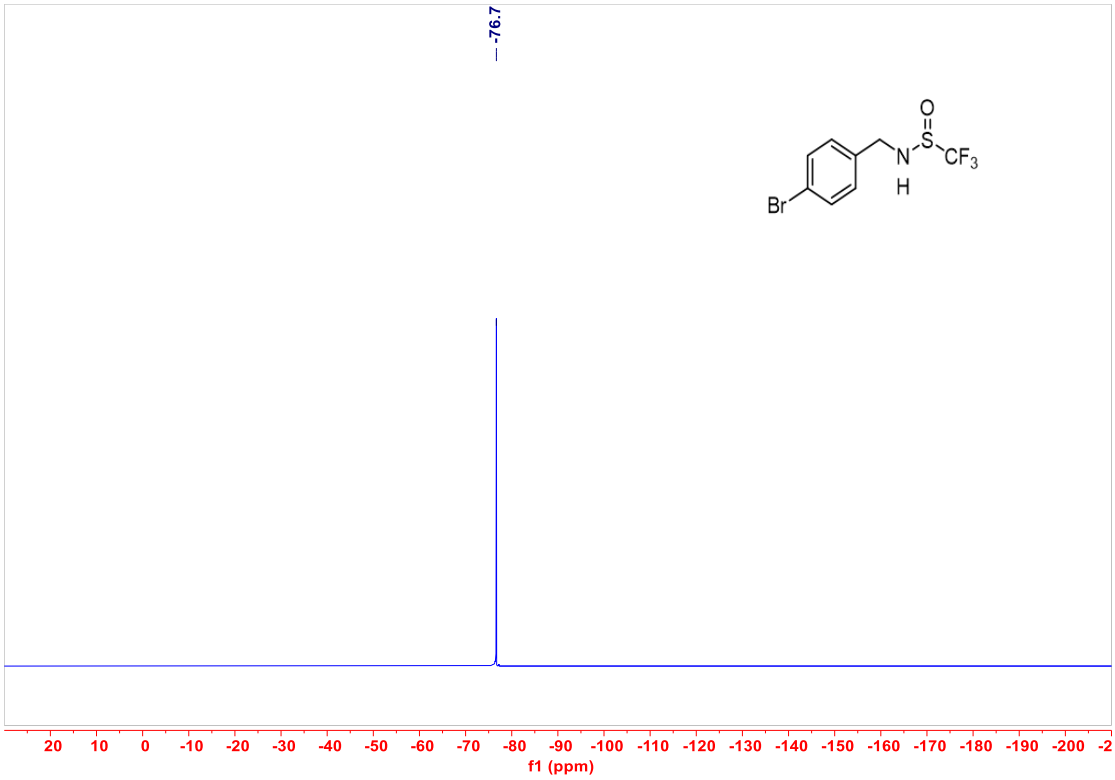
7.47
7.21
7.19
4.76
4.44
4.42
4.40
4.39
4.29
4.28
4.26
4.24
Br
N
H
S
O
CF3
1.05
1.05
1.01
1.02
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-76.7
Br
N
H
S
O
CF3
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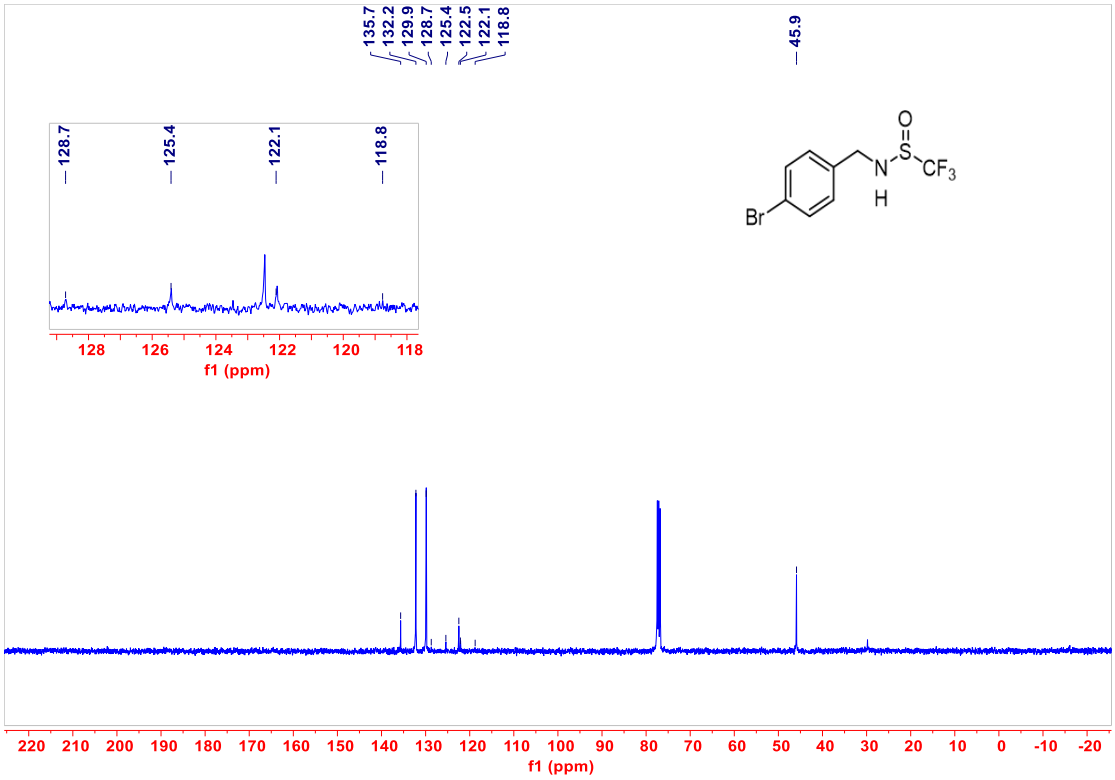
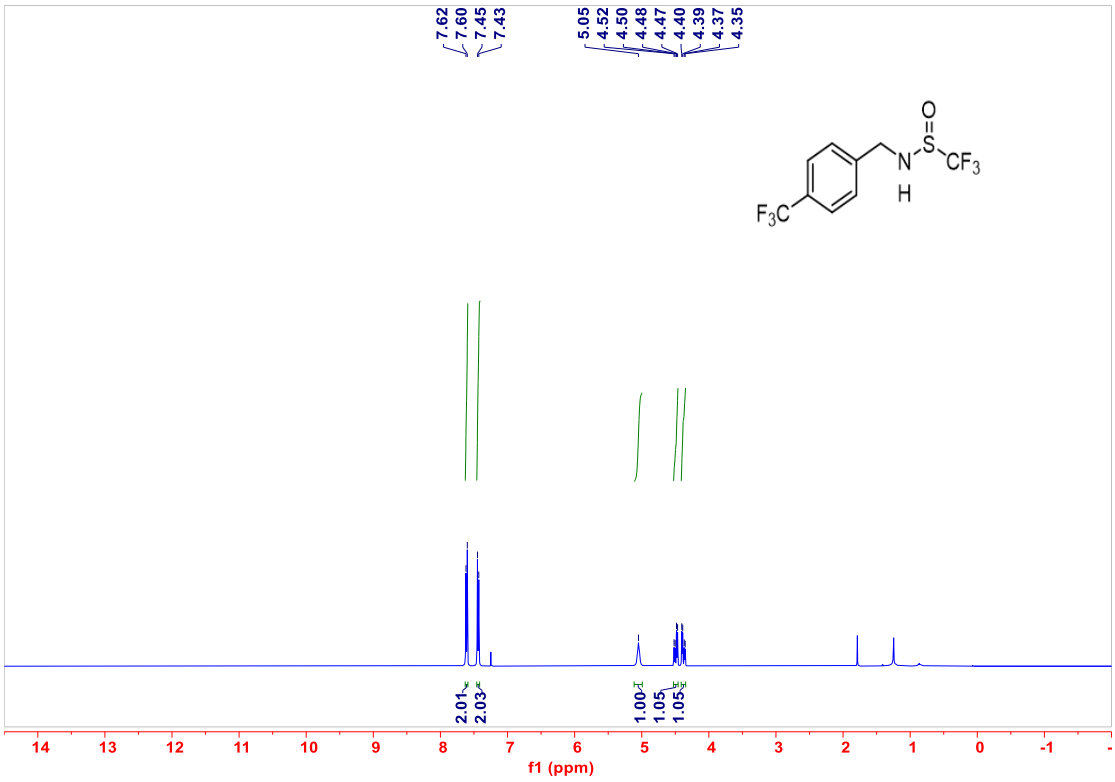
f1 (ppm)


135.7
132.2
129.9
128.7
125.4
122.5
122.1
118.8
45.9
128.7
125.4
122.1
118.8
128 126 124 122 120 118
f1 (ppm)
Br
N
H
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.60
7.45
7.43
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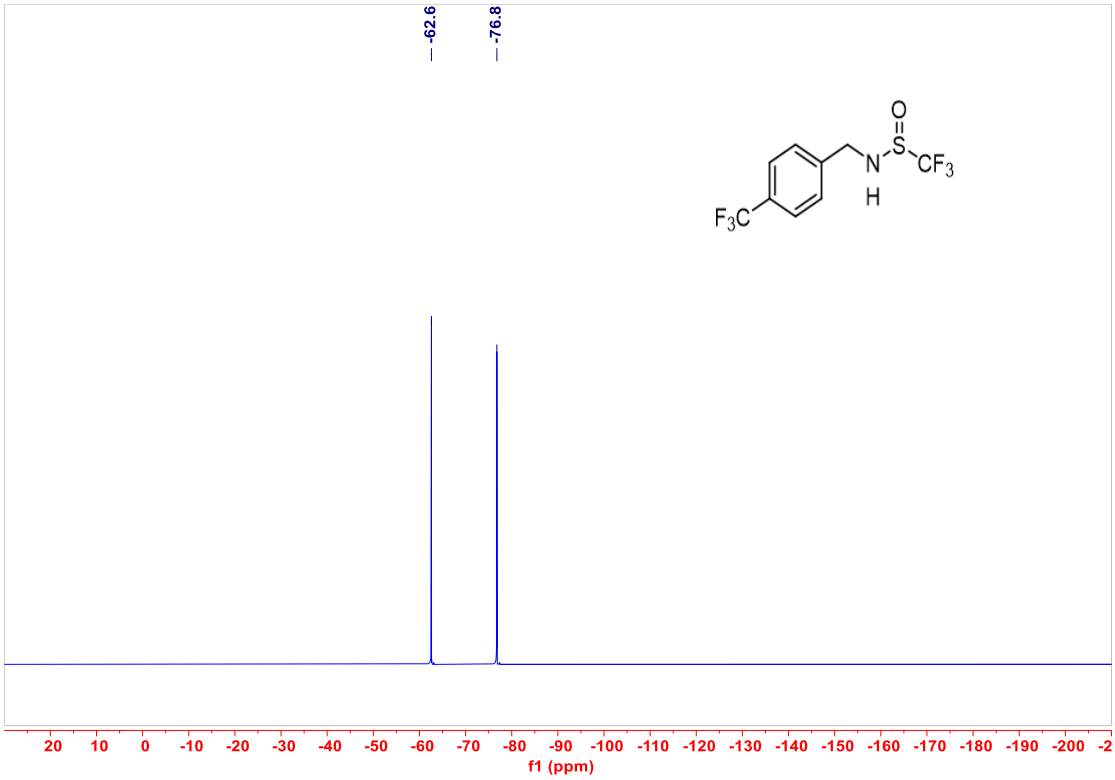
4.52
4.50
4.48
4.47
4.40
4.39
4.37
4.35
F3C
N
H
S
O
CF3
2.01
2.03
1.00
1.05
1.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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-76.8
O
S
N
H
CF3
F3C
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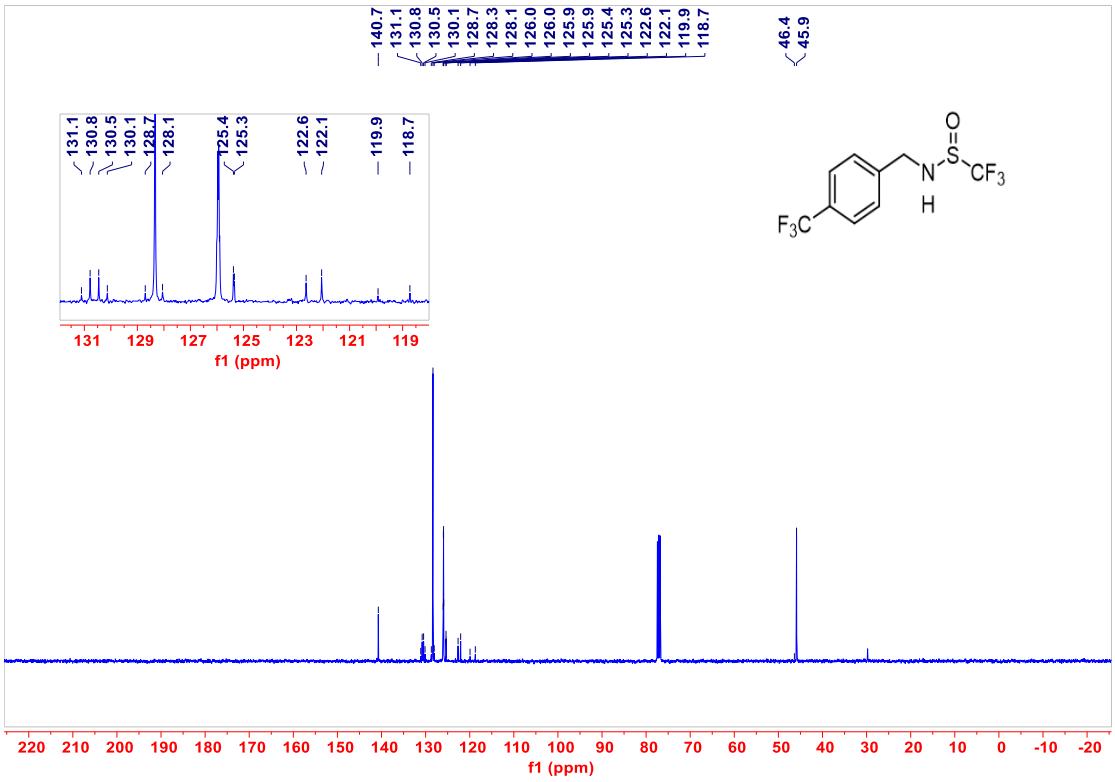
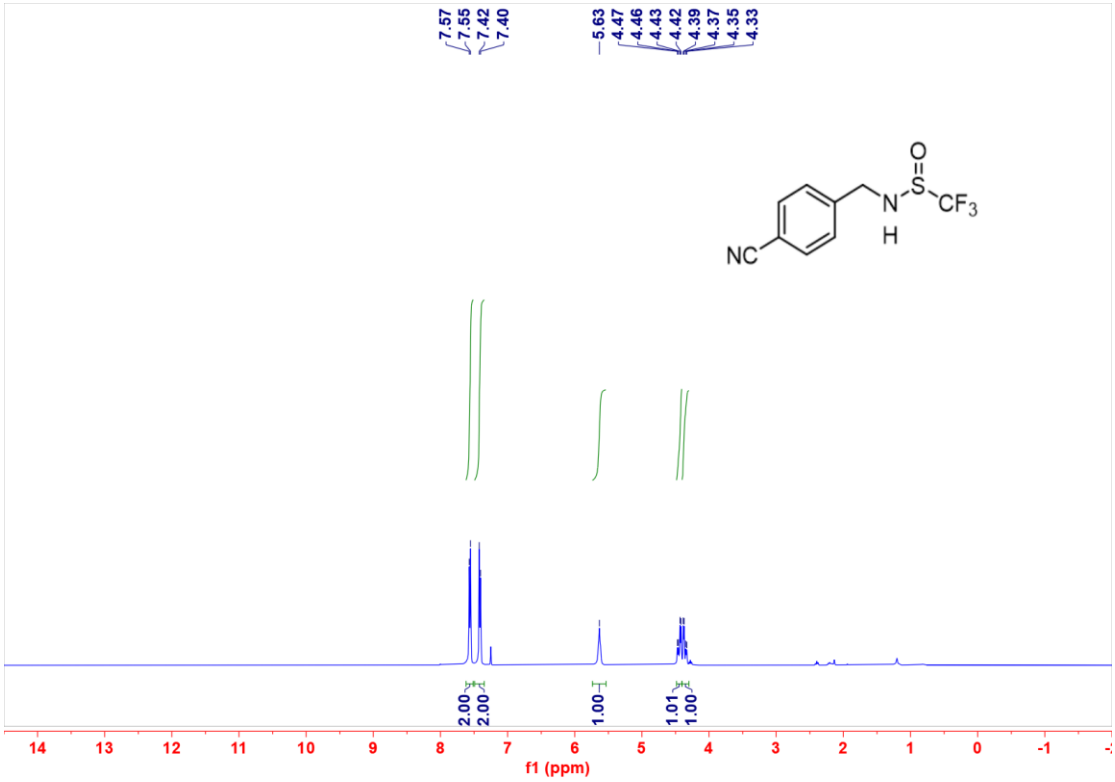
f1 (ppm)


140.7
131.1
130.8
130.5
130.1
128.7
128.3
128.1
126.0
125.9
125.9
125.4
125.3
122.6
122.1
119.9
118.7
46.4
45.9
131.1
130.8
130.5
130.1
128.7
128.1
125.4
125.3
122.6
122.1
119.9
118.7
131 129 127 125 123 121 119
f1 (ppm)
O
S
N
H
CF3
F3C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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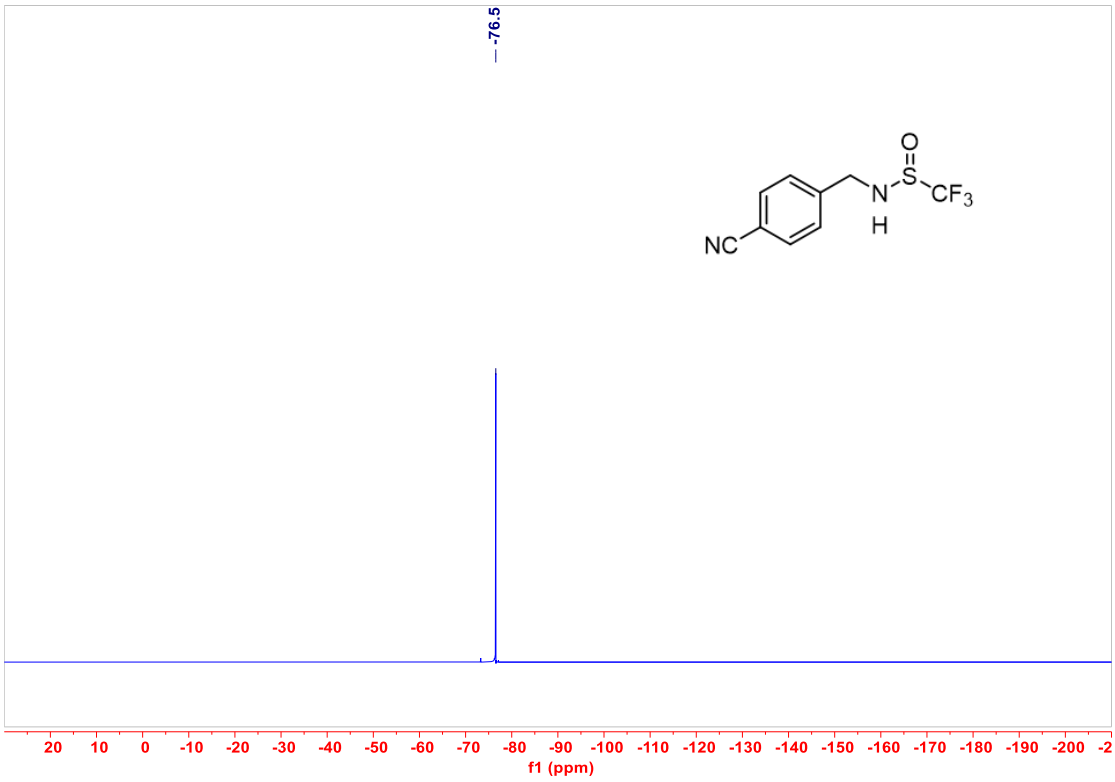
4.43
4.42
4.39
4.37
4.35
4.33
O
S
N
H
CF3
NC
2.00
2.00
1.00
1.01
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
H
CF3
NC
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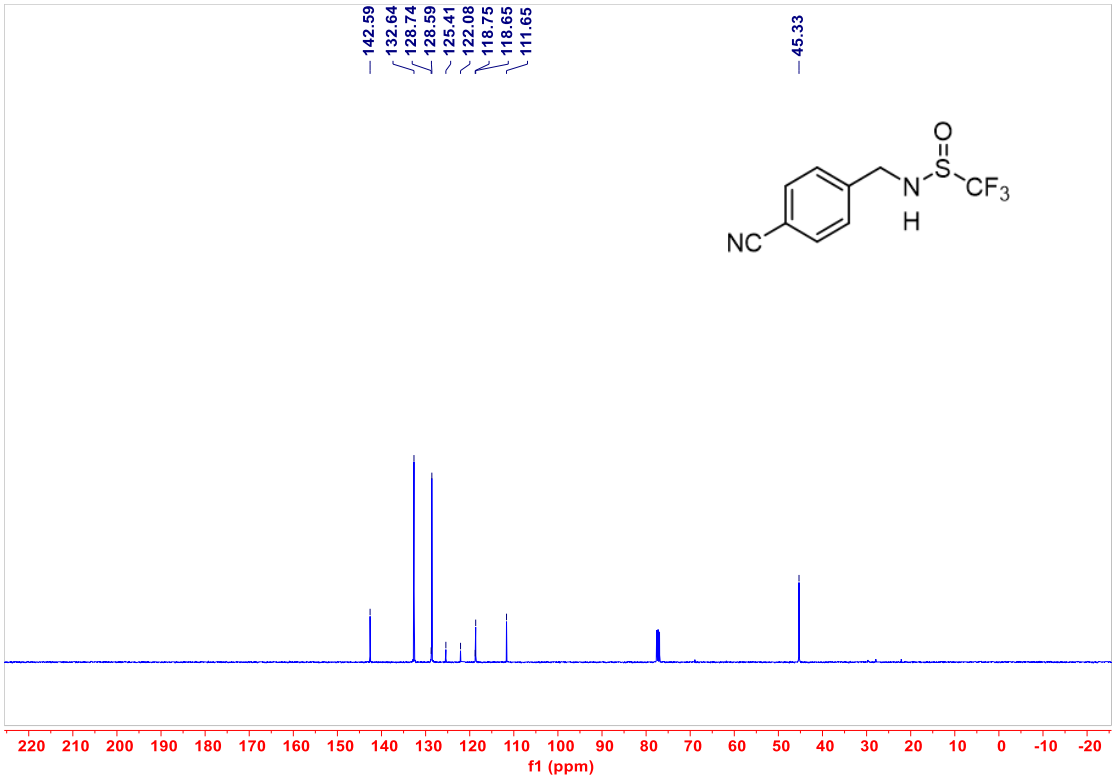
f1 (ppm)


142.59
132.64
128.74
128.59
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122.08
118.75
118.65
111.65
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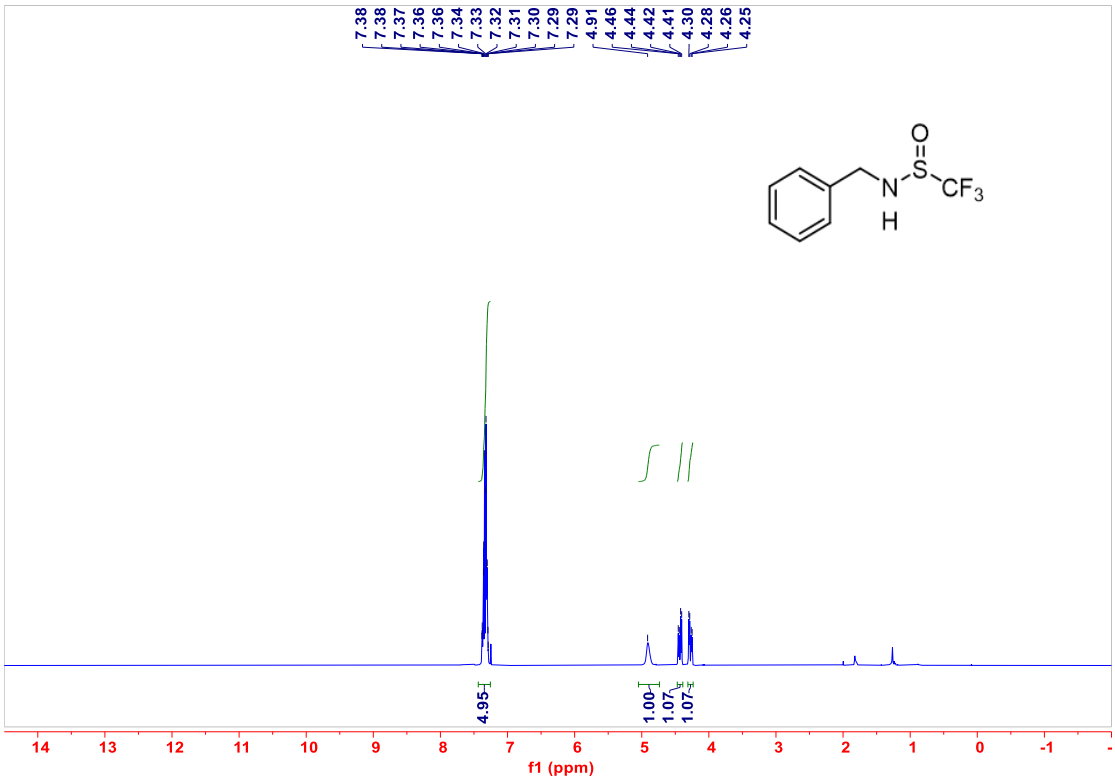
NC
N
H
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.38
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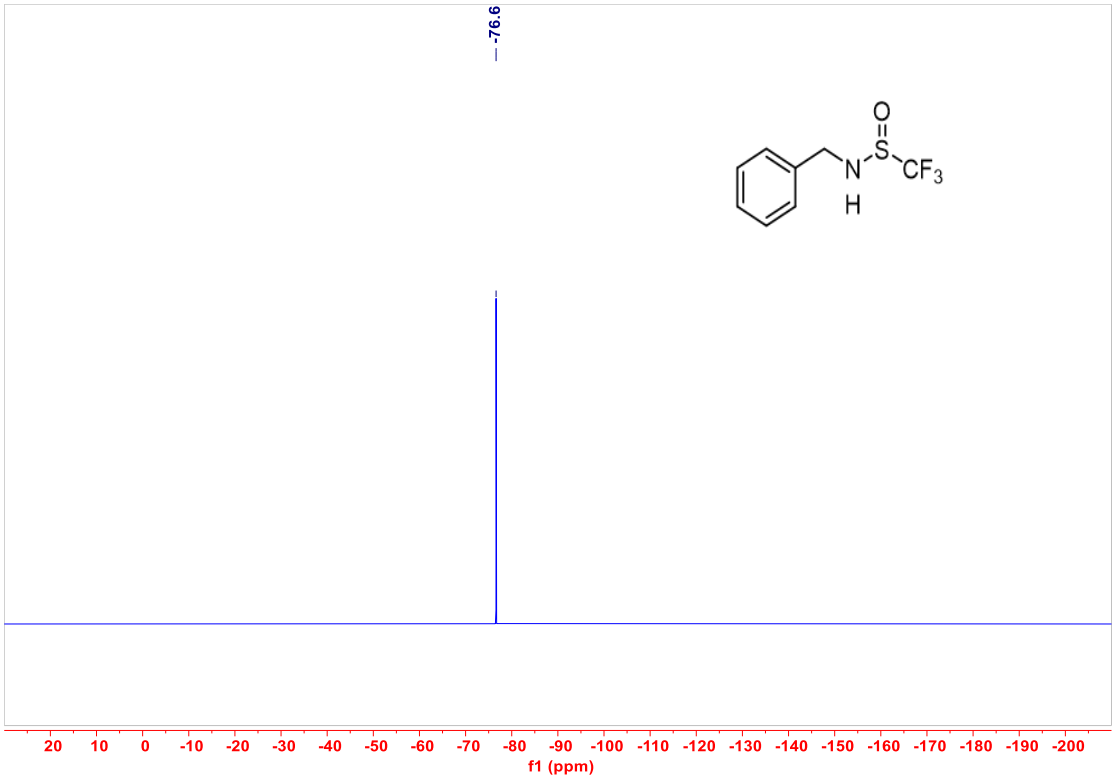
7.34
7.33
7.32
7.31
7.30
7.29
7.29
4.91
4.46
4.44
4.42
4.41
4.30
4.28
4.26
4.25
N
H
S
O
CF3
4.95
1.00
1.07
1.07
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-76.6
O
S
N
H
CF3
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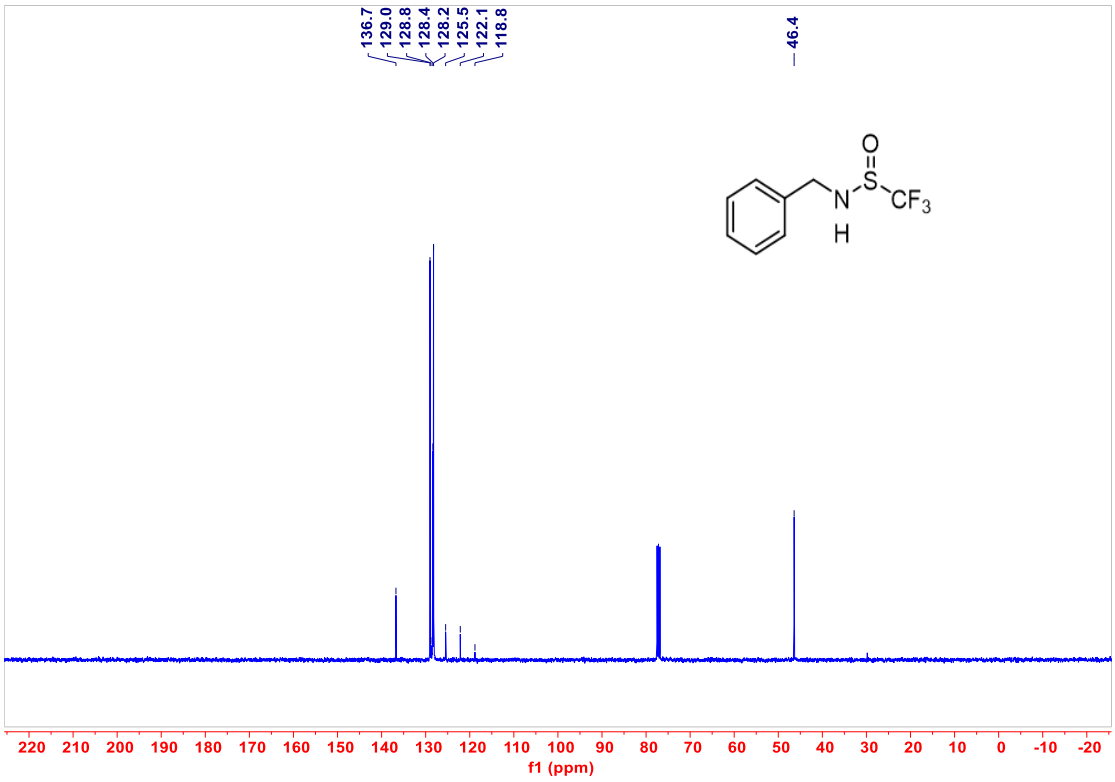
f1 (ppm)


136.7
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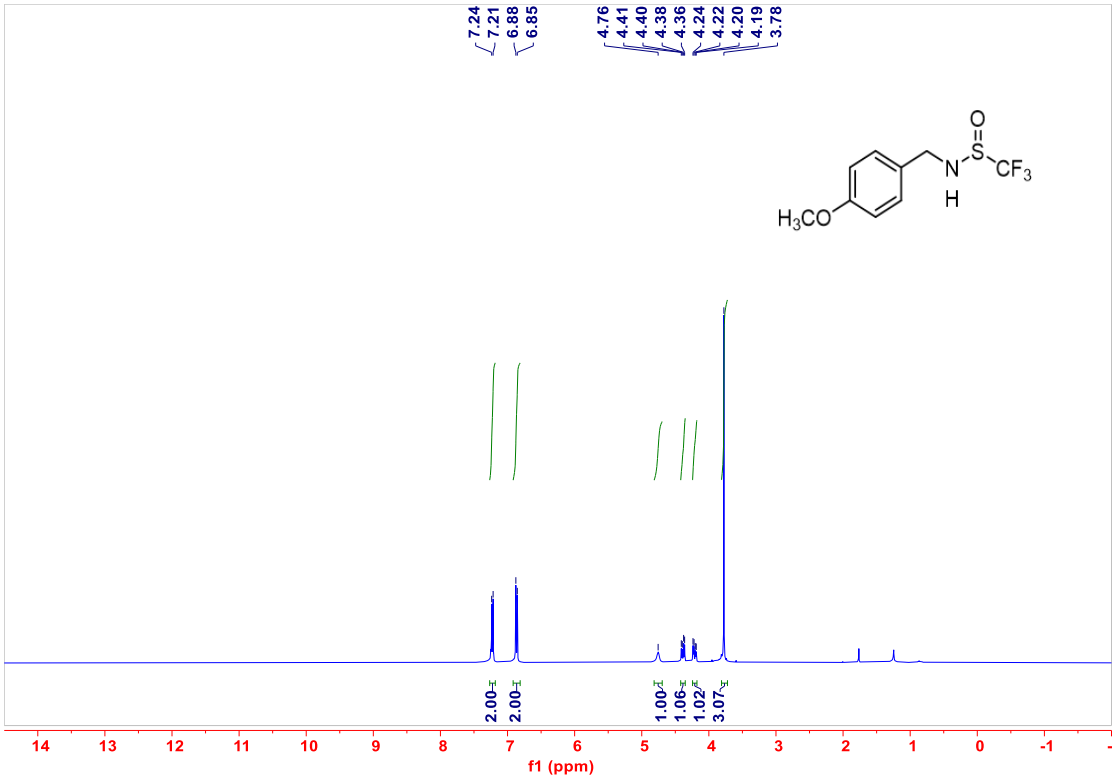
128.8
128.4
128.2
125.5
122.1
118.8
46.4
O
S
N
H
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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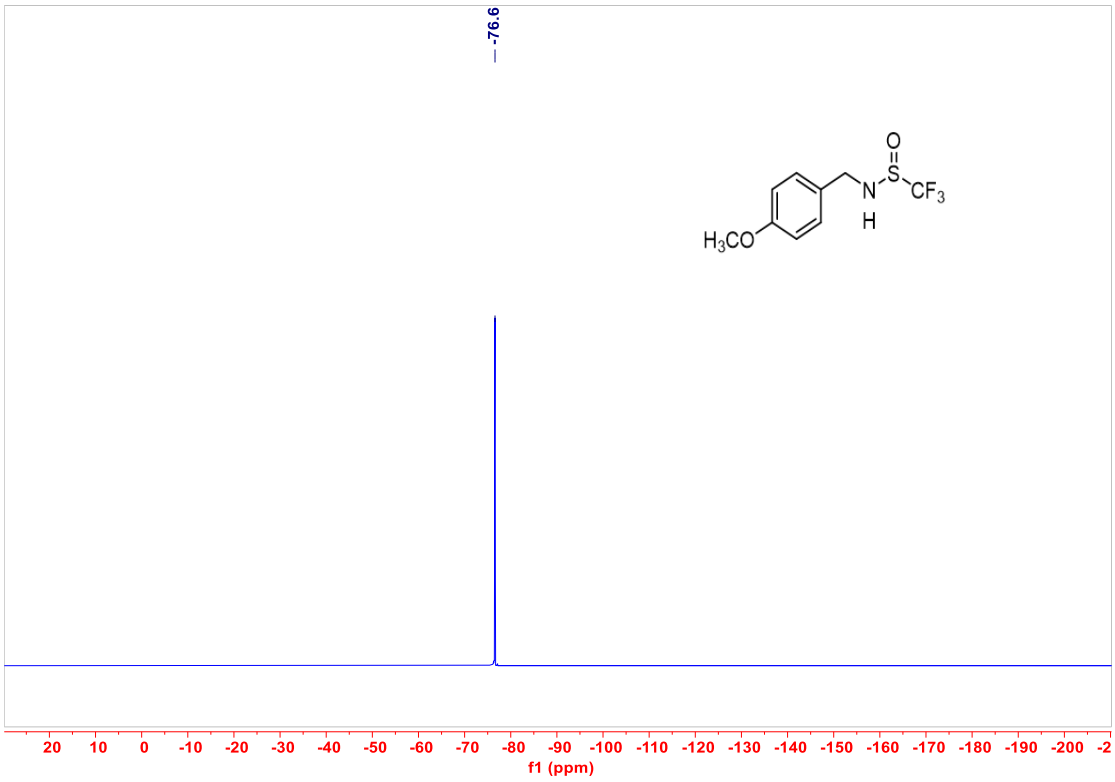
4.76
4.41
4.40
4.38
4.36
4.24
4.22
4.20
4.19
3.78
O
S
N
H
CF3
H3CO
2.00
2.00
1.00
1.06
1.02
3.07
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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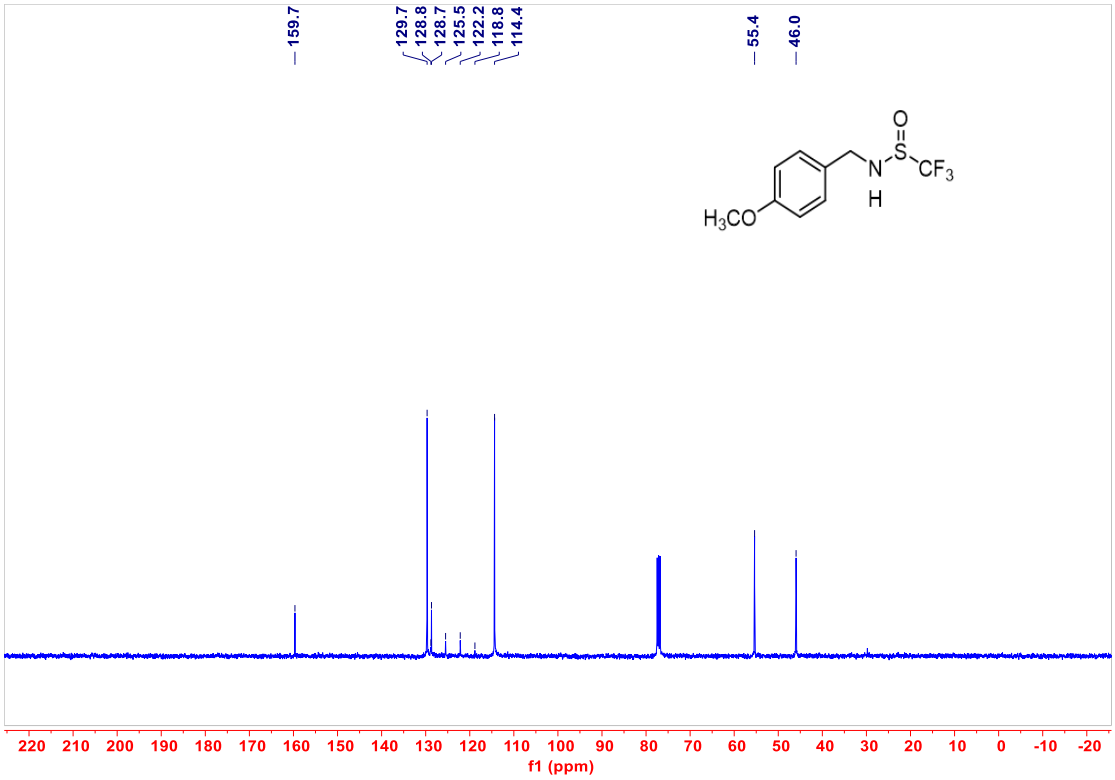
O
S
N
H
CF3
H3CO
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)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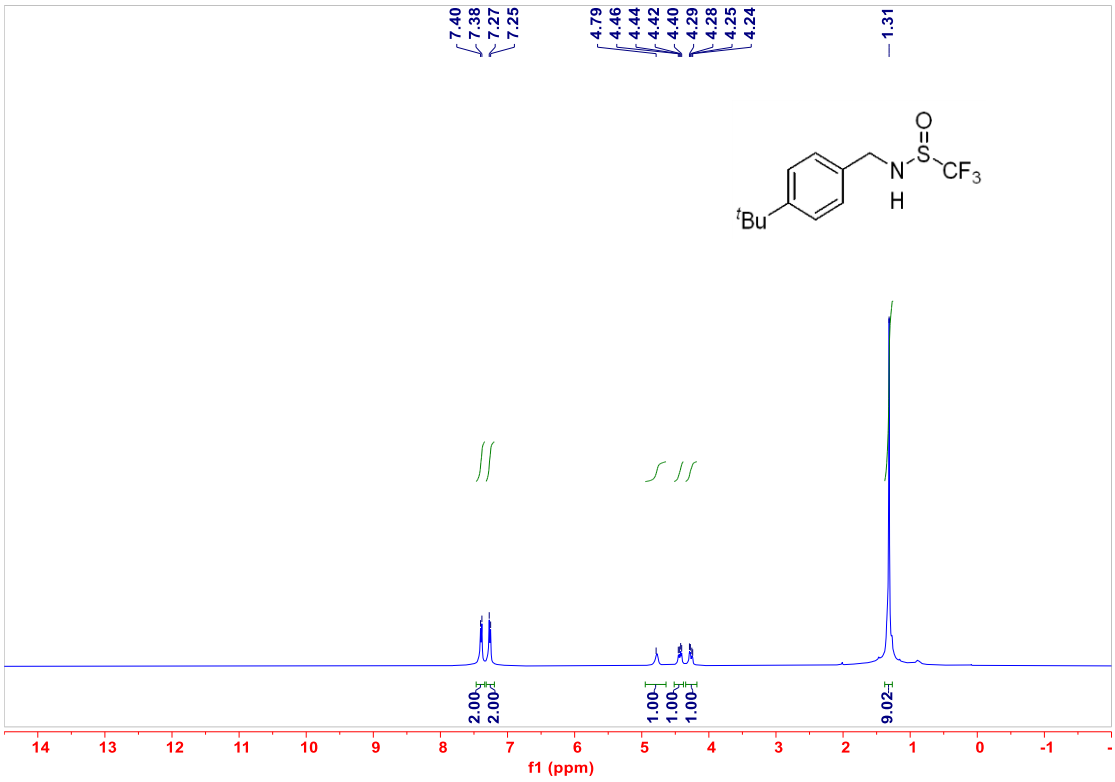
128.7
125.5
122.2
118.8
114.4
55.4
46.0
O
S
N
H
CF3
H3CO
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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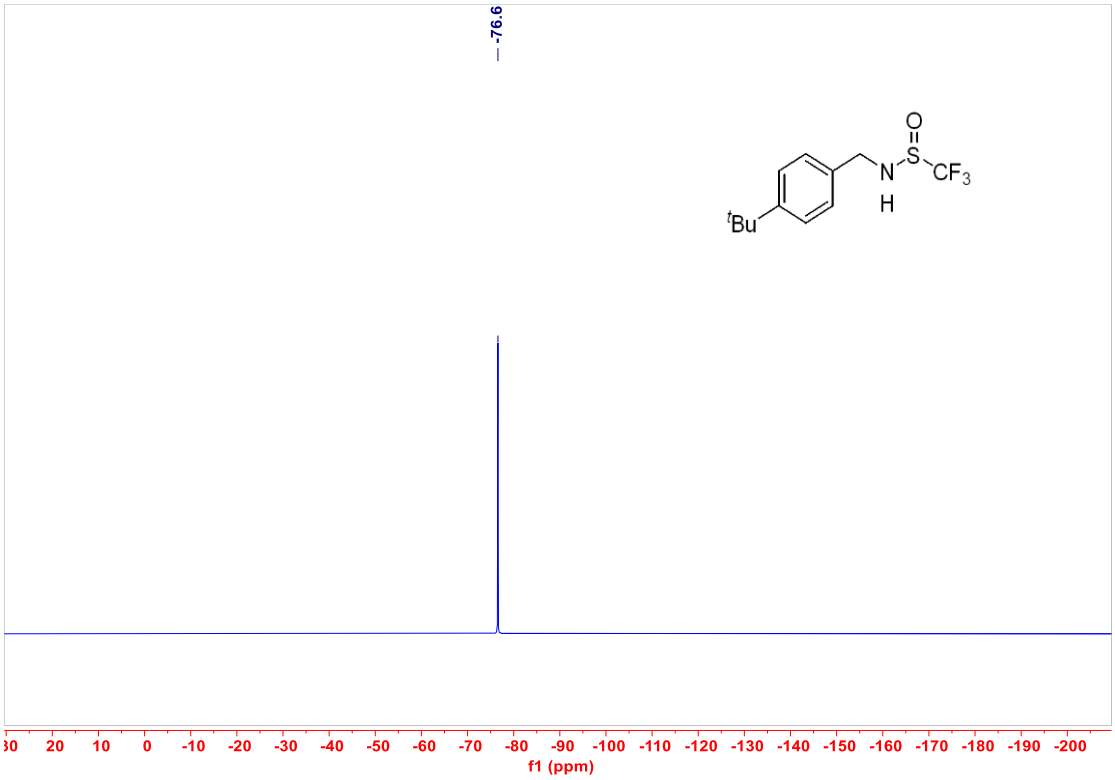
4.46
4.44
4.42
4.40
4.29
4.28
4.25
4.24
1.31
O
S
N
H
CF3
tBu
2.00
2.00
1.00
1.00
1.00
9.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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O
S
N
H
CF3
tBu
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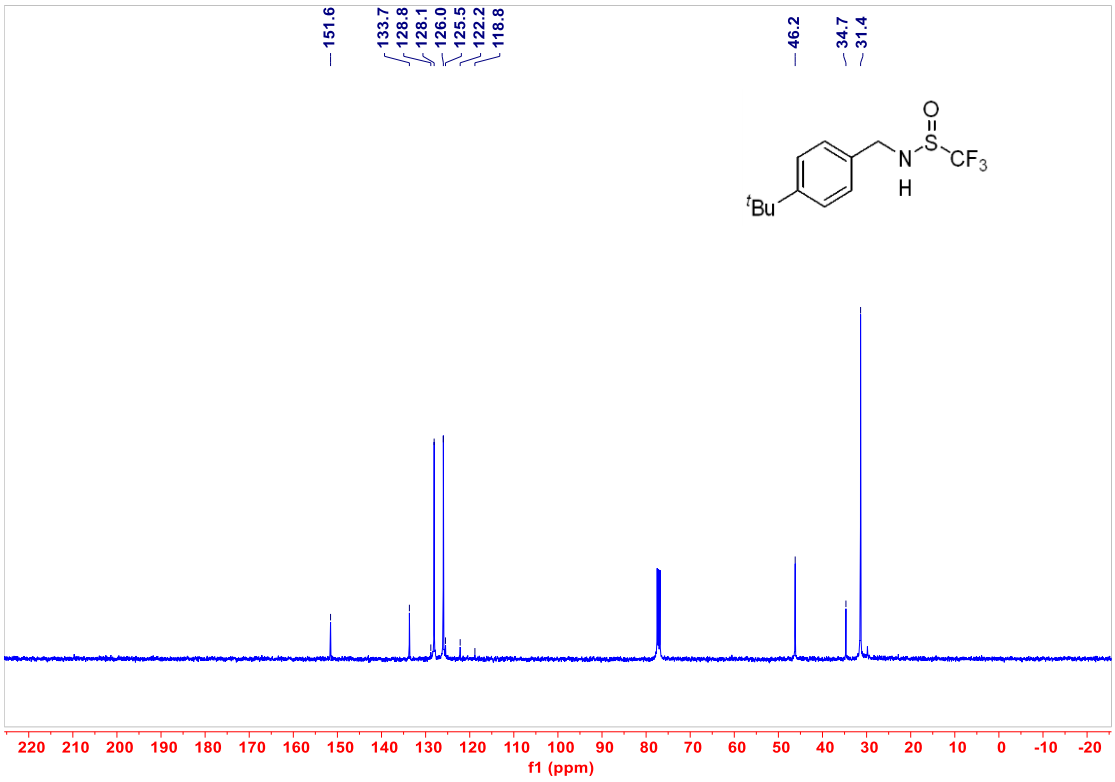
f1 (ppm)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133.7
128.8
128.1
126.0
125.5
122.2
118.8
46.2
34.7
31.4
O
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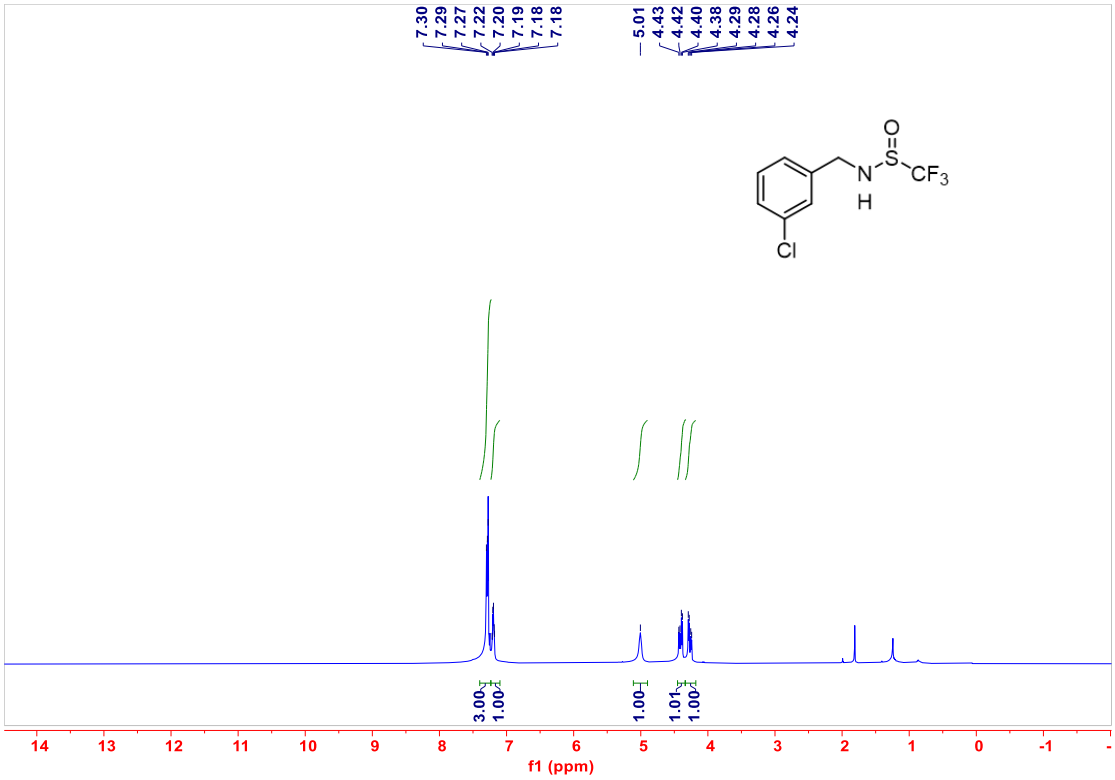
N
H
CF3
tBu
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.27
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7.19
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7.18
5.01
4.43
4.42
4.40
4.38
4.29
4.28
4.26
4.24
O
S
N
H
CF3
Cl
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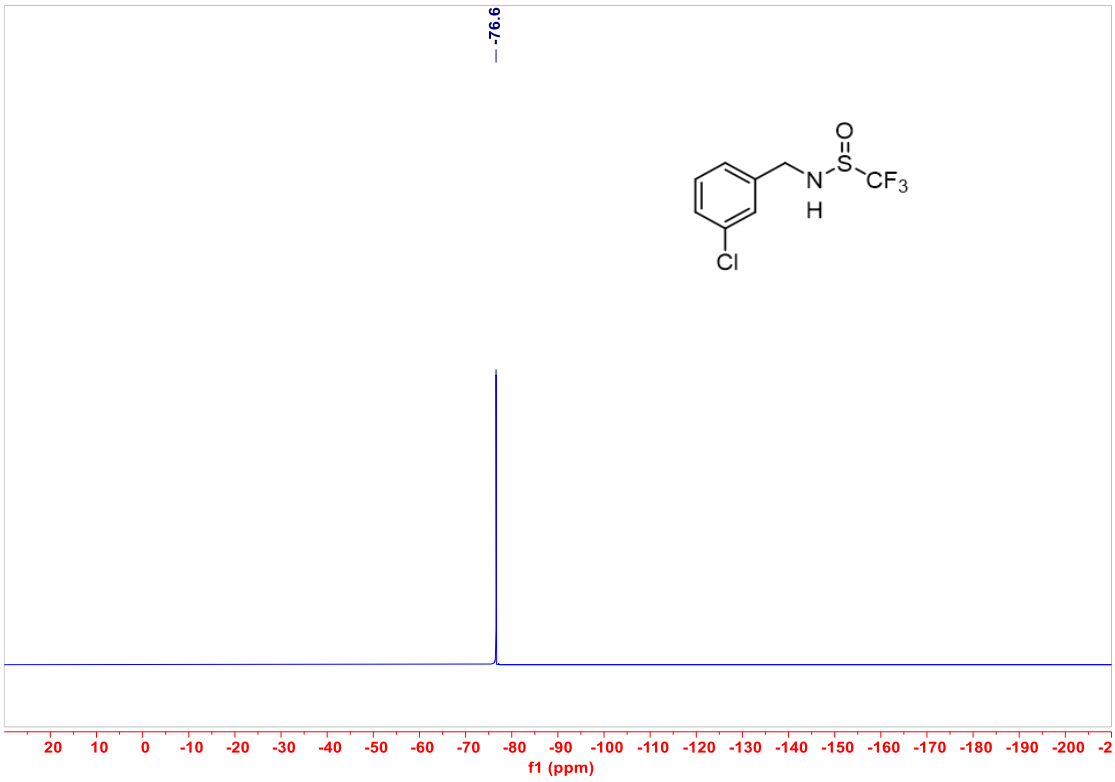
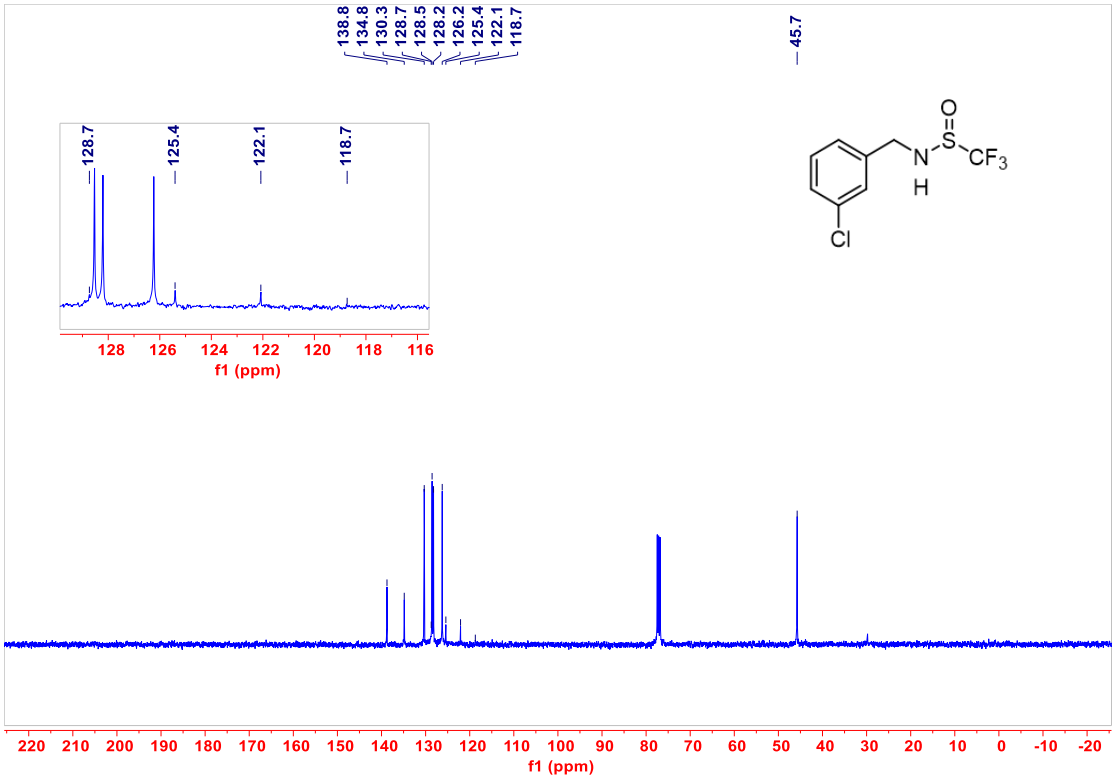
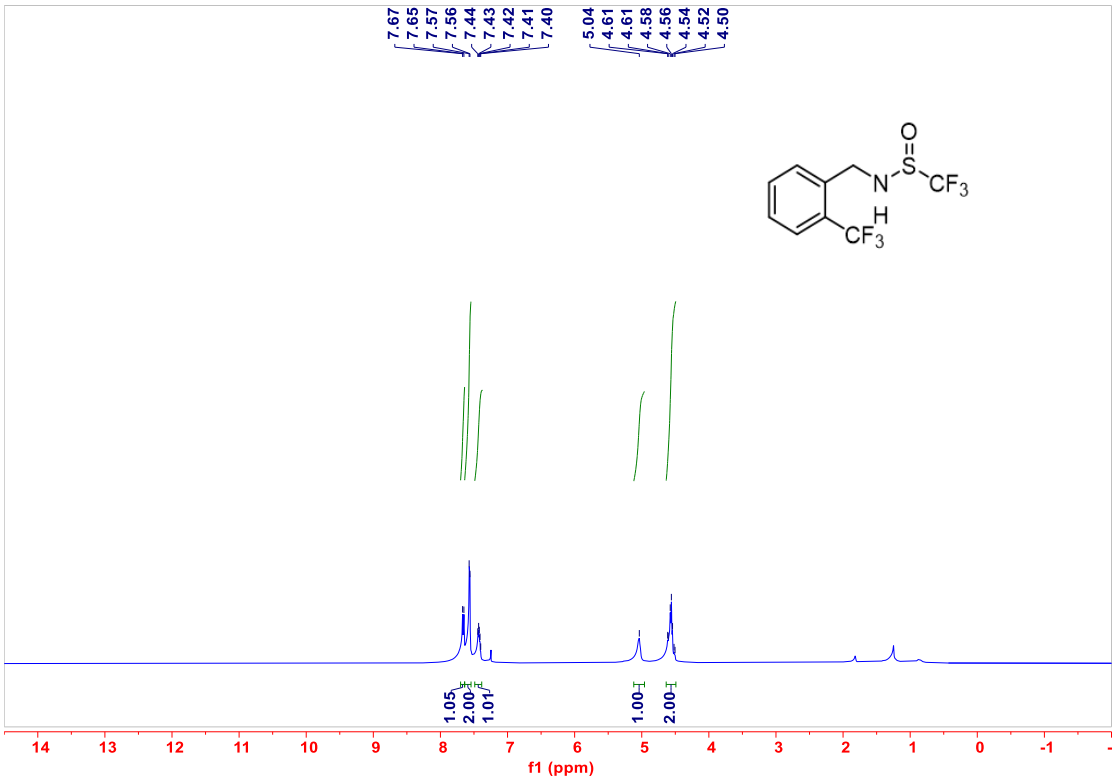
1.00
1.00
1.01
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-76.6
O
S
N
H
CF3
Cl
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


138.8
134.8
130.3
128.7
128.5
128.2
126.2
125.4
122.1
118.7
45.7
128.7
125.4
122.1
118.7
128 126 124 122 120 118 116
f1 (ppm)
O
S
N
H
CF3
Cl
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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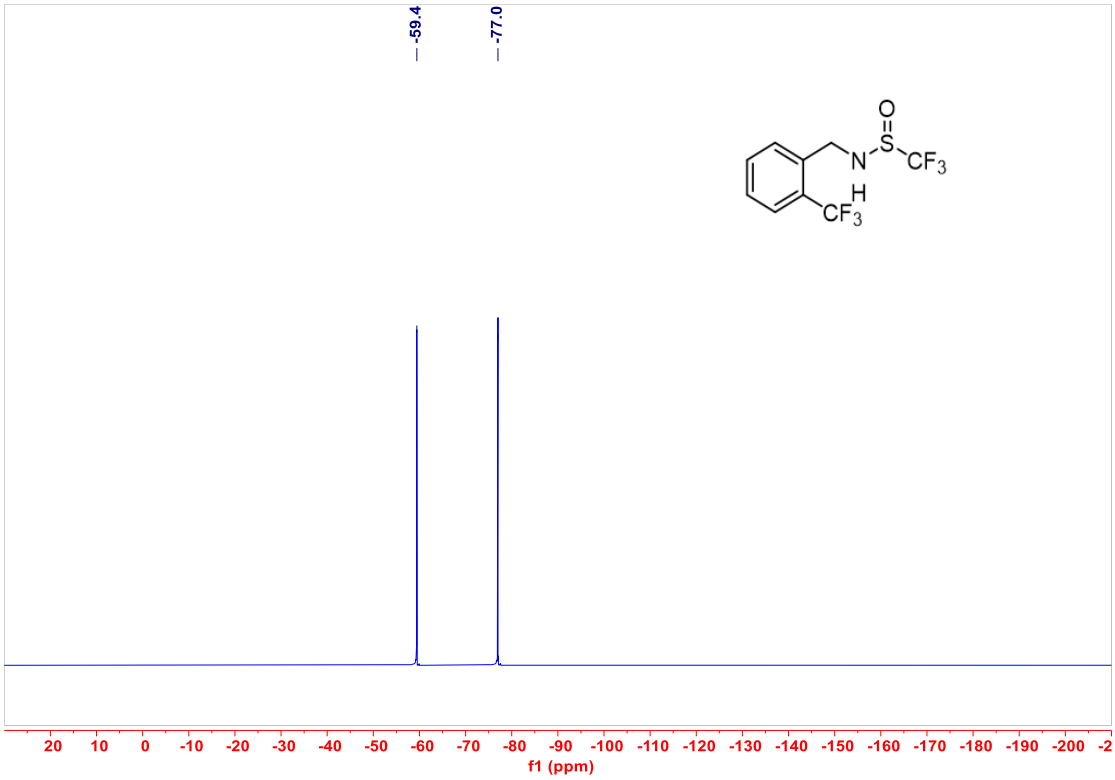
7.42
7.41
7.40
5.04
4.61
4.61
4.58
4.56
4.54
4.52
4.50
O
S
N
H
CF3
CF3
1.05
2.00
1.01
1.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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O
S
N
H
CF3
CF3
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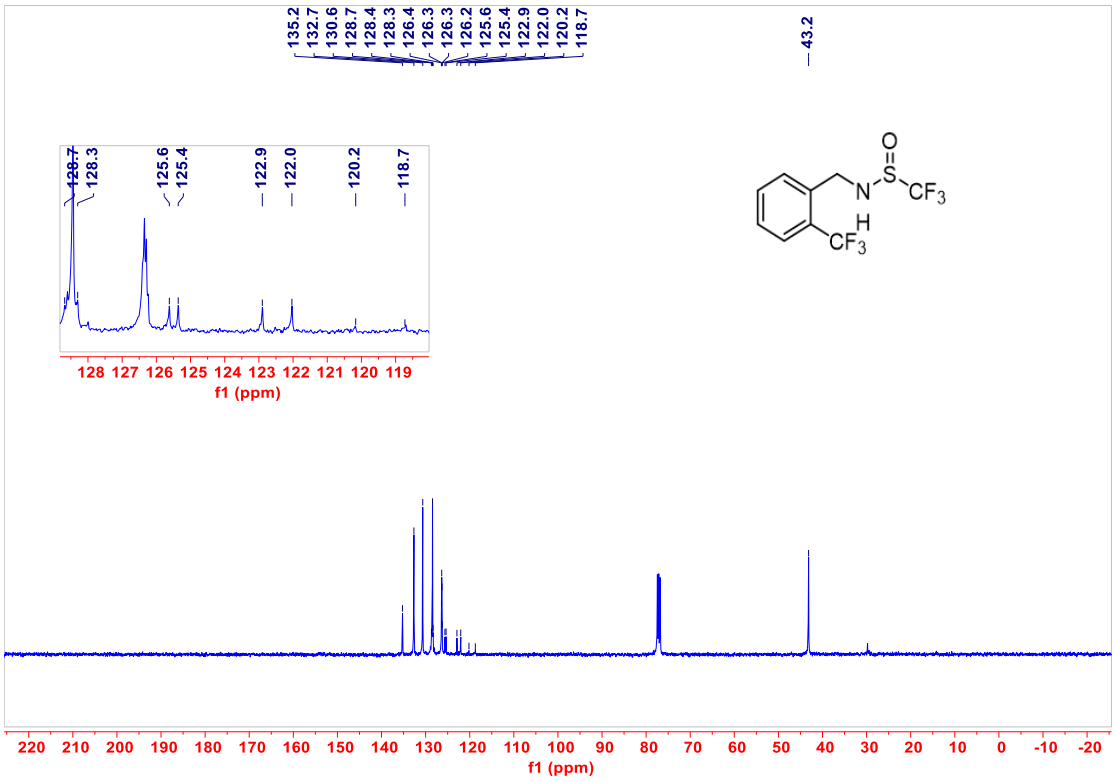
f1 (ppm)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128.4
128.3
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126.3
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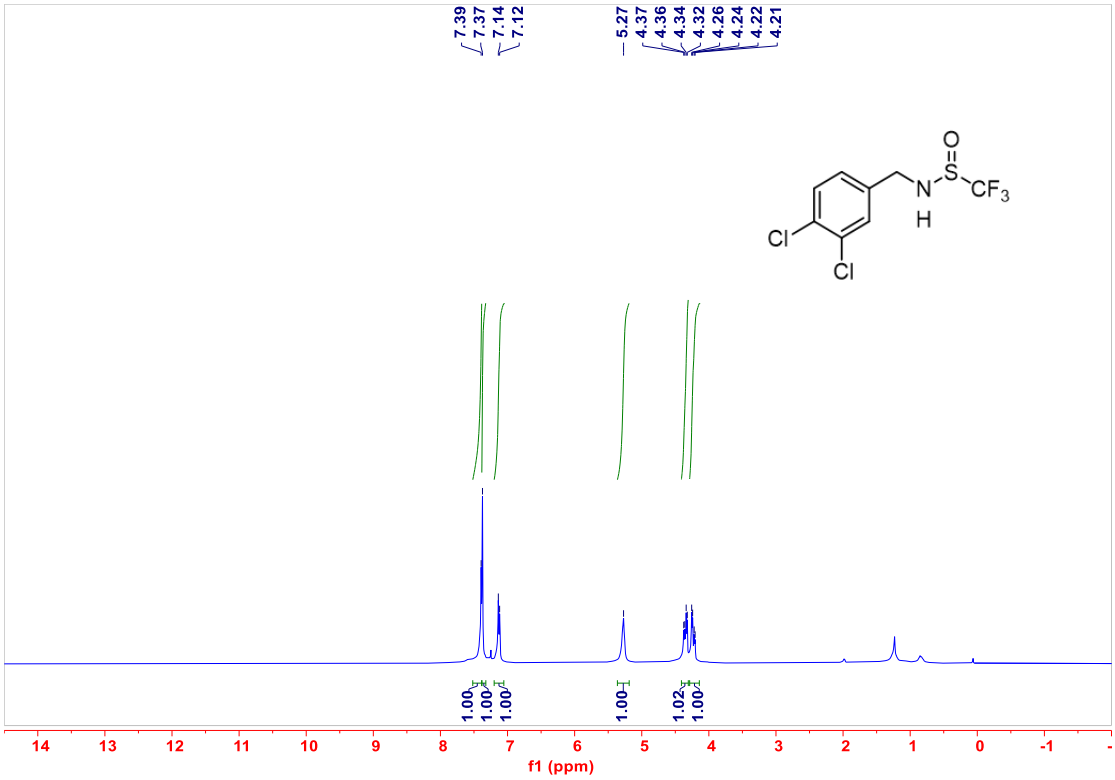
126.2
125.6
125.4
122.9
122.0
120.2
118.7
43.2
128.7
128.3
125.6
125.4
122.9
122.0
120.2
118.7
128 127 126 125 124 123 122 121 120 119
f1 (ppm)
O
S
N
H
CF3
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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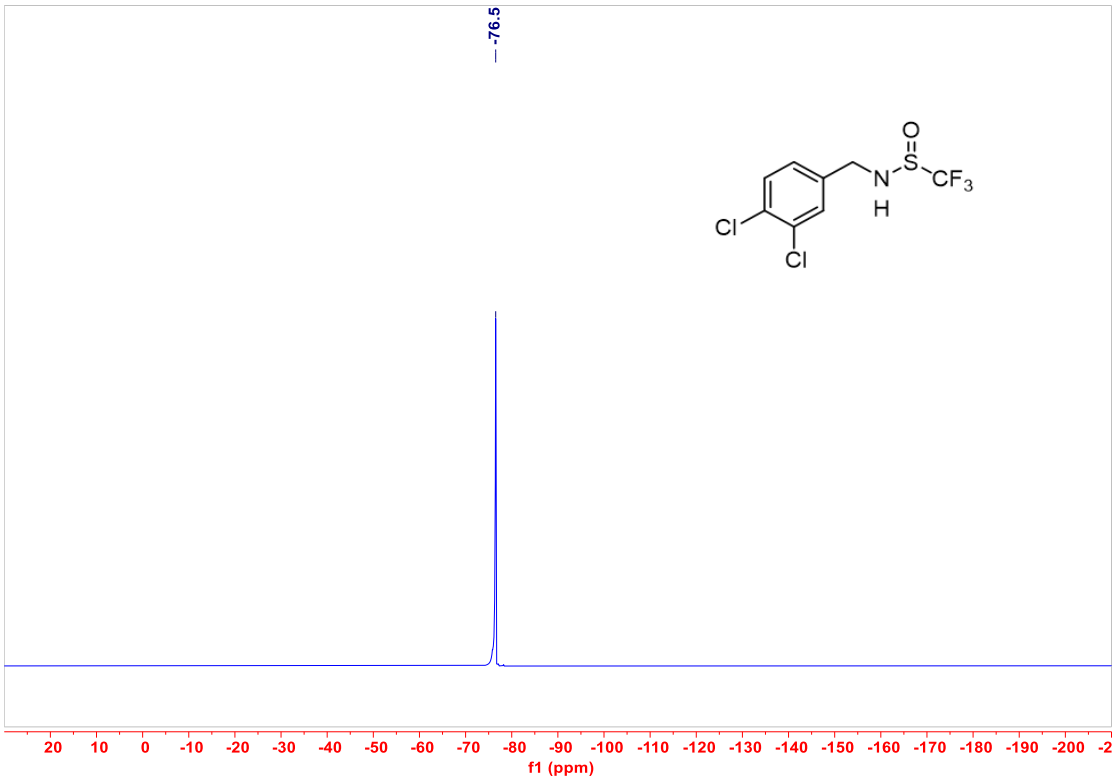
4.26
4.24
4.22
4.21
O
S
N
H
CF3
Cl
Cl
1.00
1.00
1.00
1.00
1.02
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
H
CF3
Cl
Cl
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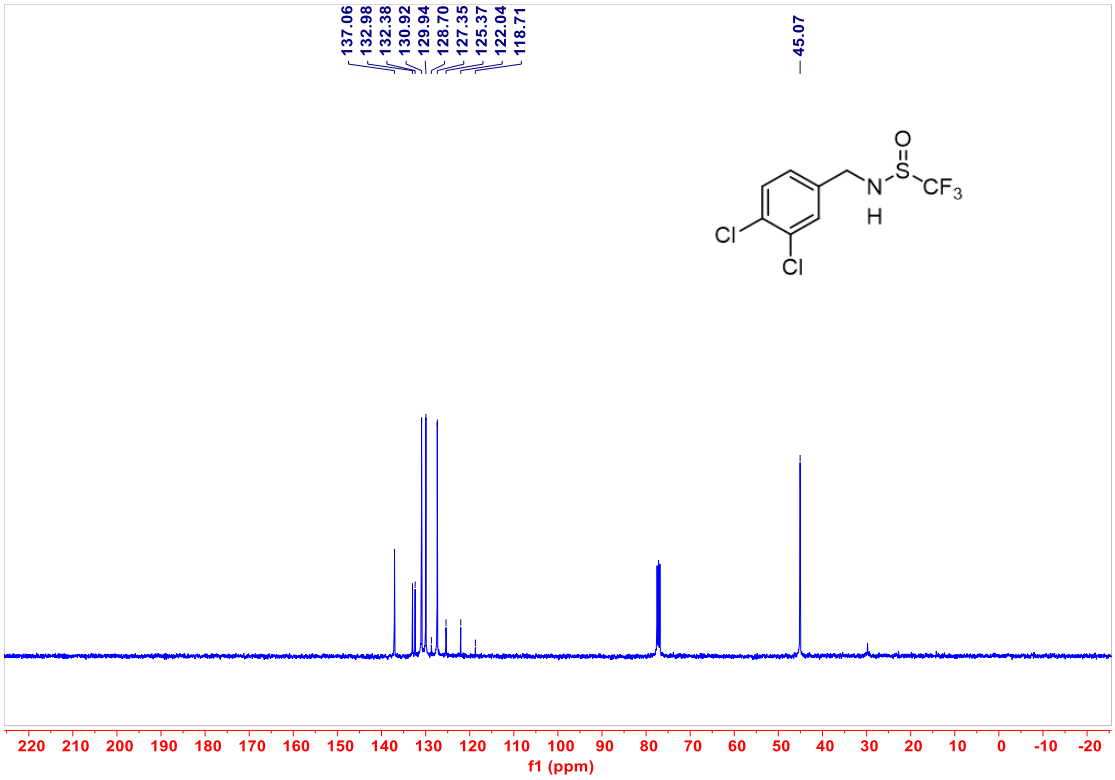
f1 (ppm)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128.70
127.35
125.37
122.04
118.71
45.07
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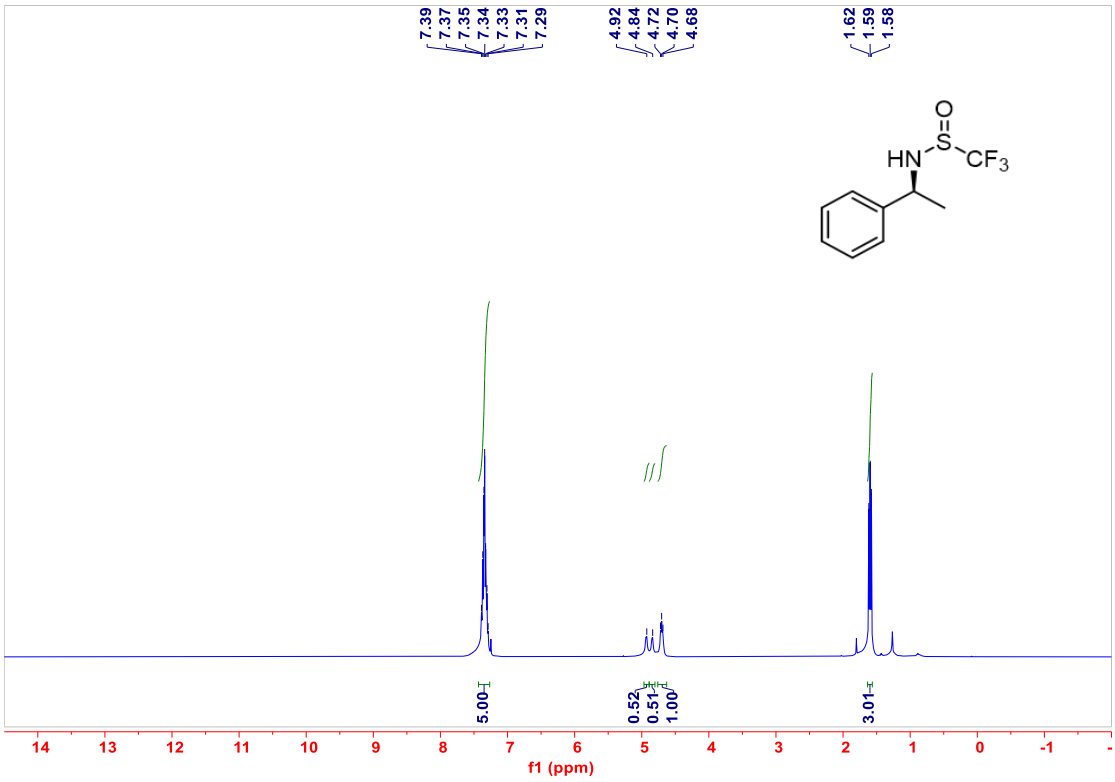
N
H
CF3
Cl
Cl
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.29
4.92
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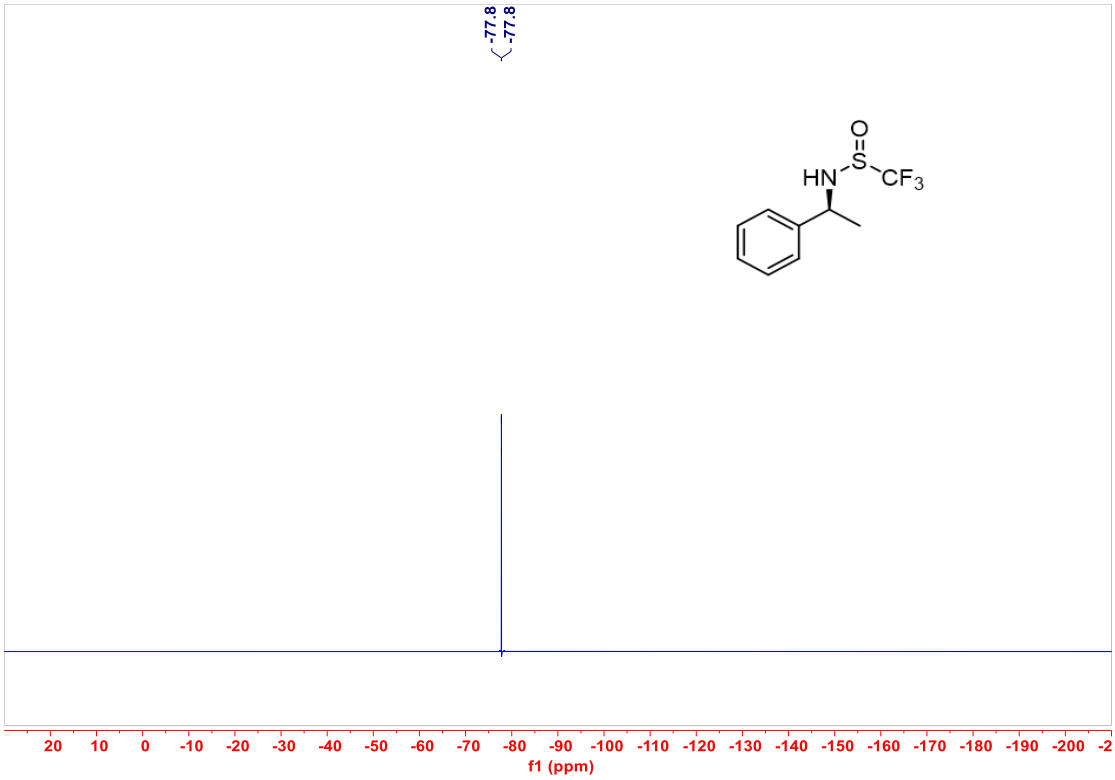
4.72
4.70
4.68
1.62
1.59
1.58
O
S
HN
CF3
5.00
0.52
0.51
1.00
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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-77.8
HN
S
O
CF3
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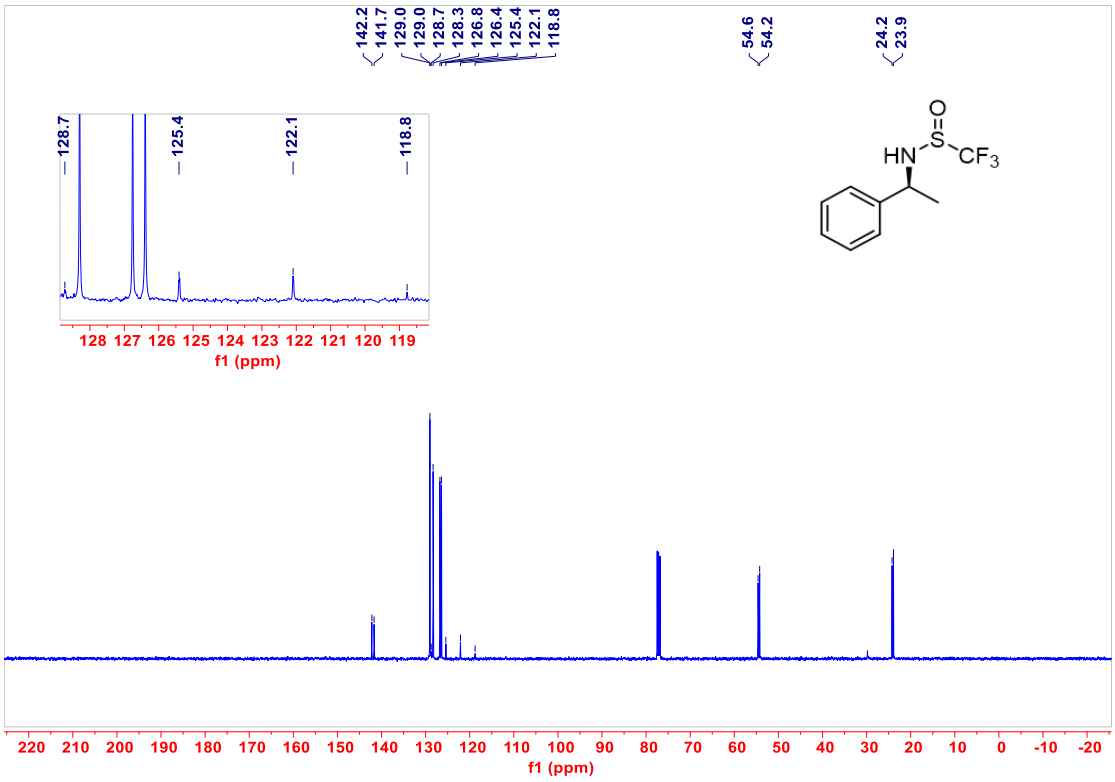
f1 (ppm)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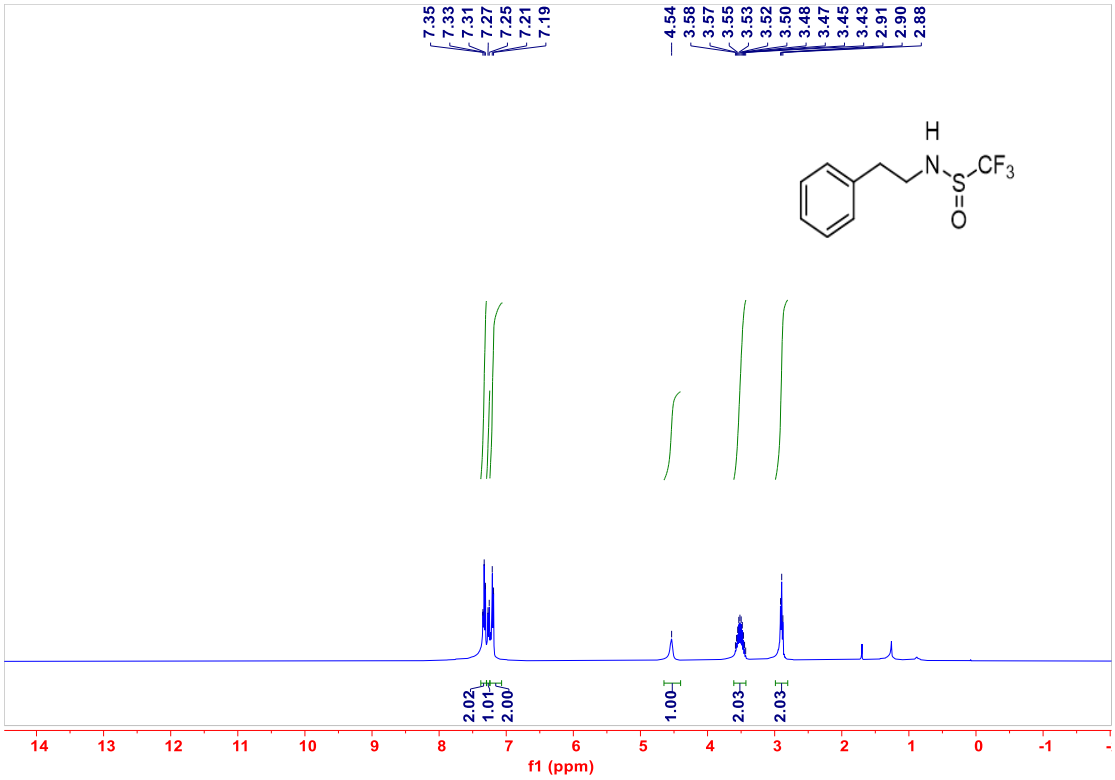
126.8
126.4
125.4
122.1
118.8
54.6
54.2
24.2
23.9
128.7
125.4
122.1
118.8
128 127 126 125 124 123 122 121 120 119
f1 (ppm)
HN
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.33
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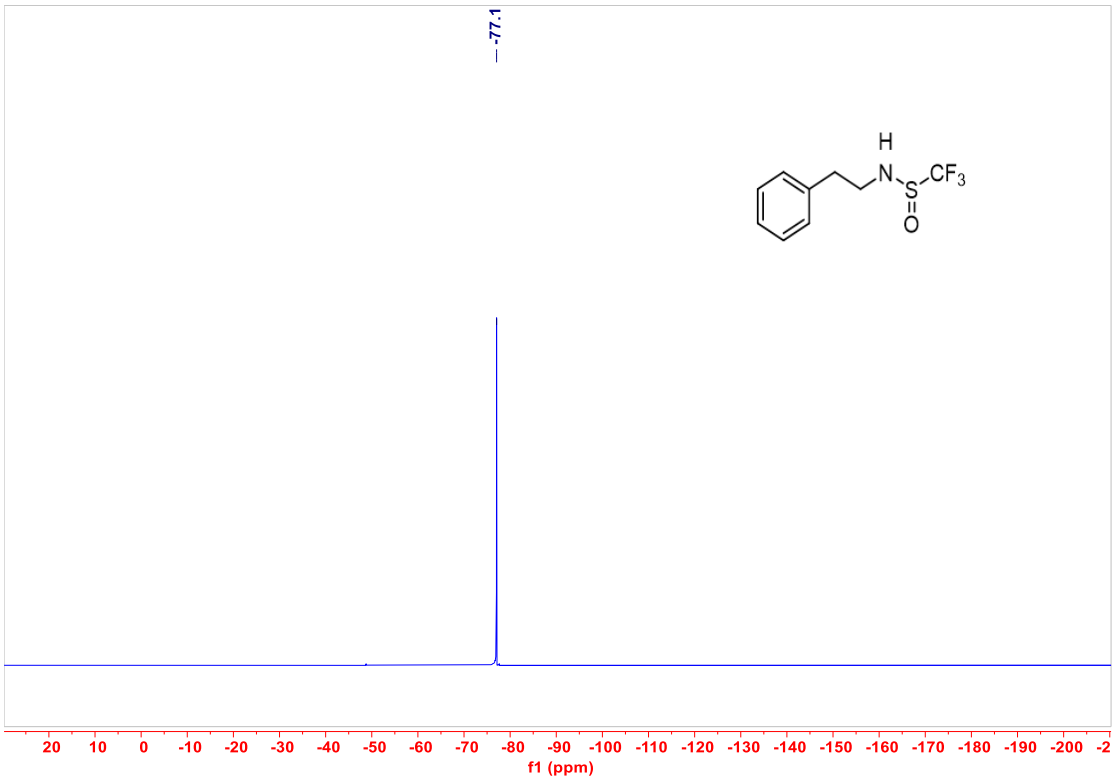
3.57
3.55
3.53
3.52
3.50
3.48
3.47
3.45
3.43
2.91
2.90
2.88
H
N
S
CF3
O
2.02
1.01
2.00
1.00
2.03
2.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
S
CF3
O
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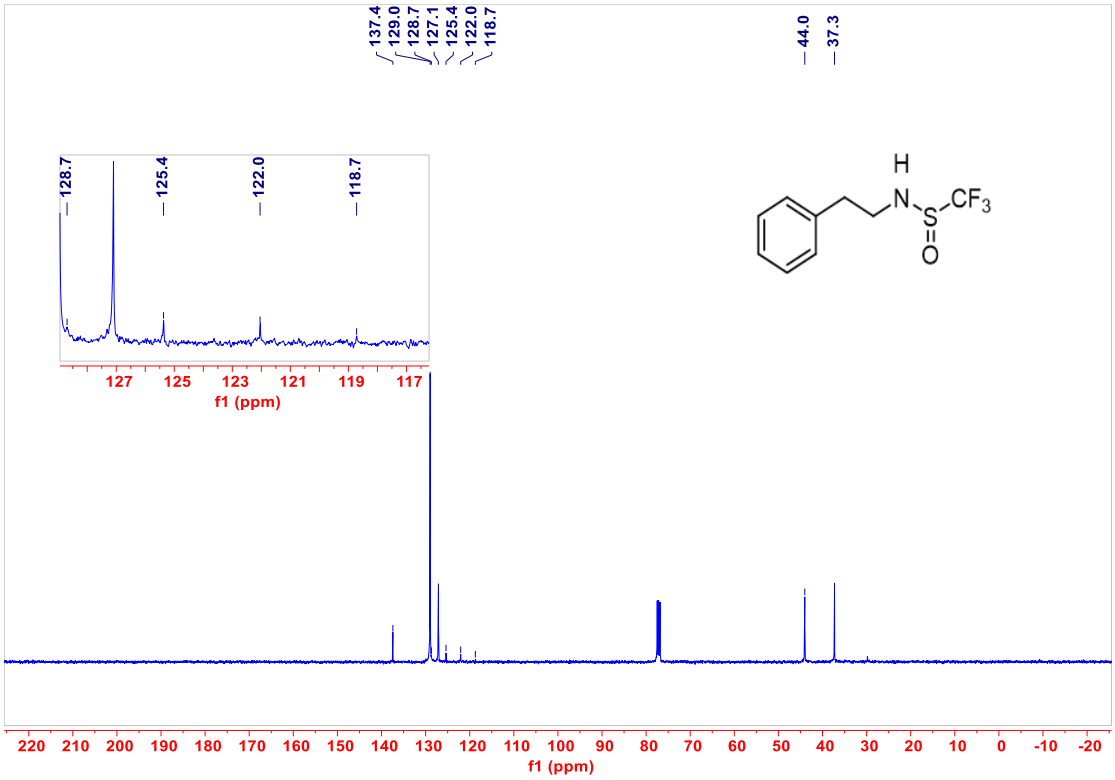
f1 (ppm)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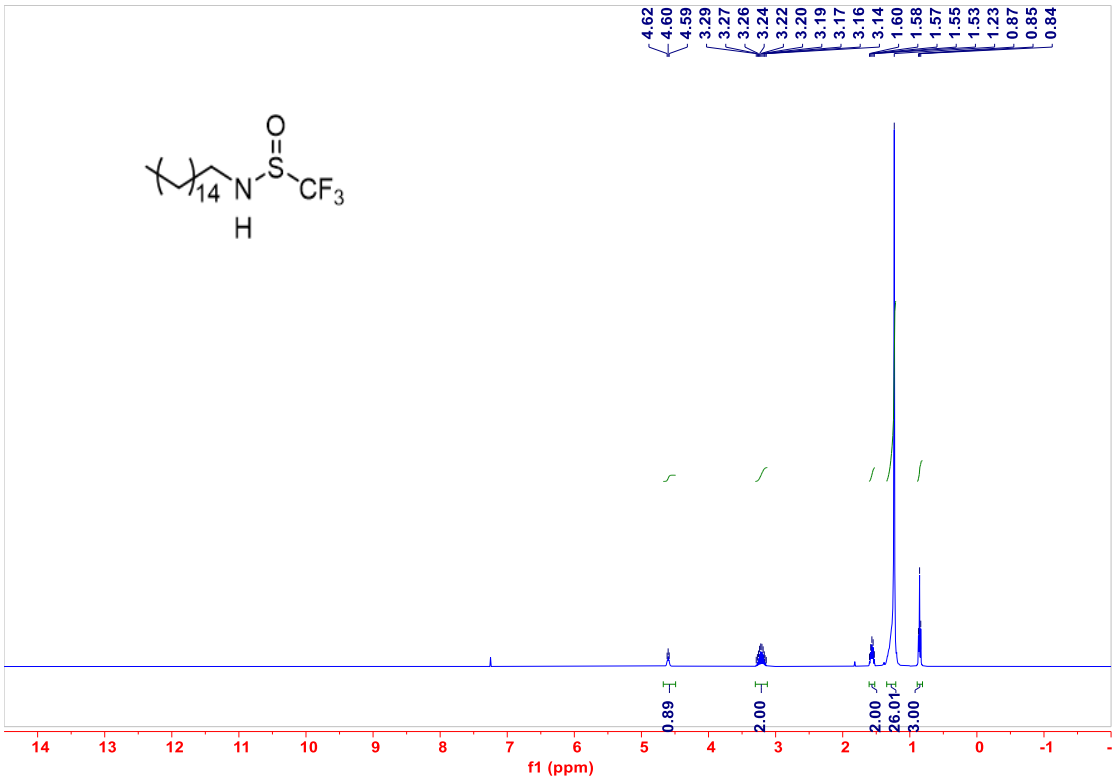
128.7
127.1
125.4
122.0
118.7
44.0
37.3
128.7
125.4
122.0
118.7
127 125 123 121 119 117
f1 (ppm)
H
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


4.62
4.60
4.59
3.29
3.27
3.26
3.24
3.22
3.20
3.19
3.17
3.16
3.14
1.60
1.58
1.57
1.55
1.53
1.23
0.87
0.85
0.84
O
S
CF3
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N
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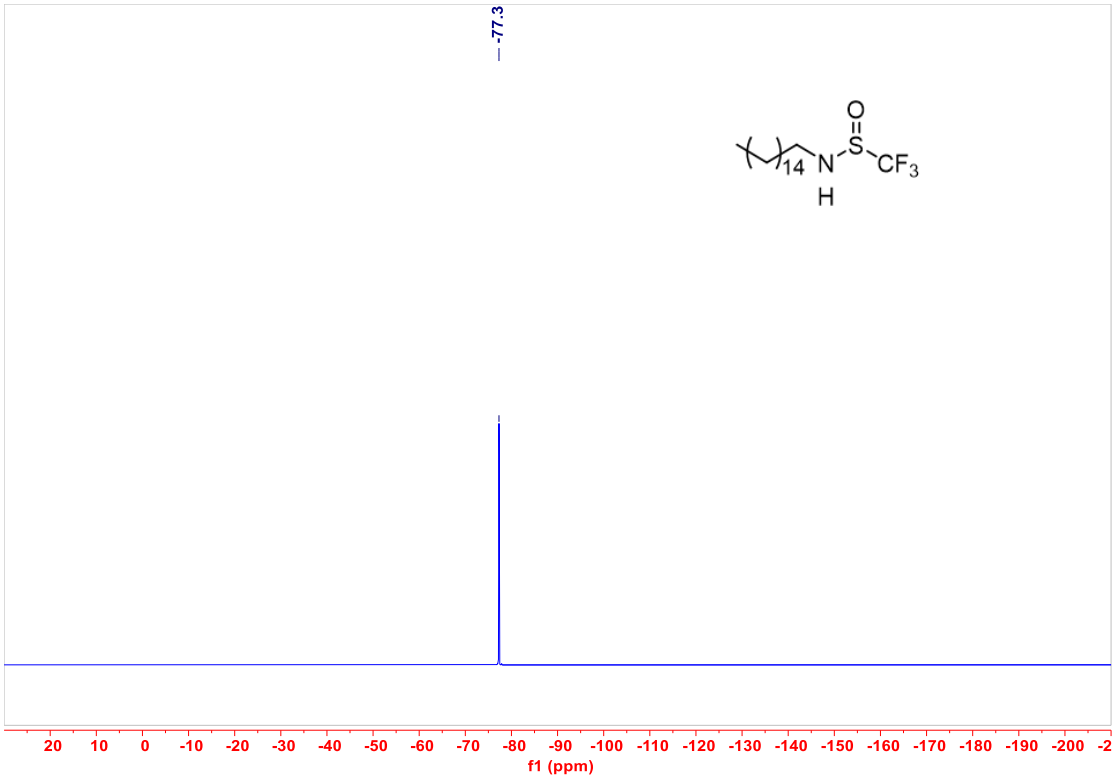
2.00
2.00
26.01
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.3
14
N
H
S
O
CF3
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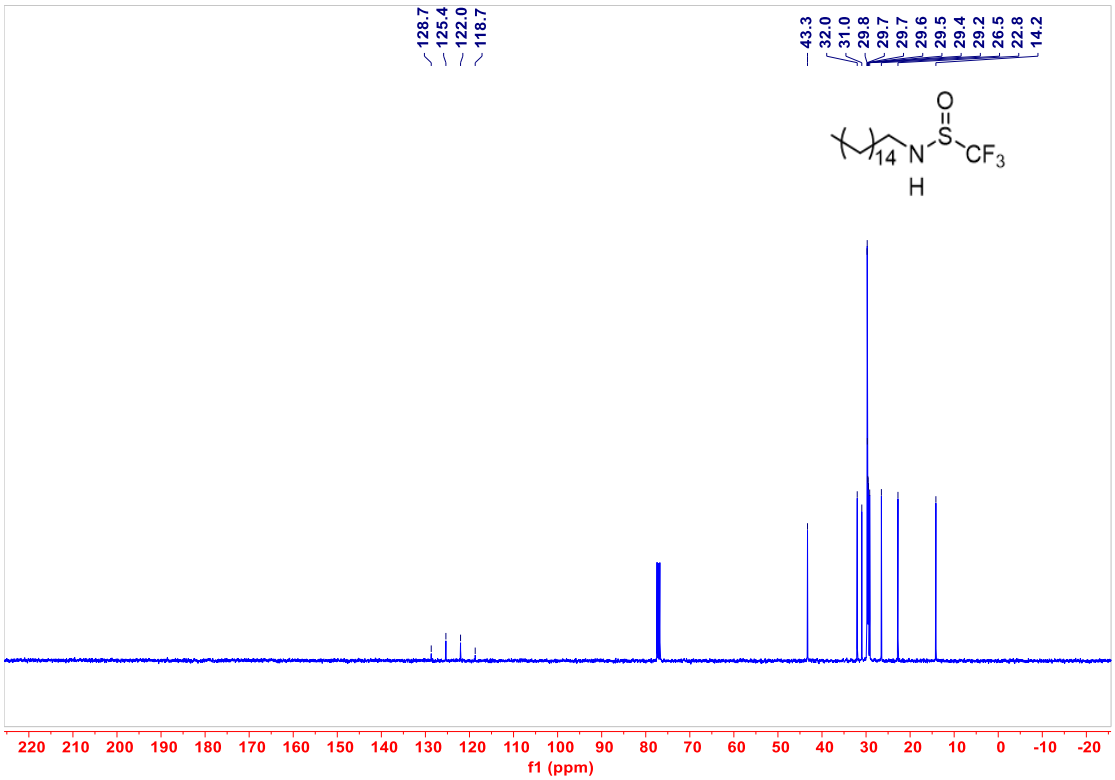
f1 (ppm)


128.7
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122.0
118.7
43.3
32.0
31.0
29.8
29.7
29.7
29.6
29.5
29.4
29.2
26.5
22.8
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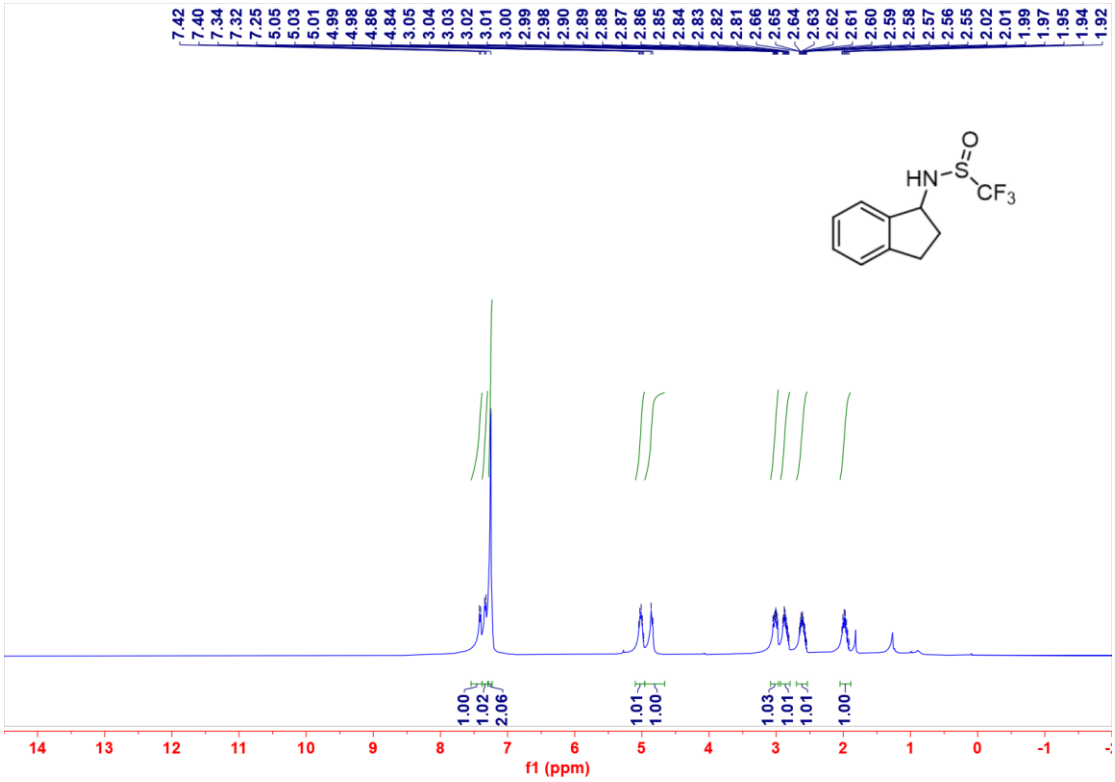
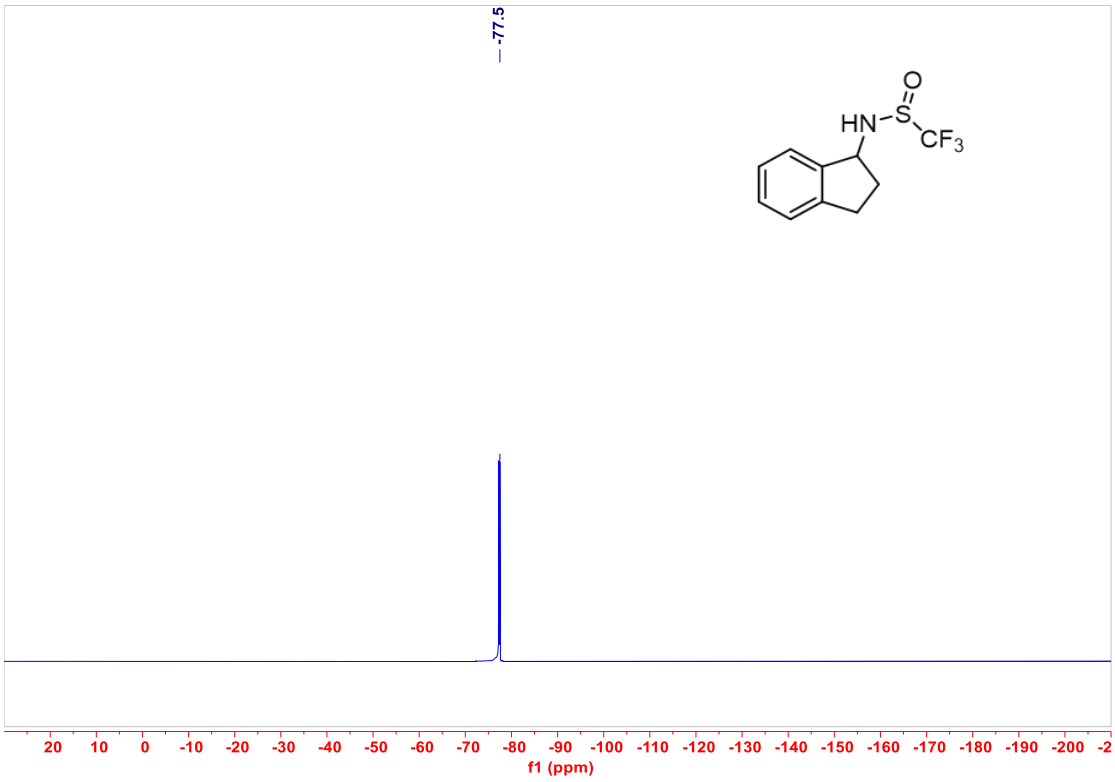
14
N
H
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.42 7.40 7.34 7.32 7.25 5.05 5.03 5.01 4.99 4.98 4.86 4.84 3.05 3.04 3.03 3.02 3.01 3.00 2.99 2.98 2.90 2.89 2.88 2.87 2.86 2.85 2.84 2.83 2.82 2.81 2.66 2.65 2.64 2.63 2.62 2.61 2.60 2.59 2.58 2.57 2.56 2.55 2.02 2.01 1.99 1.97 1.95 1.94 1.92
HN
S
O
CF3
1.00 1.02 2.06 1.01 1.00 1.03 1.01 1.01 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.5
HN
S
O
CF3
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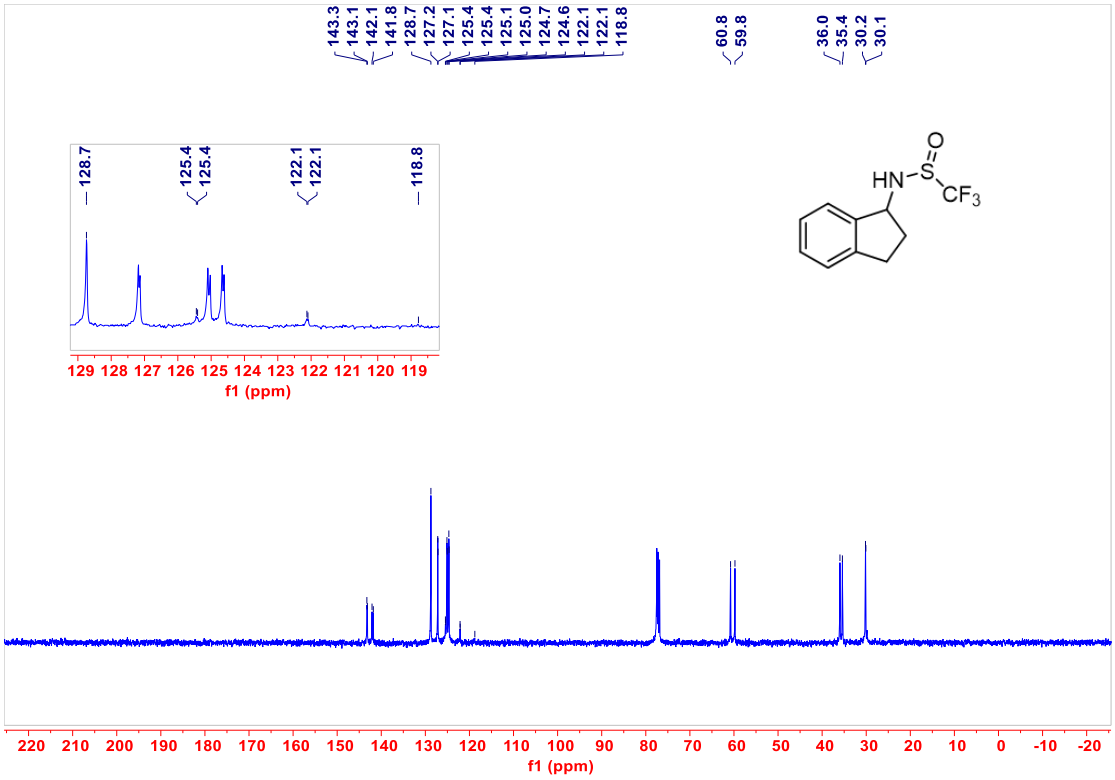
f1 (ppm)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142.1
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125.4
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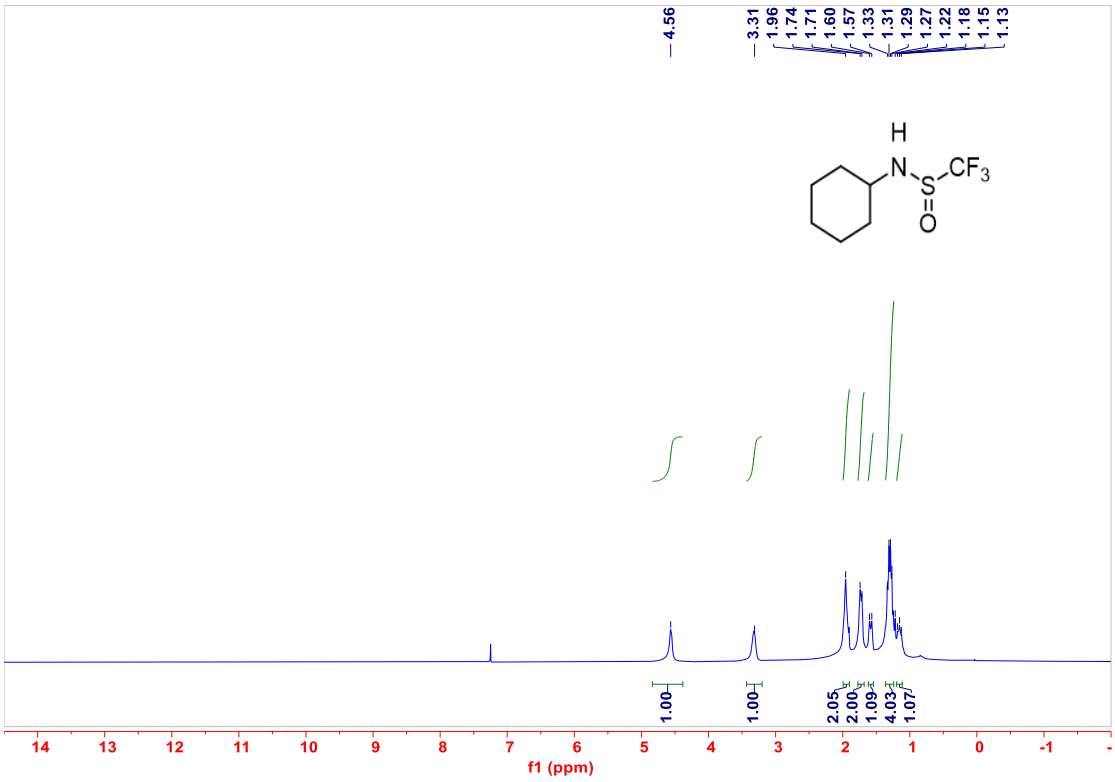
125.1
125.0
124.7
124.6
122.1
122.1
118.8
60.8
59.8
36.0
35.4
30.2
30.1
128.7
125.4
125.4
122.1
122.1
118.8
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
HN
S
O
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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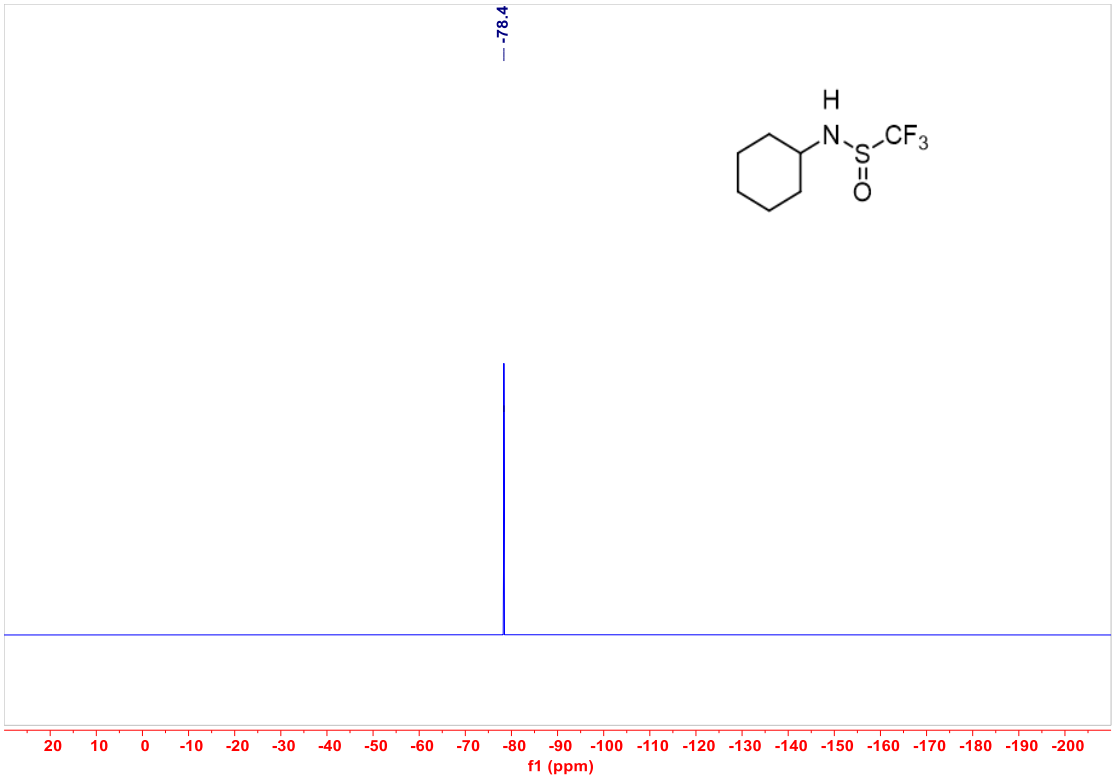
1.57
1.33
1.31
1.29
1.27
1.22
1.18
1.15
1.13
H
N
S
CF3
O
O
1.00
1.00
2.05
2.00
1.09
4.03
1.07
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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S
CF3
O
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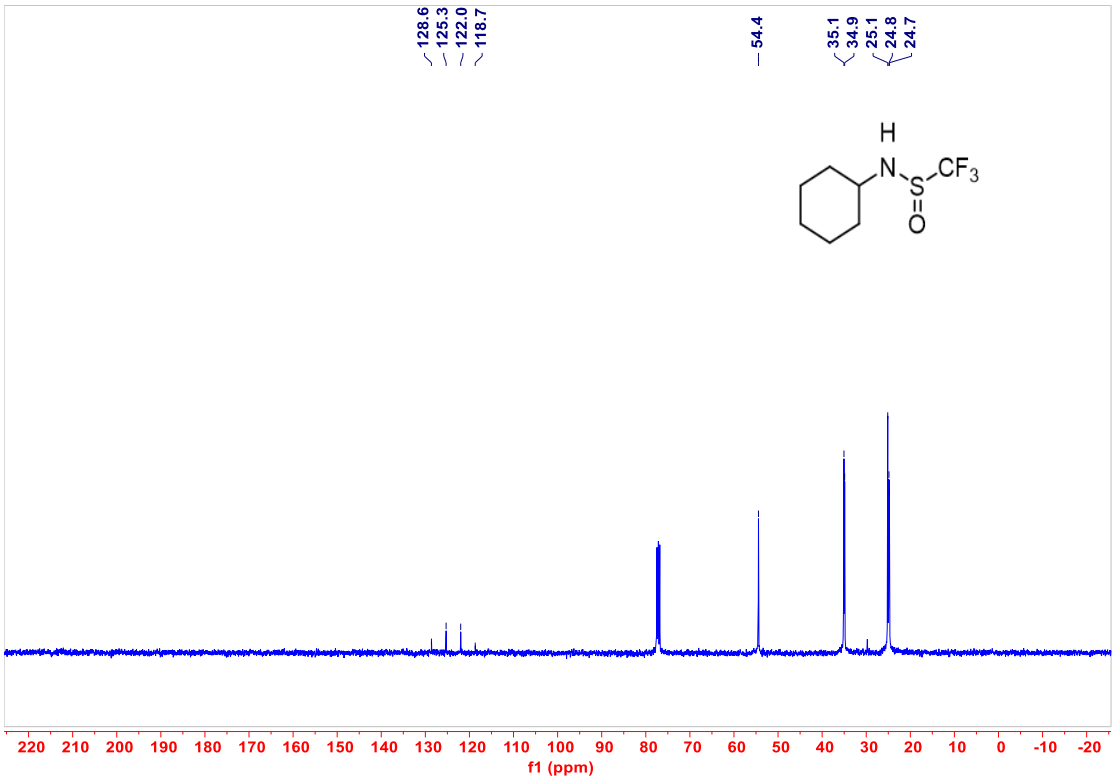
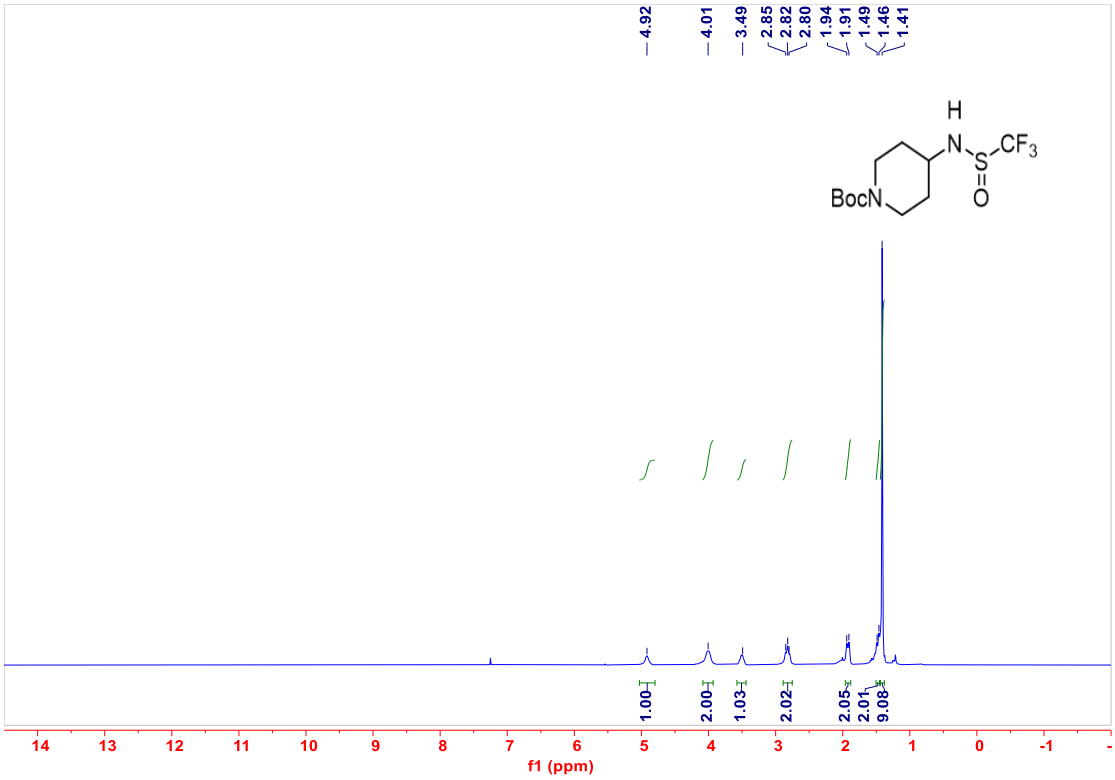
f1 (ppm)


128.6
125.3
122.0
118.7
54.4
35.1
34.9
25.1
24.8
24.7
H
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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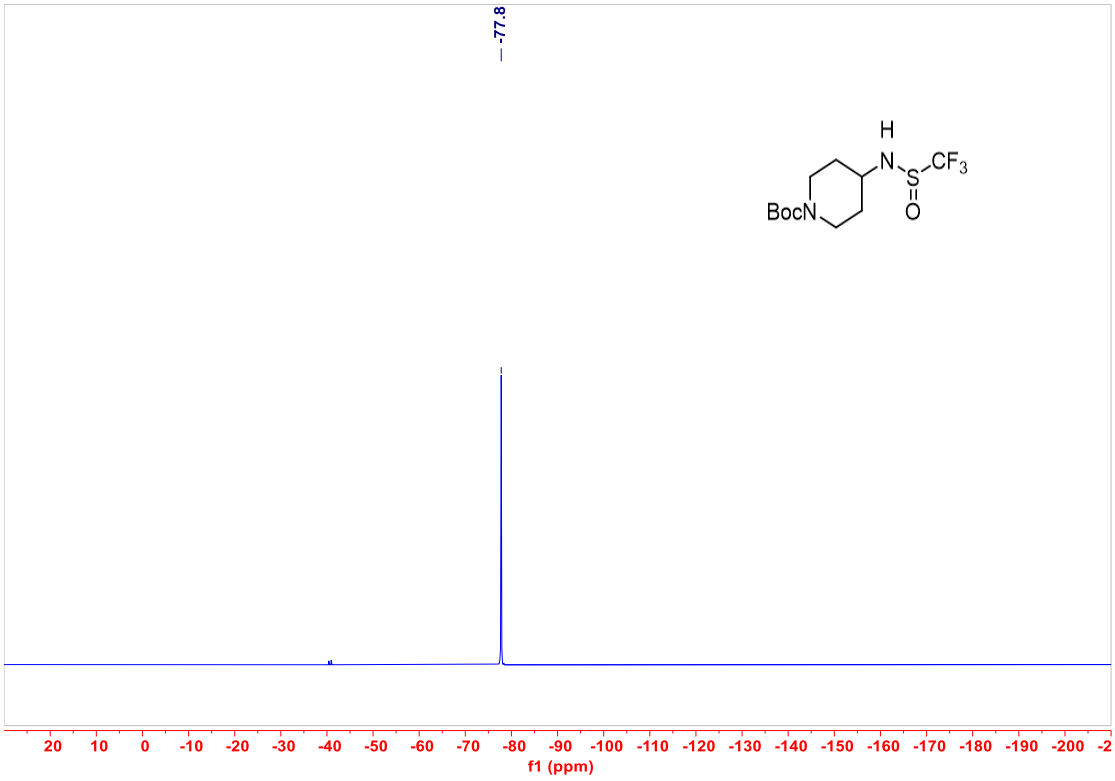
2.82
2.80
1.94
1.91
1.49
1.46
1.41
H
N
S
CF3
O
BocN
1.00
2.00
1.03
2.02
2.05
2.01
9.08
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.8
H
N
S
CF3
O
BocN
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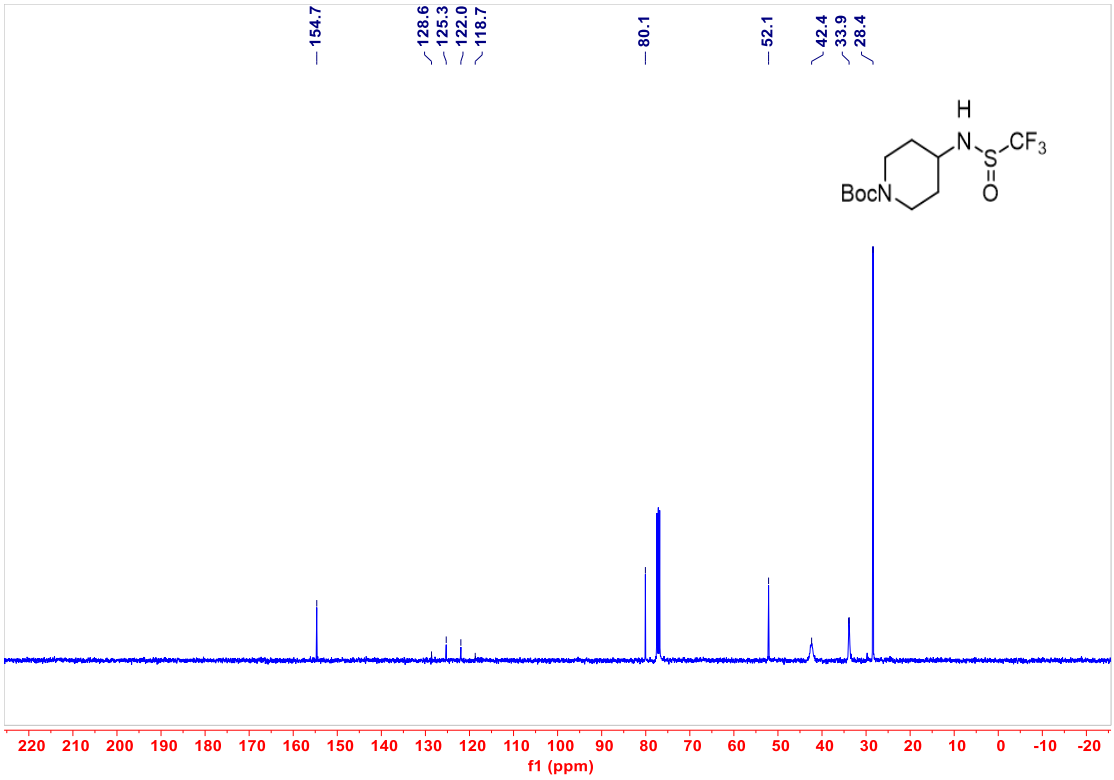
f1 (ppm)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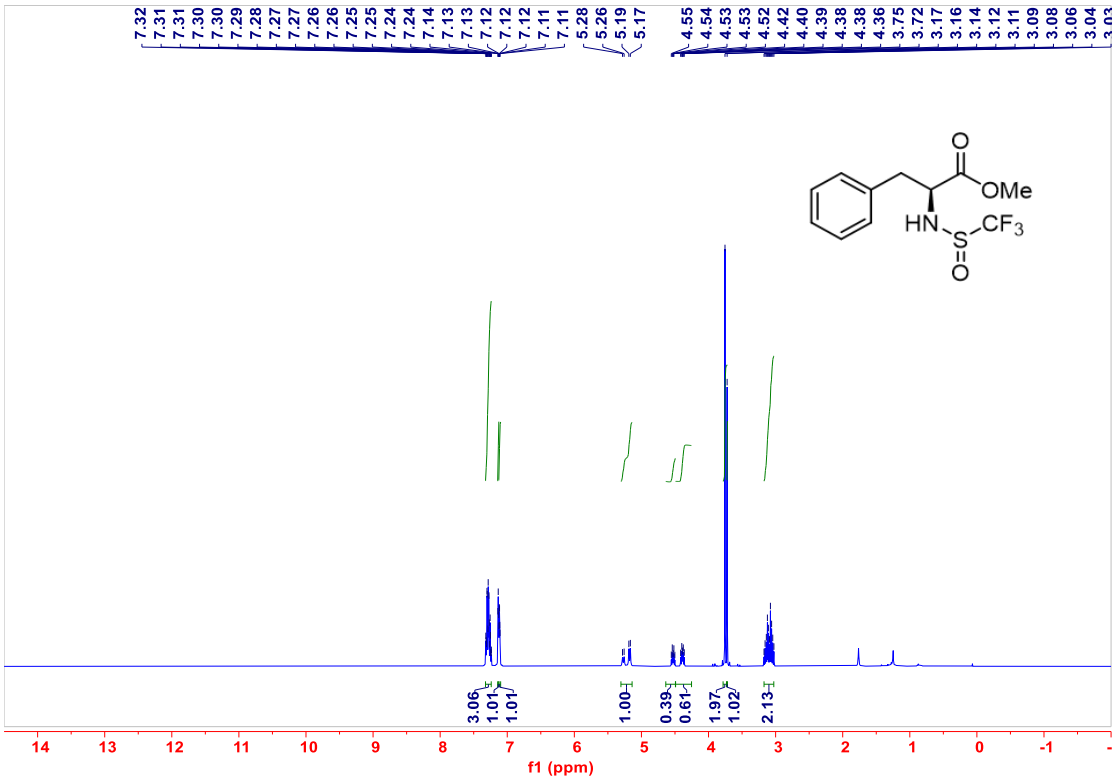
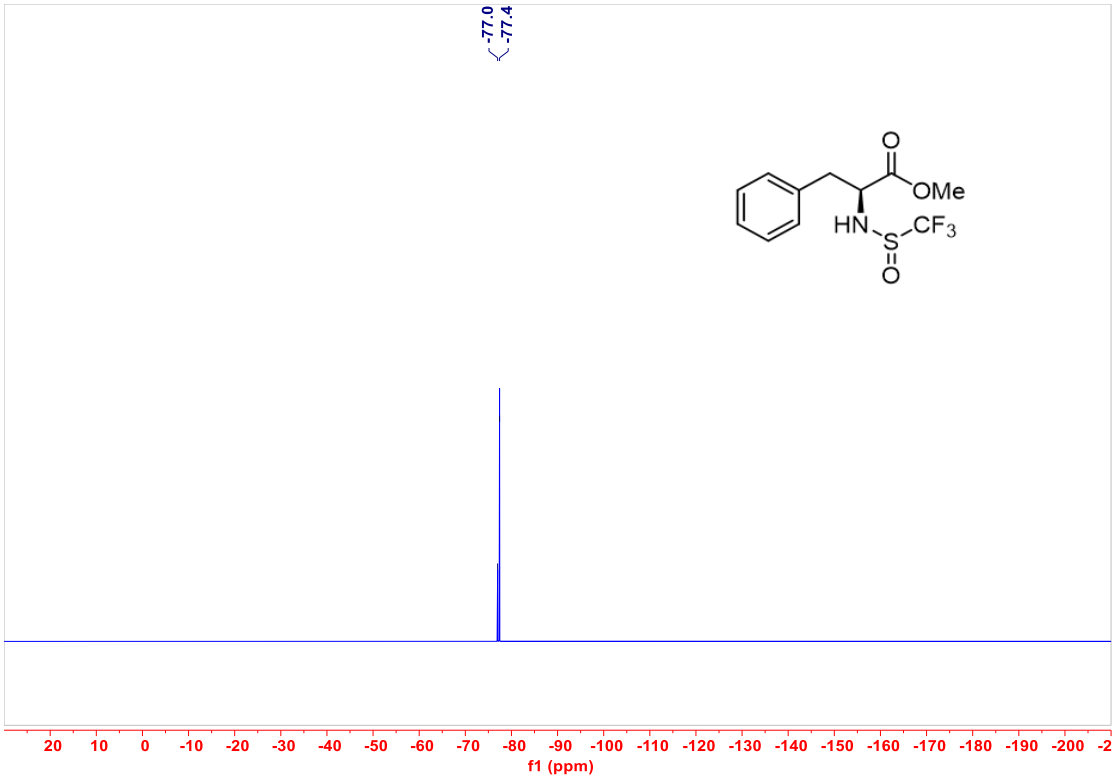
122.0
118.7
80.1
52.1
42.4
33.9
28.4
H
N
CF3
S
O
BocN
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 7.14 7.13 7.13 7.12 7.12 7.12 7.11 7.11
5.28 5.26 5.19 5.17
4.55 4.54 4.53 4.53 4.52 4.42 4.40 4.39 4.38 4.38 4.36 3.75 3.72 3.17 3.16 3.14 3.12 3.11 3.09 3.08 3.06 3.04
O
OMe
HN
CF3
S
O
3.06 1.01 1.01 1.00 0.39 0.61 1.97 1.02 2.13
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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-77.4
O
OMe
HN
S
CF3
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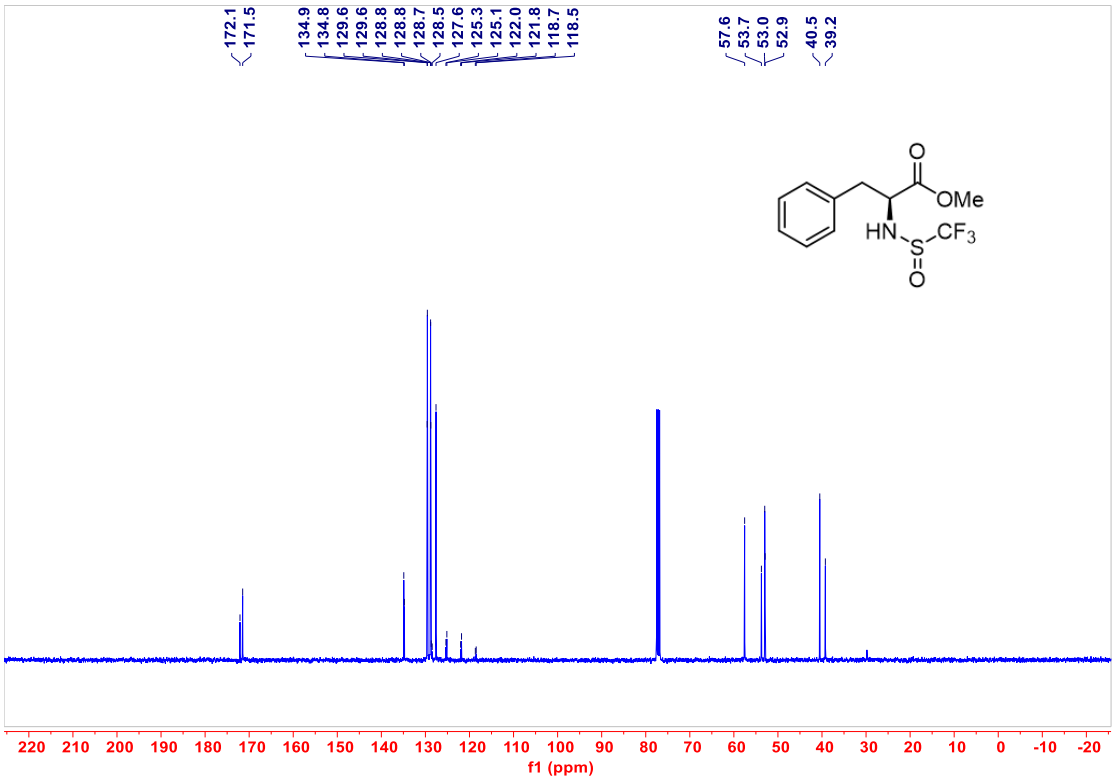
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)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171.5
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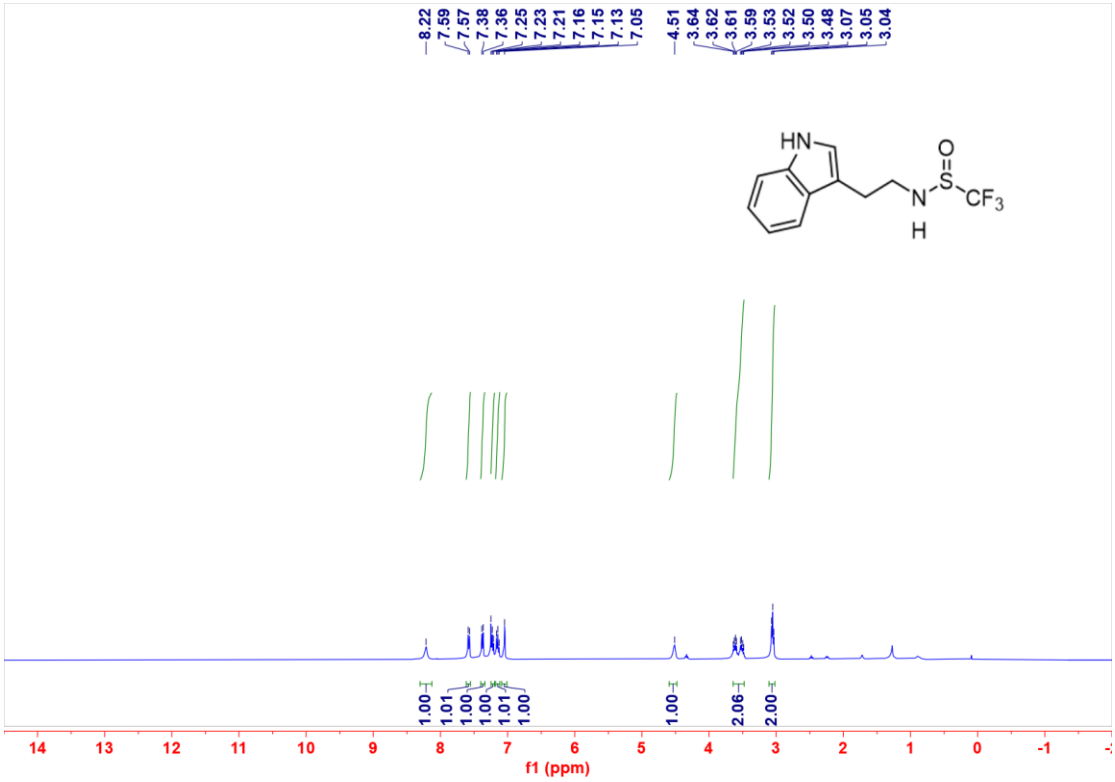
129.6
128.8
128.8
128.7
128.5
127.6
125.3
125.1
122.0
121.8
118.7
118.5
57.6
53.7
53.0
52.9
40.5
39.2
O
OMe
HN
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.05
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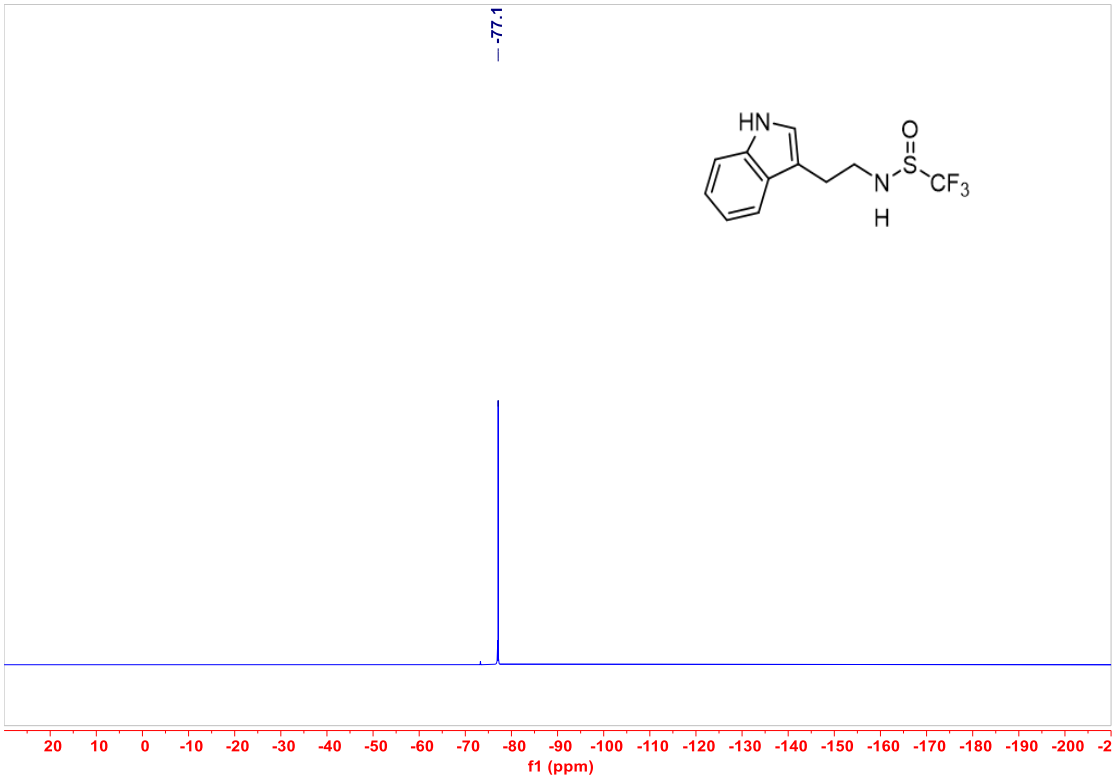
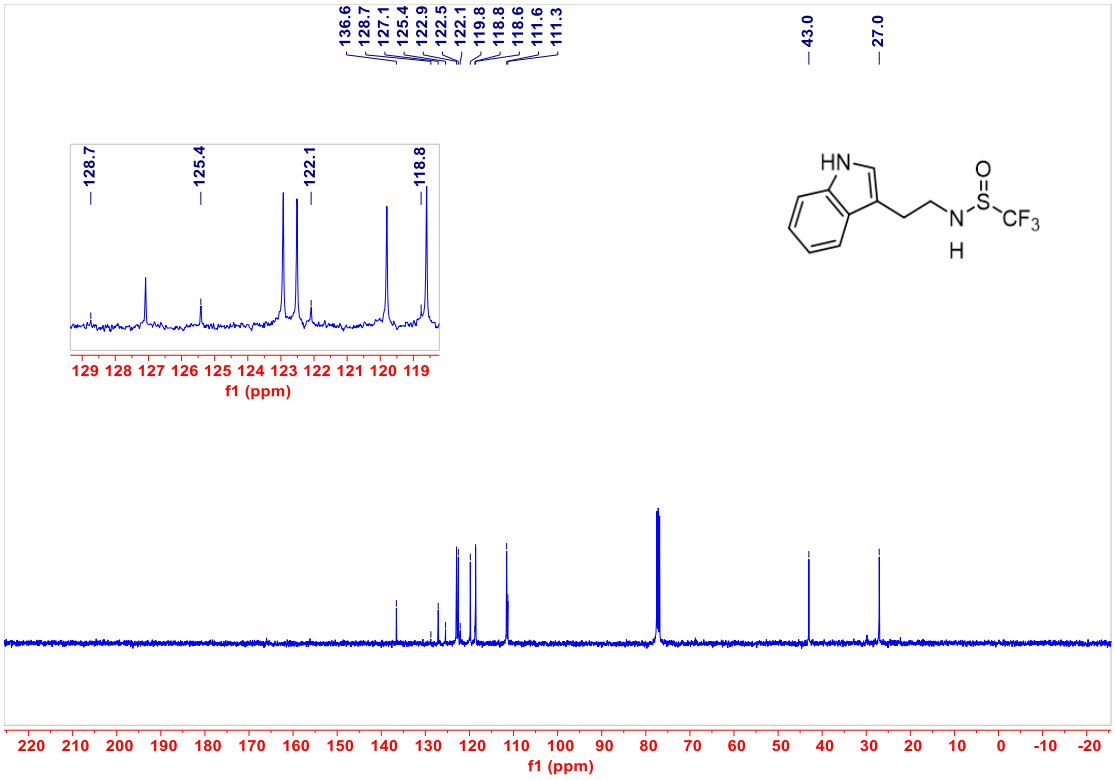
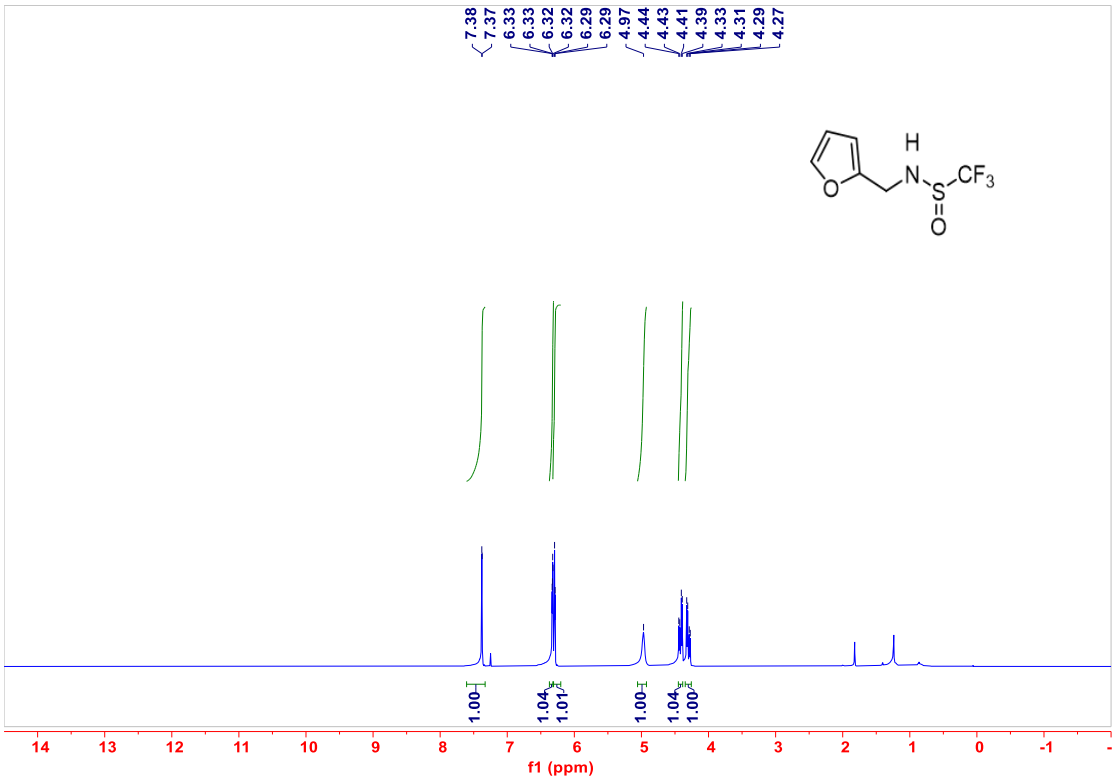
3.64
3.62
3.61
3.59
3.53
3.52
3.50
3.48
3.07
3.05
3.04
HN
O
S
N
CF3
H
1.00
1.01
1.00
1.01
1.00
1.00
2.06
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.1
HN
O
S
N
CF3
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


136.6
128.7
127.1
125.4
122.9
122.5
122.1
119.8
118.8
118.6
111.6
111.3
43.0
27.0
128.7
125.4
122.1
118.8
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
HN
O
S
N
CF3
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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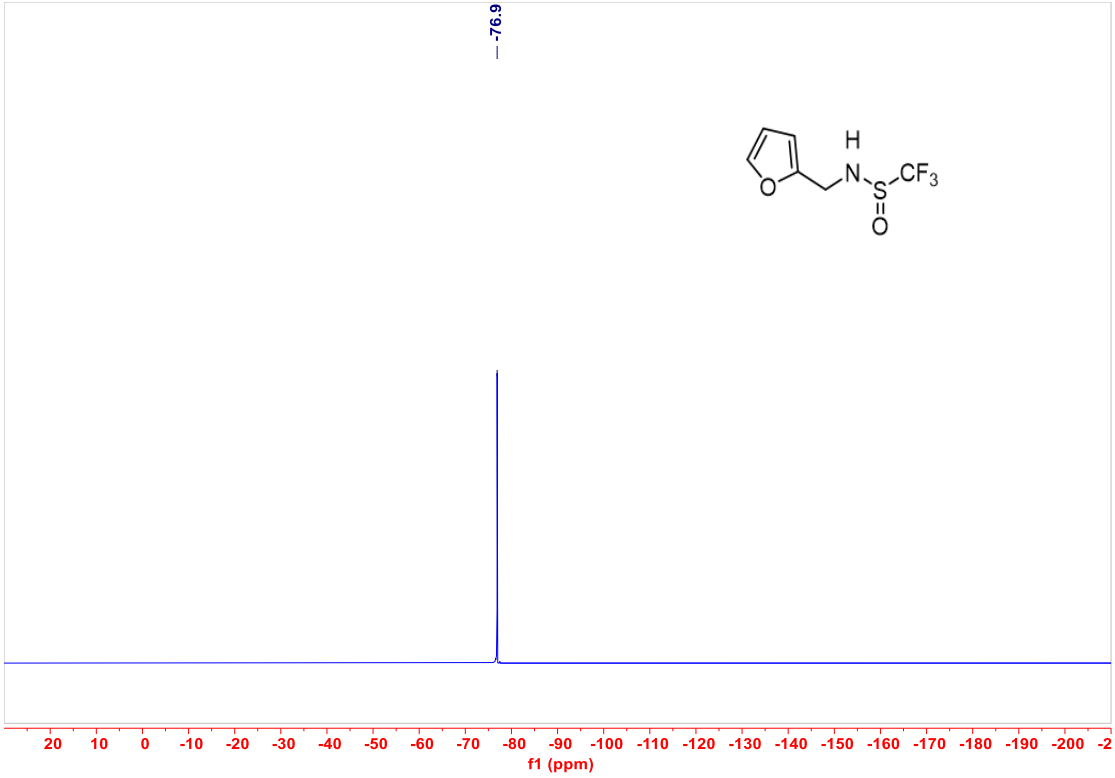
4.43
4.41
4.39
4.33
4.31
4.29
4.27
H
N
CF3
S
O
O
1.00
1.04
1.01
1.00
1.04
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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H
N
S
CF3
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O
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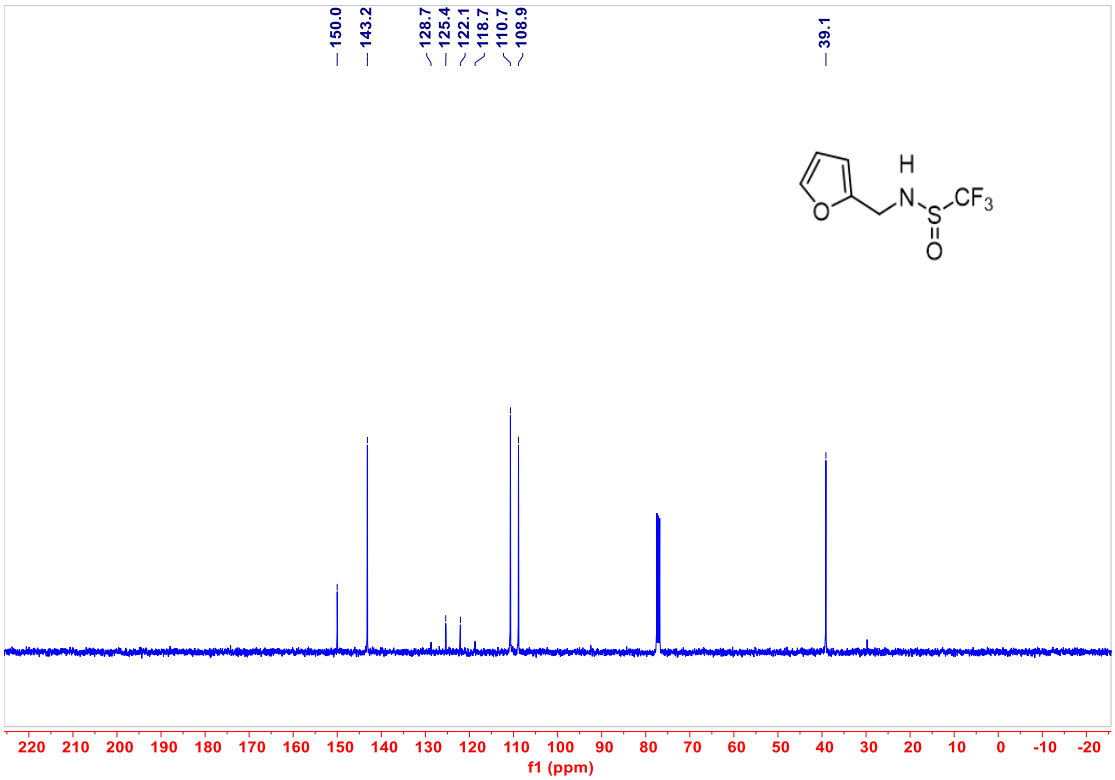
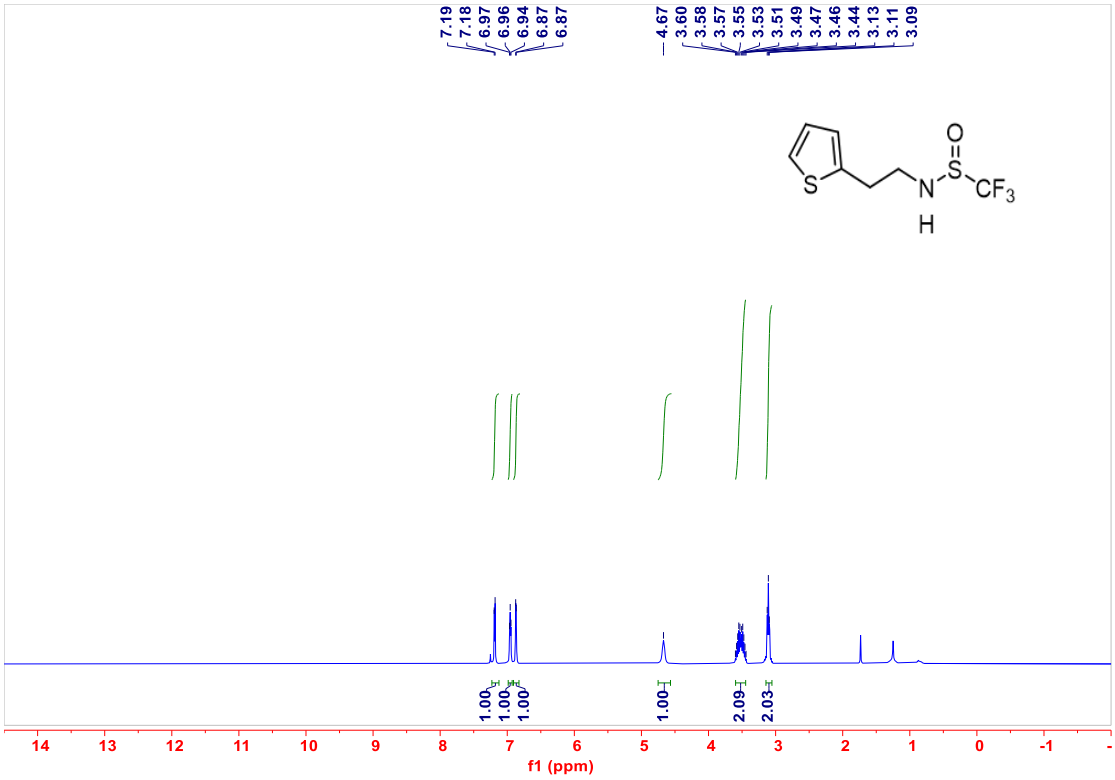
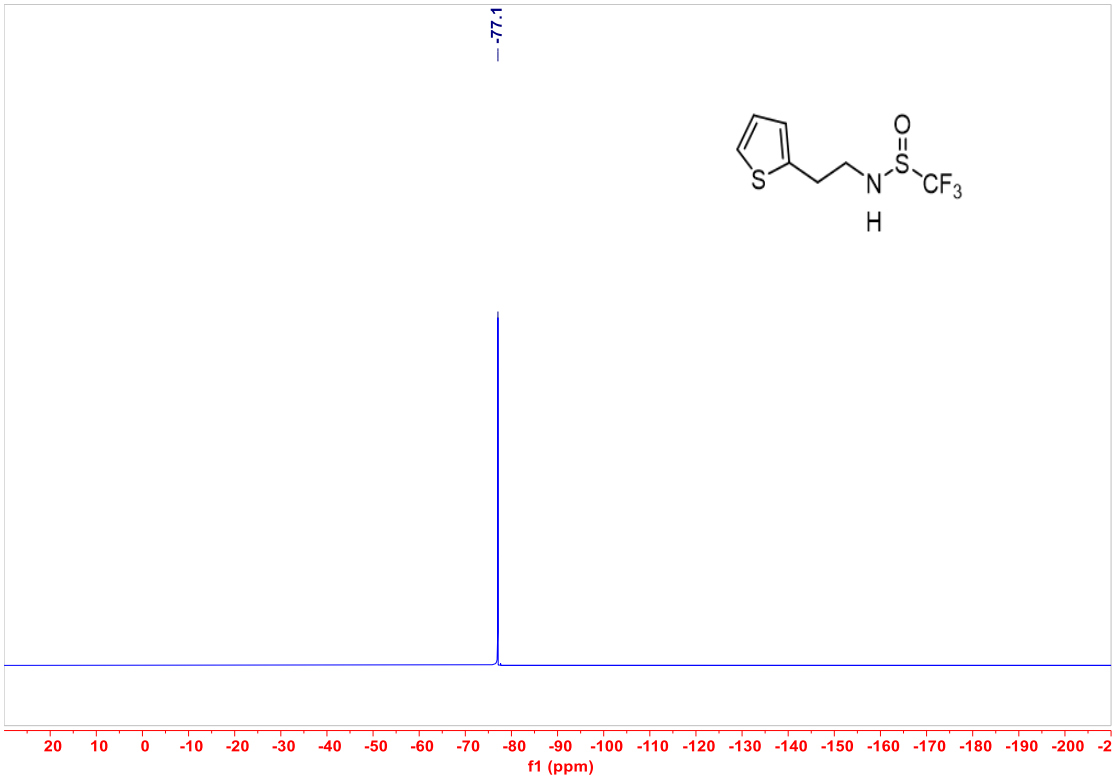
f1 (ppm)


150.0
143.2
128.7
125.4
122.1
118.7
110.7
108.9
39.1
H
N
S
CF3
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.19
7.18
6.97
6.96
6.94
6.87
6.87
4.67
3.60
3.58
3.57
3.55
3.53
3.51
3.49
3.47
3.46
3.44
3.13
3.11
3.09
S
N
H
O
S
CF3
1.00
1.00
1.00
1.00
2.09
2.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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S
N
H
O
S
CF3
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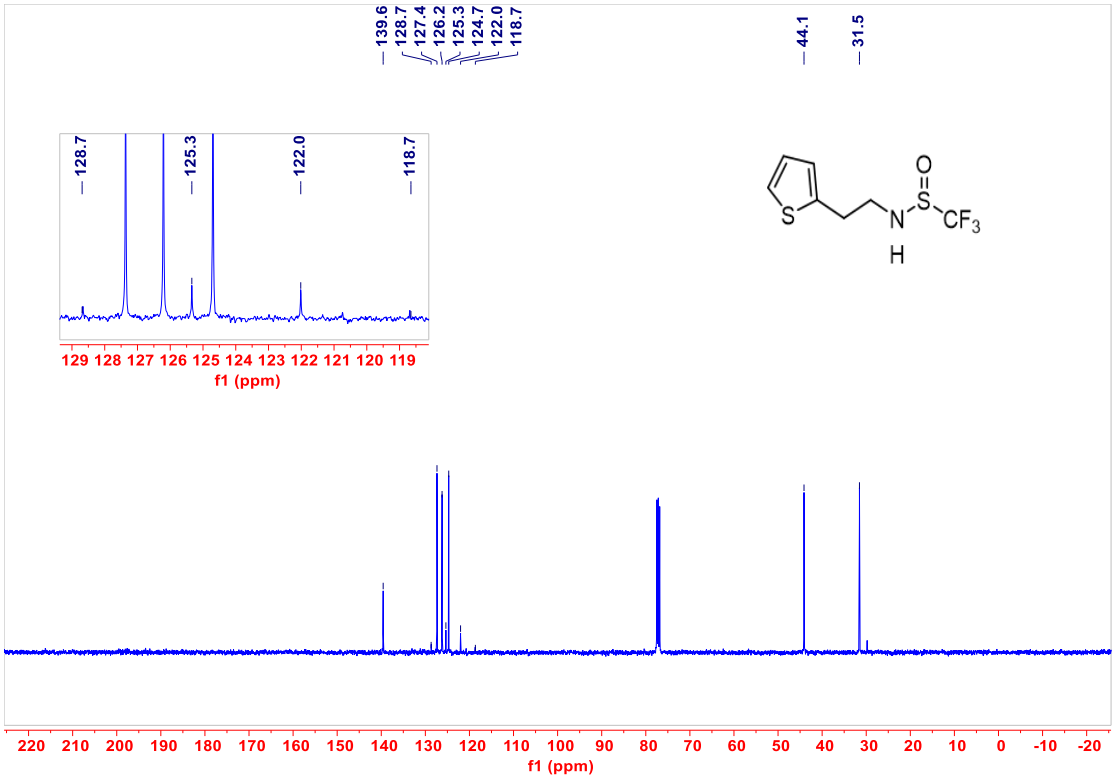
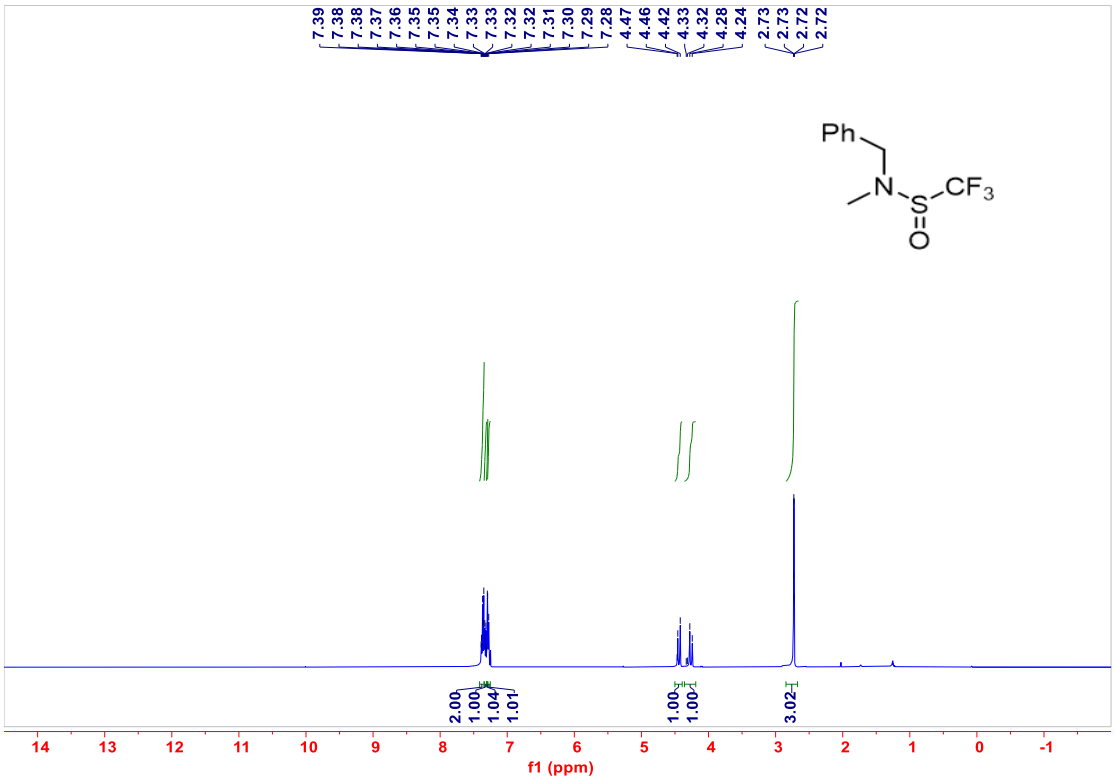
f1 (ppm)


139.6
128.7
127.4
126.2
125.3
124.7
122.0
118.7
44.1
31.5
128.7
125.3
122.0
118.7
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
S
N
H
O
S
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.38
7.38
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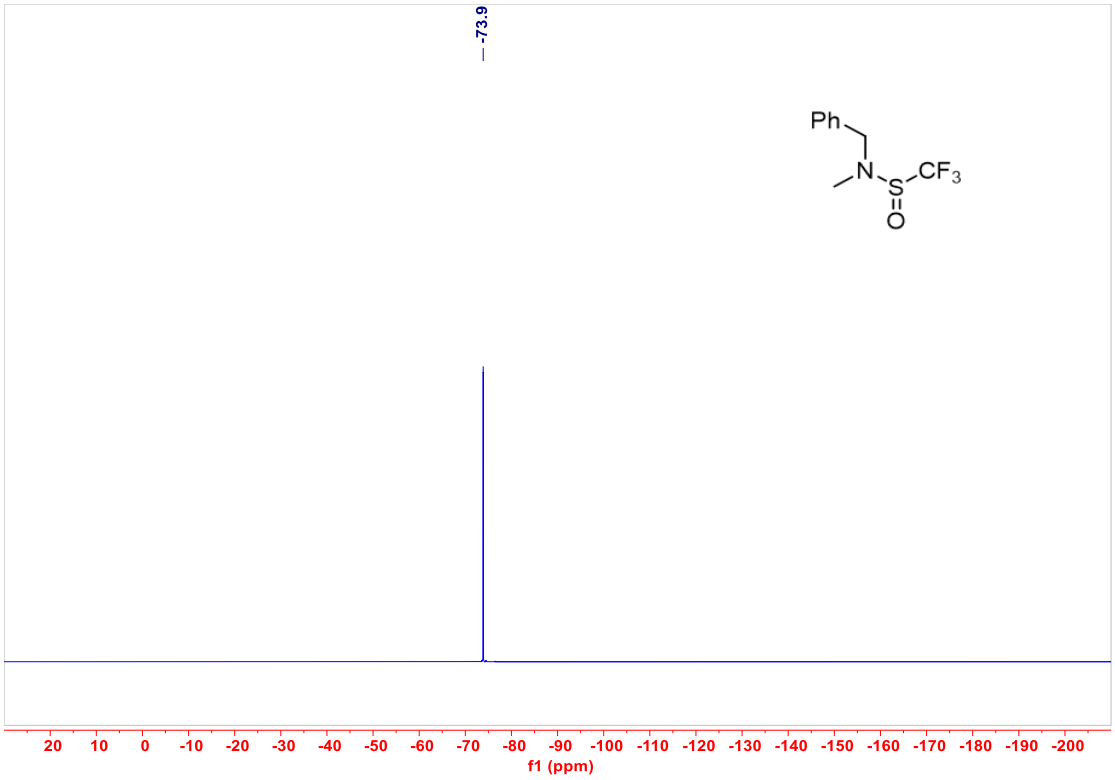
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.29
7.28
4.47
4.46
4.42
4.33
4.32
4.28
4.24
2.73
2.73
2.72
2.72
Ph
N
S
CF3
O
2.00
1.00
1.04
1.01
1.00
1.00
3.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-73.9
Ph
N
S
O
CF3
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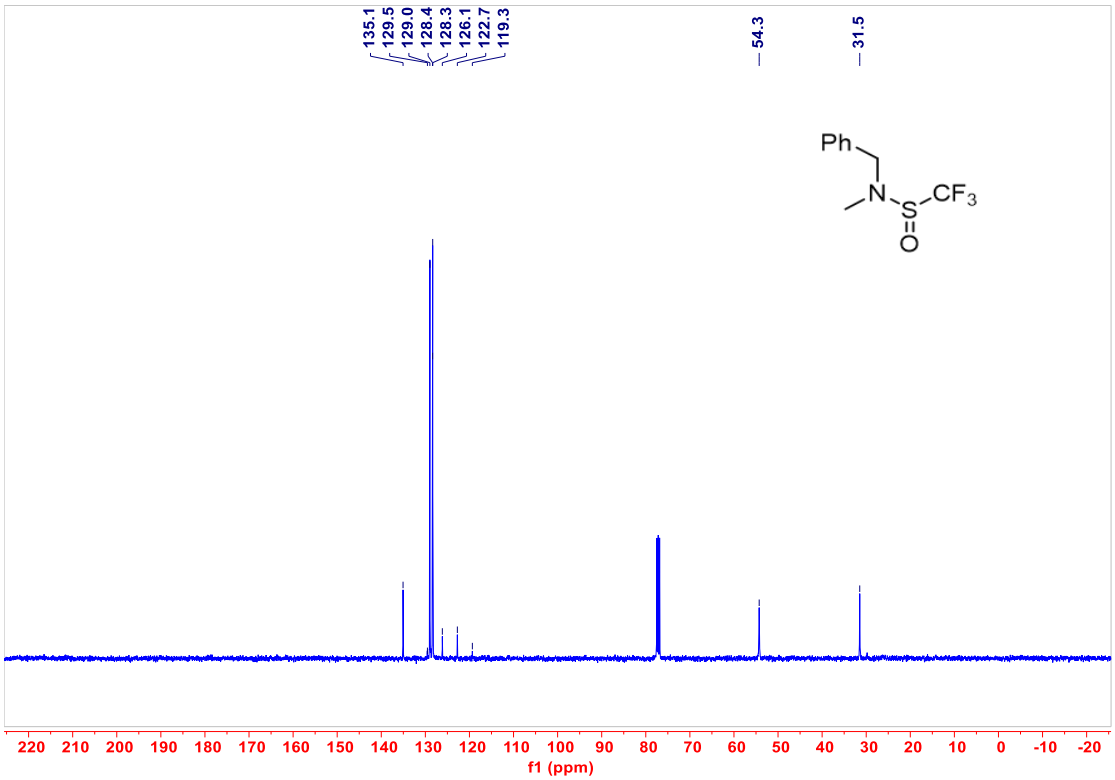
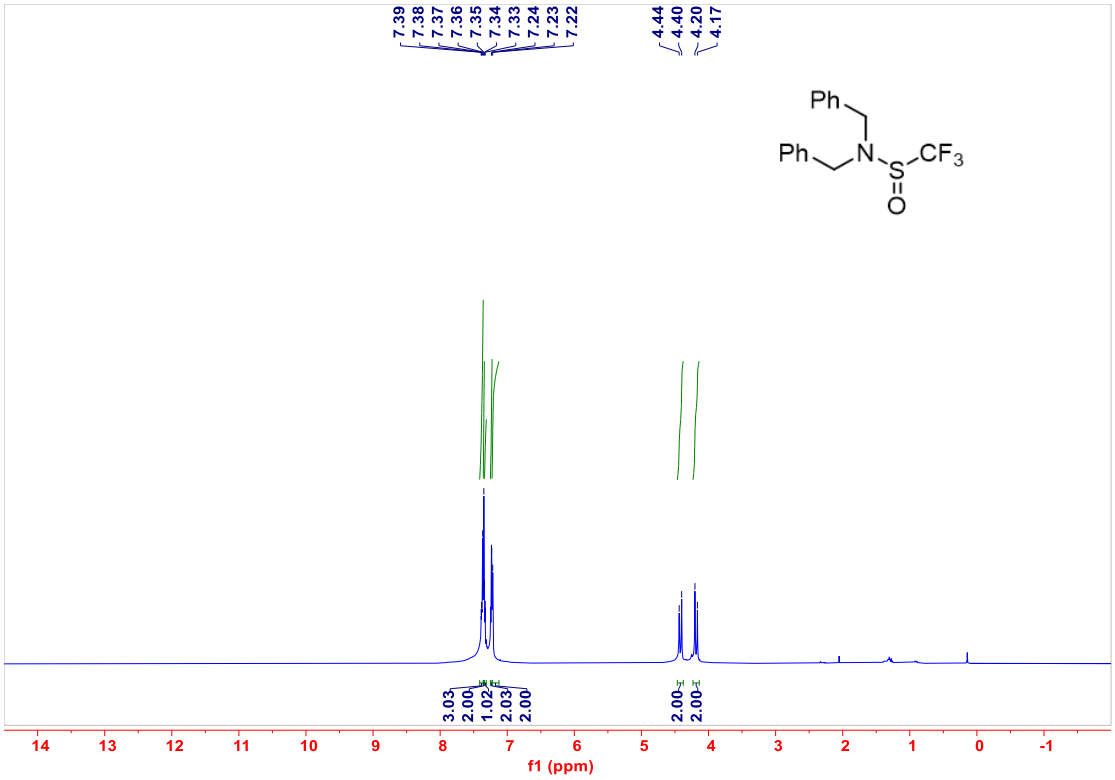
f1 (ppm)


135.1
129.5
129.0
128.4
128.3
126.1
122.7
119.3
54.3
31.5
Ph
N
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.39
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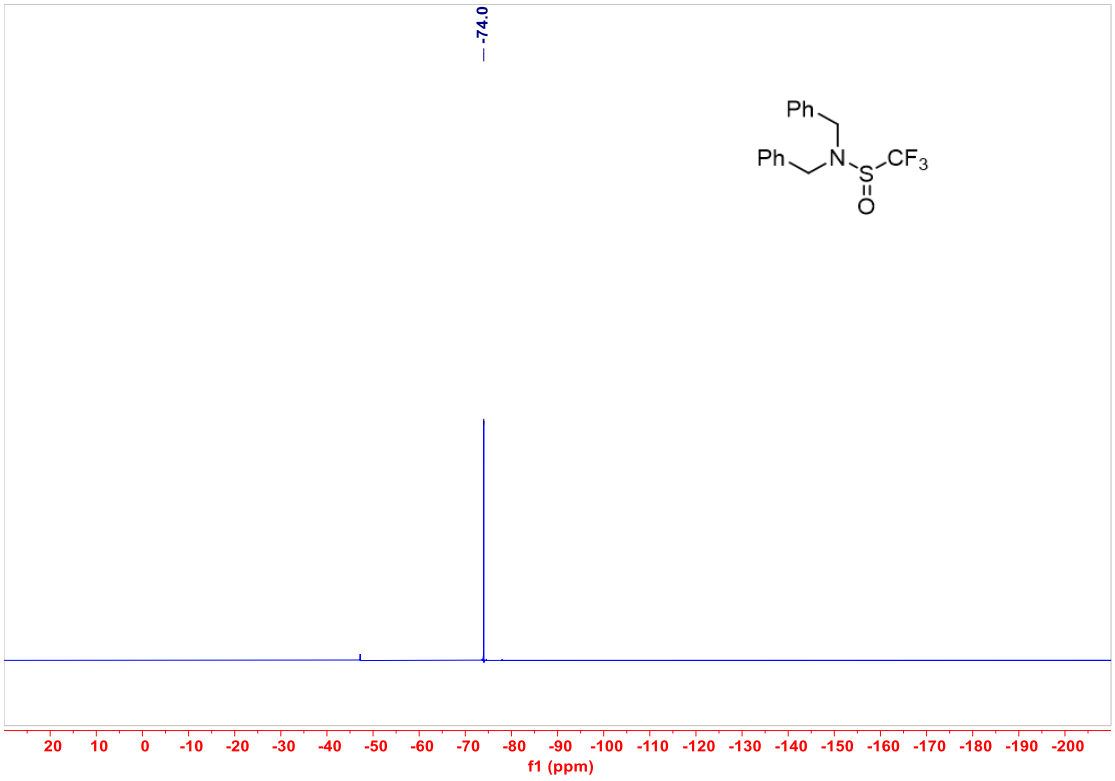
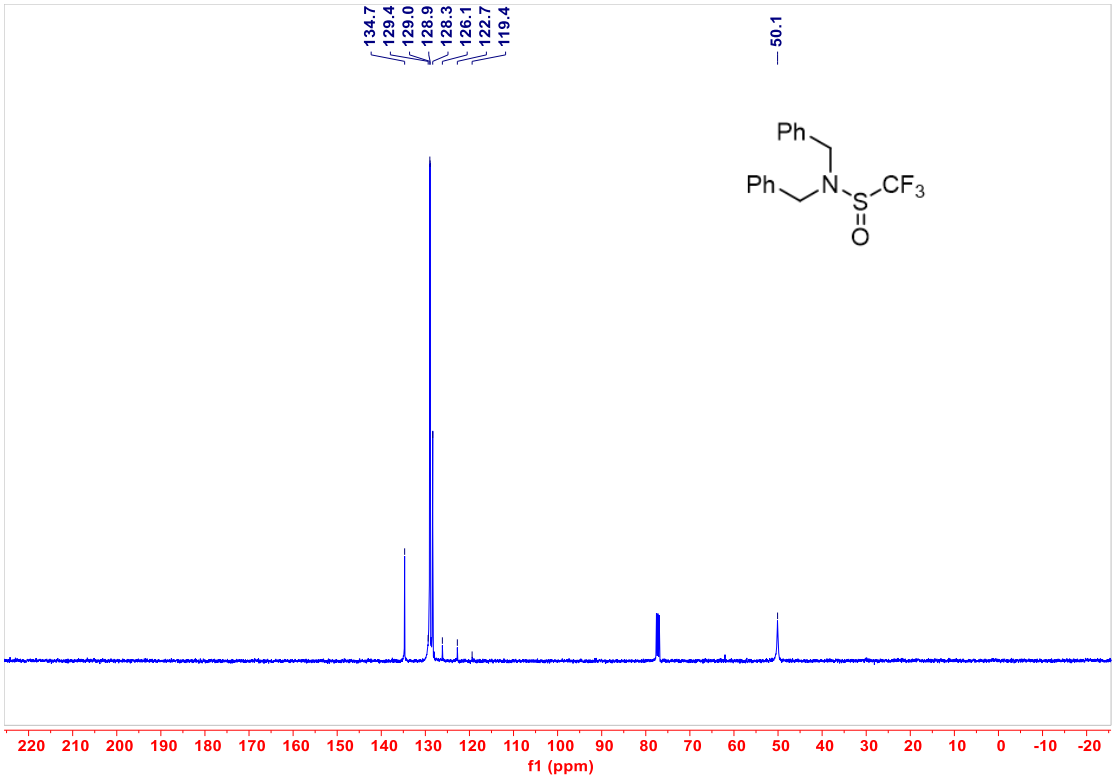
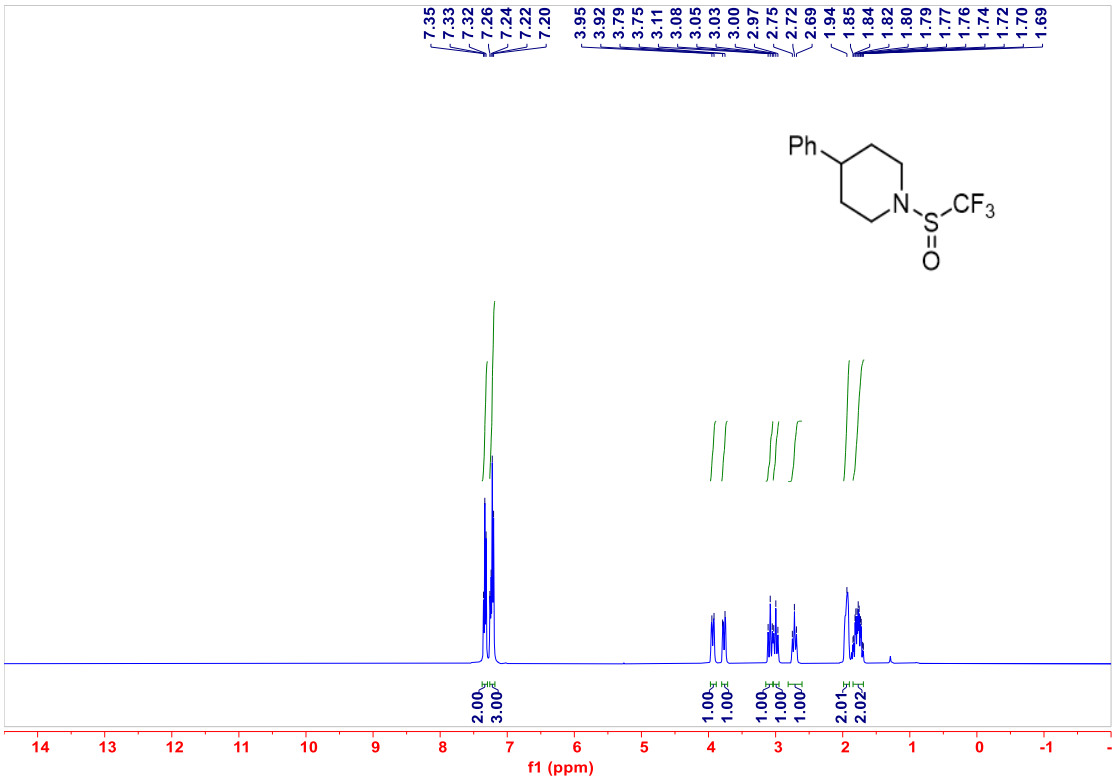
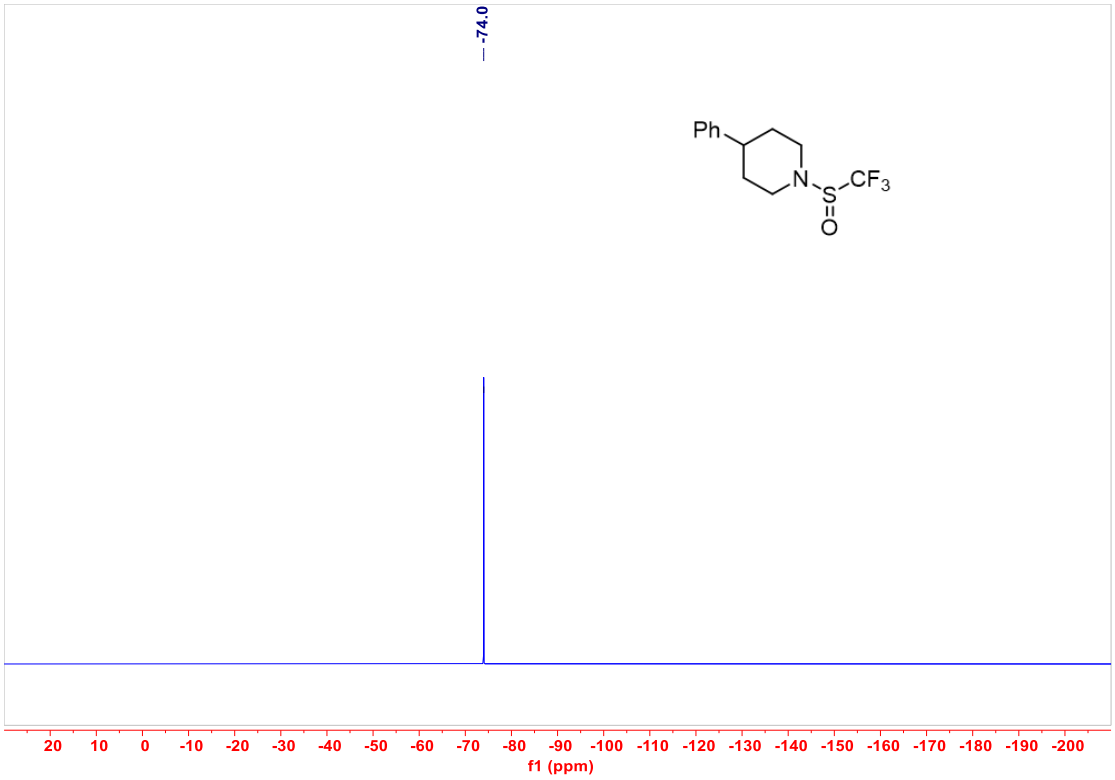
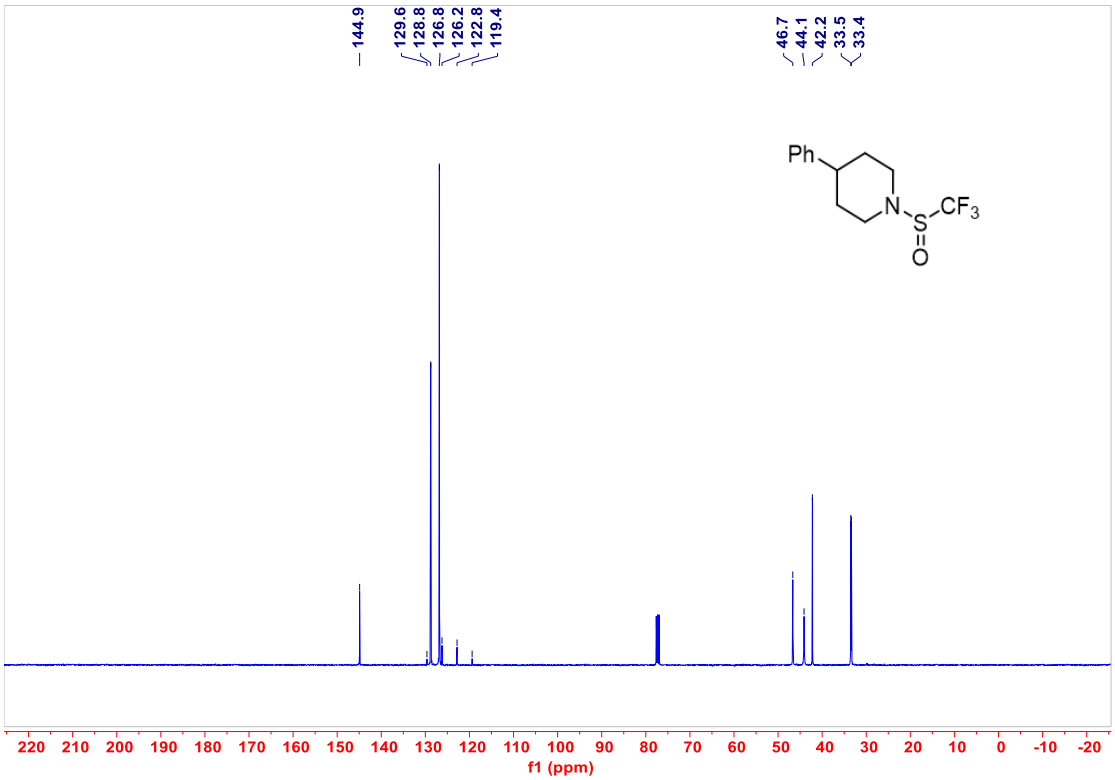
7.36
7.35
7.34
7.33
7.24
7.23
7.22
4.44
4.40
4.20
4.17
Ph
Ph
N
S
O
CF3
3.03
2.00
1.02
2.03
2.00
2.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

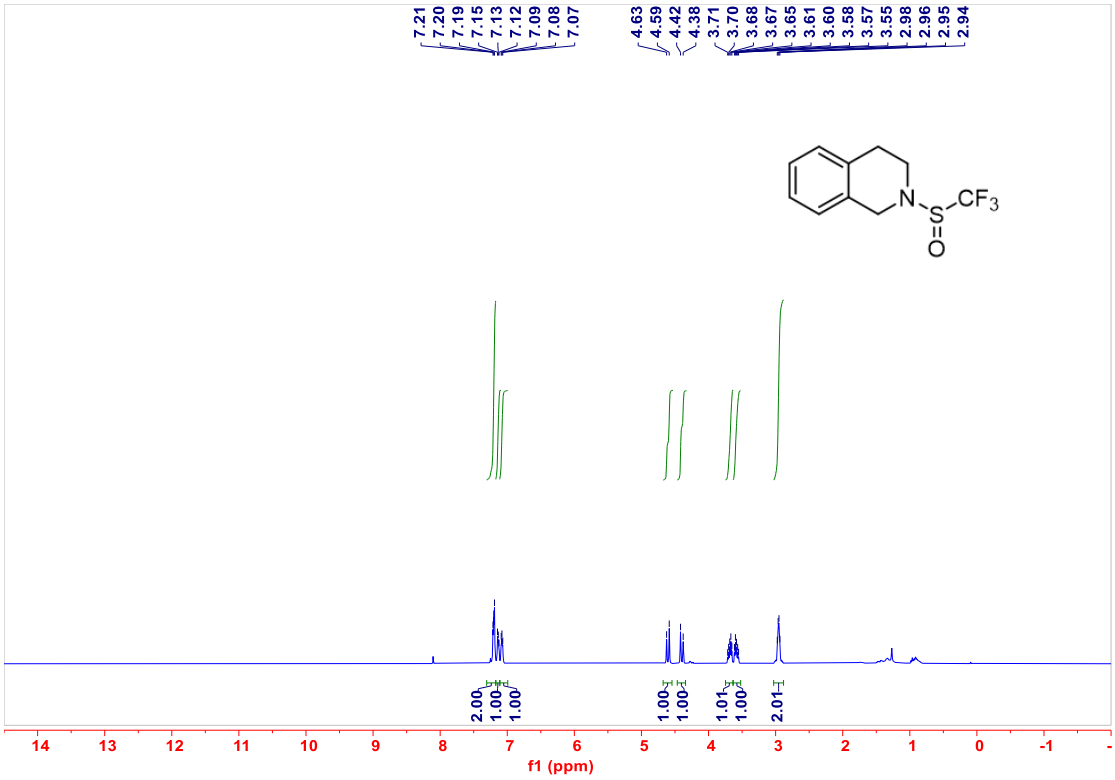

-74.0
Ph
Ph
N
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

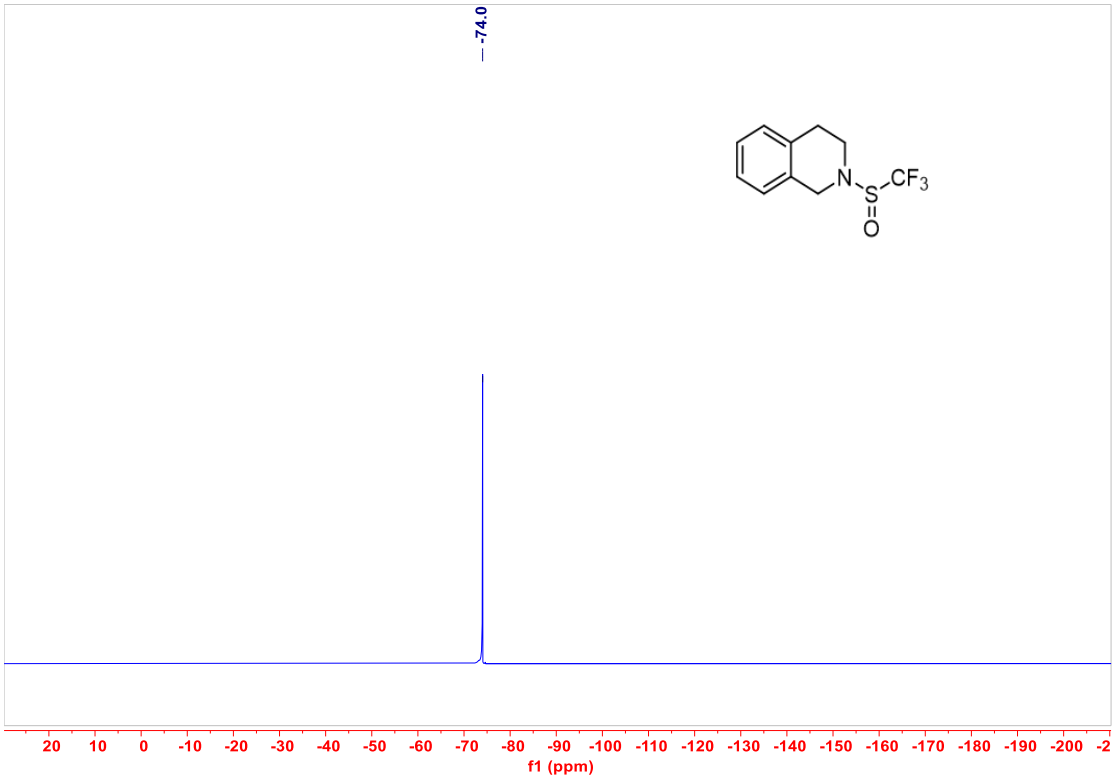

134.7
129.4
129.0
128.9
128.3
126.1
122.7
119.4
50.1
Ph
Ph
N
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

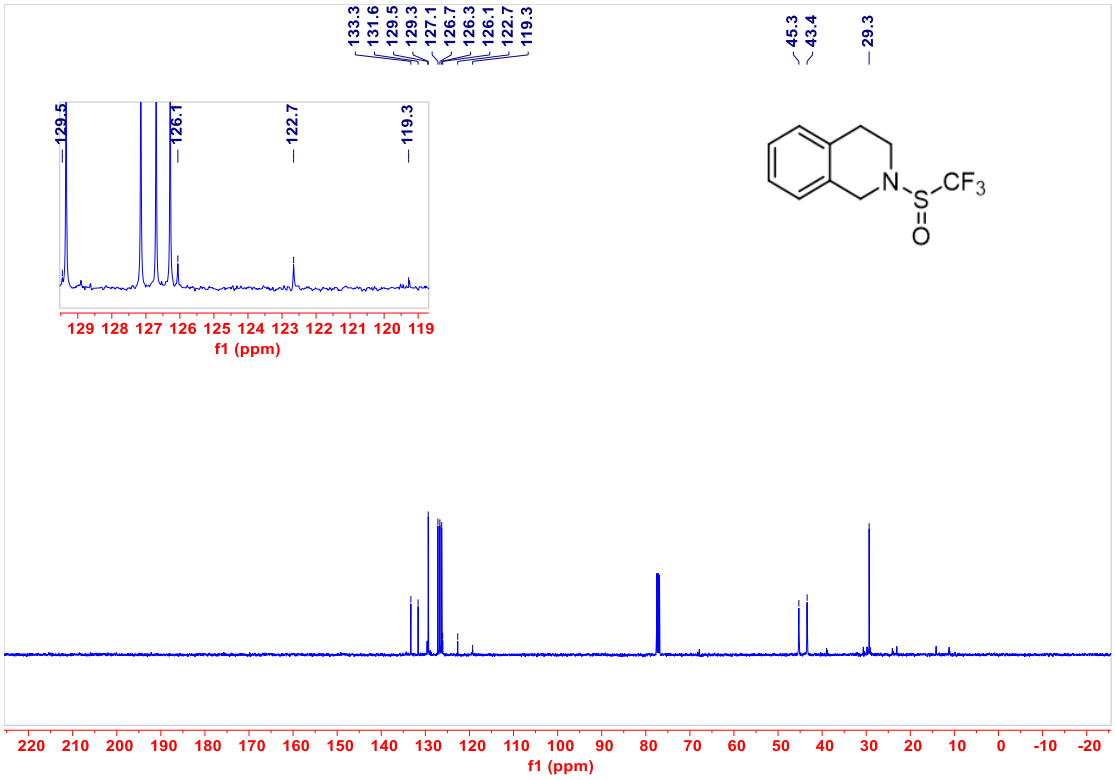

7.35
7.33
7.32
7.26
7.24
7.22
7.20
3.95
3.92
3.79
3.75
3.11
3.08
3.05
3.03
3.00
2.97
2.75
2.72
2.69
1.94
1.85
1.84
1.82
1.80
1.79
1.77
1.76
1.74
1.72
1.70
1.69
Ph
N
S
O
CF3
2.00
3.00
1.00
1.00
1.00
1.00
1.00
2.01
2.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

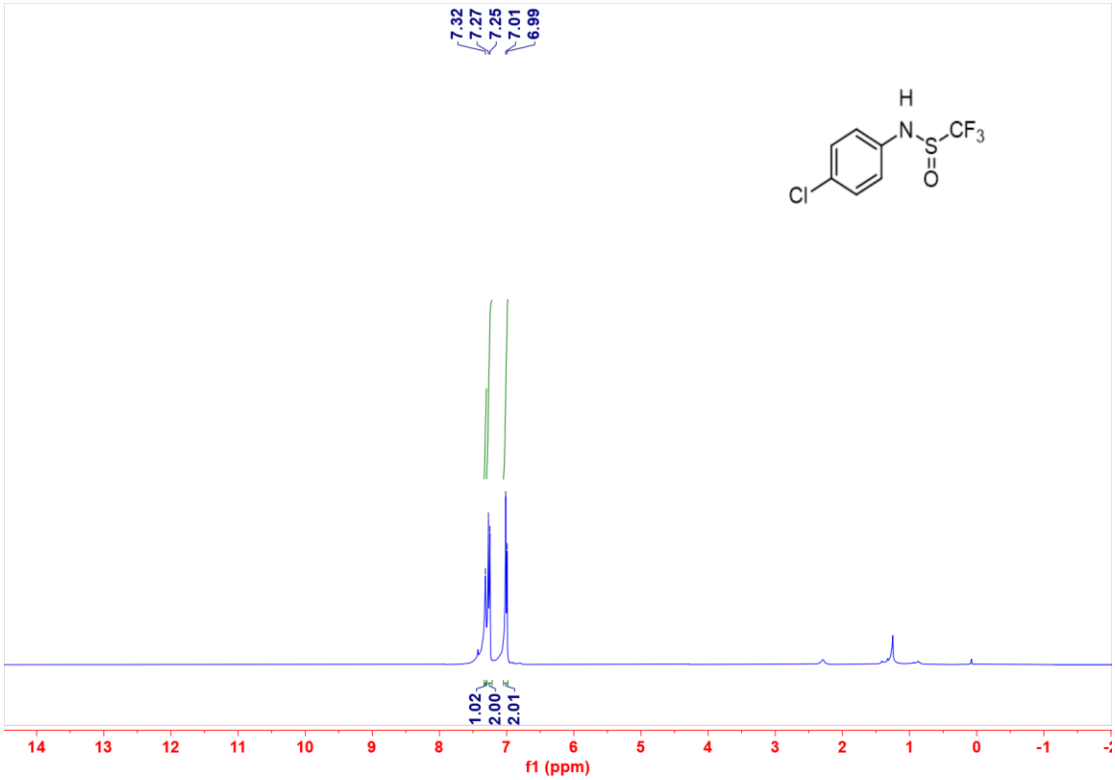

-74.0
Ph
N
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

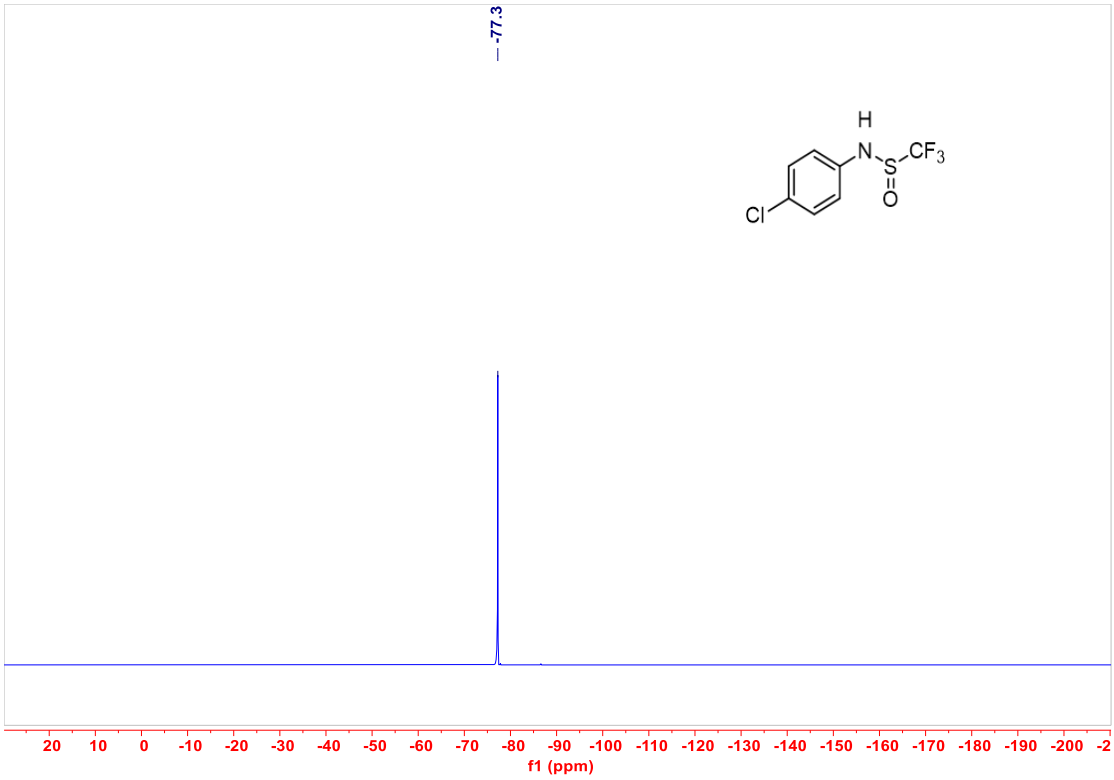

144.9
129.6
128.8
126.8
126.2
122.8
119.4
46.7
44.1
42.2
33.5
33.4
Ph
N
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

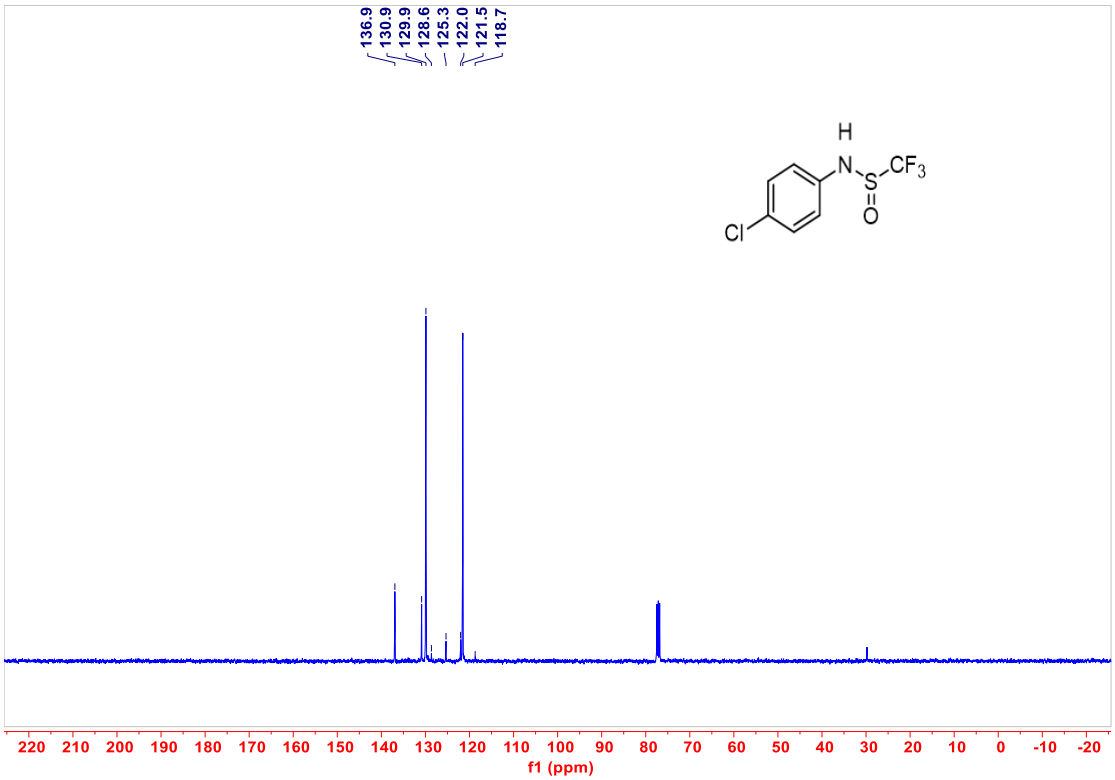

7.21
7.20
7.19
7.15
7.13
7.12
7.09
7.08
7.07
4.63
4.59
4.42
4.38
3.71
3.70
3.68
3.67
3.65
3.61
3.60
3.58
3.57
3.55
2.98
2.96
2.95
2.94
N
S
O
CF3
2.00
1.00
1.00
1.00
1.00
1.01
1.00
2.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

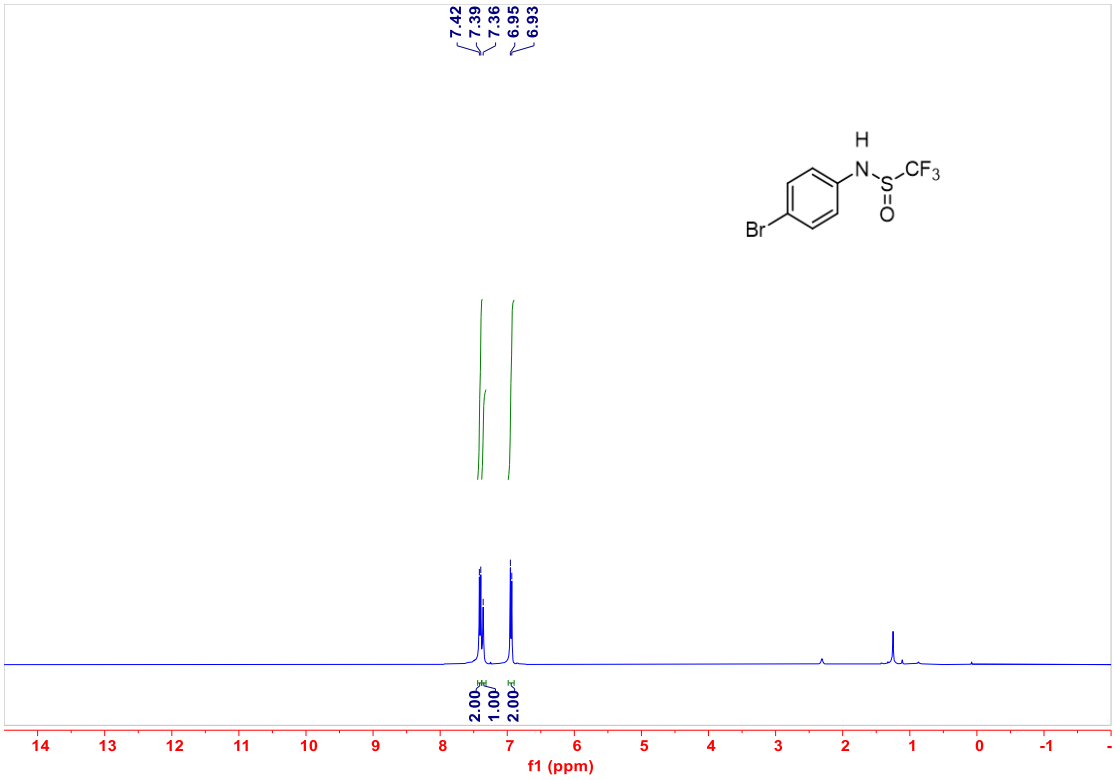

-74.0
N
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

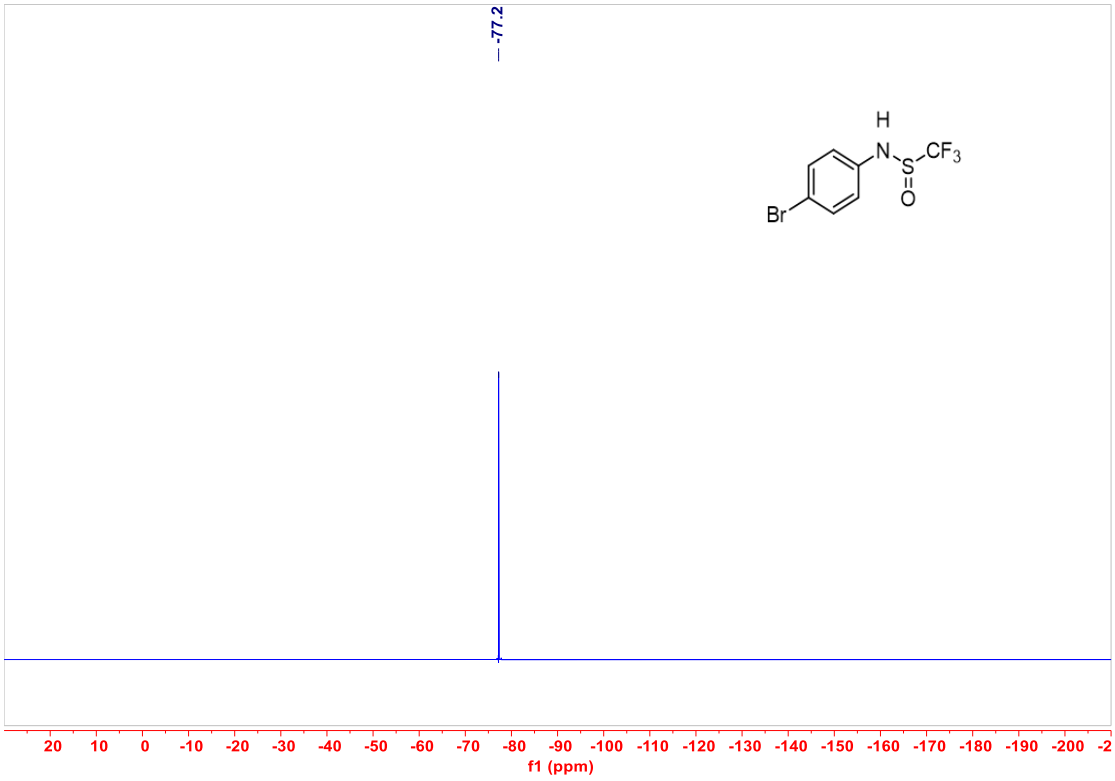

133.3
131.6
129.5
129.3
127.1
126.7
126.3
126.1
122.7
119.3
45.3
43.4
29.3
129.5
126.1
122.7
119.3
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

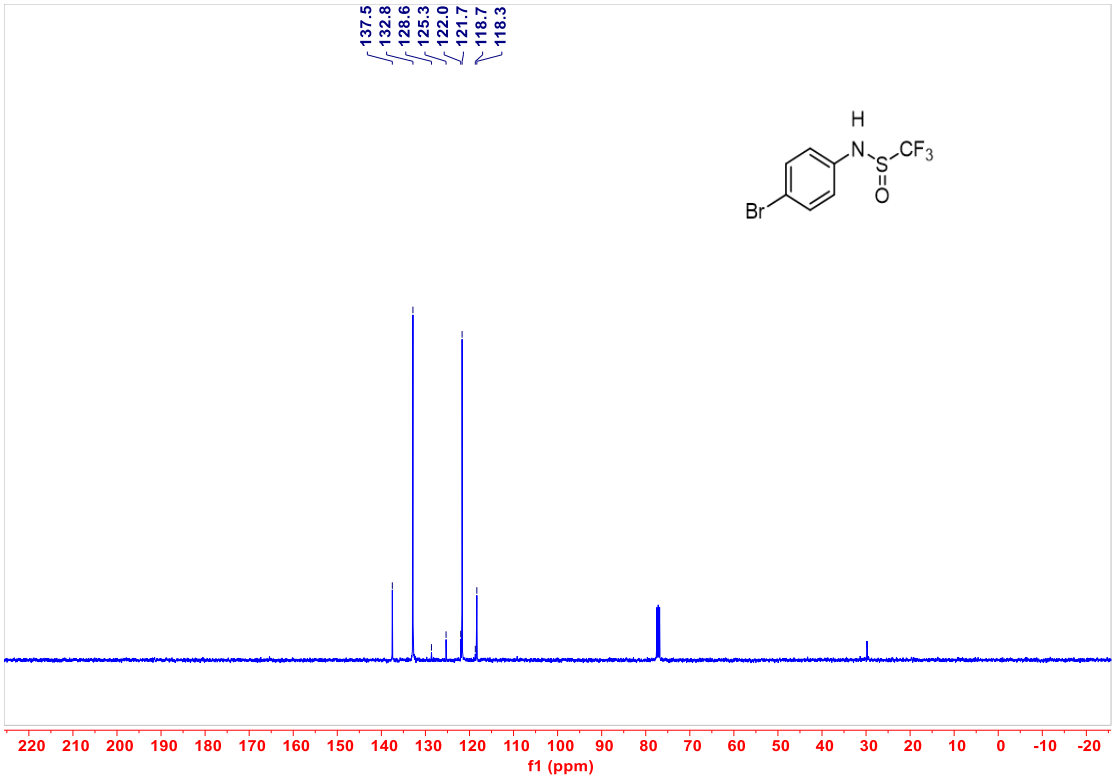

7.32
7.27
7.25
7.01
6.99
H
N
S
CF3
O
Cl
1.02
2.00
2.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

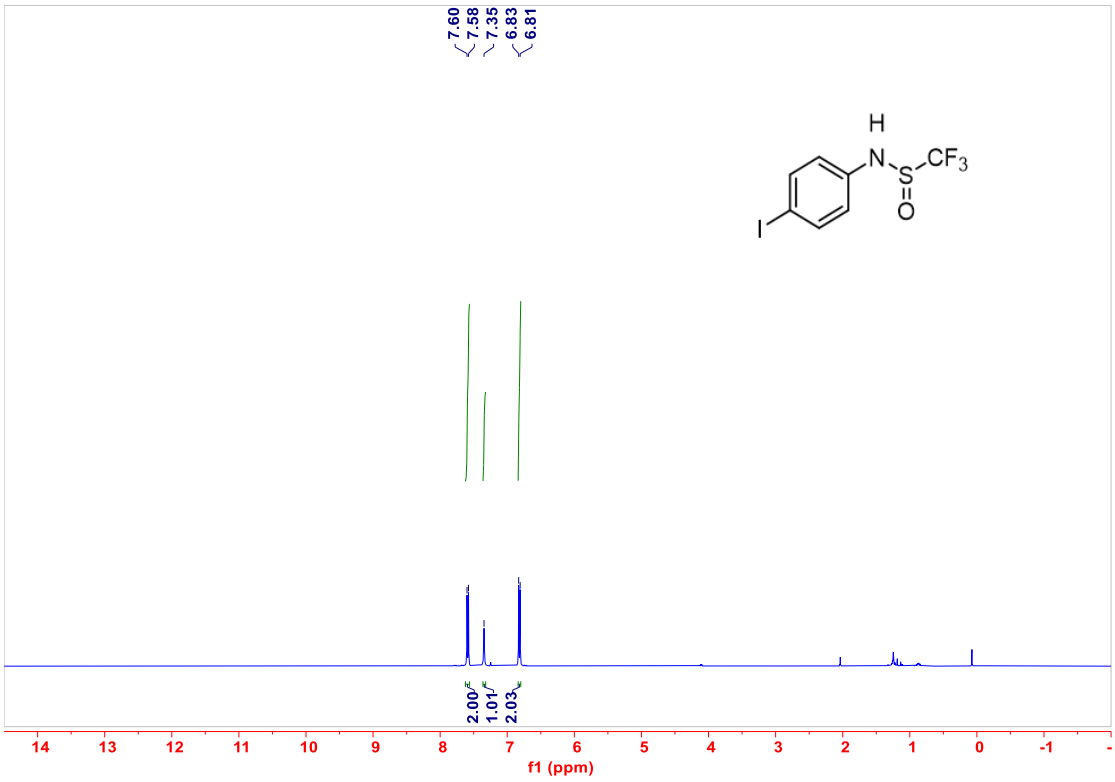

-77.3
H
N
S
CF3
O
Cl
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

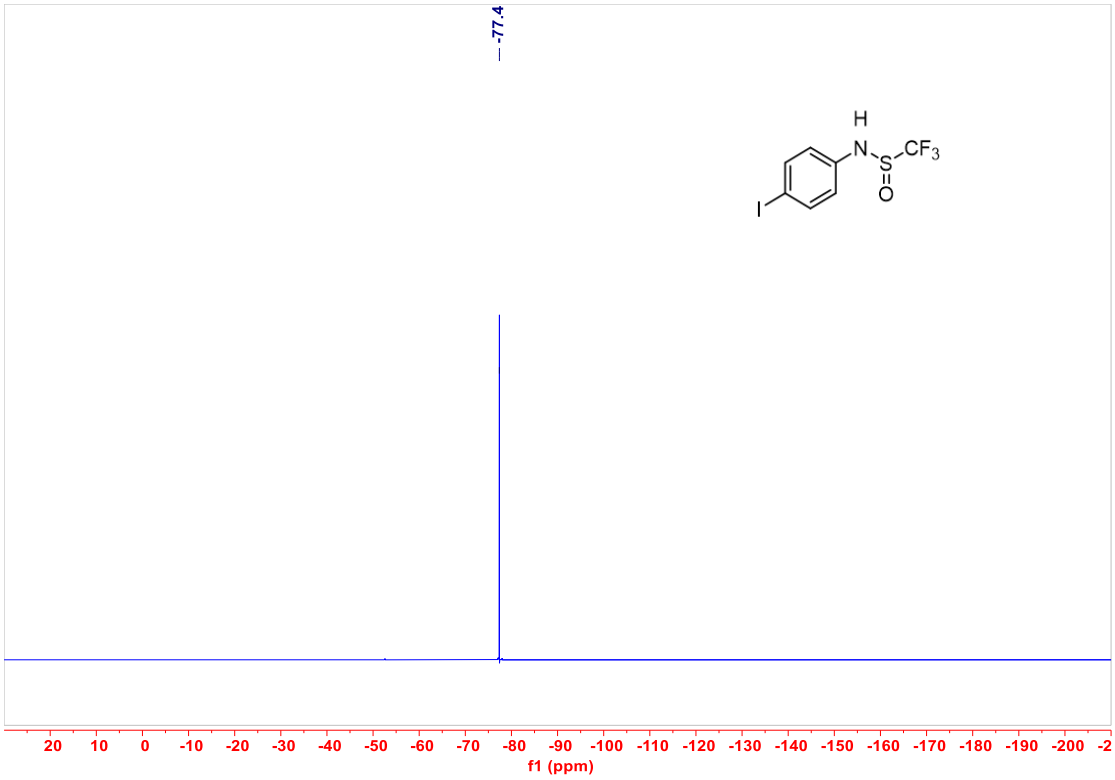

136.9
130.9
129.9
128.6
125.3
122.0
121.5
118.7
H
N
S
CF3
O
Cl
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.42
7.39
7.36
6.95
6.93
H
N
S
CF3
O
Br
2.00
1.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.2
H
N
S
CF3
O
Br
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


137.5
132.8
128.6
125.3
122.0
121.7
118.7
118.3
H
N
S
CF3
O
Br
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.60
7.58
7.35
6.83
6.81
H
N
S
CF3
O
I
2.00
1.01
2.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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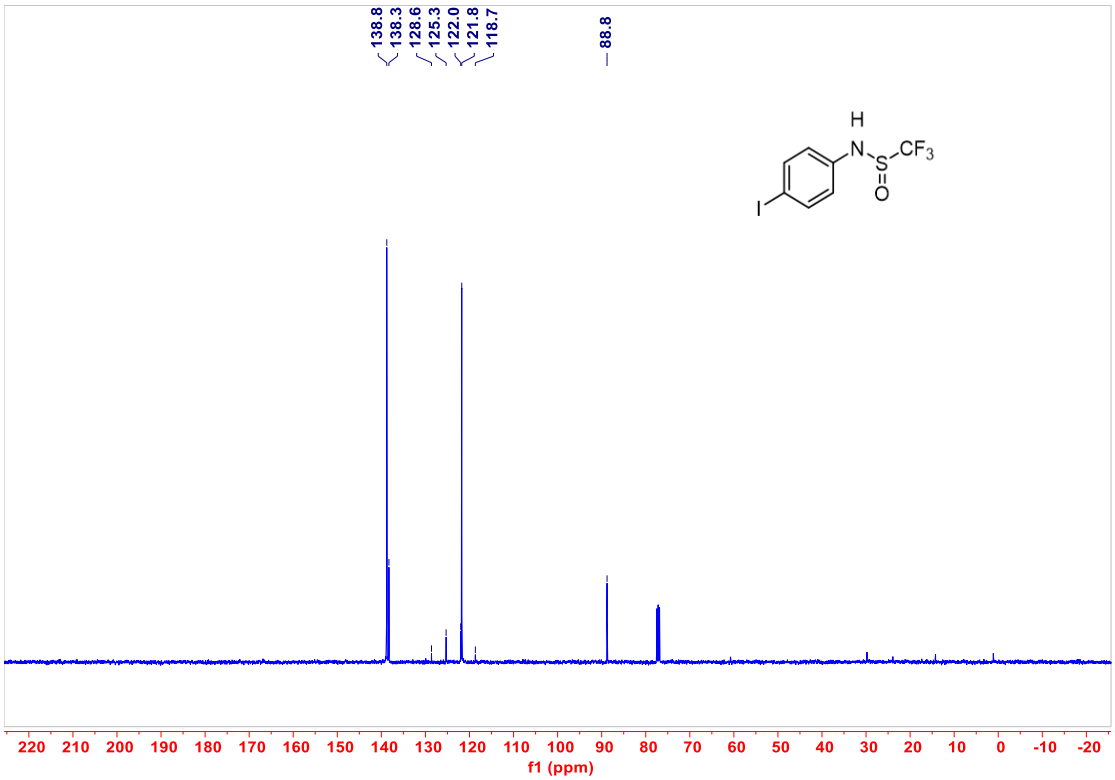
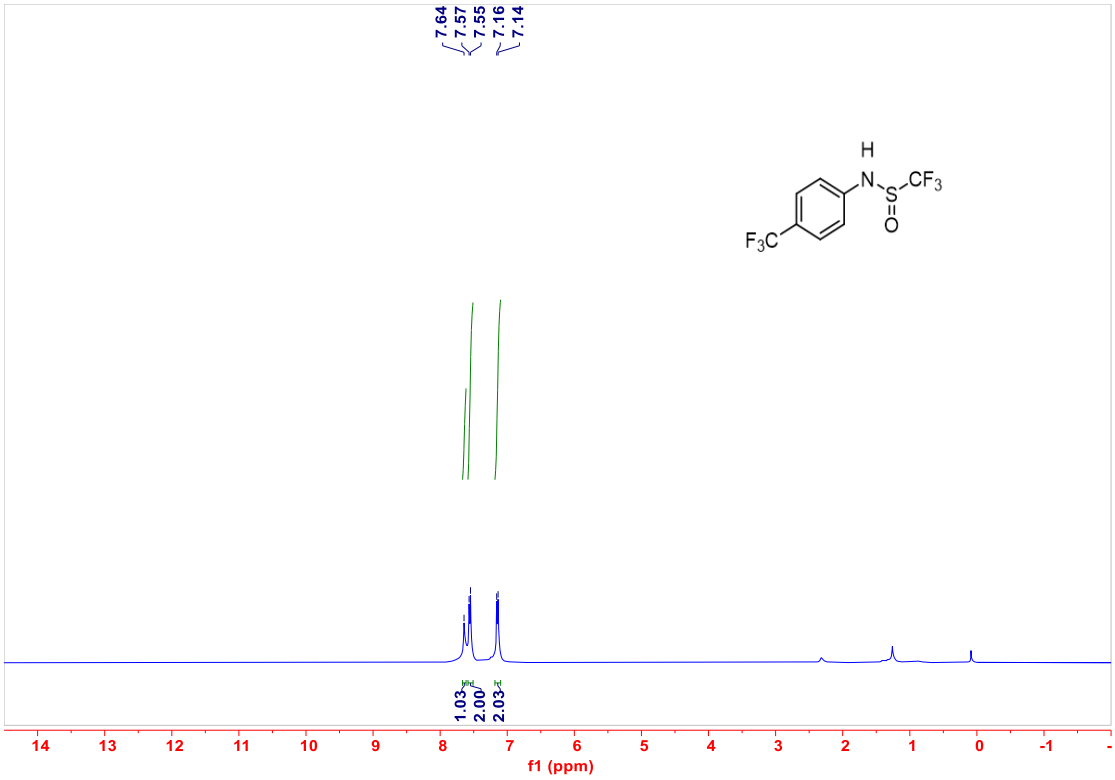
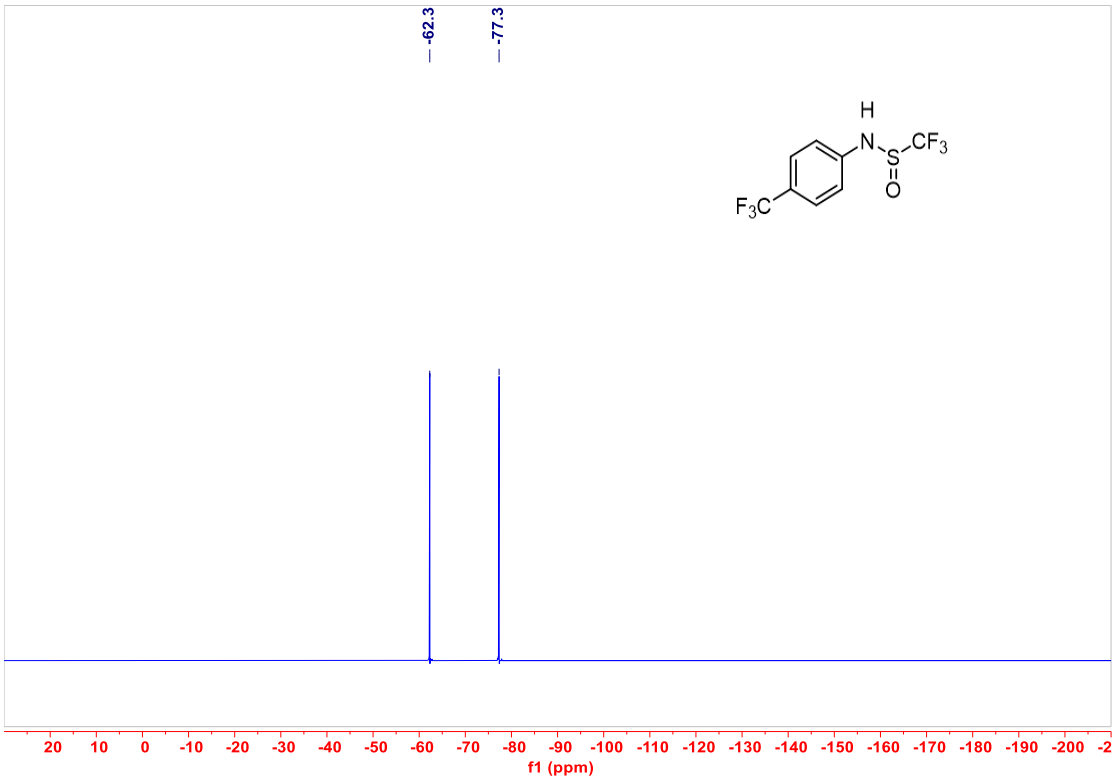
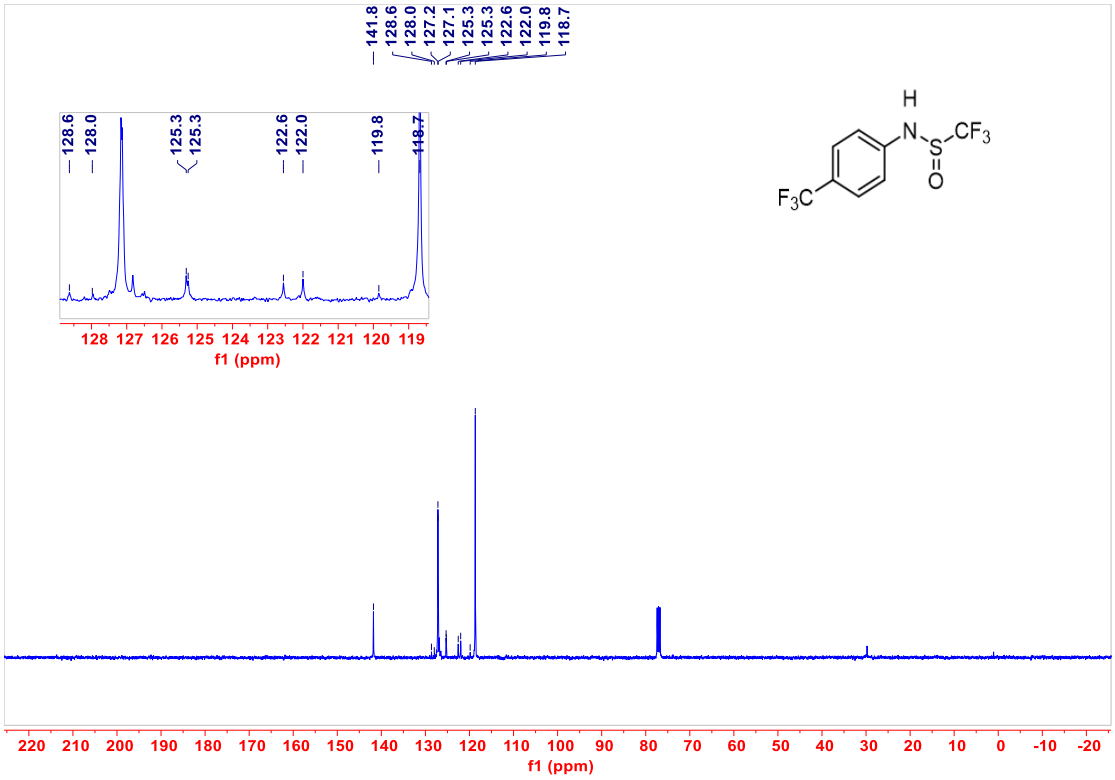
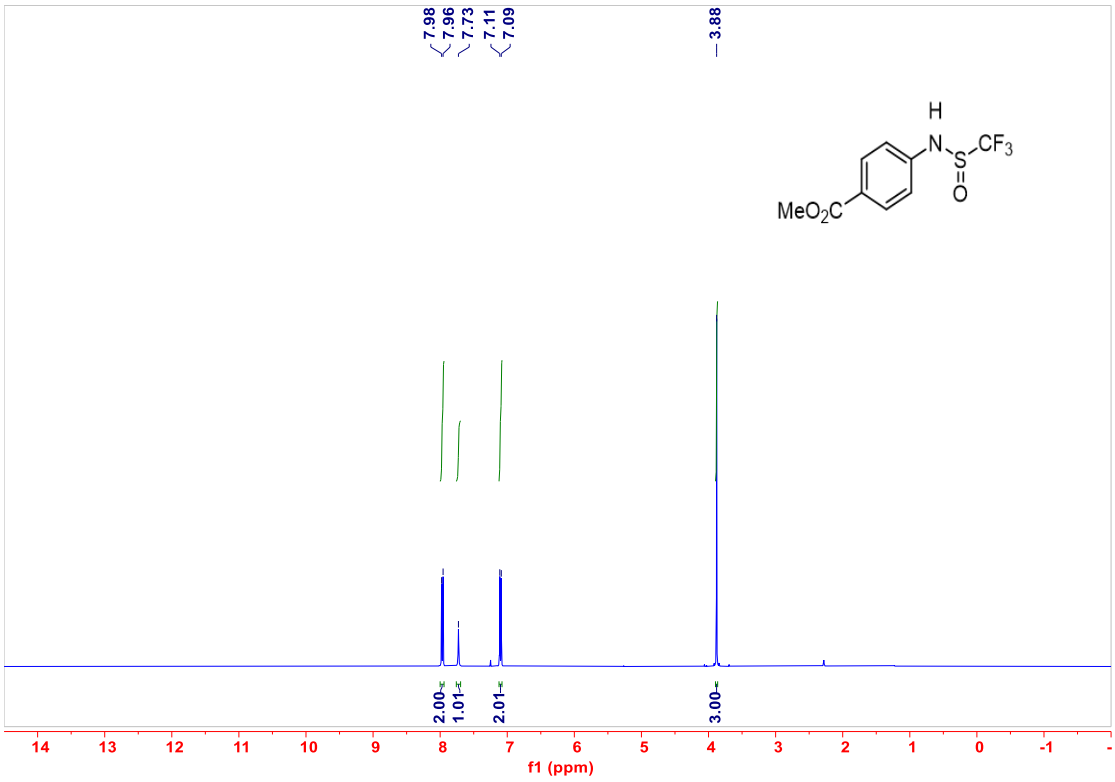
H
N
S
CF3
O
O
I
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

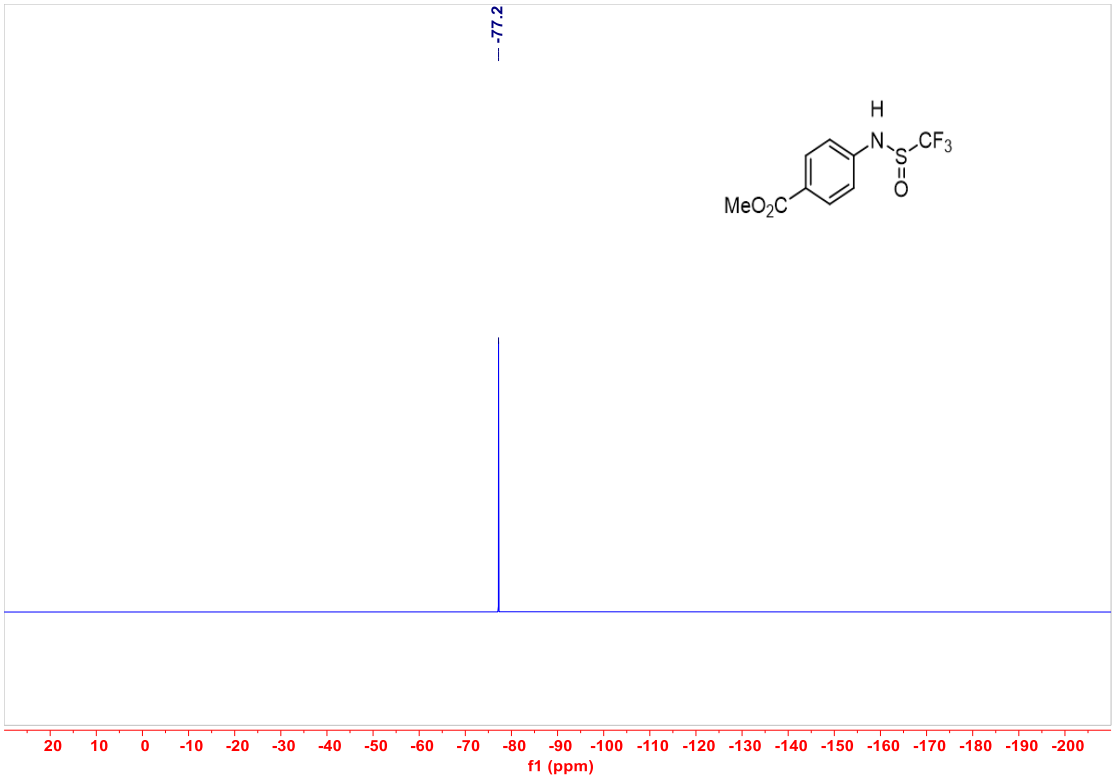

138.8
138.3
128.6
125.3
122.0
121.8
118.7
88.8
H
N
S
CF3
O
O
I
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

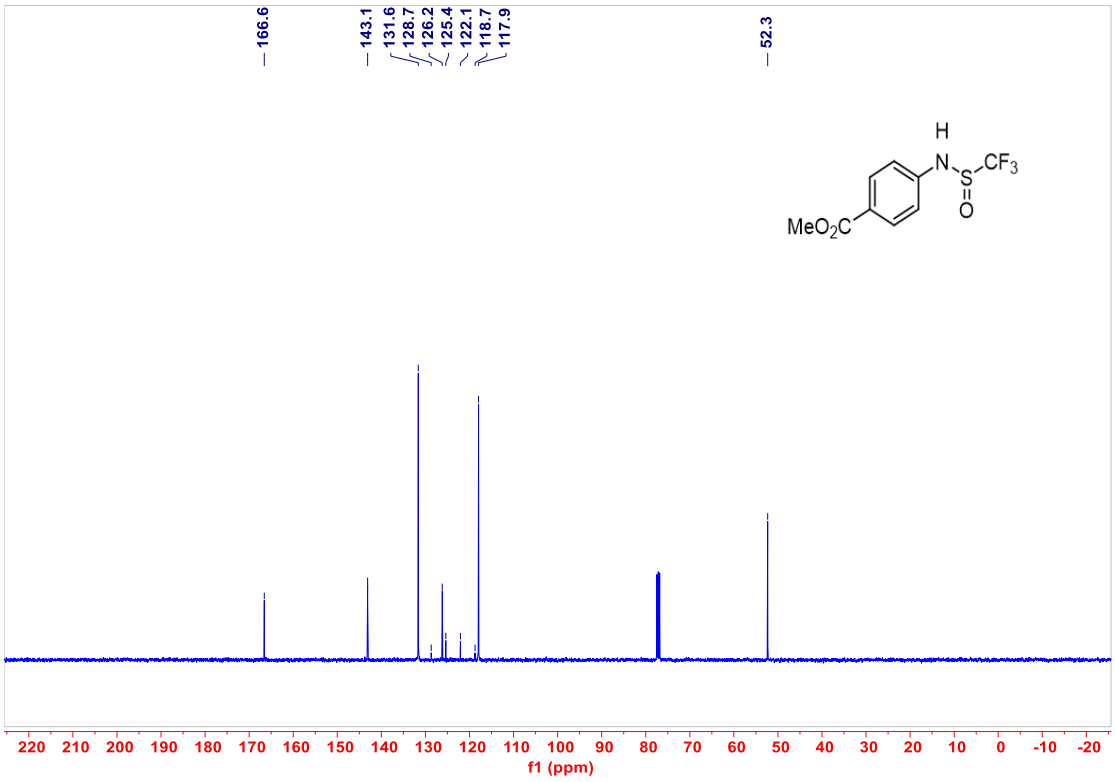

7.64
7.57
7.55
7.16
7.14
H
N
S
CF3
O
F3C
1.03
2.00
2.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

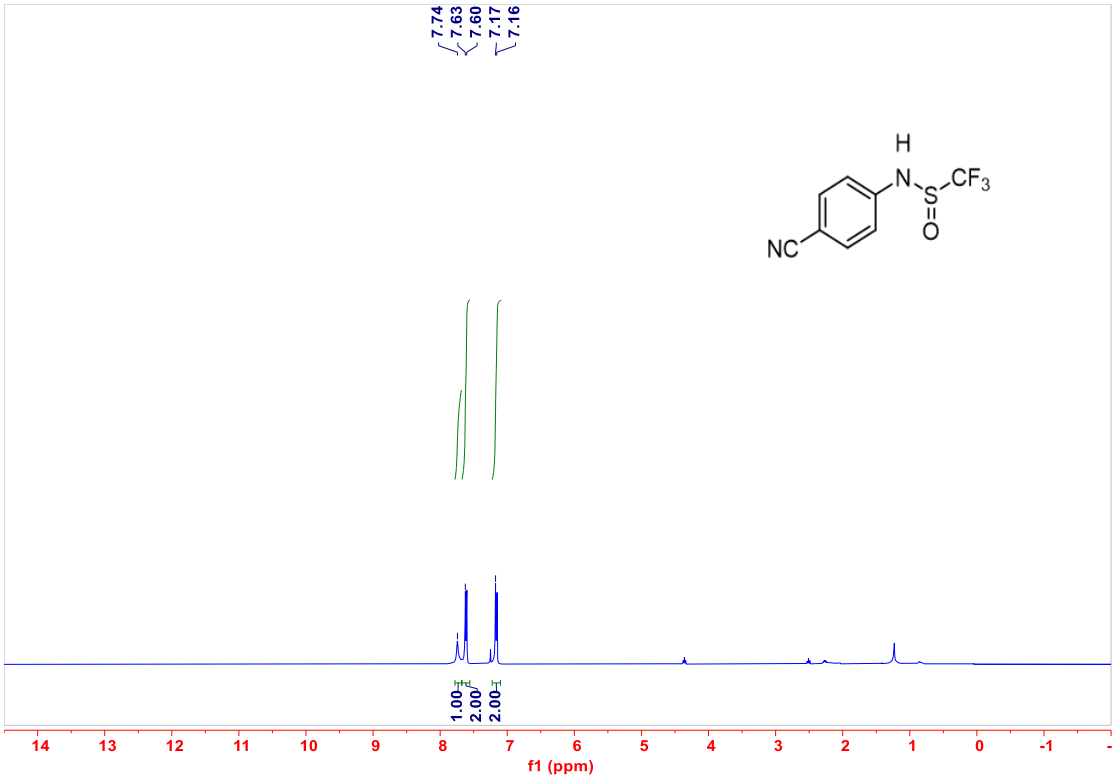

-62.3
-77.3
H
N
S
CF3
O
F3C
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

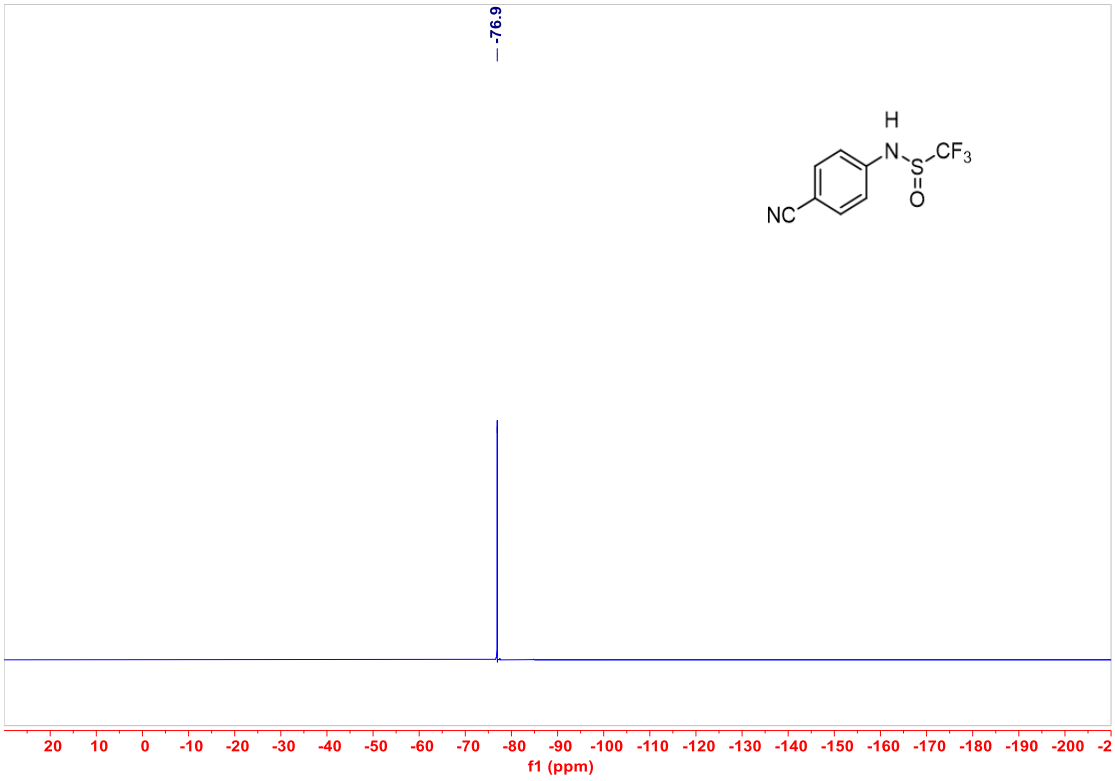

141.8
128.6
128.0
127.2
127.1
125.3
125.3
122.6
122.0
119.8
118.7
128.6
128.0
125.3
125.3
122.6
122.0
119.8
118.7
128 127 126 125 124 123 122 121 120 119
f1 (ppm)
H
N
S
CF3
O
O
F3C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

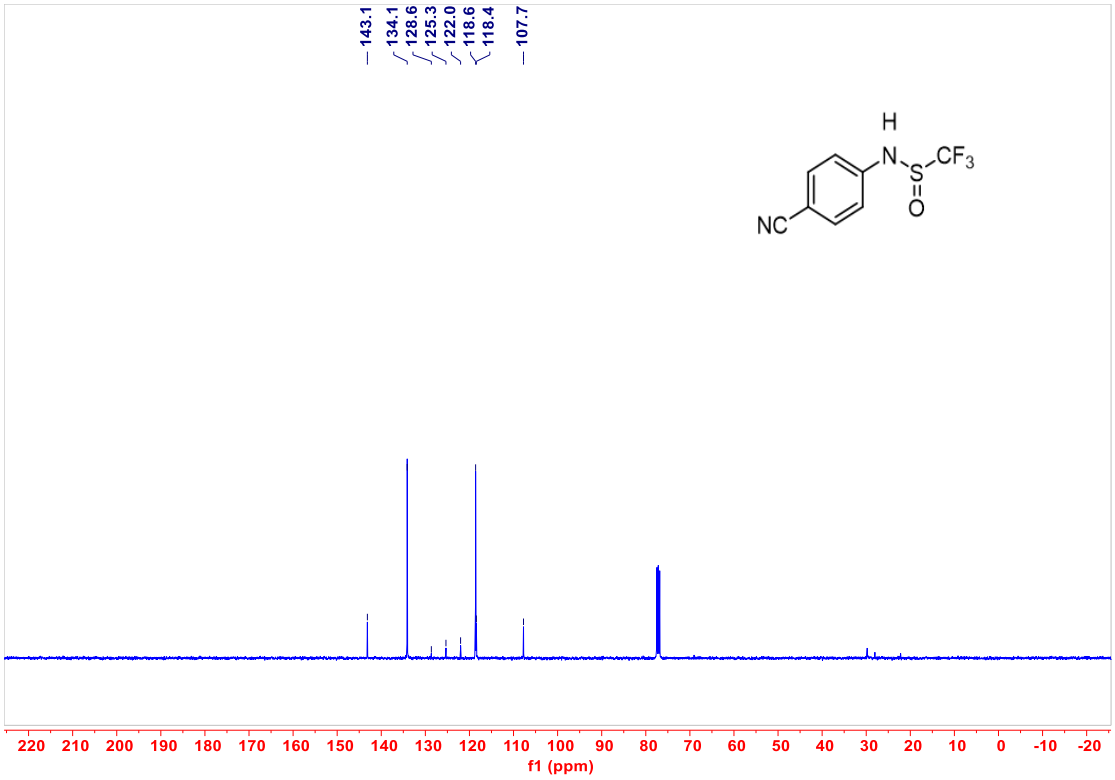

7.98
7.96
7.73
7.11
7.09
3.88
H
N
S
CF3
O
O
MeO2C
2.00
1.01
2.01
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

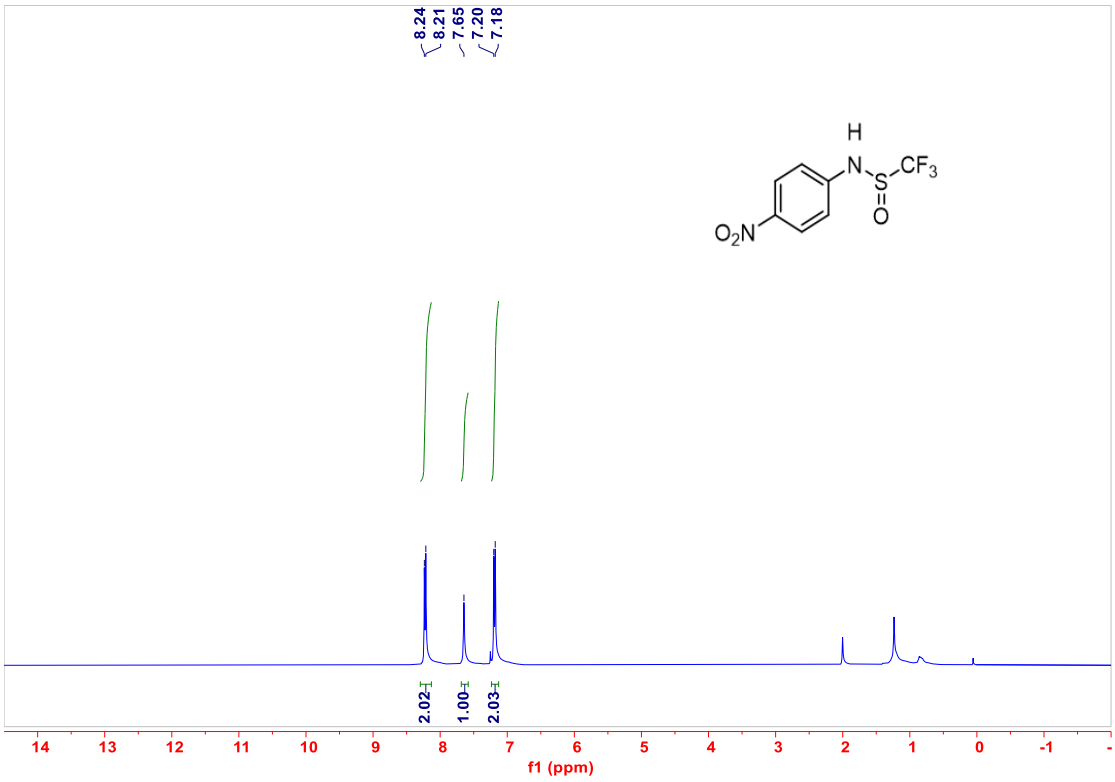

-77.2
H
N
S
CF3
O
MeO2C
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

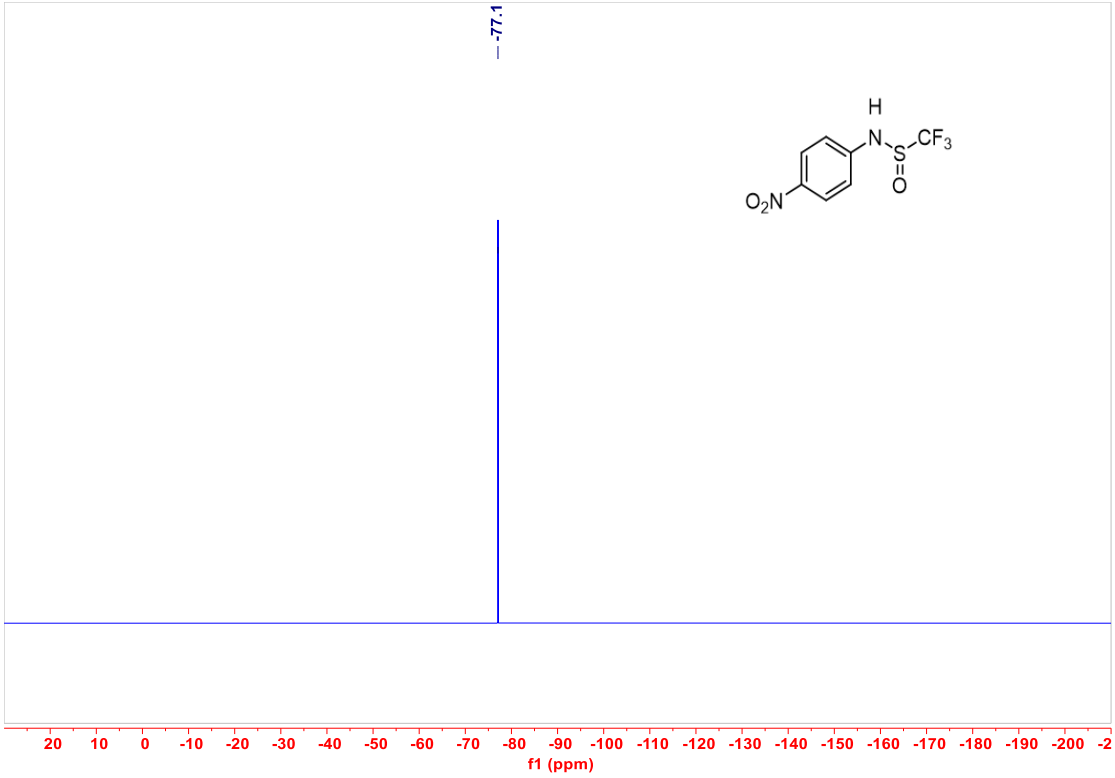

166.6
143.1
131.6
128.7
126.2
125.4
122.1
118.7
117.9
52.3
H
N
S
CF3
O
MeO2C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

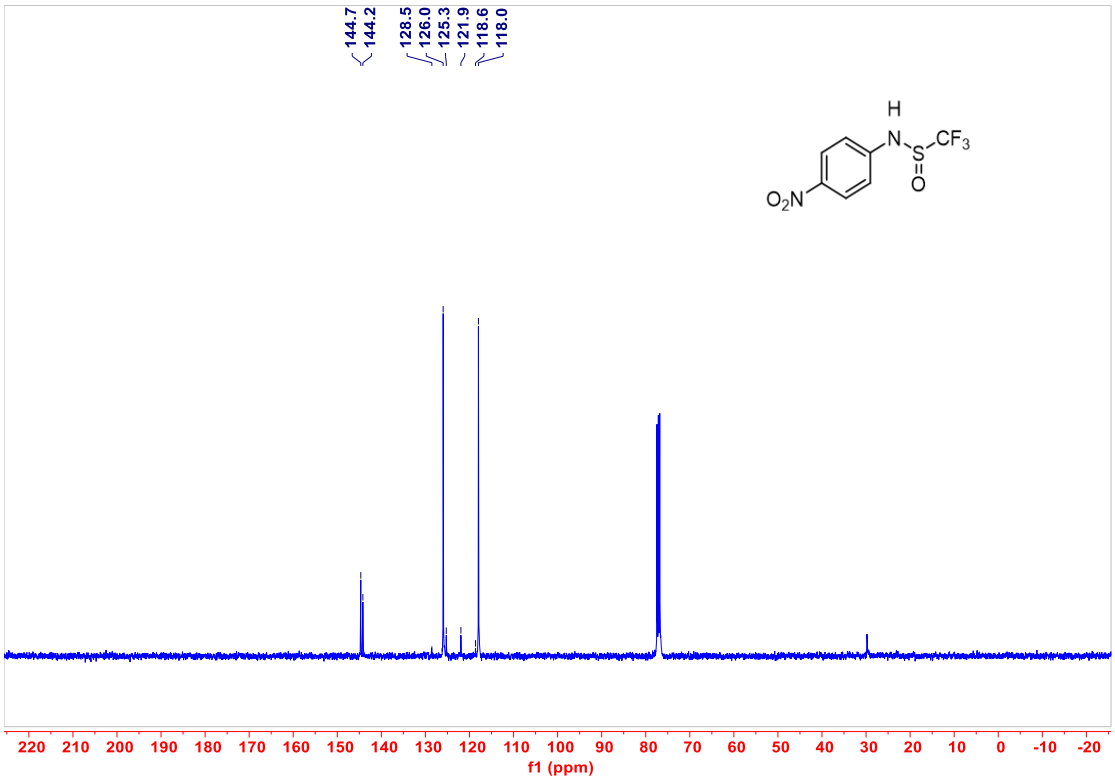

7.74
7.63
7.60
7.17
7.16
H
N
S
CF3
O
NC
1.00
2.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

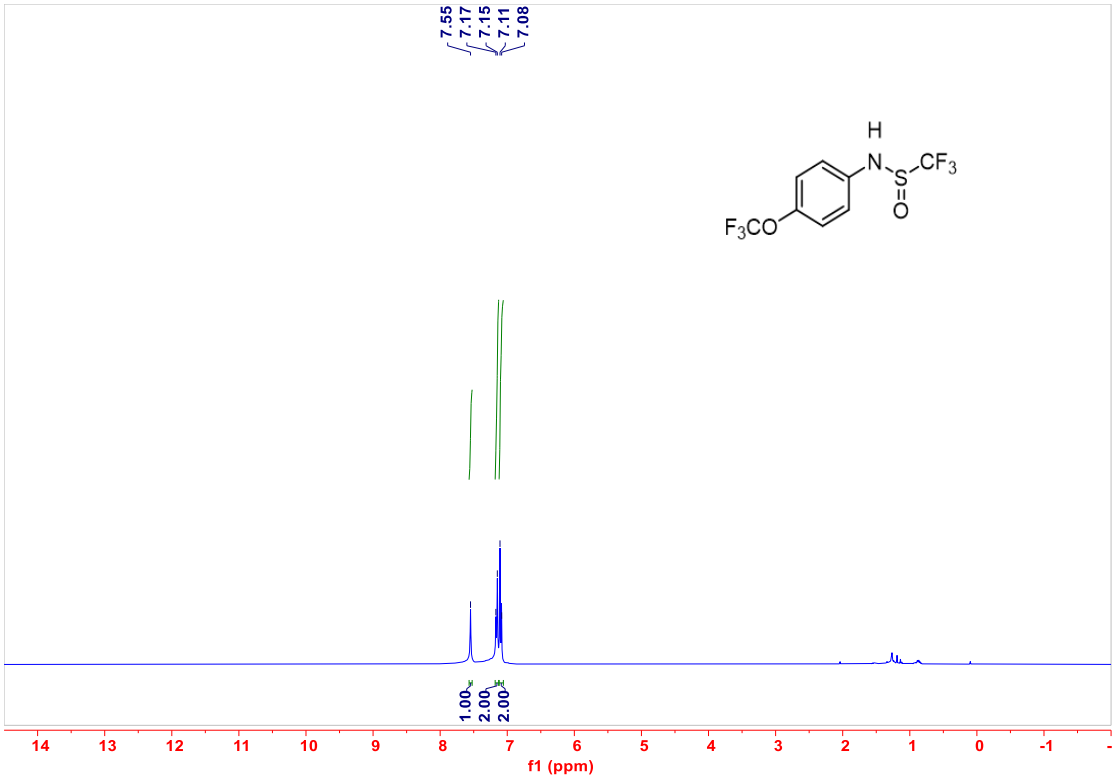

-76.9
H
N
S
CF3
O
NC
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

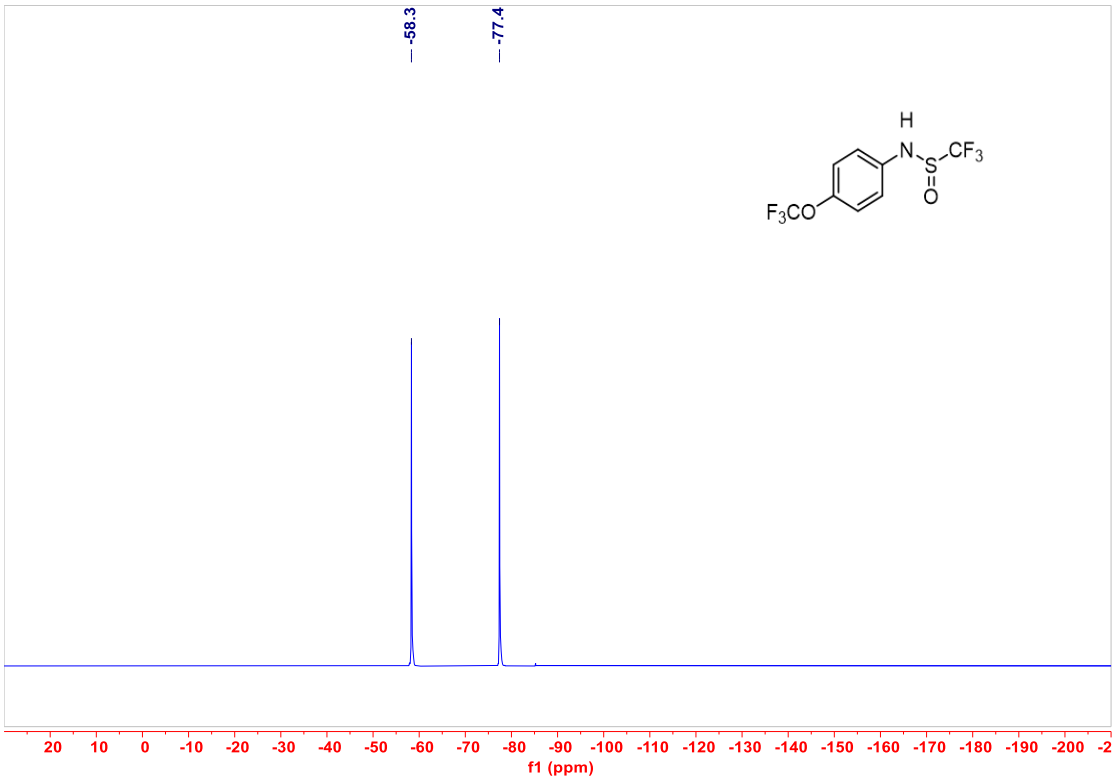

143.1
134.1
128.6
125.3
122.0
118.6
118.4
107.7
H
N
S
CF3
O
NC
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.24
8.21
7.65
7.20
7.18
H
N
S
CF3
O
O2N
2.02
1.00
2.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.1
H
N
S
CF3
O
O2N
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


144.7
144.2
128.5
126.0
125.3
121.9
118.6
118.0
H
N
S
CF3
O
O2N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.55
7.17
7.15
7.11
7.08
H
N
S
CF3
O
F3CO
1.00
2.00
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-58.3
-77.4
H
N
S
CF3
O
F3CO
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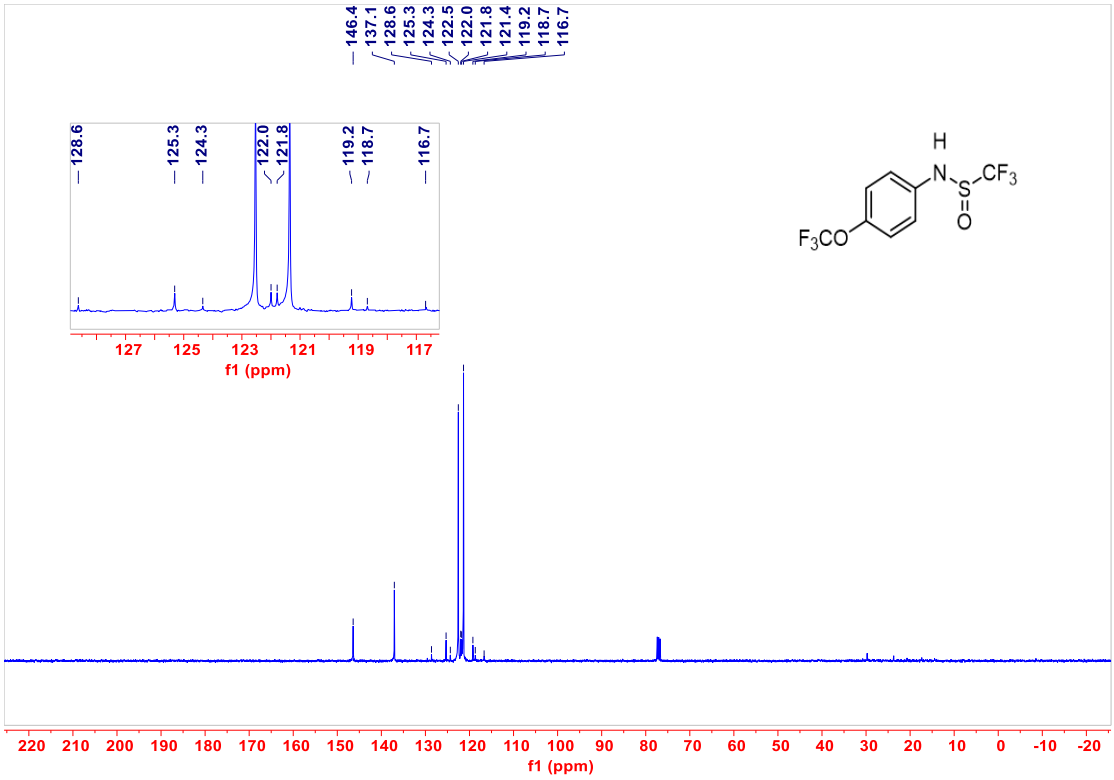
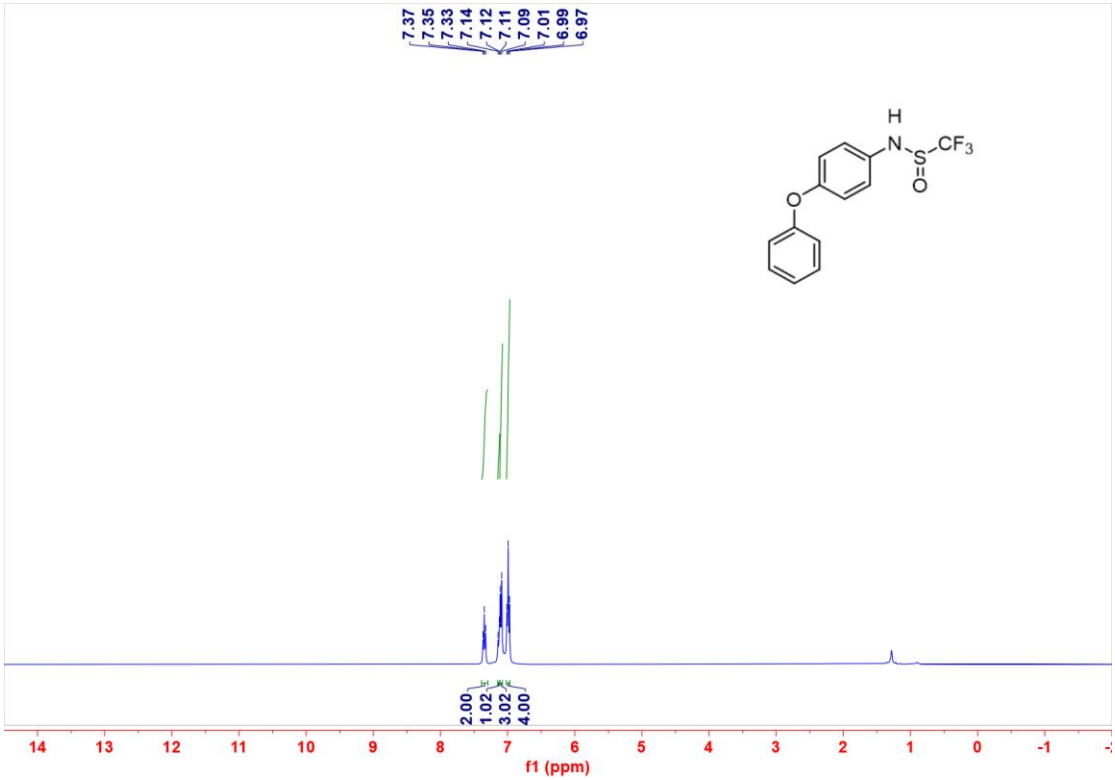
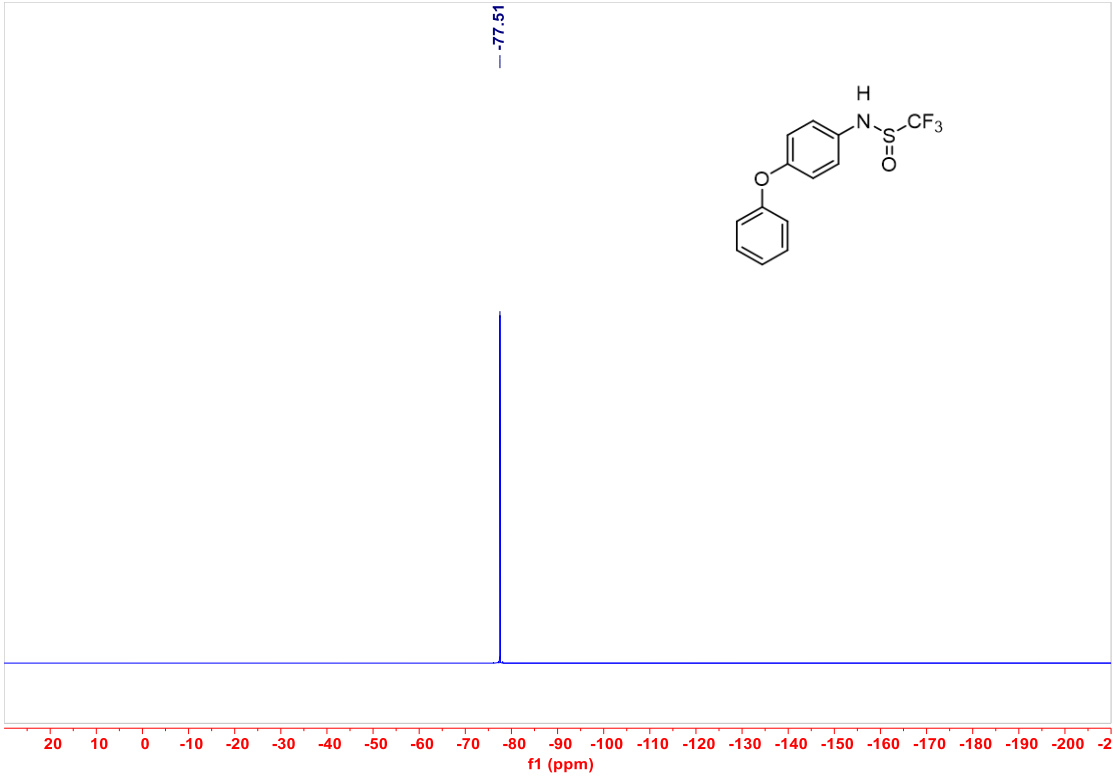
f1 (ppm)


146.4
137.1
128.6
125.3
124.3
122.5
122.0
121.8
121.4
119.2
118.7
116.7
128.6
125.3
124.3
122.0
121.8
119.2
118.7
116.7
127 125 123 121 119 117
f1 (ppm)
H
N
S
CF3
O
F3CO
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.37
7.35
7.33
7.14
7.12
7.11
7.09
7.01
6.99
6.97
H
N
S
CF3
O
O
2.00
1.02
3.02
4.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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H
N
S
CF3
O
O
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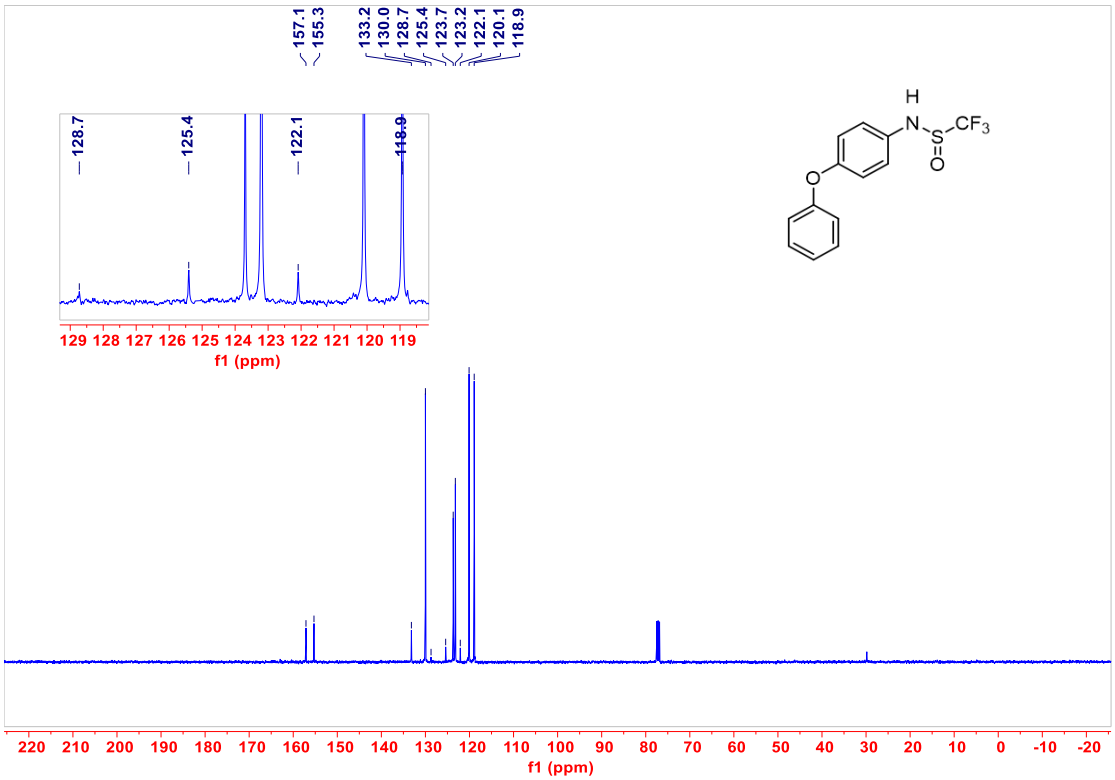
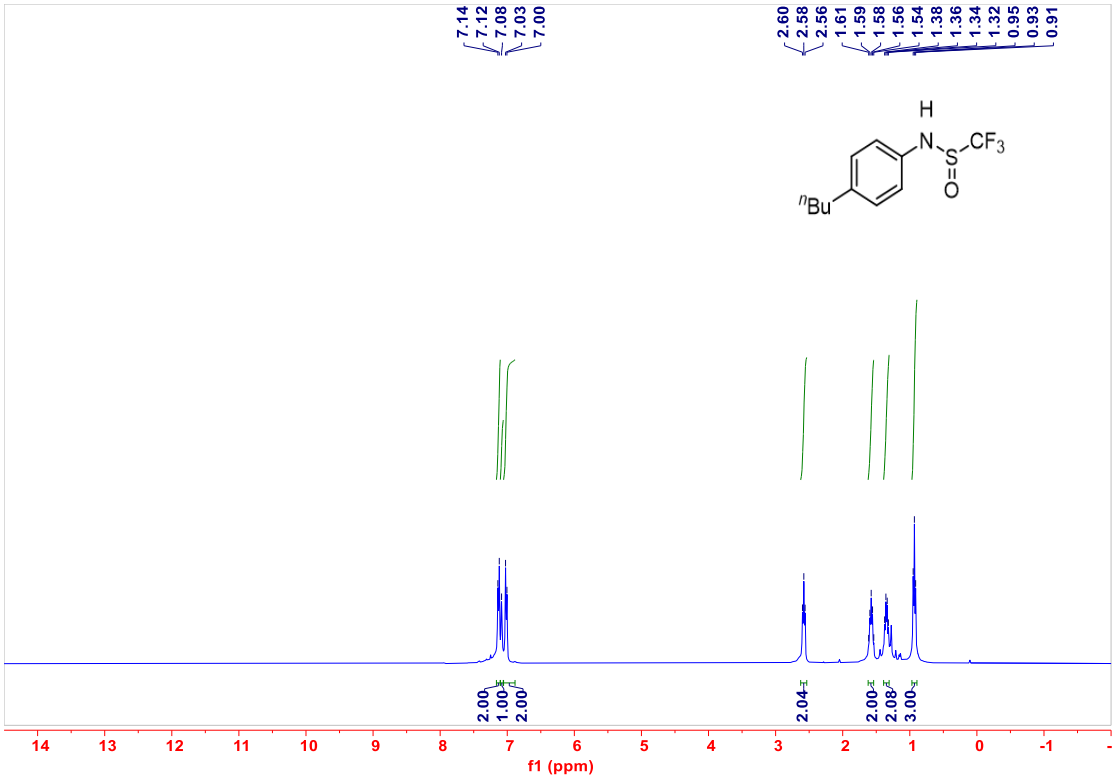
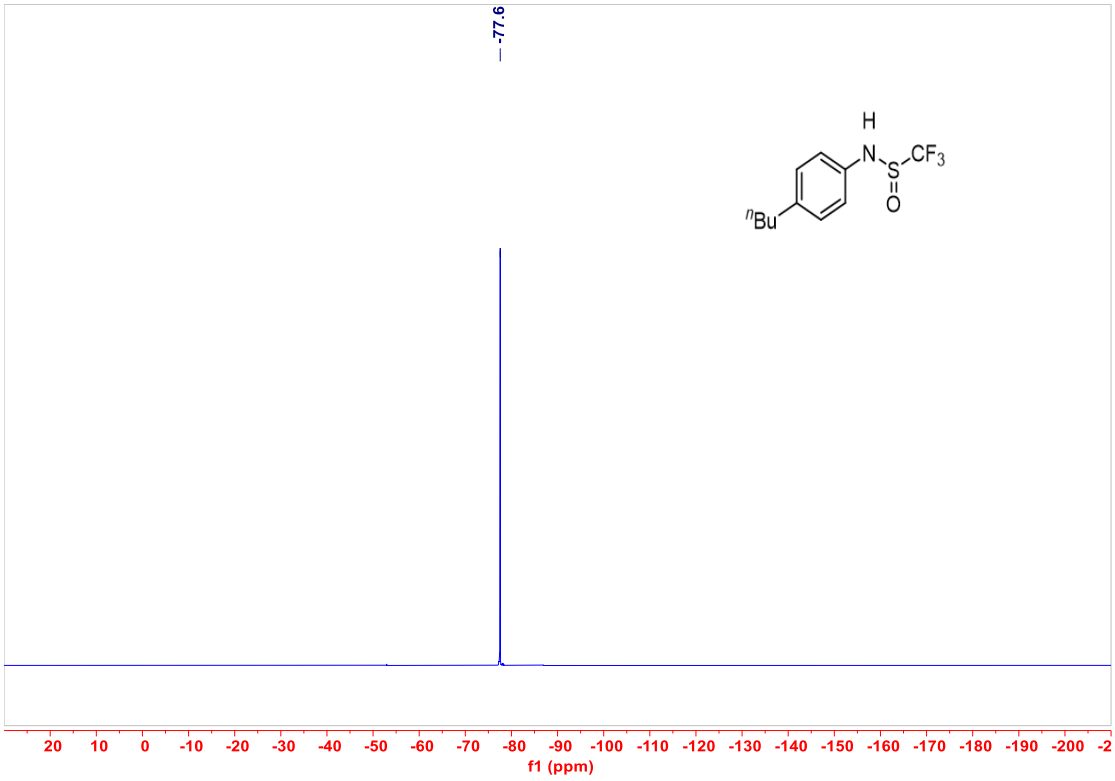
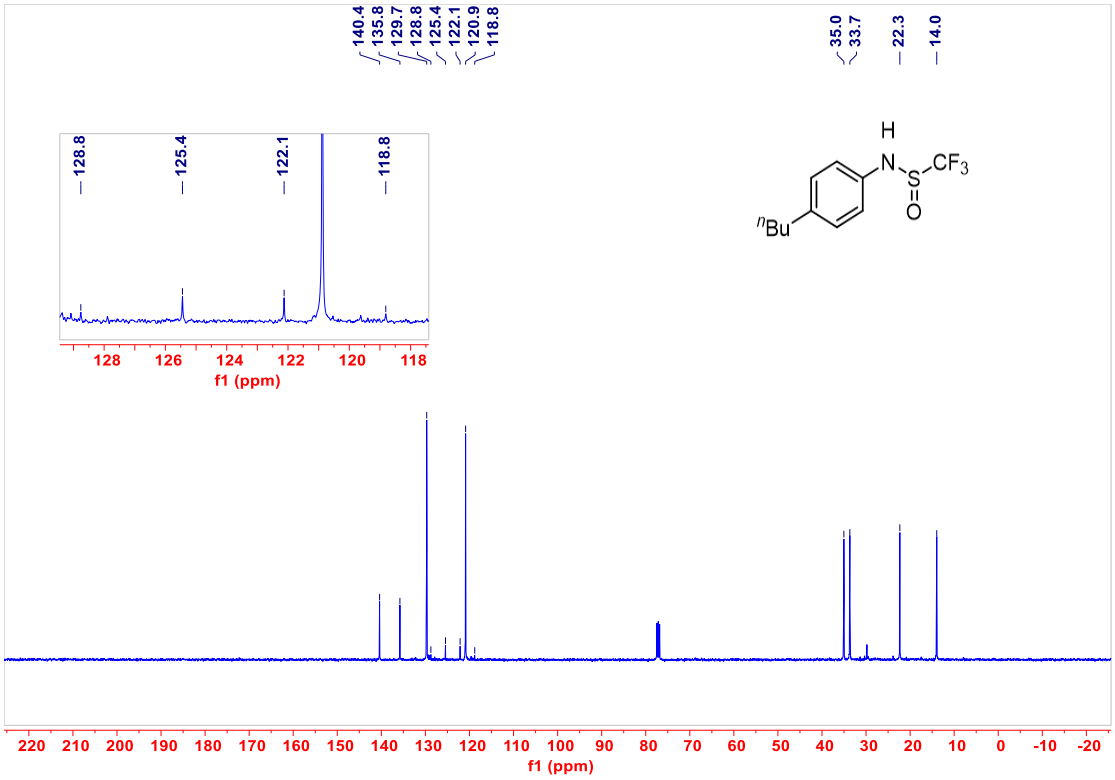
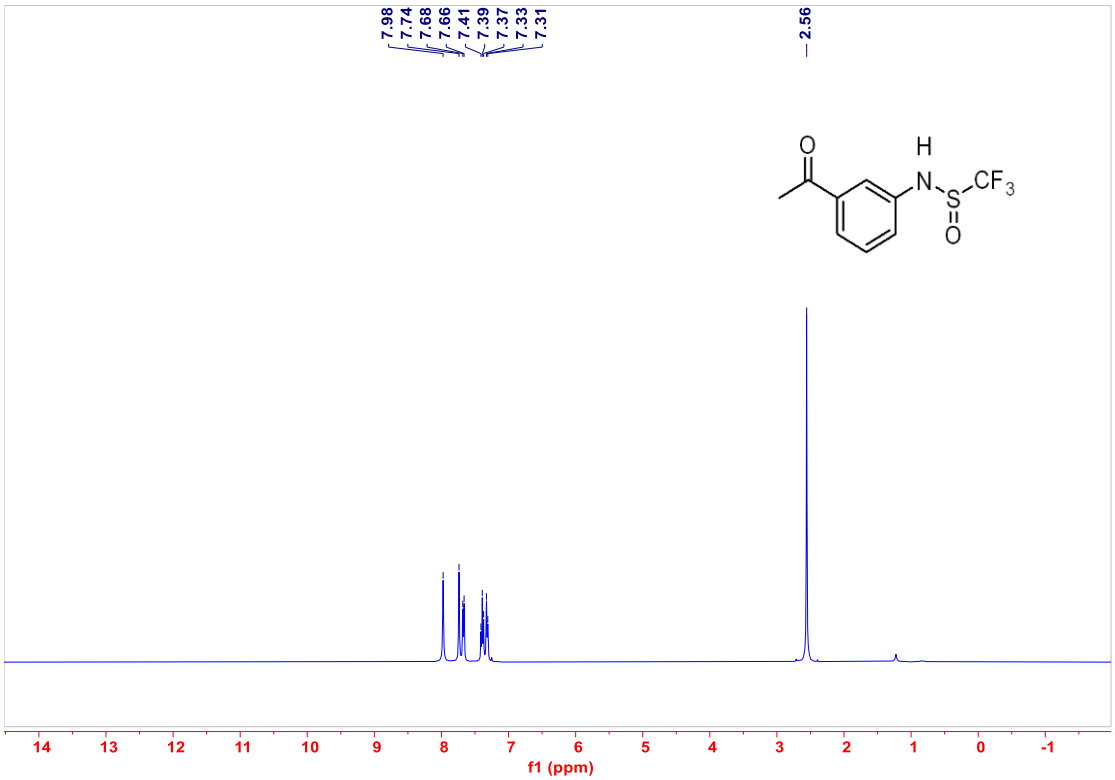
f1 (ppm)

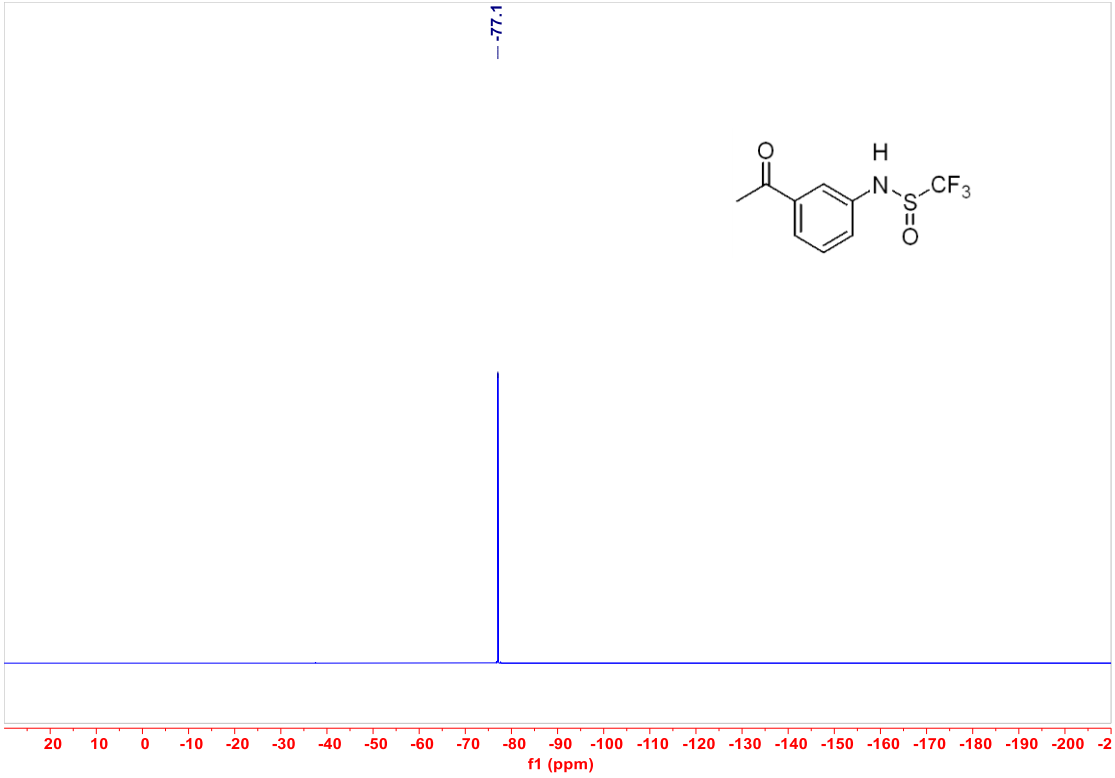

157.1
155.3
133.2
130.0
128.7
125.4
123.7
123.2
122.1
120.1
118.9
128.7
125.4
122.1
118.9
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
H
N
S
CF3
O
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

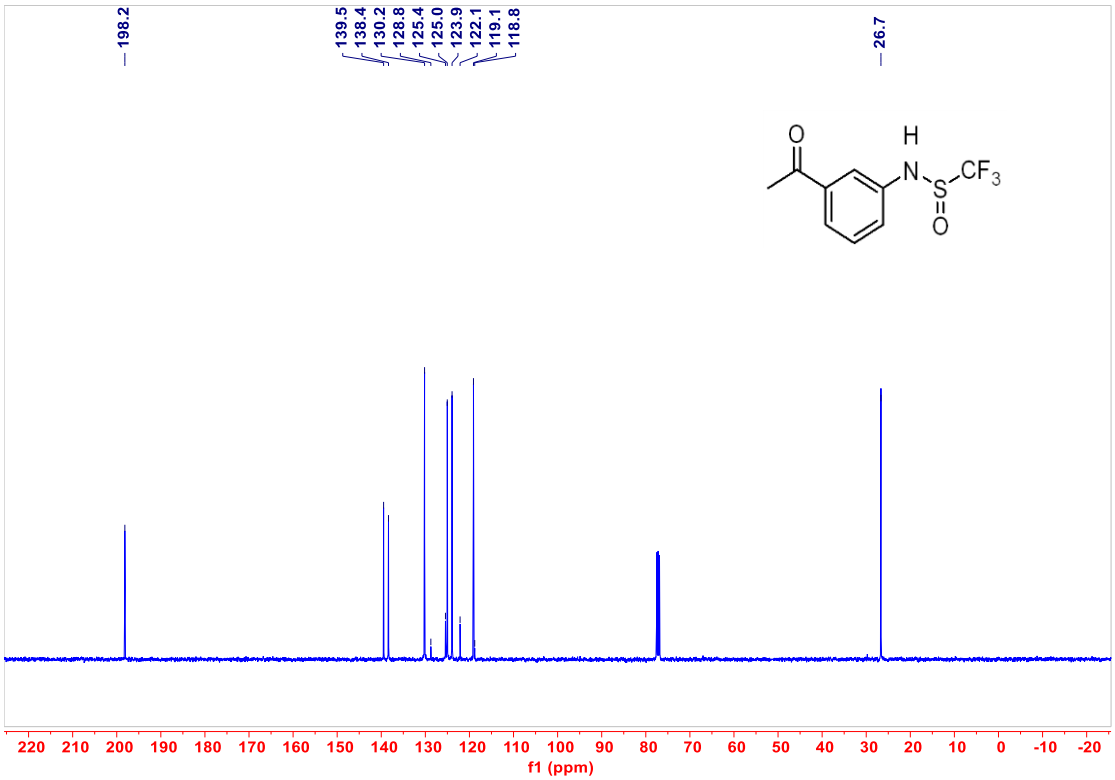

7.14
7.12
7.08
7.03
7.00
2.60
2.58
2.56
1.61
1.59
1.58
1.56
1.54
1.38
1.36
1.34
1.32
0.95
0.93
0.91
H
N
S
CF3
O
O
nBu
2.00
1.00
2.00
2.04
2.00
2.08
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

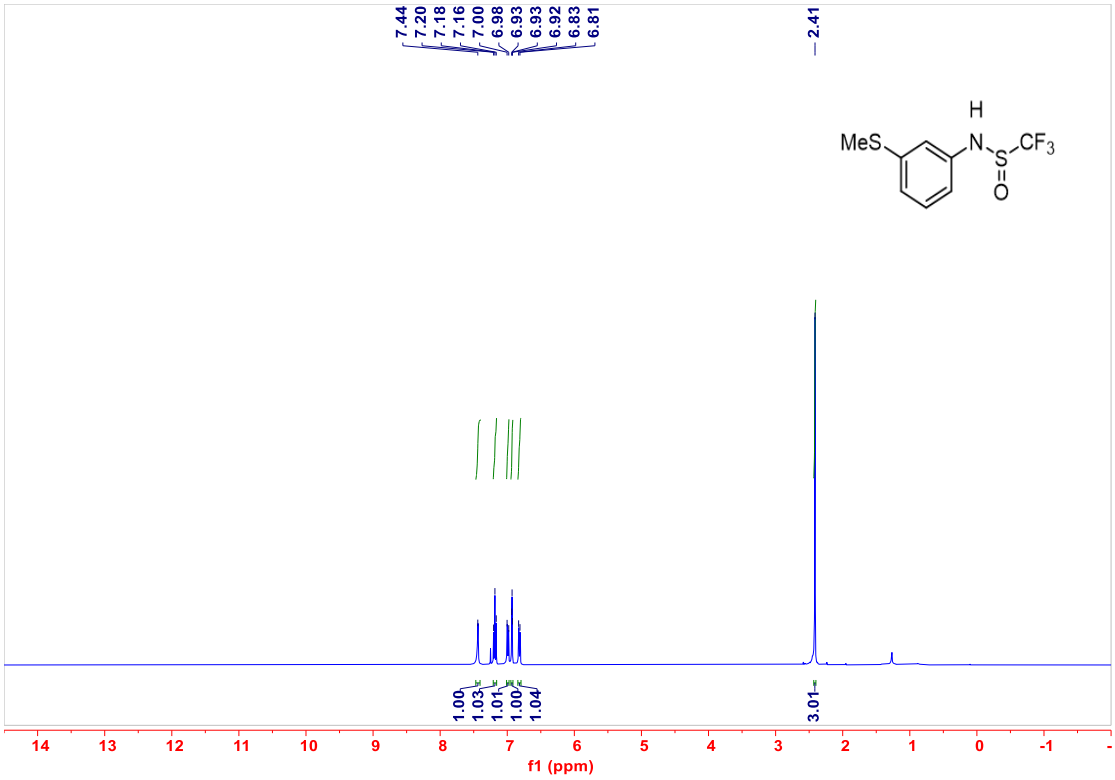

-77.6
H
N
S
CF3
O
O
nBu
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

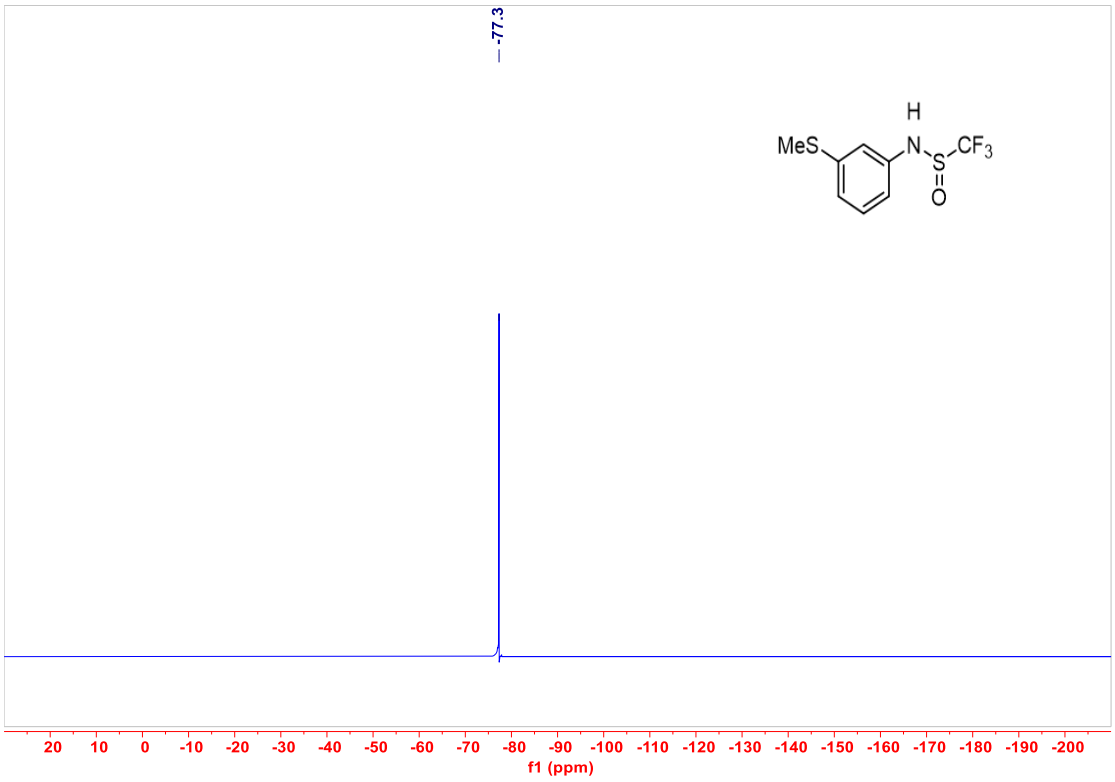

140.4
135.8
129.7
128.8
125.4
122.1
120.9
118.8
35.0
33.7
22.3
14.0
128.8
125.4
122.1
118.8
128 126 124 122 120 118
f1 (ppm)
H
N
S
CF3
O
nBu
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

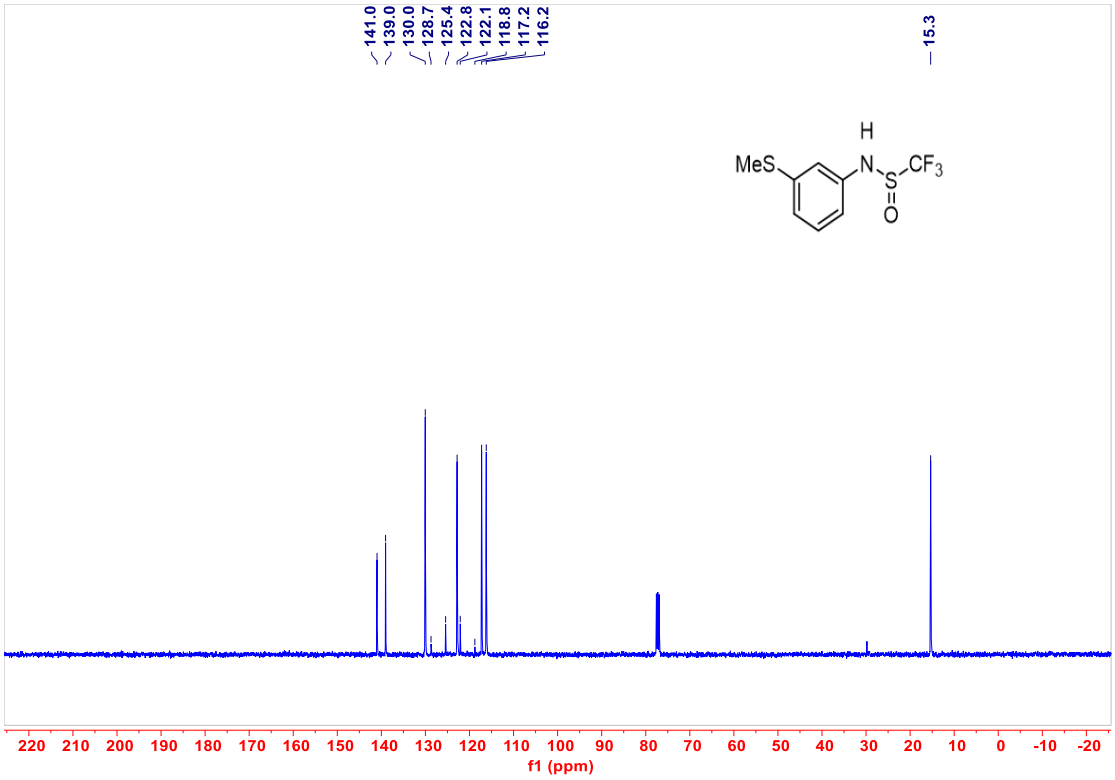

7.98
7.74
7.68
7.66
7.41
7.39
7.37
7.33
7.31
2.56
O
H
N
S
CF3
O
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

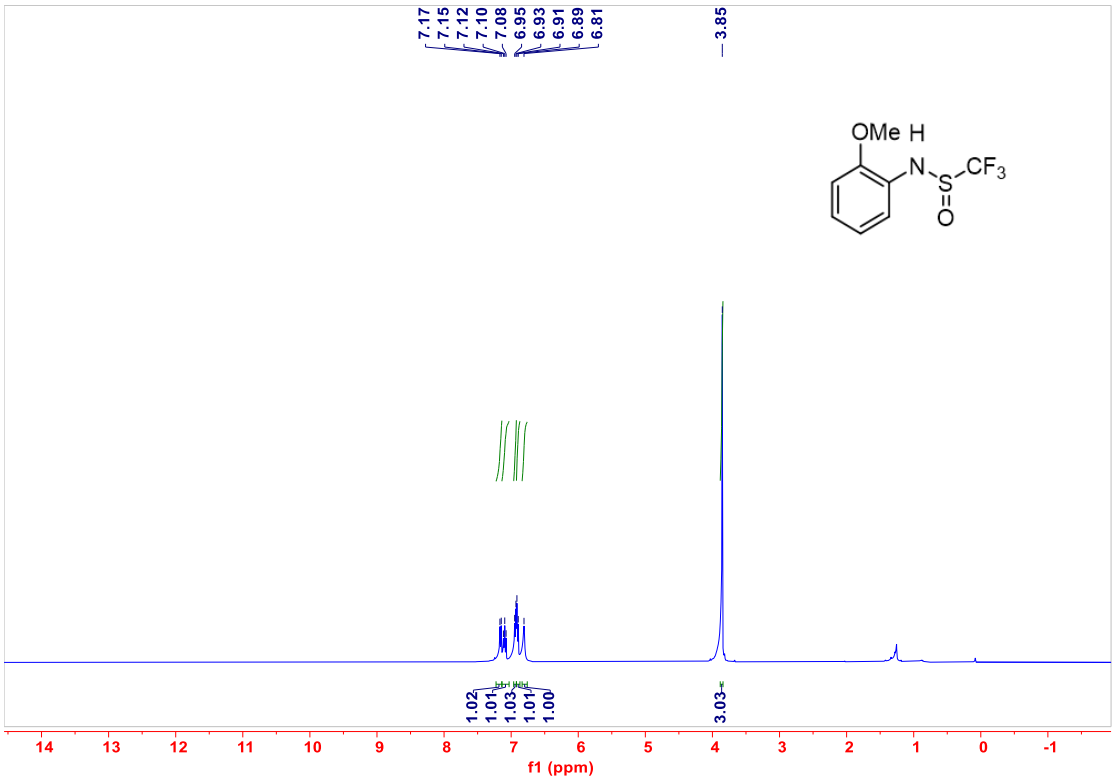

-77.1
O
H
N
S
CF3
O
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)

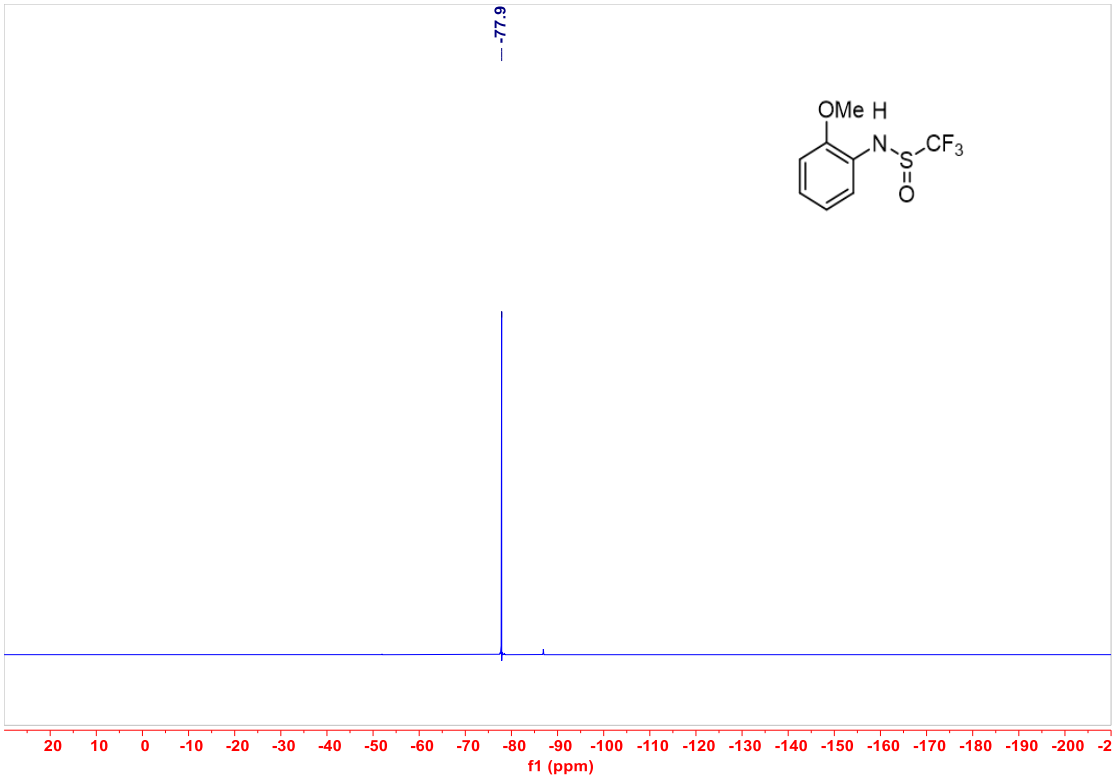

198.2
139.5
138.4
130.2
128.8
125.4
125.0
123.9
122.1
119.1
118.8
26.7
O
H
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.44
7.20
7.18
7.16
7.00
6.98
6.93
6.93
6.92
6.83
6.81
2.41
MeS
H
N
S
O
CF3
1.00
1.03
1.01
1.00
1.04
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.3
MeS
H
N
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


141.0
139.0
130.0
128.7
125.4
122.8
122.1
118.8
117.2
116.2
15.3
MeS
H
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.17
7.15
7.12
7.10
7.08
6.95
6.93
6.91
6.89
6.81
3.85
OMe H
N
S
CF3
O
1.02
1.01
1.03
1.01
1.00
3.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.9
OMe H
N
S
CF3
O
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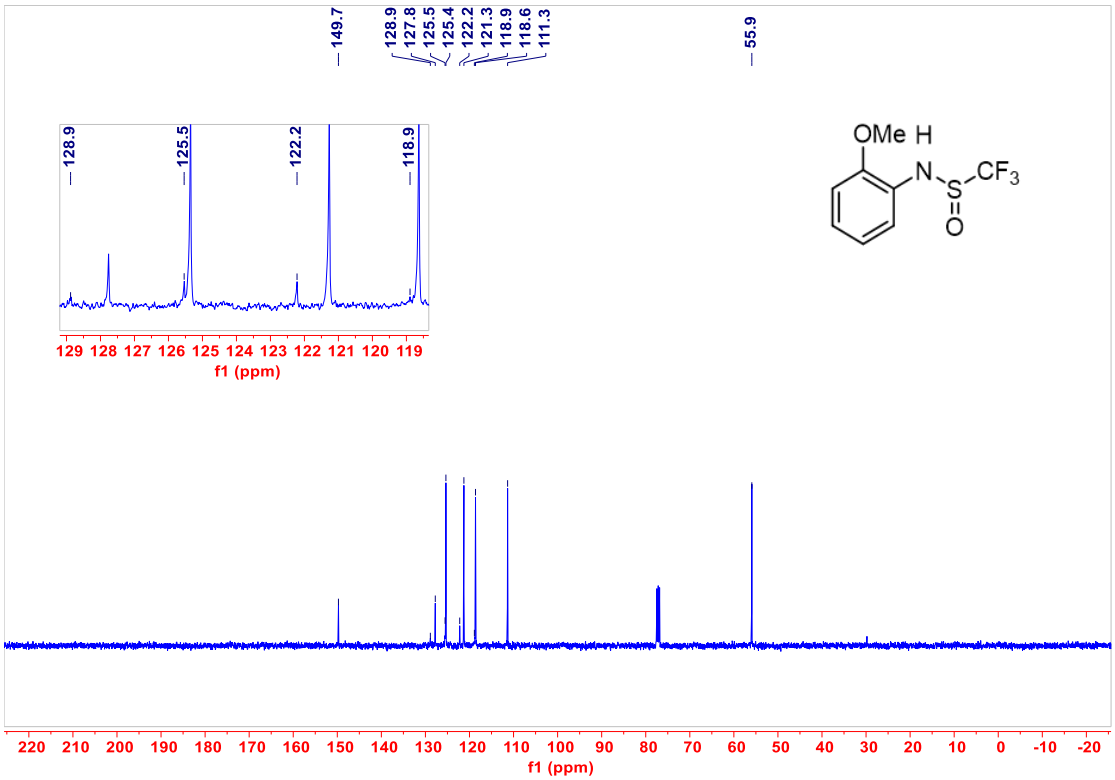
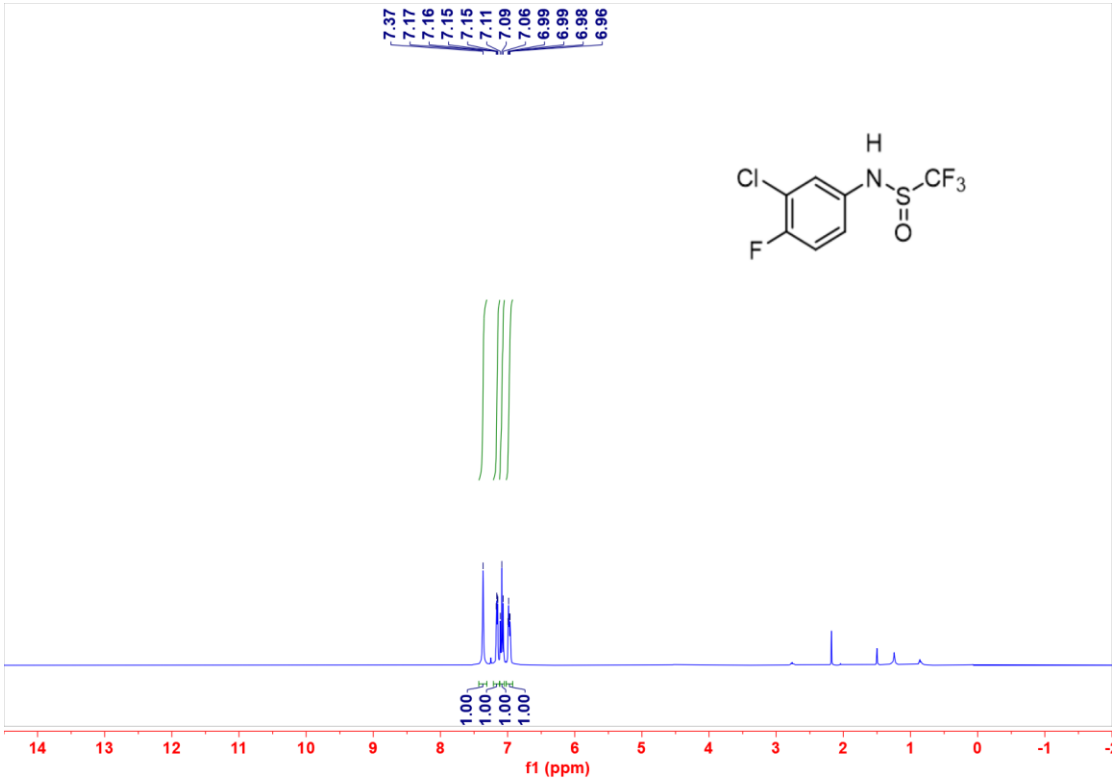
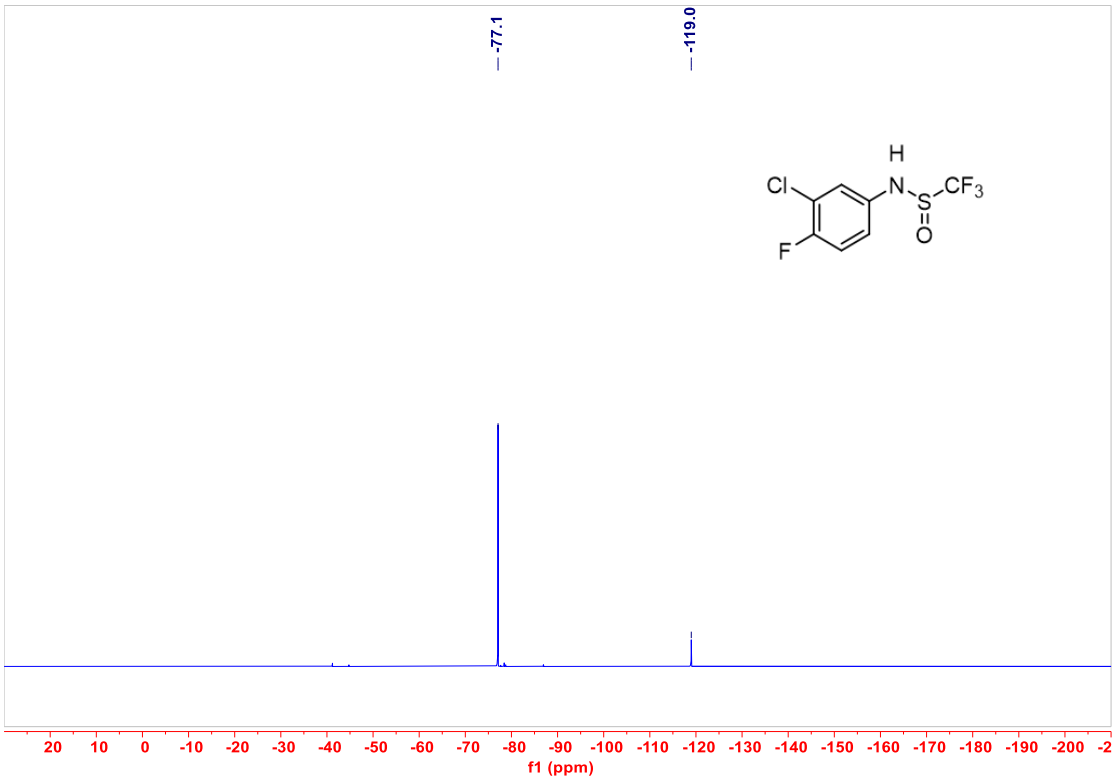
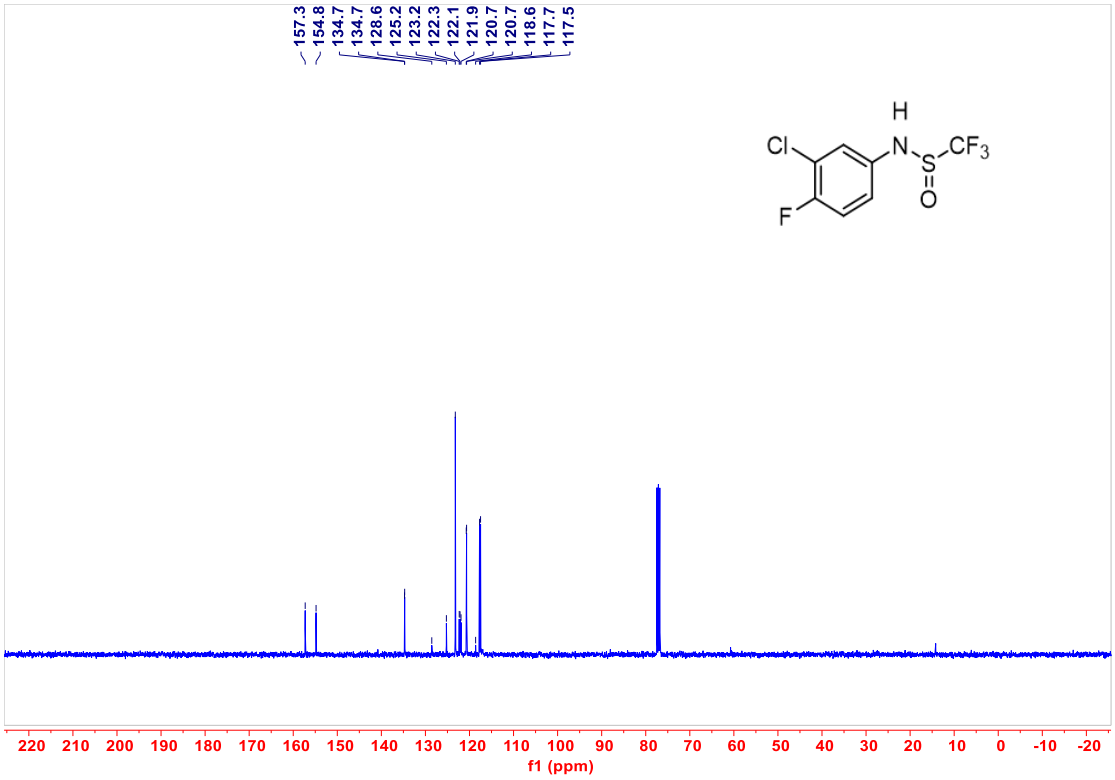
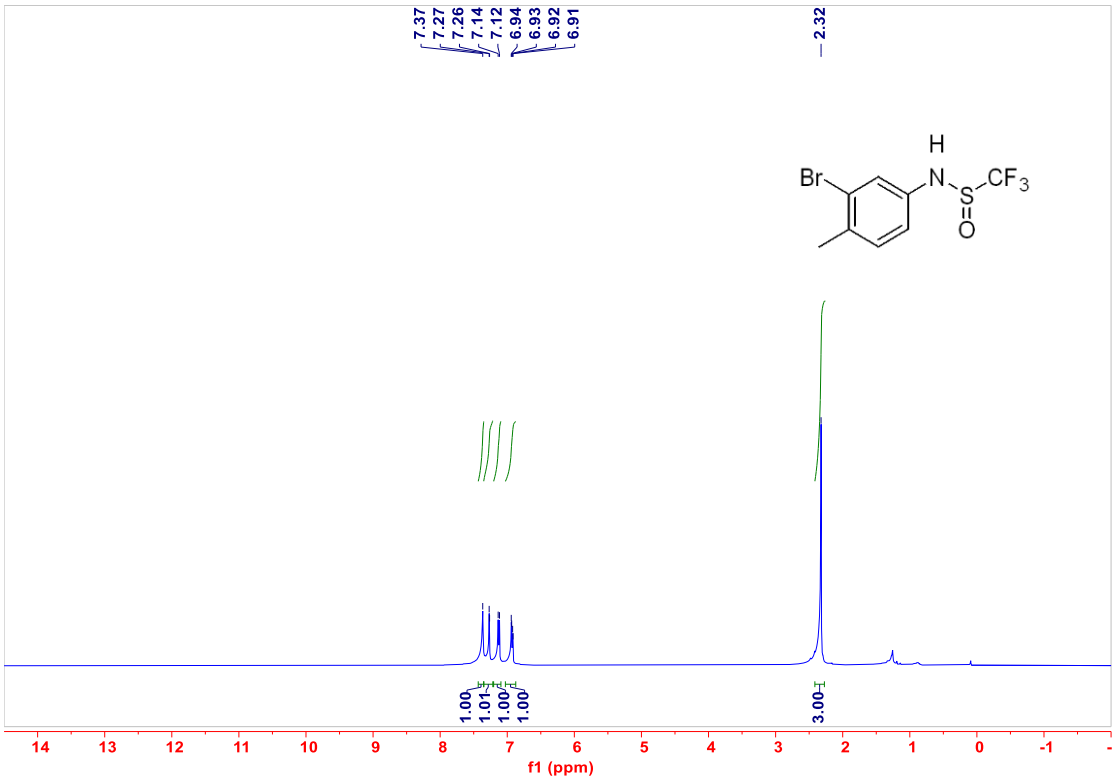
f1 (ppm)

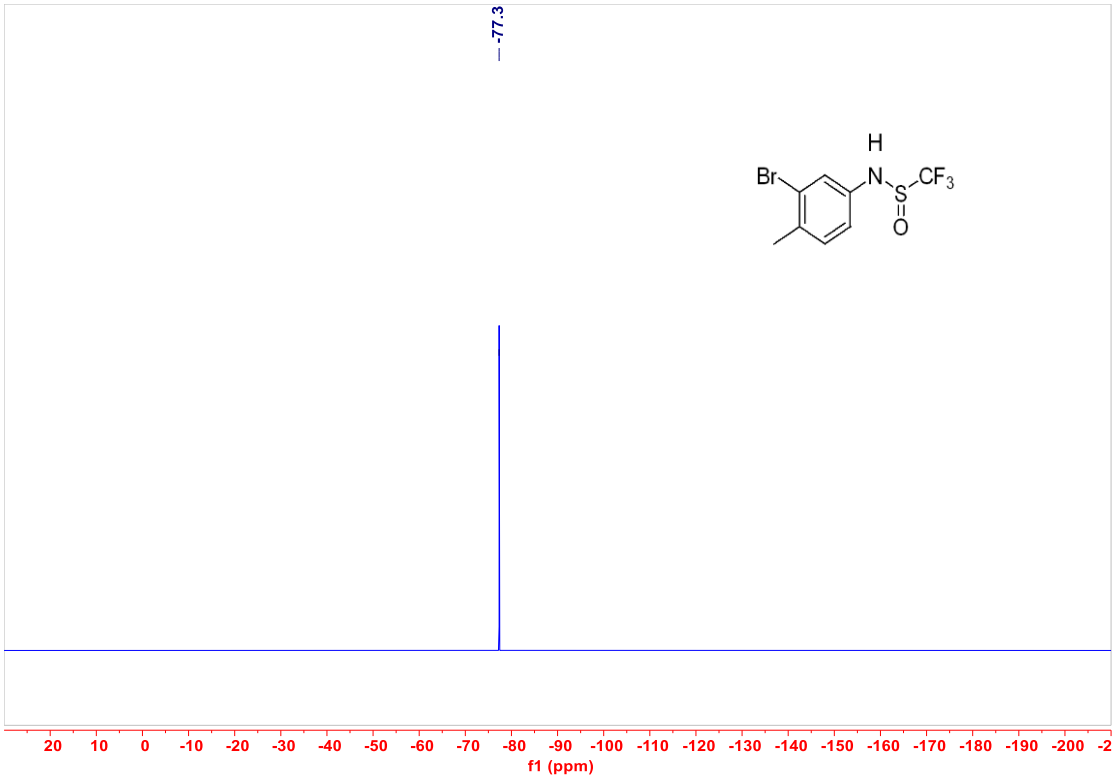

149.7
128.9
127.8
125.5
125.4
122.2
121.3
118.9
118.6
111.3
55.9
128.9
125.5
122.2
118.9
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
OMe H
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

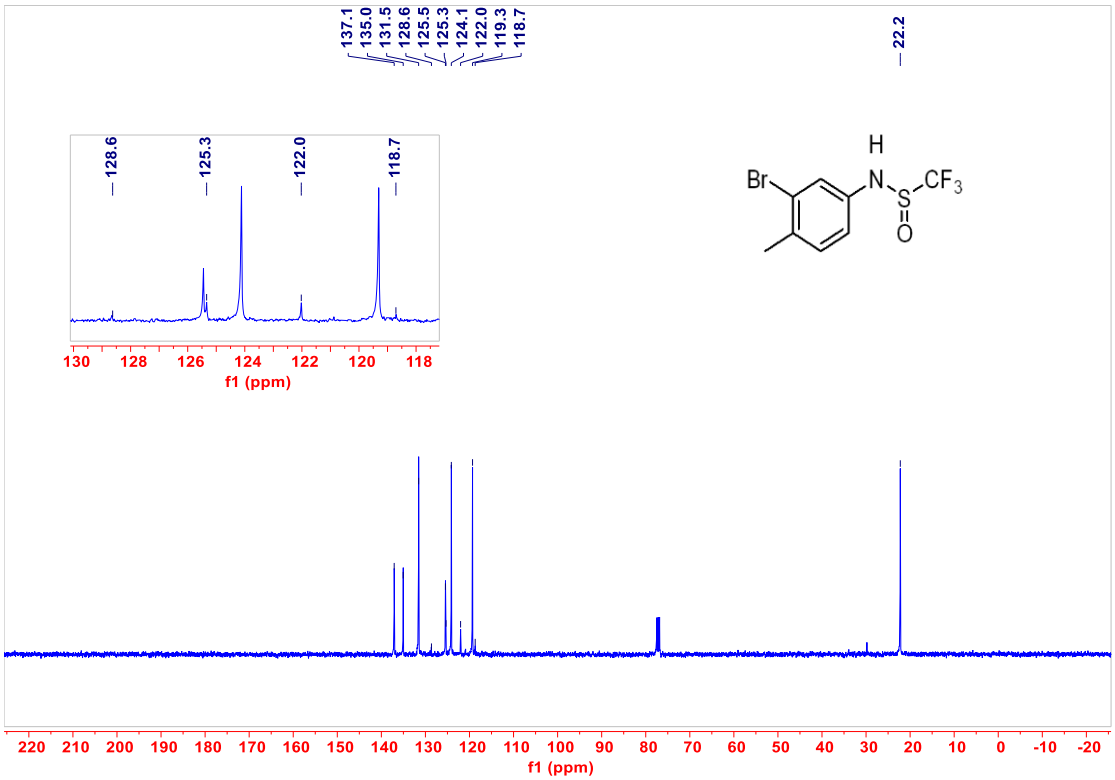

7.37
7.17
7.16
7.15
7.15
7.11
7.09
7.06
6.99
6.99
6.98
6.96
H
Cl
N
S
CF3
O
F
1.00
1.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

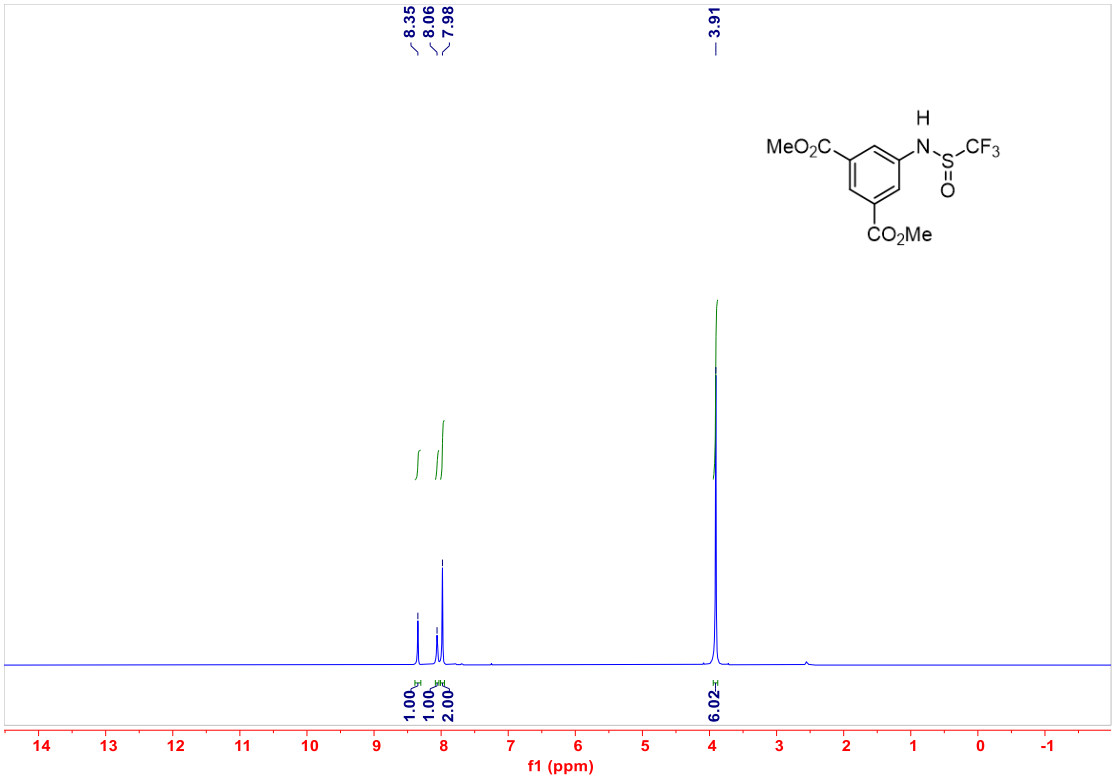

-77.1
-119.0
H
Cl
N
S
CF3
O
F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

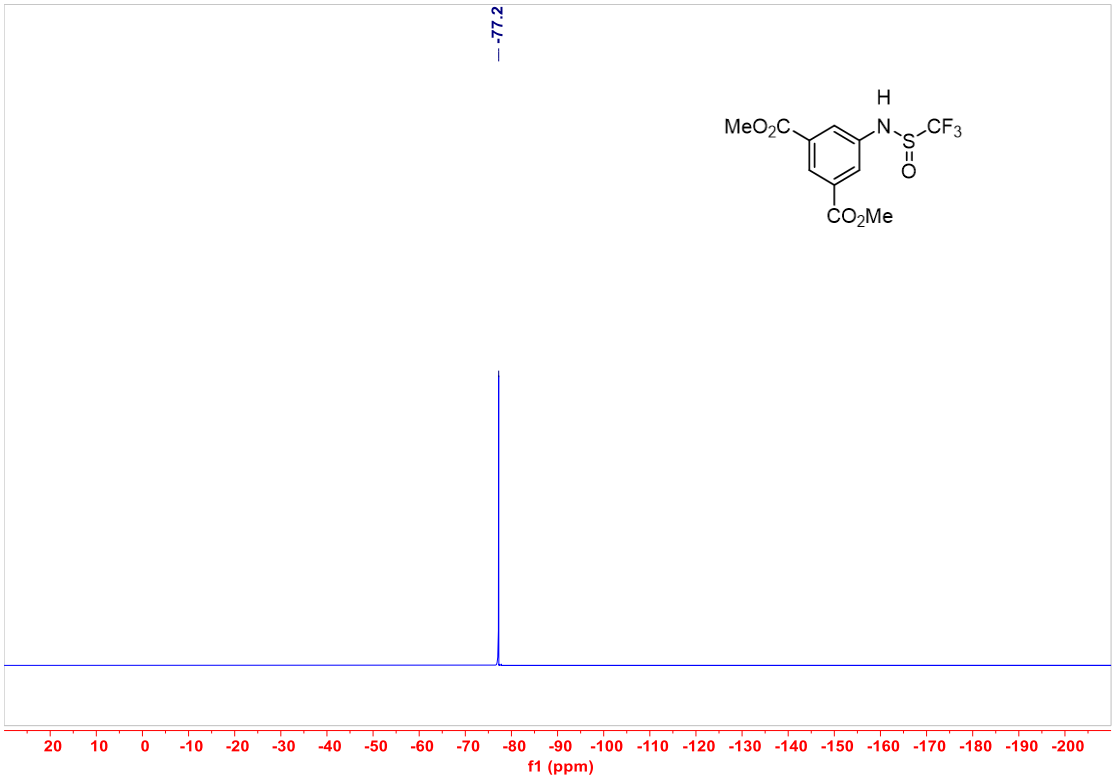

157.3
154.8
134.7
134.7
128.6
125.2
123.2
122.3
122.1
121.9
120.7
120.7
118.6
117.7
117.5
H
Cl
N
CF3
S
O
F
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.37
7.27
7.26
7.14
7.12
6.94
6.93
6.92
6.91
2.32
H
Br
N
CF3
S
O
1.00
1.01
1.00
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.3
H
Br
N
S
CF3
O
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


137.1
135.0
131.5
128.6
125.5
125.3
124.1
122.0
119.3
118.7
22.2
128.6
125.3
122.0
118.7
130 128 126 124 122 120 118
f1 (ppm)
H
Br
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.35
8.06
7.98
3.91
H
MeO2C
N
S
CF3
O
CO2Me
1.00
1.00
2.00
6.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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H
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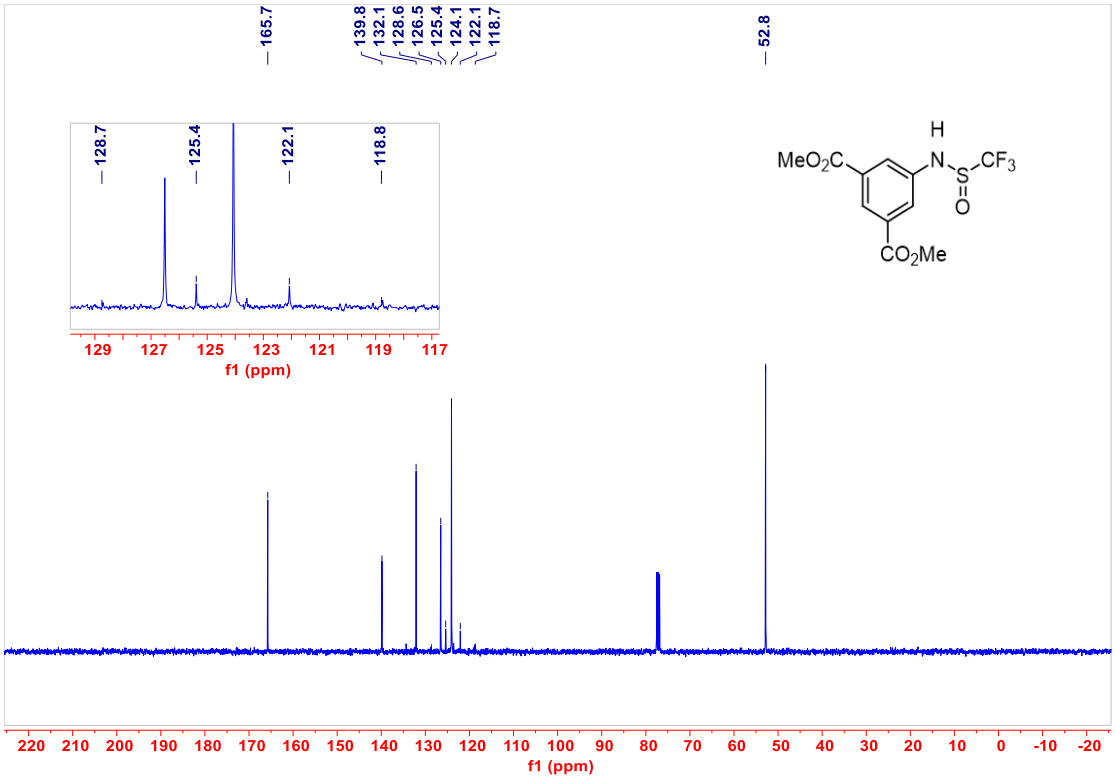
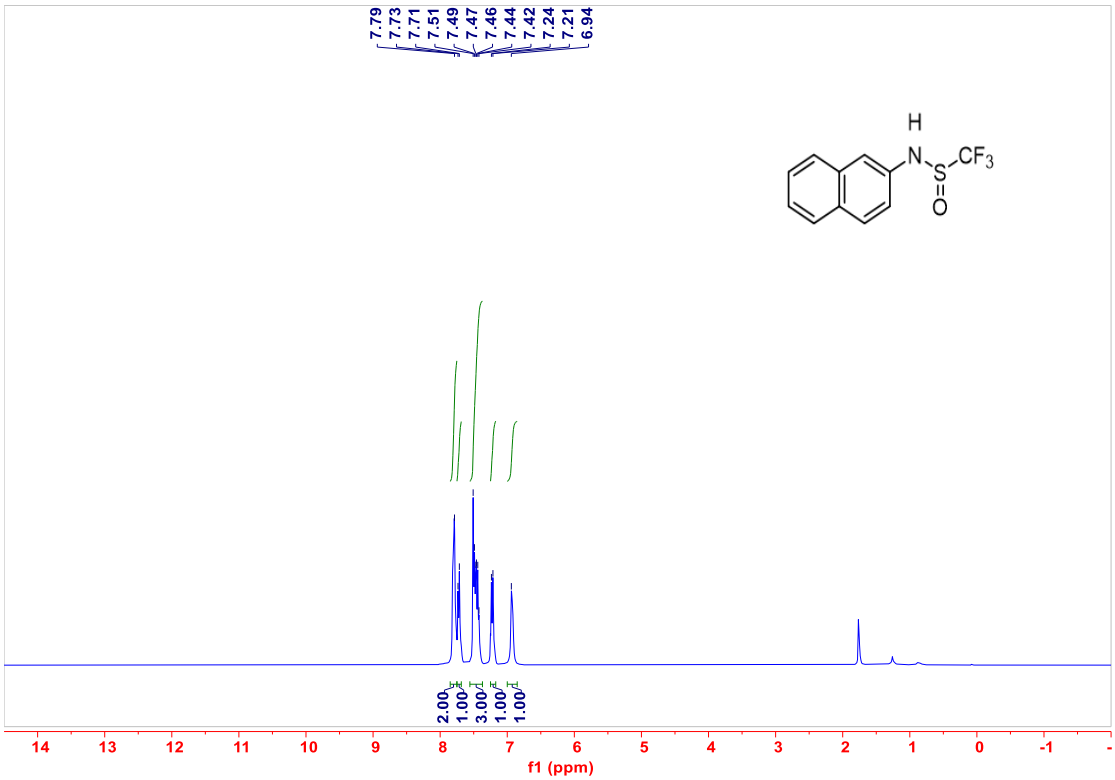
N
S
CF3
O
CO2Me
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


165.7
139.8
132.1
128.6
126.5
125.4
124.1
122.1
118.7
52.8
128.7
125.4
122.1
118.8
129 127 125 123 121 119 117
f1 (ppm)
MeO2C
H
N
S
CF3
O
CO2Me
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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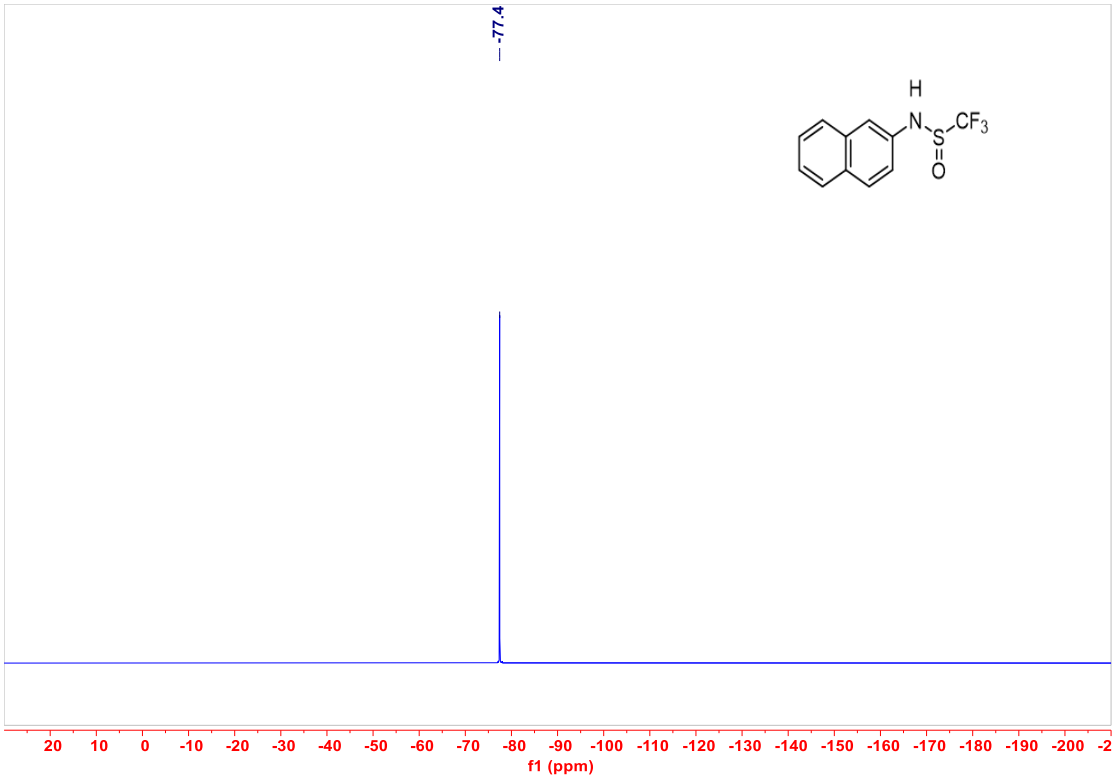
7.49
7.47
7.46
7.44
7.42
7.24
7.21
6.94
H
N
S
CF3
O
2.00
1.00
3.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.4
H
N
S
CF3
O
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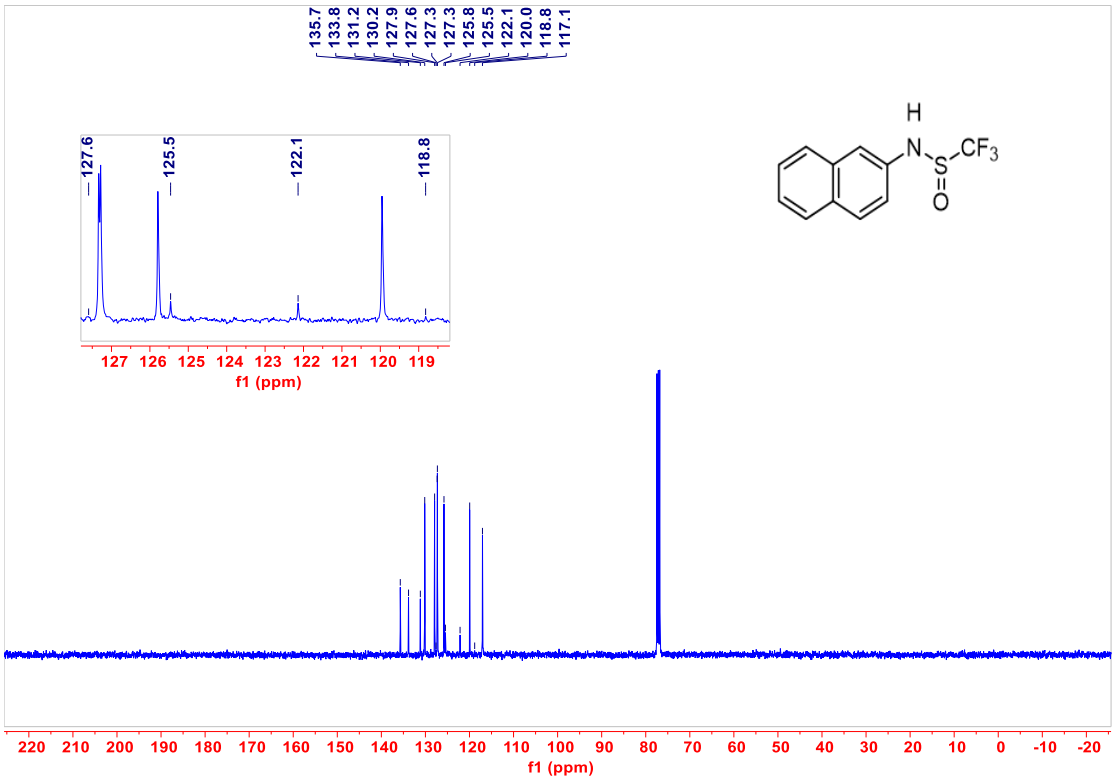
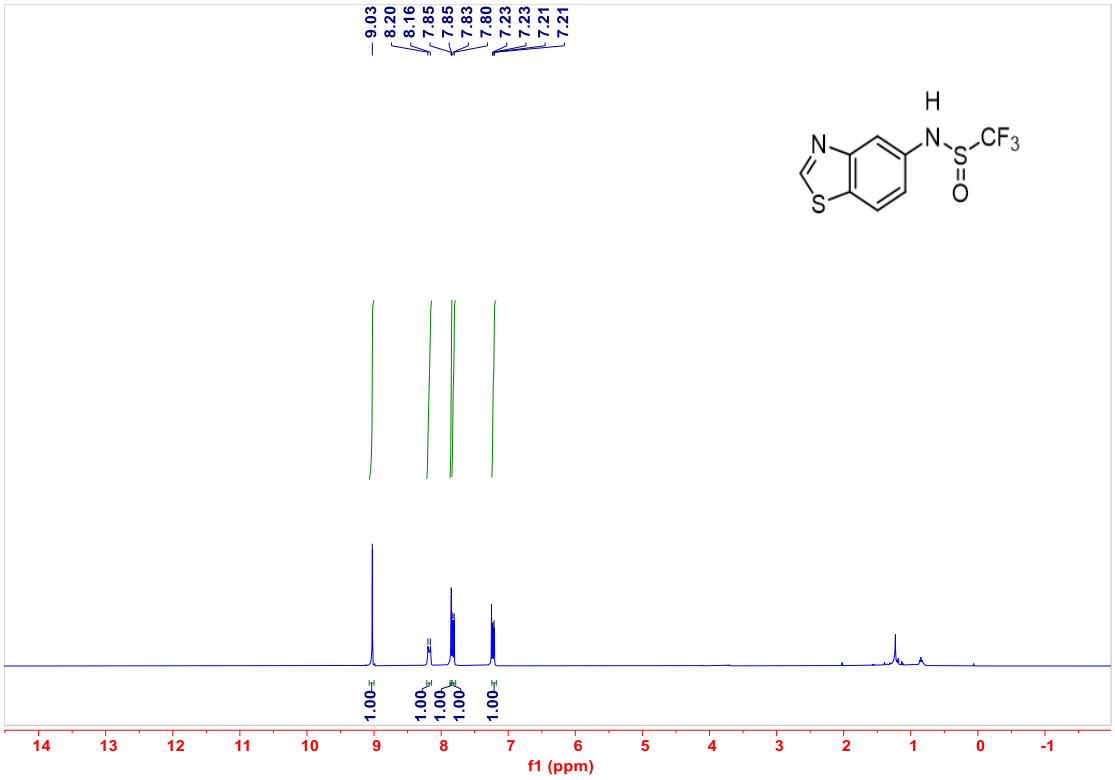
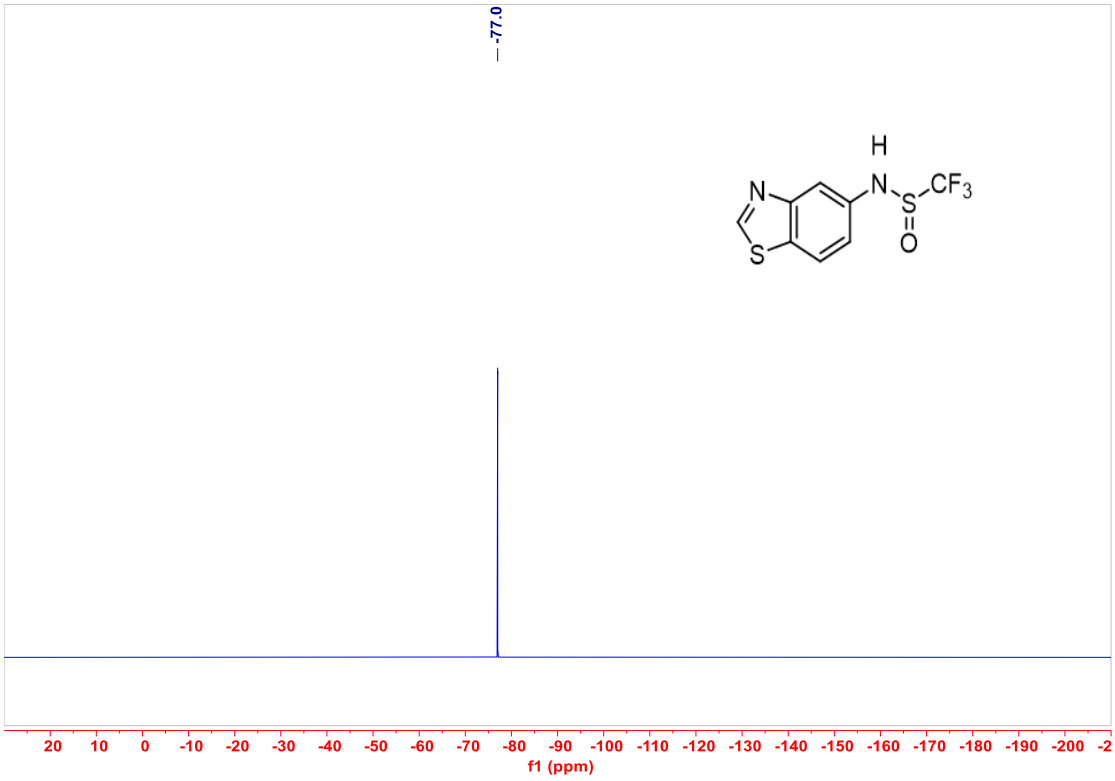
f1 (ppm)


135.7
133.8
131.2
130.2
127.9
127.6
127.3
127.3
125.8
125.5
122.1
120.0
118.8
117.1
127.6
125.5
122.1
118.8
127 126 125 124 123 122 121 120 119
f1 (ppm)
H
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.03
8.20
8.16
7.85
7.85
7.83
7.80
7.23
7.23
7.21
7.21
H
N
S
CF3
O
1.00
1.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.0
H
N
S
CF3
O
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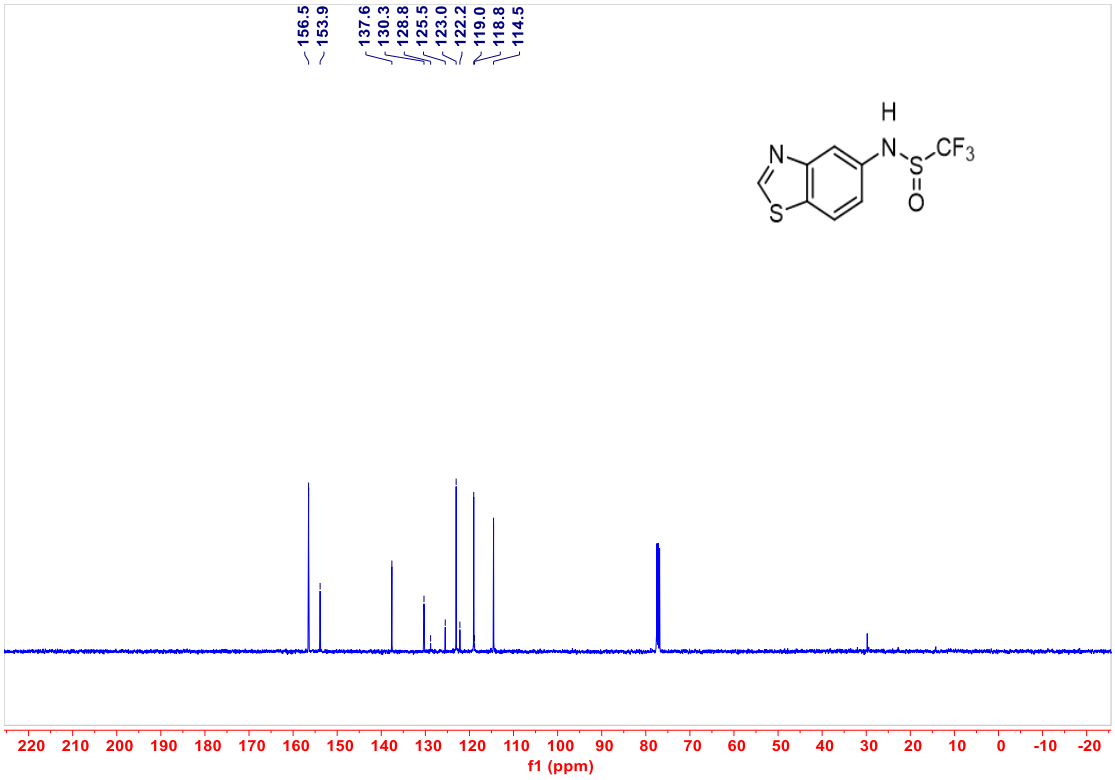
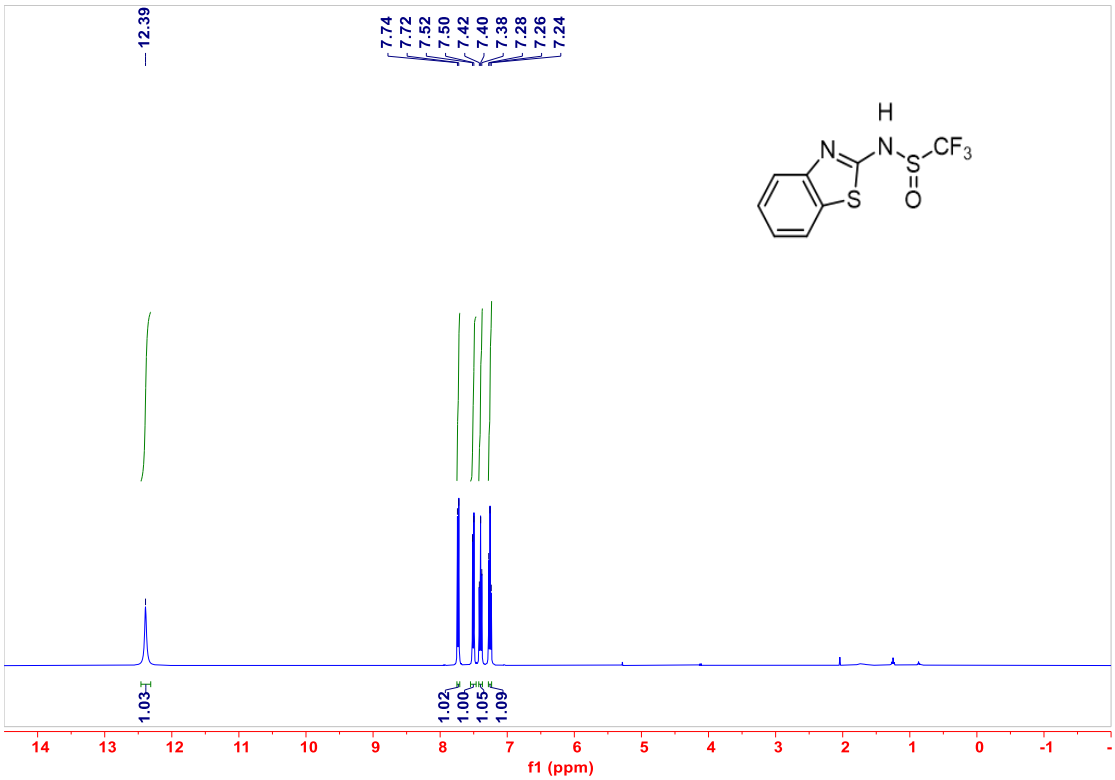
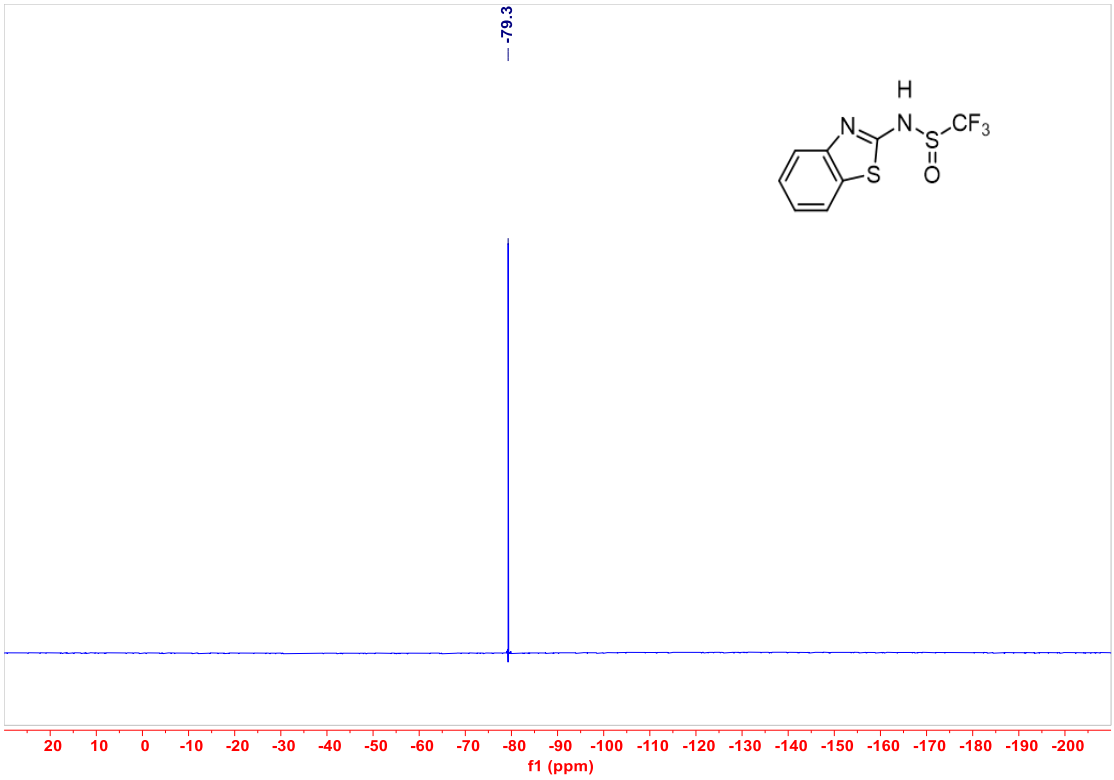
f1 (ppm)


156.5
153.9
137.6
130.3
128.8
125.5
123.0
122.2
119.0
118.8
114.5
H
N
S
CF3
O
N
S
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


12.39
7.74
7.72
7.52
7.50
7.42
7.40
7.38
7.28
7.26
7.24
H
N
S
CF3
O
N
S
1.03
1.02
1.00
1.05
1.09
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
S
CF3
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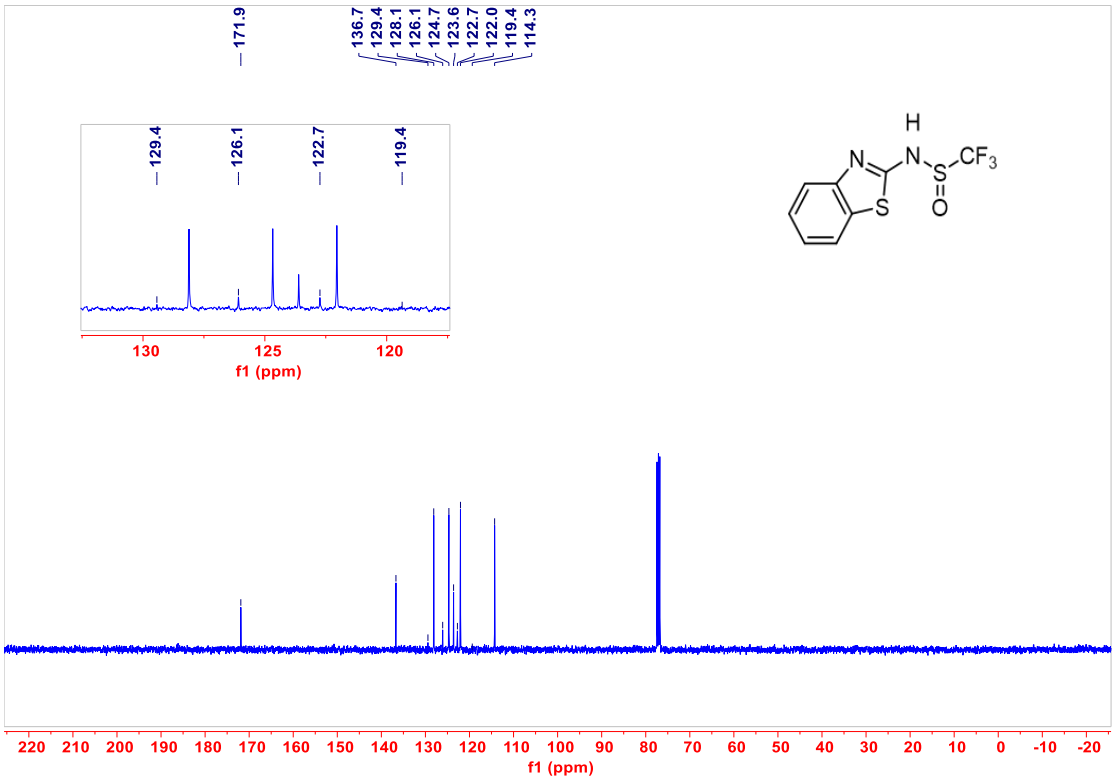
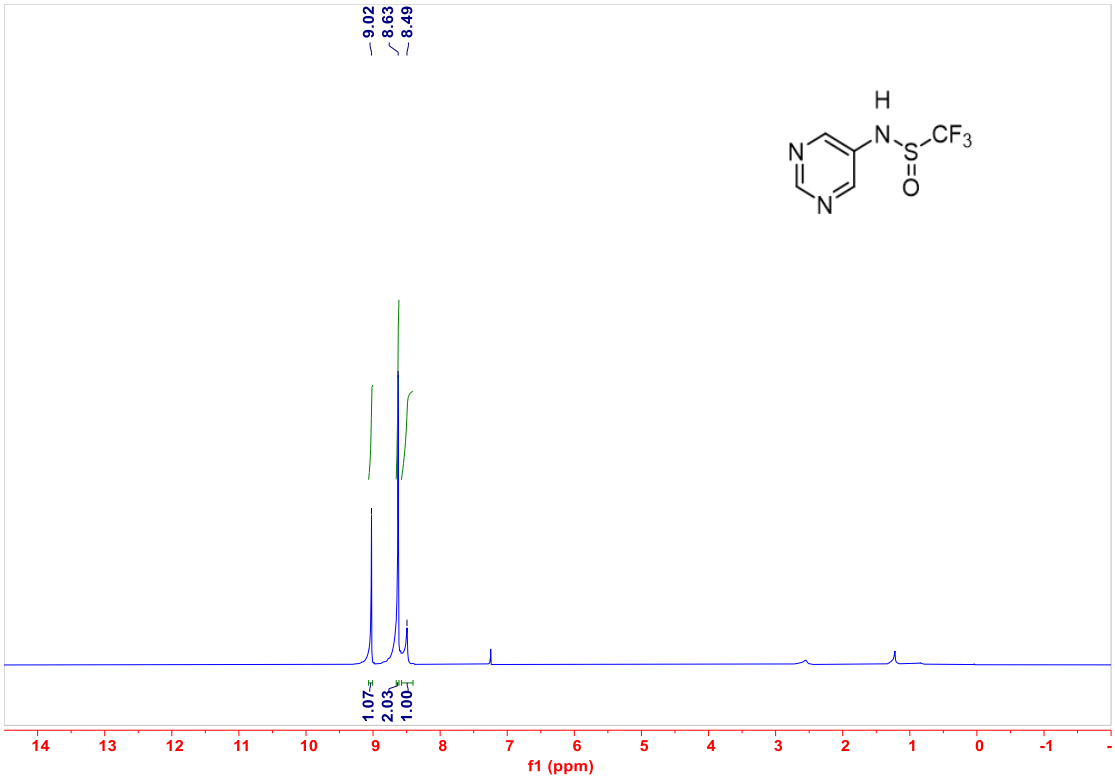
f1 (ppm)


171.9
136.7
129.4
128.1
126.1
124.7
123.6
122.7
122.0
119.4
114.3
129.4
126.1
122.7
119.4
130 125 120
f1 (ppm)
H
N
N
S
CF3
O
S
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.02
8.63
8.49
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CF3
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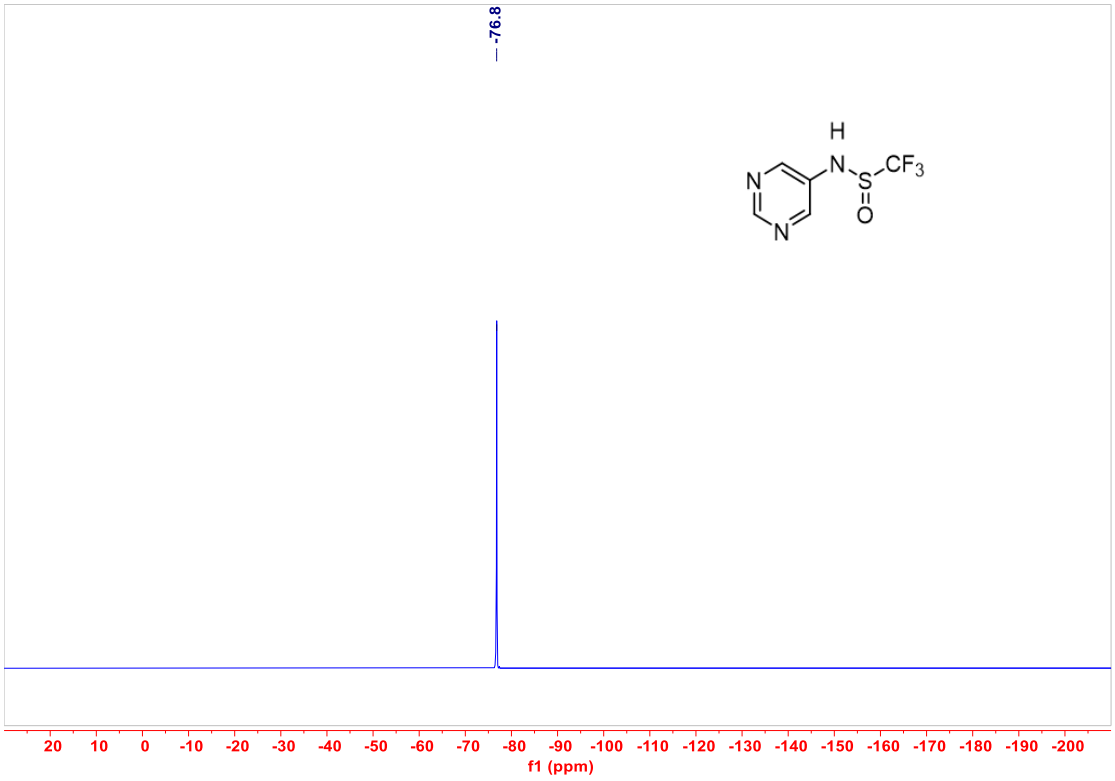
N
N
1.07
2.03
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
CF3
S
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N
N
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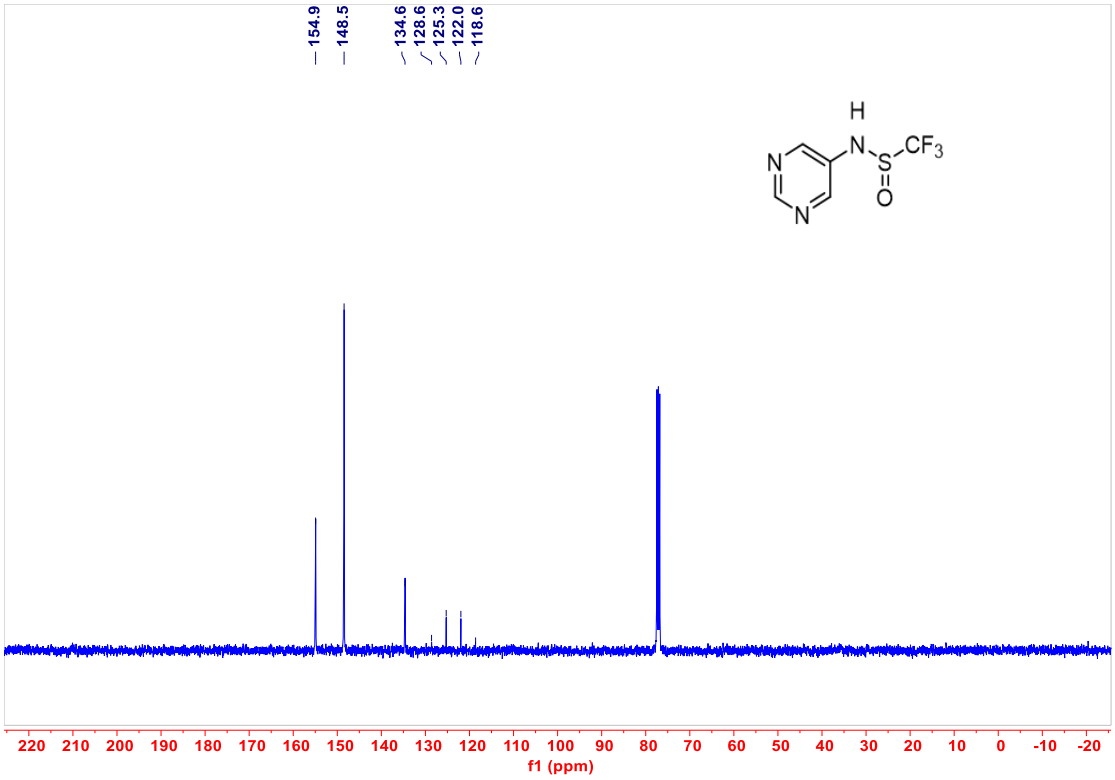
f1 (ppm)


154.9
148.5
134.6
128.6
125.3
122.0
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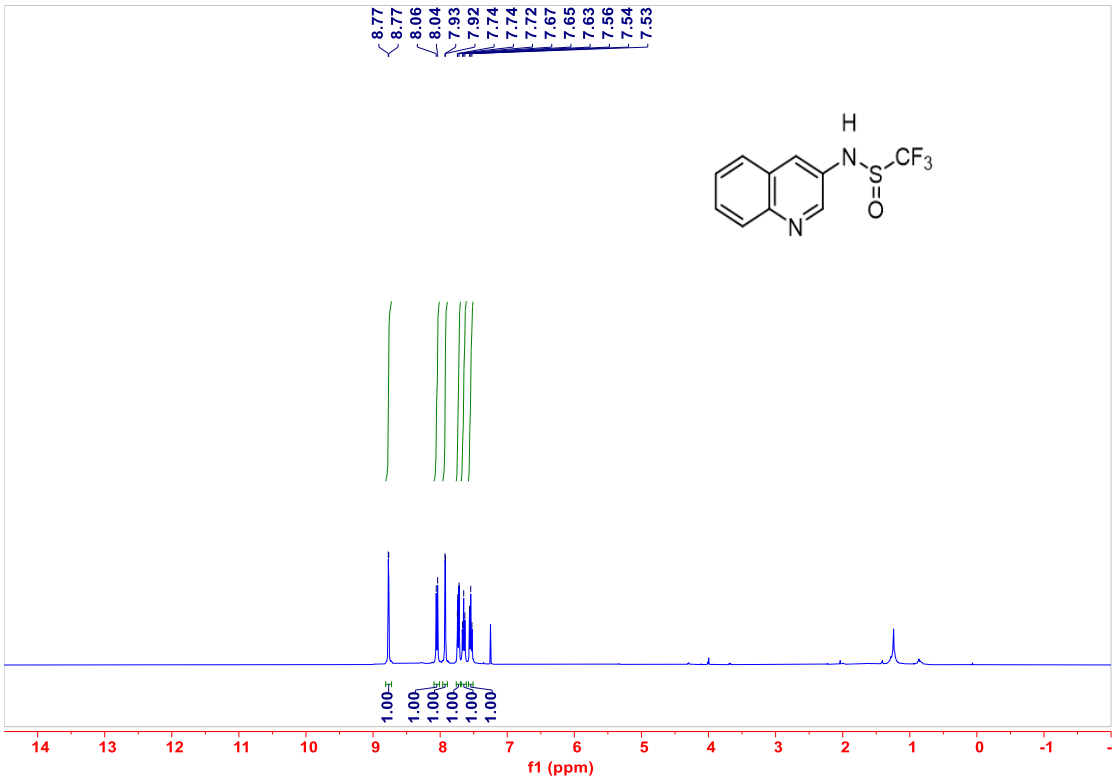
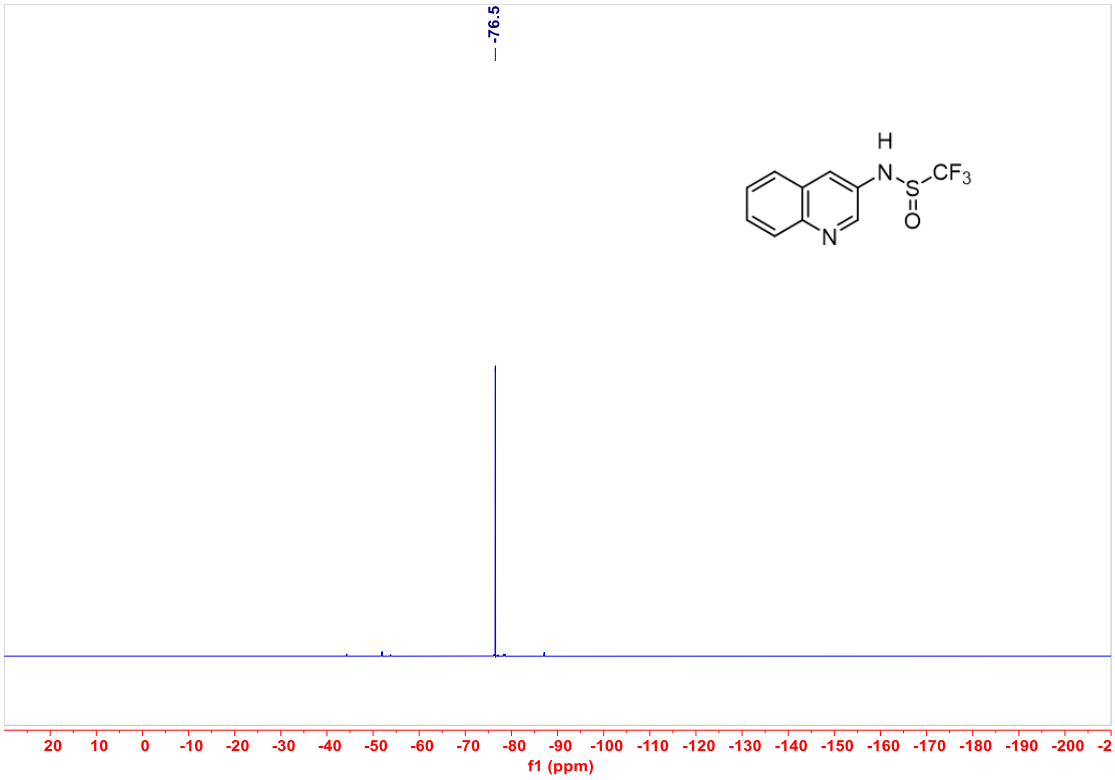
H
N
S
CF3
O
N
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.77
8.77
8.06
8.04
7.93
7.92
7.74
7.74
7.72
7.67
7.65
7.63
7.56
7.54
7.53
H
N
S
CF3
O
N
1.00
1.00
1.00
1.00
1.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-76.5
H
N
S
CF3
O
N
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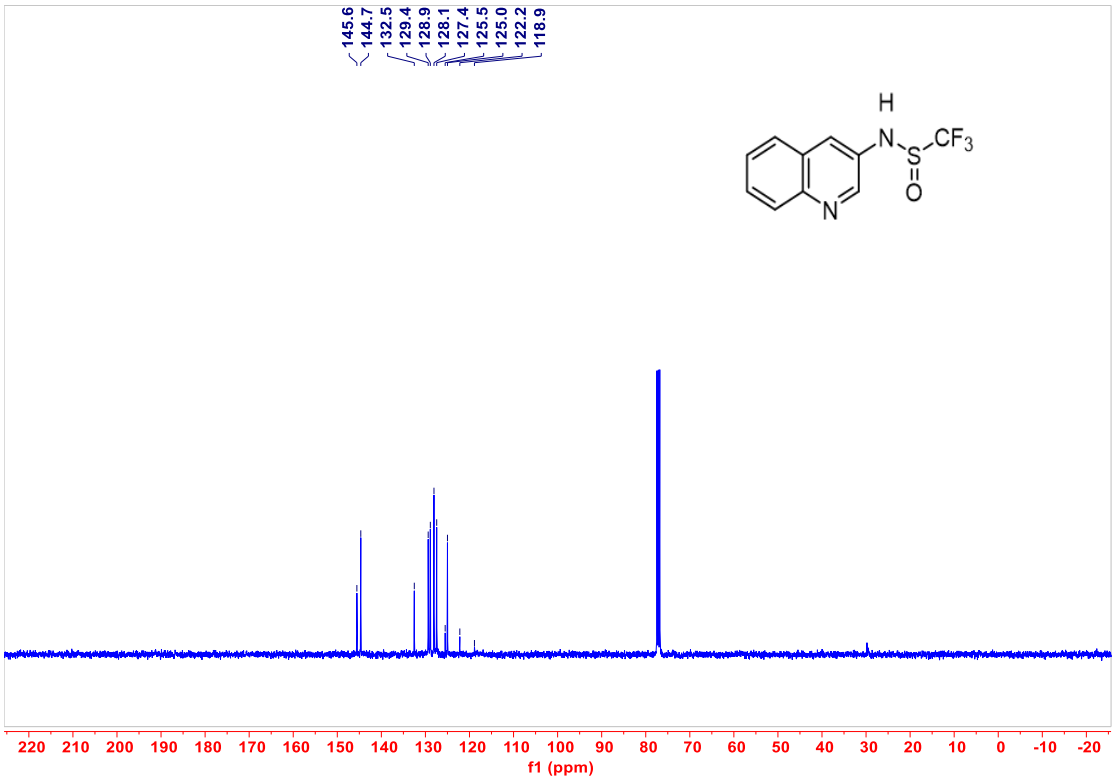
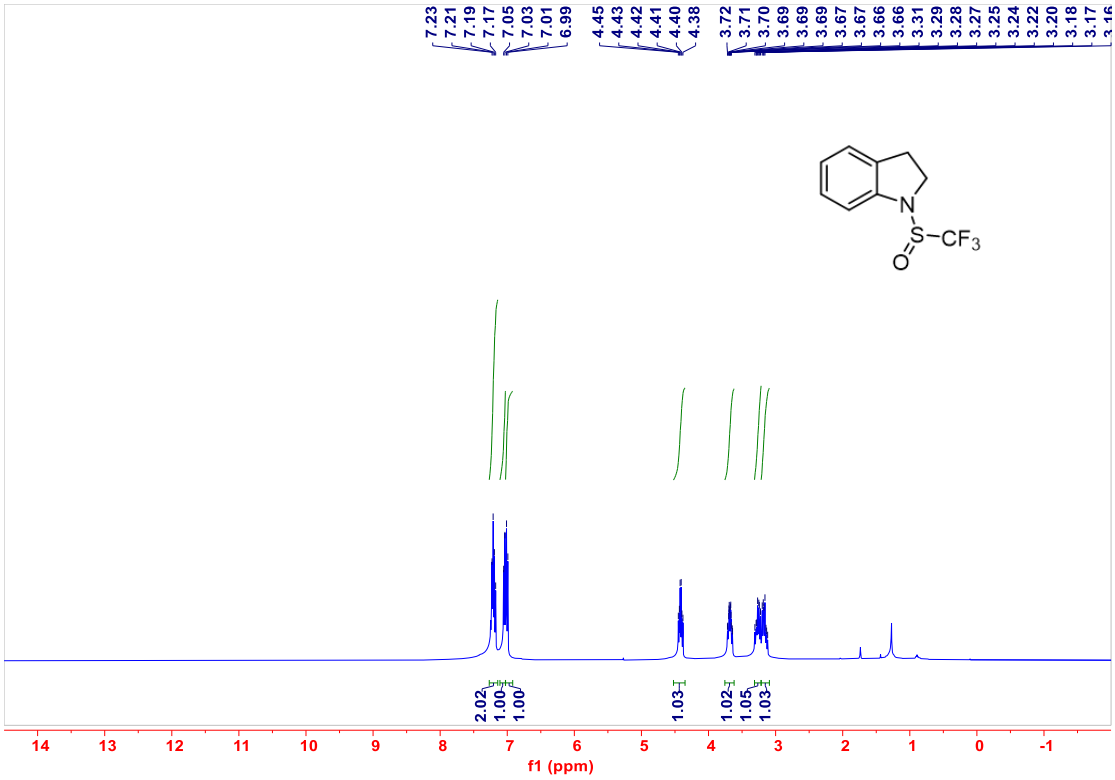
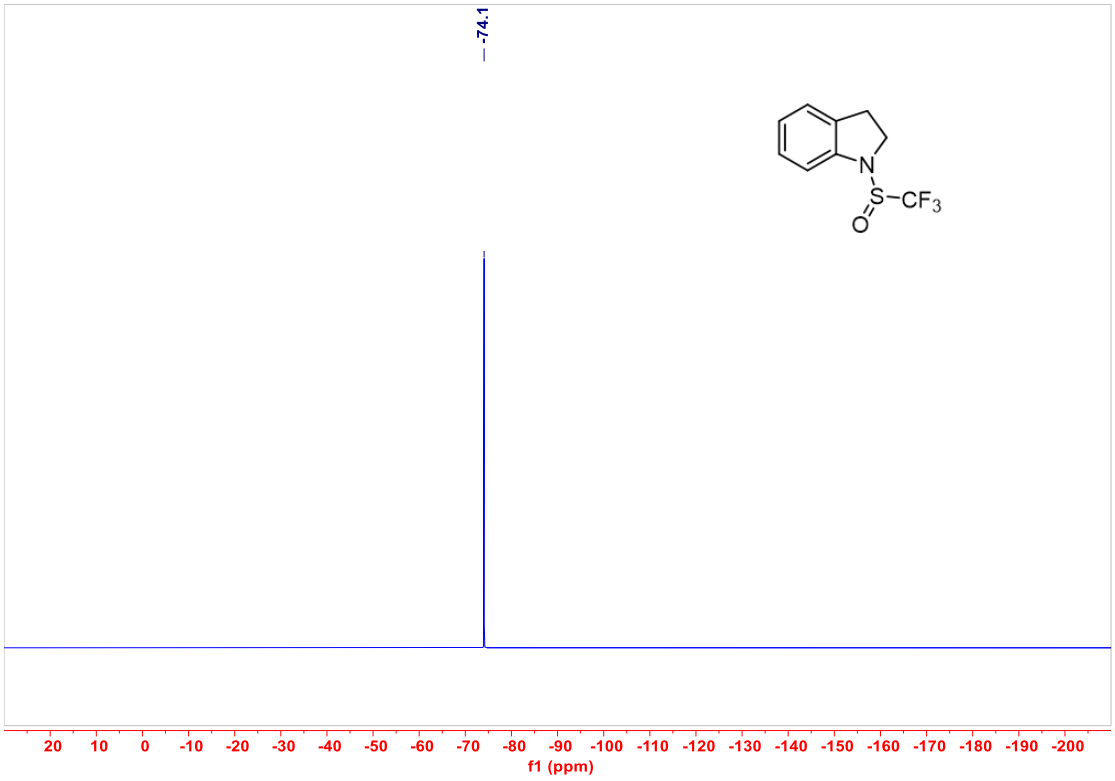
f1 (ppm)


145.6
144.7
132.5
129.4
128.9
128.1
127.4
125.5
125.0
122.2
118.9
H
N
S
CF3
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.23
7.21
7.19
7.17
7.05
7.03
7.01
6.99
4.45
4.43
4.42
4.41
4.40
4.38
3.72
3.71
3.70
3.69
3.69
3.67
3.67
3.66
3.66
3.31
3.29
3.28
3.27
3.25
3.24
3.22
3.20
3.18
3.17
N
S
CF3
O
2.02
1.00
1.00
1.03
1.02
1.05
1.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-74.1
N
S
CF3
O
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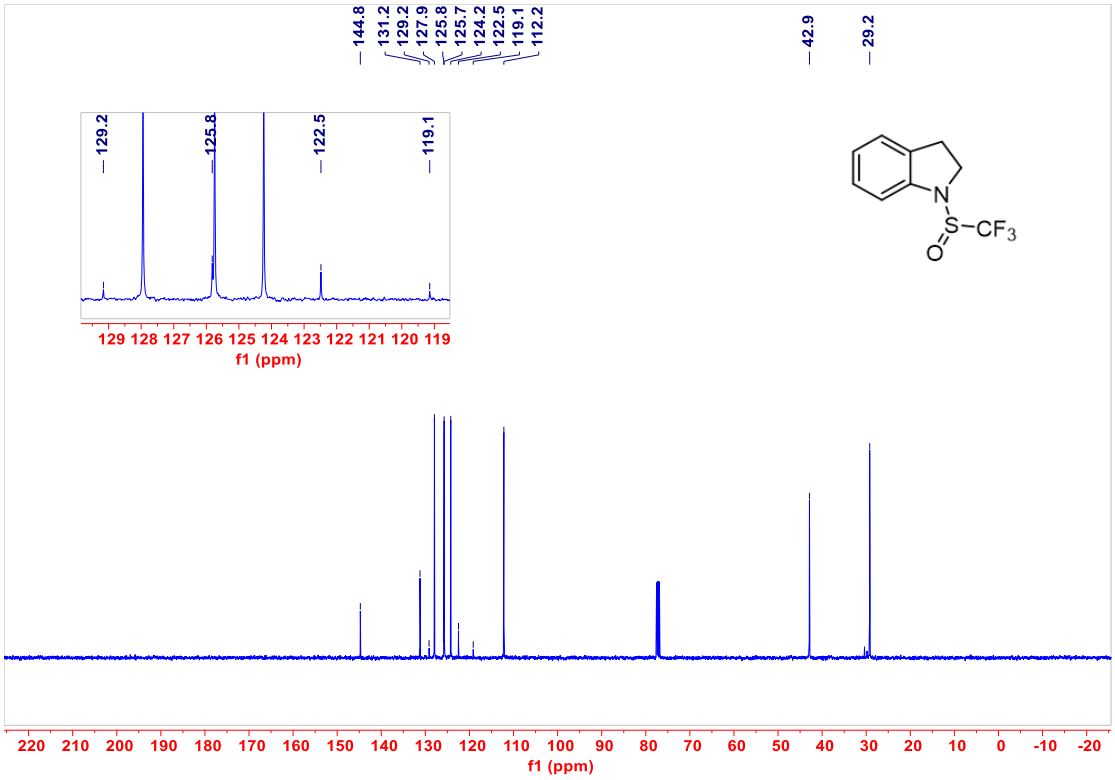
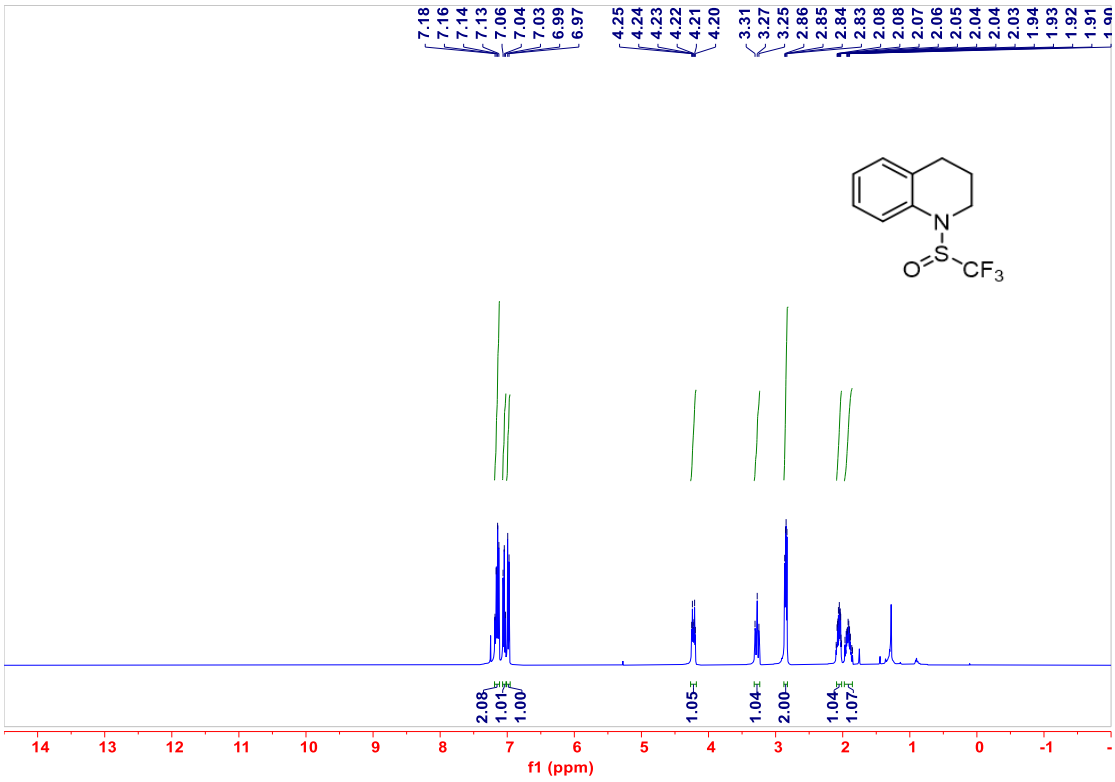
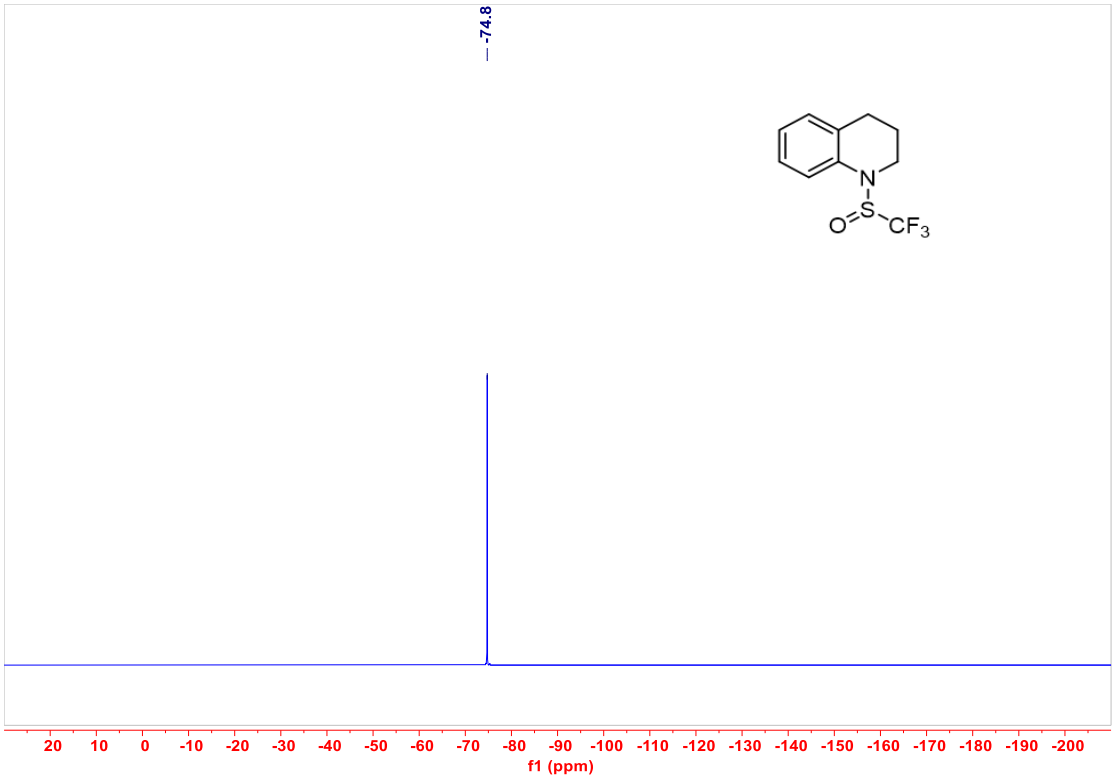
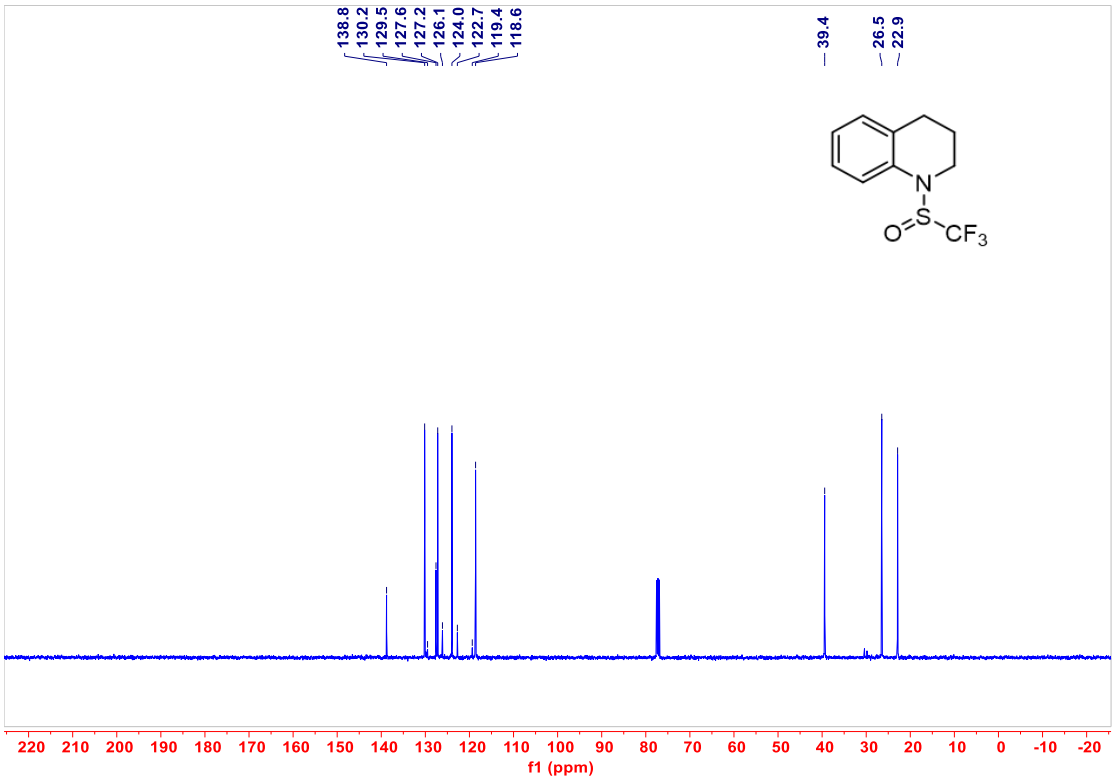
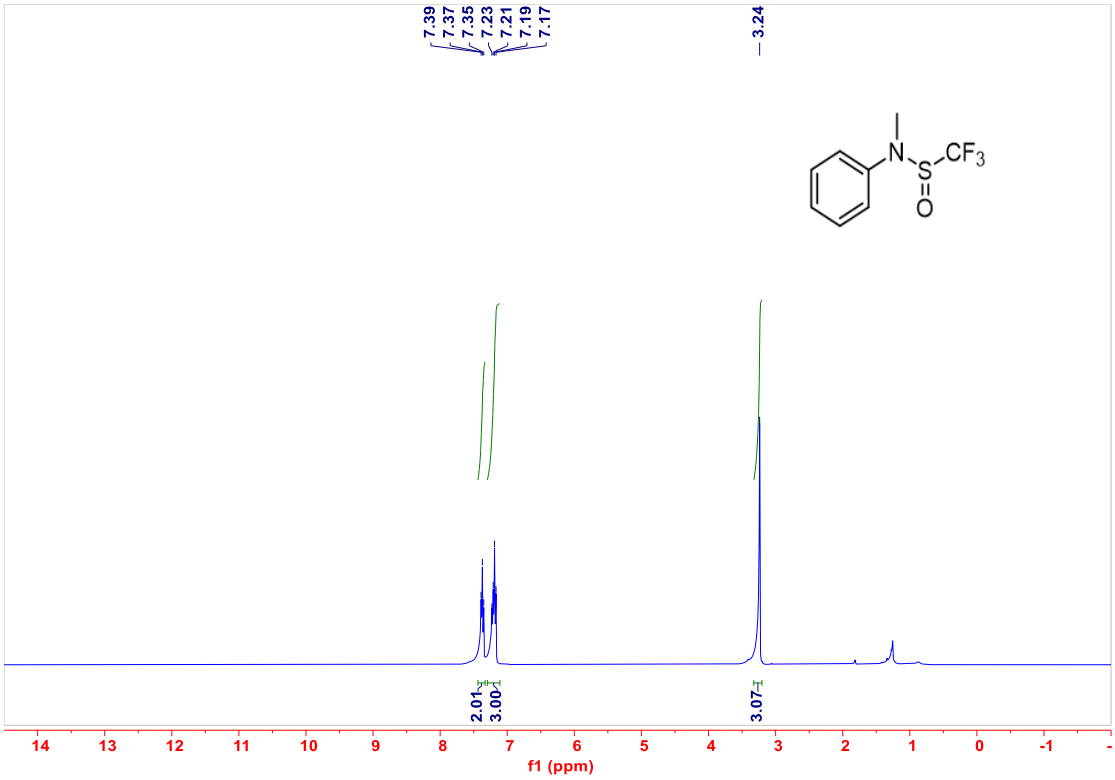
f1 (ppm)

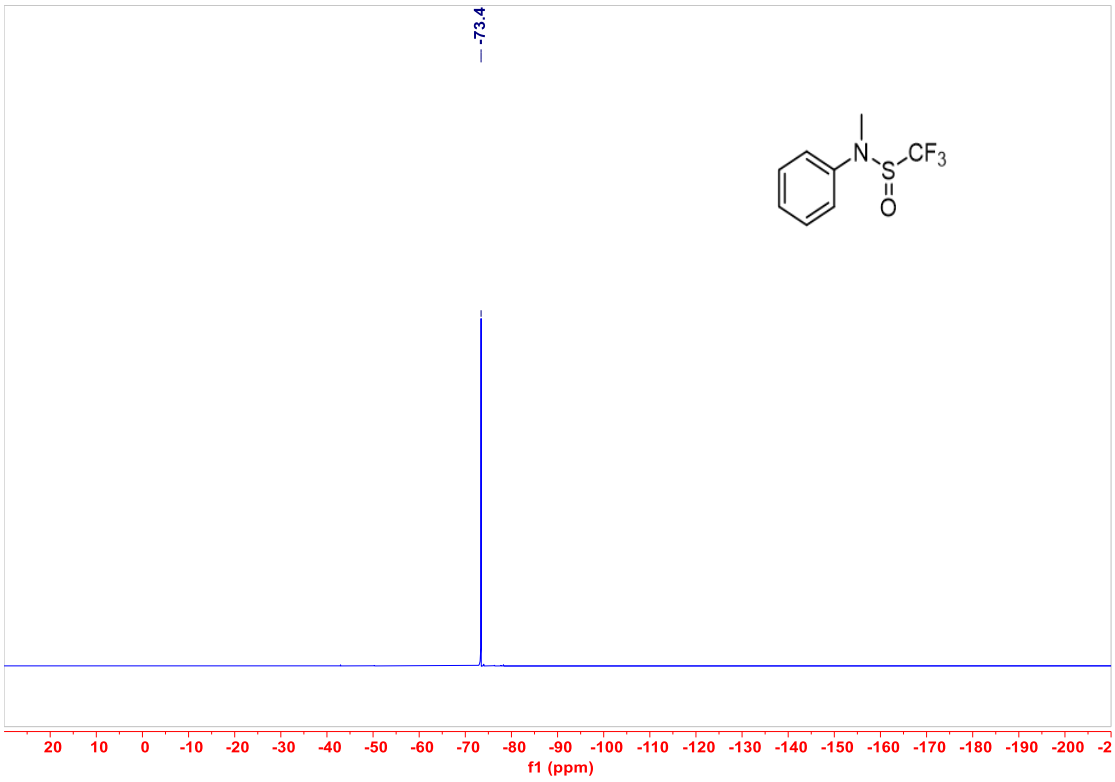

144.8
131.2
129.2
127.9
125.8
125.7
124.2
122.5
119.1
112.2
42.9
29.2
129.2
125.8
122.5
119.1
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.18
7.16
7.14
7.13
7.06
7.04
7.03
6.99
6.97
4.25
4.24
4.23
4.22
4.21
4.20
3.31
3.27
3.25
2.86
2.85
2.84
2.83
2.08
2.08
2.07
2.06
2.05
2.04
2.04
2.03
1.94
1.93
1.92
1.91
N
S
CF3
O
2.08
1.01
1.00
1.05
1.04
2.00
1.04
1.07
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-74.8
N
O
S
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


138.8
130.2
129.5
127.6
127.2
126.1
124.0
122.7
119.4
118.6
39.4
26.5
22.9
N
O
S
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.39
7.37
7.35
7.23
7.21
7.19
7.17
3.24
N
S
CF3
O
2.01
3.00
3.07
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
S
CF3
O
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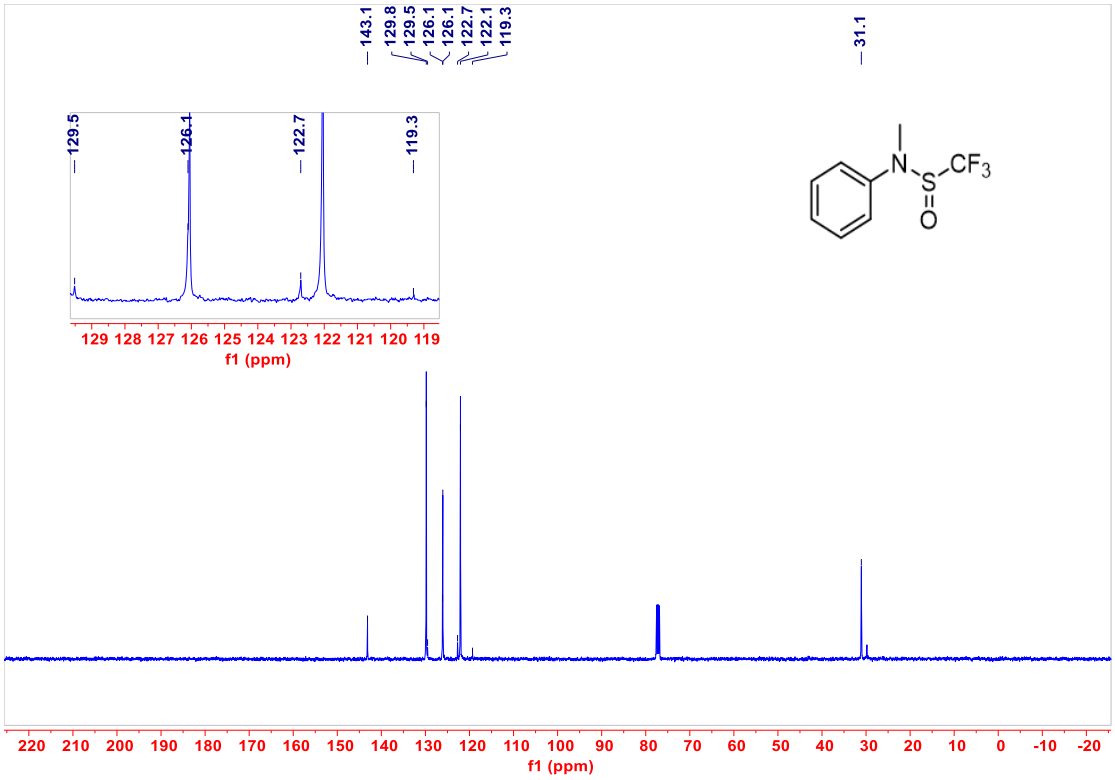
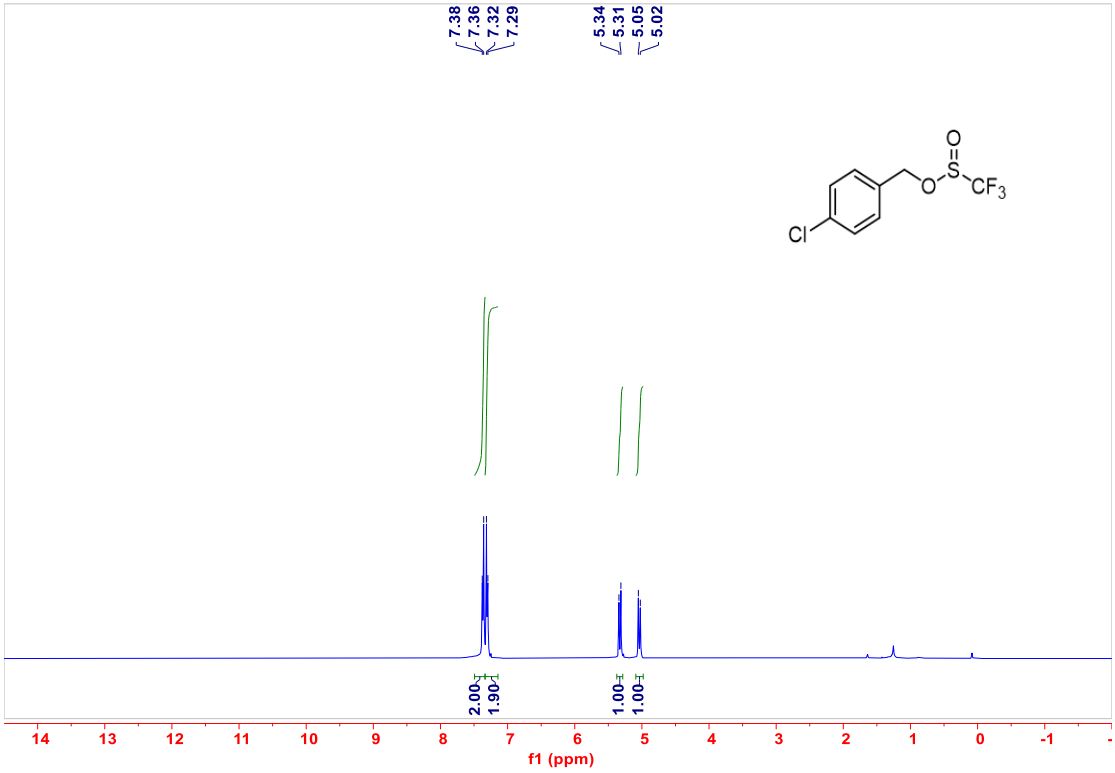
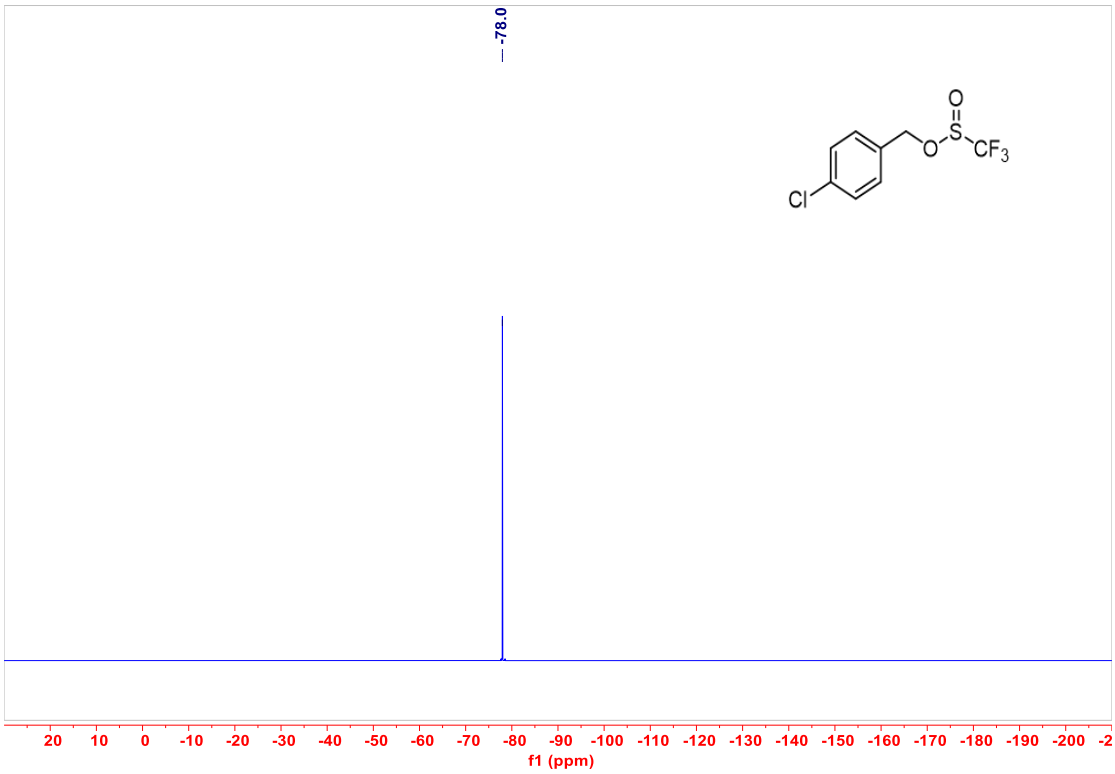
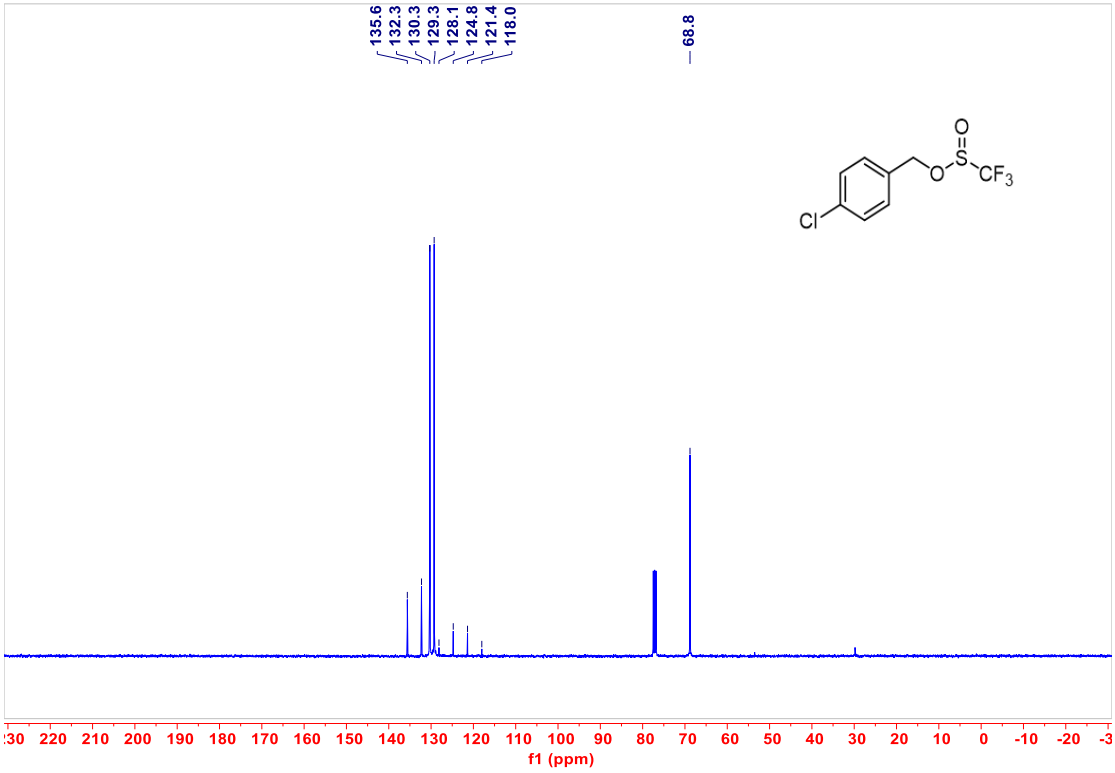
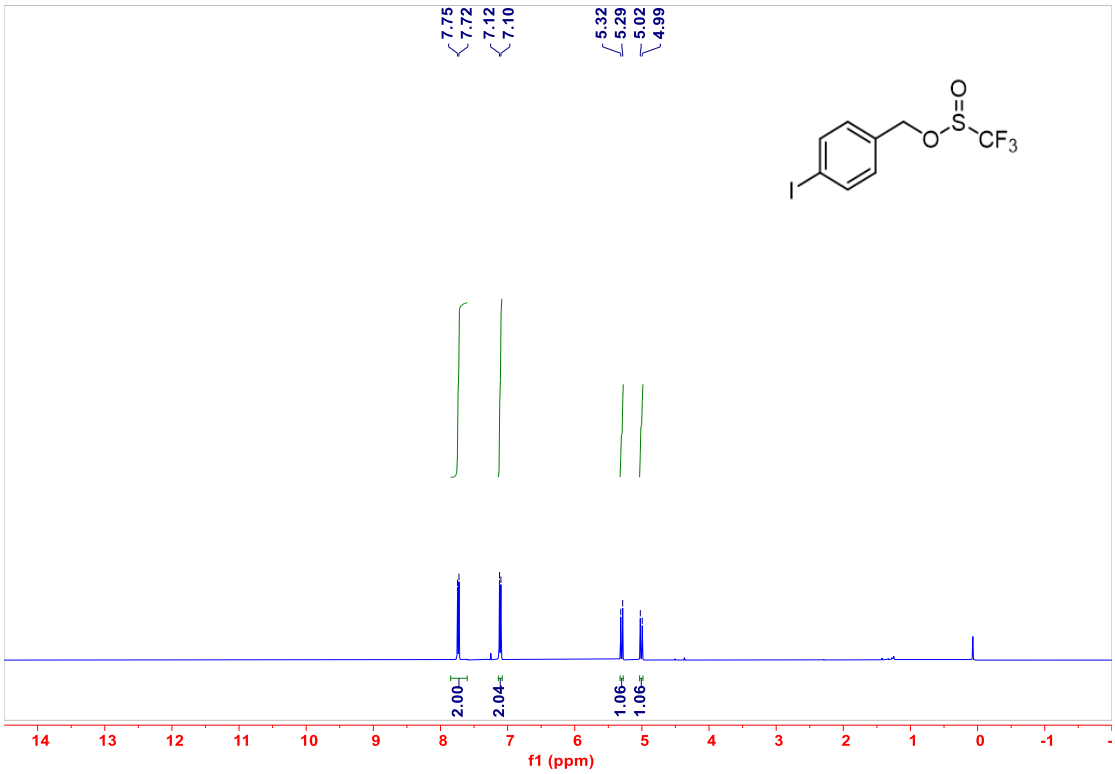
f1 (ppm)


143.1
129.8
129.5
126.1
126.1
122.7
122.1
119.3
31.1
129.5
126.1
122.7
119.3
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
N
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.38
7.36
7.32
7.29
5.34
5.31
5.05
5.02
O
S
CF3
O
Cl
2.00
1.90
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.0
Cl
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


135.6
132.3
130.3
129.3
128.1
124.8
121.4
118.0
68.8
Cl
O
S
O
CF3
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.75
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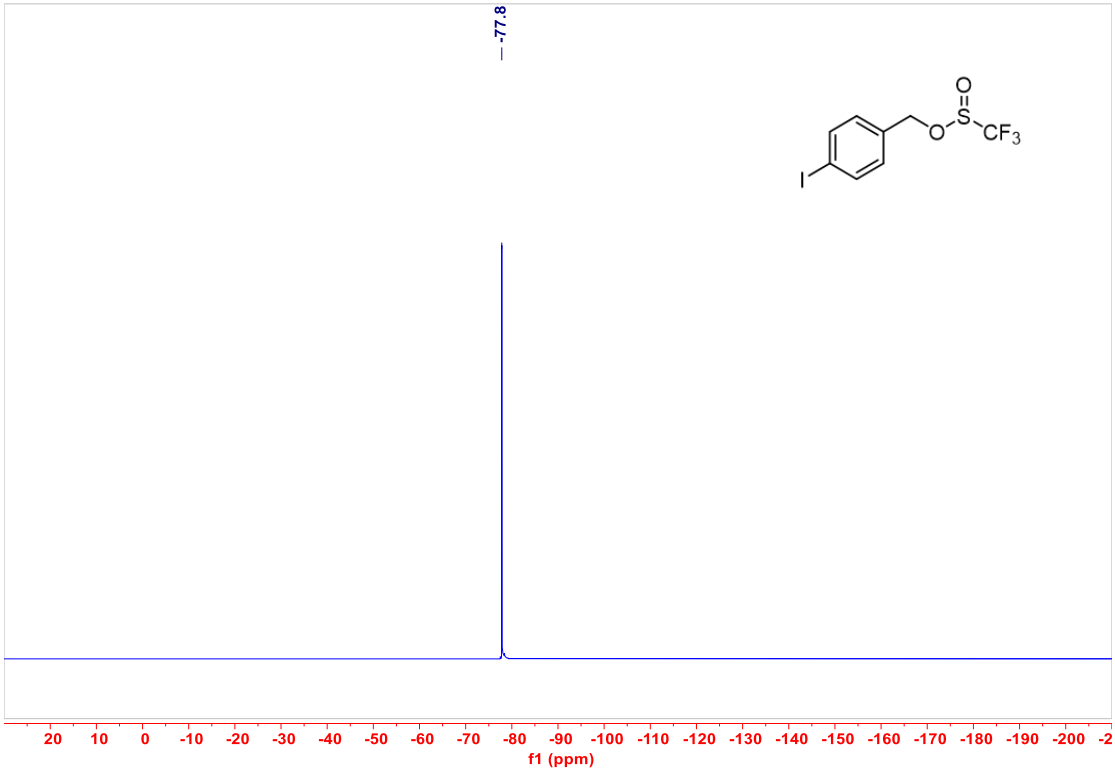
7.12
7.10
5.32
5.29
5.02
4.99
O
S
O
CF3
I
2.00
2.04
1.06
1.06
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.8
O
S
O
CF3
I
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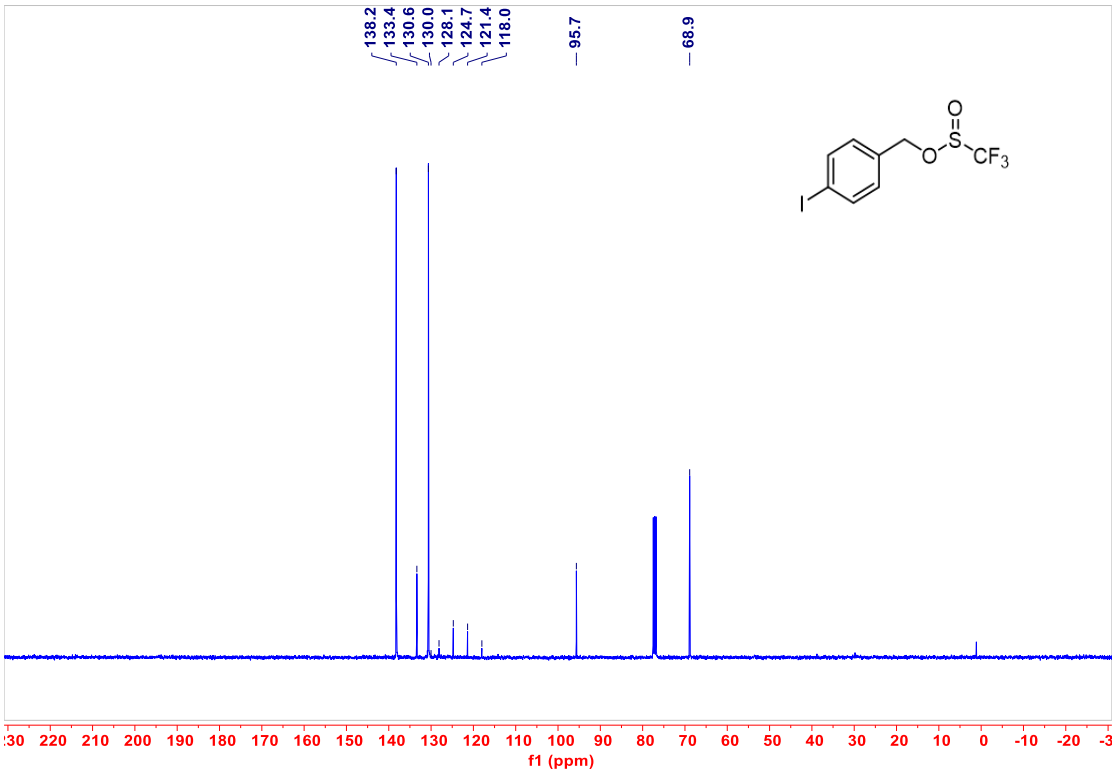
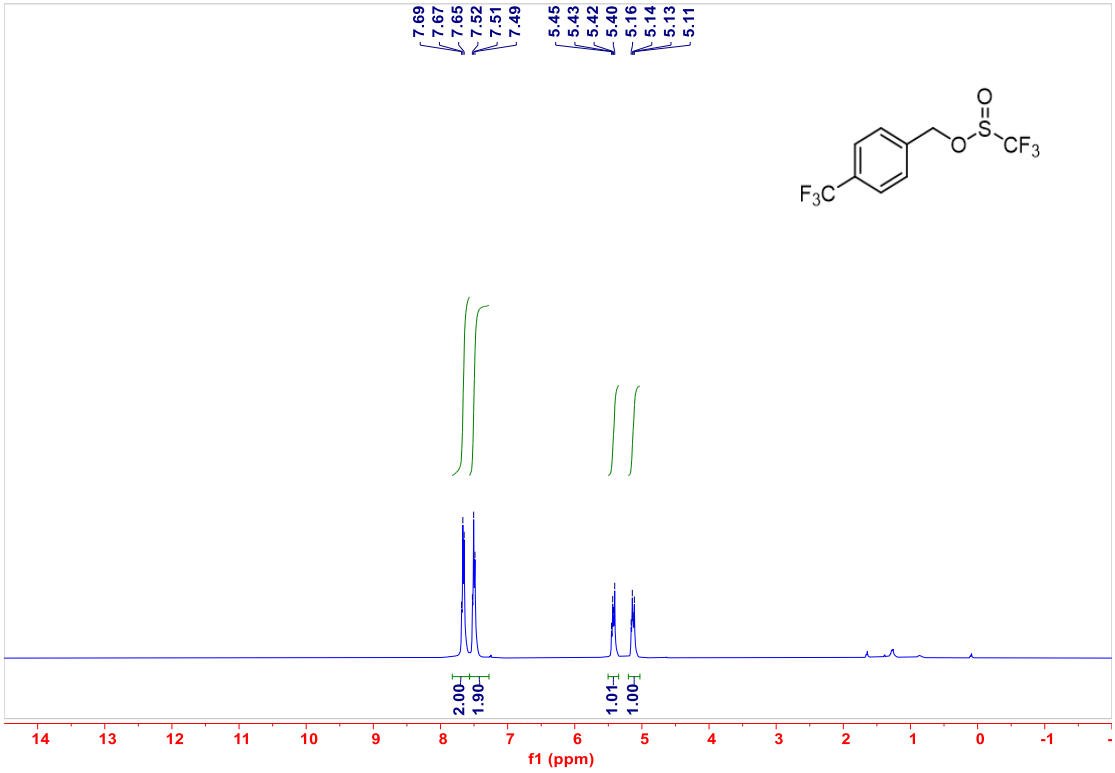
f1 (ppm)


138.2
133.4
130.6
130.0
128.1
124.7
121.4
118.0
95.7
68.9
O
S
O
CF3
I
f1 (ppm)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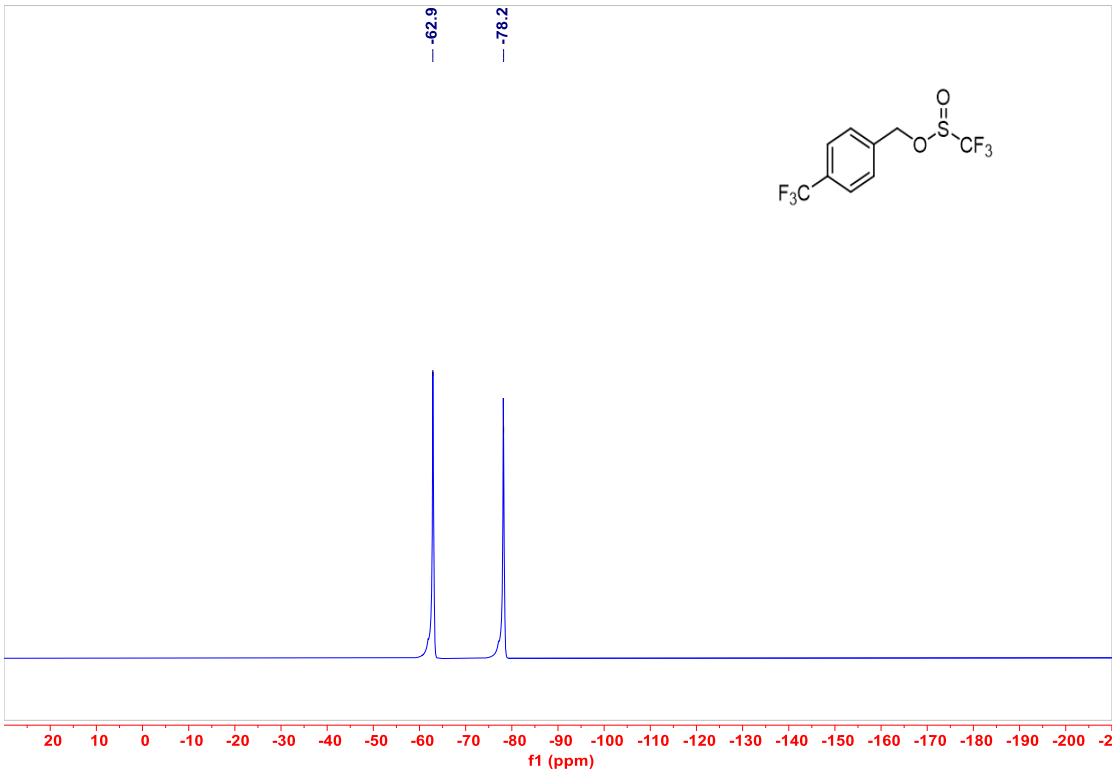
7.51
7.49
5.45
5.43
5.42
5.40
5.16
5.14
5.13
5.11
O
S
O
CF3
F3C
2.00
1.90
1.01
1.00
f1 (ppm)


-62.9
-78.2
O
S
O
CF3
F3C
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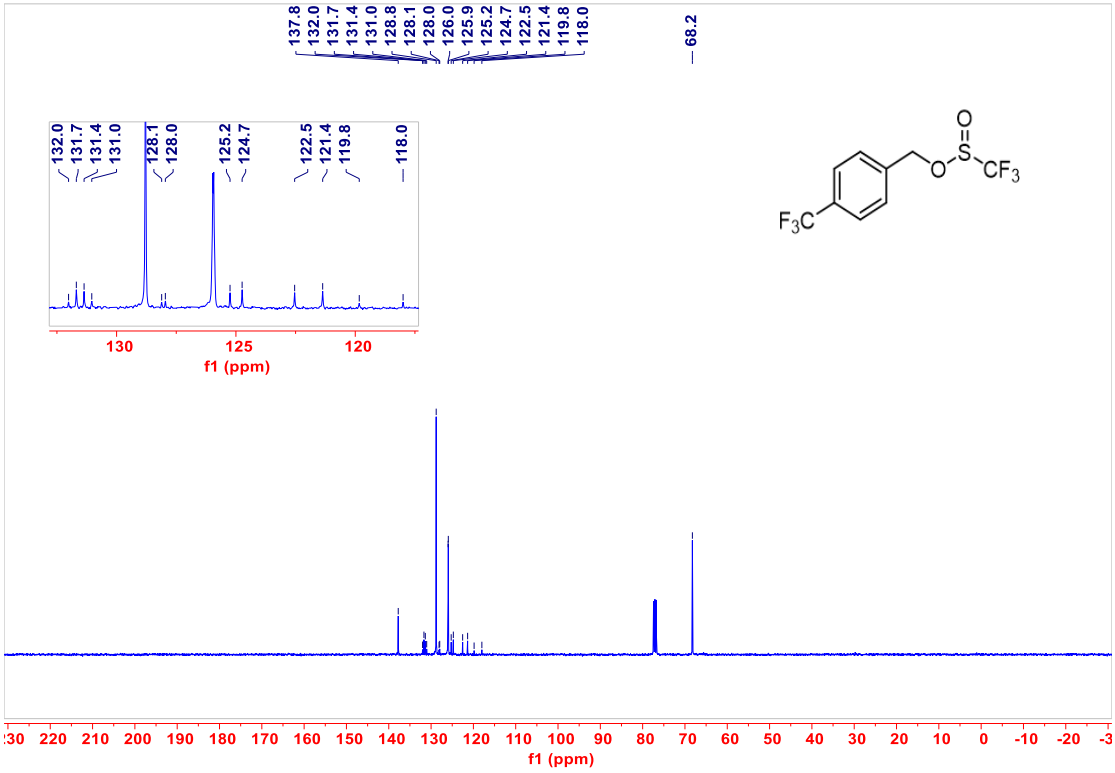
f1 (ppm)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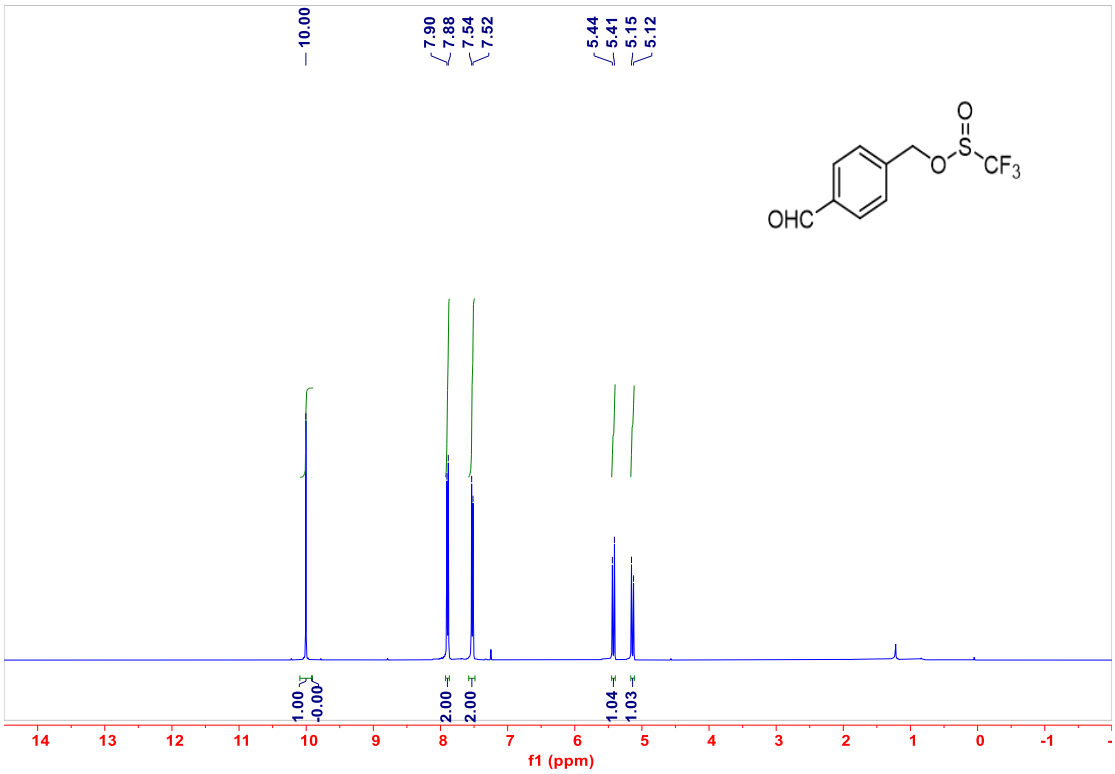
132.0
131.7
131.4
131.0
128.8
128.1
128.0
126.0
125.9
125.2
124.7
122.5
121.4
119.8
118.0
68.2
132.0
131.7
131.4
131.0
128.1
128.0
125.2
124.7
122.5
121.4
119.8
118.0
130
125
120
f1 (ppm)
O
S
O
CF3
F3C
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)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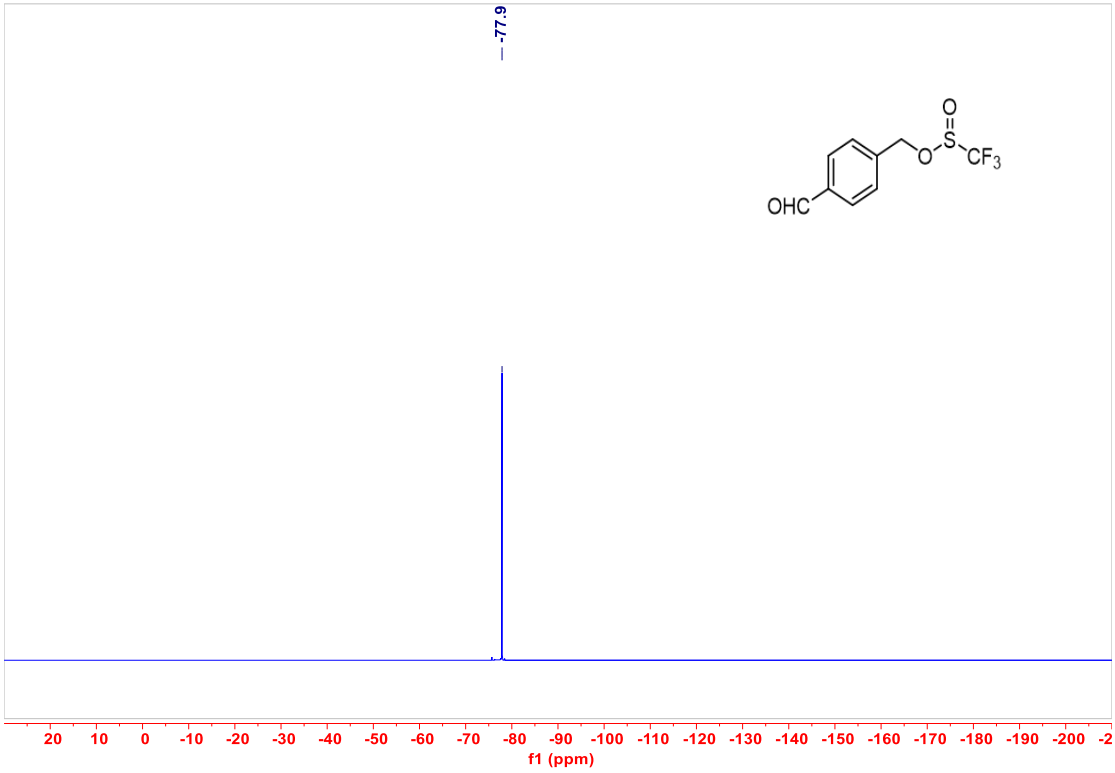
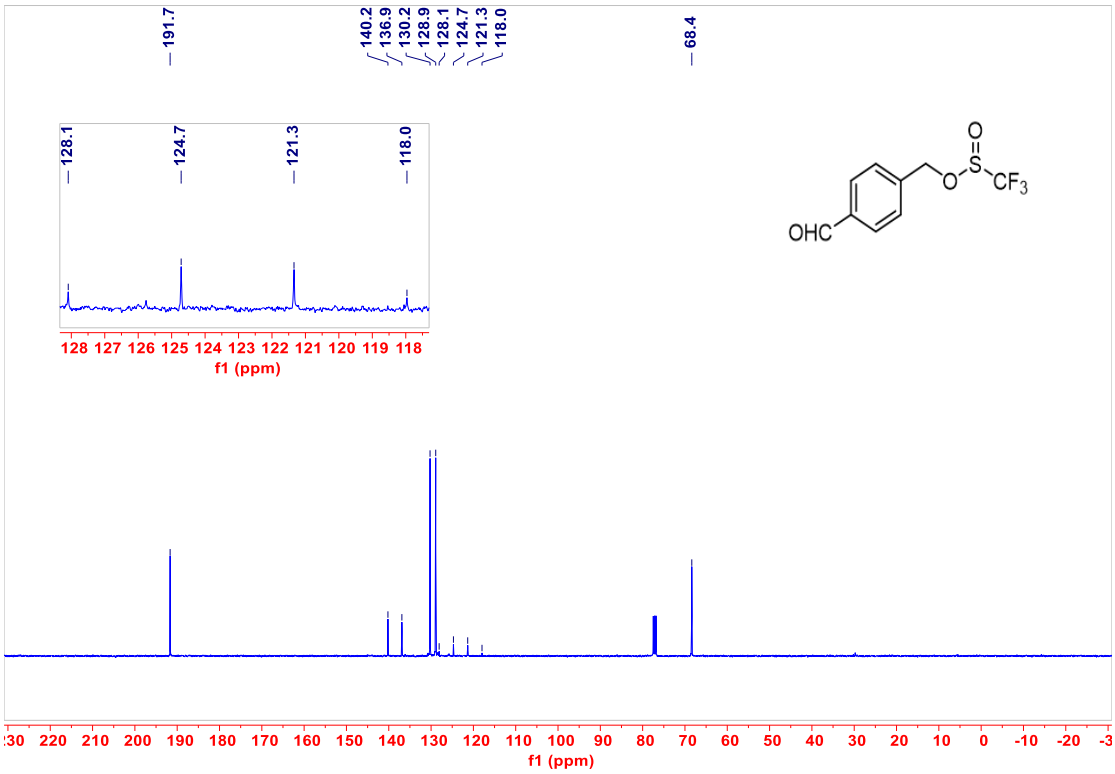
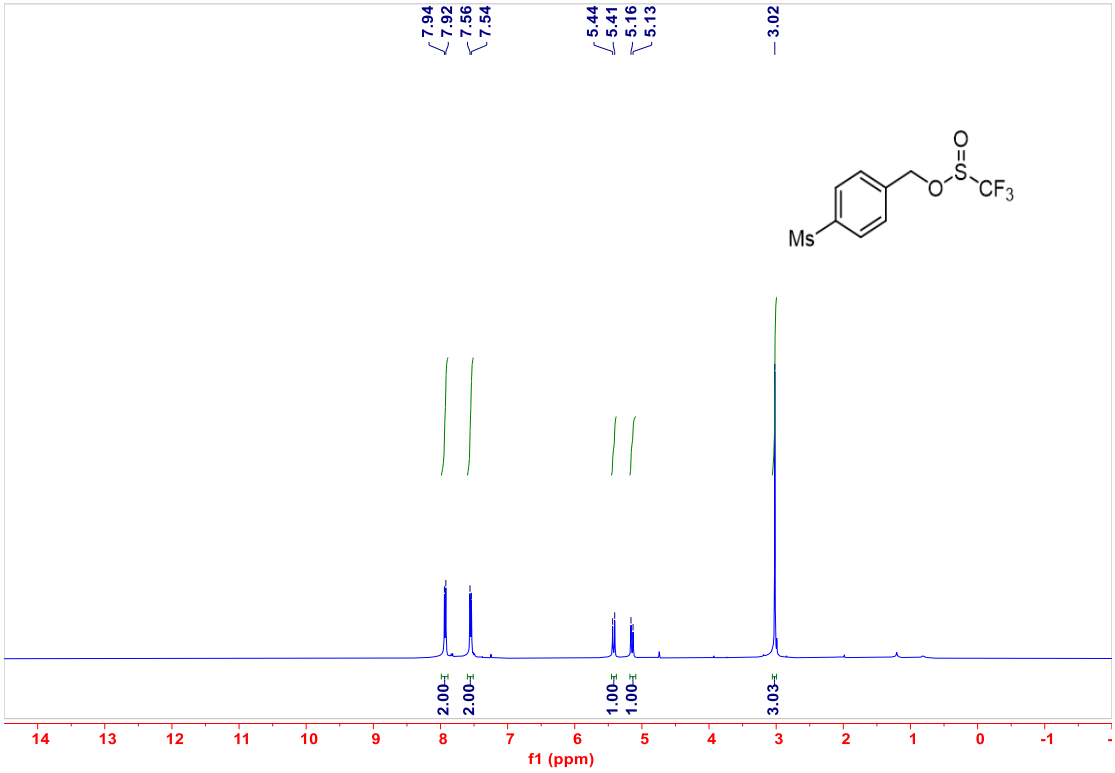
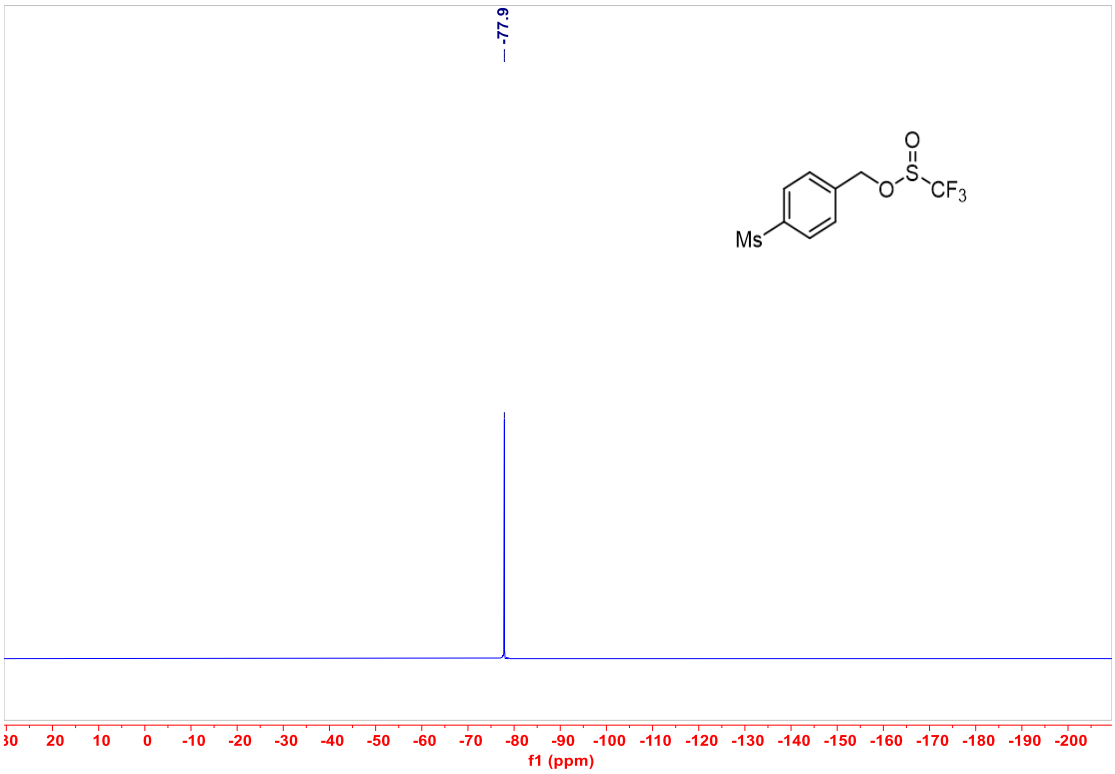
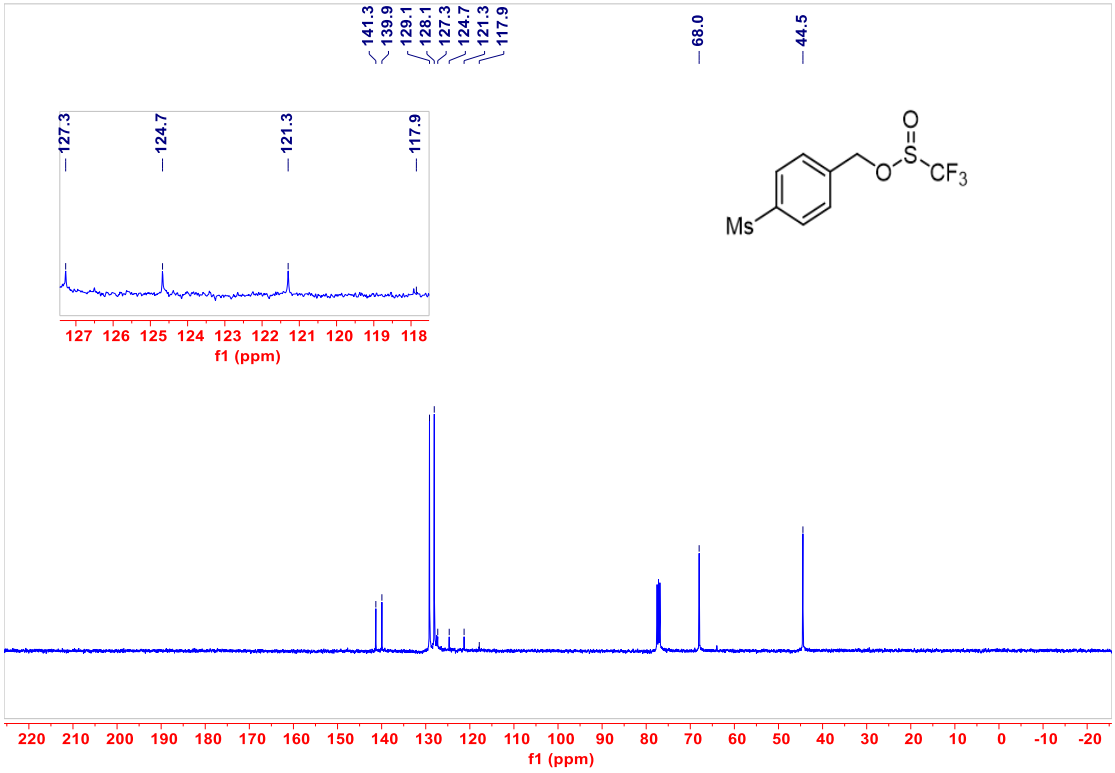
7.88
7.54
7.52
5.44
5.41
5.15
5.12
OHC
O
S
O
CF3
1.00
0.00
2.00
2.00
1.04
1.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

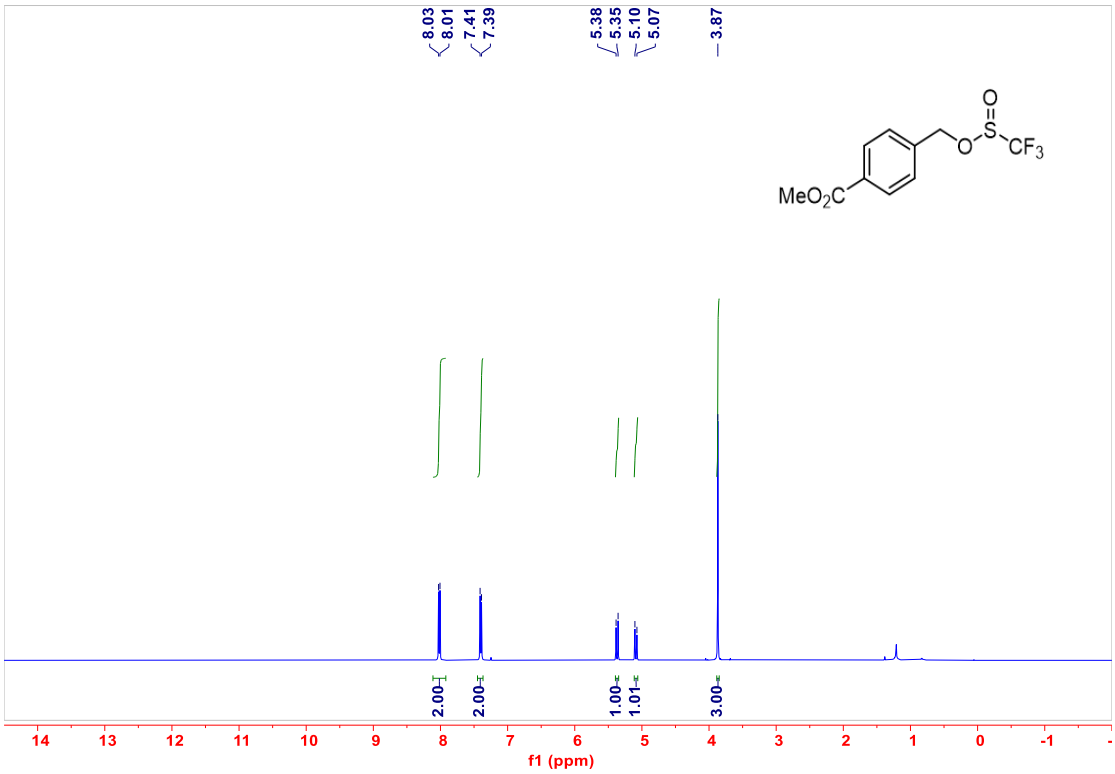

-77.9
OHC
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

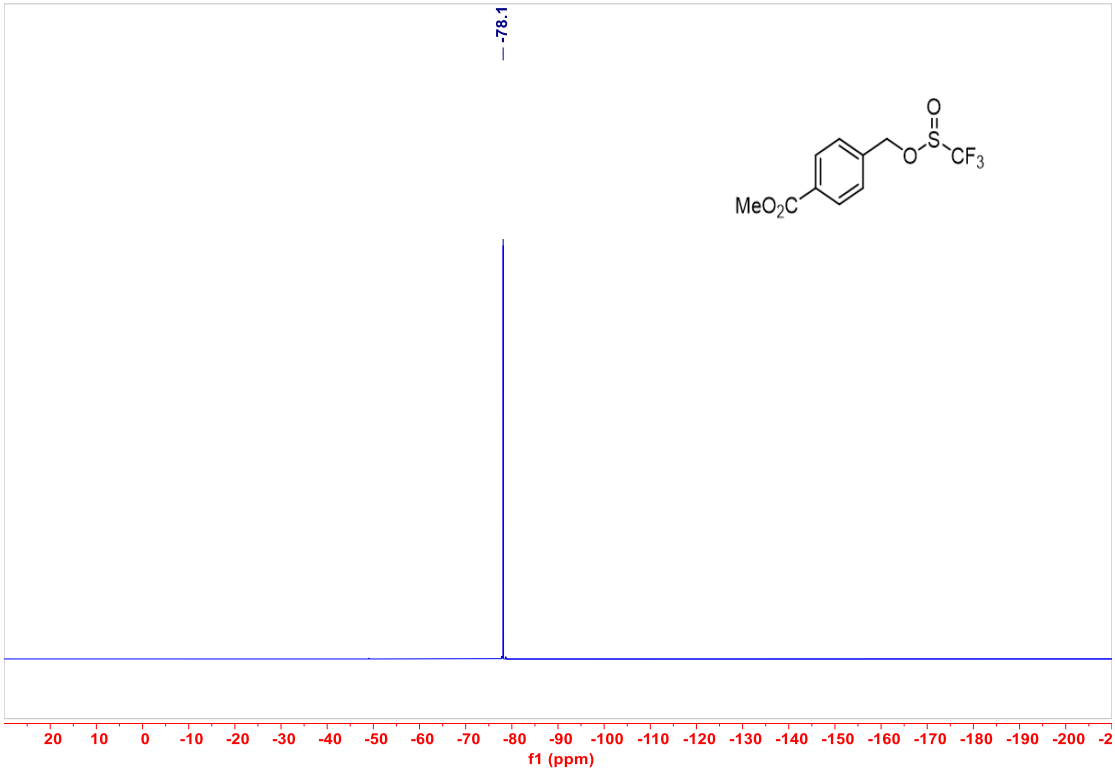

191.7
140.2
136.9
130.2
128.9
128.1
124.7
121.3
118.0
68.4
128.1
124.7
121.3
118.0
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
OHC
O
S
CF3
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.94
7.92
7.56
7.54
5.44
5.41
5.16
5.13
3.02
Ms
O
S
CF3
O
2.00
2.00
1.00
1.00
3.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-77.9
Ms
O
S
O
CF3
f1 (ppm)


141.3
139.9
129.1
128.1
127.3
124.7
121.3
117.9
68.0
44.5
127.3
124.7
121.3
117.9
Ms
O
S
O
CF3
f1 (ppm)


8.03
8.01
7.41
7.39
5.38
5.35
5.10
5.07
3.87
MeO2C
O
S
CF3
2.00
2.00
1.00
1.01
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.1
MeO2C
O
S
CF3
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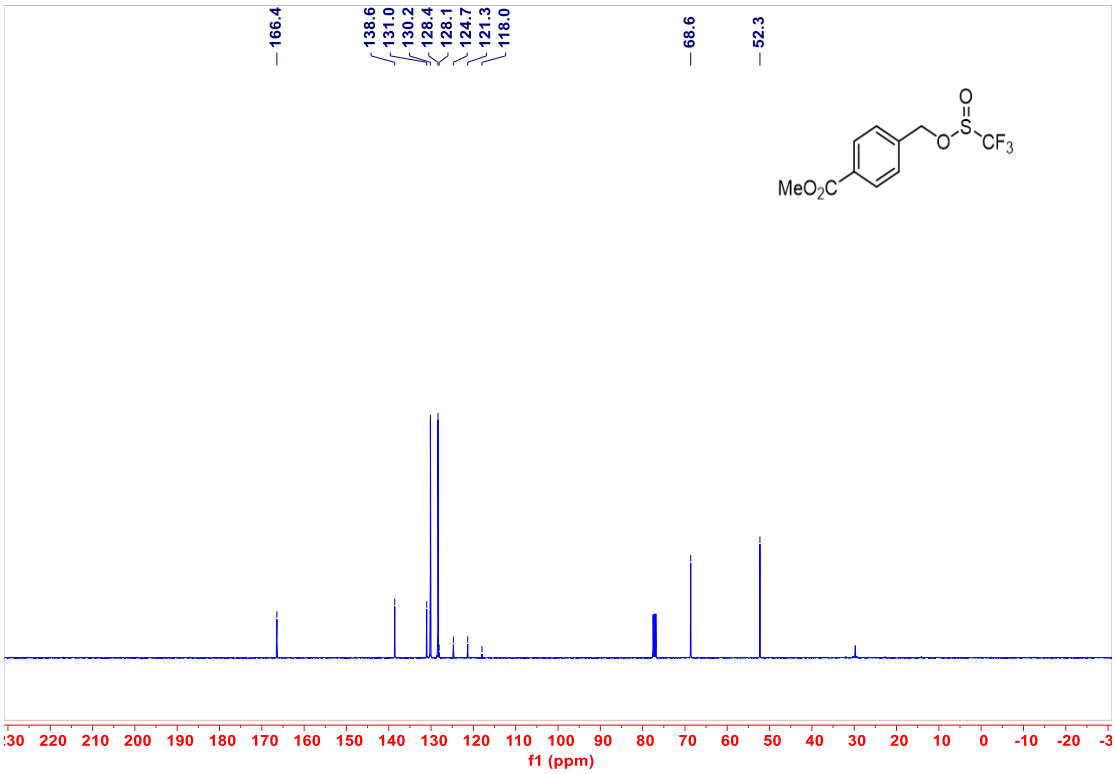
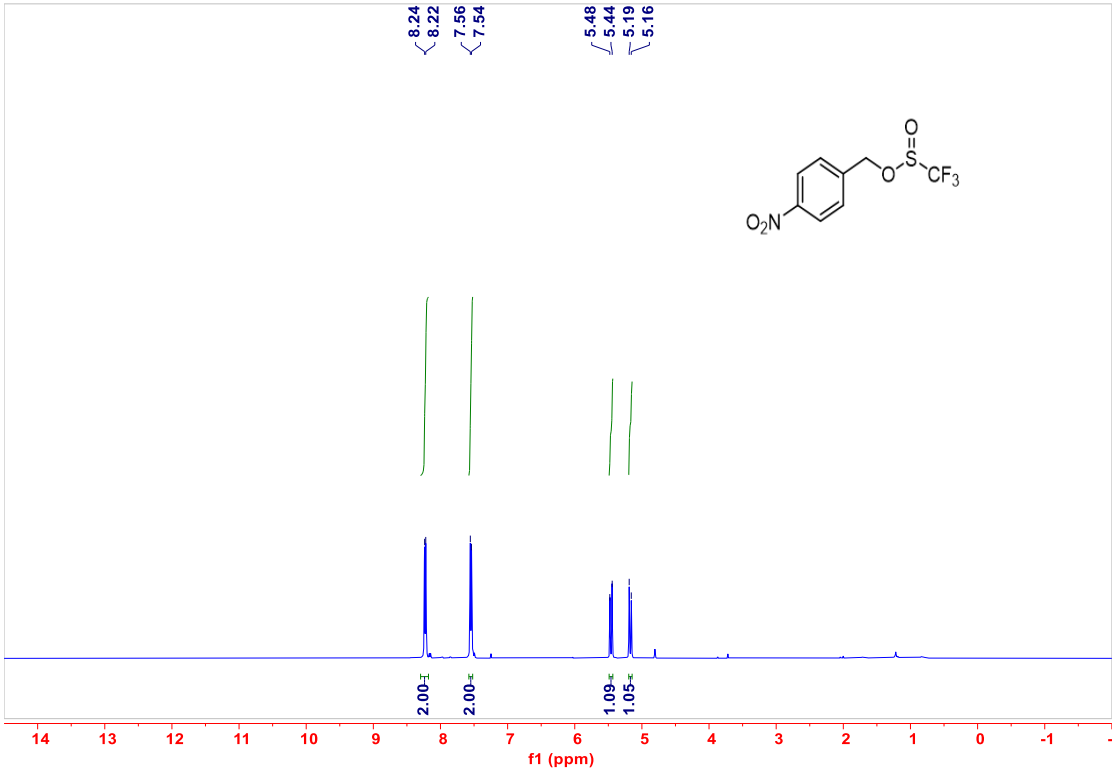
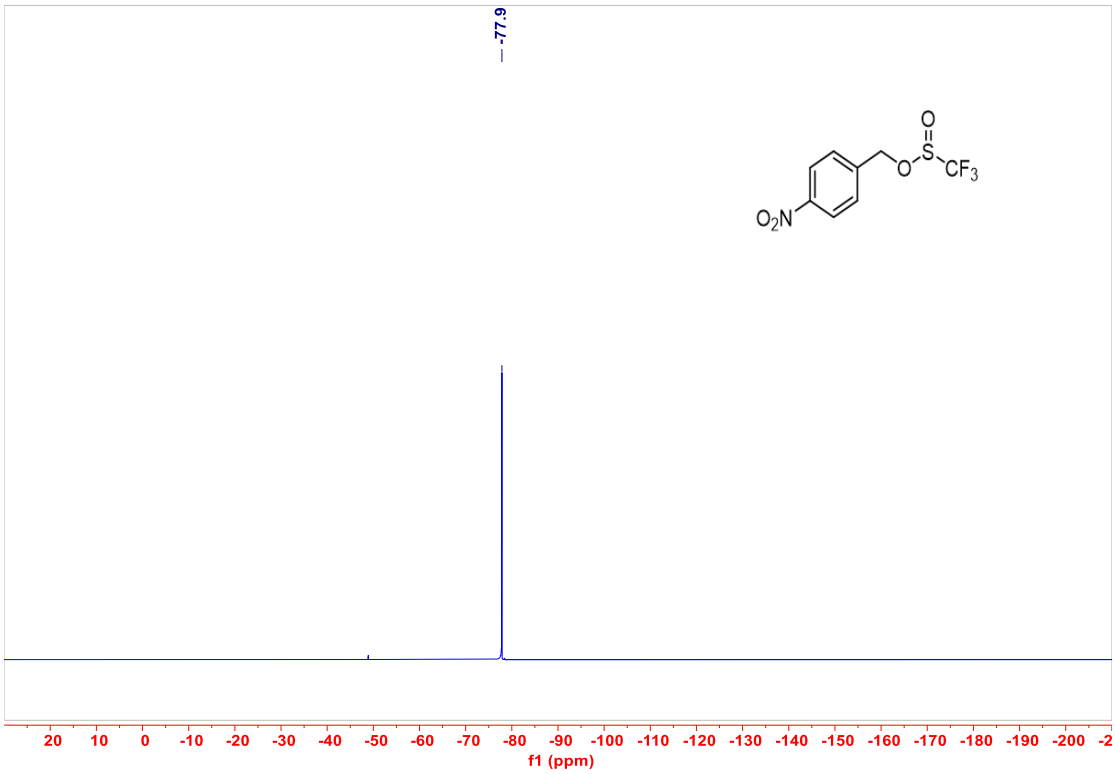
f1 (ppm)


166.4
138.6
131.0
130.2
128.4
128.1
124.7
121.3
118.0
68.6
52.3
MeO2C
O
S
CF3
f1 (ppm)


8.24
8.22
7.56
7.54
5.48
5.44
5.19
5.16
O2N
O
S
CF3
2.00
2.00
1.09
1.05
f1 (ppm)


-77.9
O
S
O
CF3
O2N
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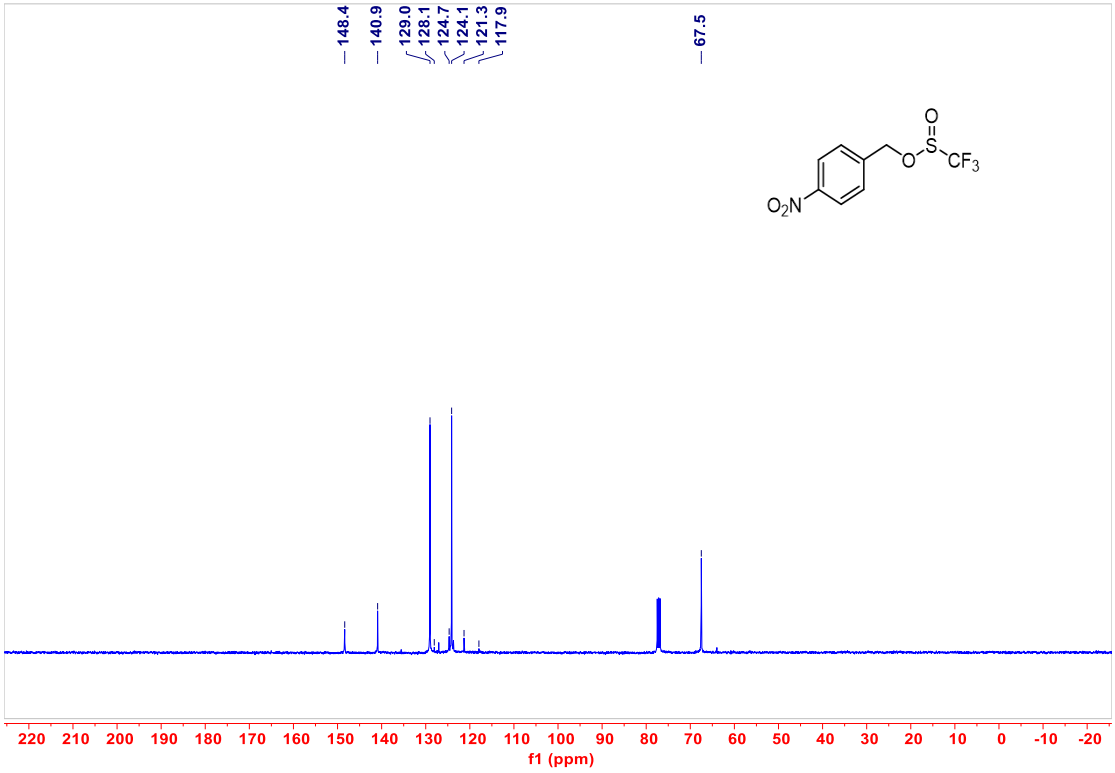
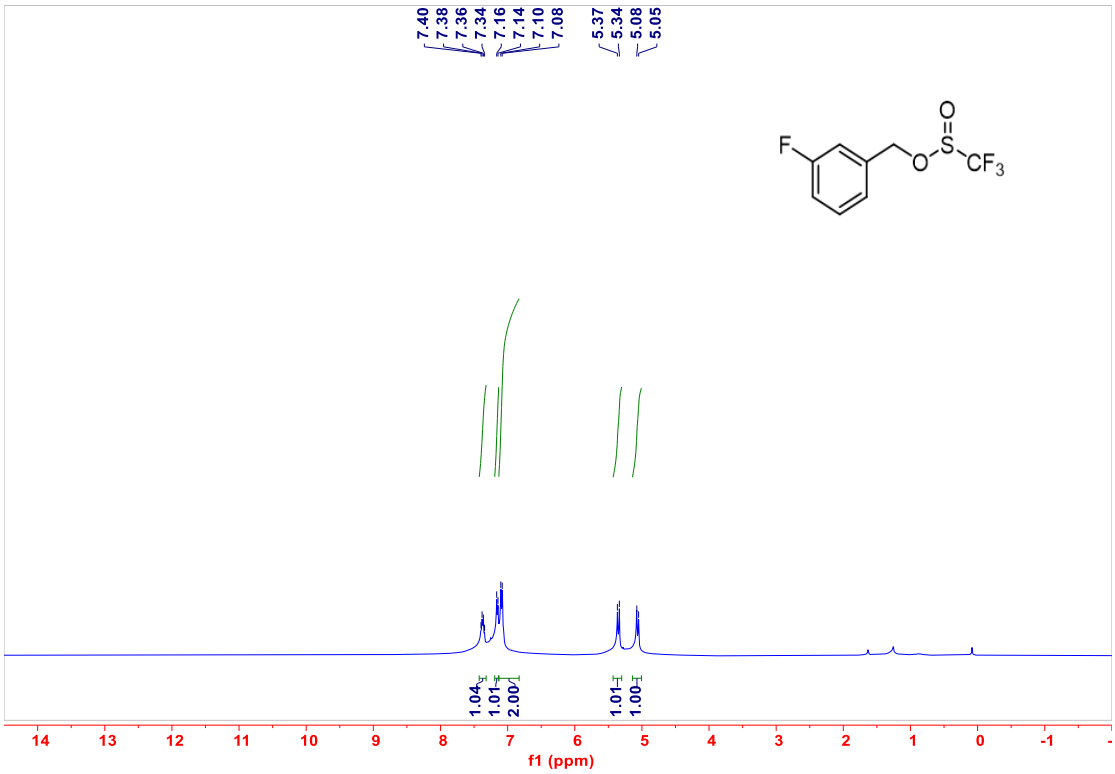
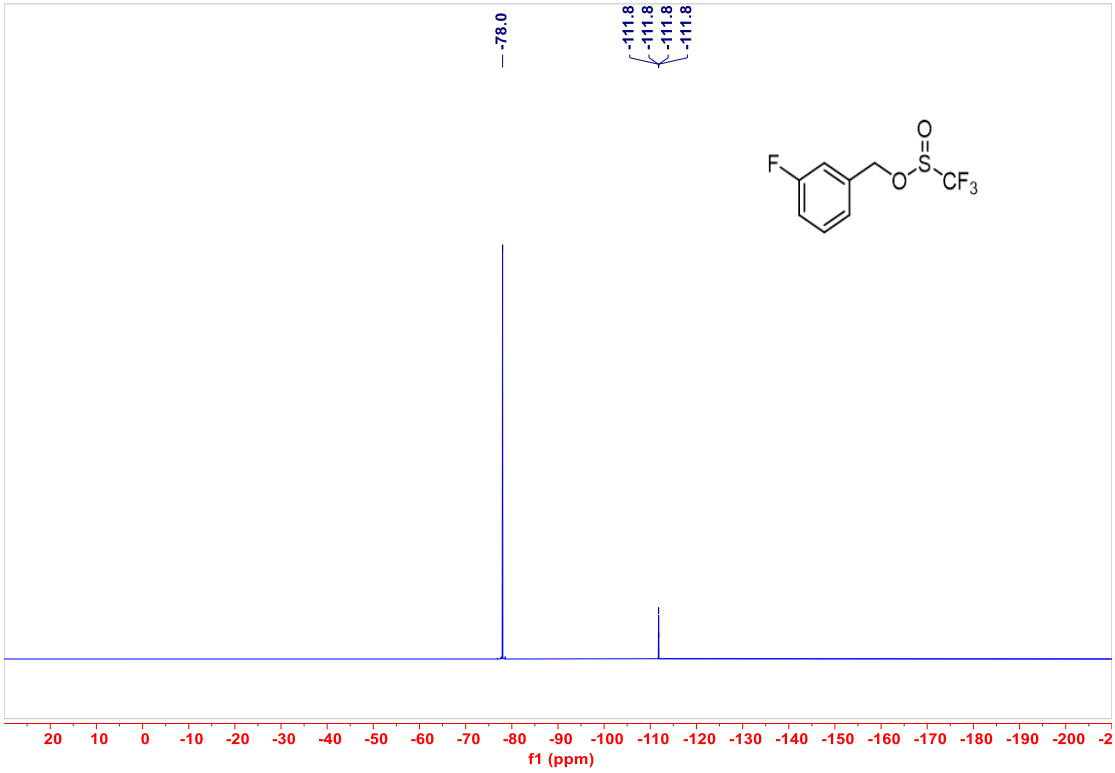
f1 (ppm)


148.4
140.9
129.0
128.1
124.7
124.1
121.3
117.9
67.5
O
S
O
CF3
O2N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.40
7.38
7.36
7.34
7.16
7.14
7.10
7.08
5.37
5.34
5.08
5.05
F
O
S
O
CF3
1.04
1.01
2.00
1.01
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.0
-111.8
-111.8
-111.8
-111.8
F
O
S
O
CF3
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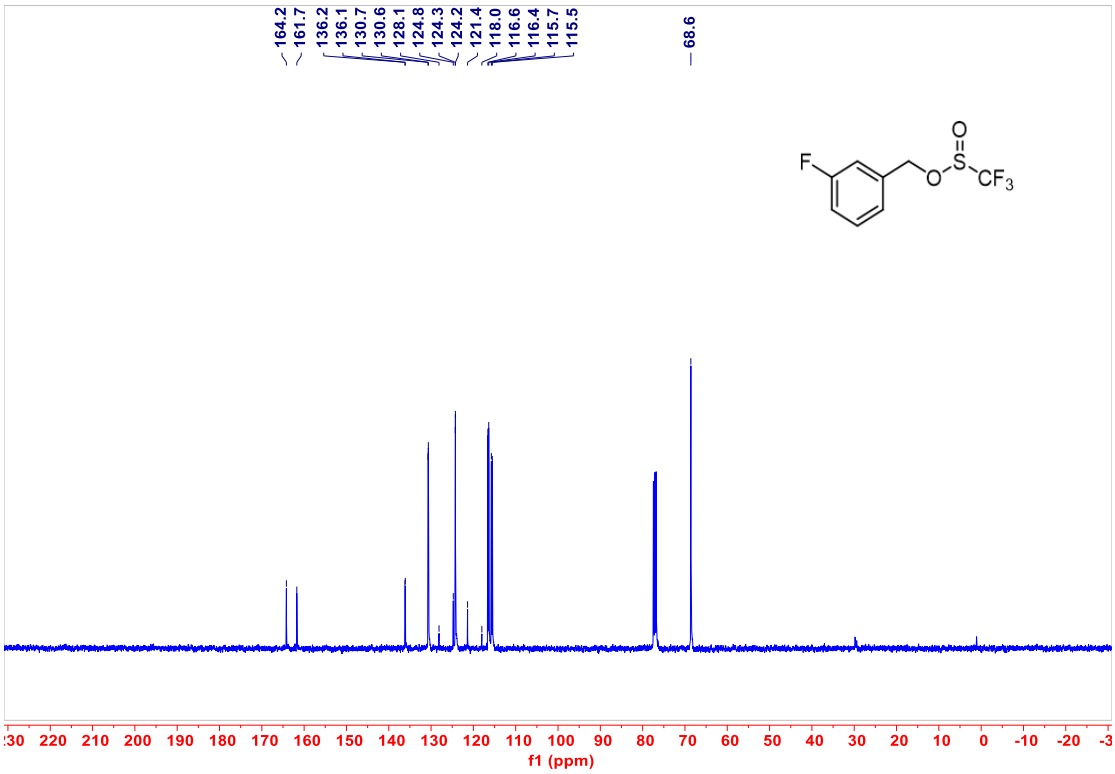
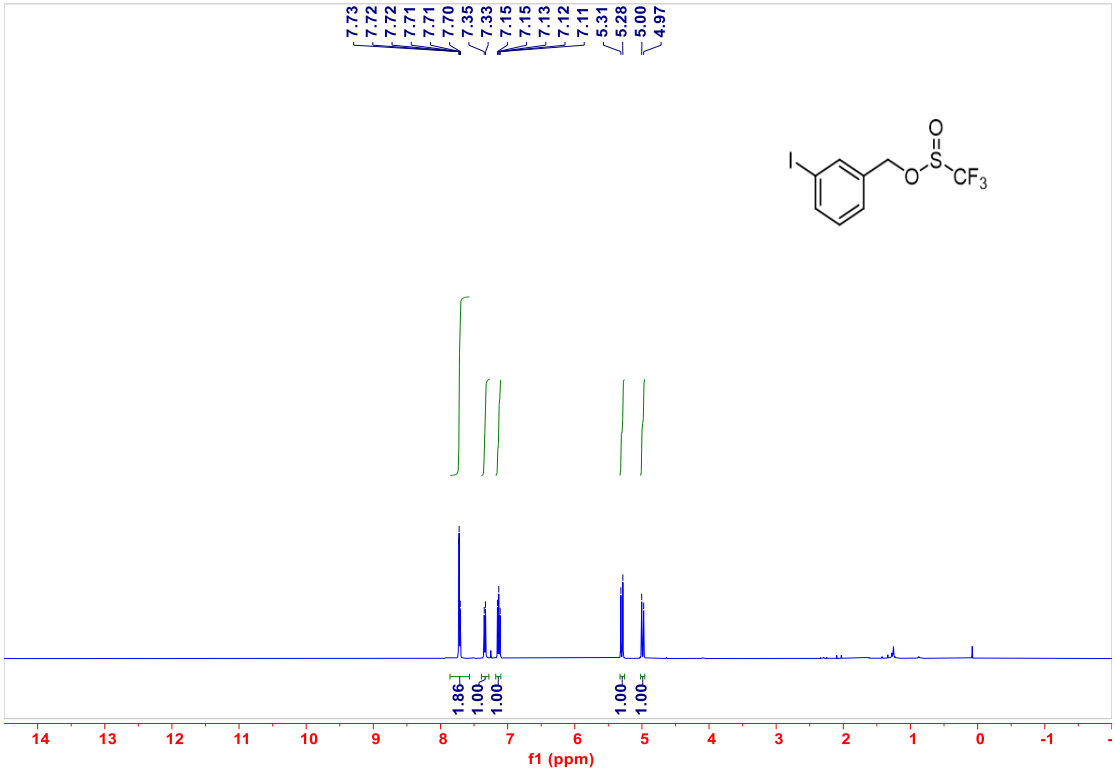
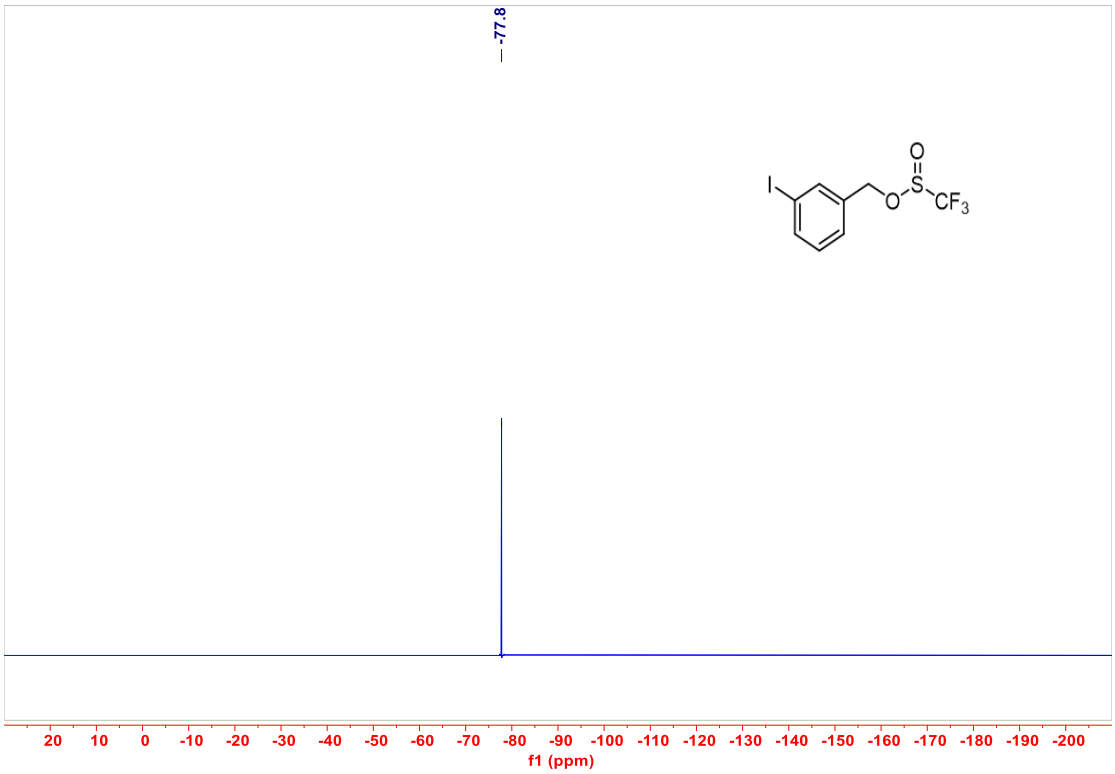
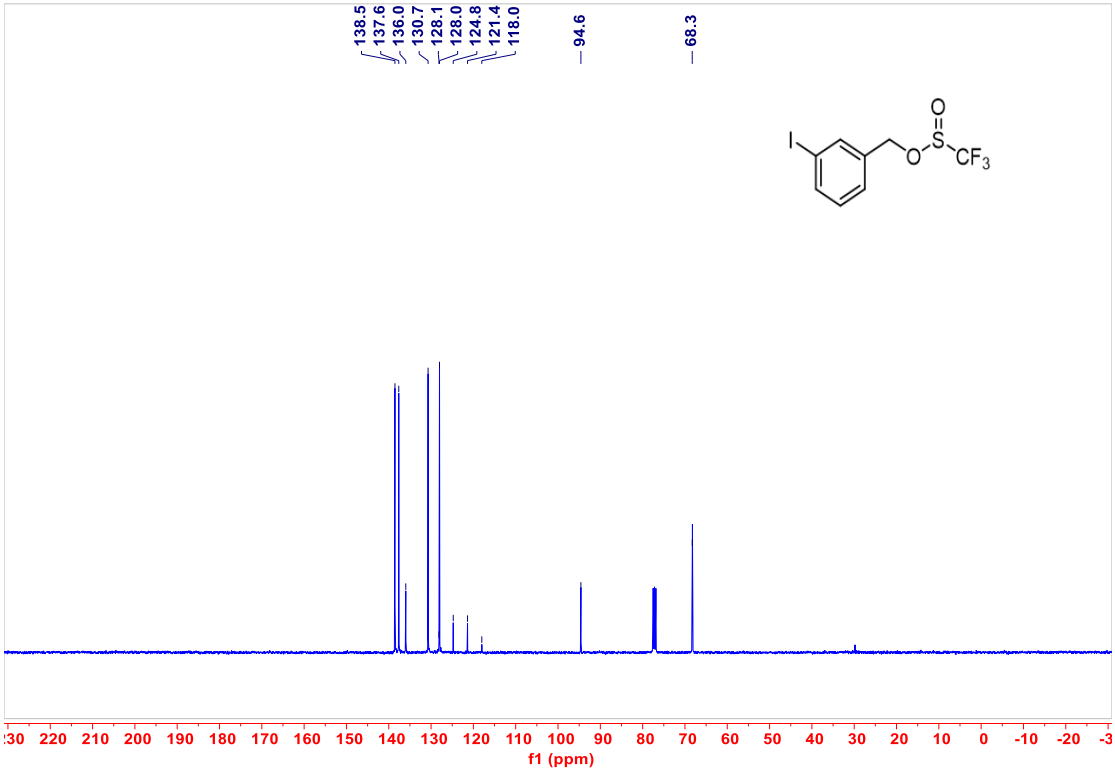
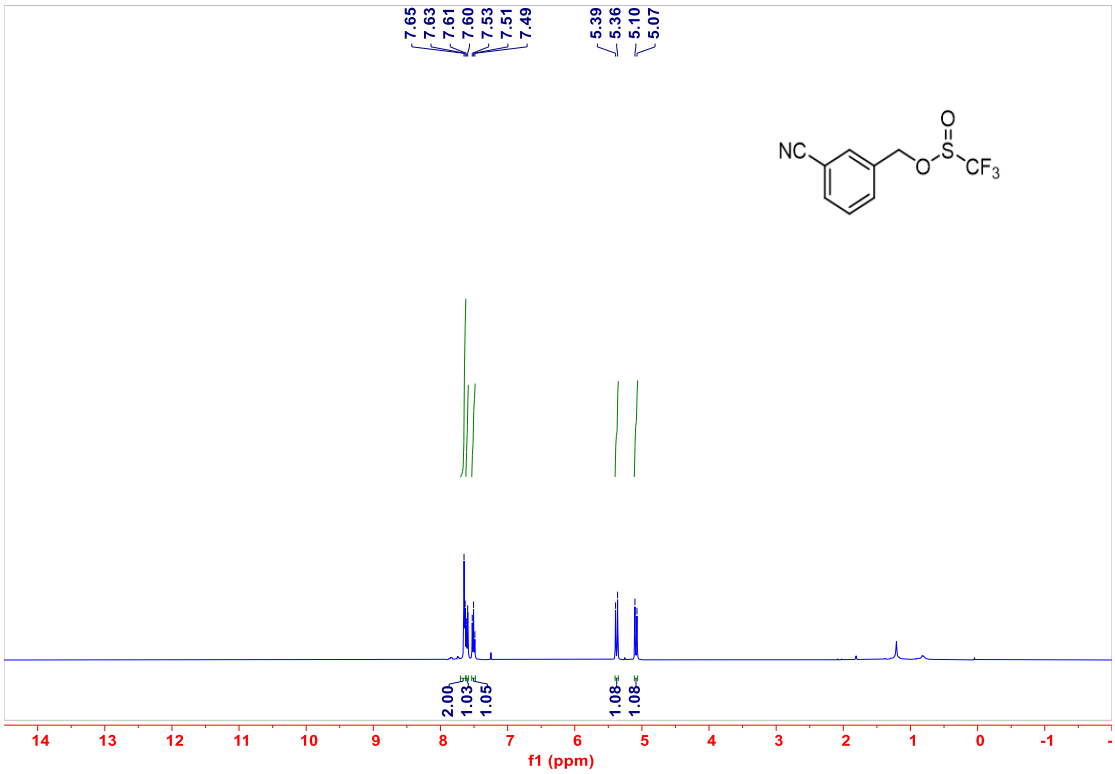
f1 (ppm)

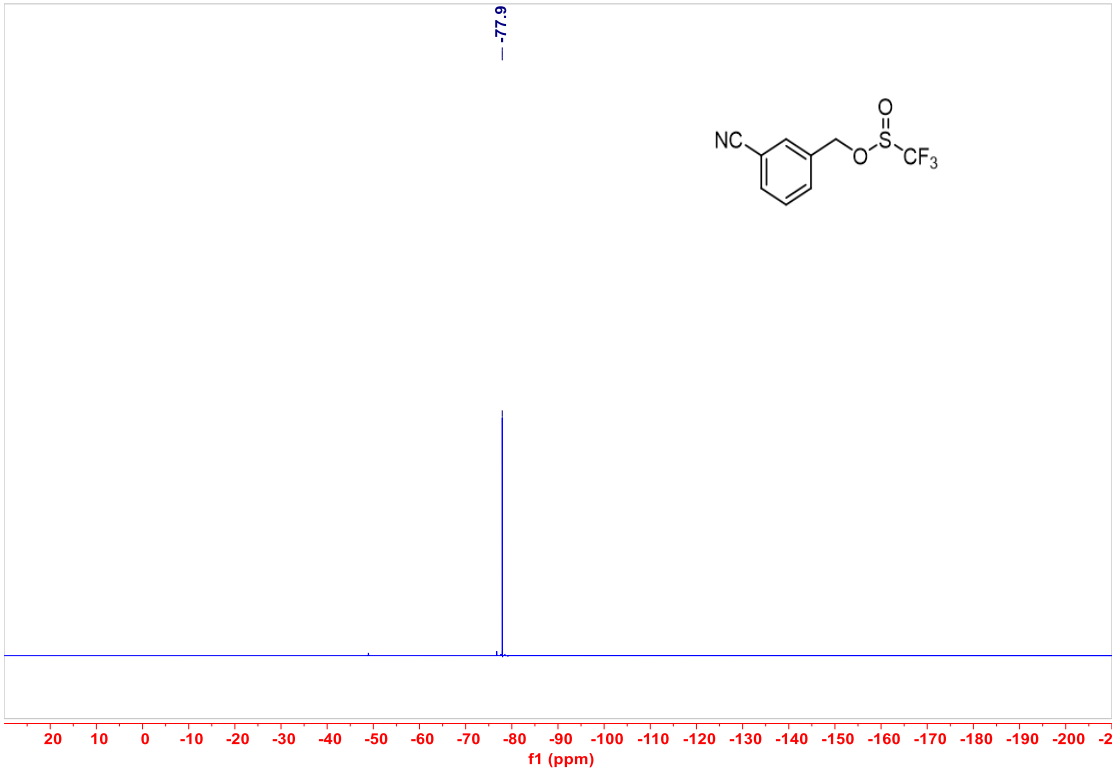

164.2
161.7
136.2
136.1
130.7
130.6
128.1
124.8
124.3
124.2
121.4
118.0
116.6
116.4
115.7
115.5
68.6
F
O
S
O
CF3
f1 (ppm)

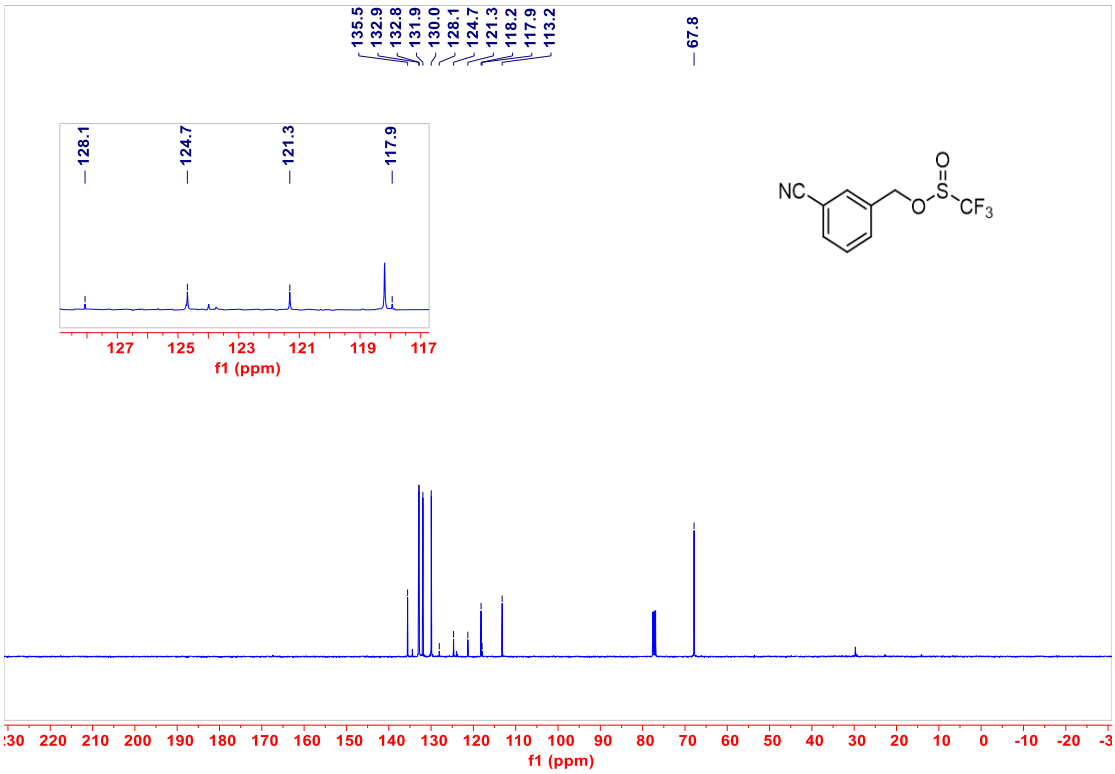

7.73
7.72
7.72
7.71
7.71
7.70
7.35
7.33
7.15
7.15
7.13
7.12
7.11
5.31
5.28
5.00
4.97
I
O
S
O
CF3
1.86
1.00
1.00
1.00
1.00
f1 (ppm)

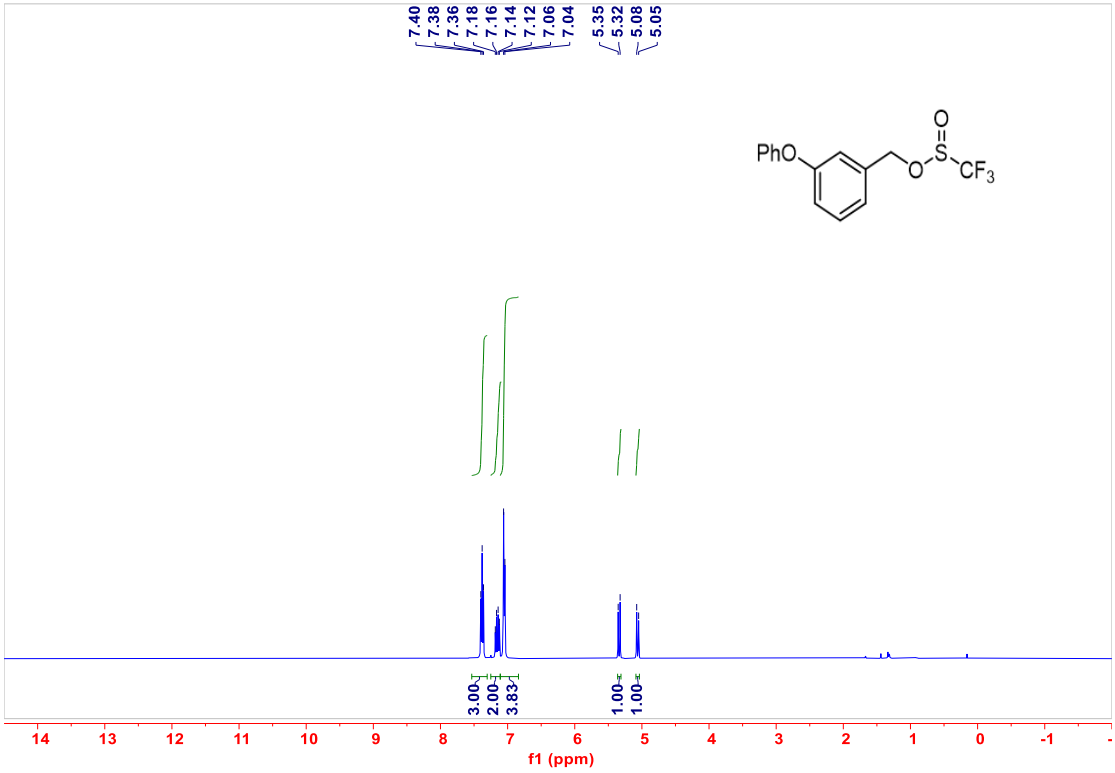

-77.8
I
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

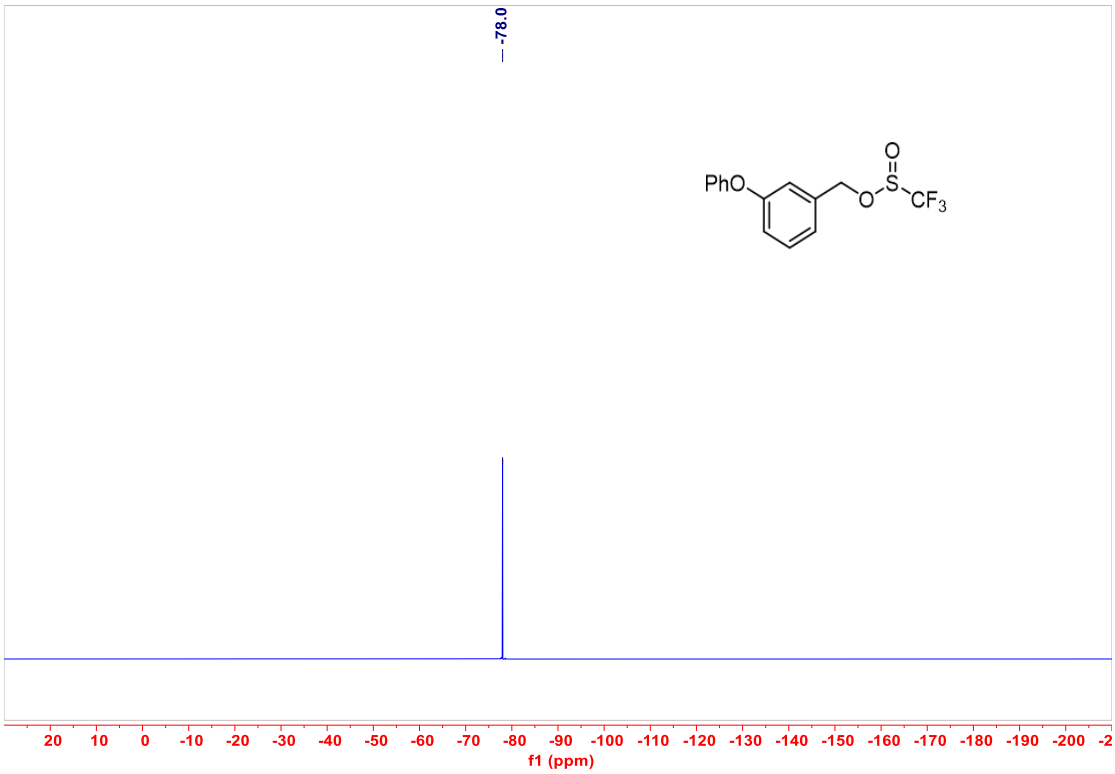

138.5
137.6
136.0
130.7
128.1
128.0
124.8
121.4
118.0
94.6
68.3
I
O
S
O
CF3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)

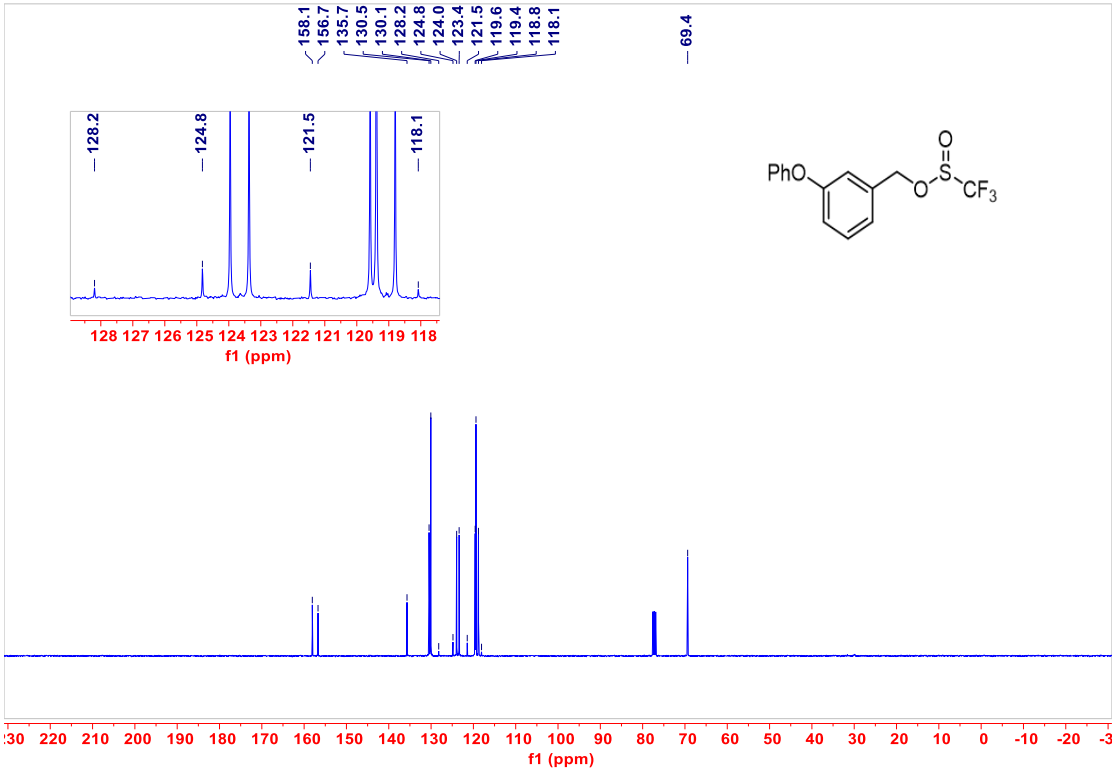

7.65
7.63
7.61
7.60
7.53
7.51
7.49
5.39
5.36
5.10
5.07
NC
O
S
O
CF3
2.00
1.03
1.05
1.08
1.08
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

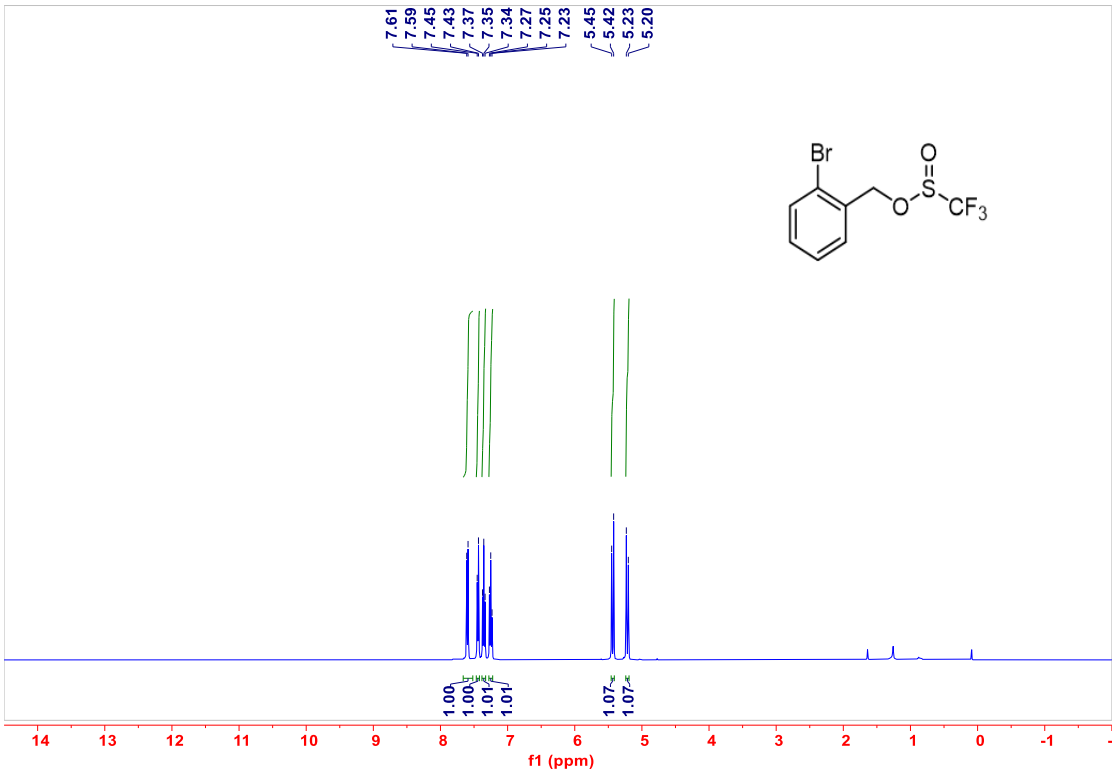

-77.9
NC
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


135.5
132.9
132.8
131.9
130.0
128.1
124.7
121.3
118.2
117.9
113.2
67.8
128.1
124.7
121.3
117.9
127 125 123 121 119 117
f1 (ppm)
NC
O
S
O
CF3
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.40
7.38
7.36
7.18
7.16
7.14
7.12
7.06
7.04
5.35
5.32
5.08
5.05
PhO
O
S
O
CF3
3.00
2.00
3.83
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.0
PhO
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


158.1
156.7
135.7
130.5
130.1
128.2
124.8
124.0
123.4
121.5
119.6
119.4
118.8
118.1
69.4
128.2
124.8
121.5
118.1
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
PhO
O
S
O
CF3
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)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7.59
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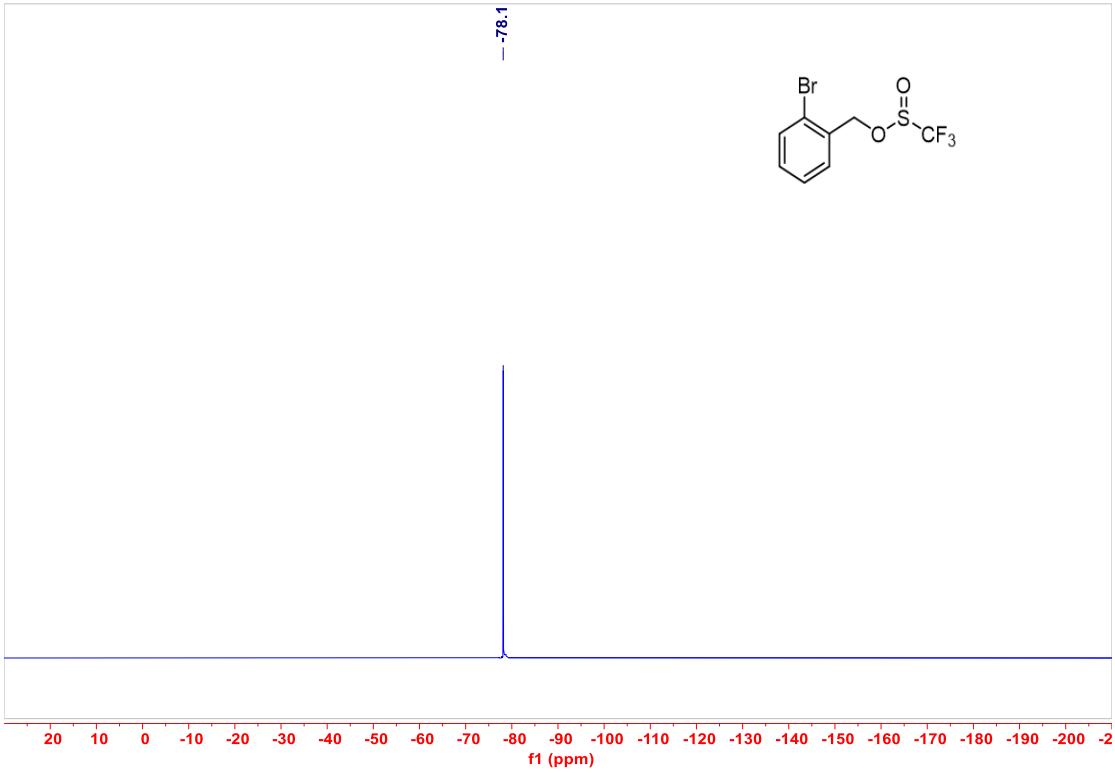
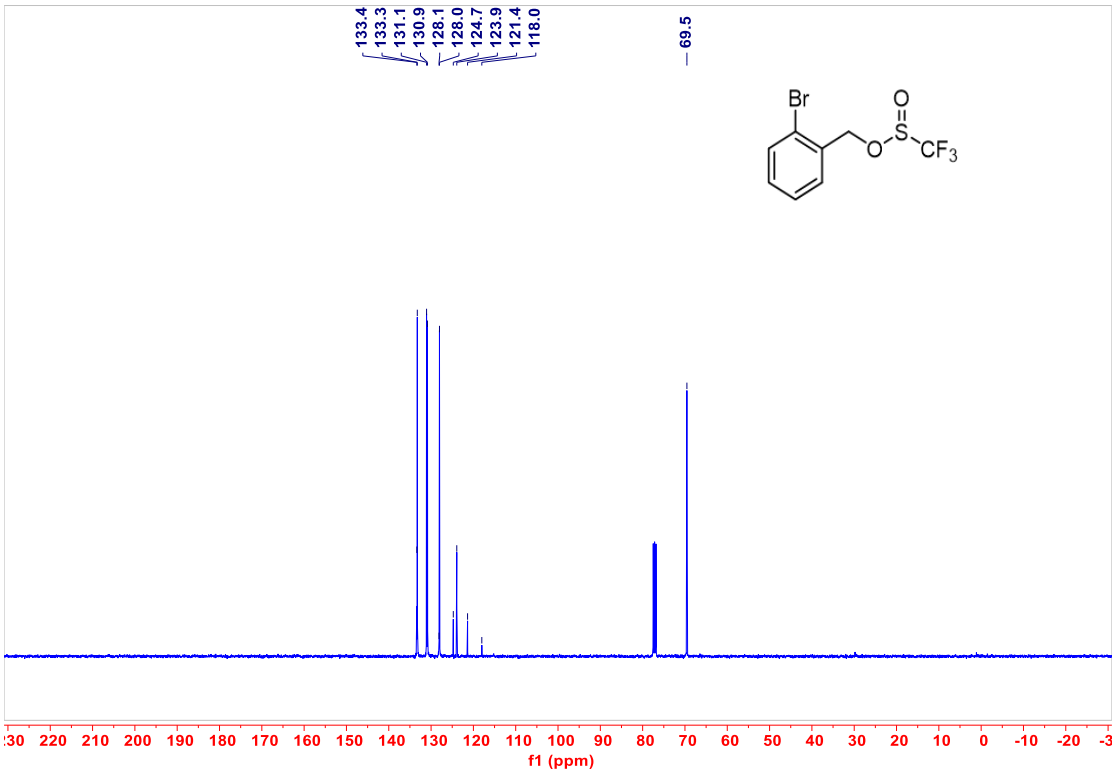
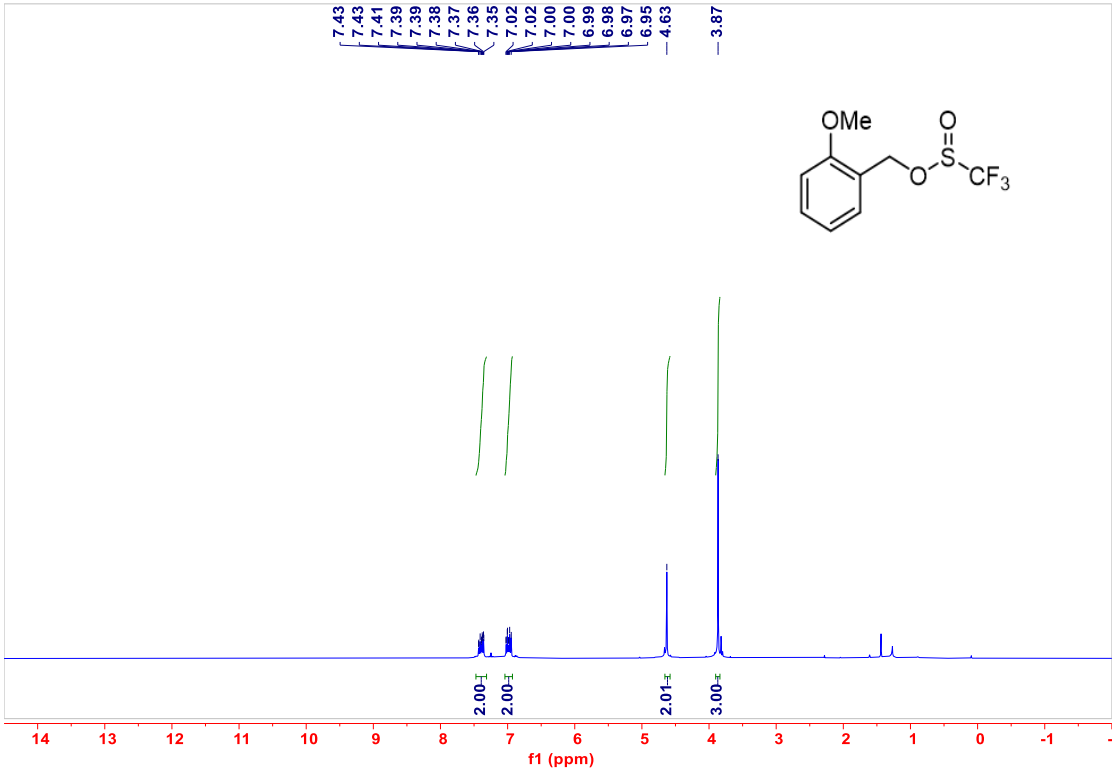
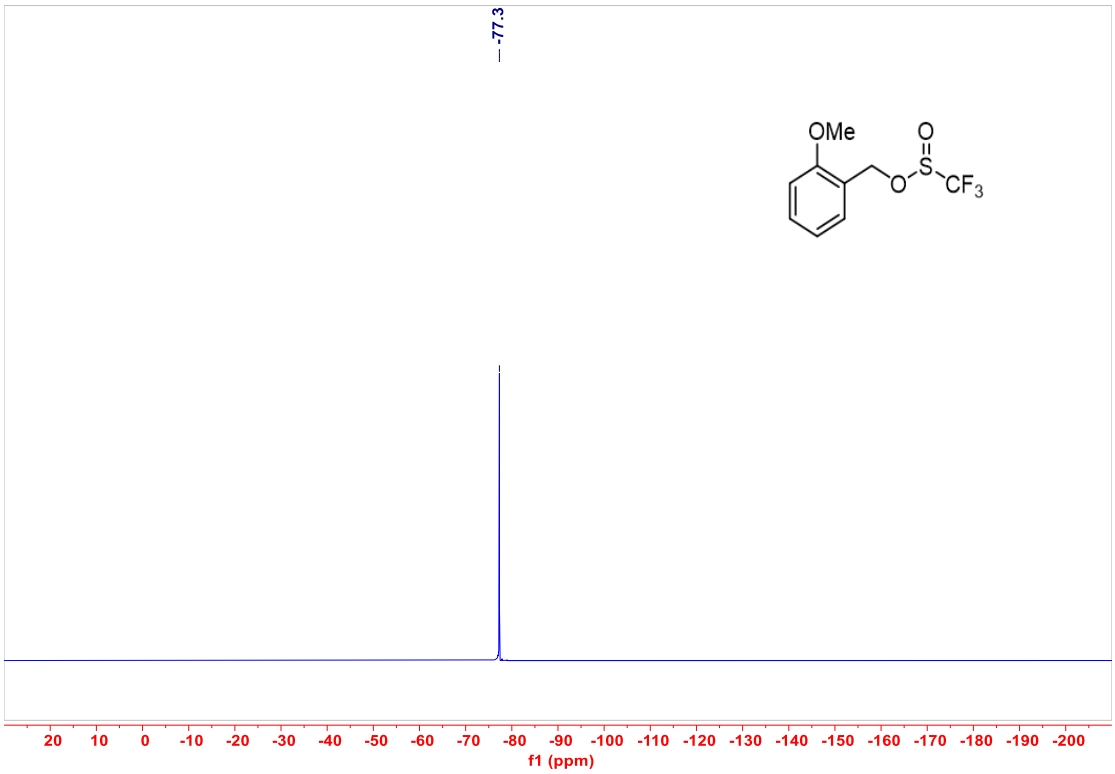
7.43
7.37
7.35
7.34
7.27
7.25
7.23
5.45
5.42
5.23
5.20
Br
O
S
O
CF3
1.00
1.00
1.01
1.01
1.07
1.07
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.1
Br
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


133.4
133.3
131.1
130.9
128.1
128.0
124.7
123.9
121.4
118.0
69.5
Br
O
S
O
CF3
f1 (ppm)


7.43
7.43
7.41
7.39
7.39
7.38
7.37
7.36
7.35
7.02
7.02
7.00
7.00
6.99
6.98
6.97
6.95
4.63
3.87
OMe
O
S
O
CF3
2.00
2.00
2.01
3.00
f1 (ppm)


-77.3
OMe
O
S
O
CF3
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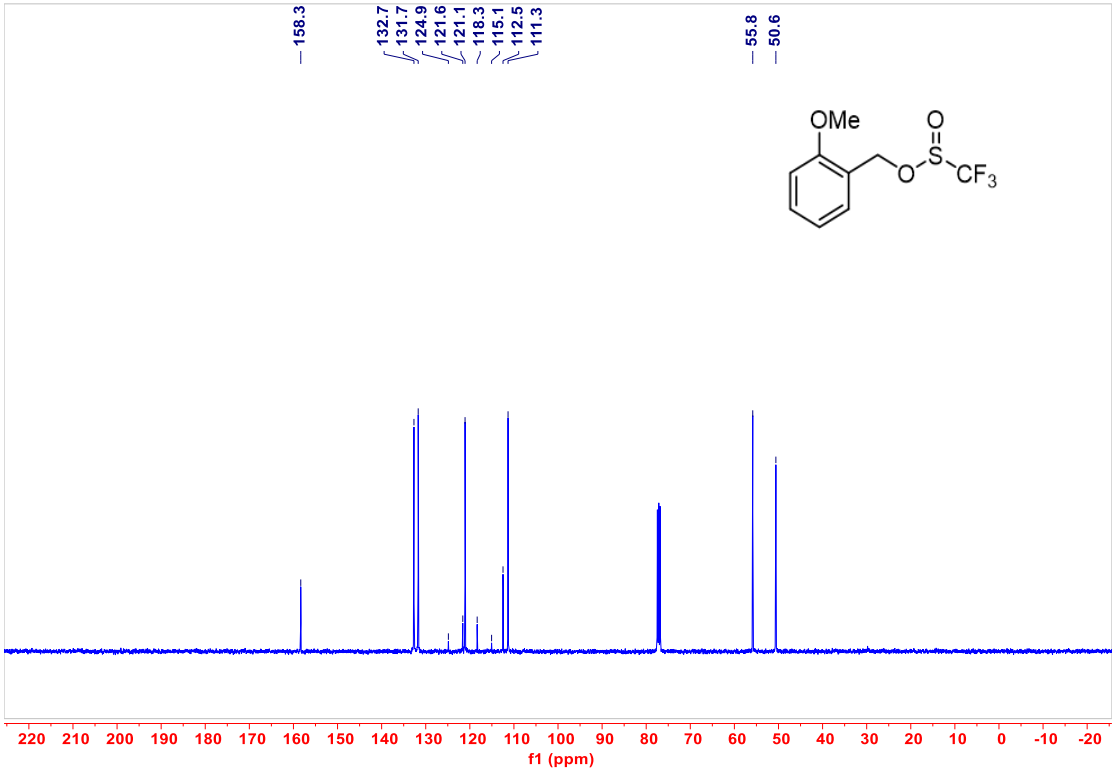
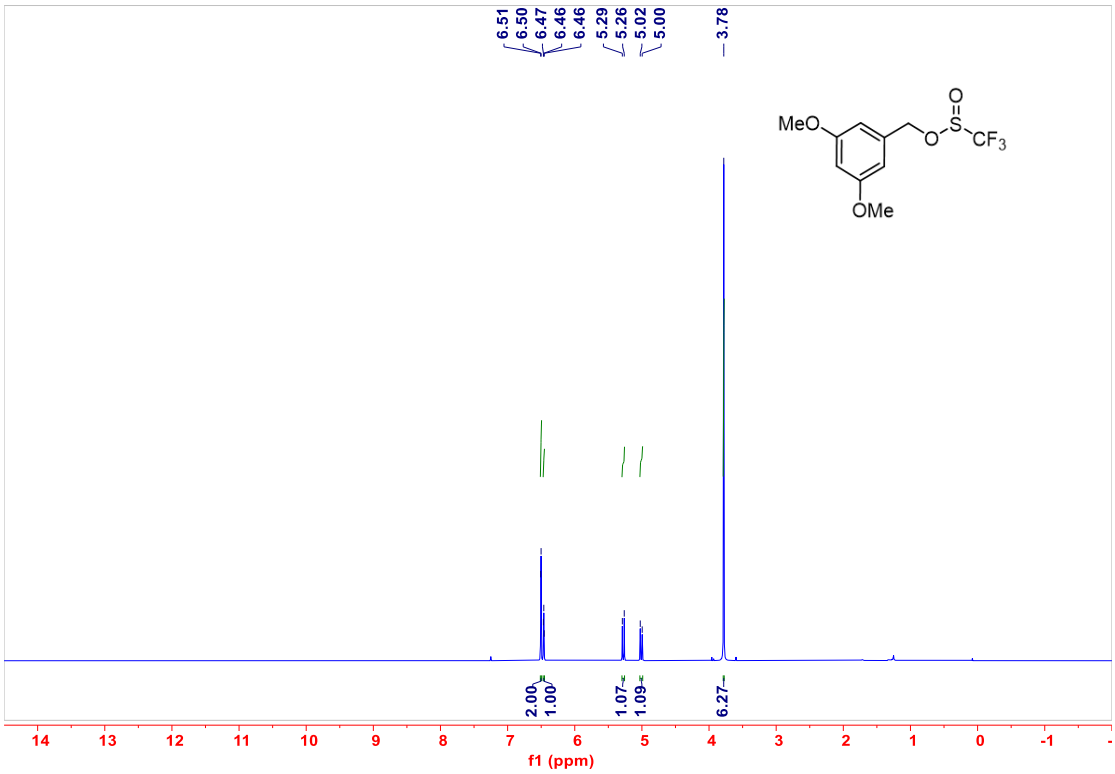
f1 (ppm)


158.3
132.7
131.7
124.9
121.6
121.1
118.3
115.1
112.5
111.3
55.8
50.6
OMe
O
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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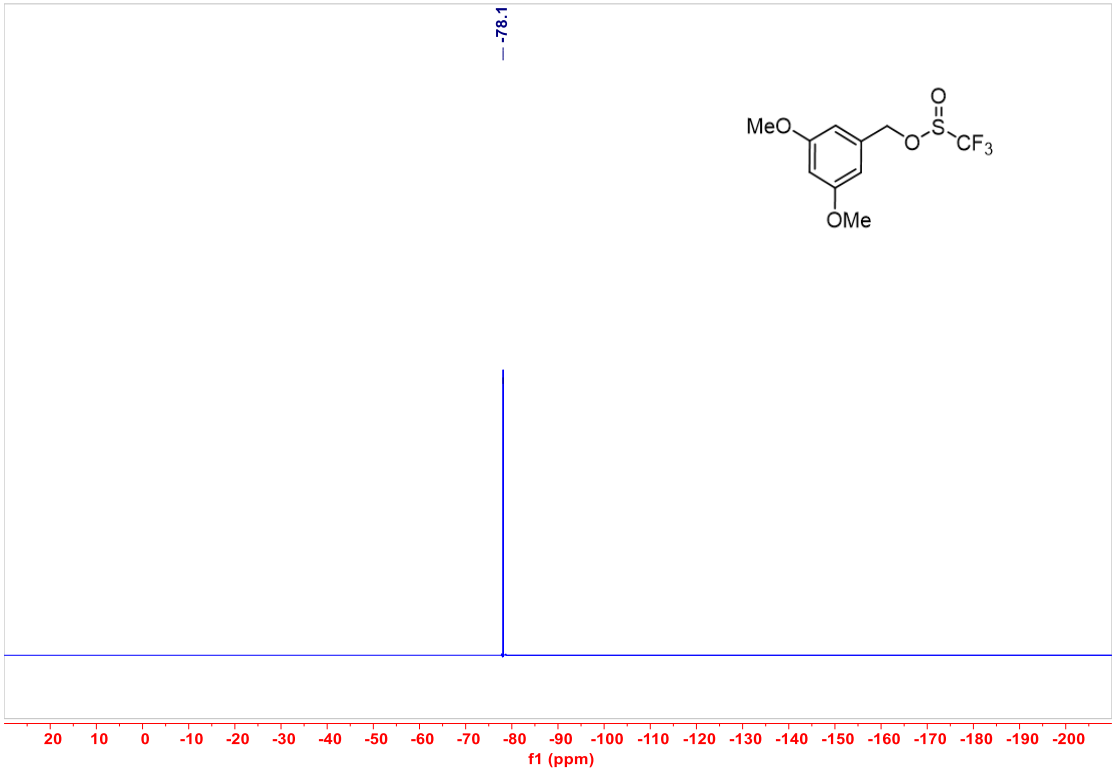
6.50
6.47
6.46
6.46
5.29
5.26
5.02
5.00
3.78
MeO
OMe
O
S
CF3
2.00
1.00
1.07
1.09
6.27
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.1
MeO
OMe
O
S
CF3
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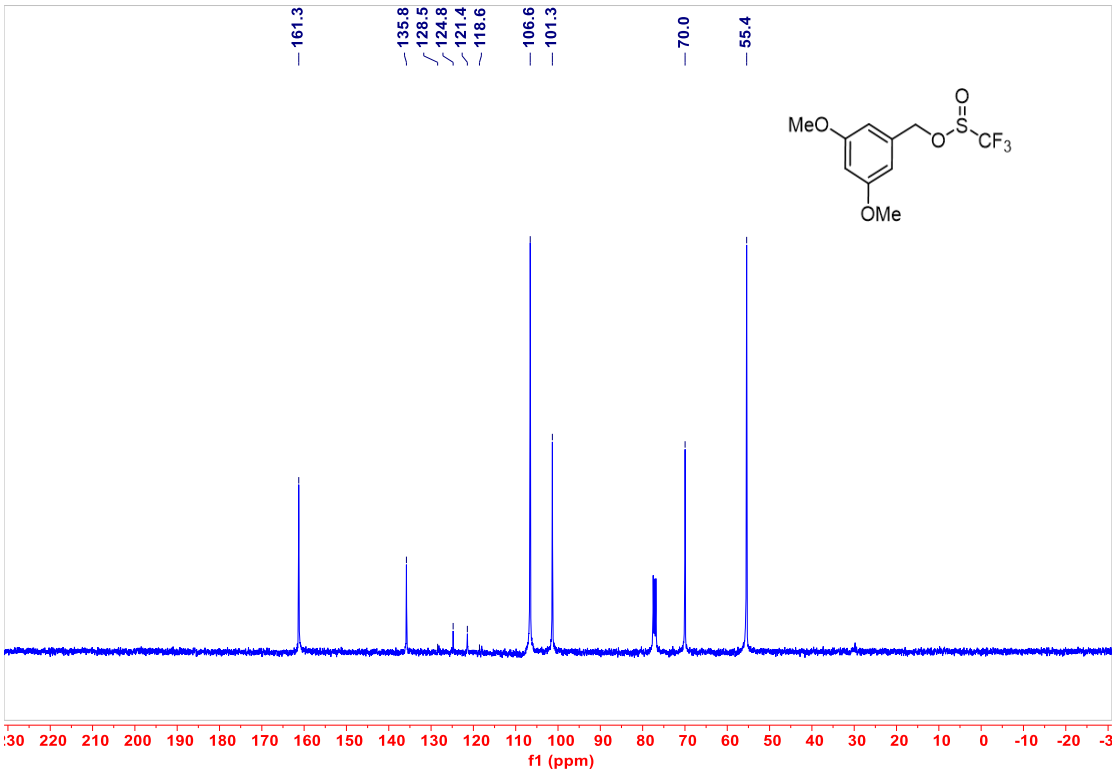
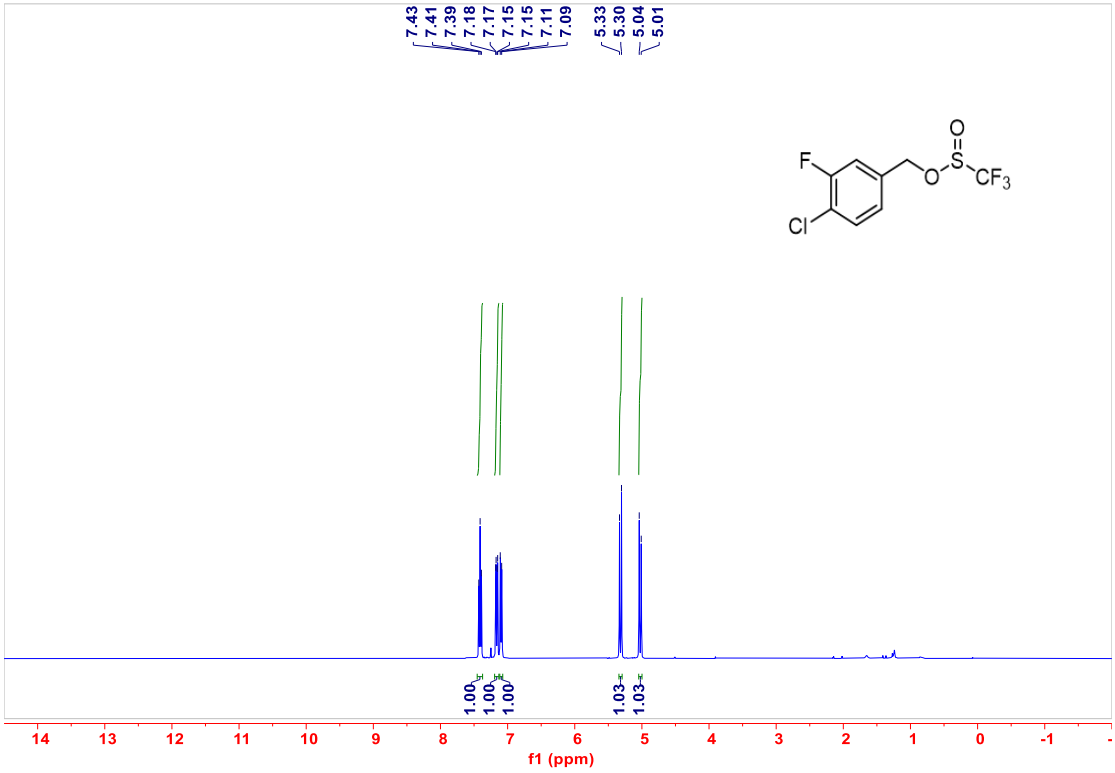
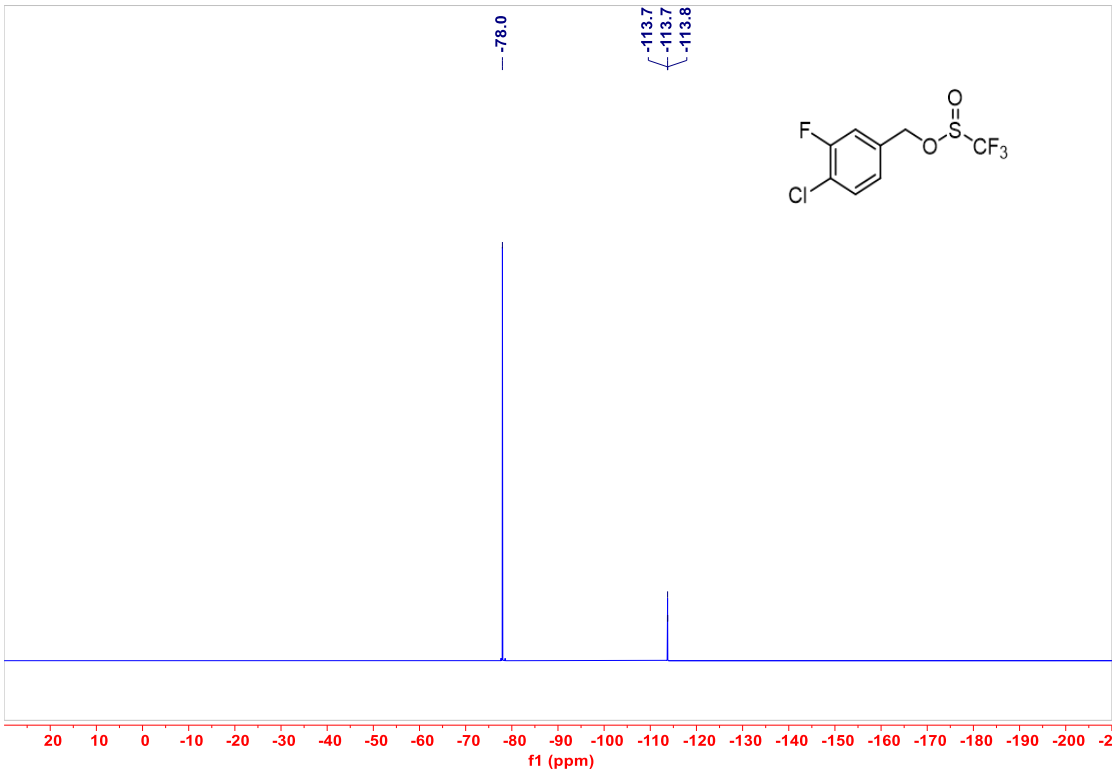
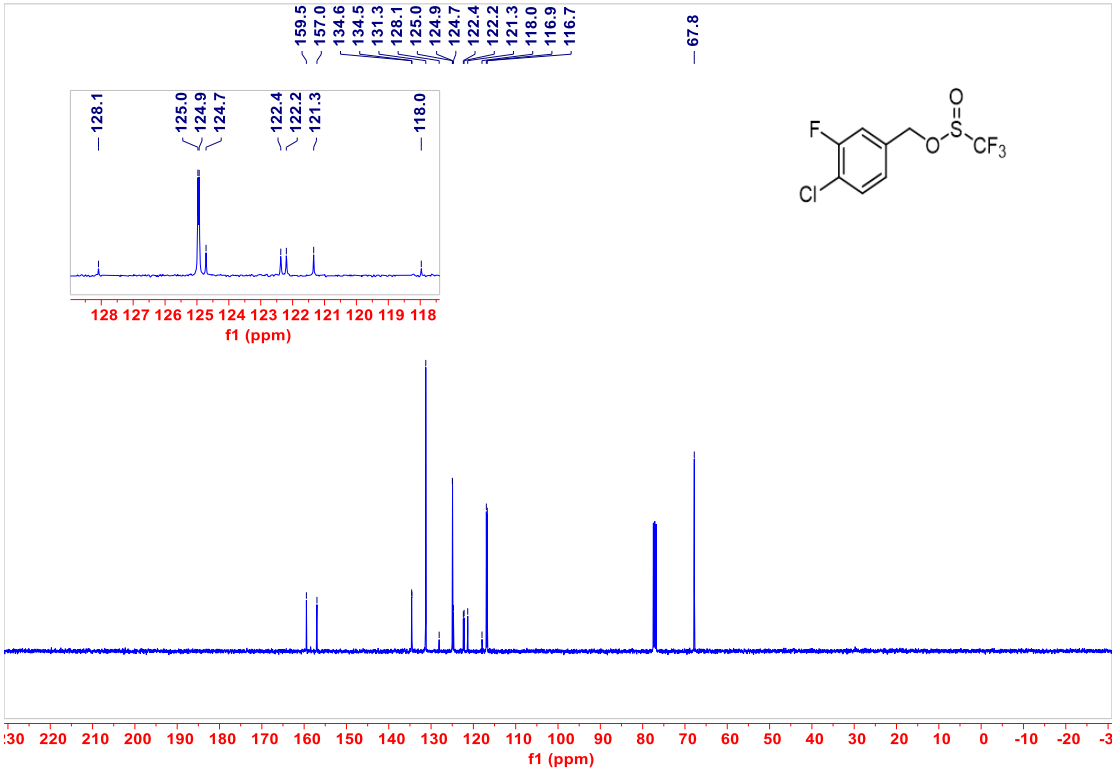
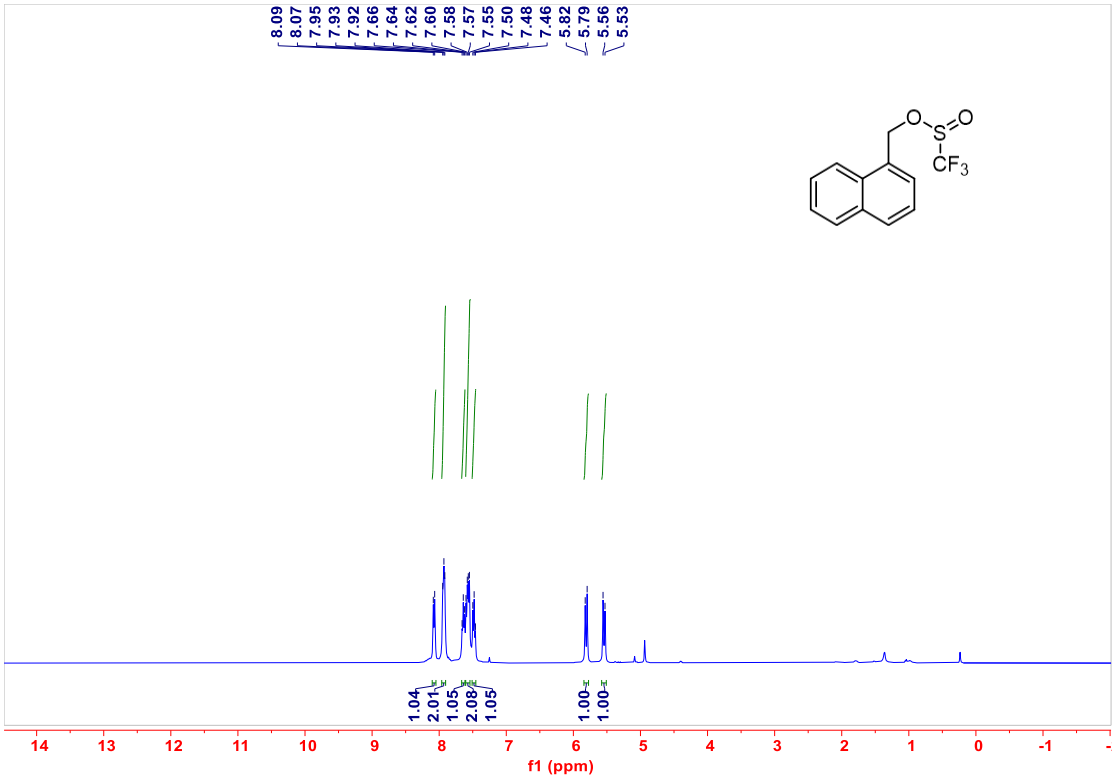
f1 (ppm)


161.3
135.8
128.5
124.8
121.4
118.6
106.6
101.3
70.0
55.4
MeO
OMe
O
S
CF3
f1 (ppm)


7.43
7.41
7.39
7.18
7.17
7.15
7.15
7.11
7.09
5.33
5.30
5.04
5.01
F
Cl
O
S
CF3
1.00
1.00
1.00
1.03
1.03
f1 (ppm)


-78.0
-113.7
-113.7
-113.8
F
Cl
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


159.5
157.0
134.6
134.5
131.3
128.1
125.0
124.9
124.7
122.4
122.2
121.3
118.0
116.9
116.7
67.8
128.1
125.0
124.9
124.7
122.4
122.2
121.3
118.0
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
F
Cl
O
S
O
CF3
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)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7.93
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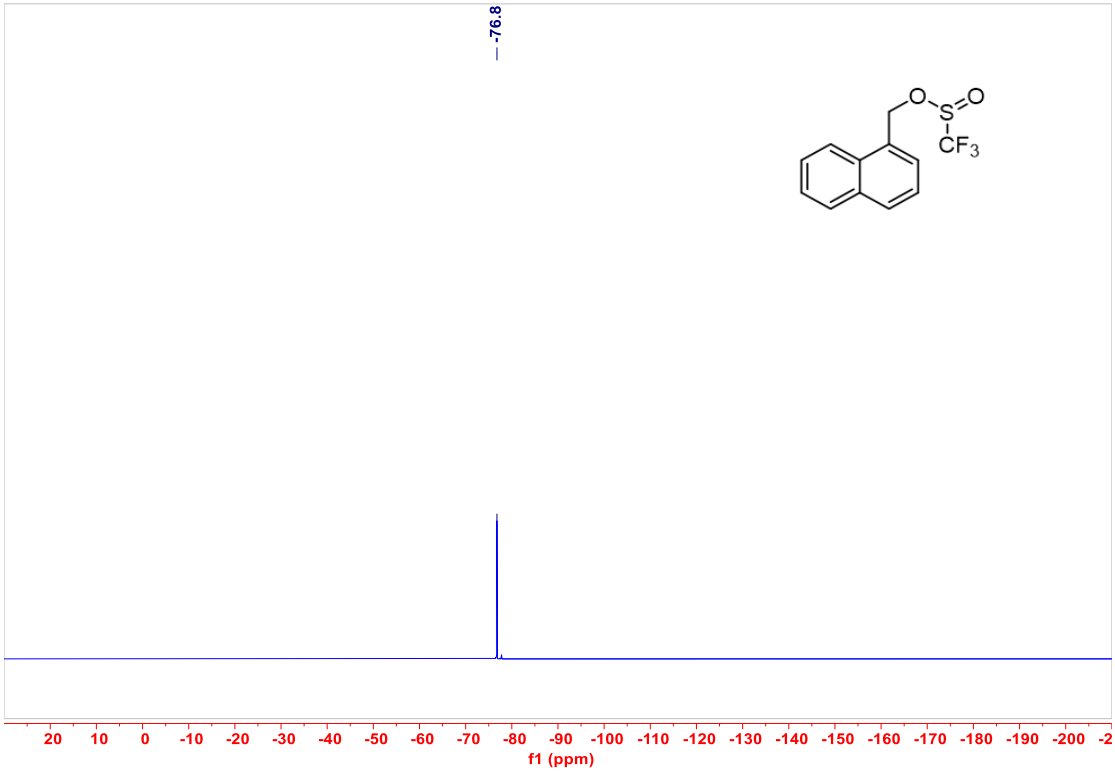
7.62
7.60
7.58
7.57
7.55
7.50
7.48
7.46
5.82
5.79
5.56
5.53
O
S
O
CF3
1.04
2.01
1.05
2.08
1.05
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-76.8
O
S
O
CF3
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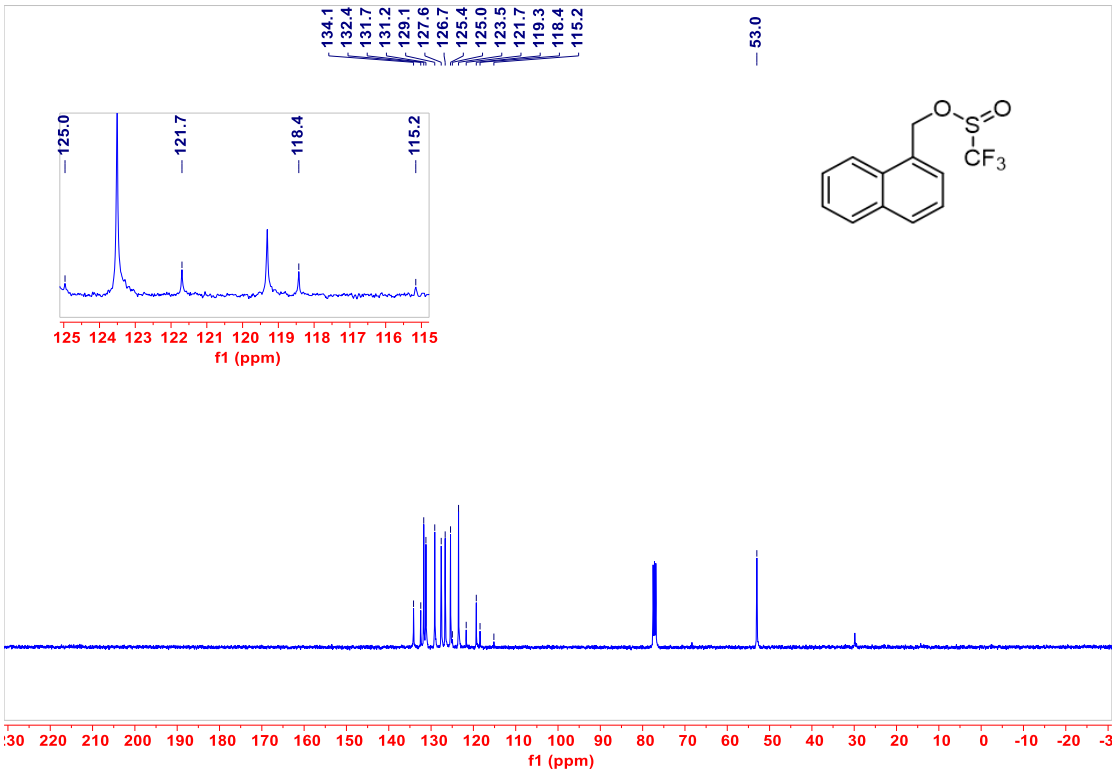
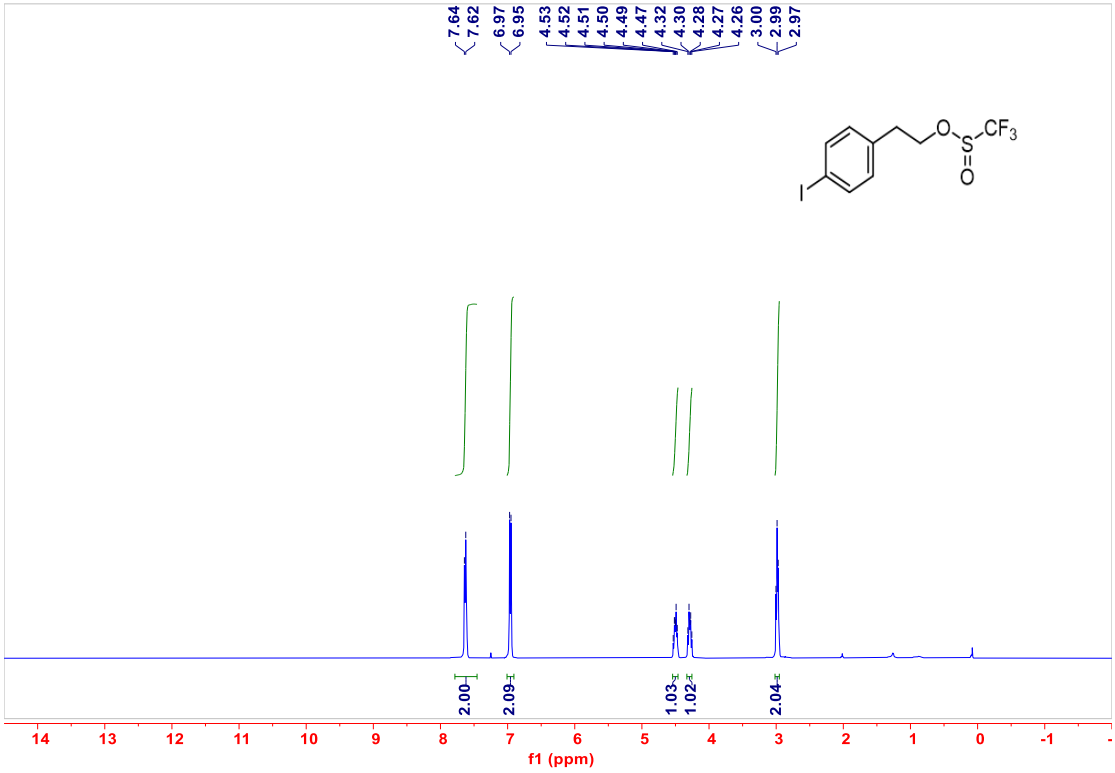
f1 (ppm)


134.1
132.4
131.7
131.2
129.1
127.6
126.7
125.4
125.0
123.5
121.7
119.3
118.4
115.2
53.0
125.0
121.7
118.4
115.2
125 124 123 122 121 120 119 118 117 116 115
f1 (ppm)
O
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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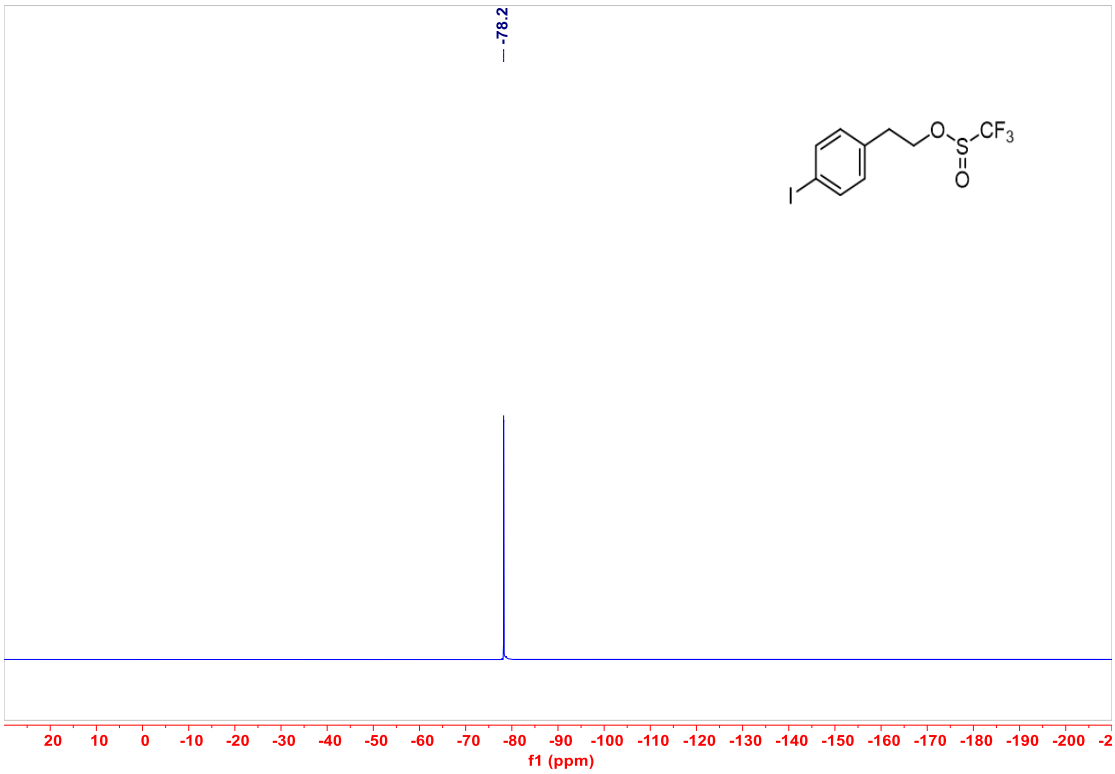
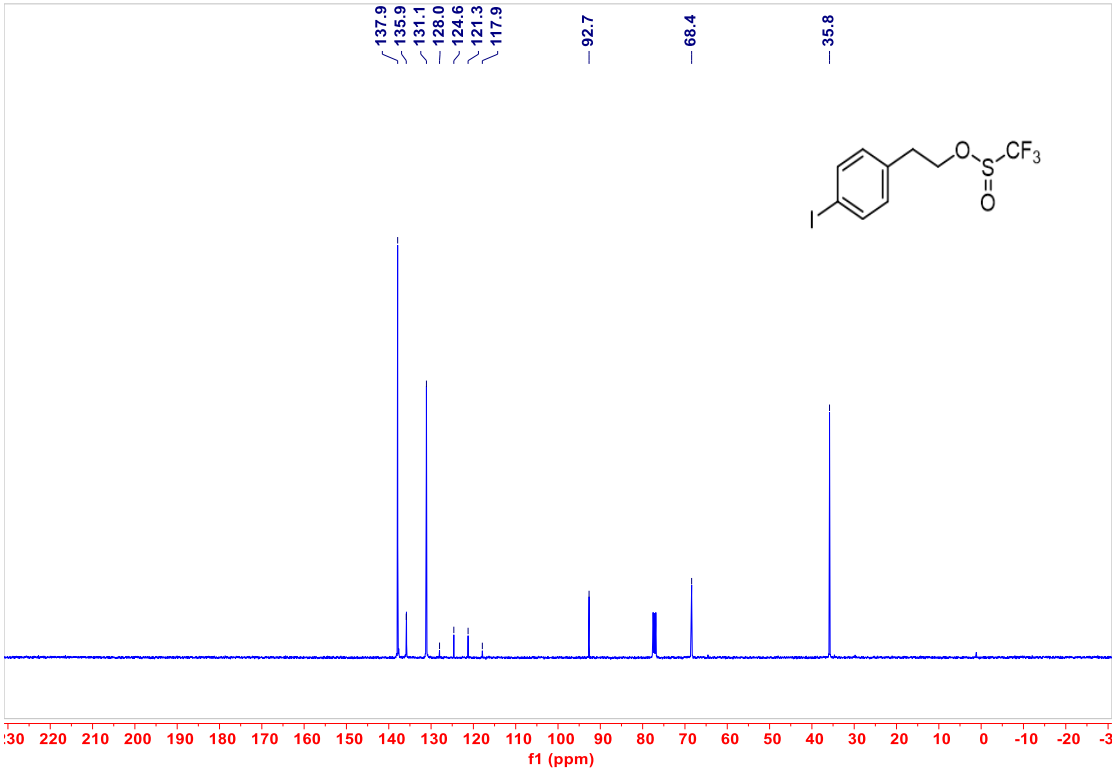
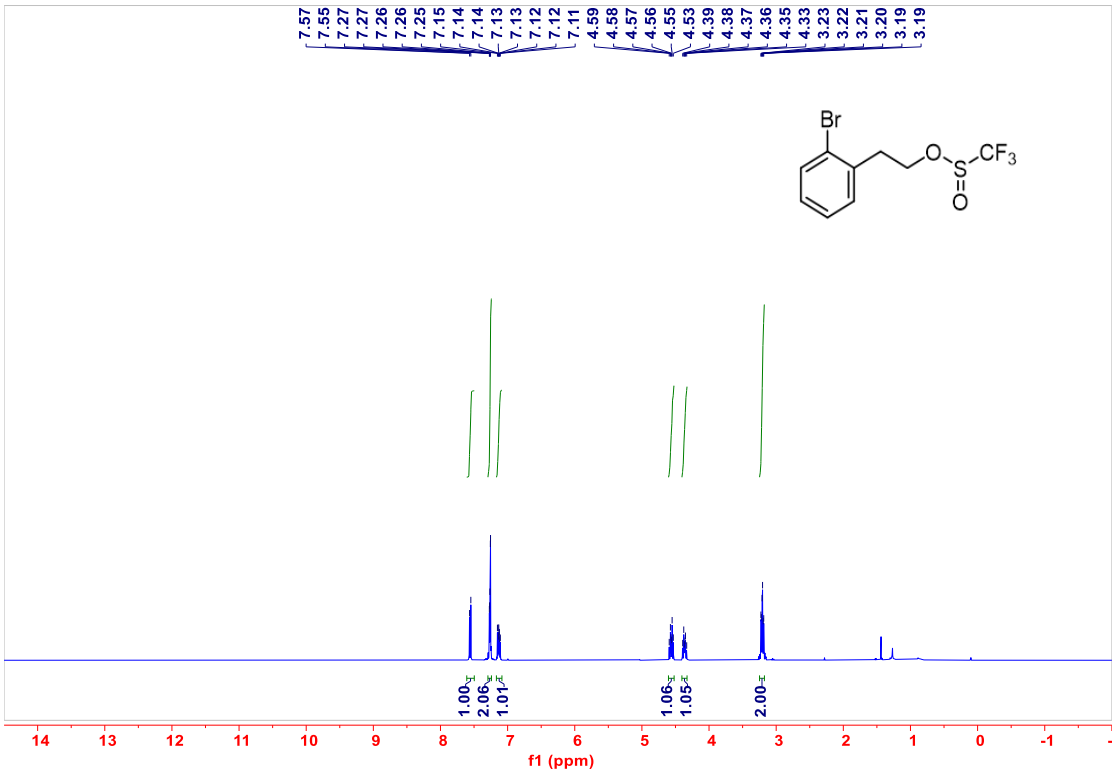
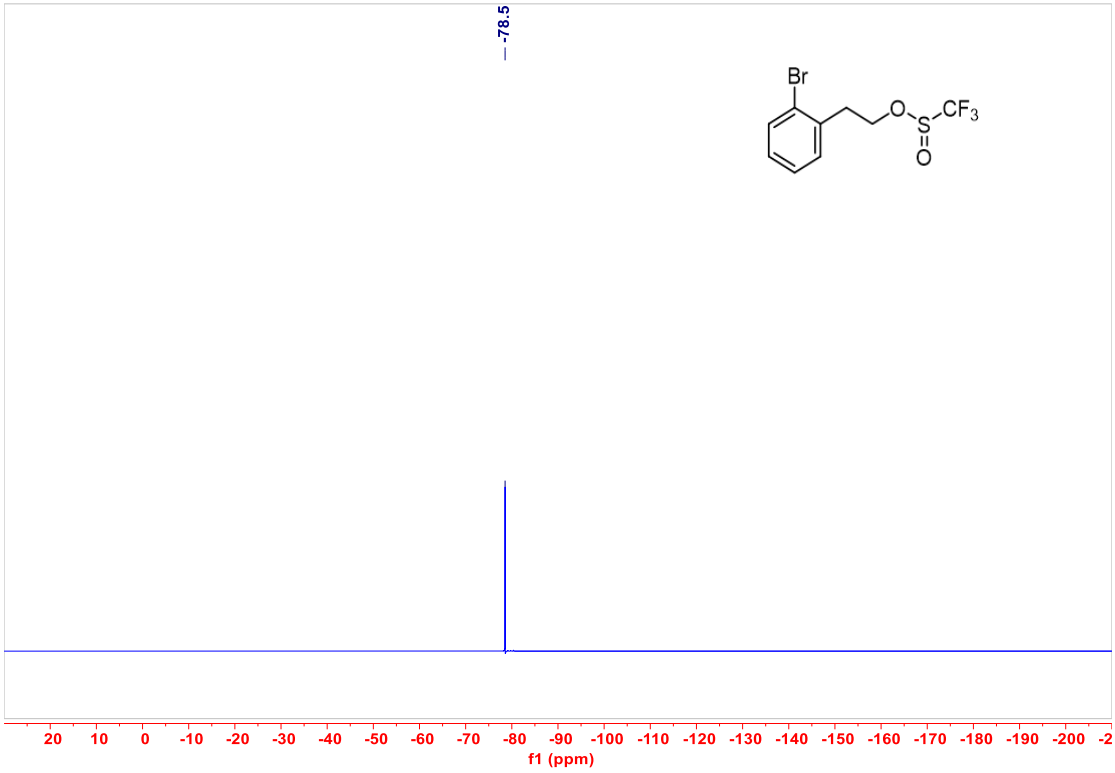
4.47
4.32
4.30
4.28
4.27
4.26
3.00
2.99
2.97
O
S
CF3
O
I
2.00
2.09
1.03
1.02
2.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.2
O
S
CF3
O
I
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


137.9
135.9
131.1
128.0
124.6
121.3
117.9
92.7
68.4
35.8
O
S
CF3
O
I
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.57 7.55 7.27 7.27 7.26 7.26 7.25 7.15 7.14 7.14 7.13 7.13 7.12 7.12 7.11 4.59 4.58 4.57 4.56 4.55 4.53 4.39 4.38 4.37 4.36 4.35 4.33 3.23 3.22 3.21 3.20 3.19 3.19
Br
O
S
CF3
O
1.00 2.06 1.01 1.06 1.05 2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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Br
O
S
CF3
O
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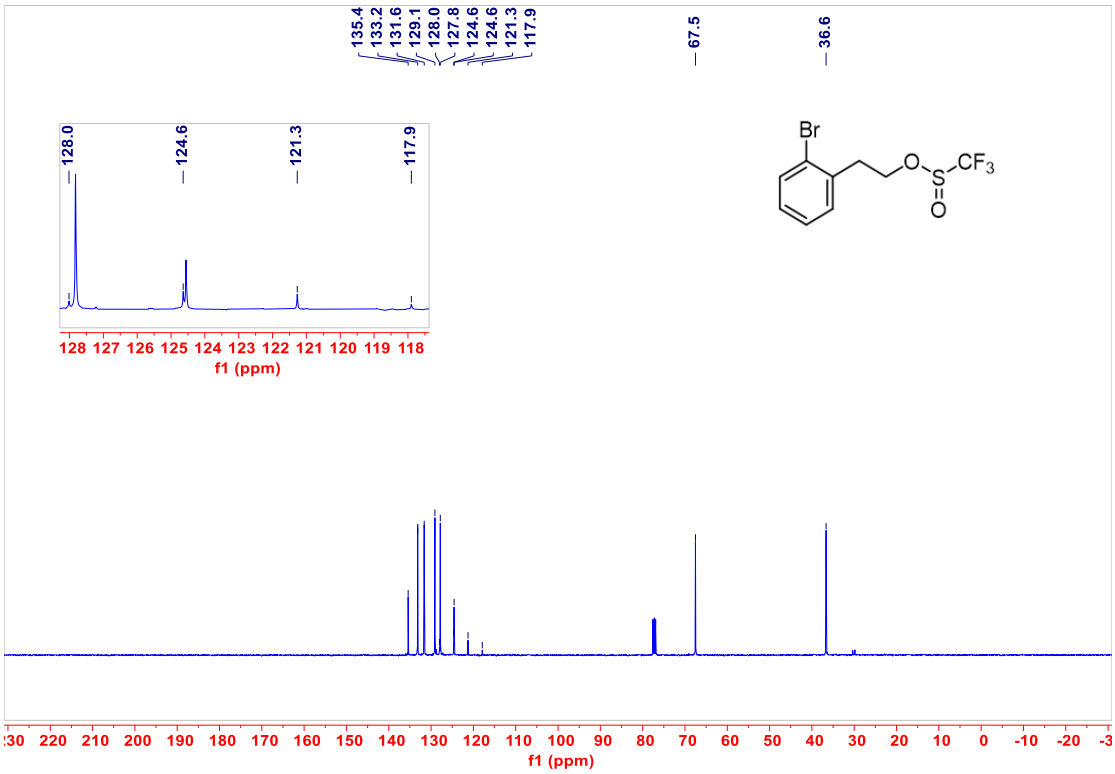
f1 (ppm)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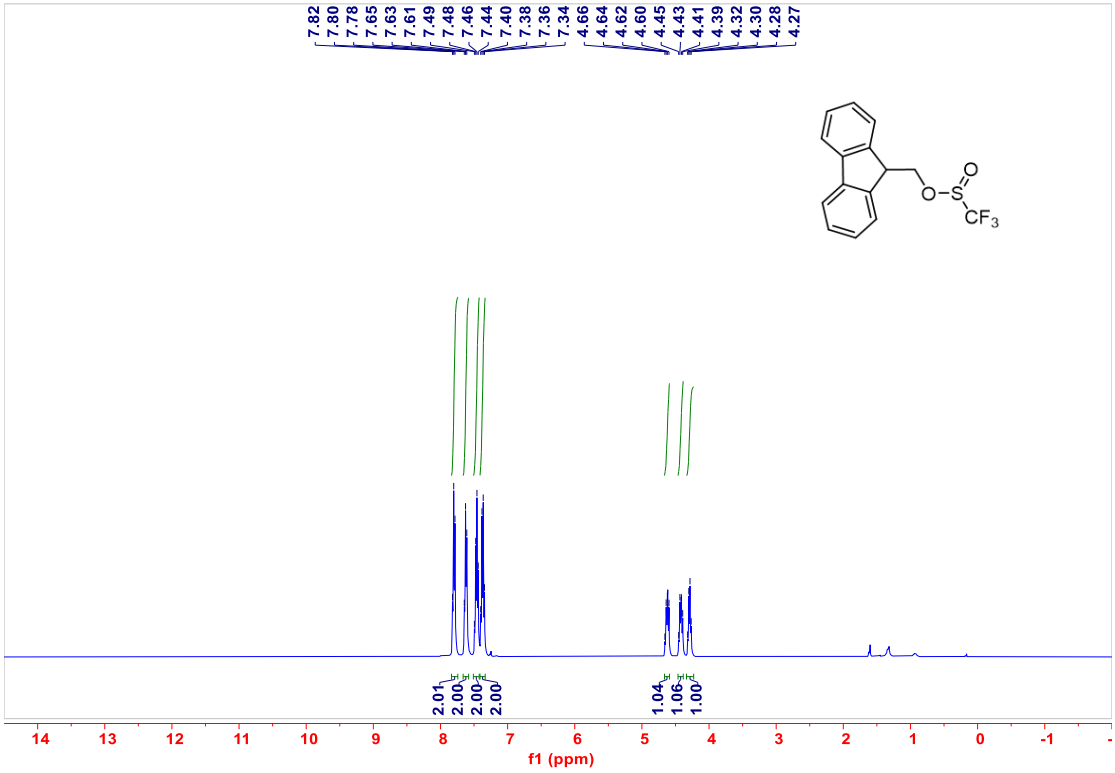
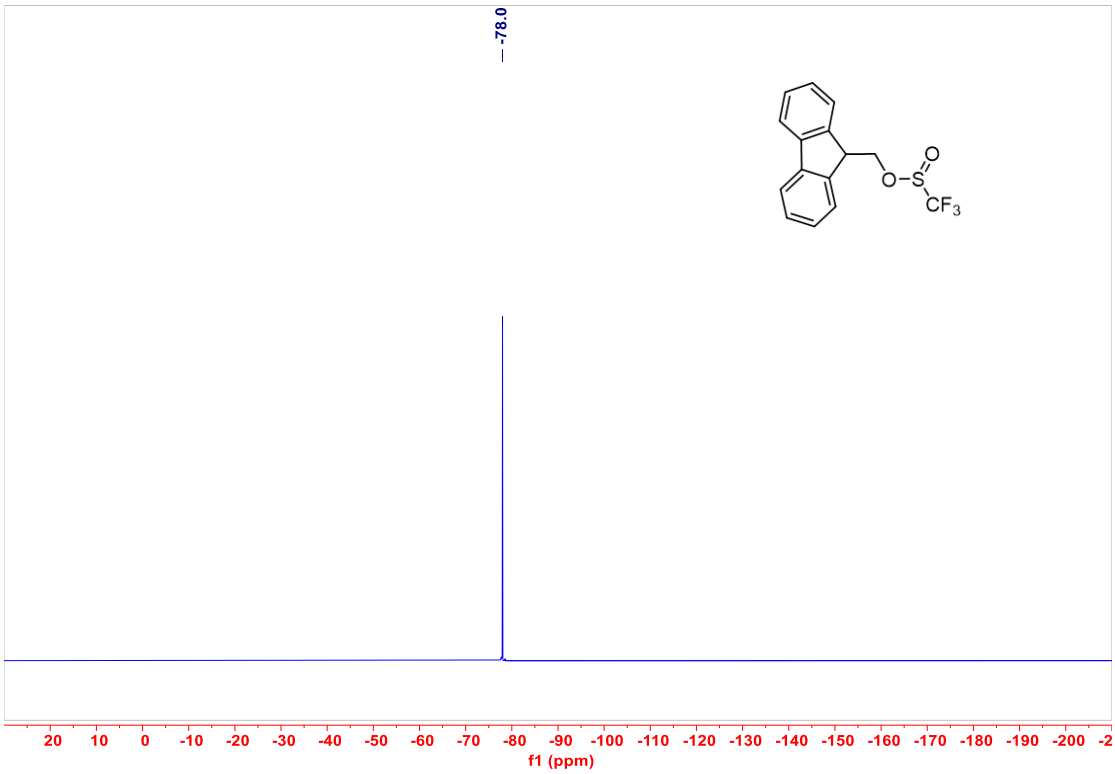
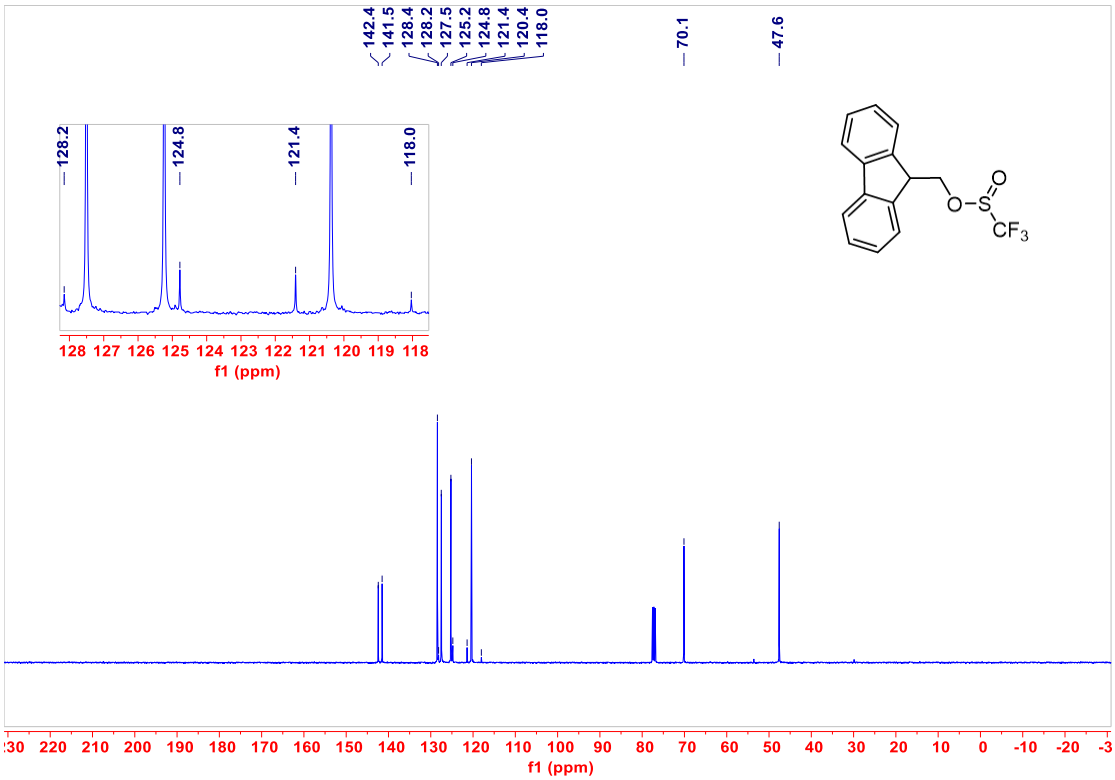
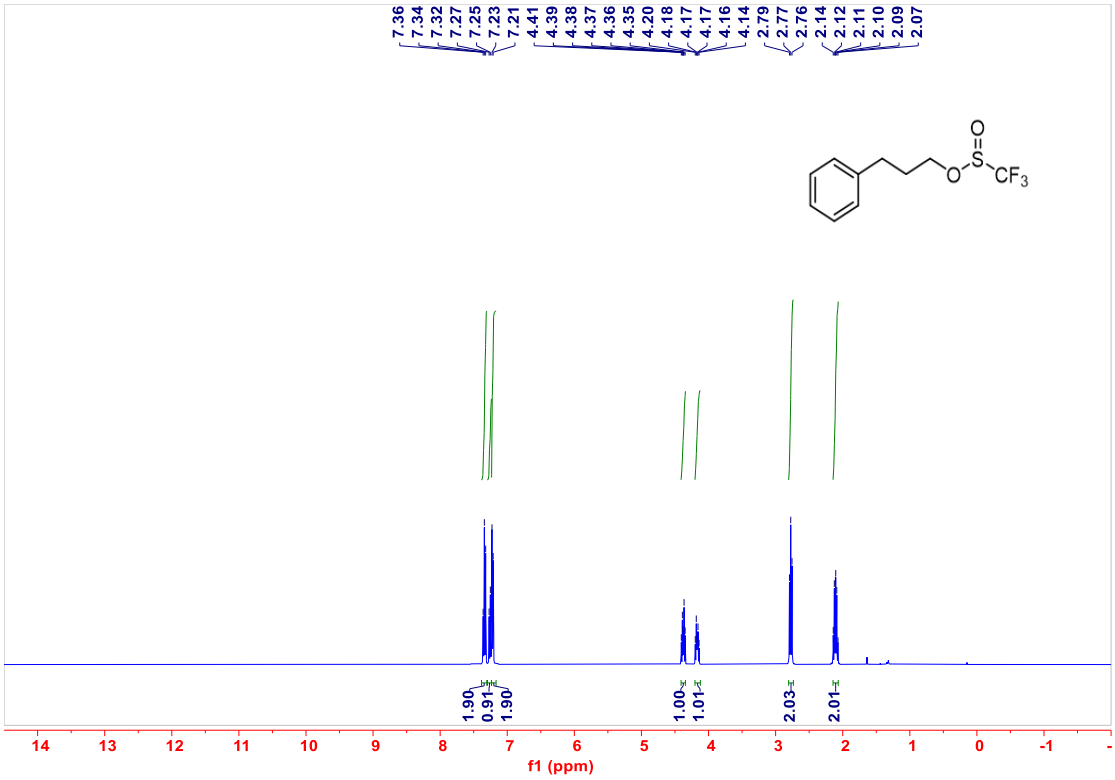
133.2
131.6
129.1
128.0
127.8
124.6
124.6
121.3
117.9
67.5
36.6
128.0
124.6
121.3
117.9
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
Br
O
S
CF3
O
f1 (ppm)


7.82
7.80
7.78
7.65
7.63
7.61
7.49
7.48
7.46
7.44
7.40
7.38
7.36
7.34
4.66
4.64
4.62
4.60
4.45
4.43
4.41
4.39
4.32
4.30
4.28
4.27
O
S
O
CF3
2.01
2.00
2.00
2.00
1.04
1.06
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.0
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


142.4
141.5
128.4
128.2
127.5
125.2
124.8
121.4
120.4
118.0
70.1
47.6
128.2
124.8
121.4
118.0
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
O
S
O
CF3
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)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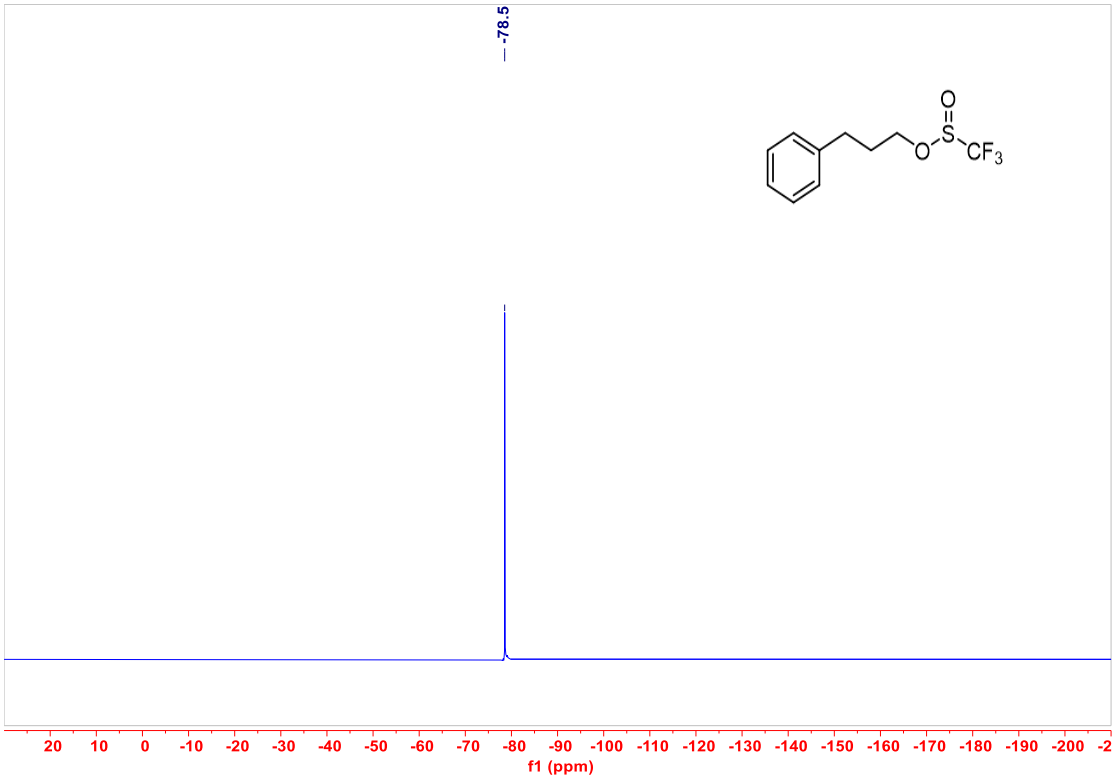
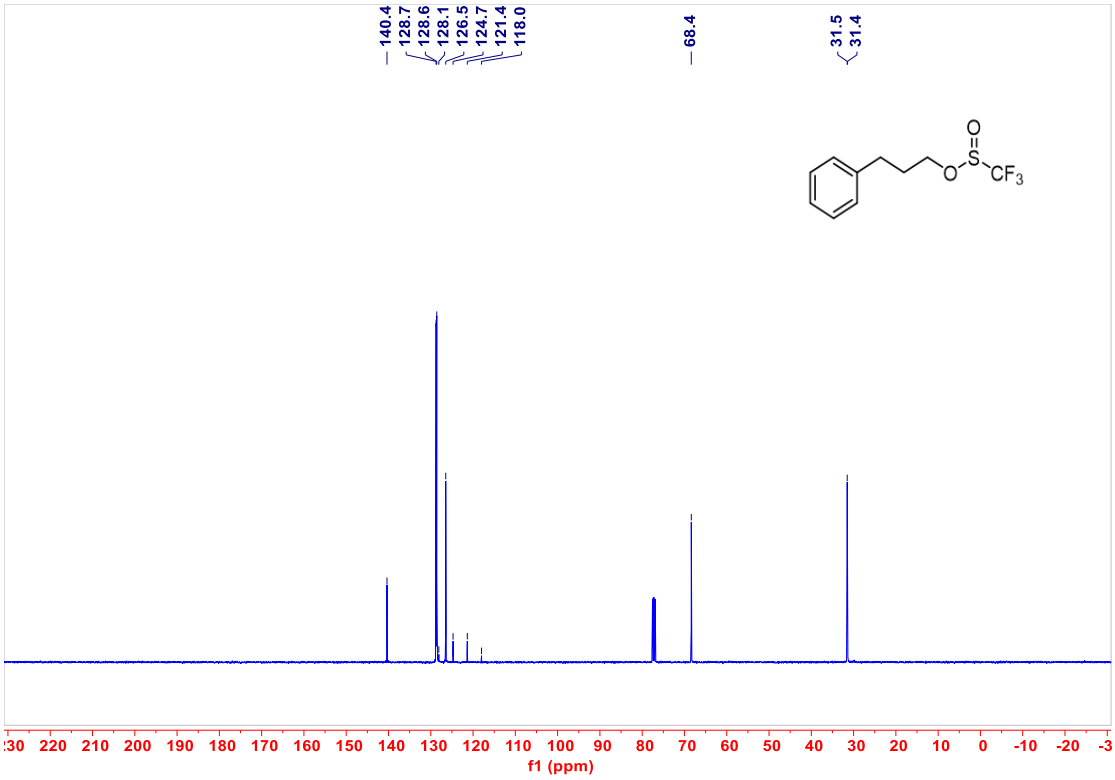
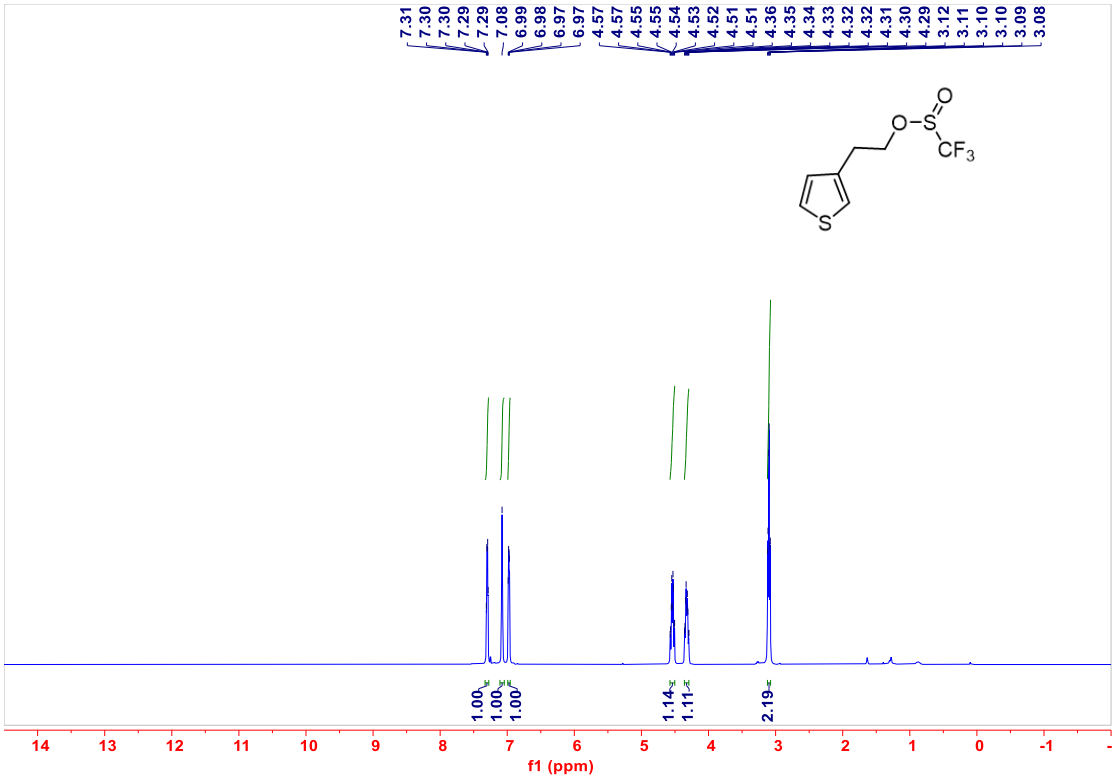
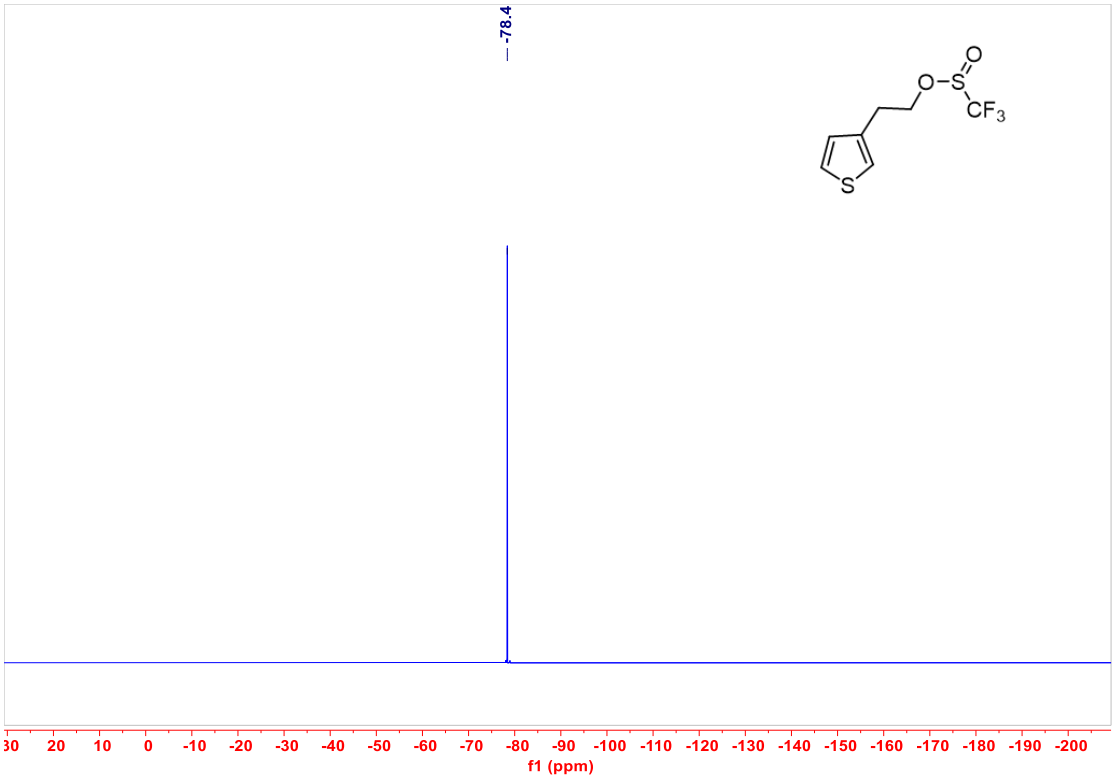
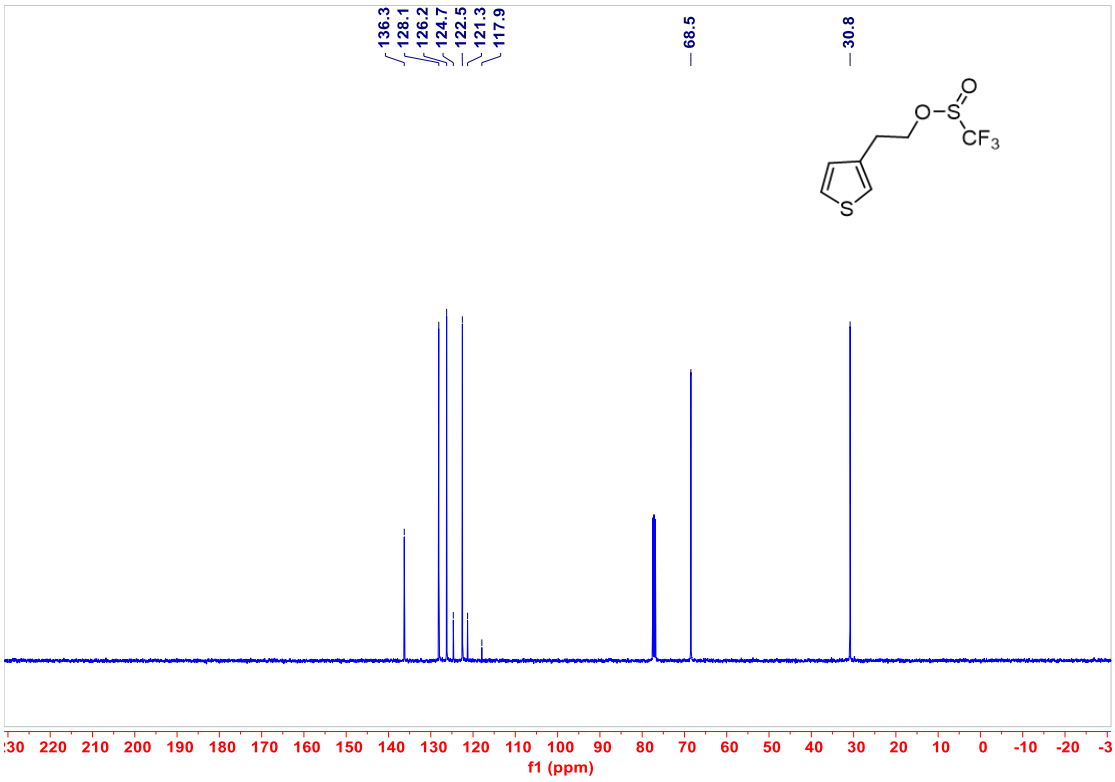
7.34
7.32
7.27
7.25
7.23
7.21
4.41
4.39
4.38
4.37
4.36
4.35
4.20
4.18
4.17
4.17
4.16
4.14
2.79
2.77
2.76
2.14
2.12
2.11
2.10
2.09
2.07
O
S
O
CF3
1.90
0.91
1.90
1.00
1.01
2.03
2.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

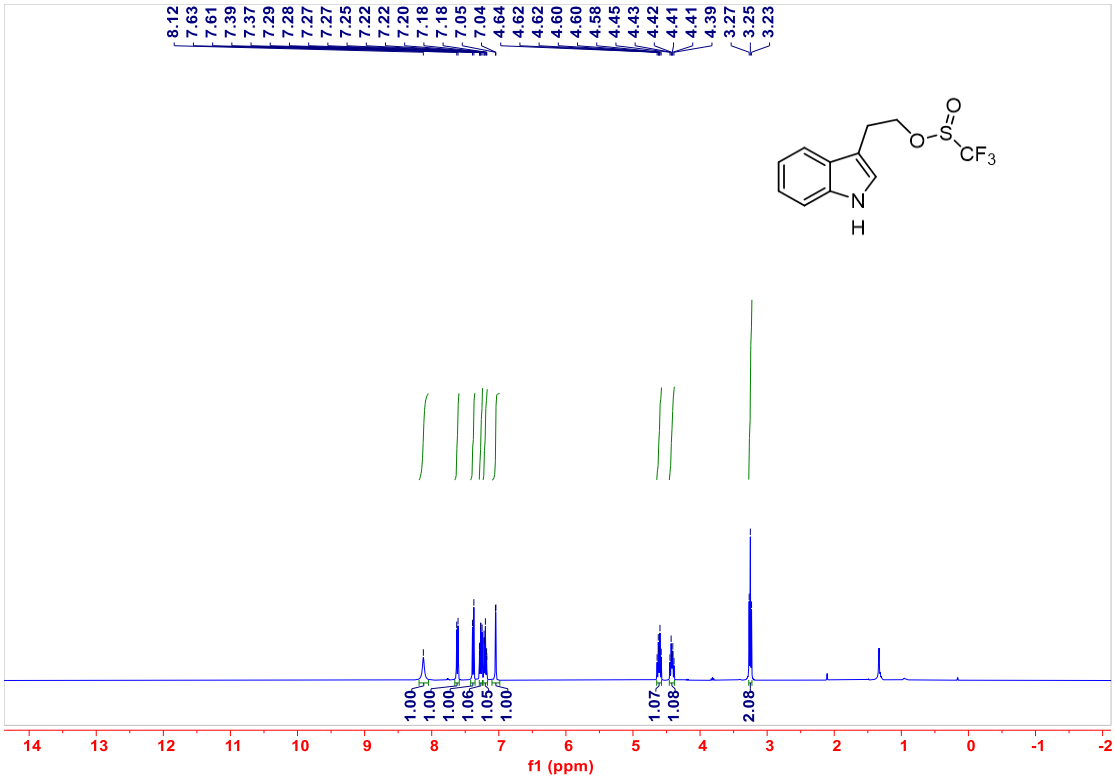

-78.5
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

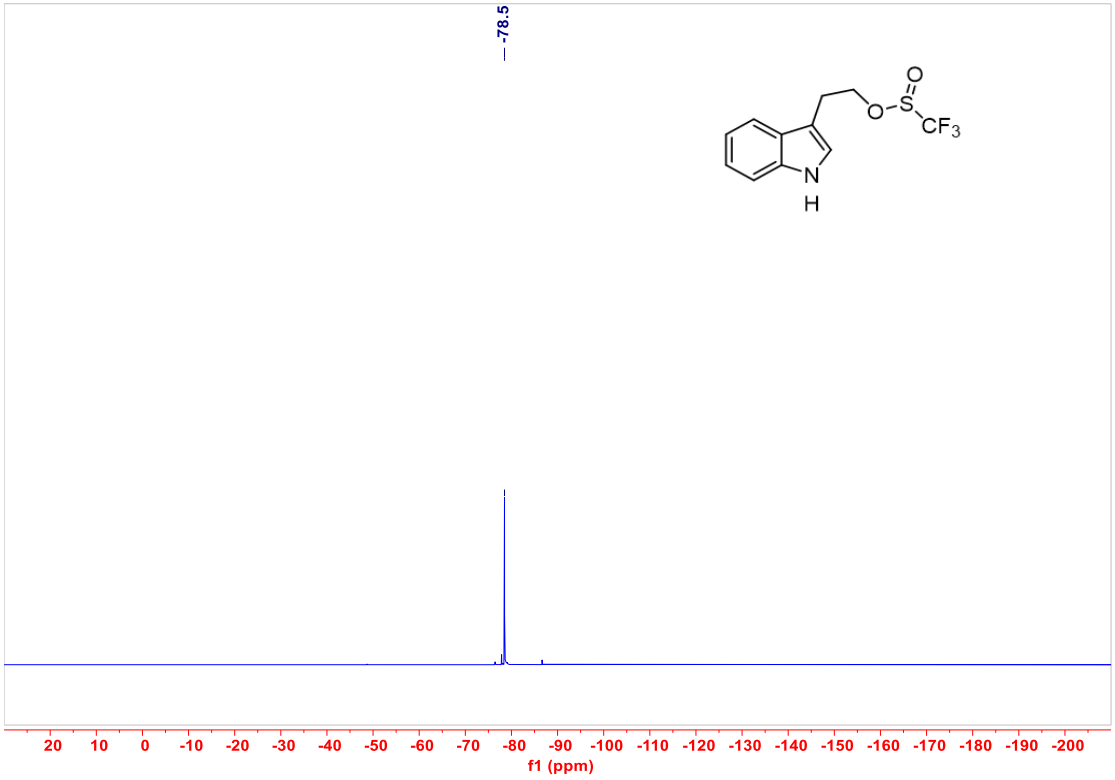

140.4
128.7
128.6
128.1
126.5
124.7
121.4
118.0
68.4
31.5
31.4
O
S
O
CF3
f1 (ppm)

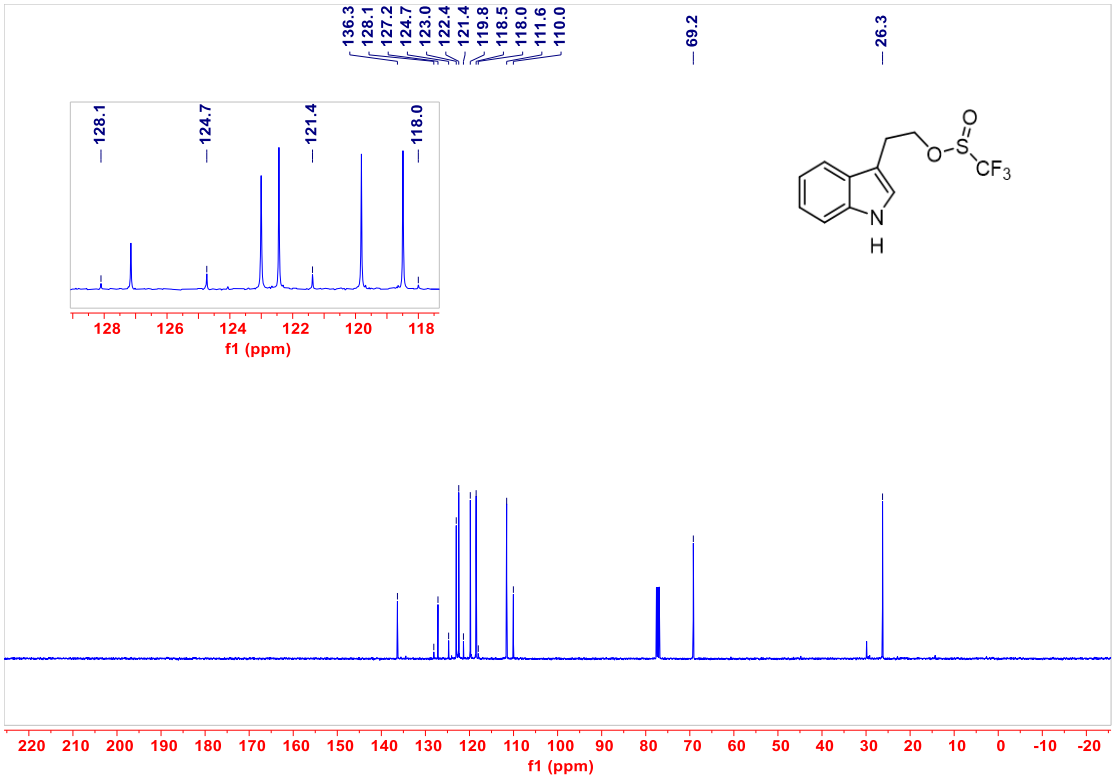

7.31
7.30
7.30
7.29
7.29
7.08
6.99
6.98
6.97
6.97
4.57
4.57
4.55
4.55
4.54
4.53
4.52
4.51
4.51
4.36
4.35
4.34
4.33
4.32
4.32
4.31
4.30
4.29
3.12
3.11
3.10
3.10
3.09
3.08
O
S
O
CF3
S
1.00
1.00
1.00
1.14
1.11
2.19
f1 (ppm)


-78.4
O
O-S
CF3
S
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


136.3
128.1
126.2
124.7
122.5
121.3
117.9
68.5
30.8
O
O-S
CF3
S
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


8.12
7.63
7.61
7.39
7.37
7.29
7.28
7.27
7.27
7.25
7.22
7.22
7.20
7.18
7.18
7.05
7.04
4.64
4.62
4.62
4.60
4.60
4.58
4.45
4.43
4.42
4.41
4.41
4.39
3.27
3.25
3.23
1.00
1.00
1.00
1.06
1.05
1.00
1.07
1.08
2.08
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


-78.5
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)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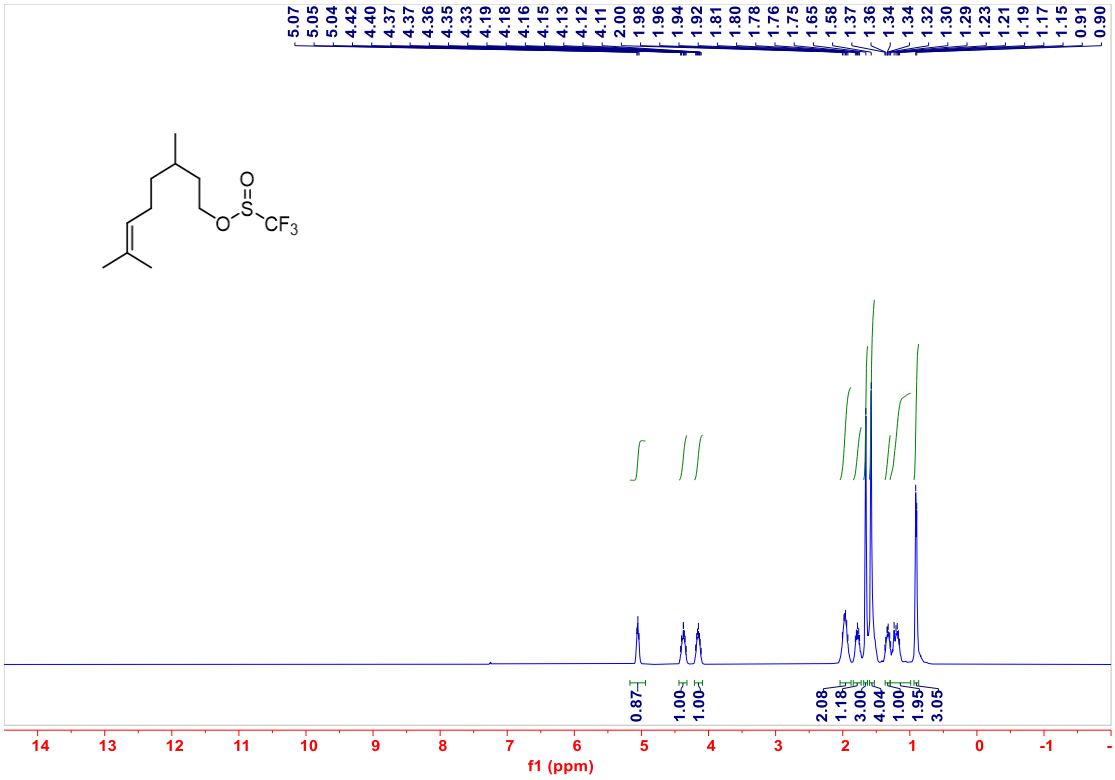
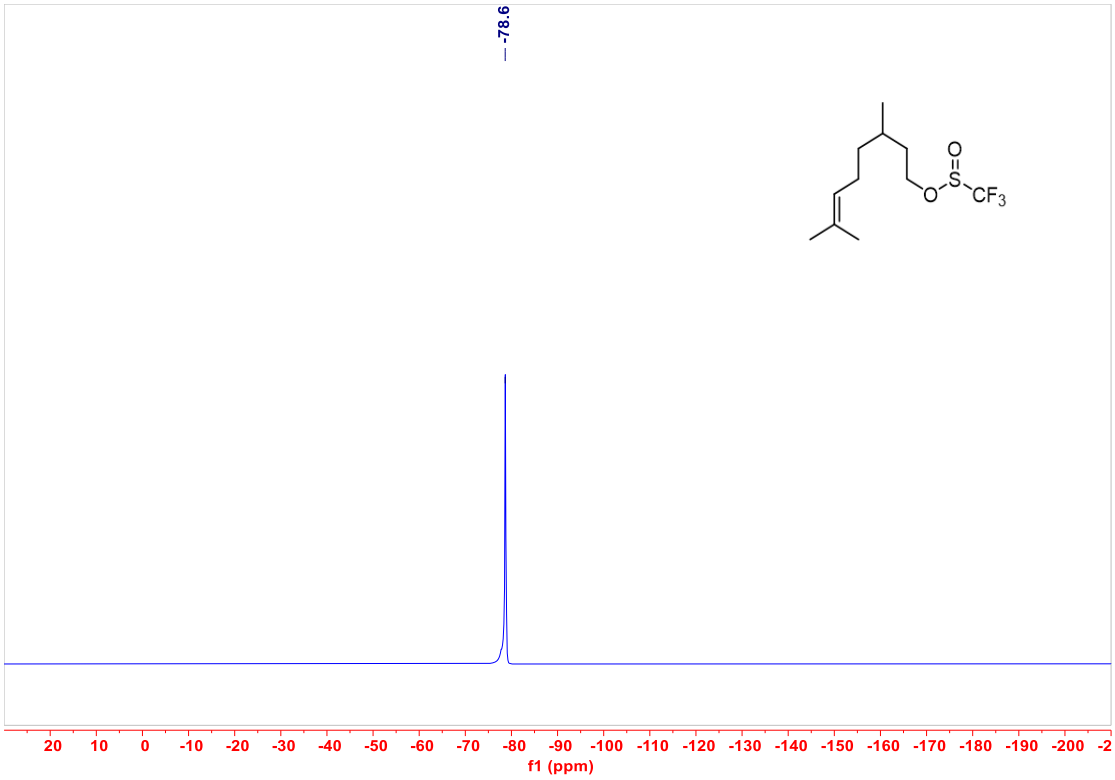
127.2
124.7
123.0
122.4
121.4
119.8
118.5
118.0
111.6
110.0
69.2
26.3
128.1
124.7
121.4
118.0
128 126 124 122 120 118
f1 (ppm)
O
S
O
CF3
N
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


5.07
5.05
5.04
4.42
4.40
4.37
4.37
4.36
4.35
4.33
4.19
4.18
4.16
4.15
4.13
4.12
4.11
2.00
1.98
1.96
1.94
1.92
1.81
1.80
1.78
1.76
1.75
1.65
1.58
1.37
1.36
1.34
1.34
1.32
1.30
1.29
1.23
1.21
1.19
1.17
1.15
0.91
0.90
O
S
O
CF3
0.87
1.00
1.00
2.08
1.18
3.00
4.04
1.00
1.95
3.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.6
O
S
O
CF3
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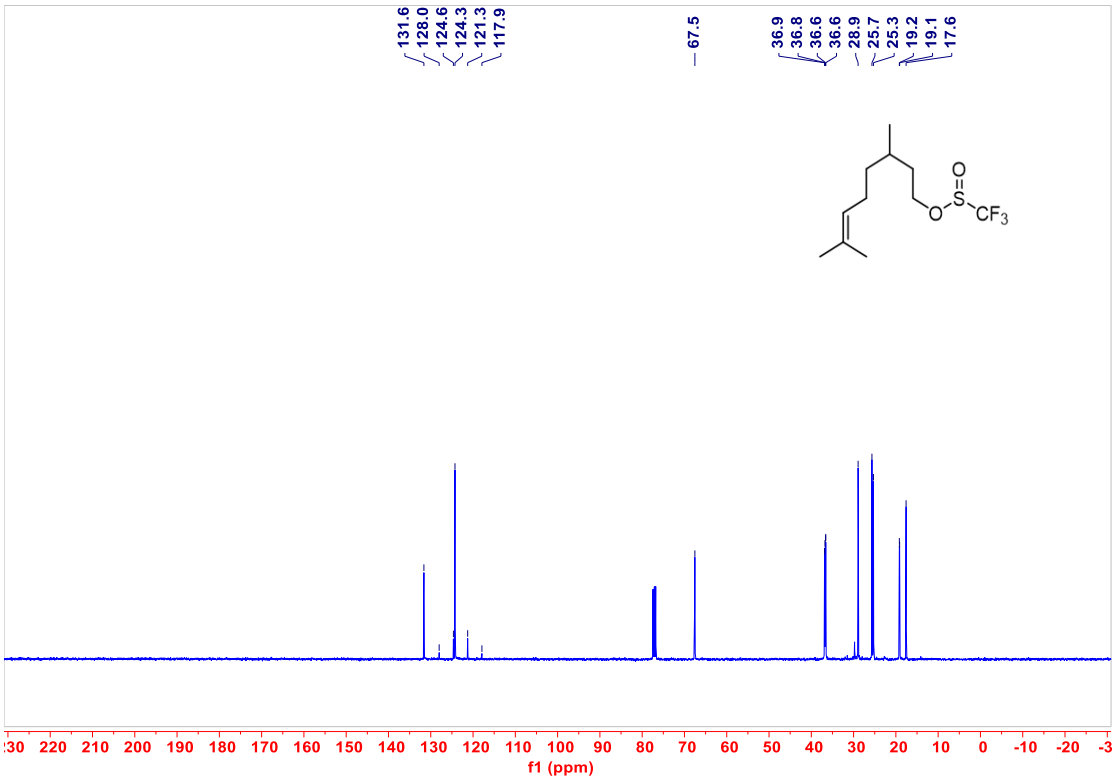
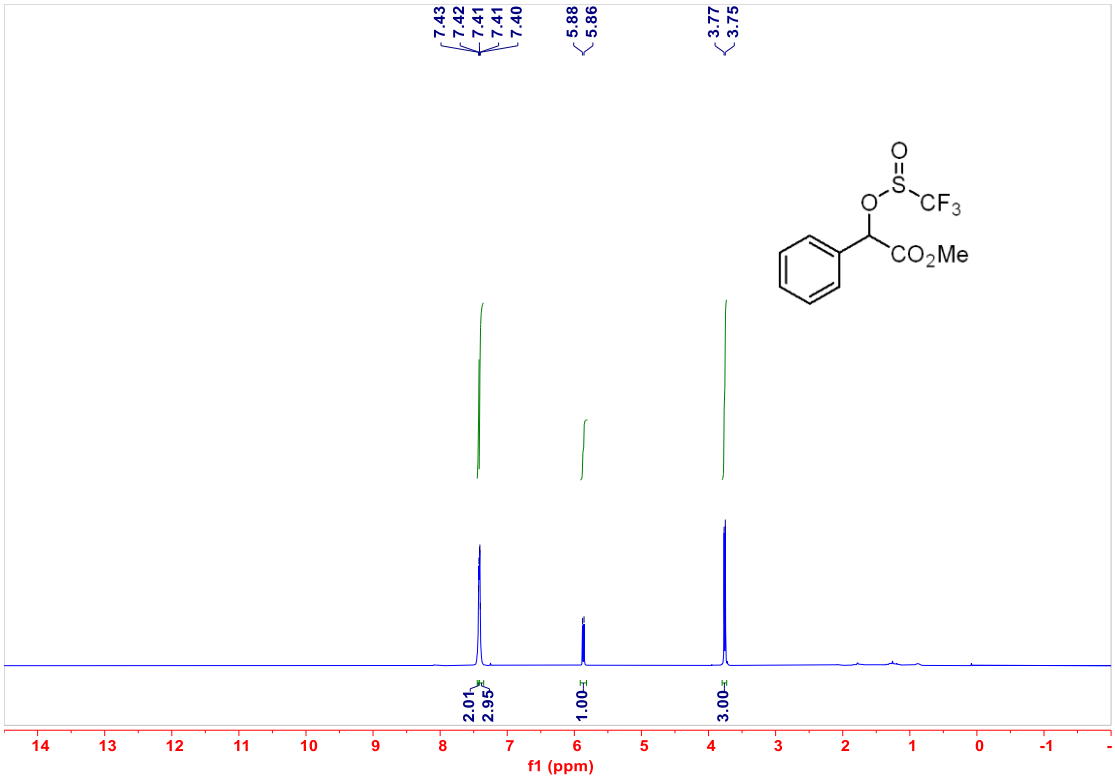
f1 (ppm)


131.6
128.0
124.6
124.3
121.3
117.9
67.5
36.9
36.8
36.6
36.6
28.9
25.7
25.3
19.2
19.1
17.6
O
S
O
CF3
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.43
7.42
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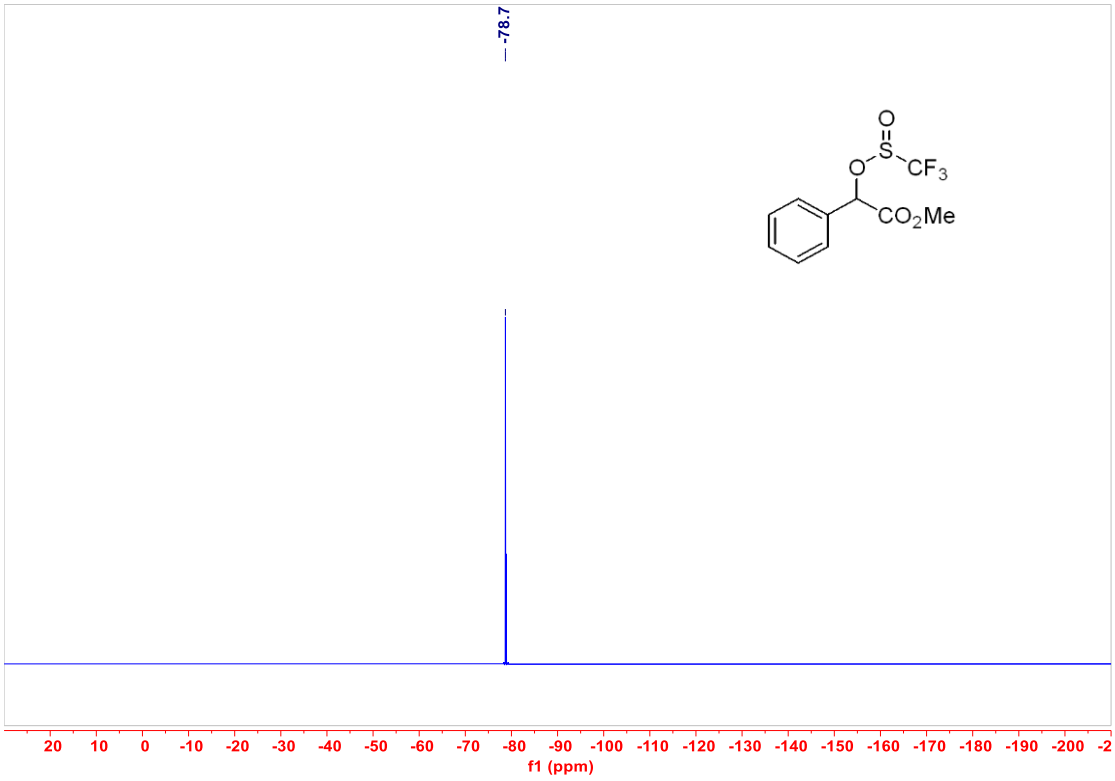
7.41
7.40
5.88
5.86
3.77
3.75
O
S
CF3
O
CO2Me
2.01
2.95
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.7
O
S
CF3
O
CO2Me
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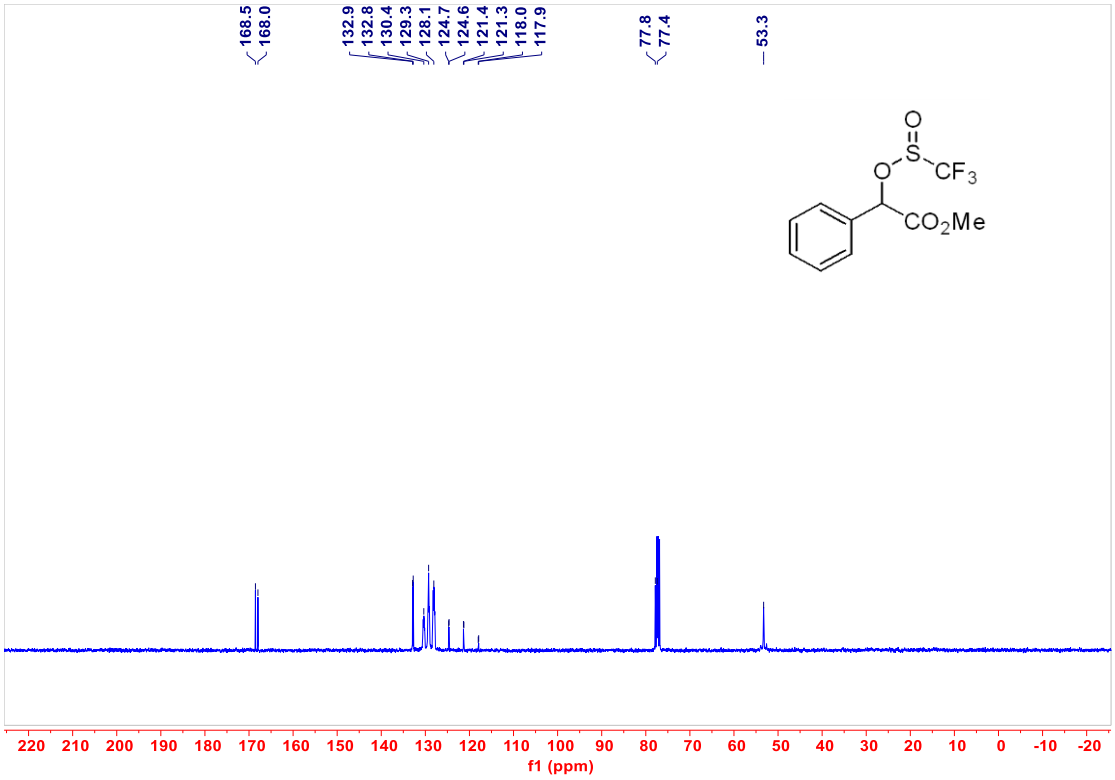
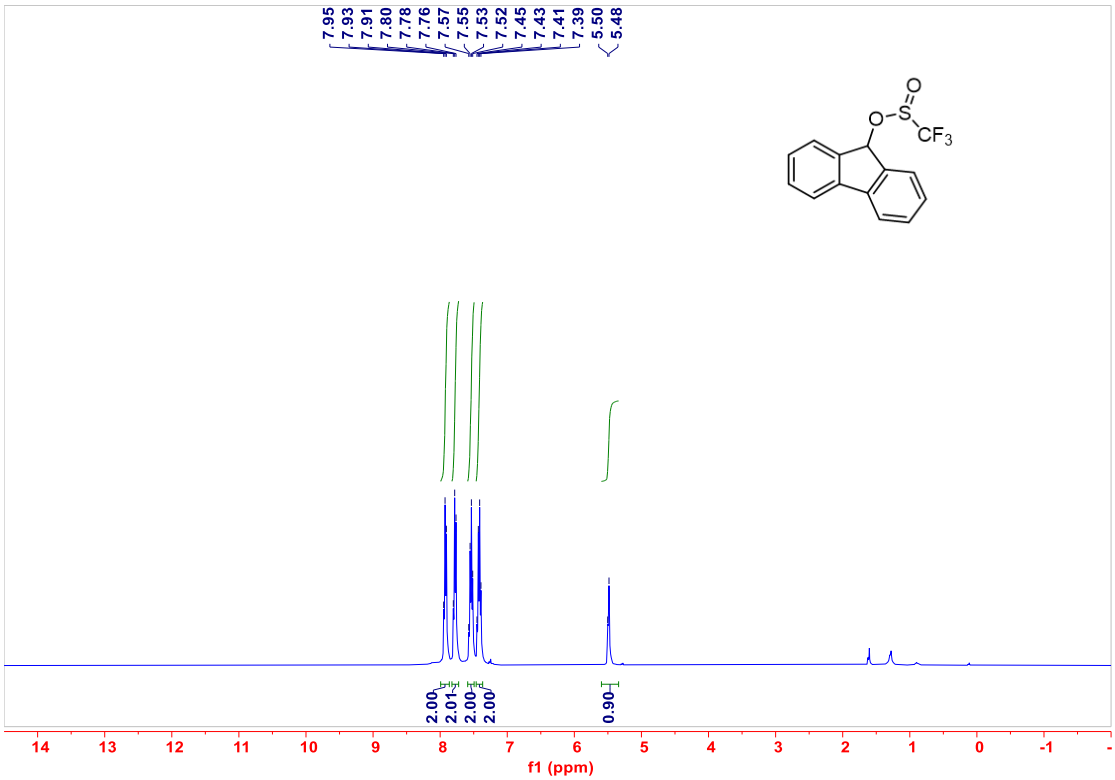
f1 (ppm)


168.5
168.0
132.9
132.8
130.4
129.3
128.1
124.7
124.6
121.4
121.3
118.0
117.9
77.8
77.4
53.3
O
S
O
CF3
CO2Me
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.93
7.91
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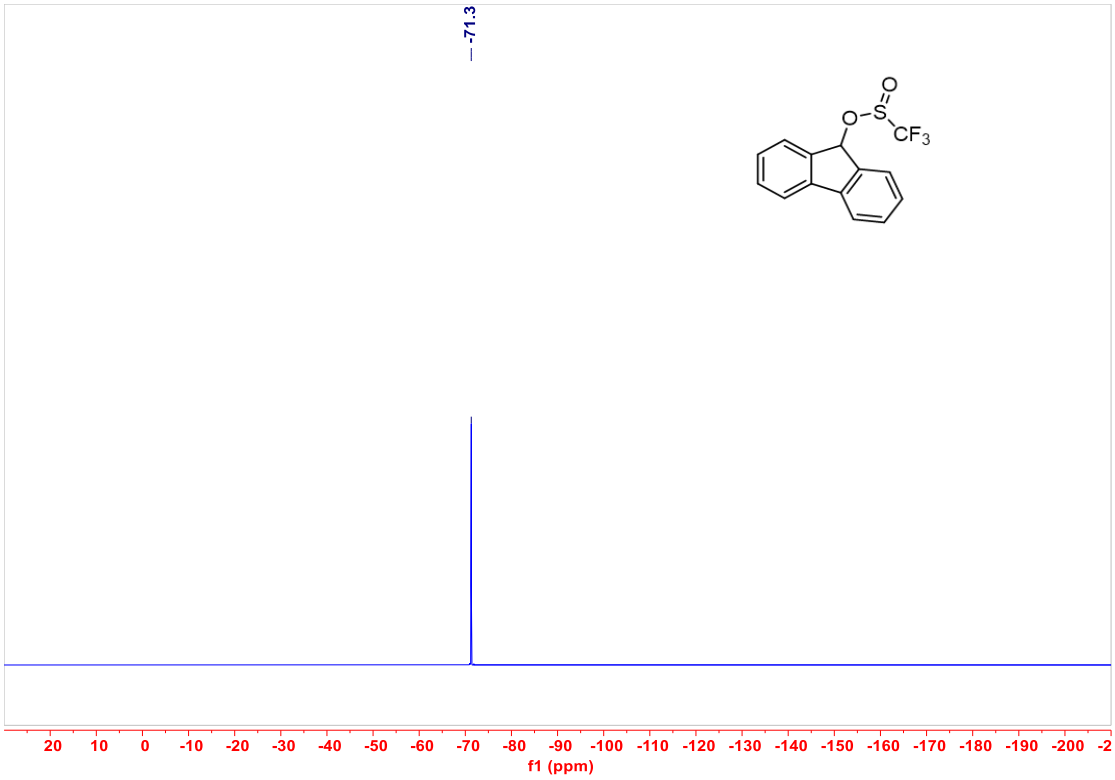
7.76
7.57
7.55
7.53
7.52
7.45
7.43
7.41
7.39
5.50
5.48
O
S
O
CF3
2.00
2.01
2.00
2.00
0.90
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-71.3
O
S
O
CF3
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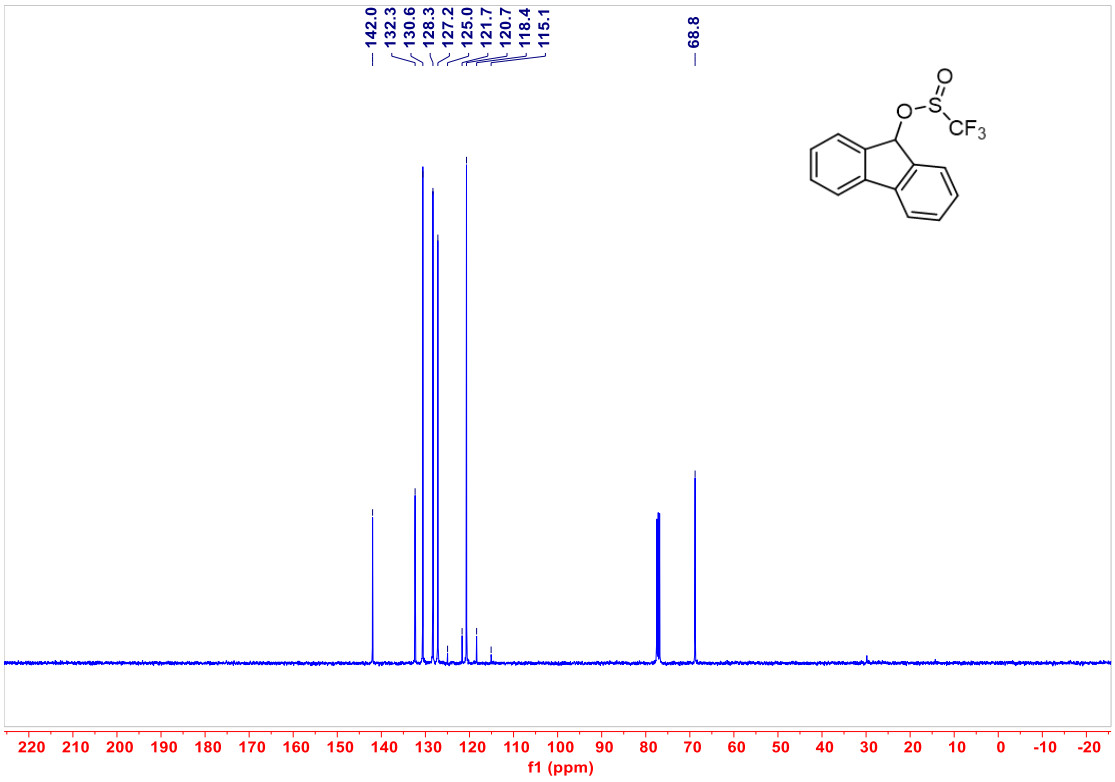
f1 (ppm)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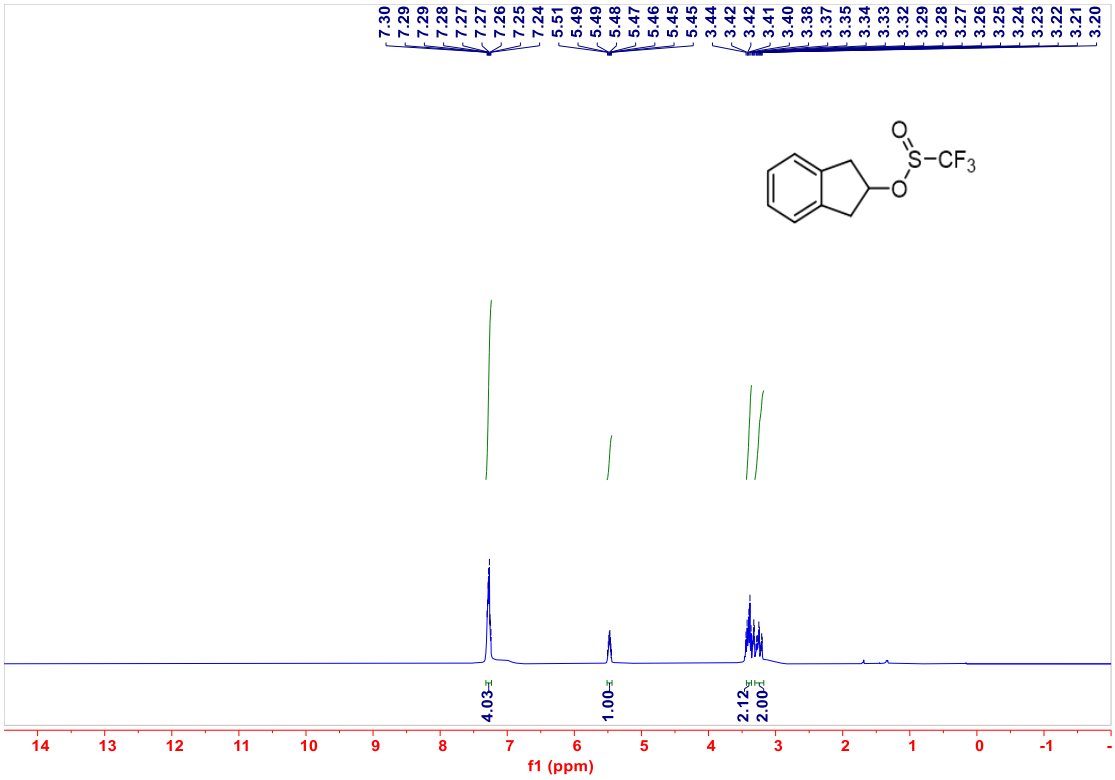
132.3
130.6
128.3
127.2
125.0
121.7
120.7
118.4
115.1
68.8
O
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.29
7.28
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7.26
7.25
7.24
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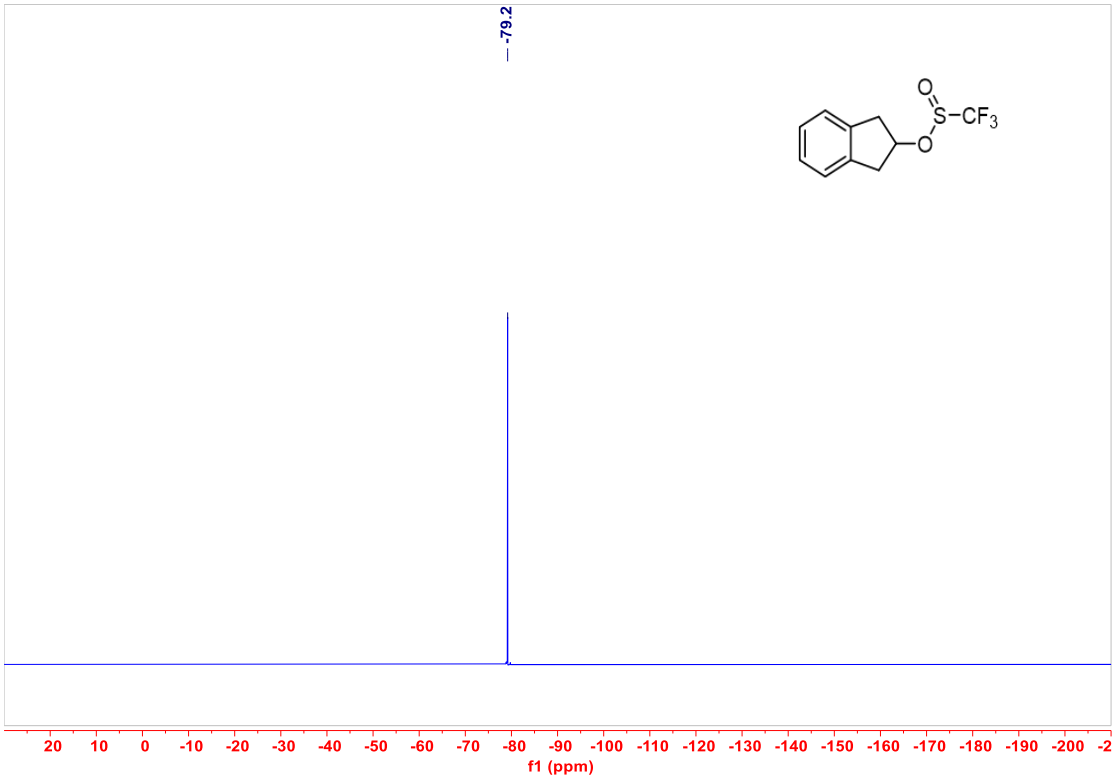
5.48
5.47
5.46
5.45
5.45
3.44
3.42
3.42
3.41
3.40
3.38
3.37
3.35
3.34
3.33
3.32
3.29
3.28
3.27
3.26
3.25
3.24
3.23
3.22
3.21
3.20
O
S
CF3
O
4.03
1.00
2.12
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.2
O
S
CF3
O
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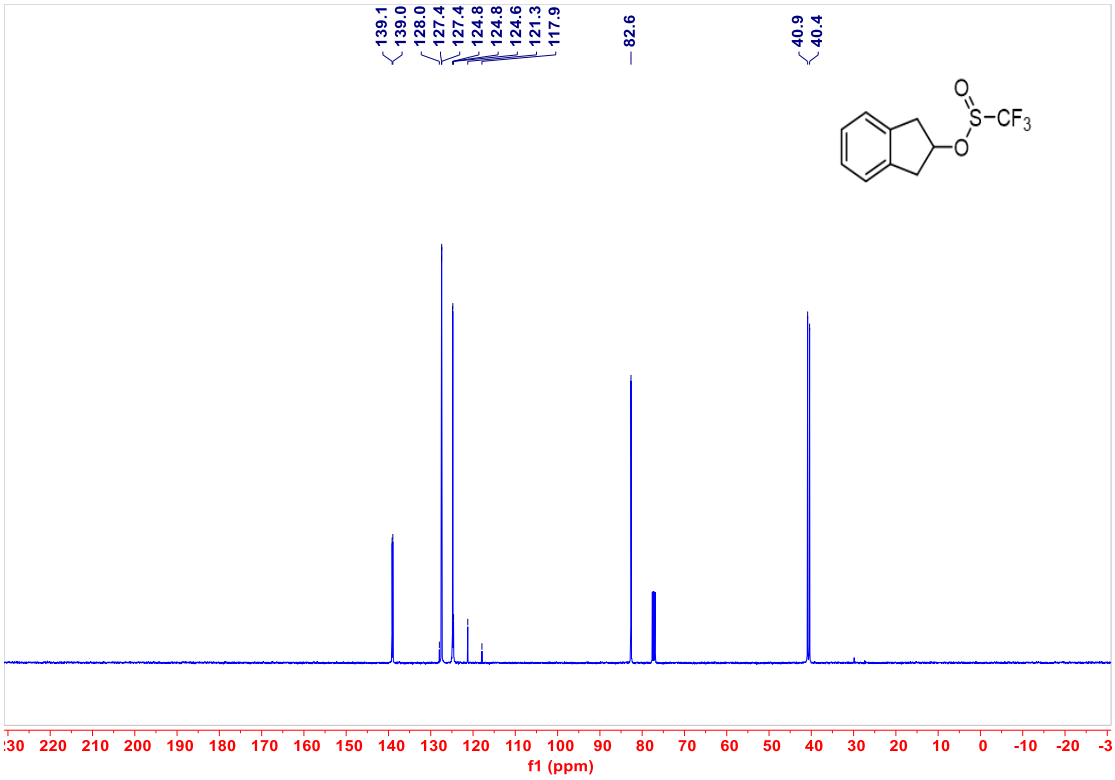
f1 (ppm)


139.1
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127.4
127.4
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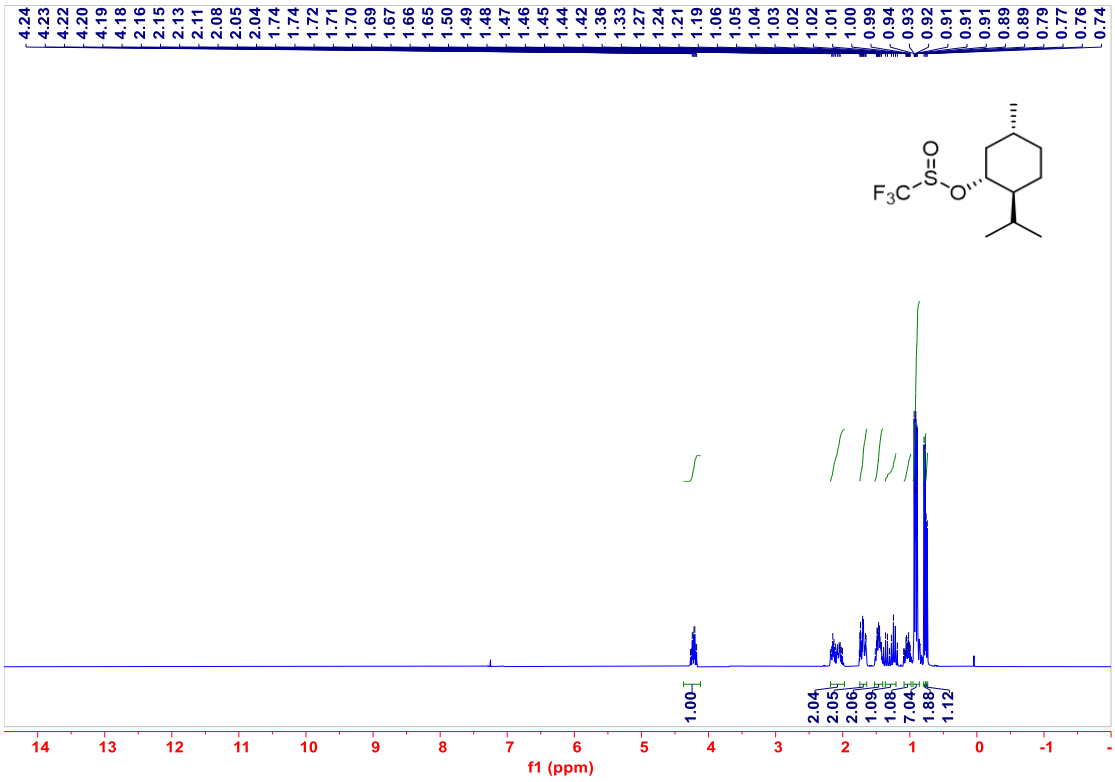
124.8
124.6
121.3
117.9
82.6
40.9
40.4
O
S
CF3
O
f1 (ppm)


4.24
4.23
4.22
4.20
4.19
4.18
2.16
2.15
2.13
2.11
2.08
2.05
2.04
1.74
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1.06
1.05
1.04
1.03
1.02
1.02
1.01
1.00
0.99
0.94
0.93
0.92
0.91
0.91
0.91
0.89
0.89
0.79
0.77
0.76
0.74
F3C
S
O
O
1.00
2.04
2.05
2.06
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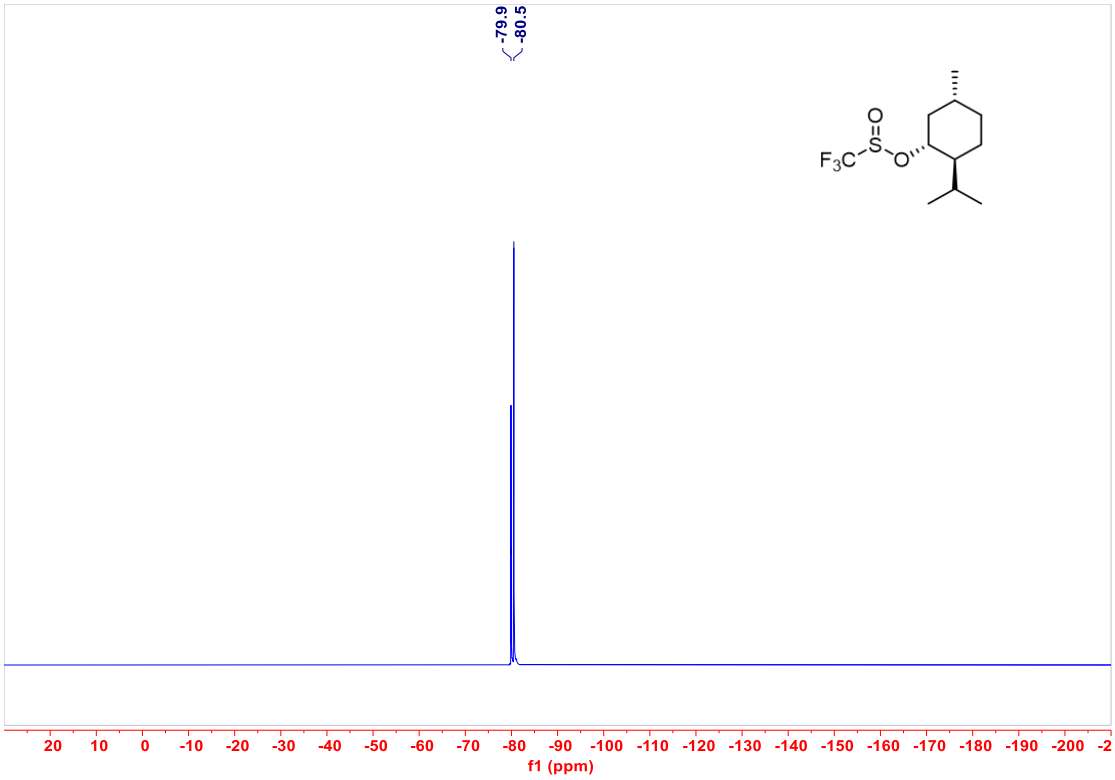
1.08
7.04
1.88
1.12
f1 (ppm)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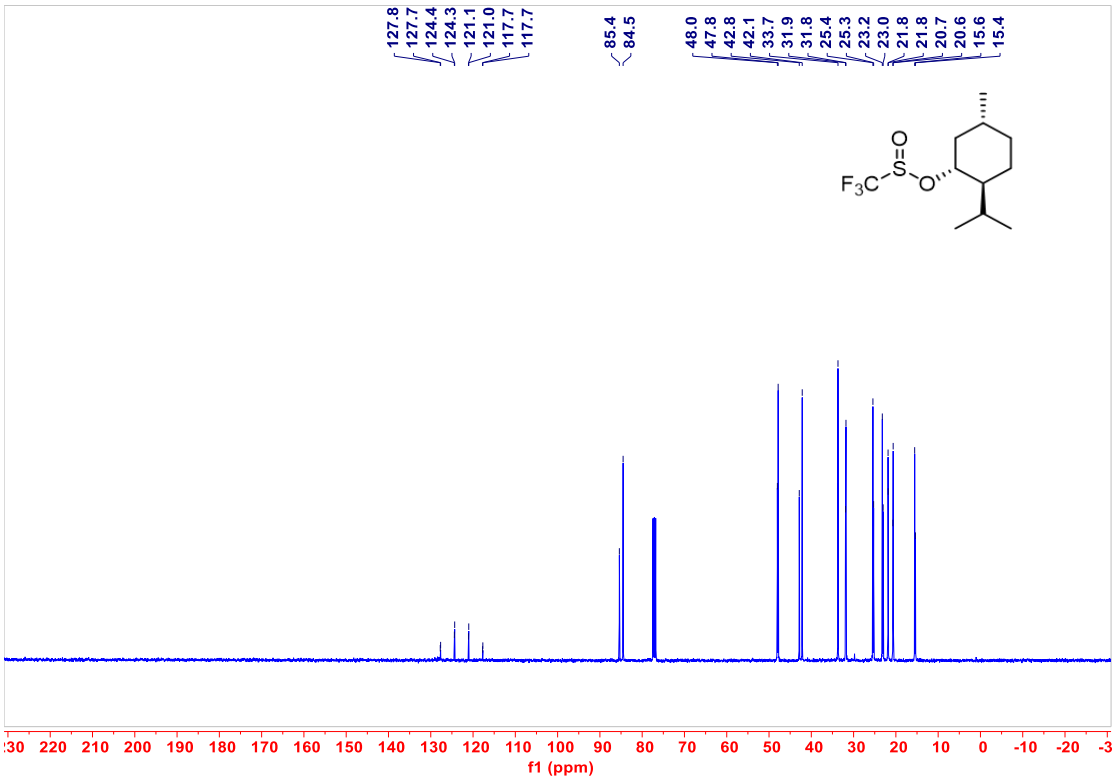
-80.5
F3C
S
O
O
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)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124.4
124.3
121.1
121.0
117.7
117.7
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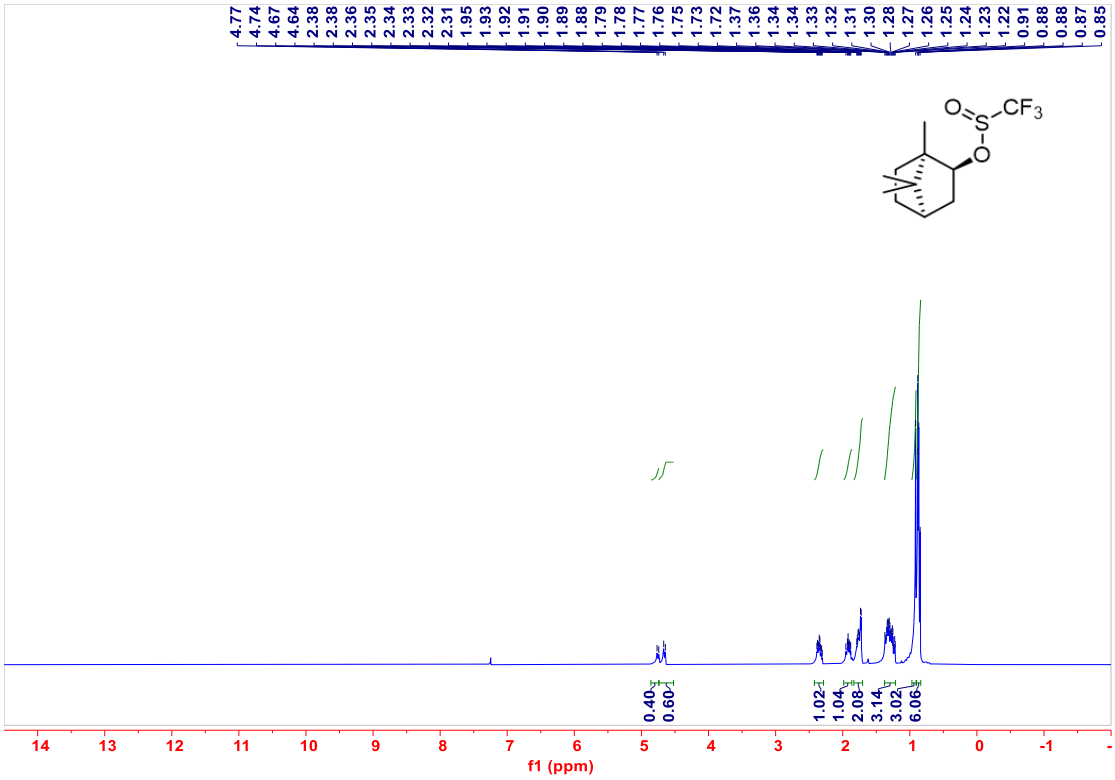
84.5
48.0
47.8
42.8
42.1
33.7
31.9
31.8
25.4
25.3
23.2
23.0
21.8
21.8
20.7
20.6
15.6
15.4
F3C
S
O
O
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)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4.74
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4.64
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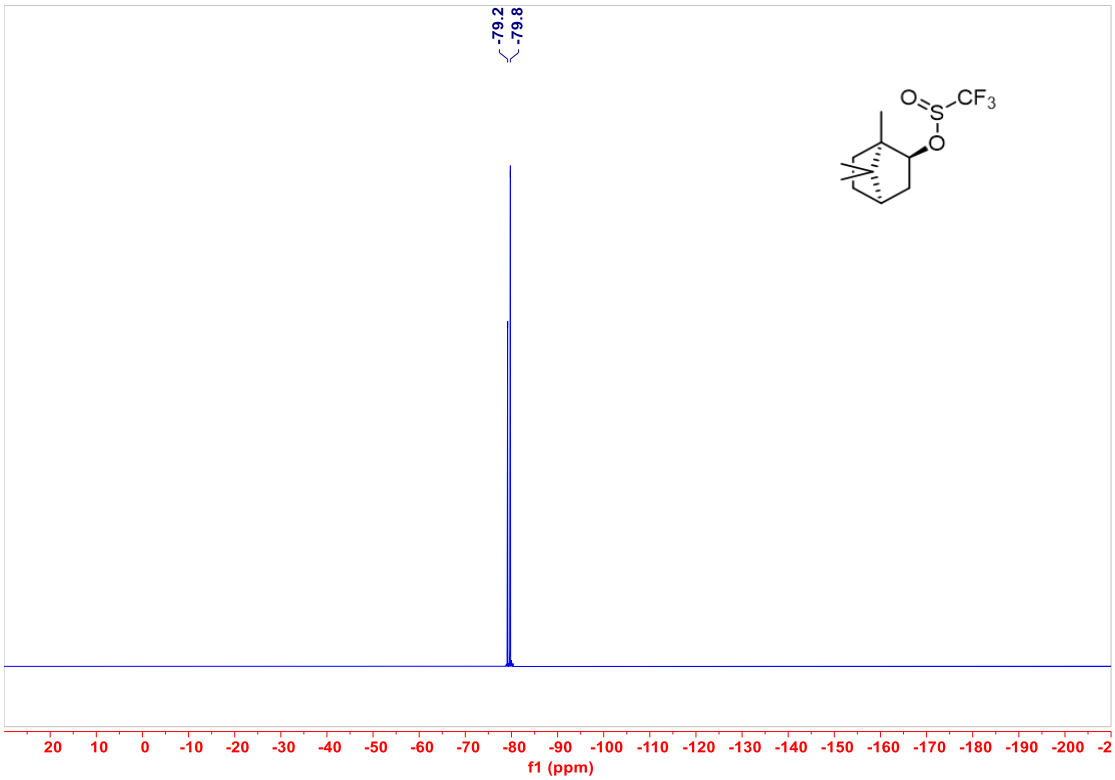
2.36
2.35
2.34
2.33
2.32
2.31
1.95
1.93
1.92
1.91
1.90
1.89
1.88
1.79
1.78
1.77
1.76
1.75
1.73
1.72
1.37
1.36
1.34
1.34
1.33
1.32
1.31
1.30
1.28
1.27
1.26
1.25
1.24
1.23
1.22
0.91
0.88
0.88
0.87
0.85
O
S
CF3
O
0.40
0.60
1.02
1.04
2.08
3.14
3.02
6.06
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.2
-79.8
O
S
CF3
O
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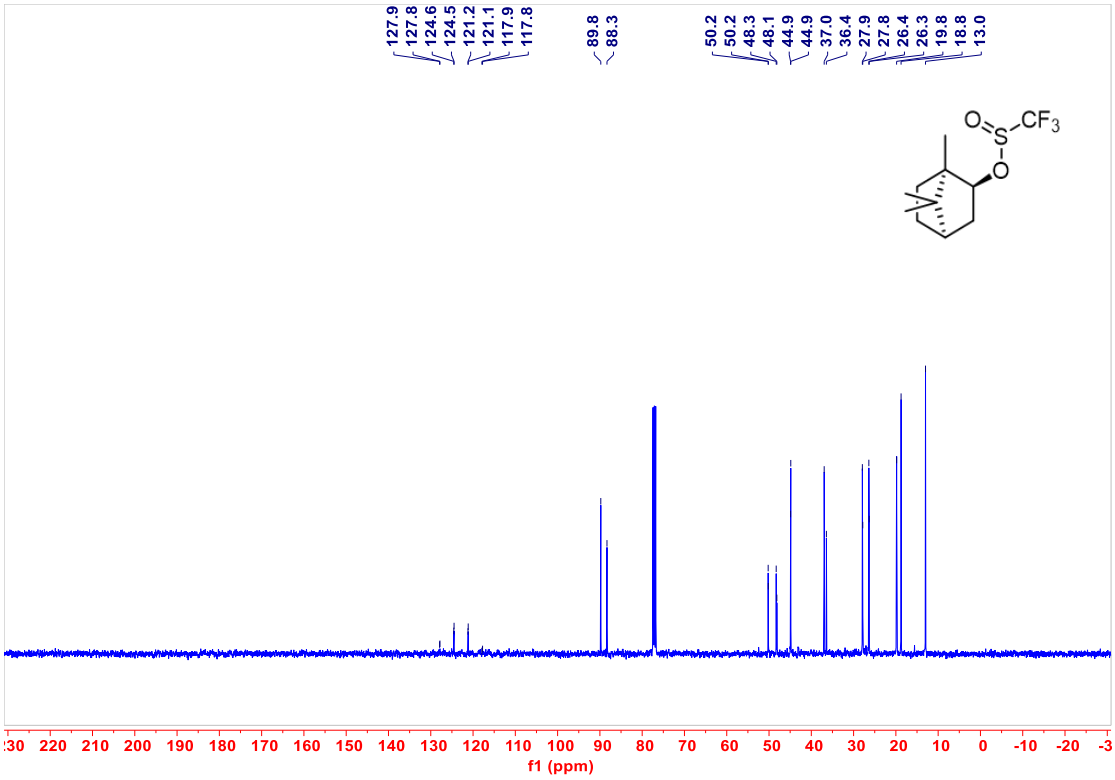
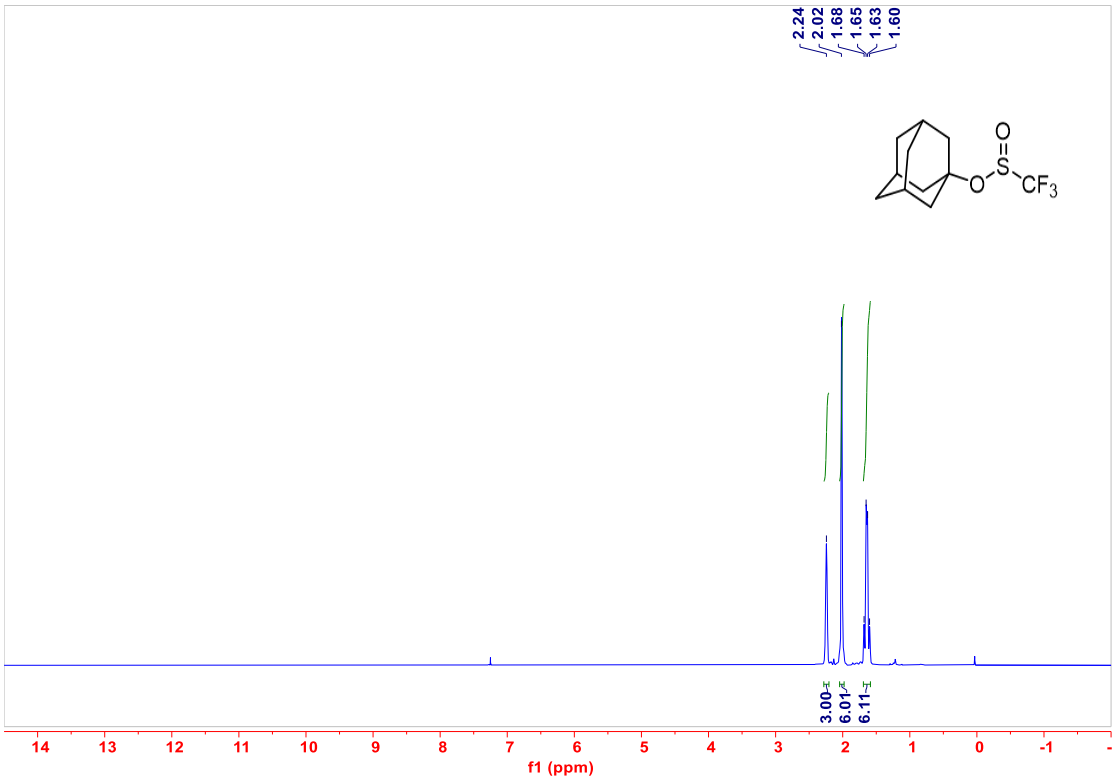
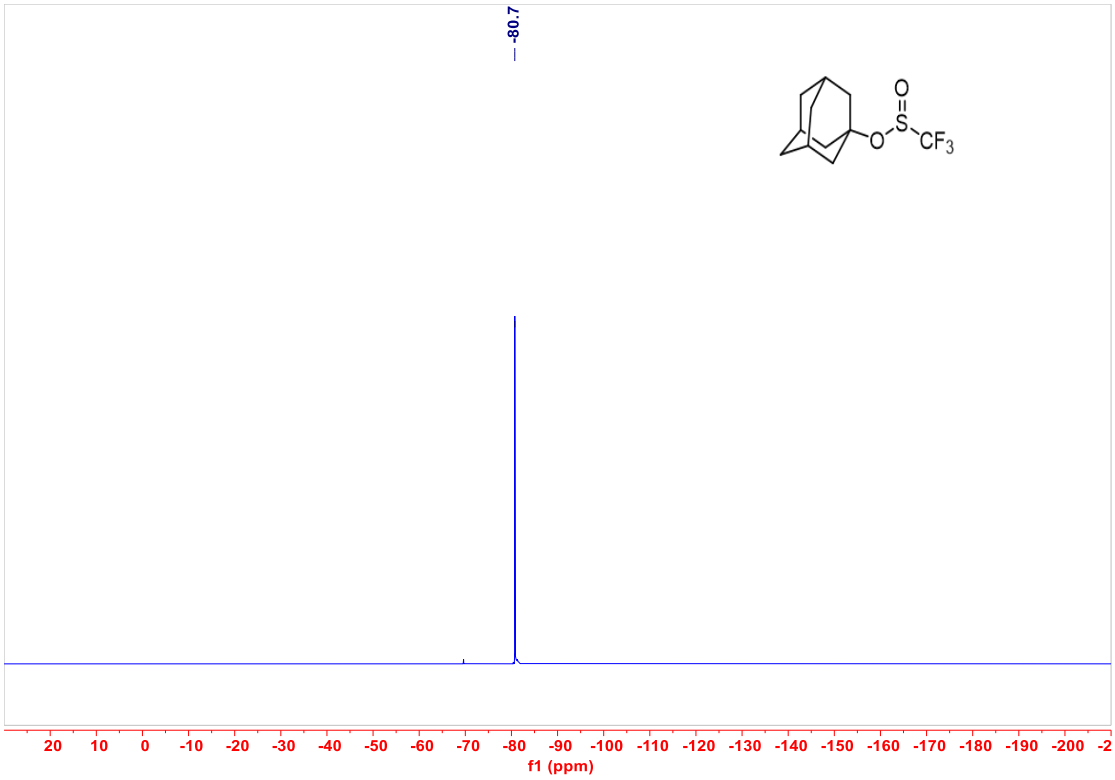
f1 (ppm)


127.9
127.8
124.6
124.5
121.2
121.1
117.9
117.8
89.8
88.3
50.2
50.2
48.3
48.1
44.9
44.9
37.0
36.4
27.9
27.8
26.4
26.3
19.8
18.8
13.0
O
S
CF3
O
f1 (ppm)


2.24
2.02
1.68
1.65
1.63
1.60
O
S
CF3
O
3.00
6.01
6.11
f1 (ppm)


-80.7
O
S
O
CF3
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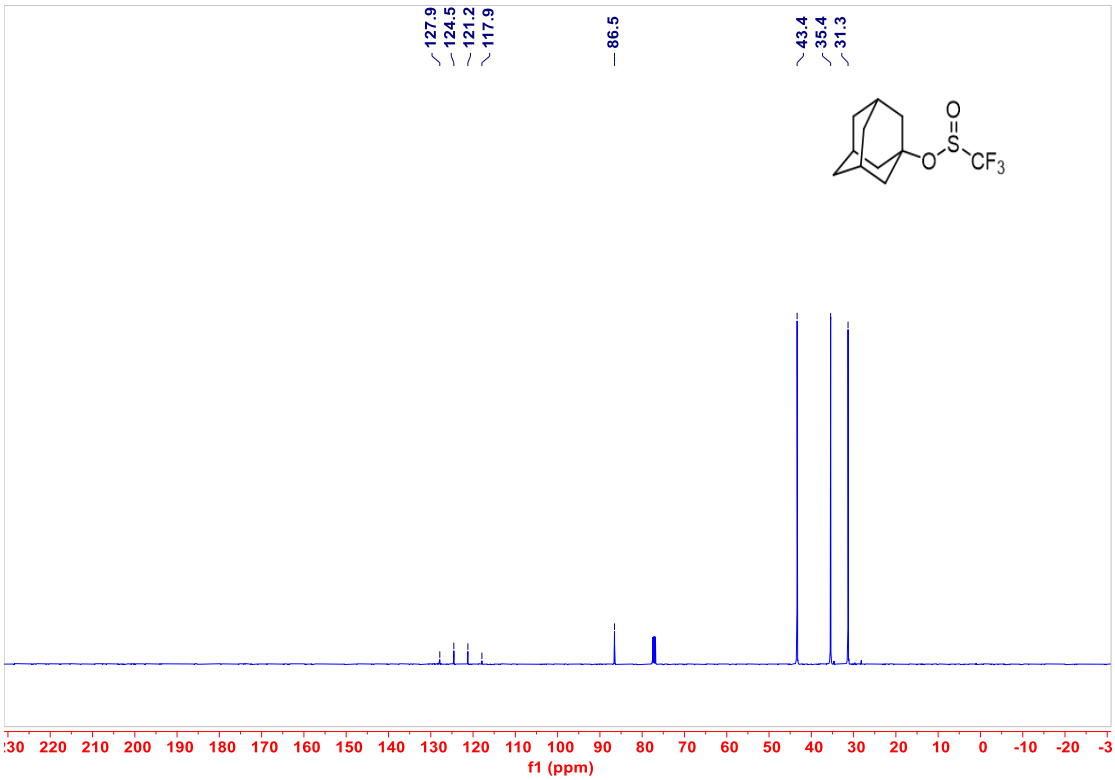
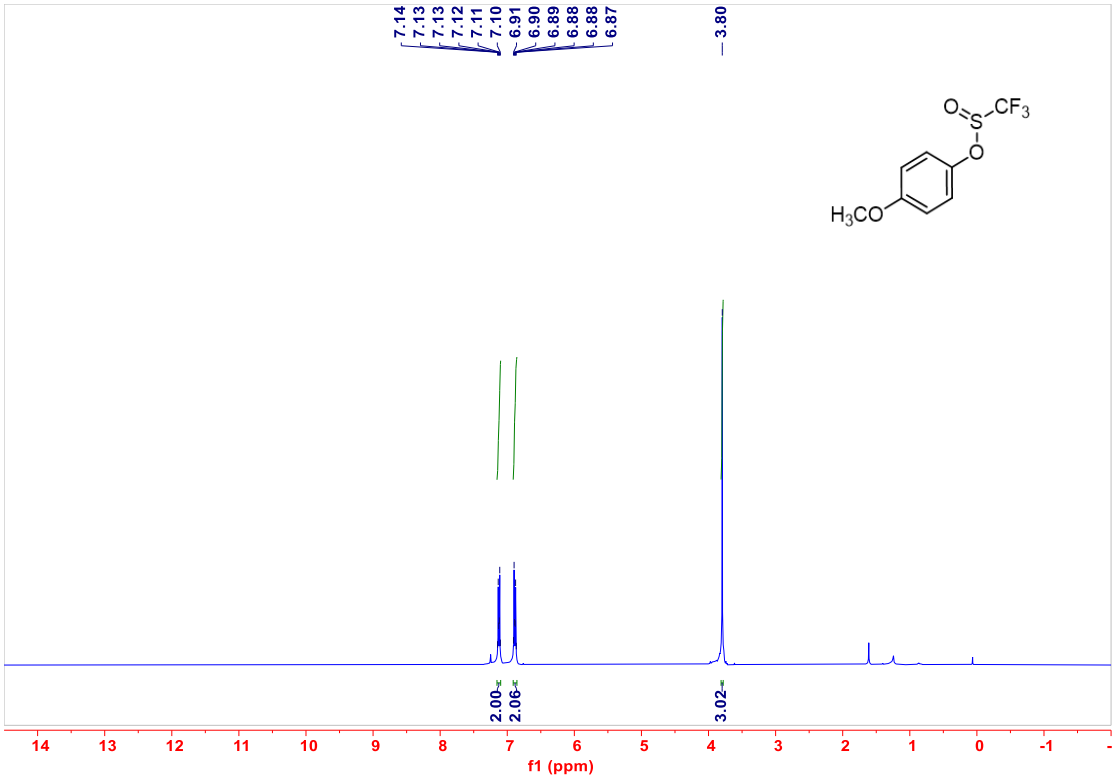
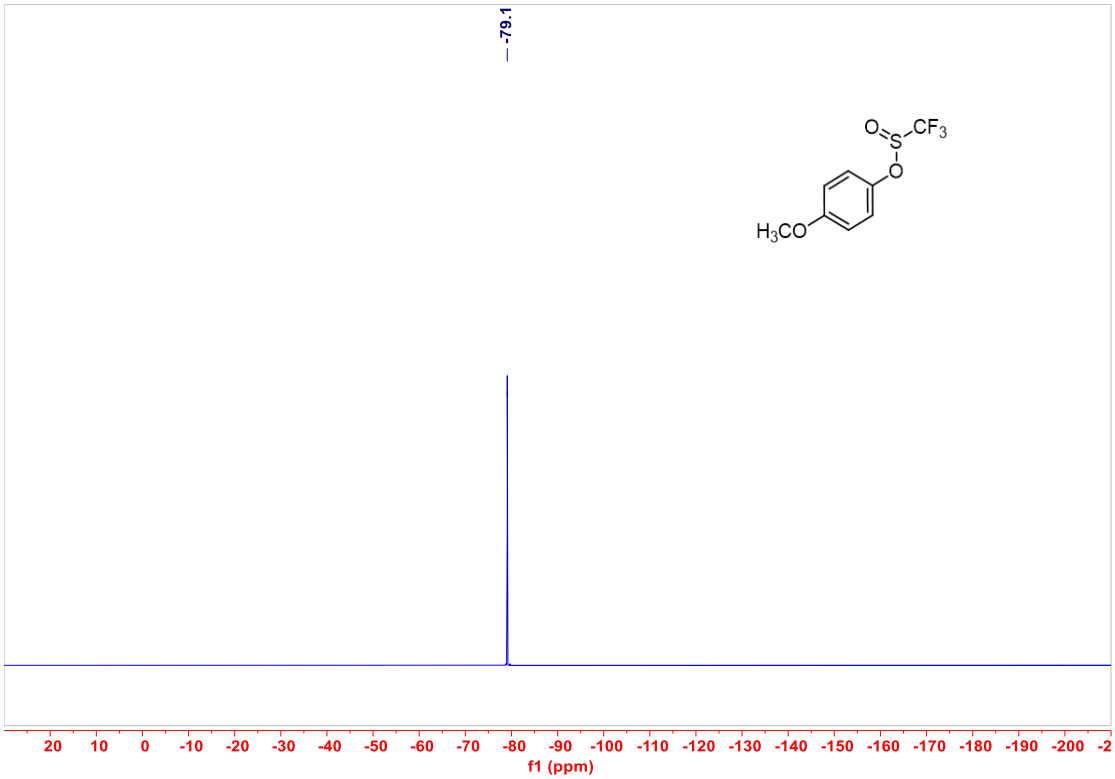
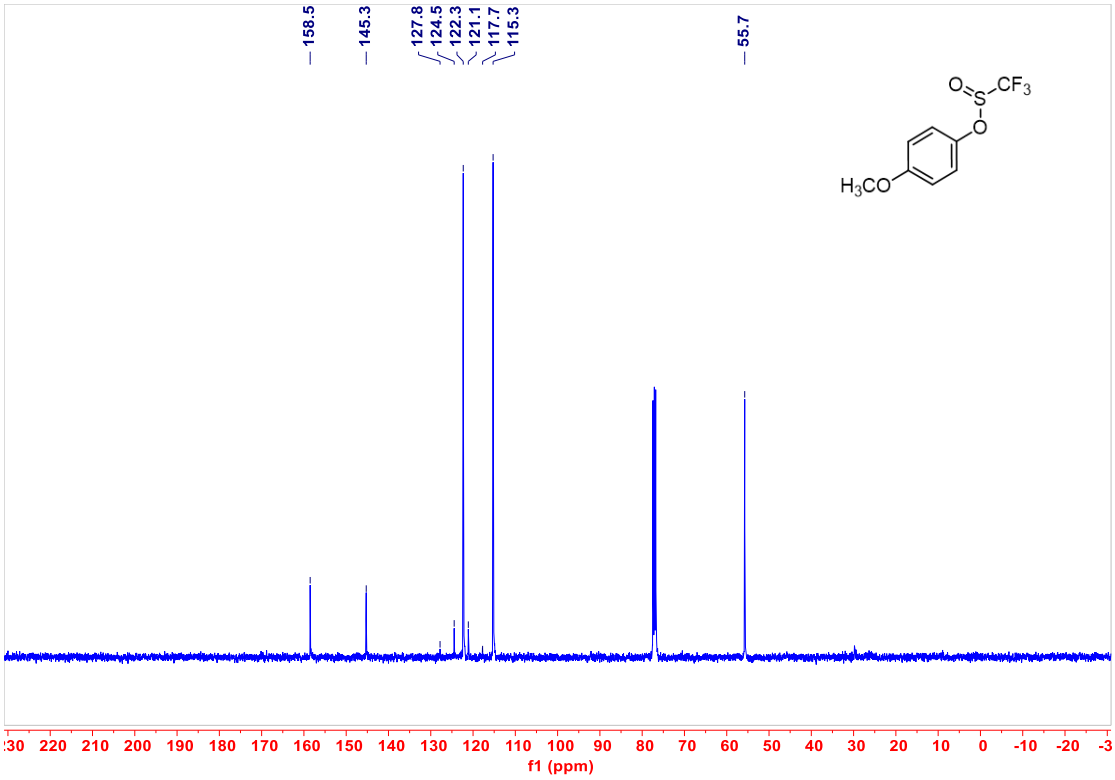
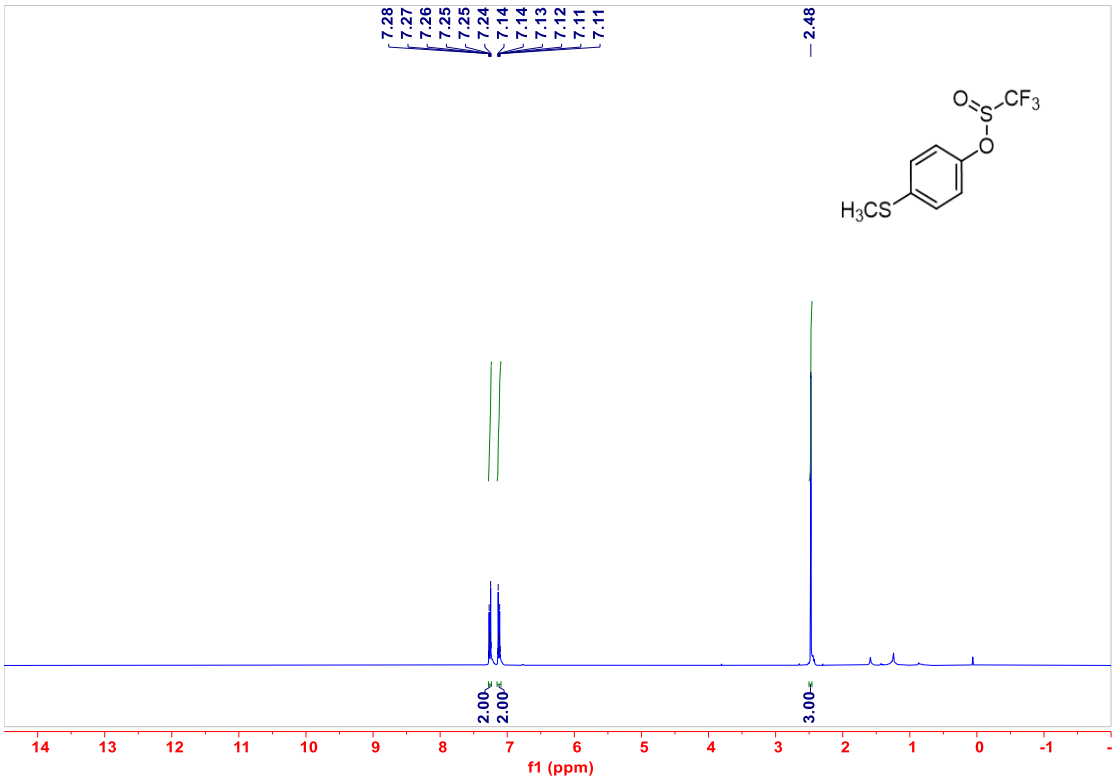
f1 (ppm)


127.9
124.5
121.2
117.9
86.5
43.4
35.4
31.3
O
S
O
CF3
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.14
7.13
7.13
7.12
7.11
7.10
6.91
6.90
6.89
6.88
6.88
6.87
3.80
2.00
2.06
3.02
f1 (ppm)


-79.1
f1 (ppm)


158.5
145.3
127.8
124.5
122.3
121.1
117.7
115.3
55.7
O
S
CF3
O
H3CO
f1 (ppm)


7.28
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7.26
7.25
7.25
7.24
7.14
7.14
7.13
7.12
7.11
7.11
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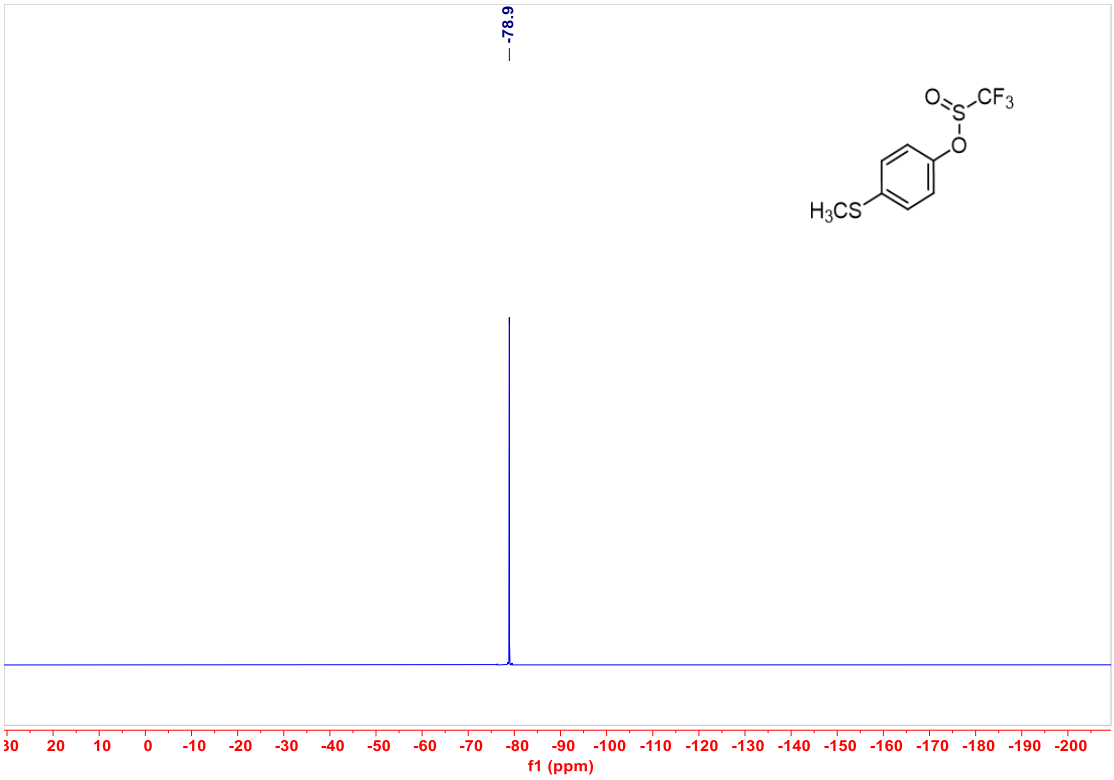
O
H3CS
2.00
2.00
3.00
f1 (ppm)


-78.9
O
S
CF3
O
H3CS
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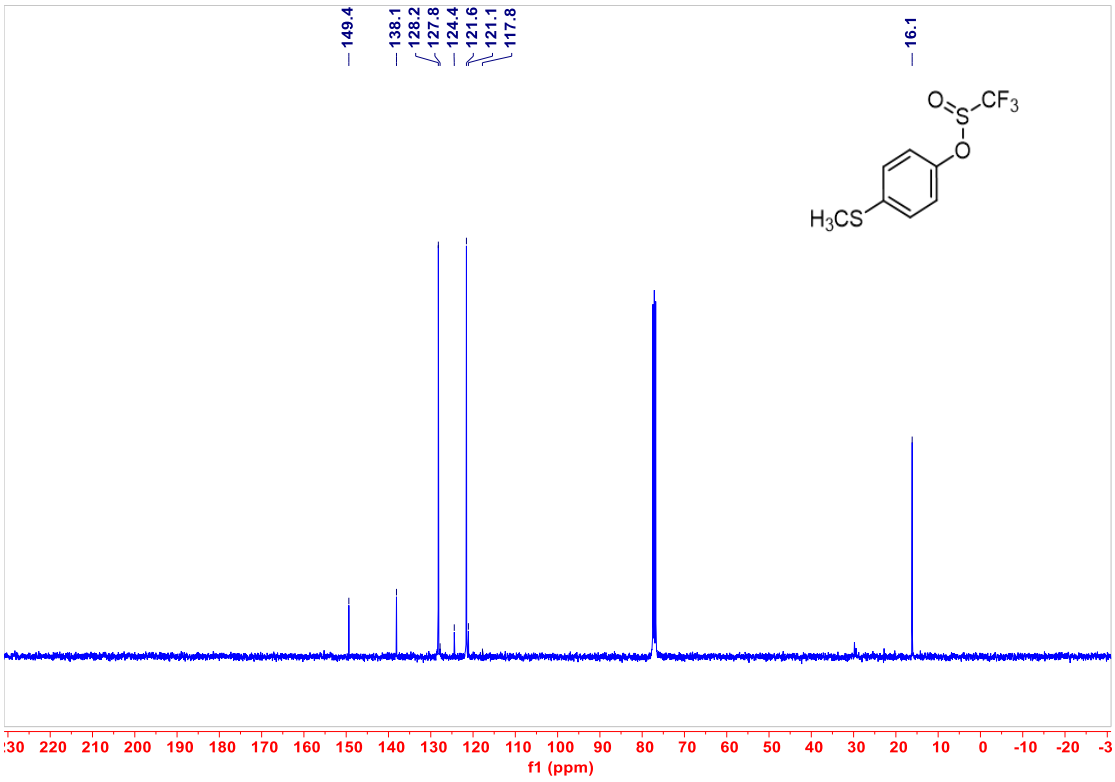
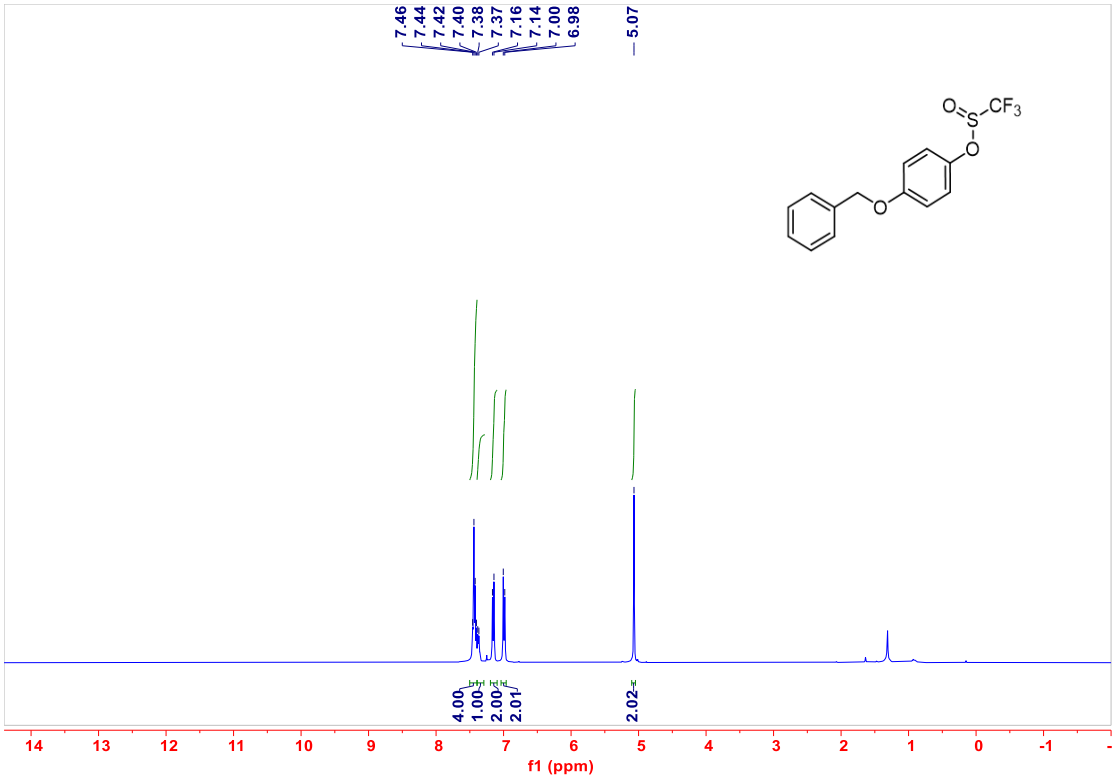
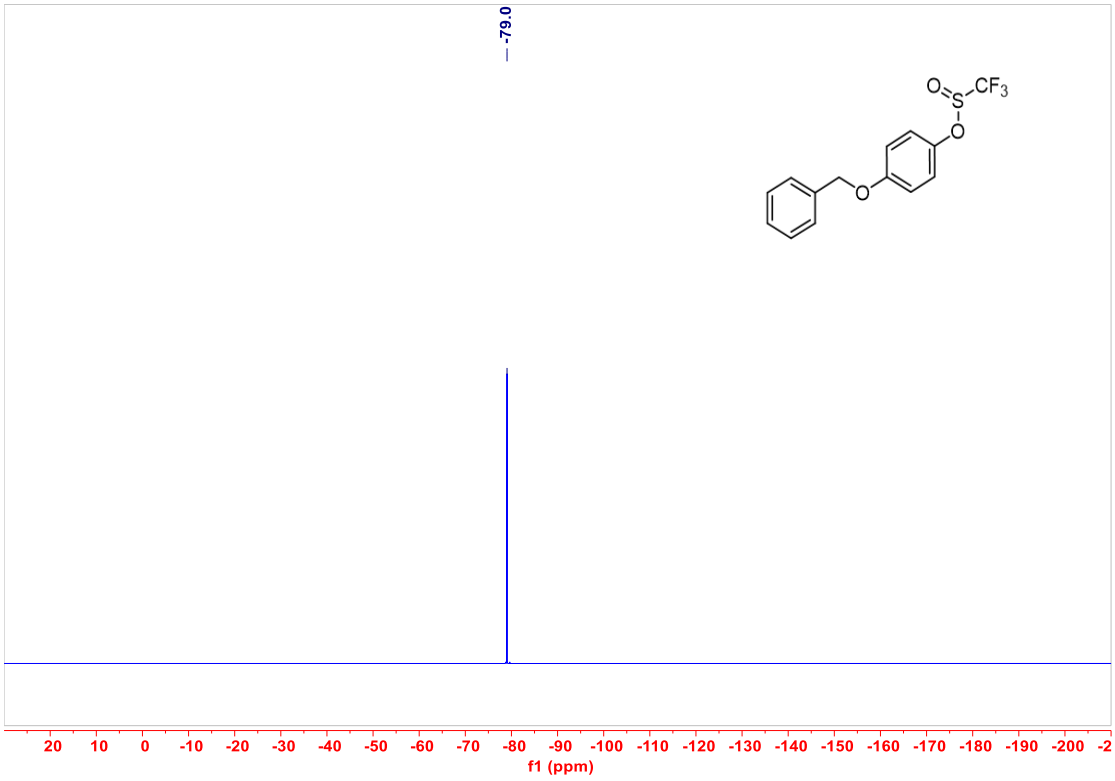
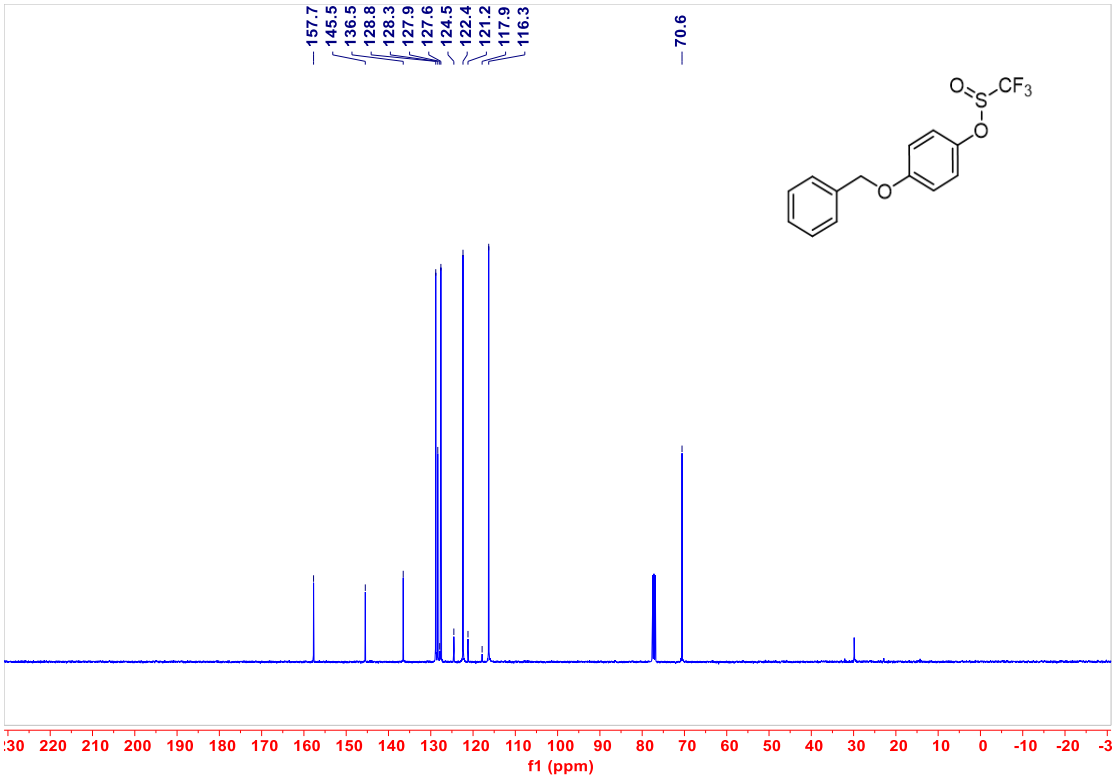
f1 (ppm)


149.4
138.1
128.2
127.8
124.4
121.6
121.1
117.8
16.1
O
S
CF3
O
H3CS
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.46
7.44
7.42
7.40
7.38
7.37
7.16
7.14
7.00
6.98
5.07
4.00
1.00
2.00
2.01
2.02
f1 (ppm)


-79.0
f1 (ppm)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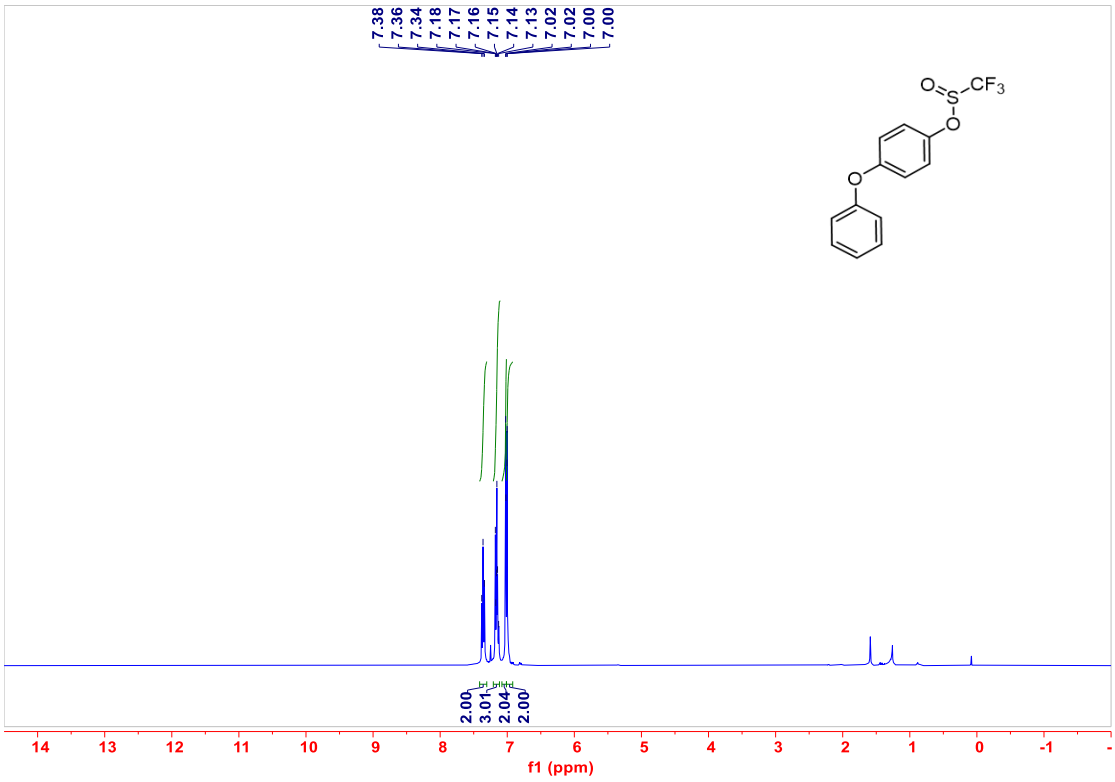
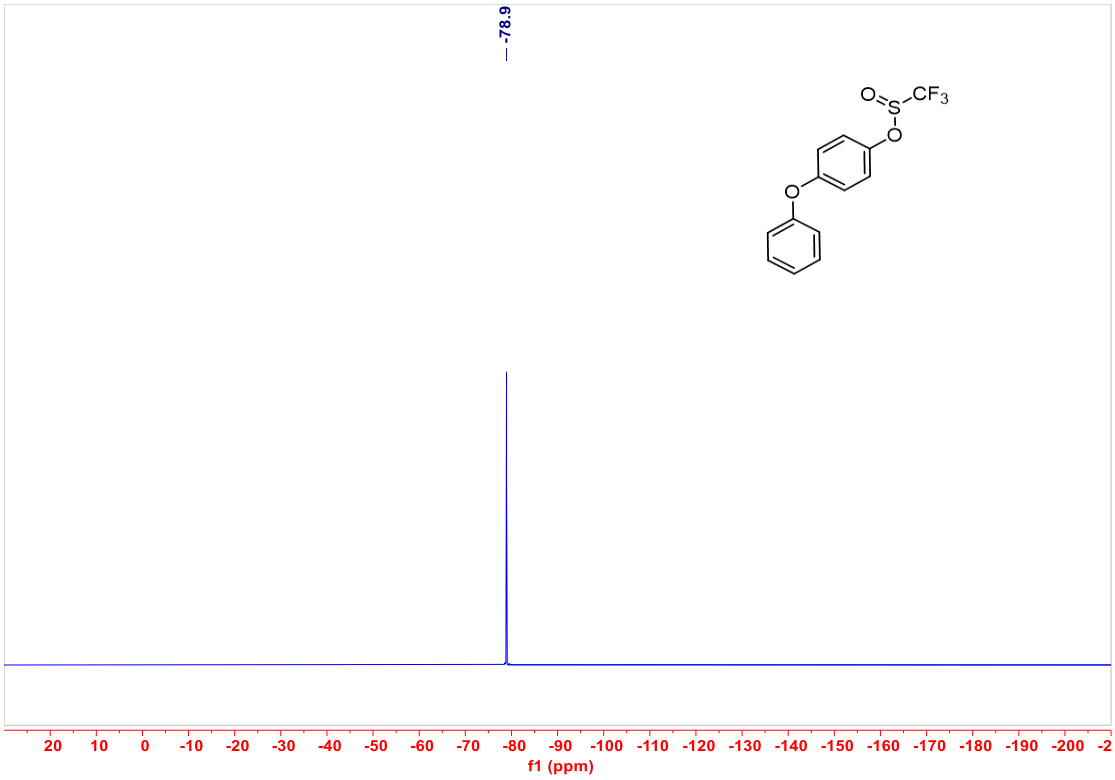
145.5
136.5
128.8
128.3
127.9
127.6
124.5
122.4
121.2
117.9
116.3
70.6
O
S
CF3
O
O
f1 (ppm)


7.38
7.36
7.34
7.18
7.17
7.16
7.15
7.14
7.13
7.02
7.02
7.00
7.00
O
S
CF3
O
O
2.00
3.01
2.04
2.00
f1 (ppm)


-78.9
O
S
CF3
O
O
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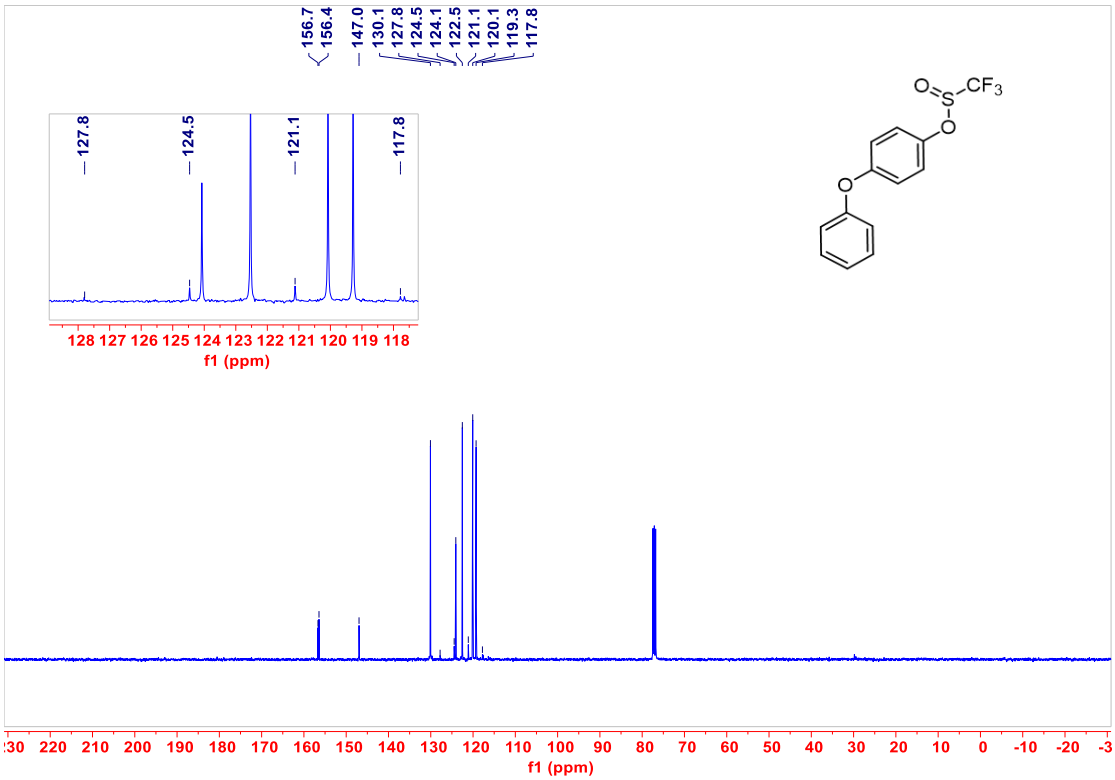
f1 (ppm)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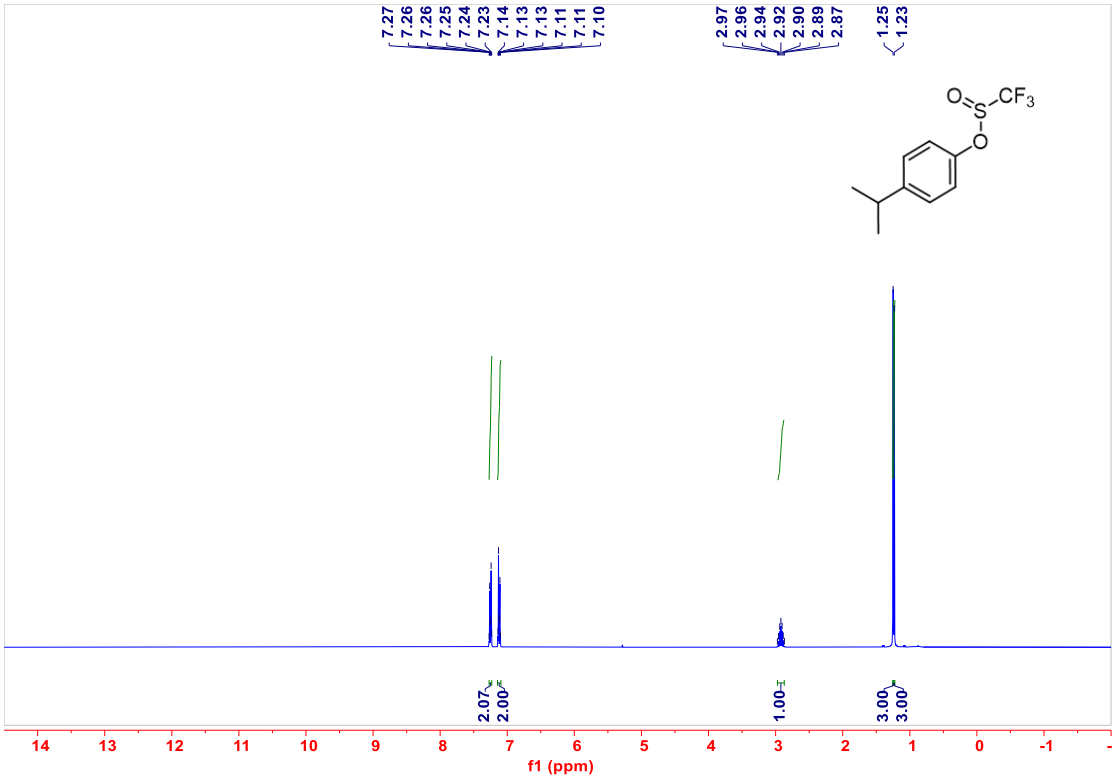
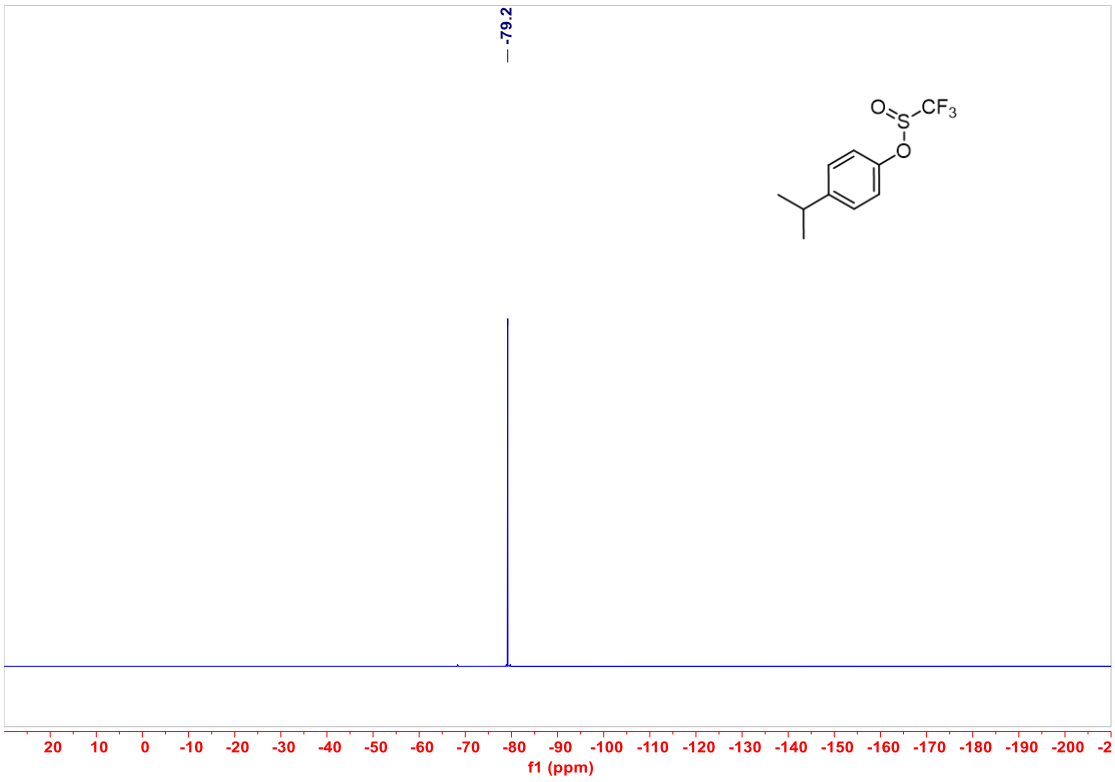
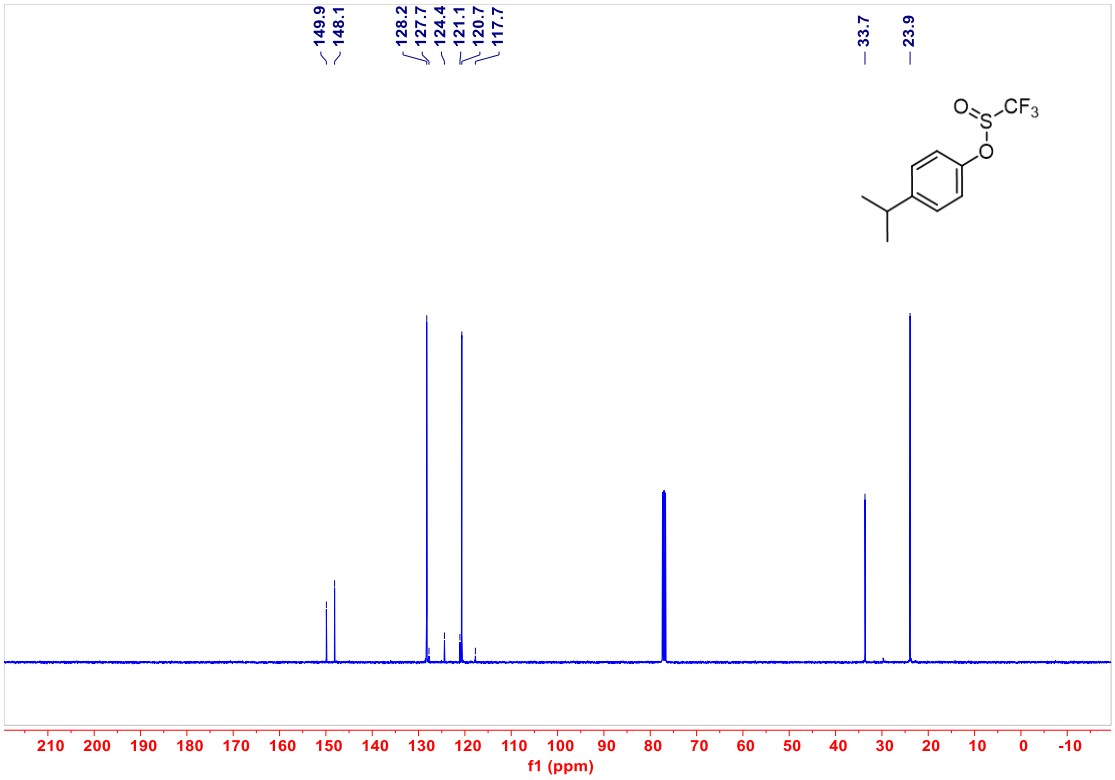
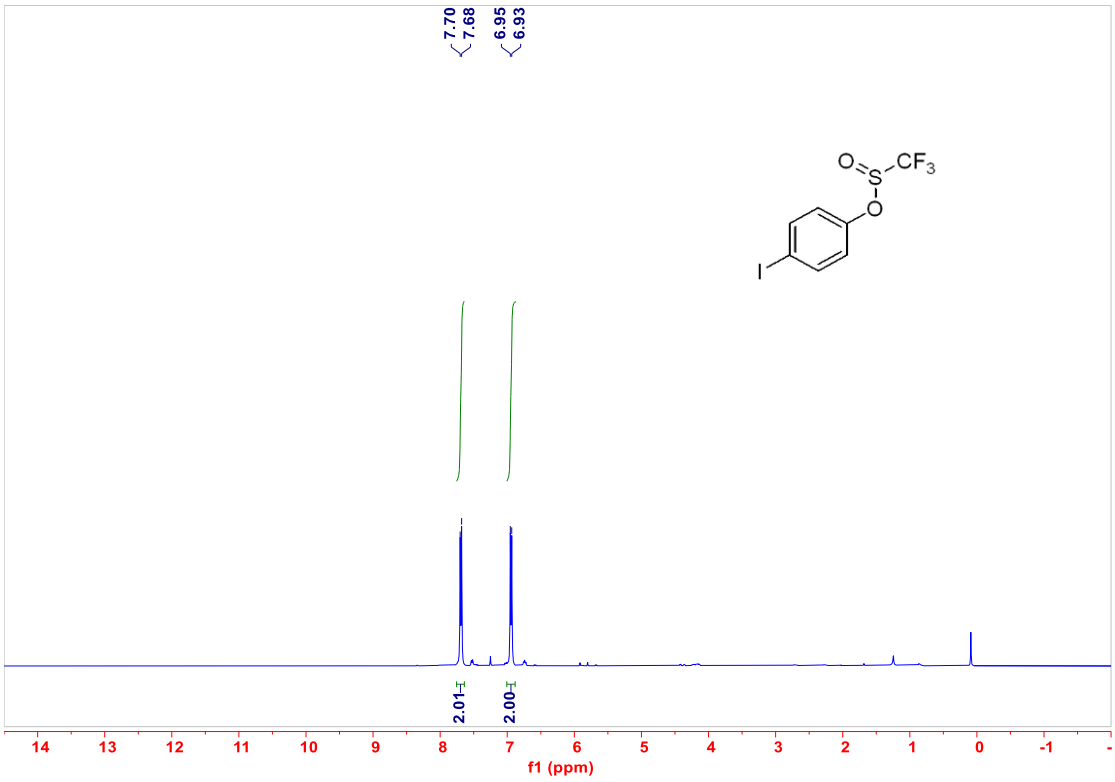
156.4
147.0
130.1
127.8
124.5
124.1
122.5
121.1
120.1
119.3
117.8
127.8
124.5
121.1
117.8
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
O
S
CF3
O
O
:30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


7.27
7.26
7.26
7.25
7.24
7.23
7.14
7.13
7.13
7.11
7.11
7.10
2.97
2.96
2.94
2.92
2.90
2.89
2.87
1.25
1.23
O
S
CF3
O
2.07
2.00
1.00
3.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.2
O
S
CF3
O
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


149.9
148.1
128.2
127.7
124.4
121.1
120.7
117.7
33.7
23.9
O
S
CF3
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)


7.70
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6.93
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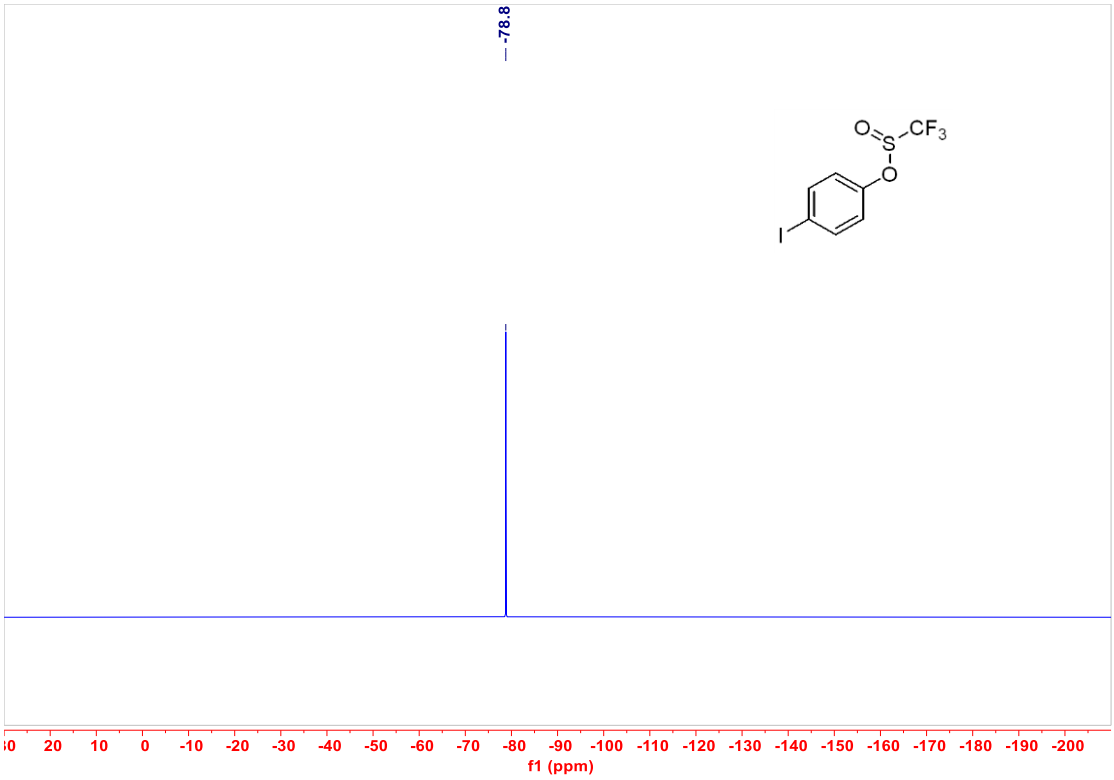
S
CF3
O
I
2.01
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.8
O
S
CF3
O
I
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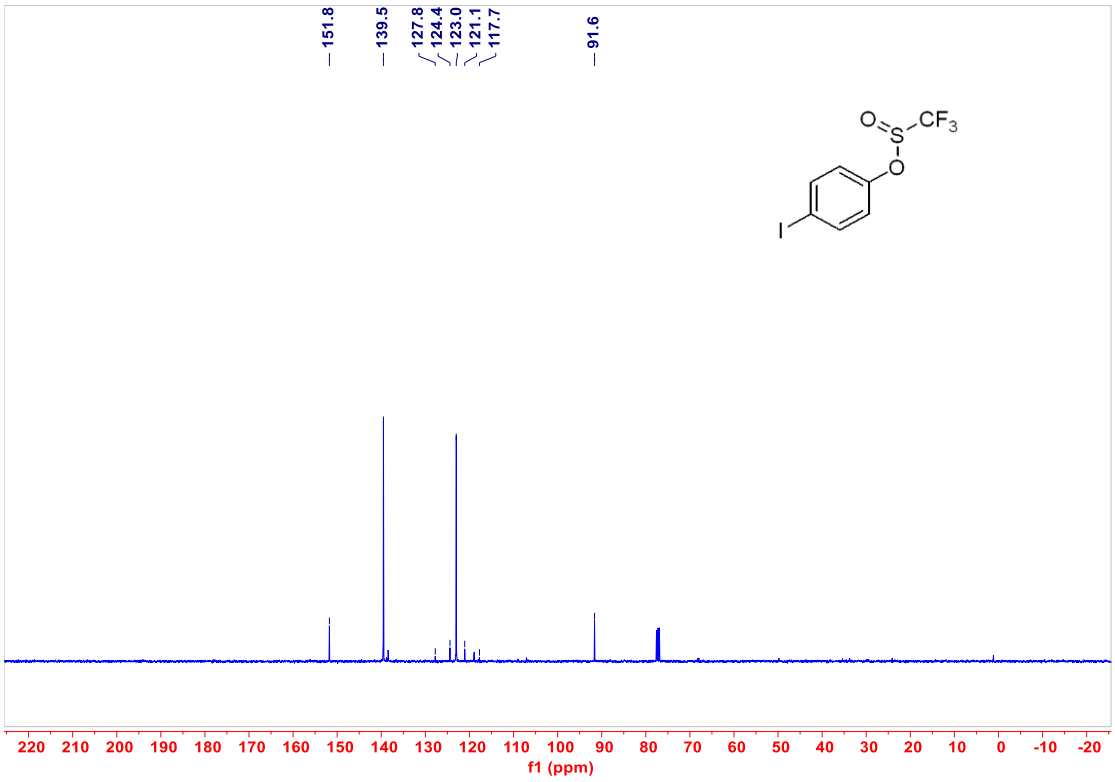
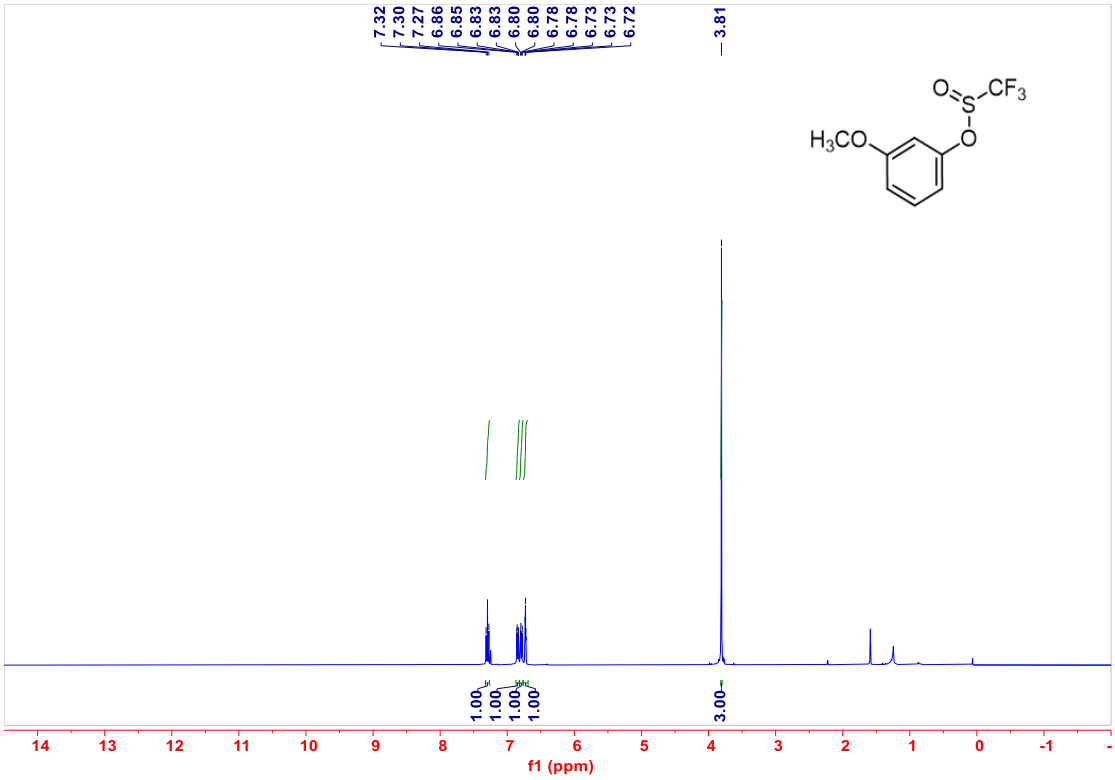
f1 (ppm)


151.8
139.5
127.8
124.4
123.0
121.1
117.7
91.6
O
S
CF3
O
I
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.27
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6.85
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6.83
6.80
6.80
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6.78
6.73
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6.72
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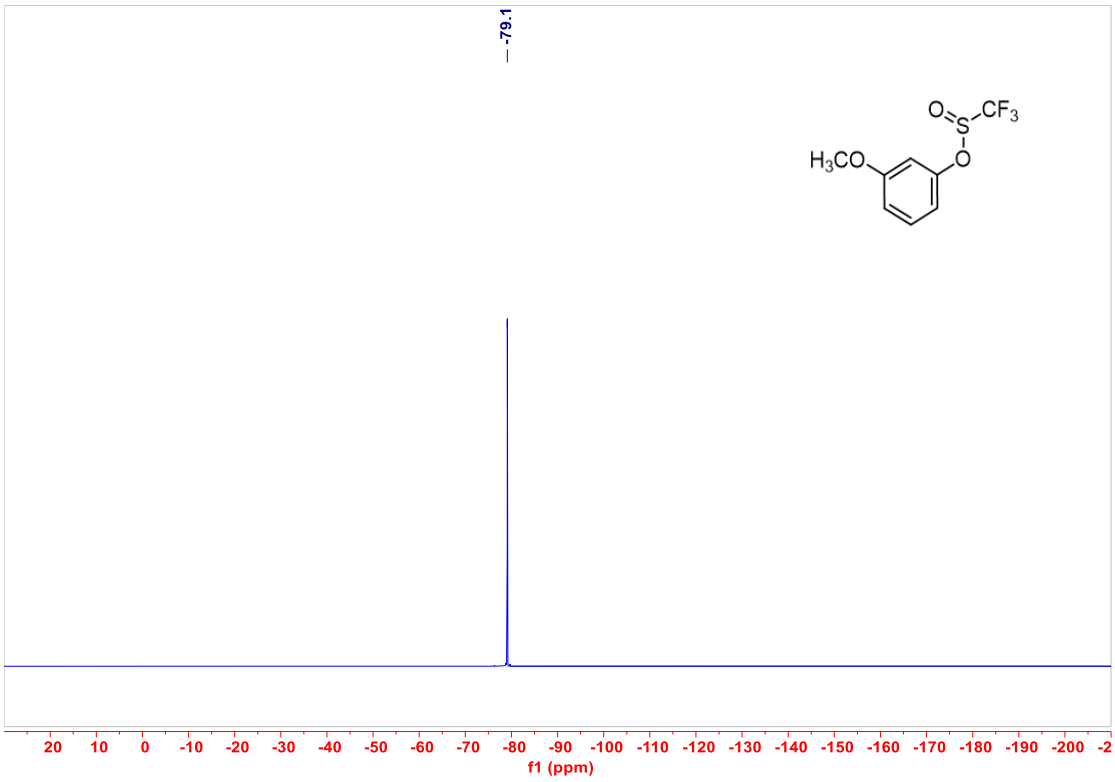
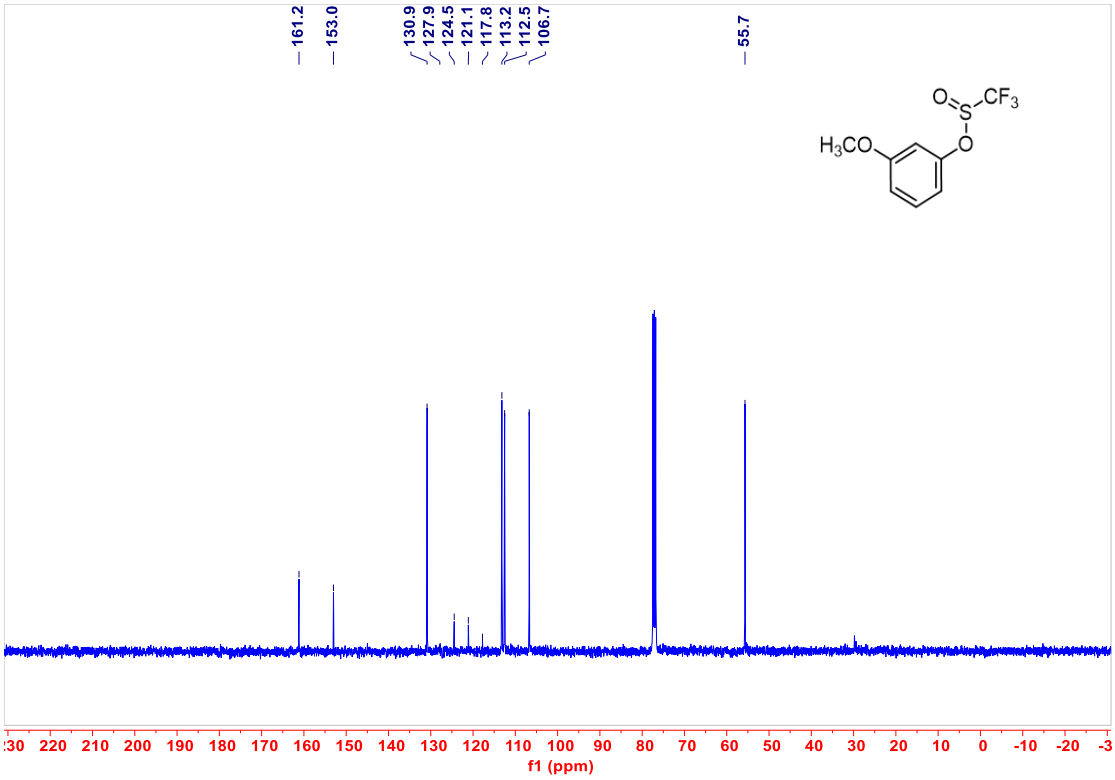
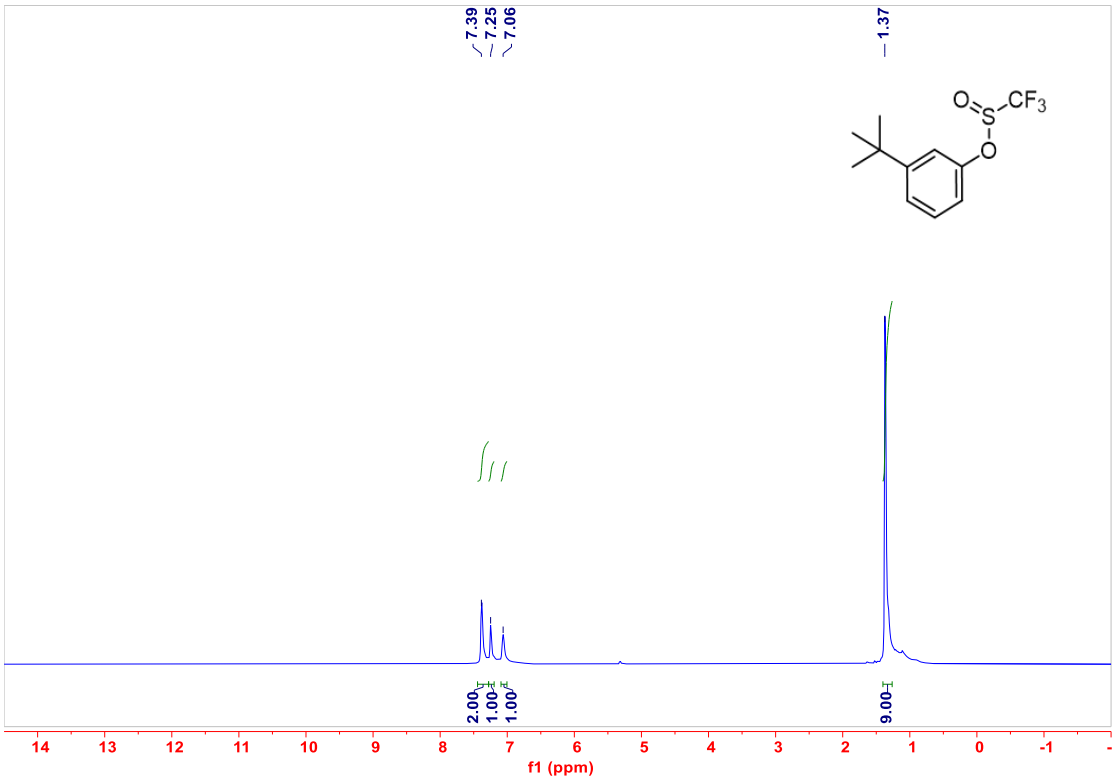
1.00
1.00
1.00
3.00
f1 (ppm)


-79.1
f1 (ppm)


161.2
153.0
130.9
127.9
124.5
121.1
117.8
113.2
112.5
106.7
55.7
O
S
CF3
H3CO
O
f1 (ppm)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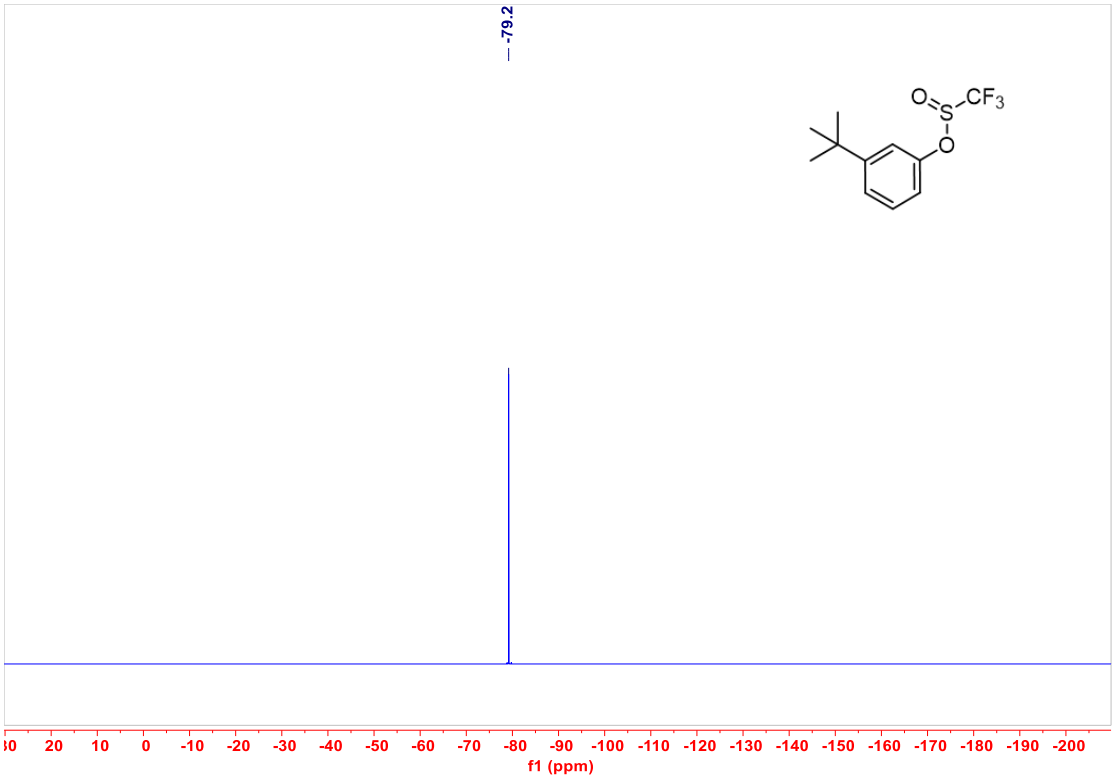
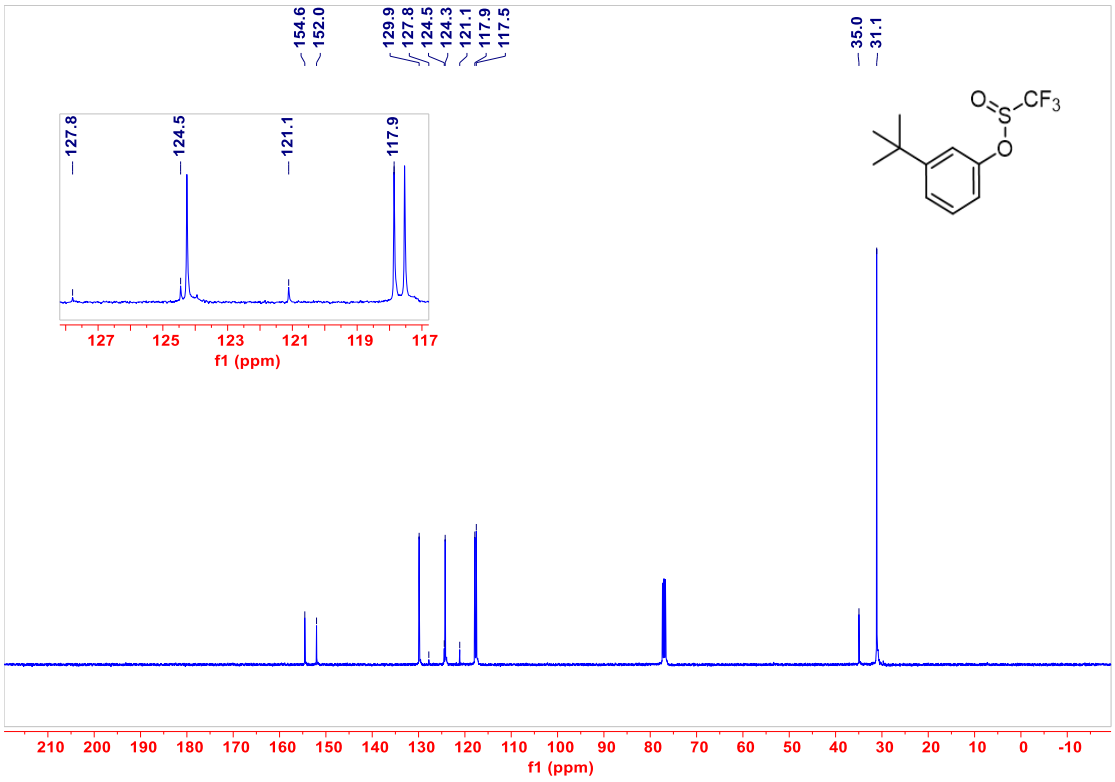
7.25
7.06
1.37
O
S
CF3
O
2.00
1.00
1.00
9.00
f1 (ppm)


-79.2
O
S
CF3
O
f1 (ppm)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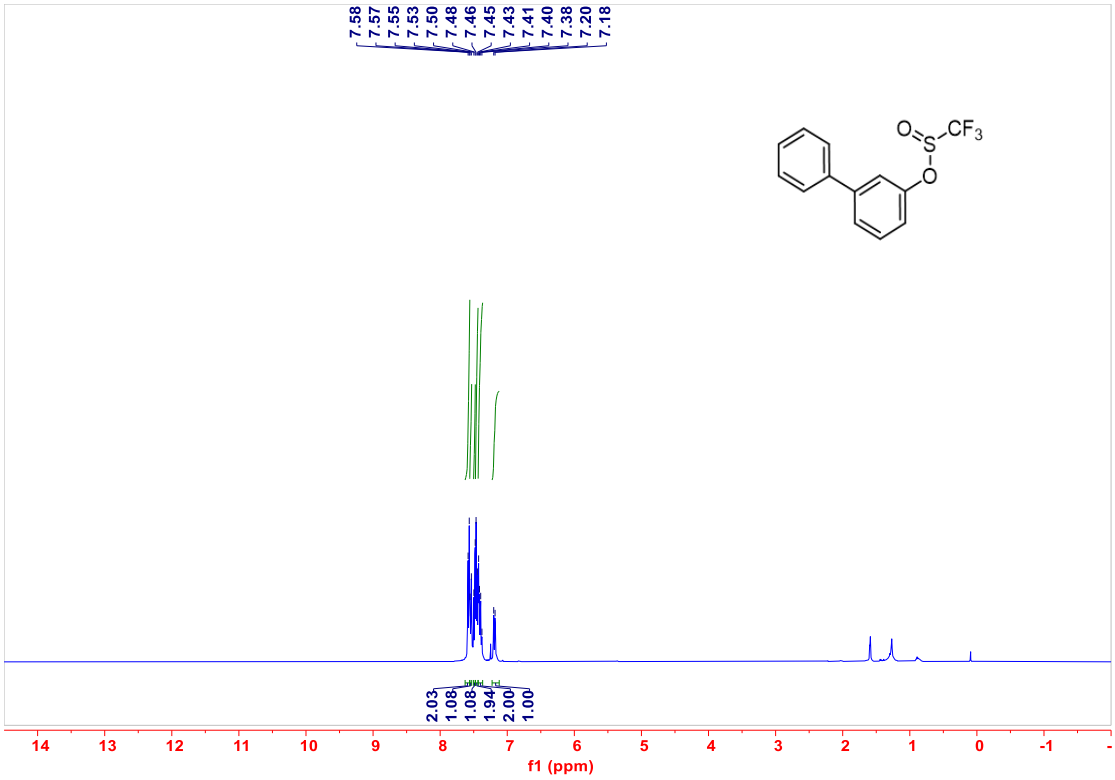
152.0
129.9
127.8
124.5
124.3
121.1
117.9
117.5
35.0
31.1
127.8
124.5
121.1
117.9
f1 (ppm)
O
S
CF3
O
f1 (ppm)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7.41
7.40
7.38
7.20
7.18
O
S
CF3
O
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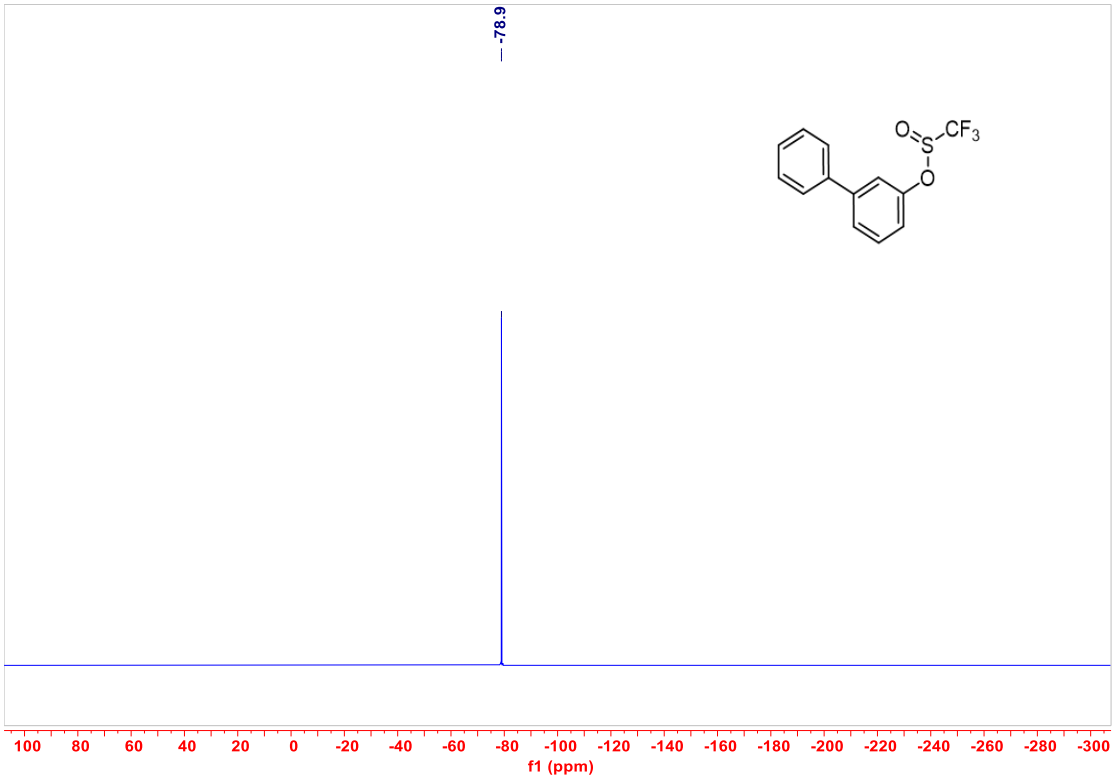
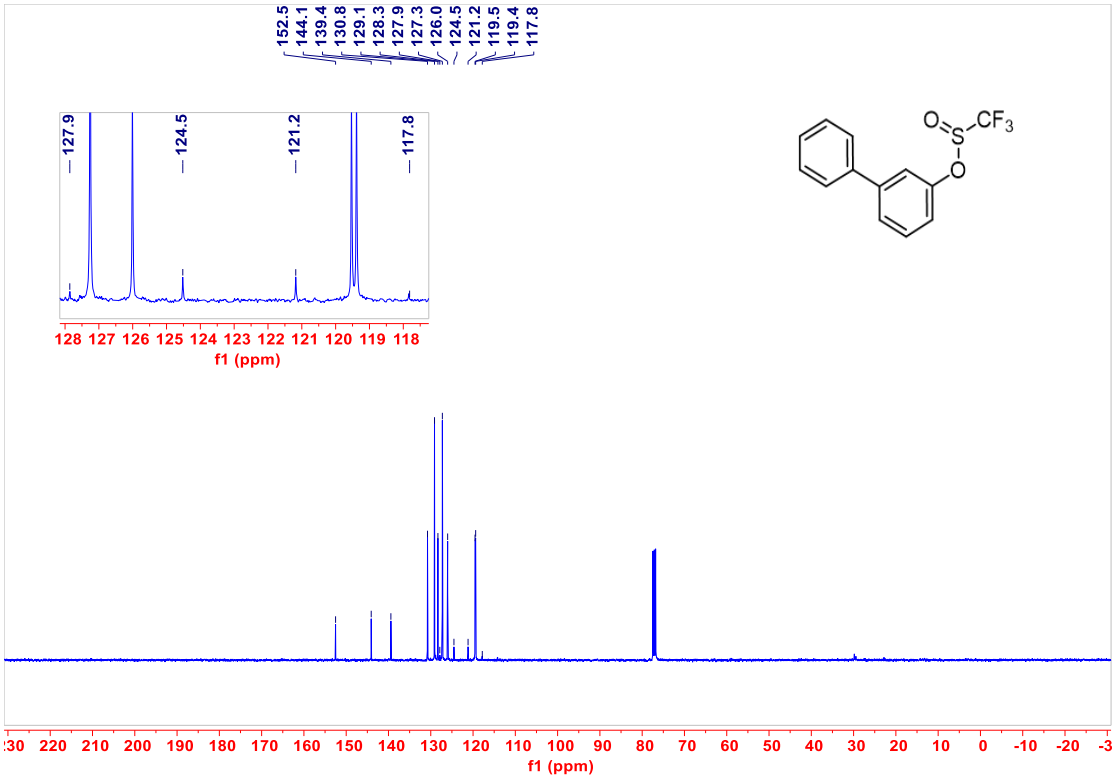
1.08
1.08
1.94
2.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.9
O
S
CF3
O
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)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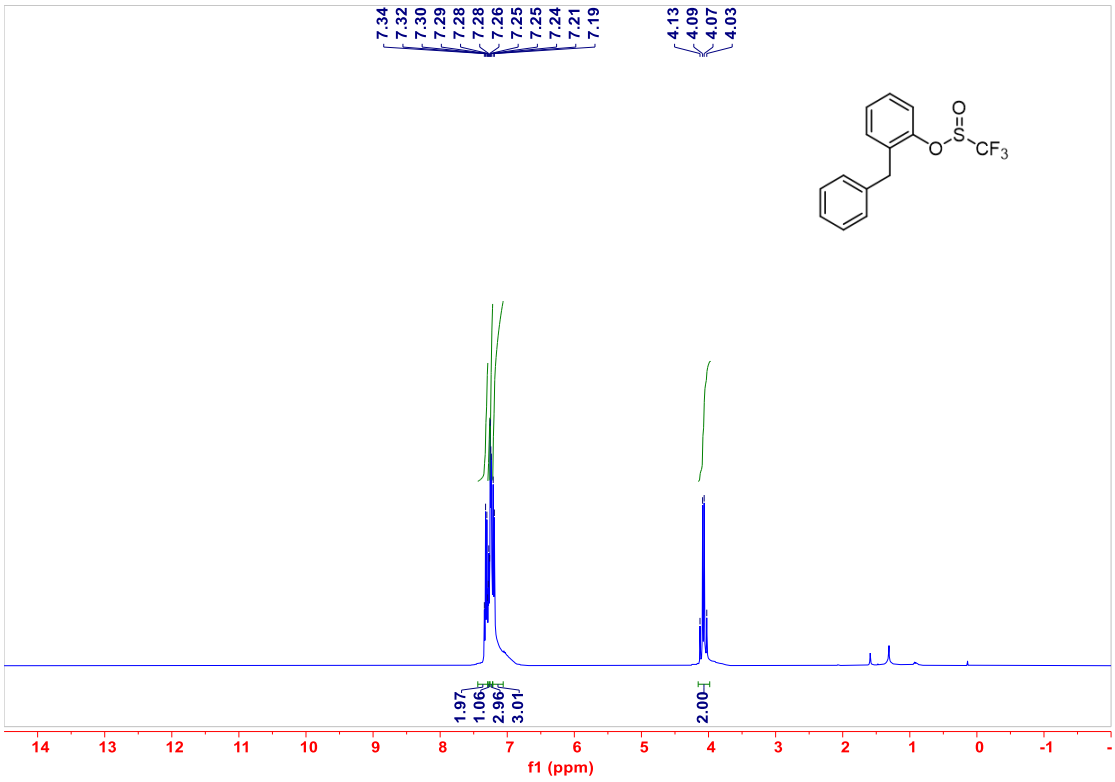
144.1
139.4
130.8
129.1
128.3
127.9
127.3
126.0
124.5
121.2
119.5
119.4
117.8
127.9
124.5
121.2
117.8
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
O
S
CF3
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.28
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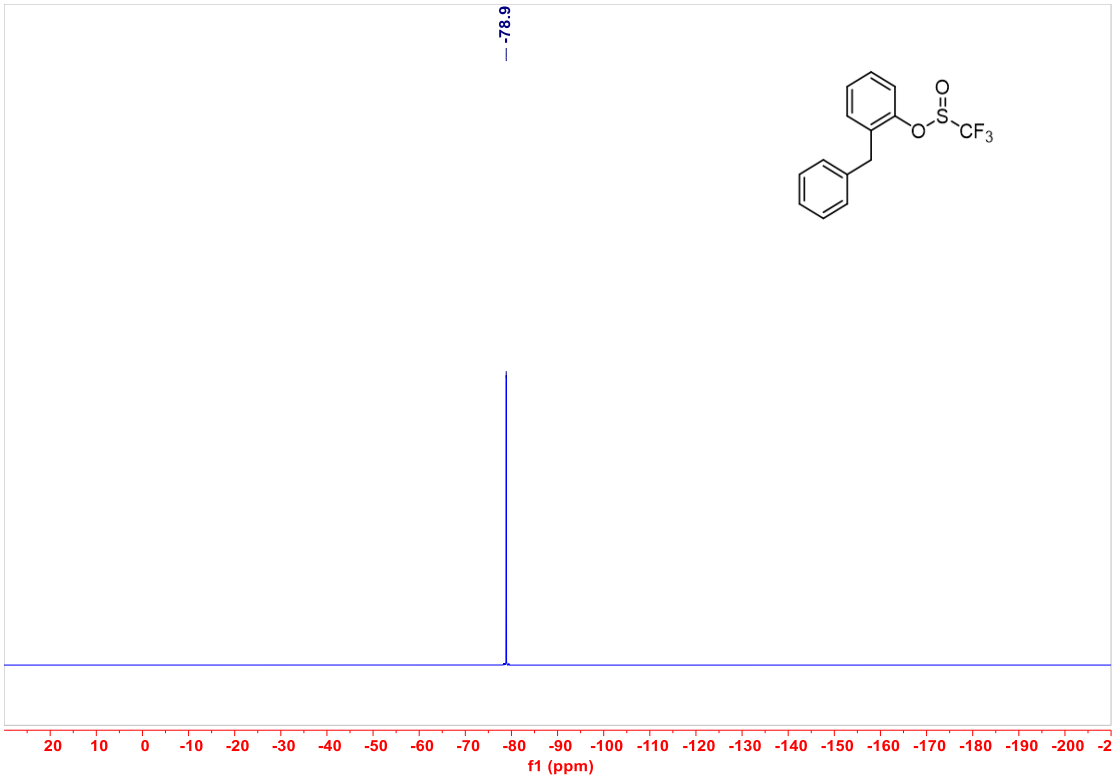
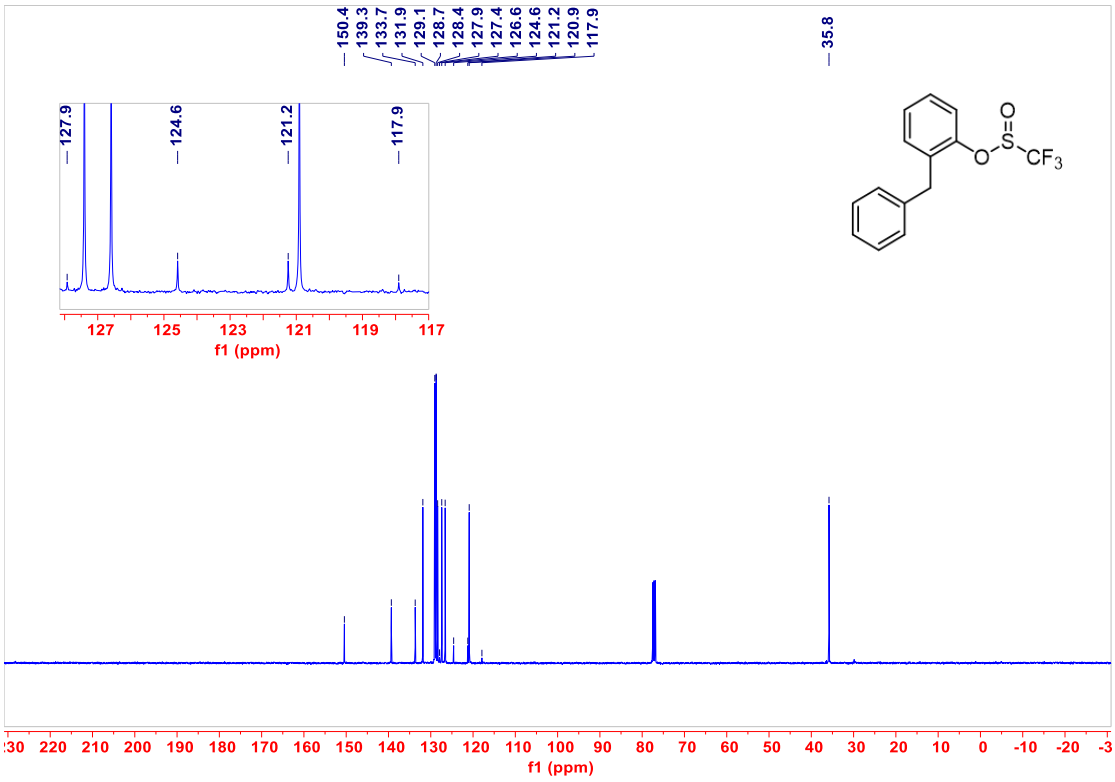
7.25
7.25
7.24
7.21
7.19
4.13
4.09
4.07
4.03
O
S
CF3
O
1.97
1.06
2.96
3.01
2.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-78.9
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)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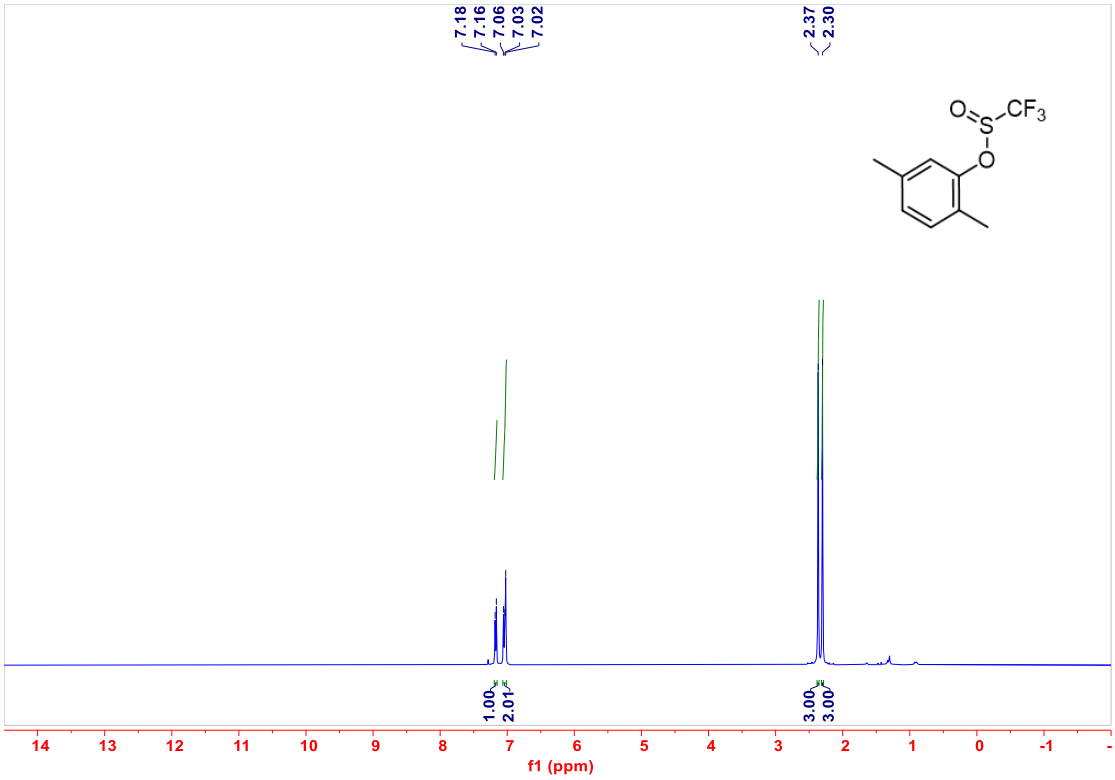
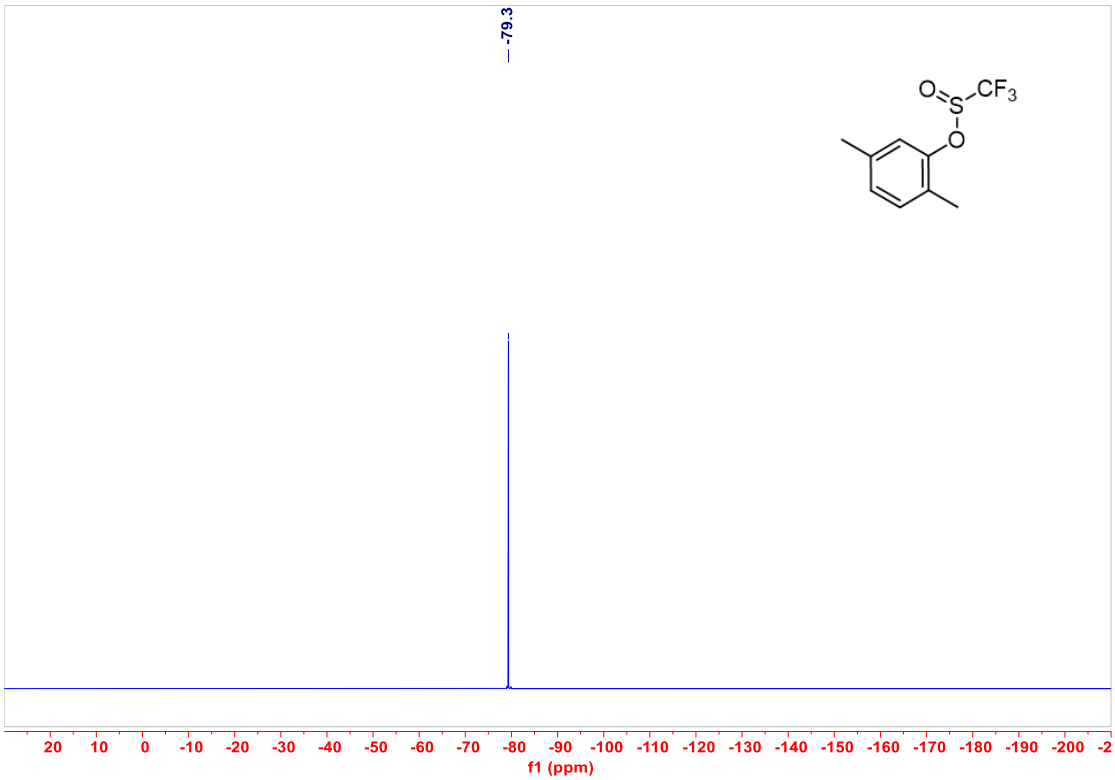
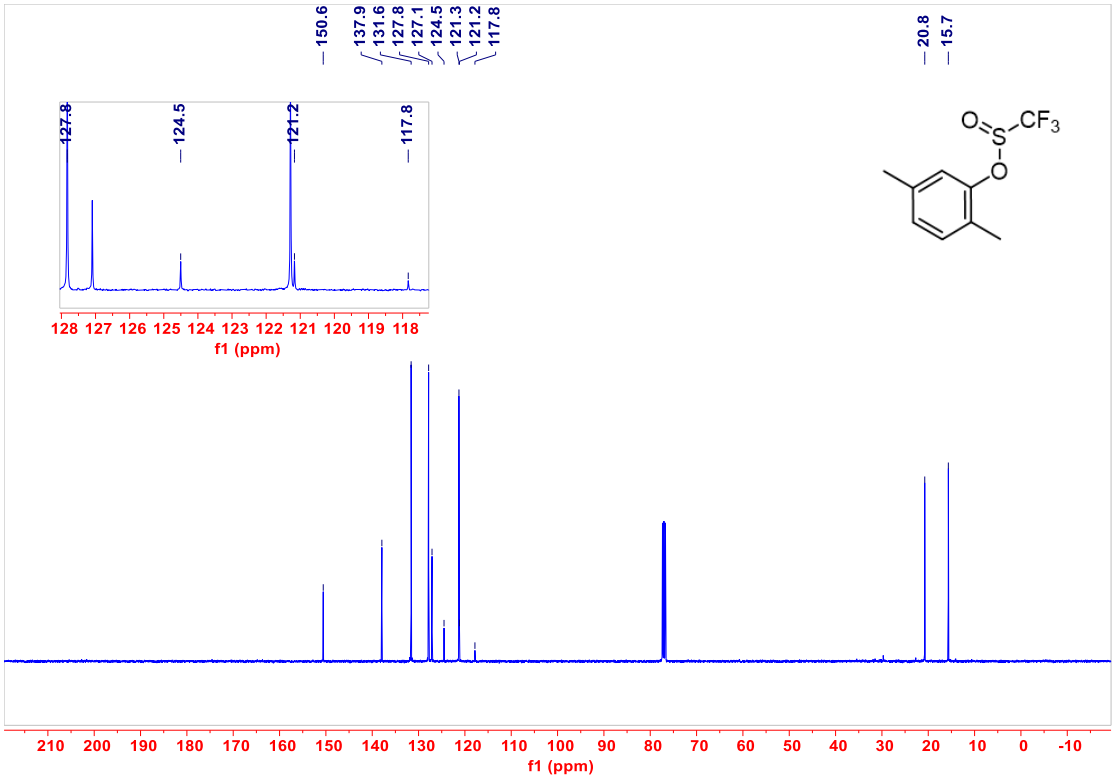
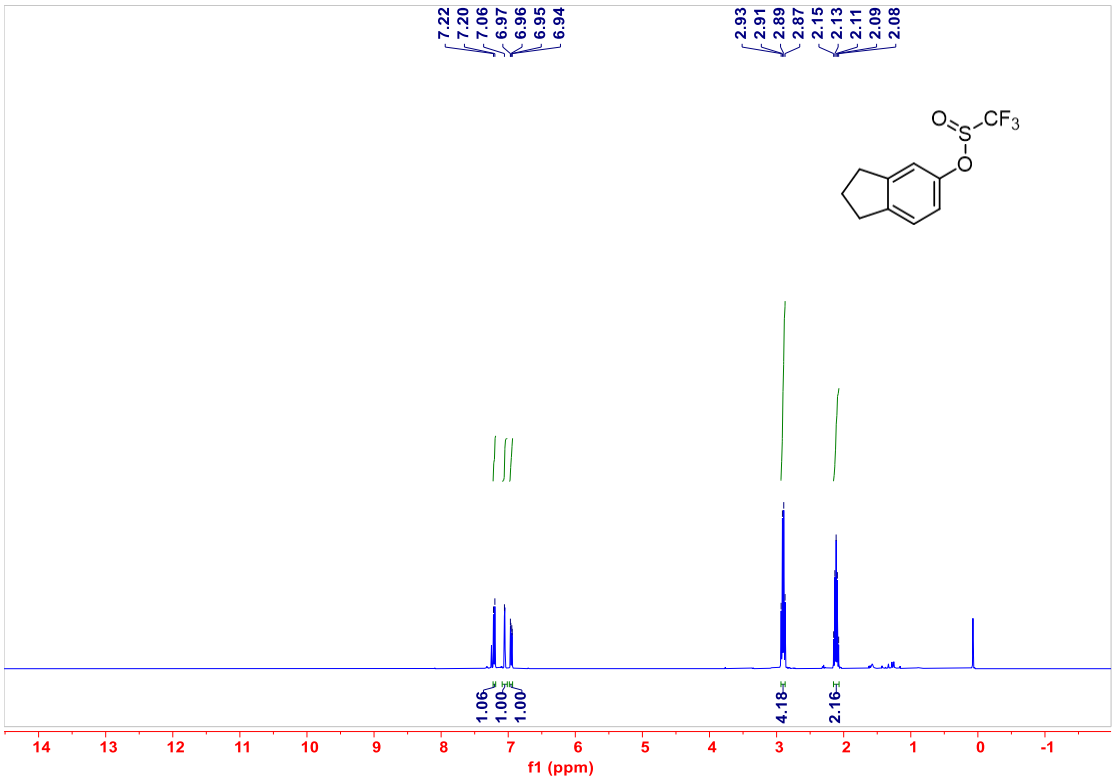
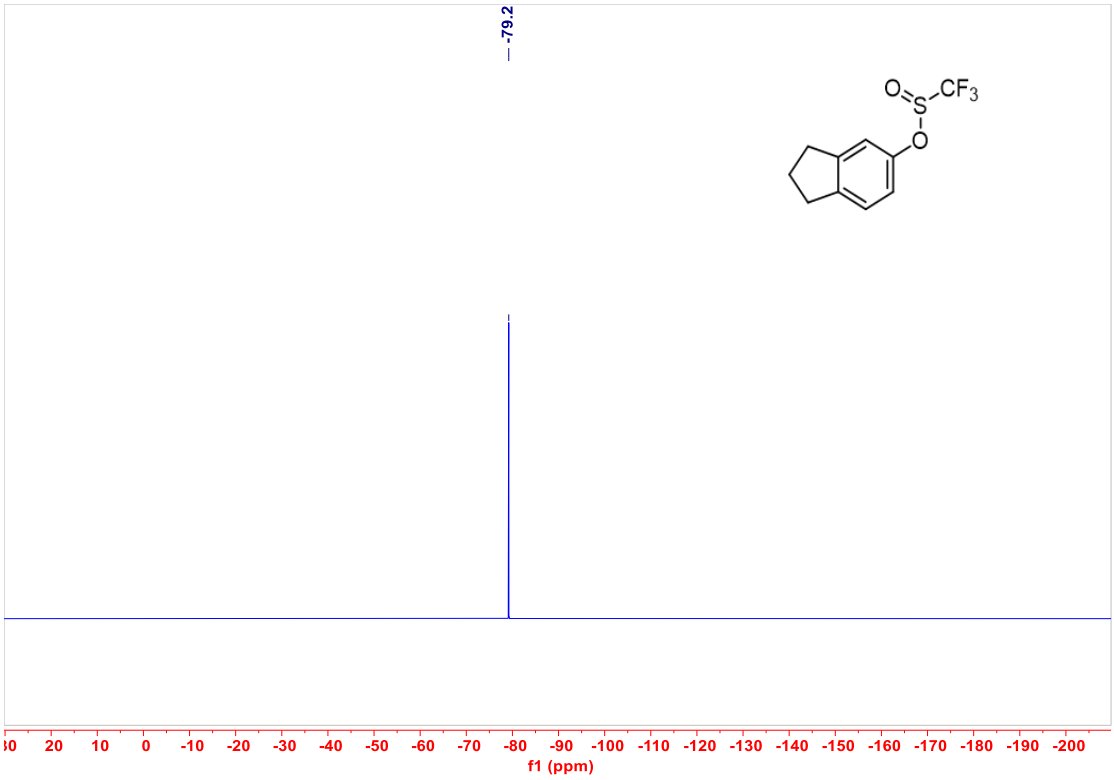
139.3
133.7
131.9
129.1
128.7
128.4
127.9
127.4
126.6
124.6
121.2
120.9
117.9
35.8
127.9
124.6
121.2
117.9
127 125 123 121 119 117
f1 (ppm)
O
S
O
CF3
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)

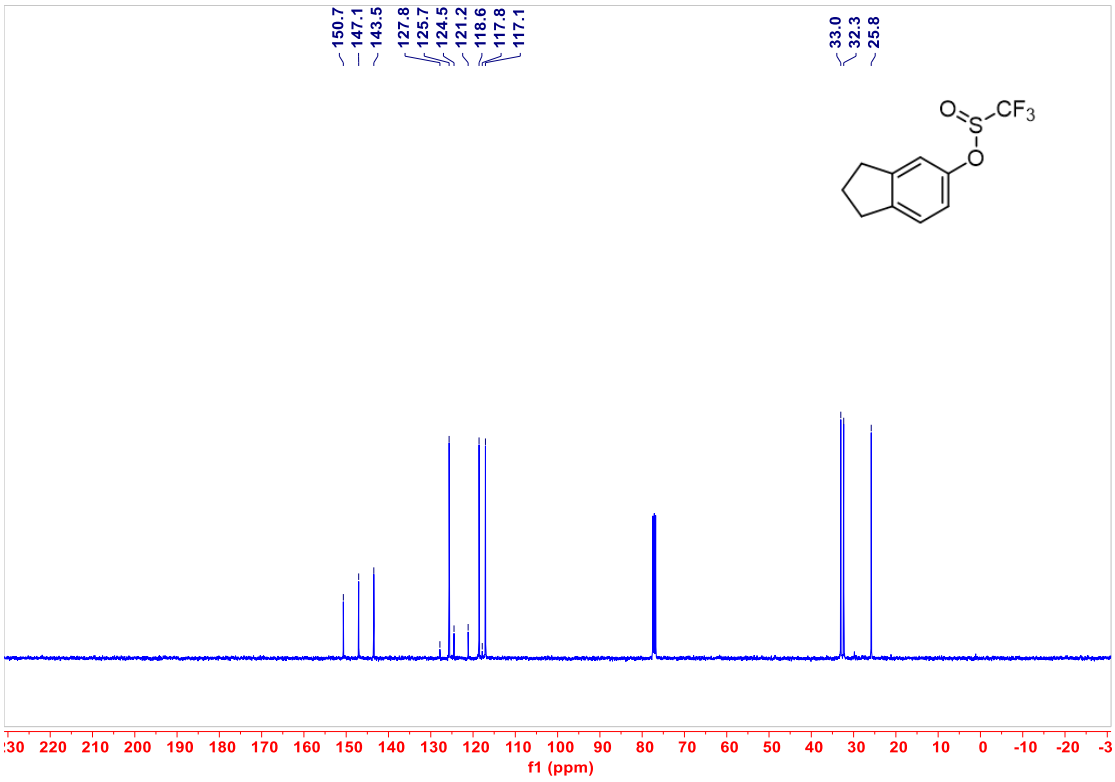

7.18
7.16
7.06
7.03
7.02
2.37
2.30
1.00
2.01
3.00
3.00
f1 (ppm)

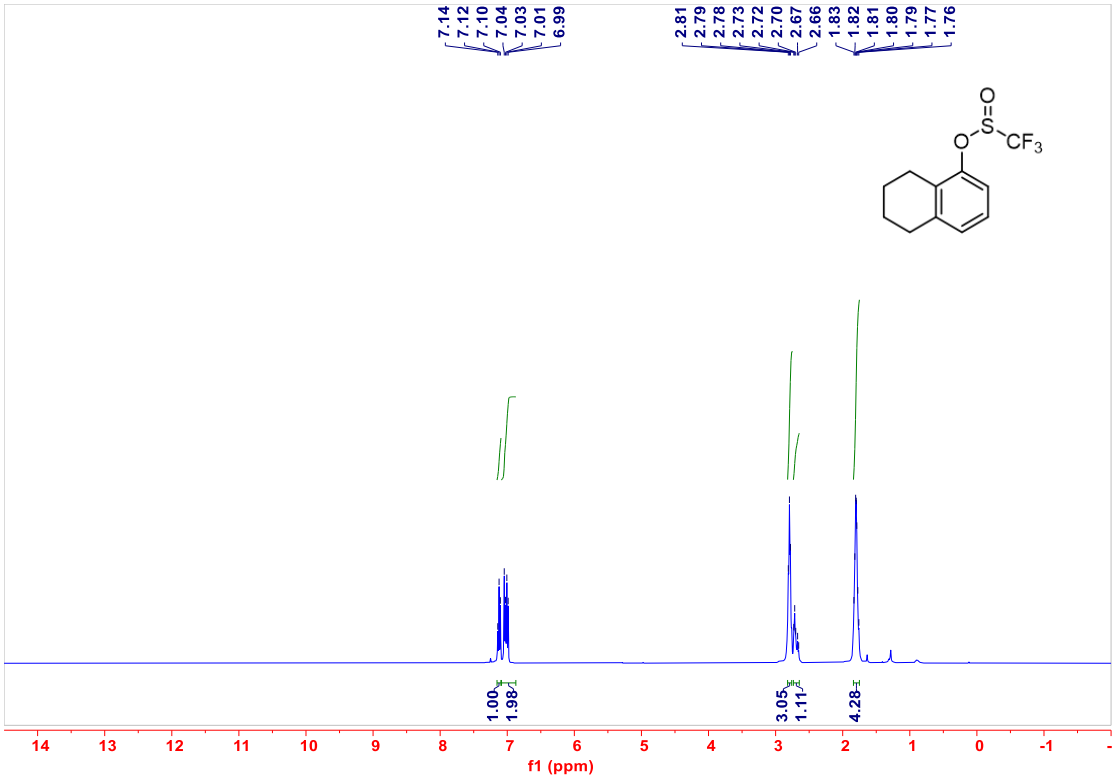

-79.3
f1 (ppm)

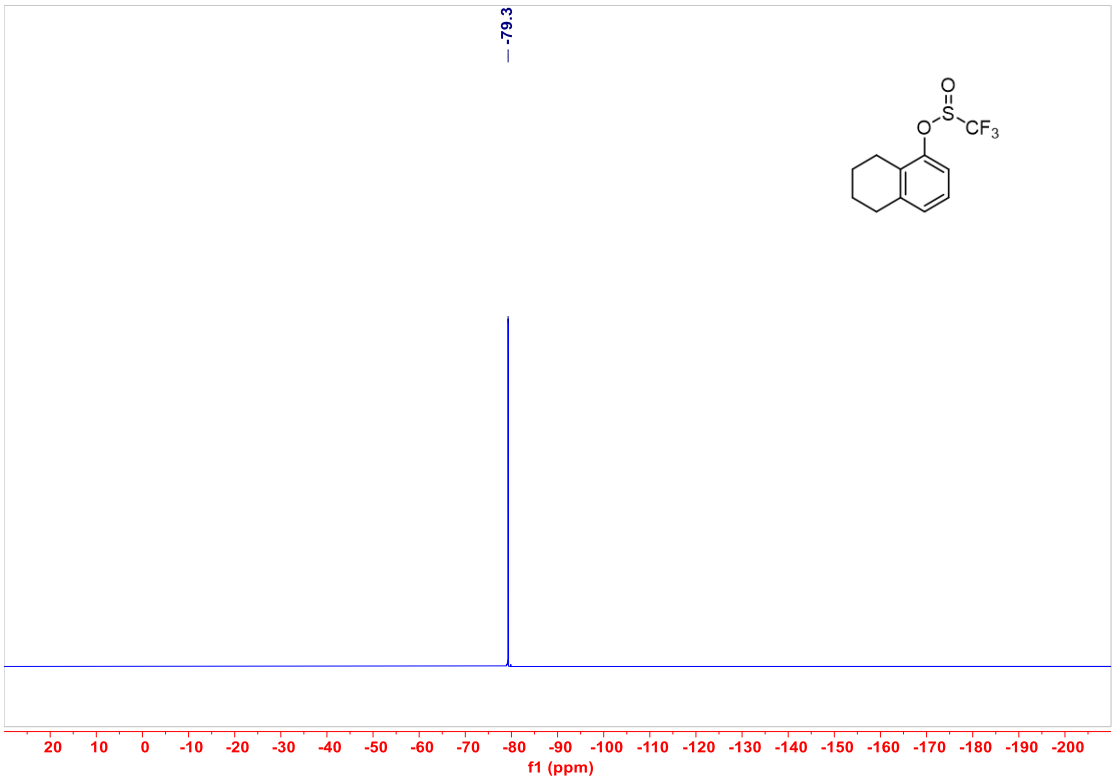

150.6
137.9
131.6
127.8
127.1
124.5
121.3
121.2
117.8
20.8
15.7
127.8
124.5
121.2
117.8
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
O
S
CF3
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

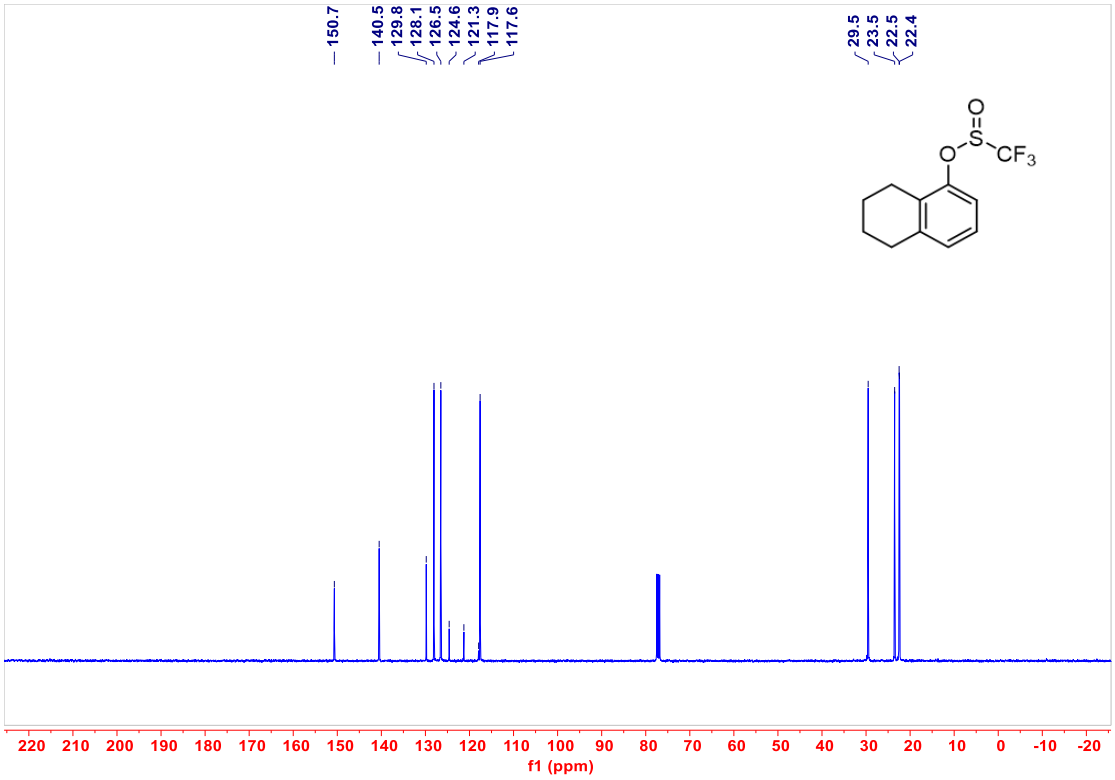

7.22
7.20
7.06
6.97
6.96
6.95
6.94
2.93
2.91
2.89
2.87
2.15
2.13
2.11
2.09
2.08
O
S
CF3
O
1.06
1.00
1.00
4.18
2.16
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

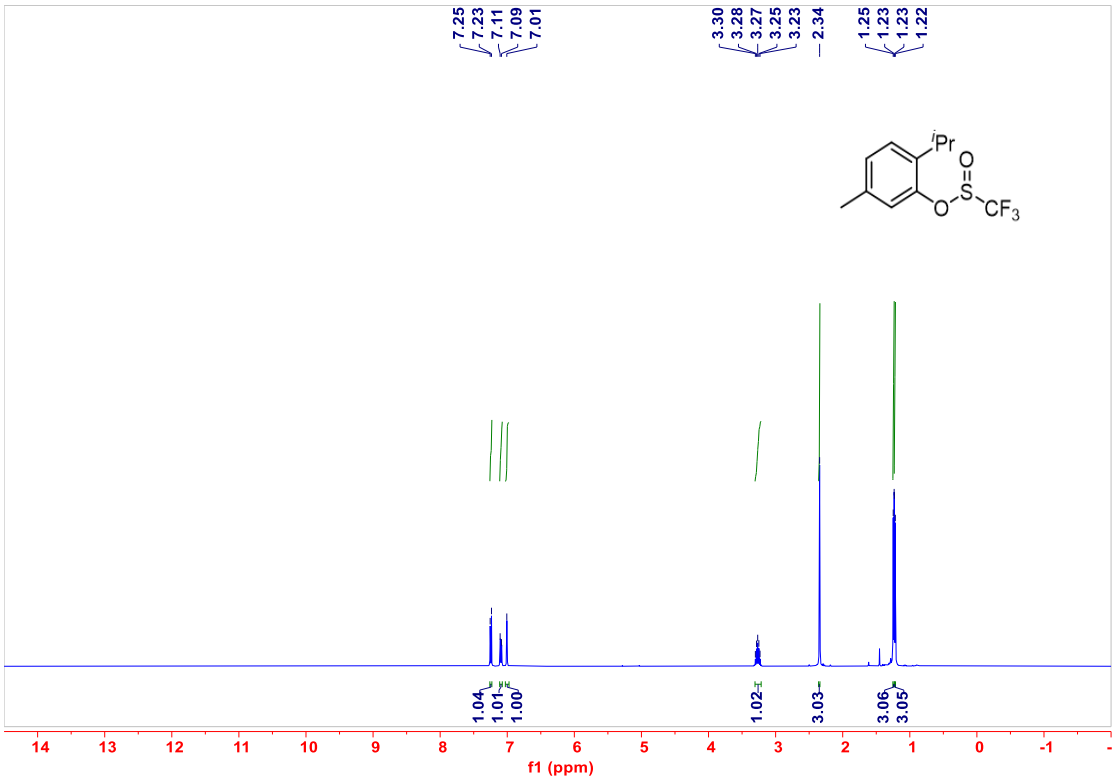

-79.2
O
S
CF3
O
f1 (ppm)

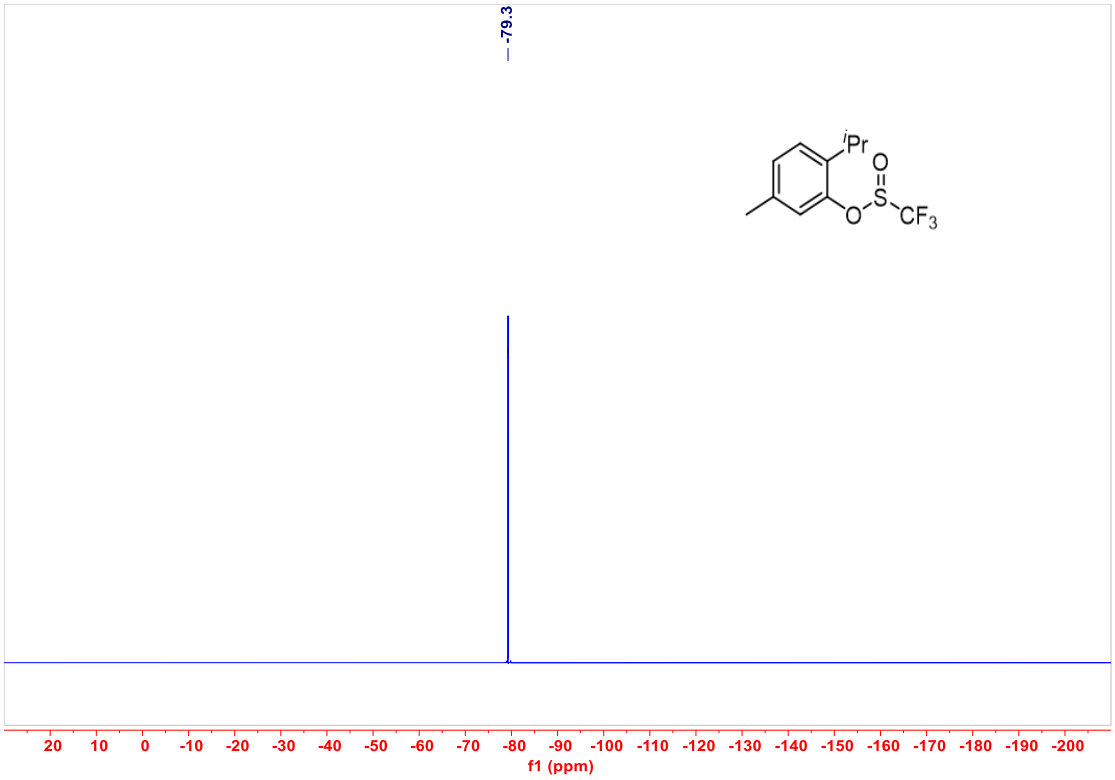

150.7
147.1
143.5
127.8
125.7
124.5
121.2
118.6
117.8
117.1
33.0
32.3
25.8
O
S
CF3
O
f1 (ppm)

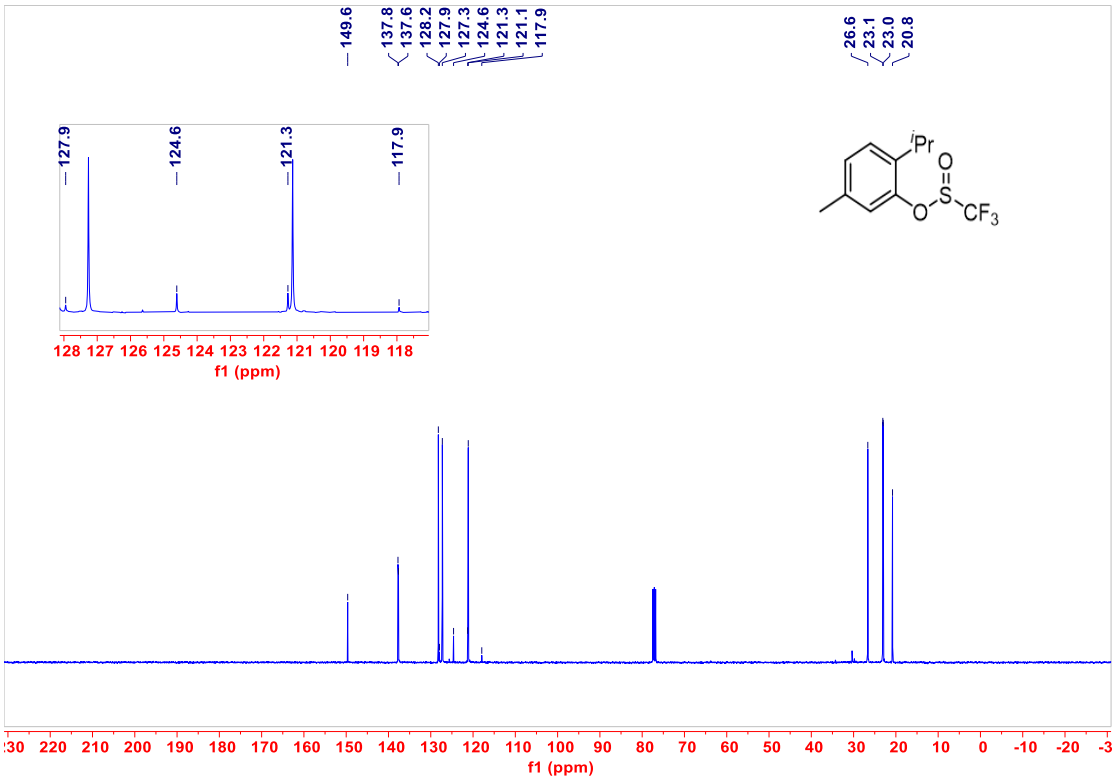

7.14
7.12
7.10
7.04
7.03
7.01
6.99
2.81
2.79
2.78
2.73
2.72
2.70
2.67
2.66
1.83
1.82
1.81
1.80
1.79
1.77
1.76
O
S
O
CF3
1.00
1.98
3.05
1.11
4.28
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

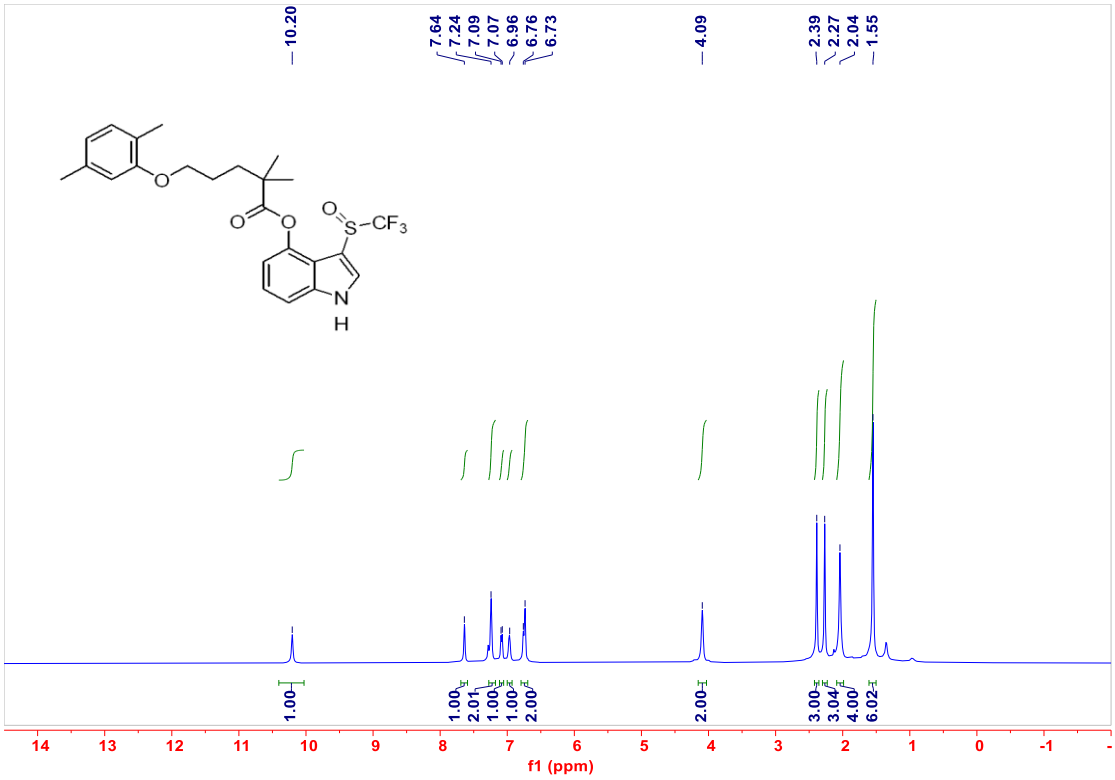

-79.3
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


150.7
140.5
129.8
128.1
126.5
124.6
121.3
117.9
117.6
29.5
23.5
22.5
22.4
O
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.25
7.23
7.11
7.09
7.01
3.30
3.28
3.27
3.25
3.23
2.34
1.25
1.23
1.23
1.22
iPr
O
S
O
CF3
1.04
1.01
1.00
1.02
3.03
3.06
3.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.3
iPr
O
S
O
CF3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


149.6
137.8
137.6
128.2
127.9
127.3
124.6
121.3
121.1
117.9
26.6
23.1
23.0
20.8
127.9
124.6
121.3
117.9
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
iPr
O
S
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


10.20
7.64
7.24
7.09
7.07
6.96
6.76
6.73
4.09
2.39
2.27
2.04
1.55
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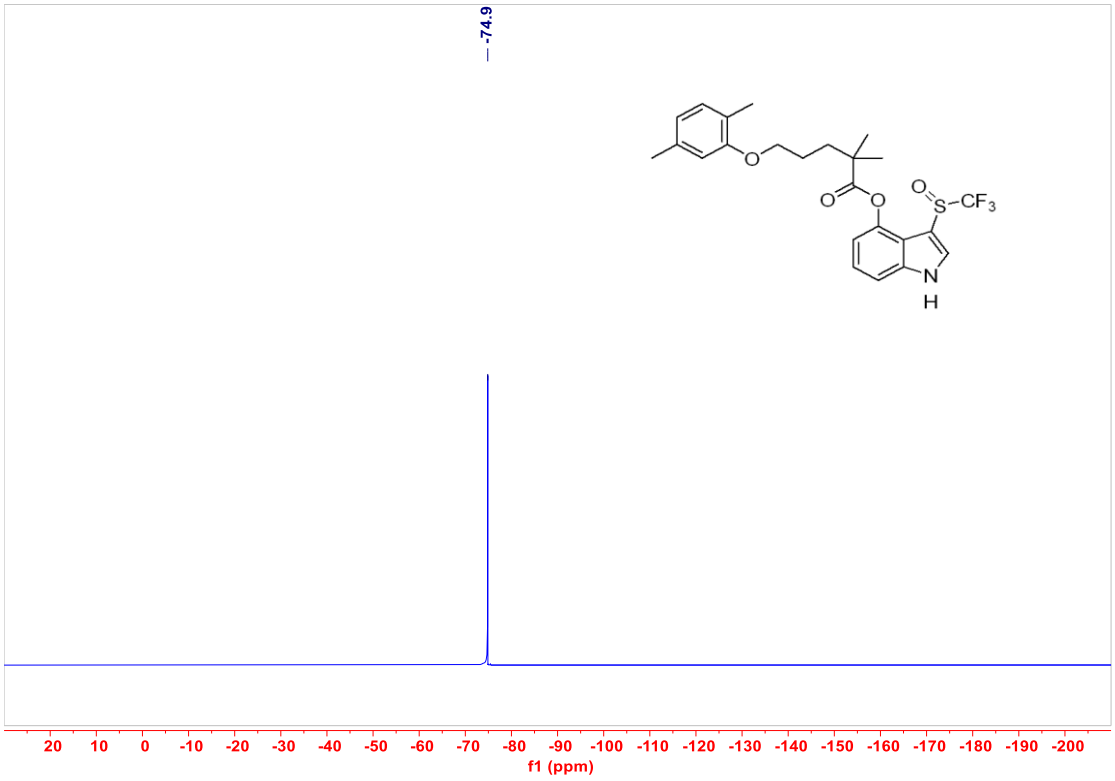
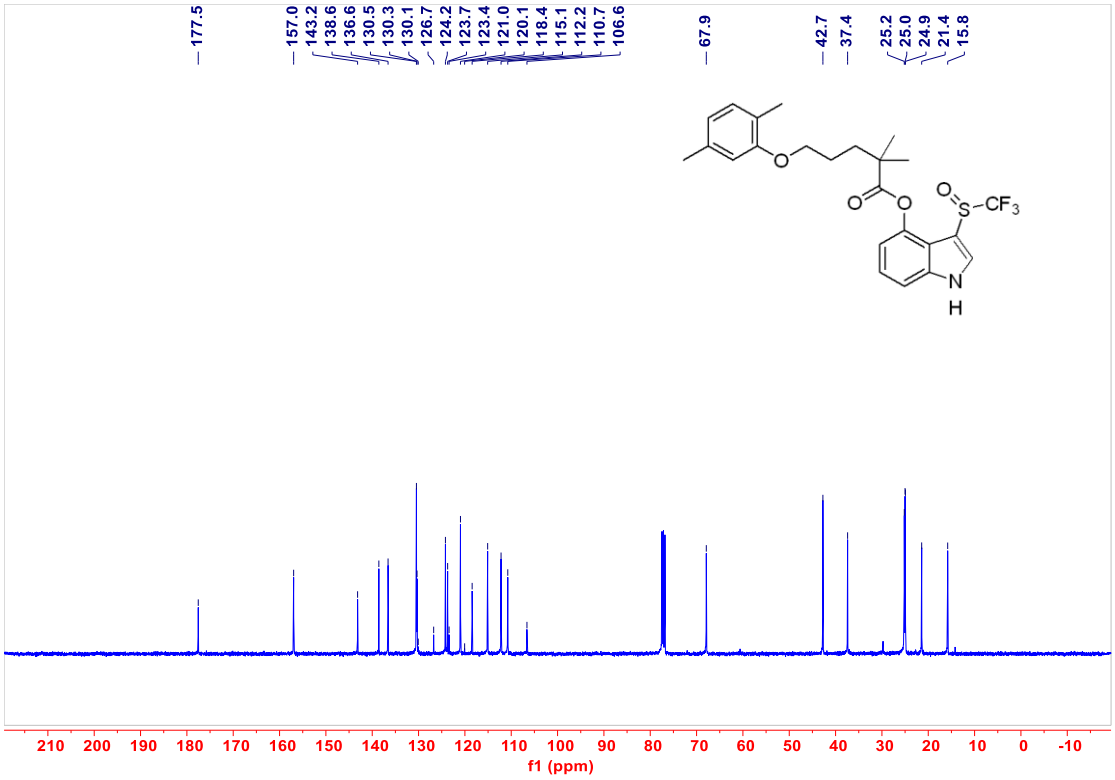
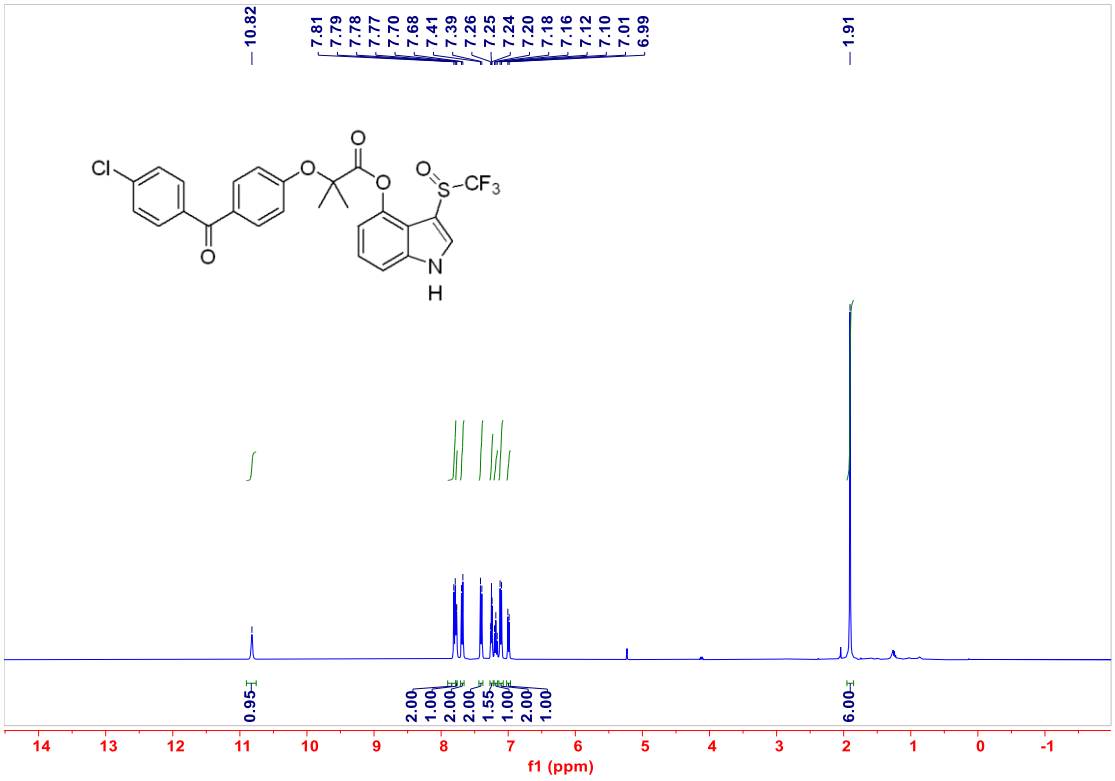
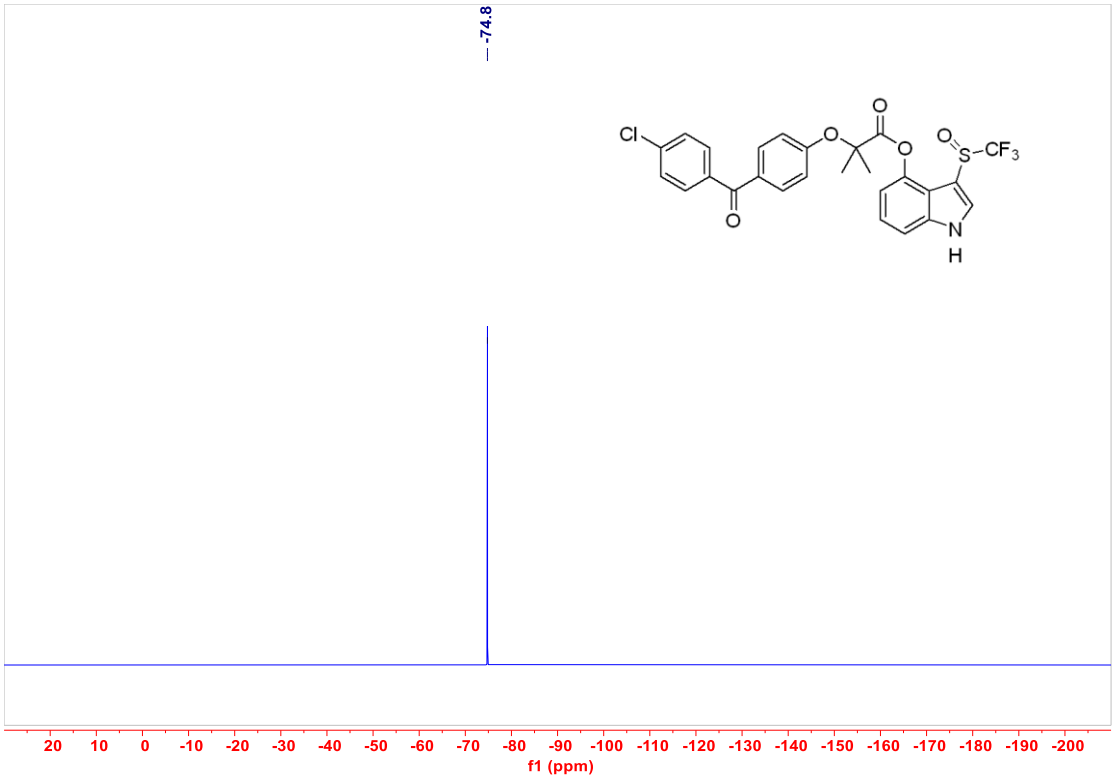
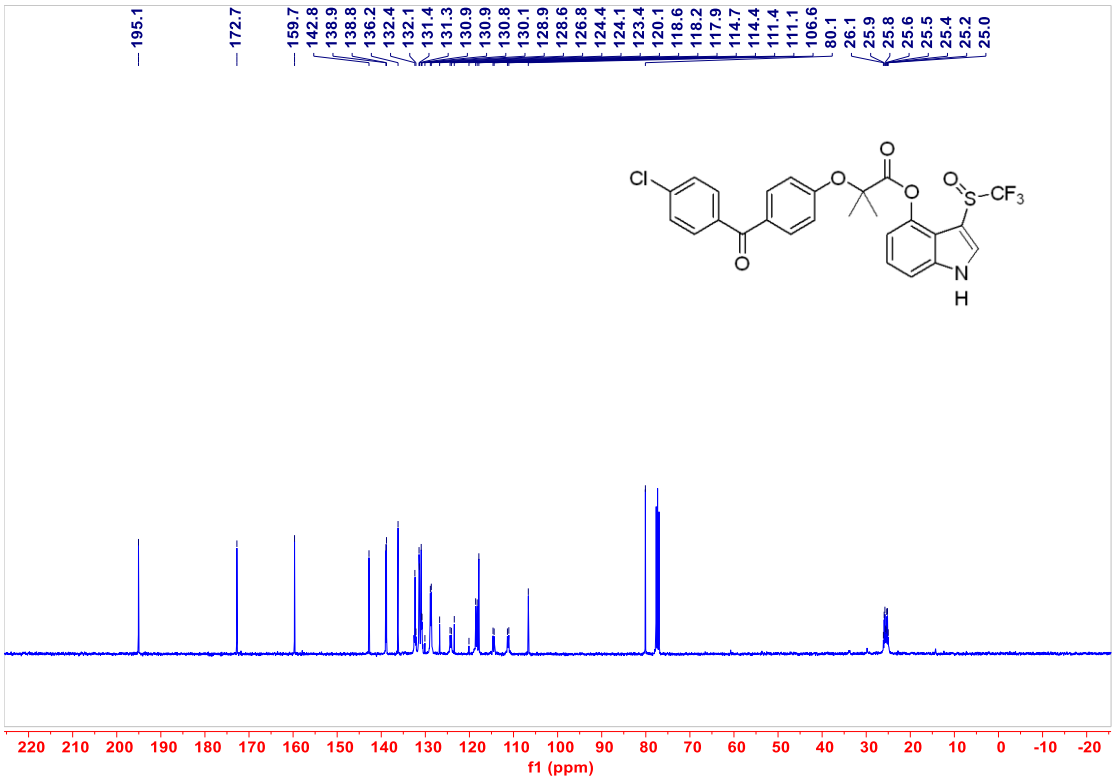
3.00
3.04
4.00
6.02
f1 (ppm)

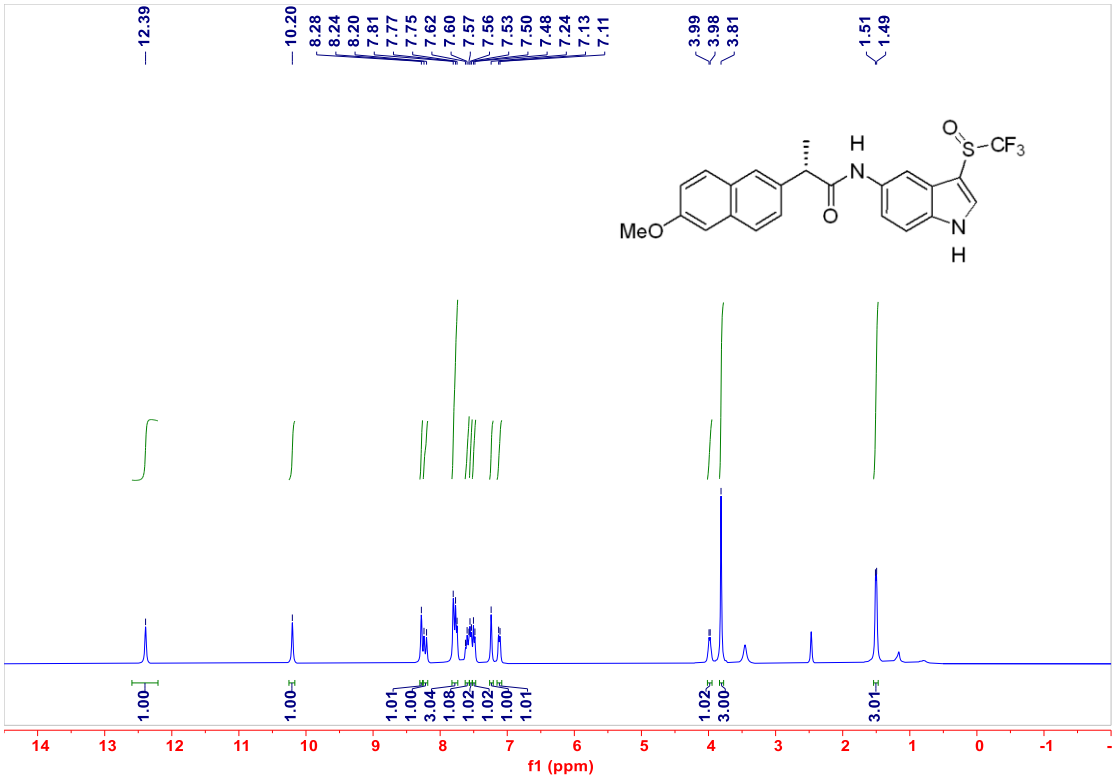

-74.9
f1 (ppm)

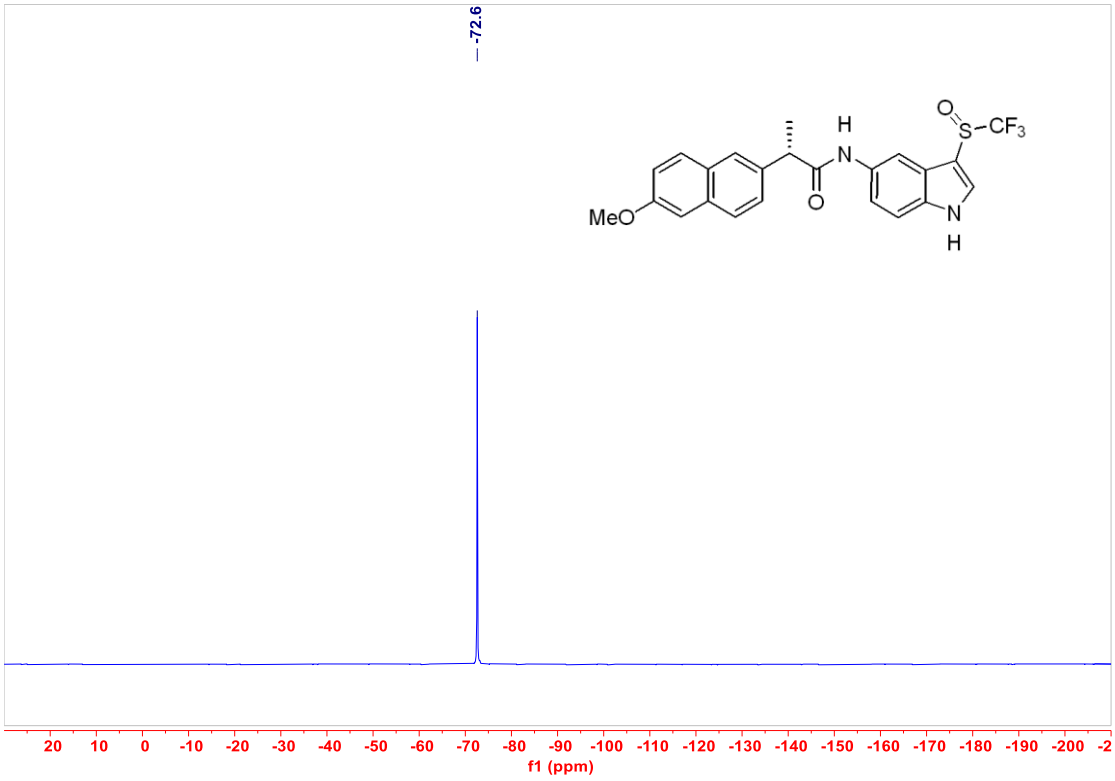

177.5
157.0
143.2
138.6
136.6
130.5
130.3
130.1
126.7
124.2
123.7
123.4
121.0
120.1
118.4
115.1
112.2
110.7
106.6
67.9
42.7
37.4
25.2
25.0
24.9
21.4
15.8
O
O
O
S
CF3
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

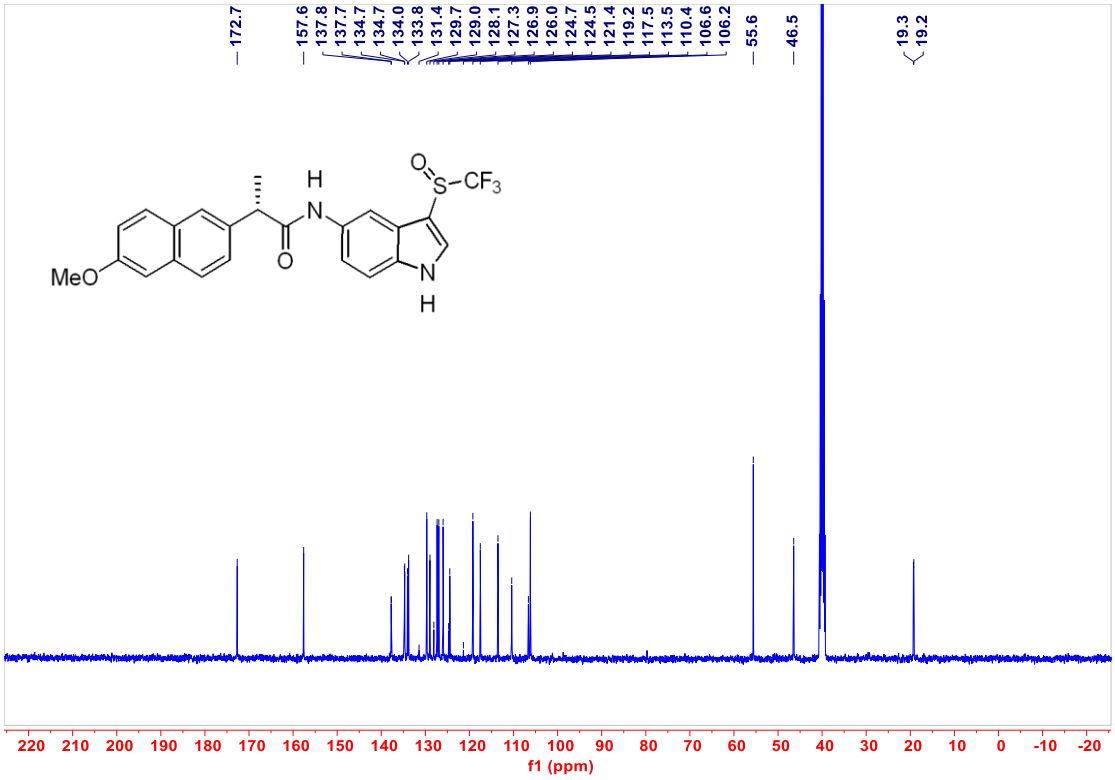

10.82
7.81
7.79
7.78
7.77
7.70
7.68
7.41
7.39
7.26
7.25
7.24
7.20
7.18
7.16
7.12
7.10
7.01
6.99
1.91
Cl
O
O
O
O
O
S
CF3
N
H
0.95
2.00
1.00
2.00
2.00
1.55
1.00
2.00
1.00
6.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

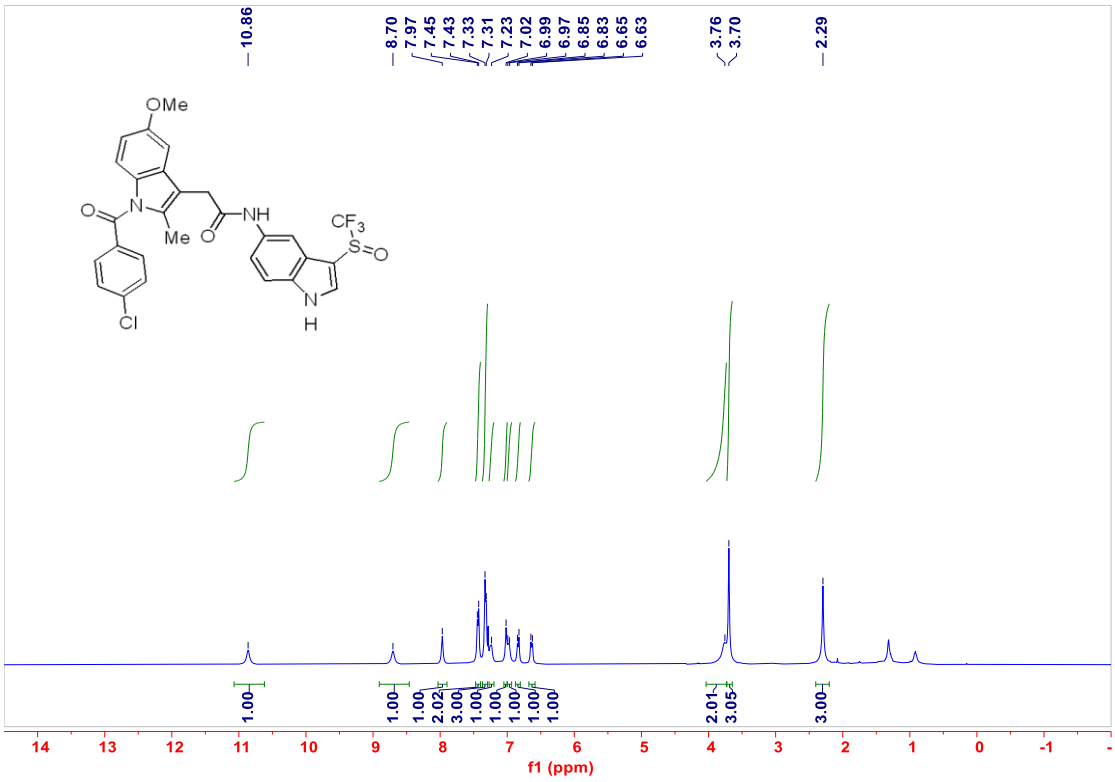

-74.8
Cl
O
O
O
O
O
S
CF3
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

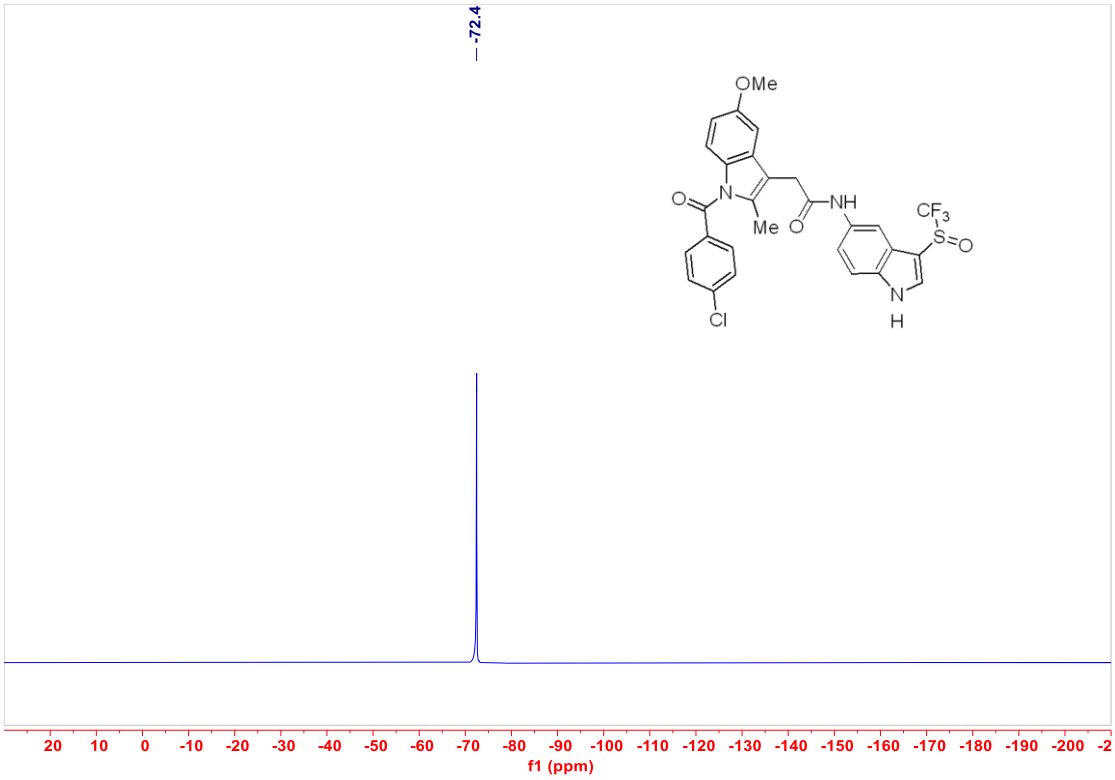

195.1
172.7
159.7
142.8
138.9
138.8
136.2
132.4
132.1
131.4
131.3
130.9
130.9
130.8
130.1
128.9
128.6
126.8
124.4
124.1
123.4
120.1
118.6
118.2
117.9
114.7
114.4
111.4
111.1
106.6
80.1
26.1
25.9
25.8
25.6
25.5
25.4
25.2
25.0
Cl
O
O
O
O
O
S
CF3
N
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


12.39
10.20
8.28
8.24
8.20
7.81
7.77
7.75
7.62
7.60
7.57
7.56
7.53
7.50
7.48
7.24
7.13
7.11
3.99
3.98
3.81
1.51
1.49
MeO
H
N
O
S
CF3
N
H
1.00
1.00
1.01
1.00
3.04
1.08
1.02
1.02
1.00
1.01
1.02
3.00
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-72.6
MeO
H
N
O
S
CF3
N
H
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


172.7
157.6
137.8
137.7
134.7
134.7
134.0
133.8
131.4
129.7
129.0
128.1
127.3
126.9
126.0
124.7
124.5
121.4
119.2
117.5
113.5
110.4
106.6
106.2
55.6
46.5
19.3
19.2
MeO
H
N
O
S
CF3
N
H
f1 (ppm)


10.86
8.70
7.97
7.45
7.43
7.33
7.31
7.23
7.02
6.99
6.97
6.85
6.83
6.65
6.63
3.76
3.70
2.29
OMe
N
O
Me
NH
O
CF3
S
O
N
H
Cl
1.00
1.00
1.00
2.02
3.00
1.00
1.00
1.00
1.00
1.00
2.01
3.05
3.00
f1 (ppm)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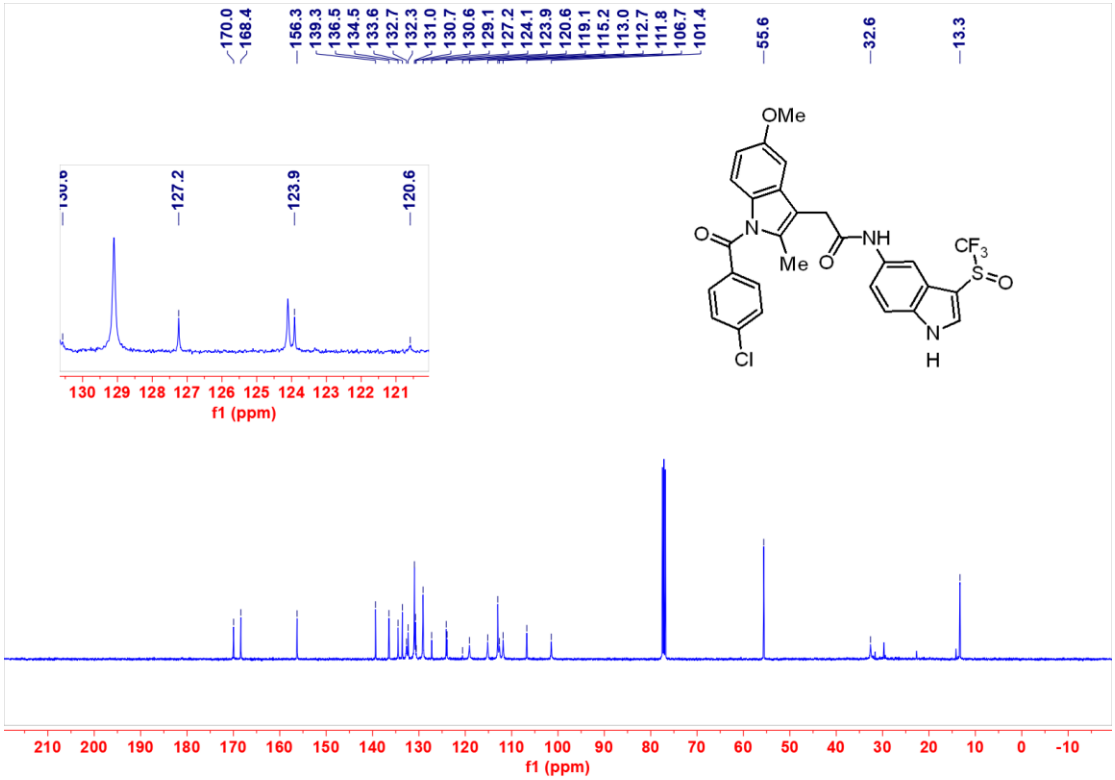
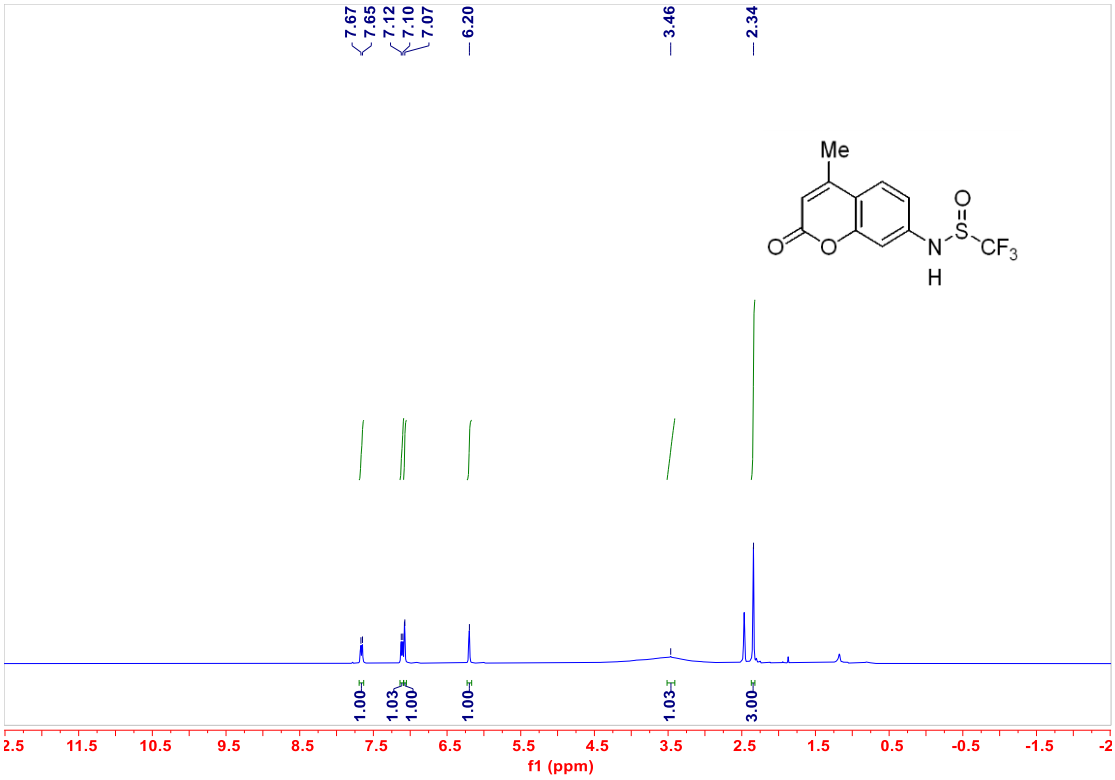
OMe
N
O
Me
O
NH
CF3
S
O
N
H
Cl
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -2
f1 (ppm)


170.0
168.4
156.3
139.3
136.5
134.5
133.6
132.7
132.3
131.0
130.7
130.6
129.1
127.2
124.1
123.9
120.6
119.1
115.2
113.0
112.7
111.8
106.7
101.4
55.6
32.6
13.3
127.2
123.9
120.6
130 129 128 127 126 125 124 123 122 121
f1 (ppm)
OMe
N
O
Me
O
NH
CF3
S
O
N
H
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)


7.67
7.65
7.12
7.10
7.07
6.20
3.46
2.34
Me
O
O
N
S
O
CF3
H
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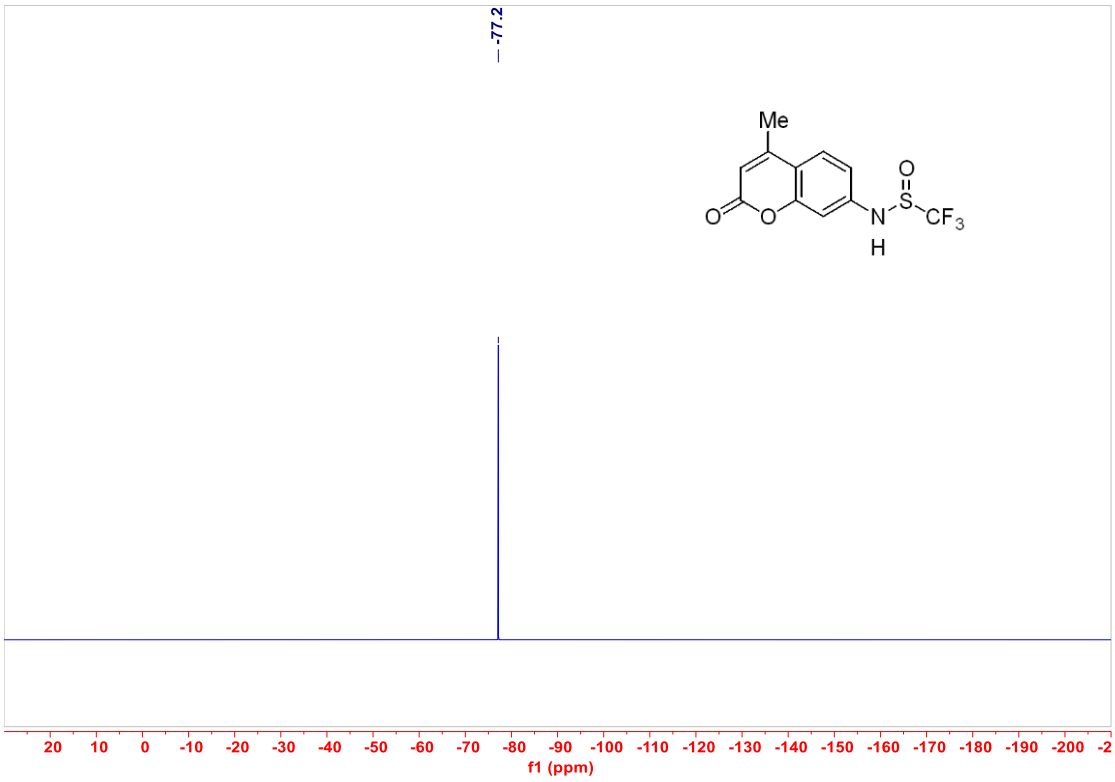
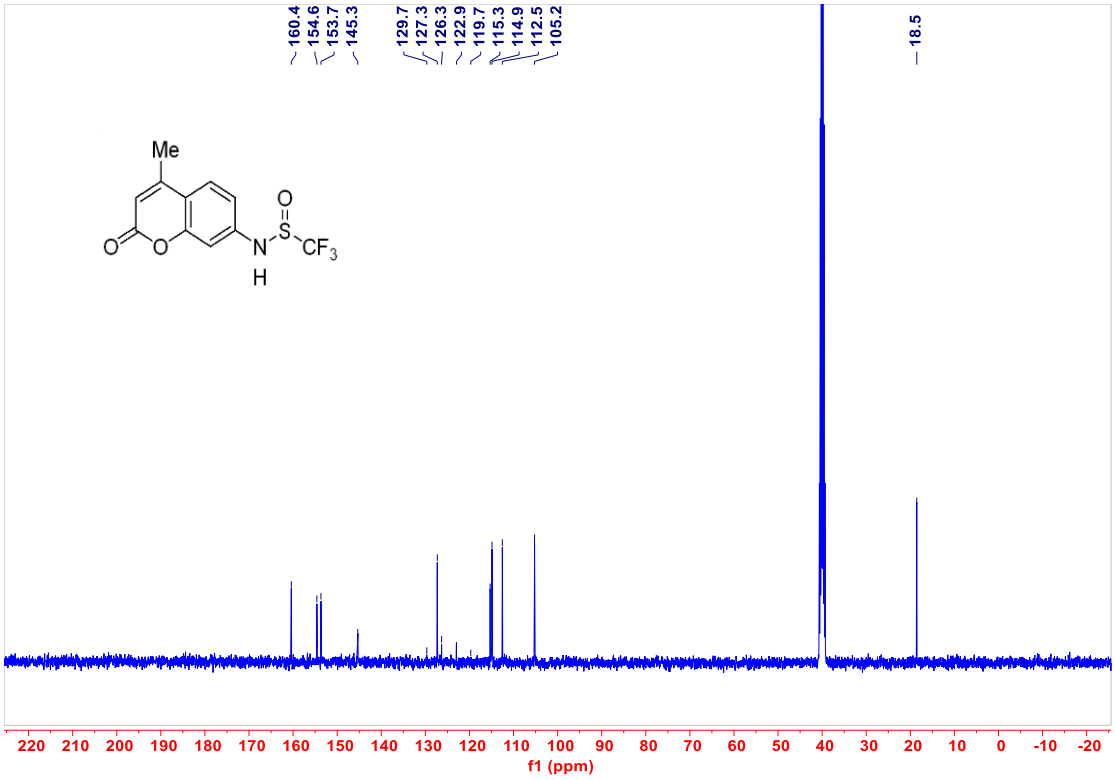
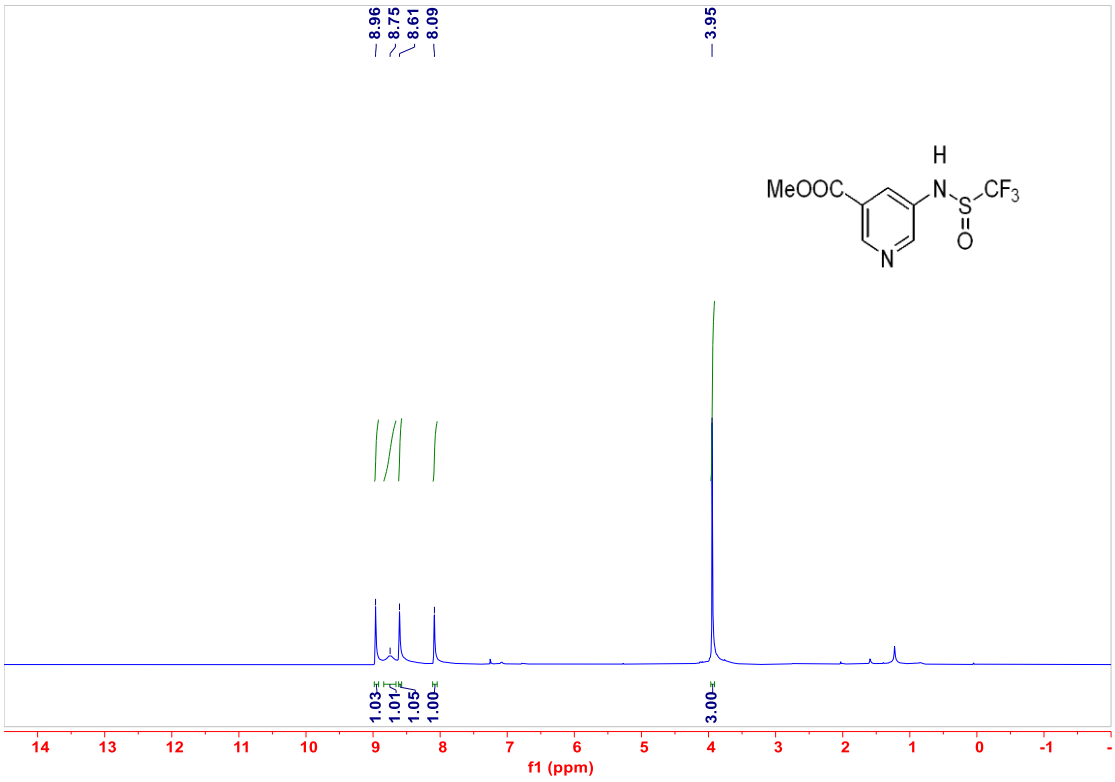
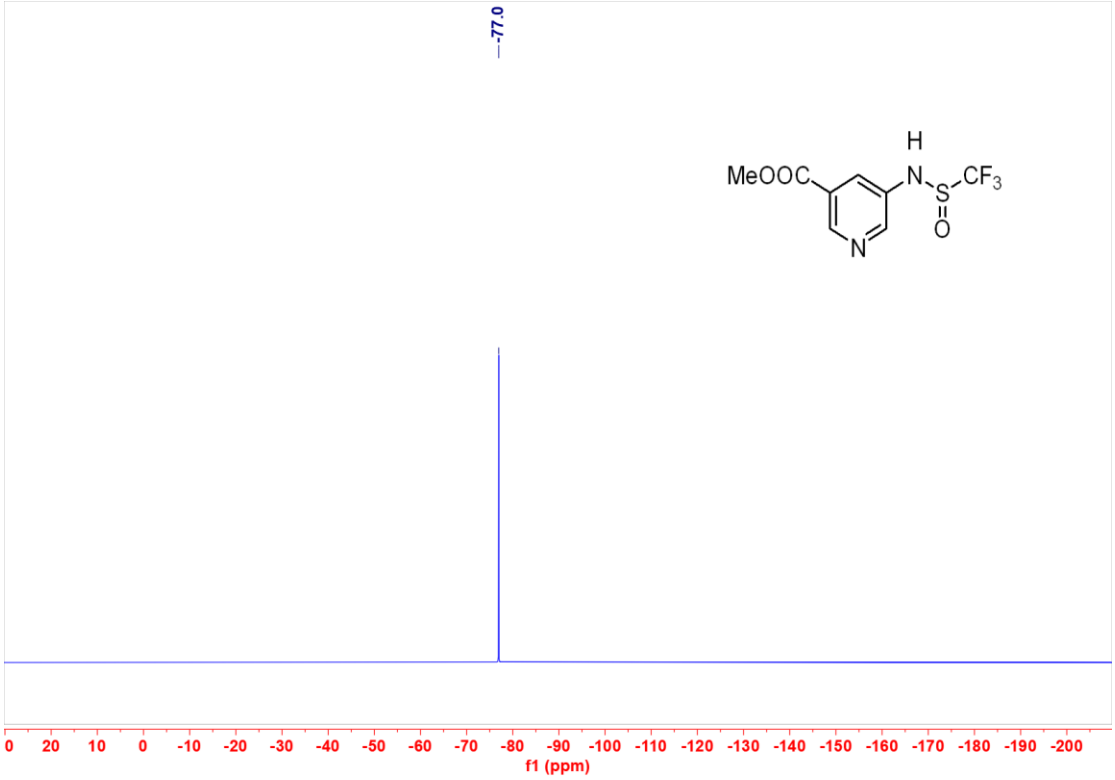
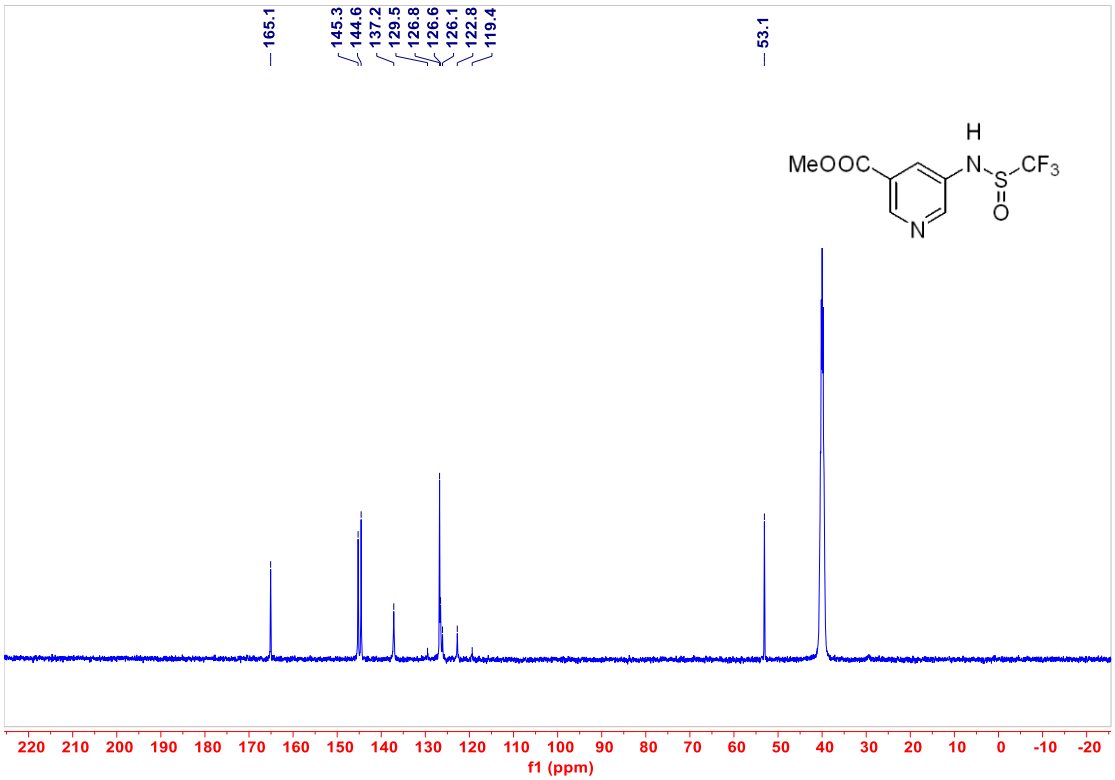
1.03
1.00
1.00
1.03
3.00
f1 (ppm)

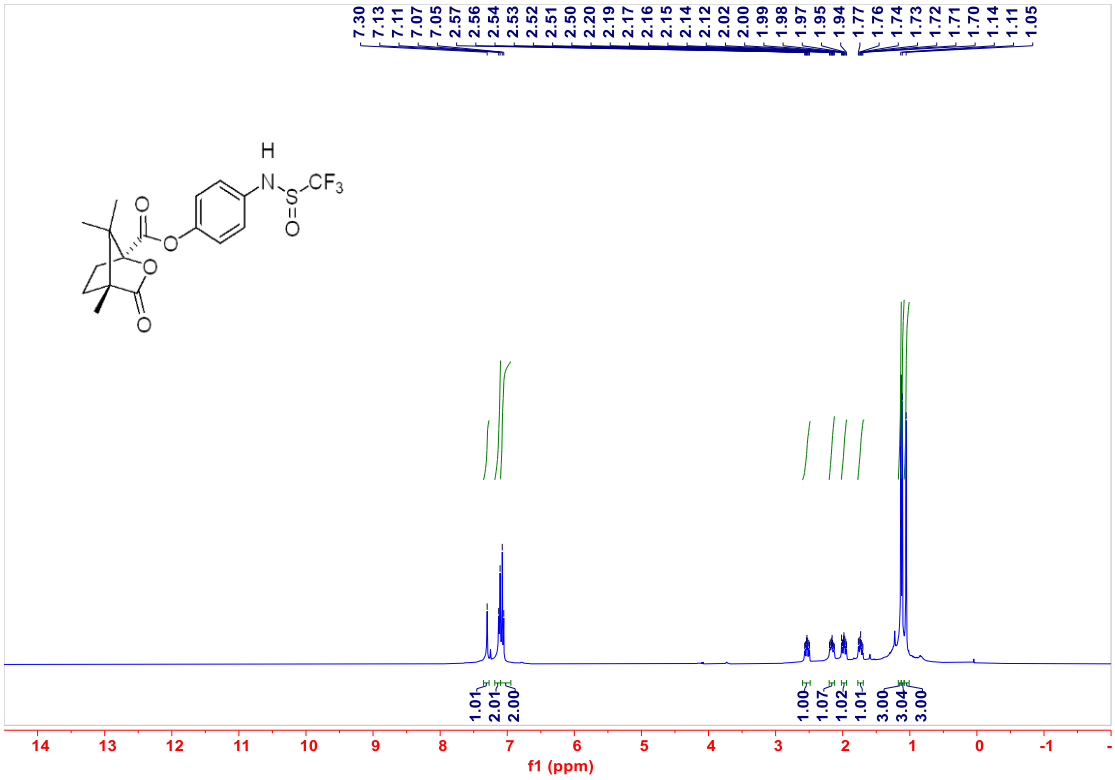

-77.2
Me
O
O
N
S
O
CF3
H
f1 (ppm)

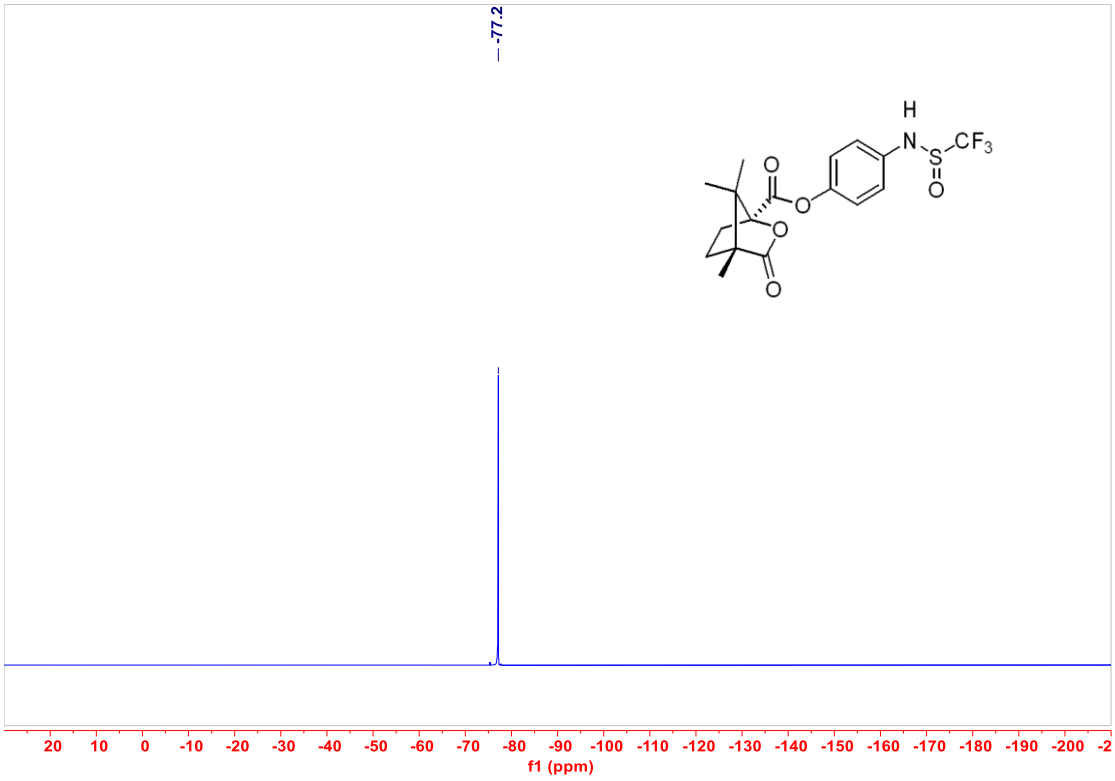

160.4
154.6
153.7
145.3
129.7
127.3
126.3
122.9
119.7
115.3
114.9
112.5
105.2
18.5
Me
O
O
O
S
N
H
CF3
f1 (ppm)


8.96
8.75
8.61
8.09
3.95
MeOOC
H
N
S
CF3
O
N
1.03
1.01
1.05
1.00
3.00
f1 (ppm)


-77.0
MeOOC
H
N
S
CF3
O
N
0 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


165.1
145.3
144.6
137.2
129.5
126.8
126.6
126.1
122.8
119.4
53.1
MeOOC
H
N
S
CF3
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.30
7.13
7.11
7.07
7.05
2.57
2.56
2.54
2.53
2.52
2.51
2.50
2.20
2.19
2.17
2.16
2.15
2.14
2.12
2.02
2.00
1.99
1.98
1.97
1.95
1.94
1.77
1.76
1.74
1.73
1.72
1.71
1.70
1.14
1.11
1.05
H
N
S
CF3
O
O
O
O
O
1.01
2.01
2.00
1.00
1.07
1.02
1.01
3.00
3.04
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
S
CF3
O
O
O
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O
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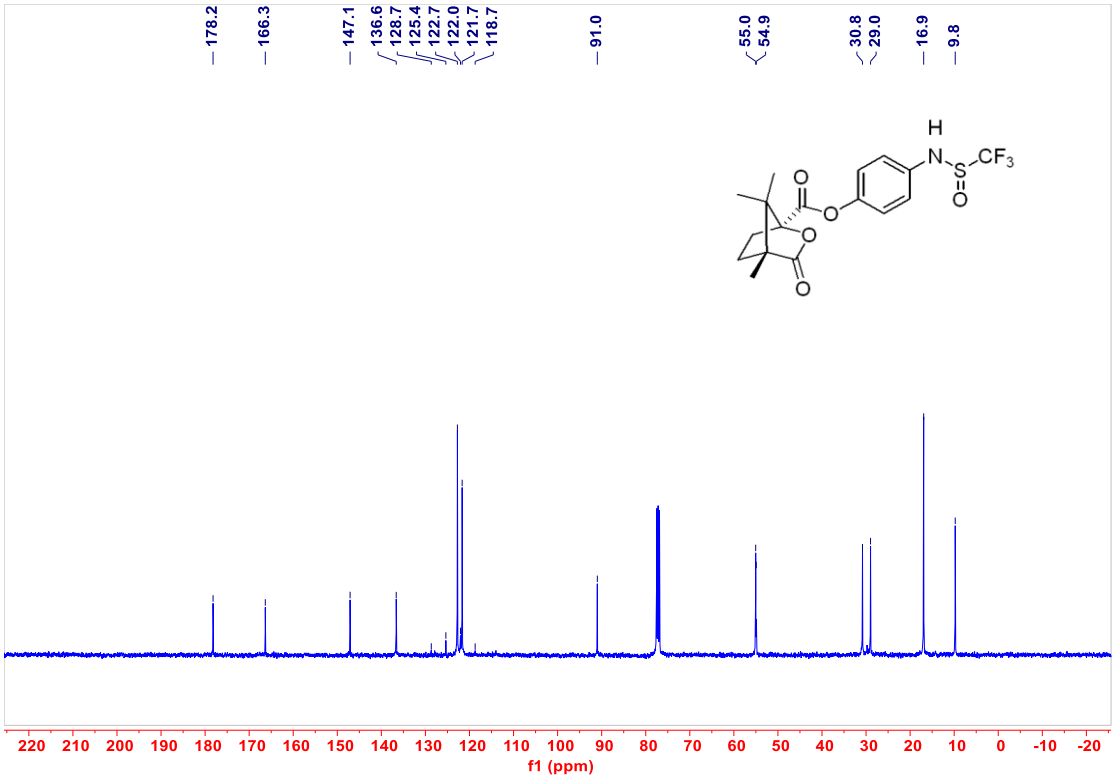
f1 (ppm)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118.7
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55.0
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29.0
16.9
9.8
H
N
S
CF3
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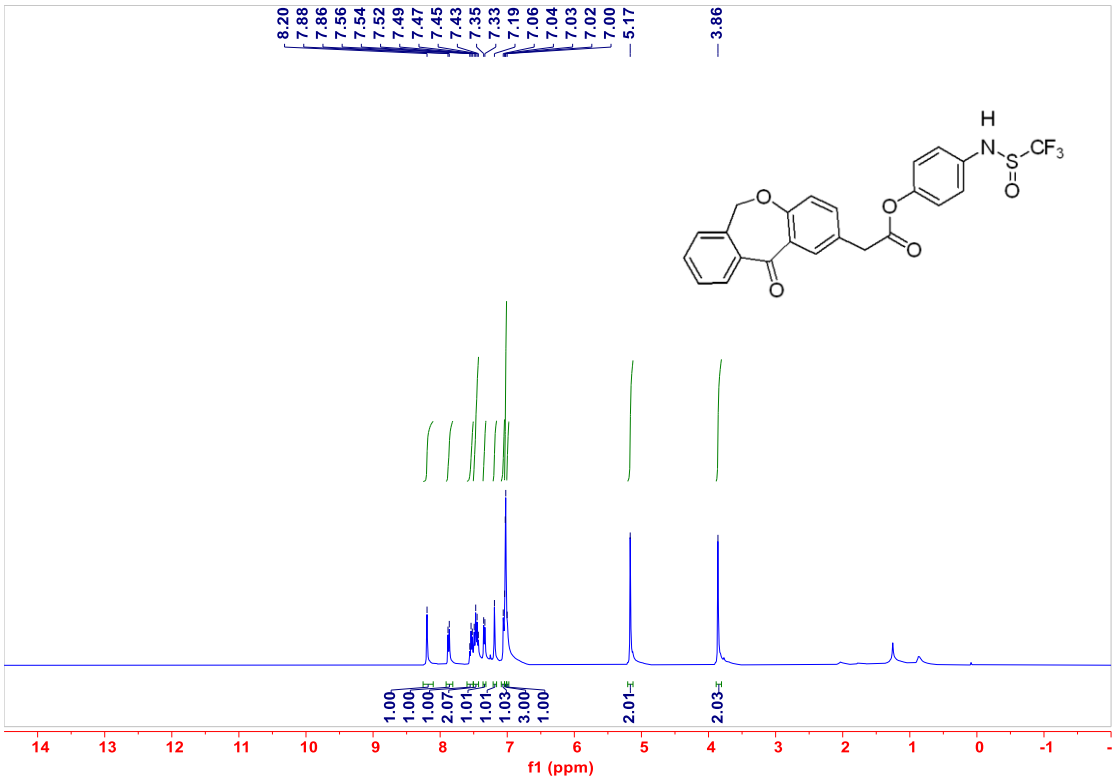
O
O
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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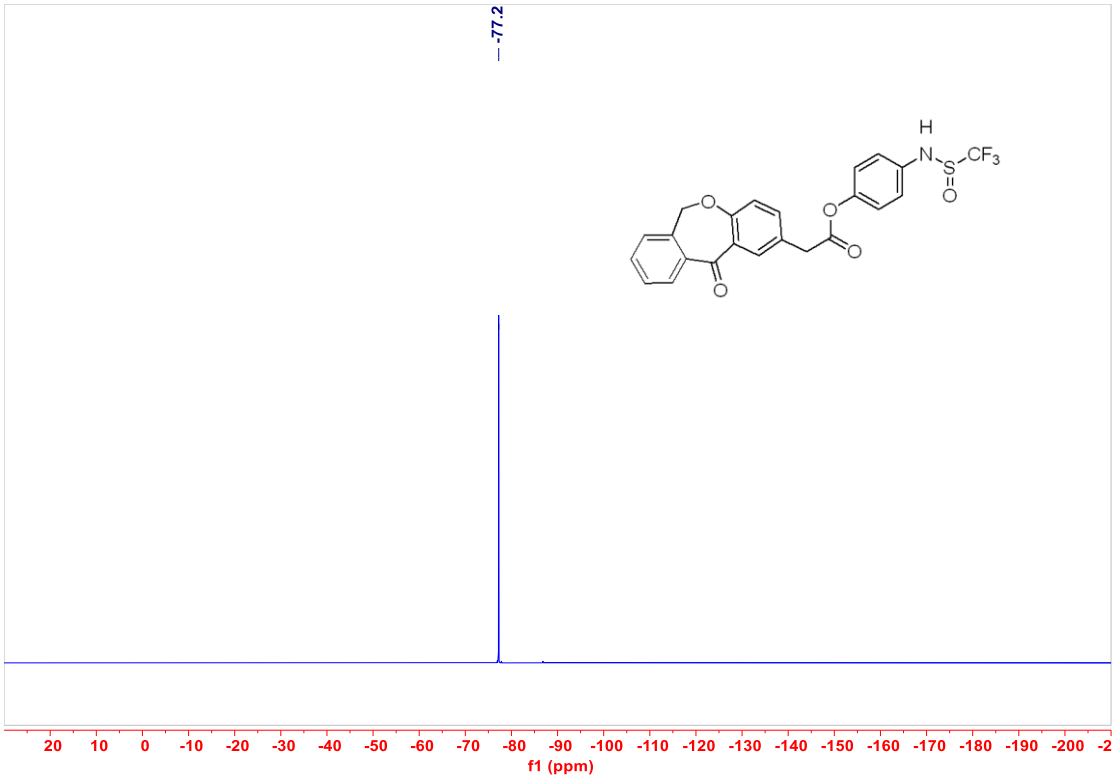
7.35
7.33
7.19
7.06
7.04
7.03
7.02
7.00
5.17
3.86
H
N
S
CF3
O
O
O
O
O
1.00
1.00
1.00
2.07
1.01
1.01
1.03
3.00
1.00
2.01
2.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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N
S
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O
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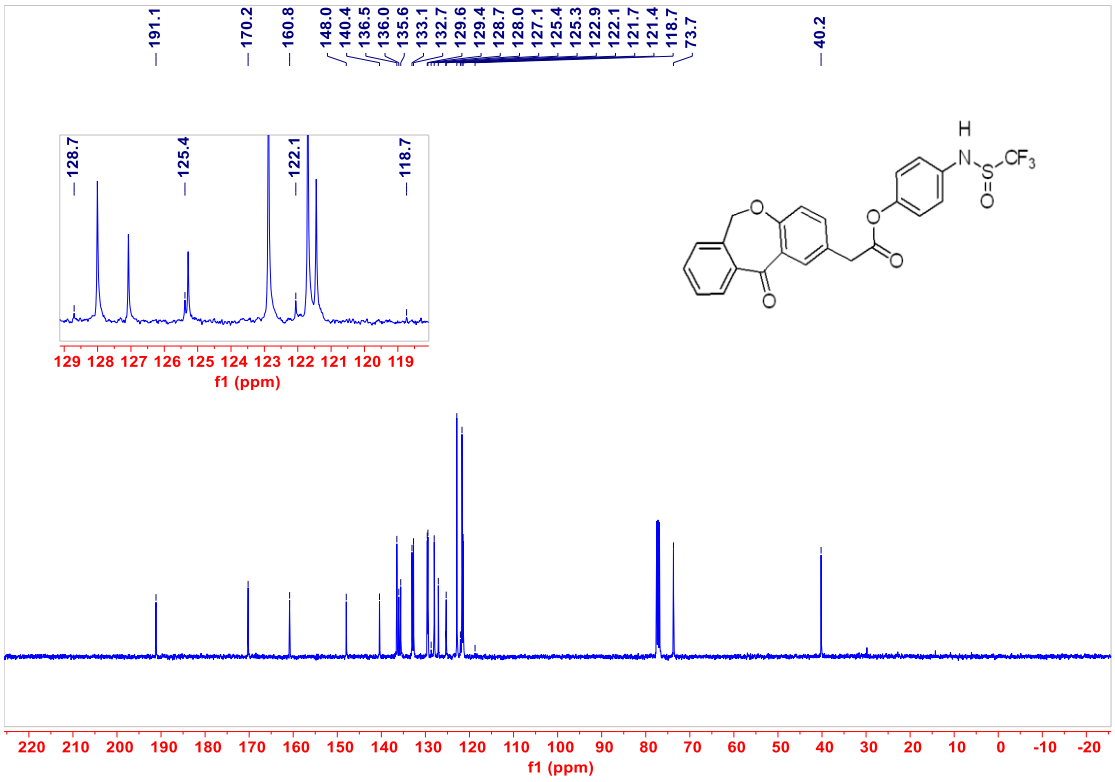
f1 (ppm)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136.0
135.6
133.1
132.7
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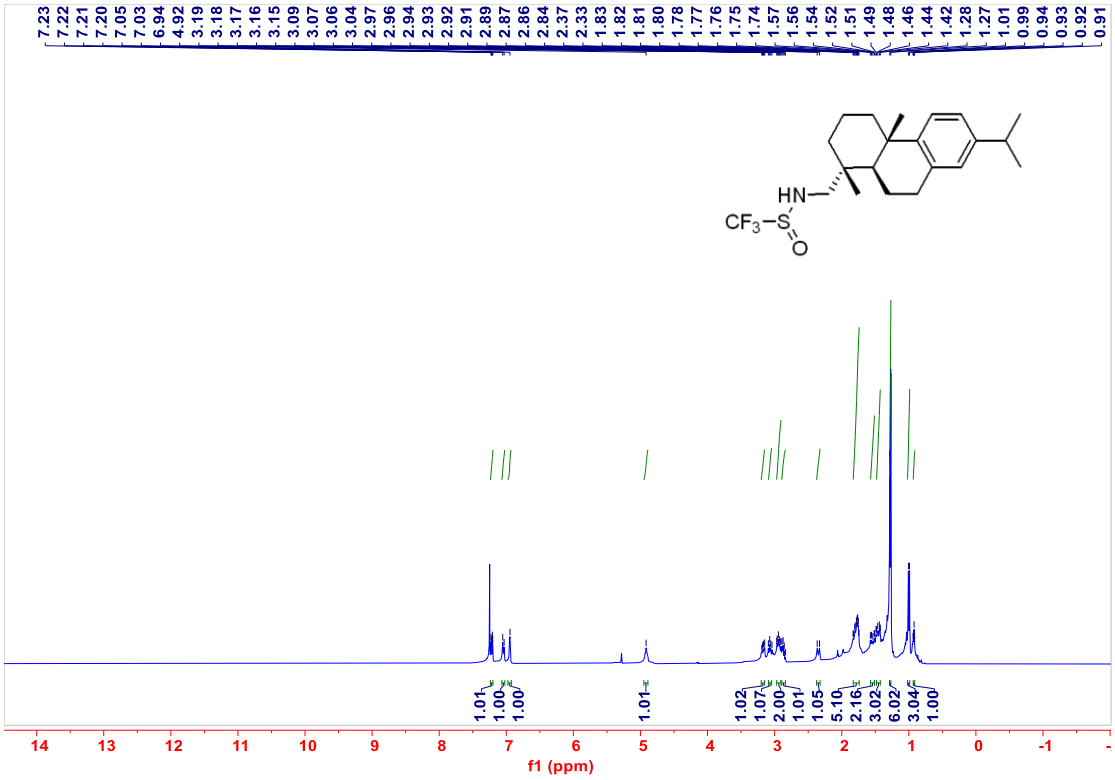
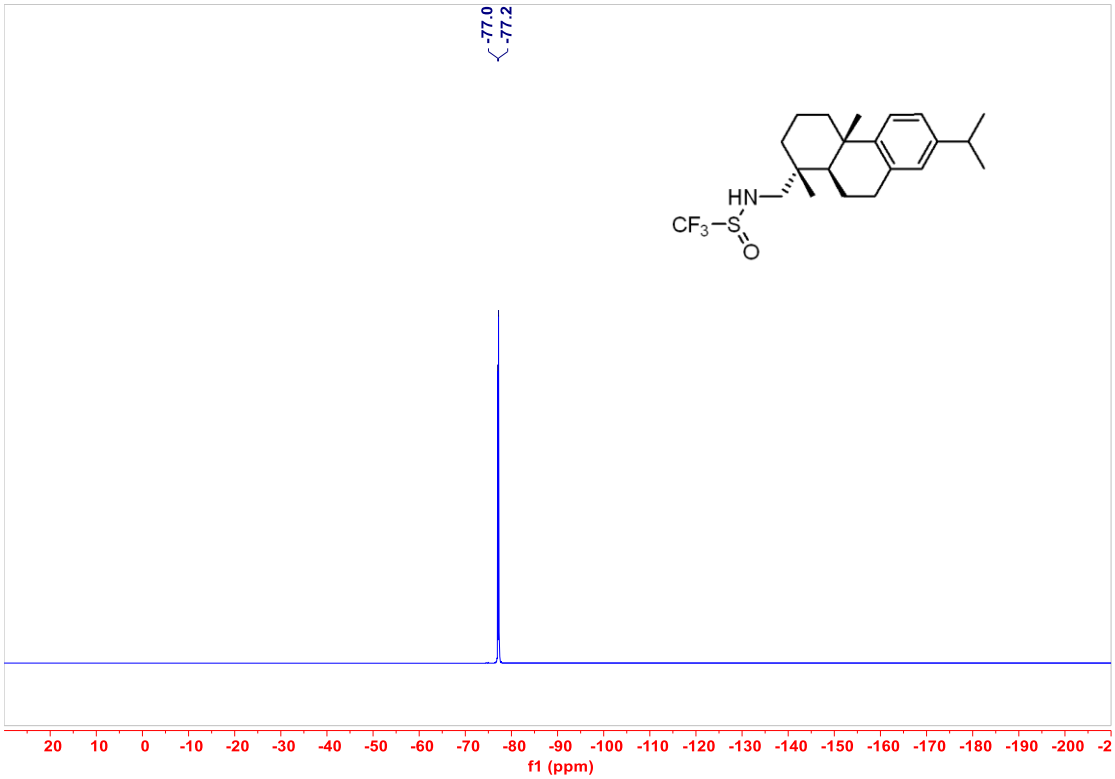
129.4
128.7
128.0
127.1
125.4
125.3
122.9
122.1
121.7
121.4
118.7
73.7
40.2
128.7
125.4
122.1
118.7
129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
H
N
S
CF3
O
O
O
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


7.23 7.22 7.21 7.20 7.05 7.03 6.94 4.92 3.19 3.18 3.17 3.16 3.15 3.09 3.07 3.06 3.04 2.97 2.96 2.94 2.93 2.92 2.91 2.89 2.87 2.86 2.84 2.37 2.33 1.83 1.82 1.81 1.80 1.78 1.77 1.76 1.75 1.74 1.57 1.56 1.54 1.52 1.51 1.49 1.48 1.46 1.44 1.42 1.28 1.27 1.01 0.99 0.94 0.93 0.92 0.91
HN
CF3–S
O
1.01 1.00 1.00 1.01 1.02 1.07 2.00 1.01 1.05 5.10 2.16 3.02 6.02 3.04 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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-77.2
HN
CF3–S
O
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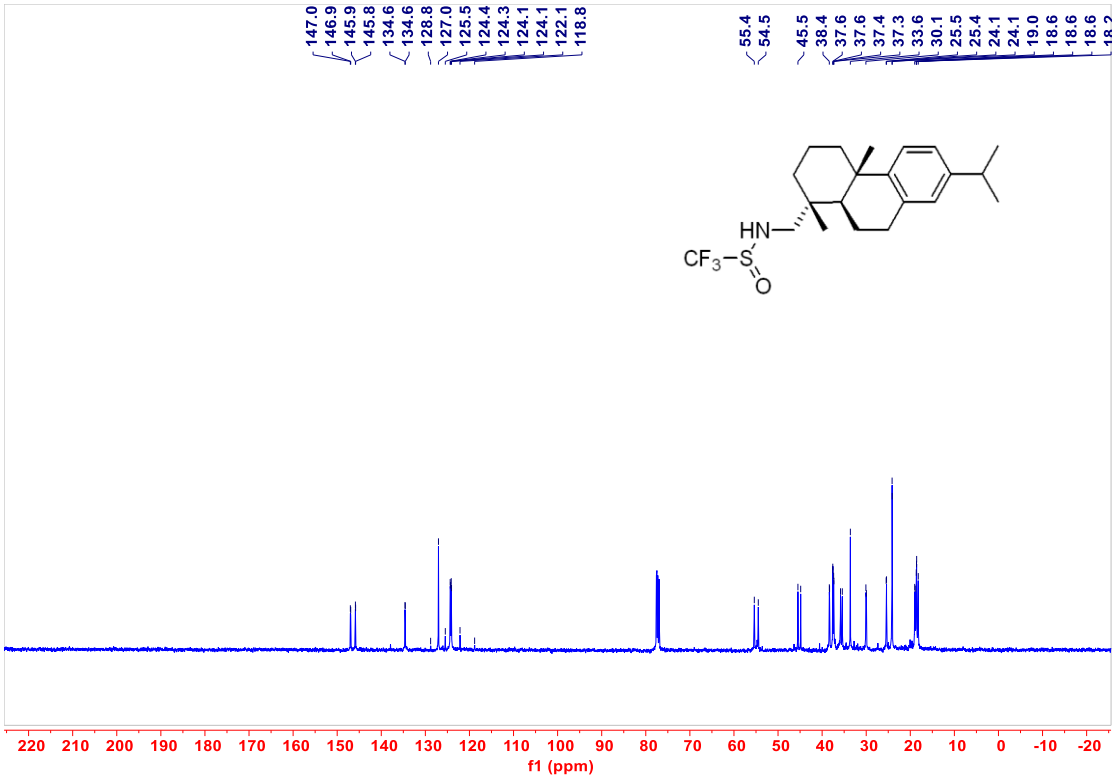
f1 (ppm)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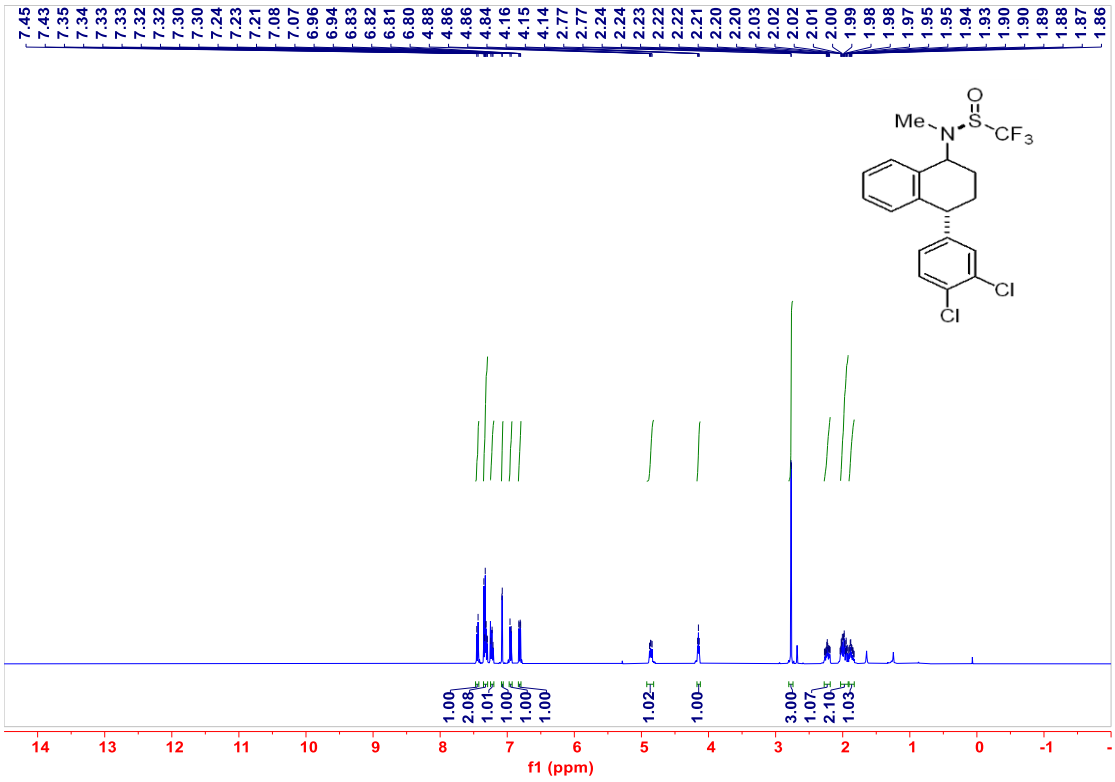
134.6
128.8
127.0
125.5
124.4
124.3
124.1
124.1
122.1
118.8
55.4
54.5
45.5
38.4
37.6
37.6
37.4
37.3
33.6
30.1
25.5
25.4
24.1
24.1
19.0
18.6
18.6
HN
CF3–S
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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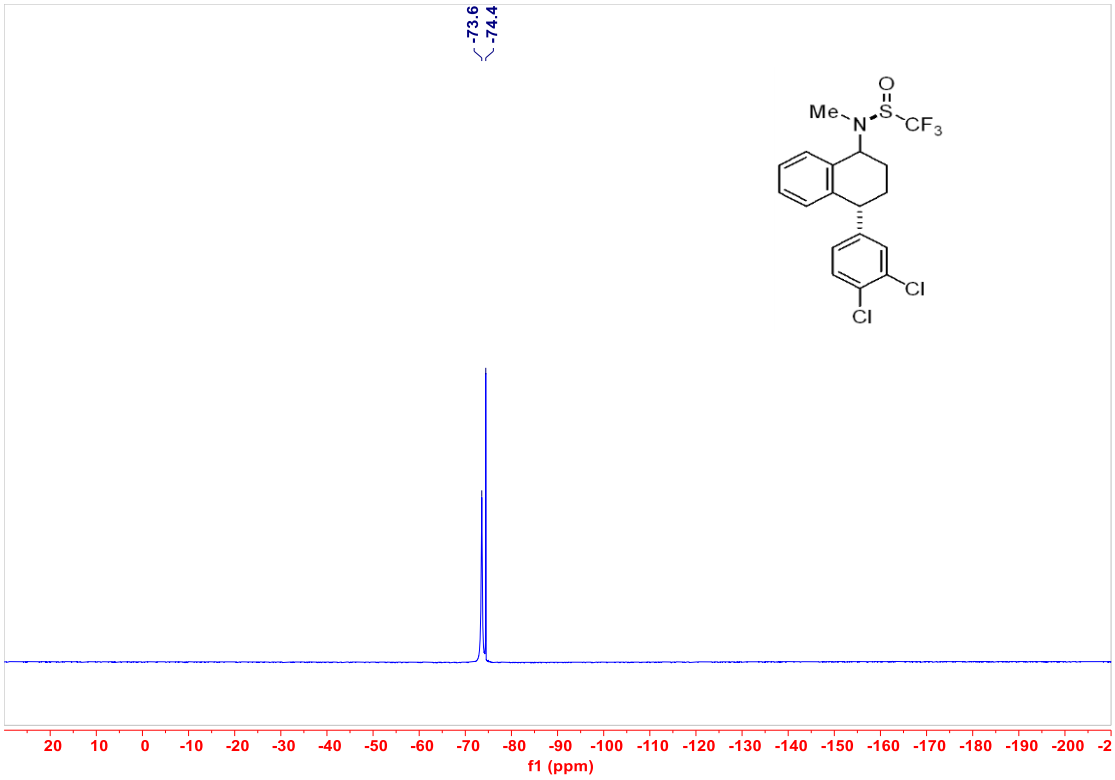
7.33
7.32
7.32
7.30
7.30
7.24
7.23
7.21
7.08
7.07
6.96
6.94
6.83
6.82
6.81
6.80
4.88
4.86
4.86
4.84
4.16
4.15
4.14
2.77
2.77
2.24
2.24
2.23
2.22
2.22
2.22
2.21
2.20
2.20
2.03
2.02
2.02
2.01
2.00
1.99
1.98
1.98
1.97
1.95
1.95
1.94
1.93
1.90
1.90
1.89
1.88
1.87
1.86
Me
N
S
O
CF3
Cl
Cl
1.00
2.08
1.01
1.00
1.00
1.00
1.02
1.00
3.00
1.07
2.10
1.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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-74.4
Me
N
O
S
CF3
Cl
Cl
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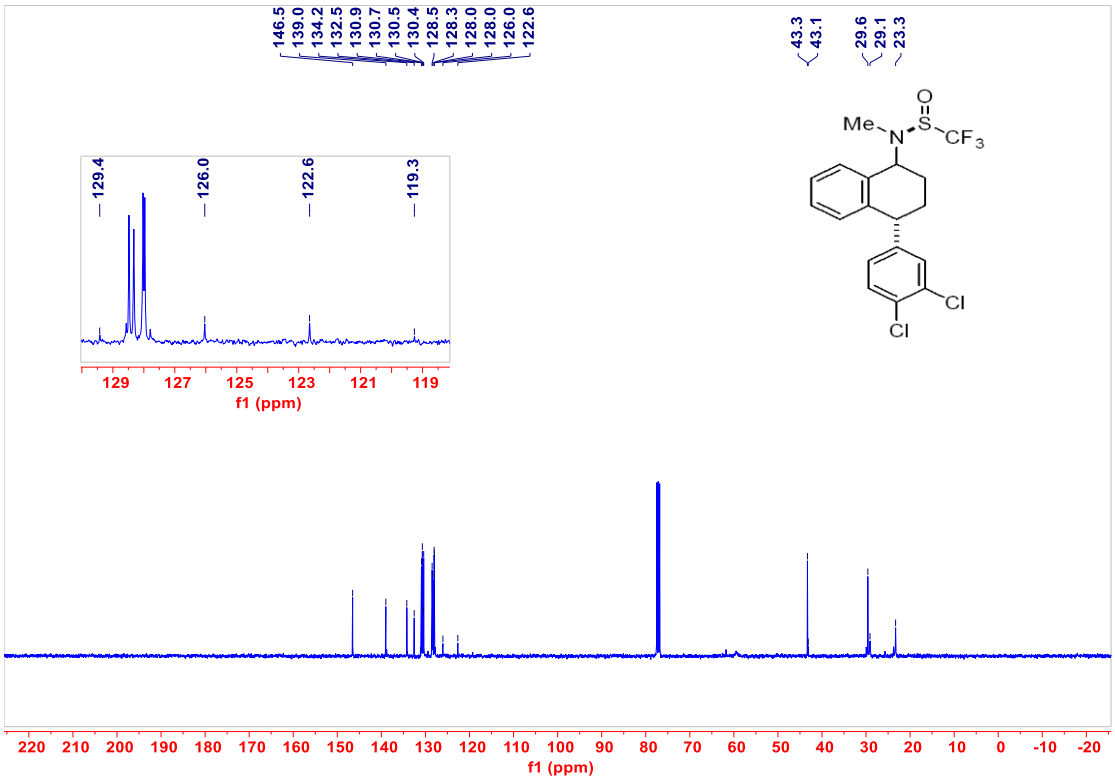
f1 (ppm)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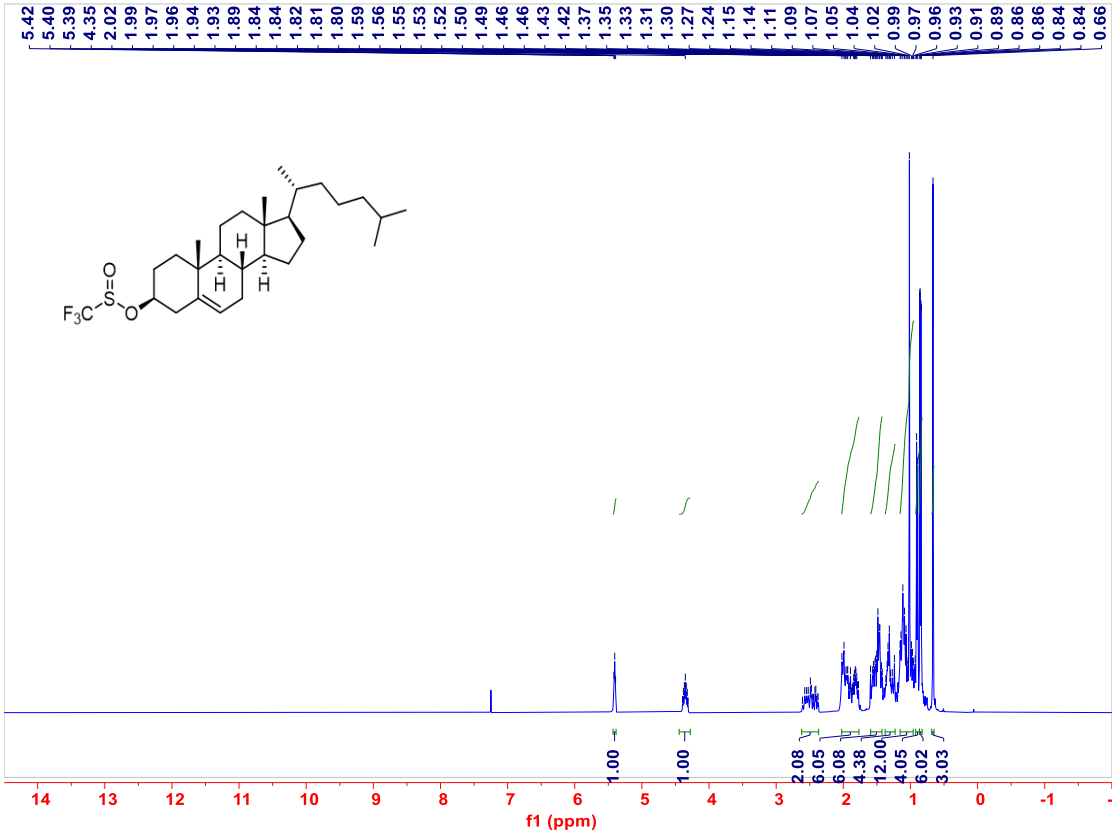
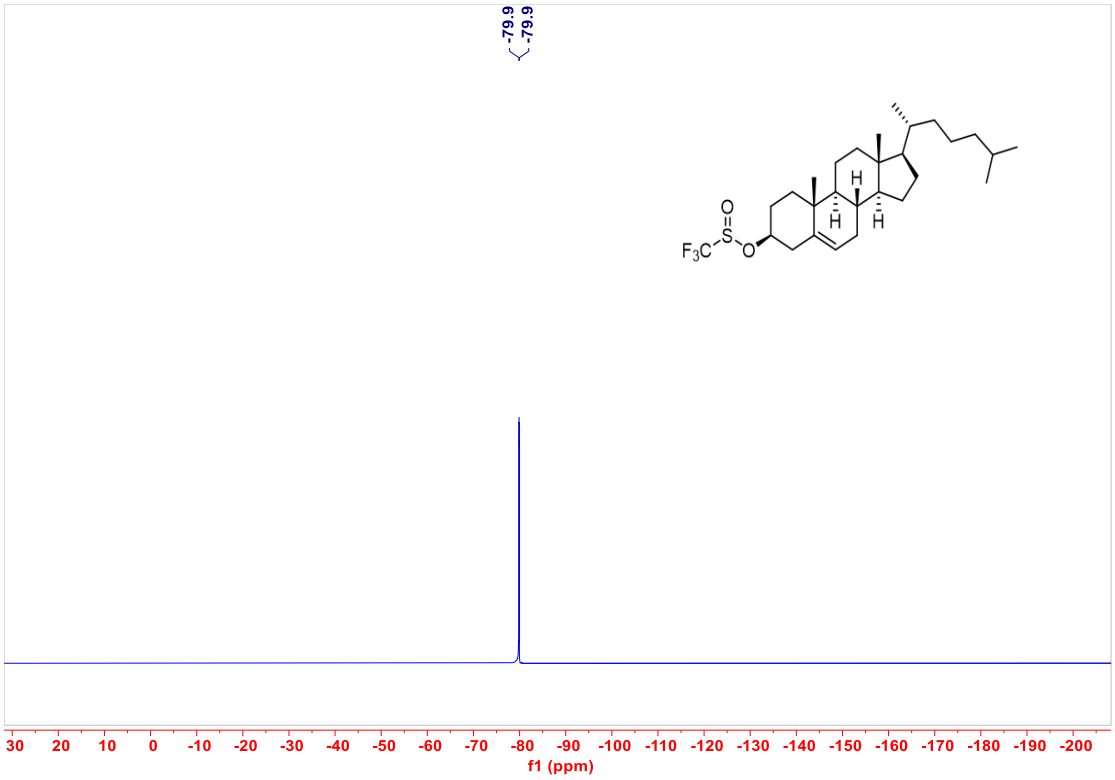
139.0
134.2
132.5
130.9
130.7
130.5
130.4
128.5
128.3
128.0
128.0
126.0
122.6
43.3
43.1
29.6
29.1
23.3
129.4
126.0
122.6
119.3
129 127 125 123 121 119
f1 (ppm)
Me
N
O
S
CF3
Cl
Cl
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


5.42 5.40 5.39 4.35 2.02 1.99 1.97 1.96 1.94 1.93 1.89 1.84 1.84 1.82 1.81 1.80 1.59 1.56 1.55 1.53 1.52 1.50 1.49 1.46 1.46 1.43 1.42 1.37 1.35 1.33 1.31 1.30 1.27 1.24 1.15 1.14 1.11 1.09 1.07 1.05 1.04 1.02 0.99 0.97 0.96 0.93 0.91 0.89 0.86 0.86 0.84 0.84 0.66
1.00 1.00 2.08 6.05 6.08 4.38 12.00 4.05 6.02 3.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.9
-79.9
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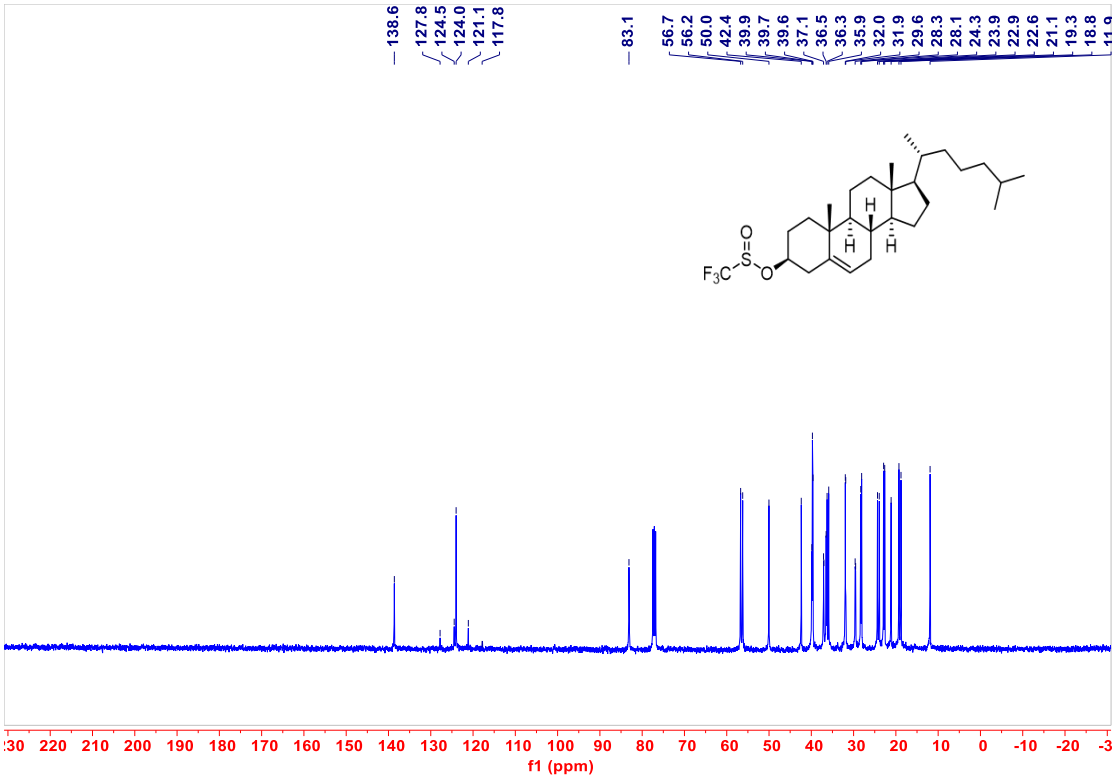
f1 (ppm)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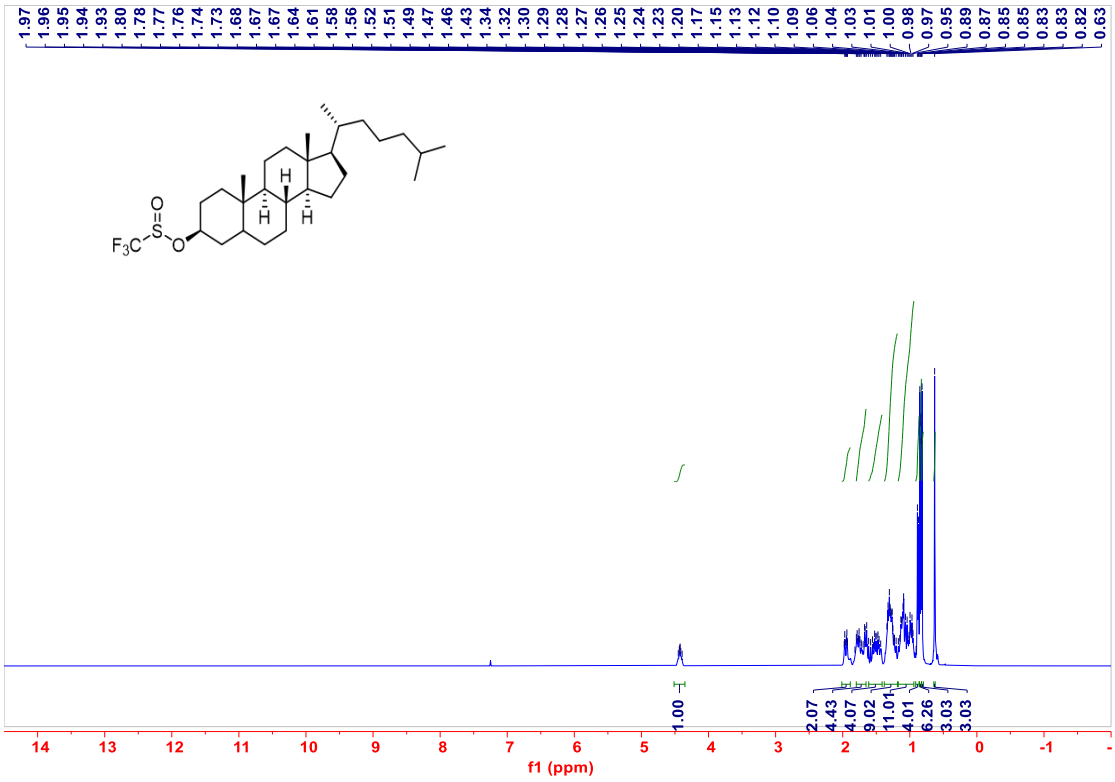
117.8
83.1
56.7
56.2
50.0
42.4
39.9
39.7
39.6
37.1
36.5
36.3
35.9
32.0
31.9
29.6
28.3
28.1
24.3
23.9
22.9
22.6
21.1
19.3
18.8
F3C
S
O
H
f1 (ppm)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1.95
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1.80
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1.77
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1.74
1.73
1.68
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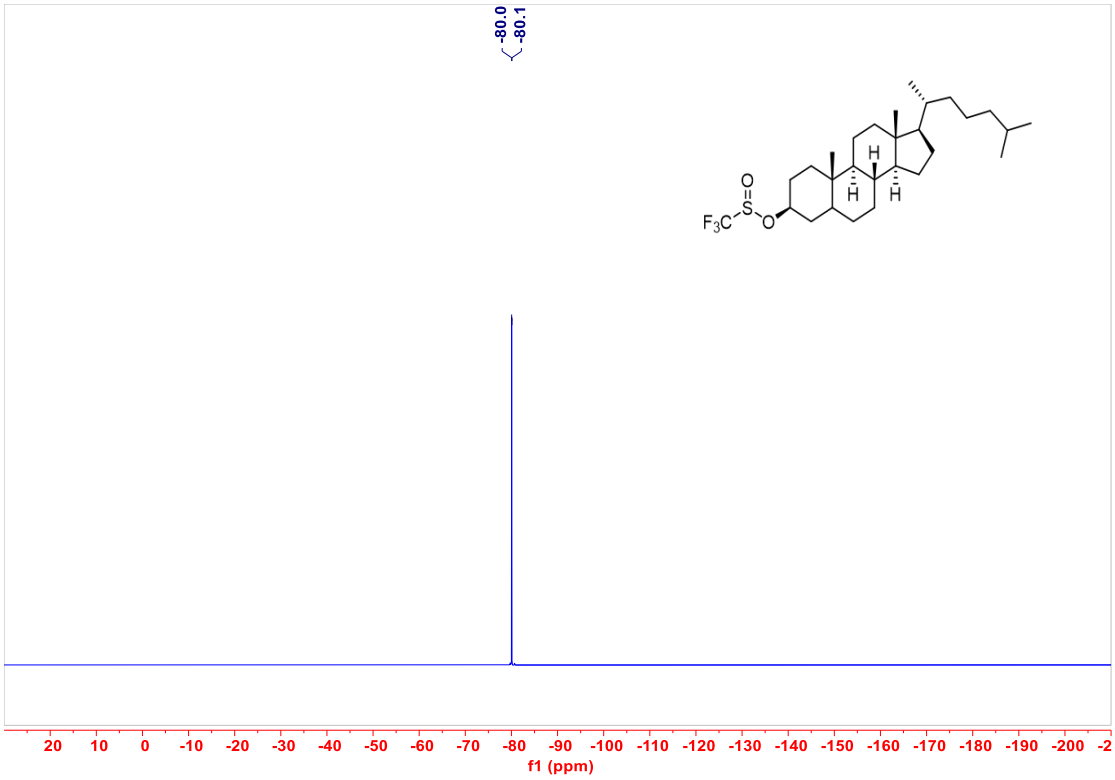
1.67
1.64
1.61
1.58
1.56
1.52
1.51
1.49
1.47
1.46
1.43
1.34
1.32
1.30
1.29
1.28
1.27
1.26
1.25
1.24
1.23
1.20
1.17
1.15
1.13
1.12
1.10
1.09
1.06
1.04
1.03
1.01
1.00
0.98
0.97
0.95
0.89
0.87
0.85
0.85
0.83
0.83
0.82
0.63
1.00
2.07
4.43
4.07
9.02
11.01
4.01
6.26
3.03
3.03
F3C
S
O
H
f1 (ppm)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O
O
H
H
H
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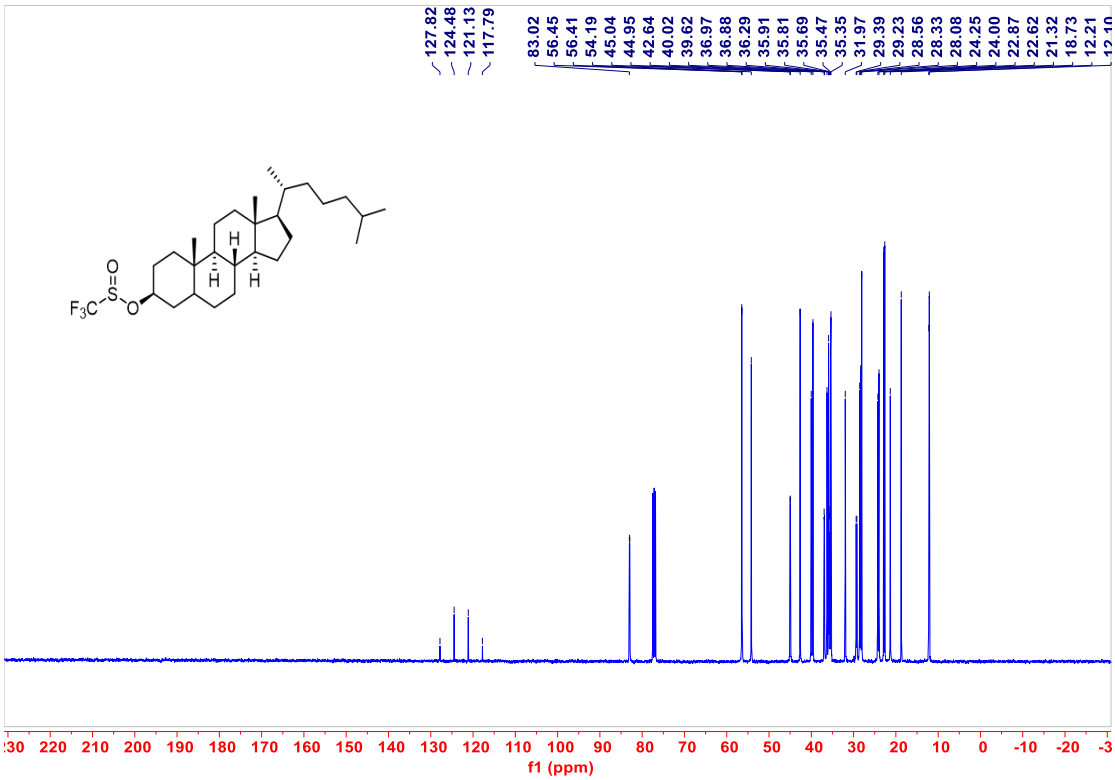
f1 (ppm)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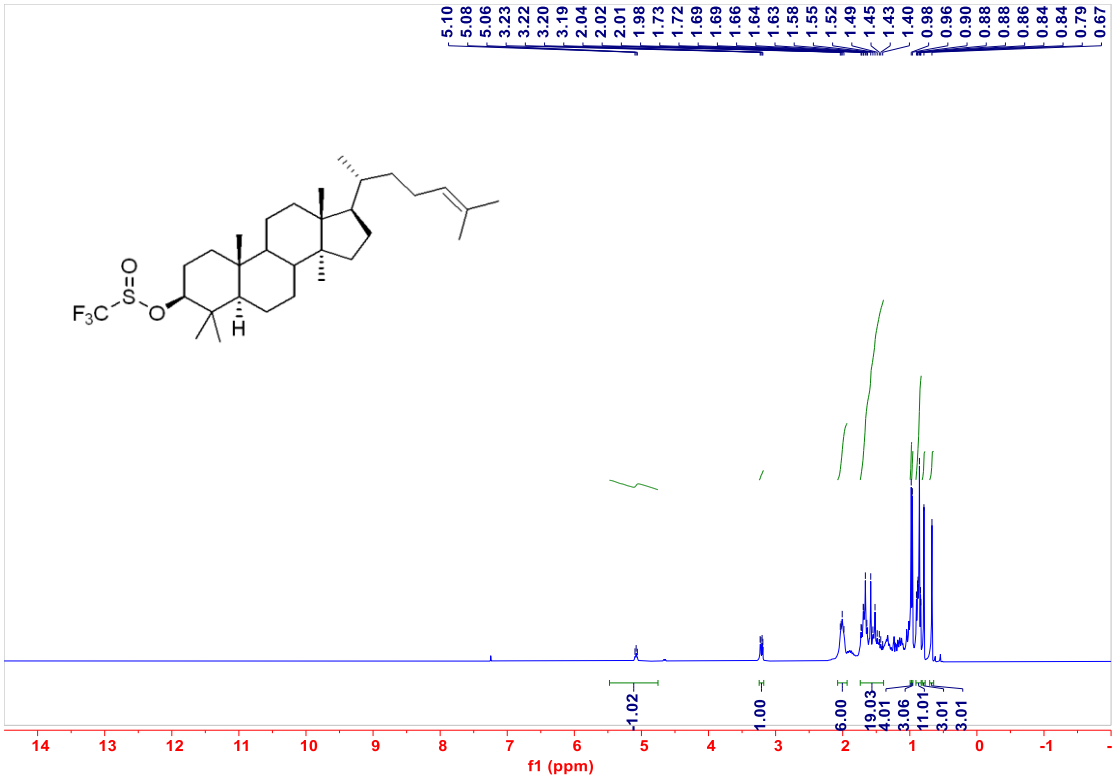
56.41
54.19
45.04
44.95
42.64
40.02
39.62
36.97
36.88
36.29
35.91
35.81
35.69
35.47
35.35
31.97
29.39
29.23
28.56
28.33
28.08
24.25
24.00
22.87
22.62
21.32
18.73
12.21
F3C
S
O
O
H
H
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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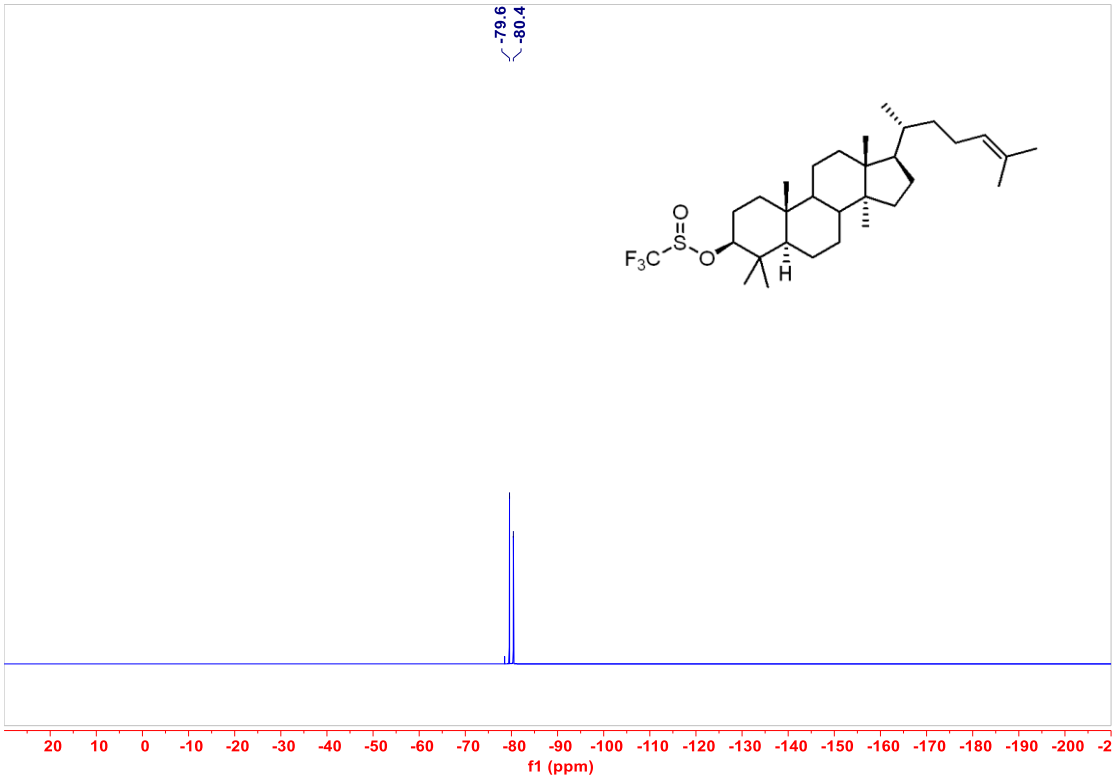
5.08
5.06
3.23
3.22
3.20
3.19
2.04
2.02
2.01
1.98
1.73
1.72
1.69
1.69
1.66
1.64
1.63
1.58
1.55
1.52
1.49
1.45
1.43
1.40
0.98
0.96
0.90
0.88
0.88
0.86
0.84
0.84
0.79
0.67
F3C
S
O
O
H
1.02
1.00
6.00
19.03
4.01
3.06
11.01
3.01
3.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.6
-80.4
F3C
S
O
O
H
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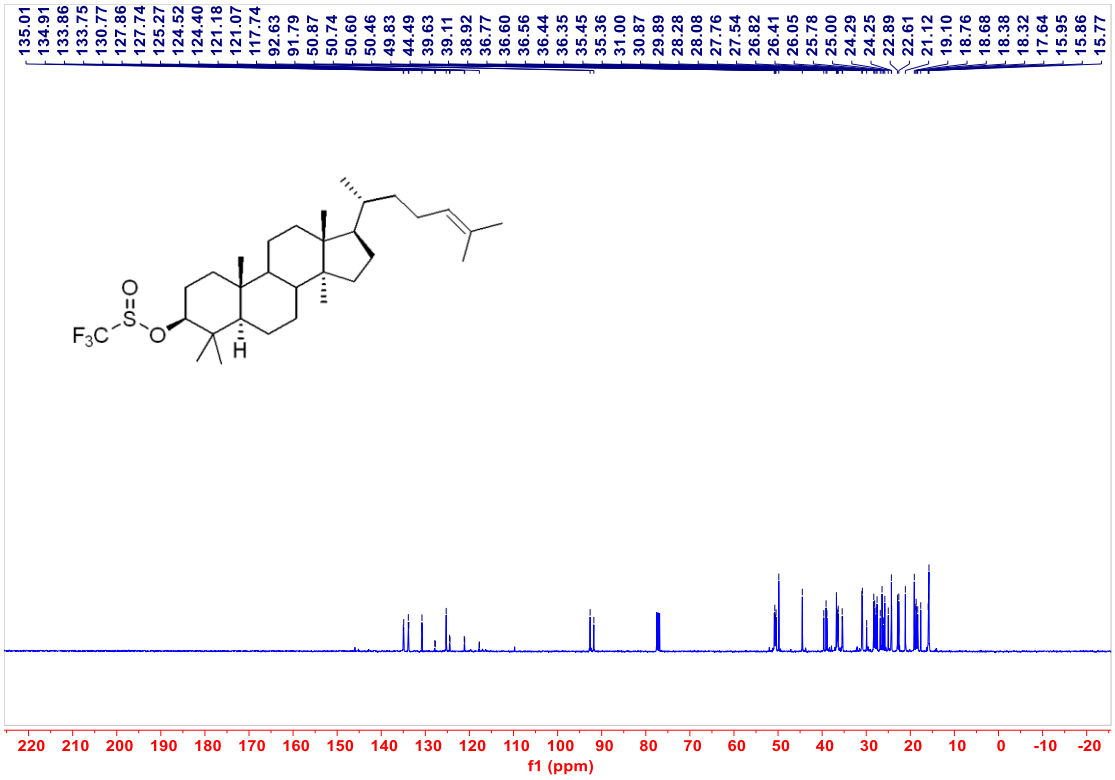
f1 (ppm)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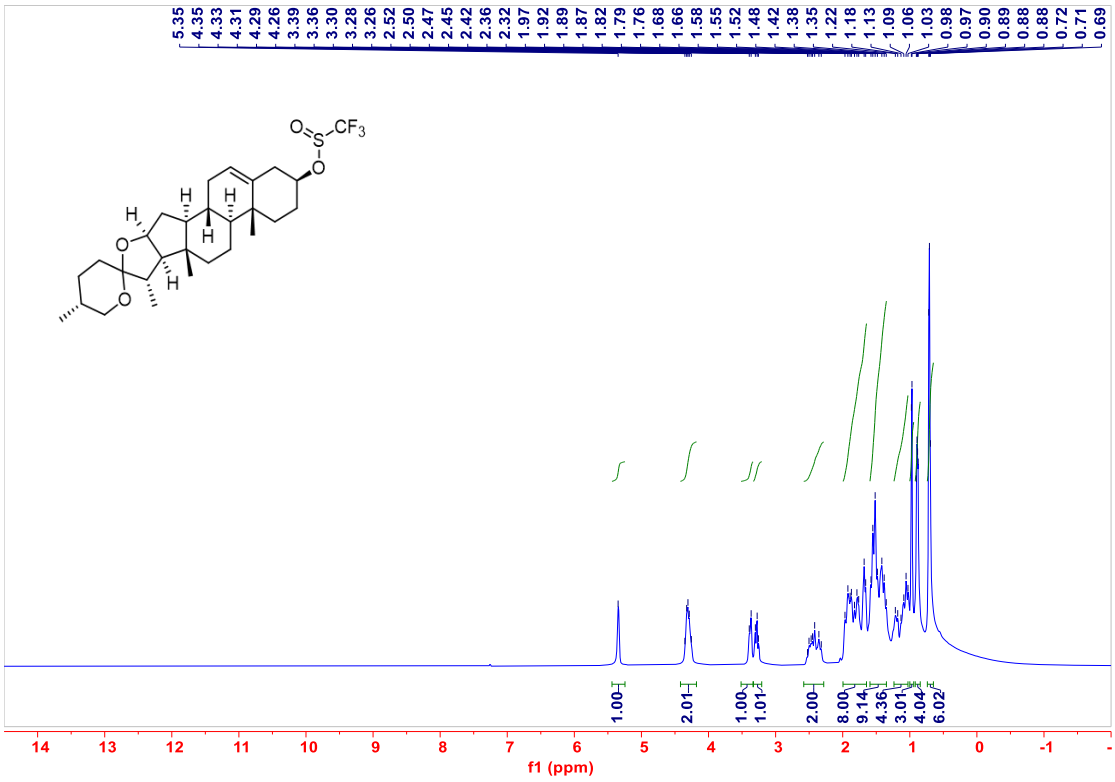
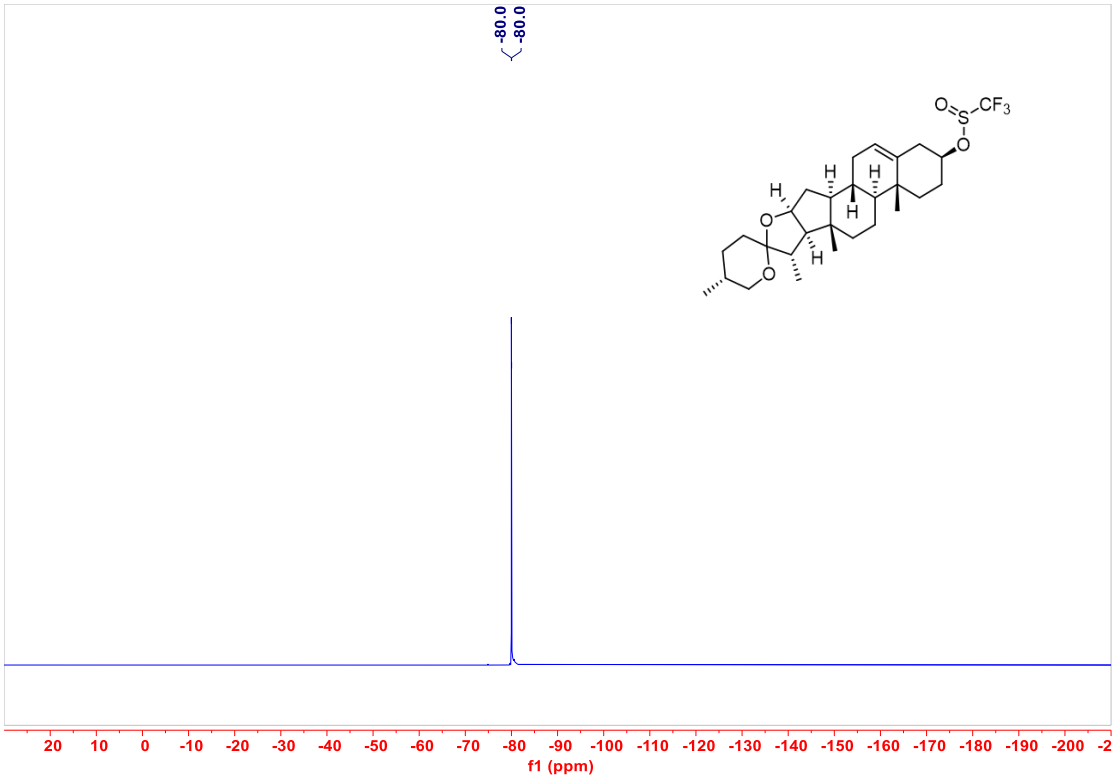
F3C
S
O
O
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


5.35 4.35 4.33 4.31 4.29 4.26 3.39 3.36 3.30 3.28 3.26 2.52 2.50 2.47 2.45 2.42 2.36 2.32 1.97 1.92 1.89 1.87 1.82 1.79 1.76 1.68 1.66 1.58 1.55 1.52 1.48 1.42 1.38 1.35 1.22 1.18 1.13 1.09 1.06 1.03 0.98 0.97 0.90 0.89 0.88 0.88 0.72 0.71 0.69
O
S
CF3
O
H
H
H
H
H
O
O
1.00 2.01 1.00 1.01 2.00 8.00 9.14 4.36 3.01 4.04 6.02
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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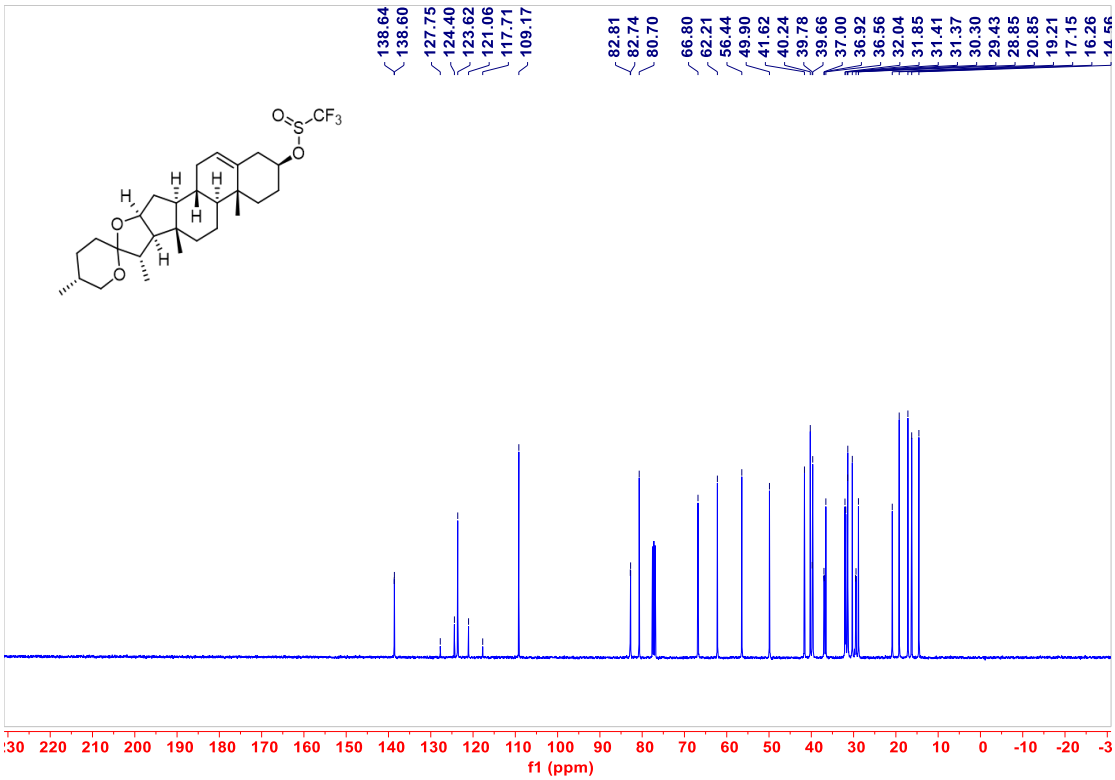
-80.0
f1 (ppm)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123.62
121.06
117.71
109.17
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82.74
80.70
66.80
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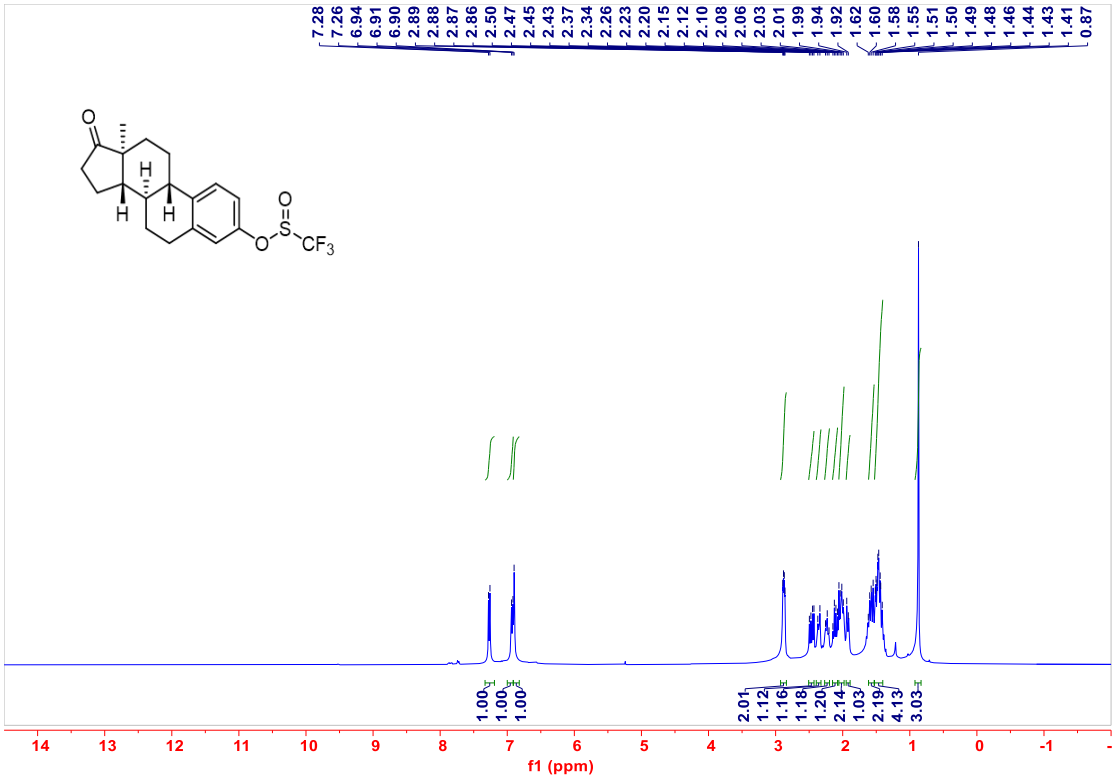
56.44
49.90
41.62
40.24
39.78
39.66
37.00
36.92
36.56
32.04
31.85
31.41
31.37
30.30
29.43
28.85
20.85
19.21
17.15
16.26
f1 (ppm)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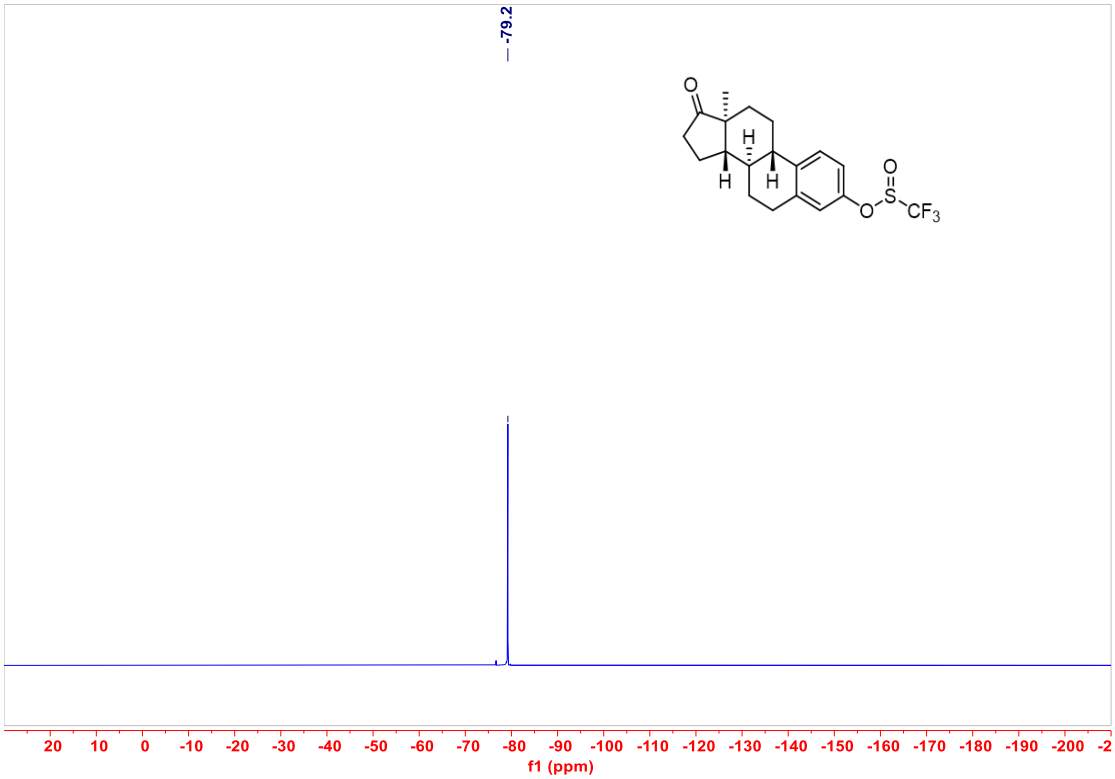
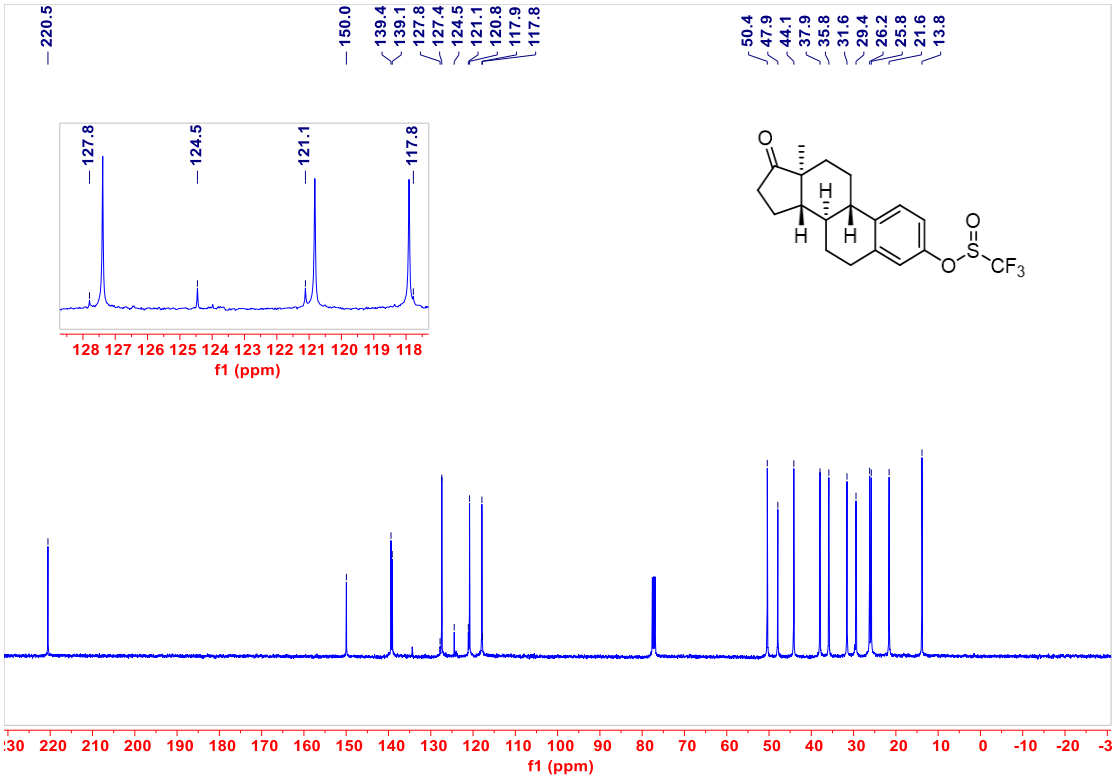
1.00 1.00 1.00
2.01 1.12 1.16 1.18 1.20 2.14 1.03 2.19 4.13 3.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


-79.2
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)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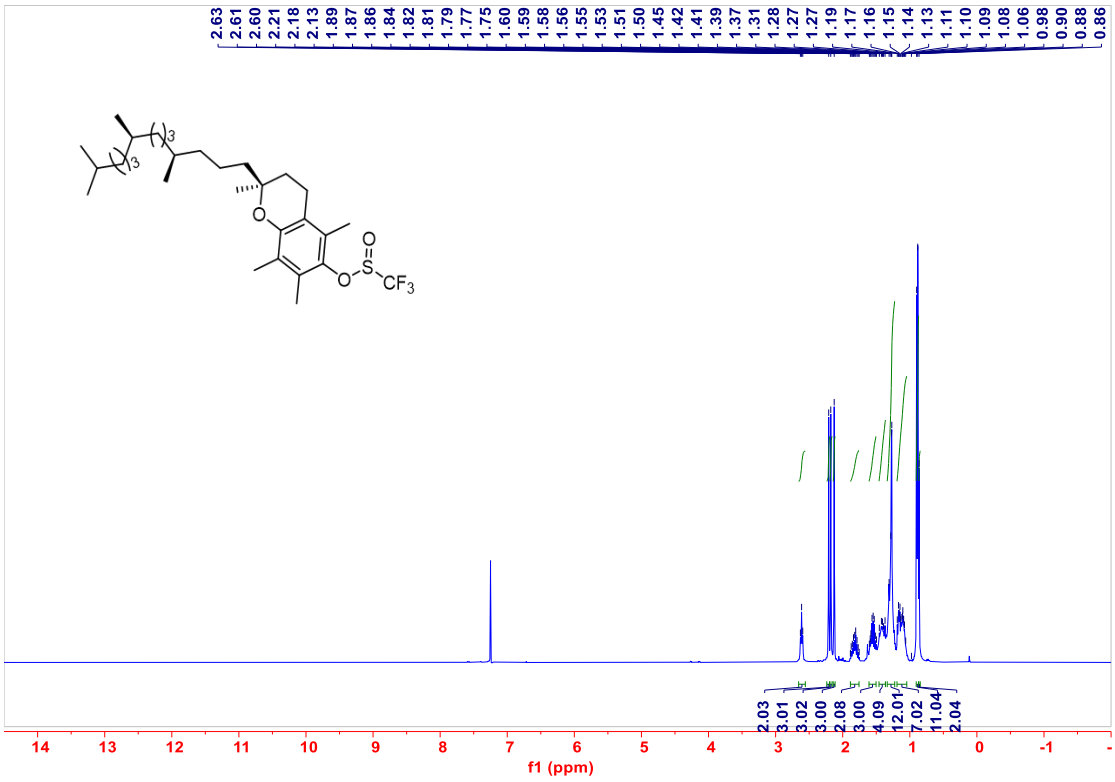
139.1
127.8
127.4
124.5
121.1
120.8
117.9
117.8
50.4
47.9
44.1
37.9
35.8
31.6
29.4
26.2
25.8
21.6
13.8
127.8
124.5
121.1
117.8
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
O
H
H
H
O
S
CF3
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)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1.84
1.82
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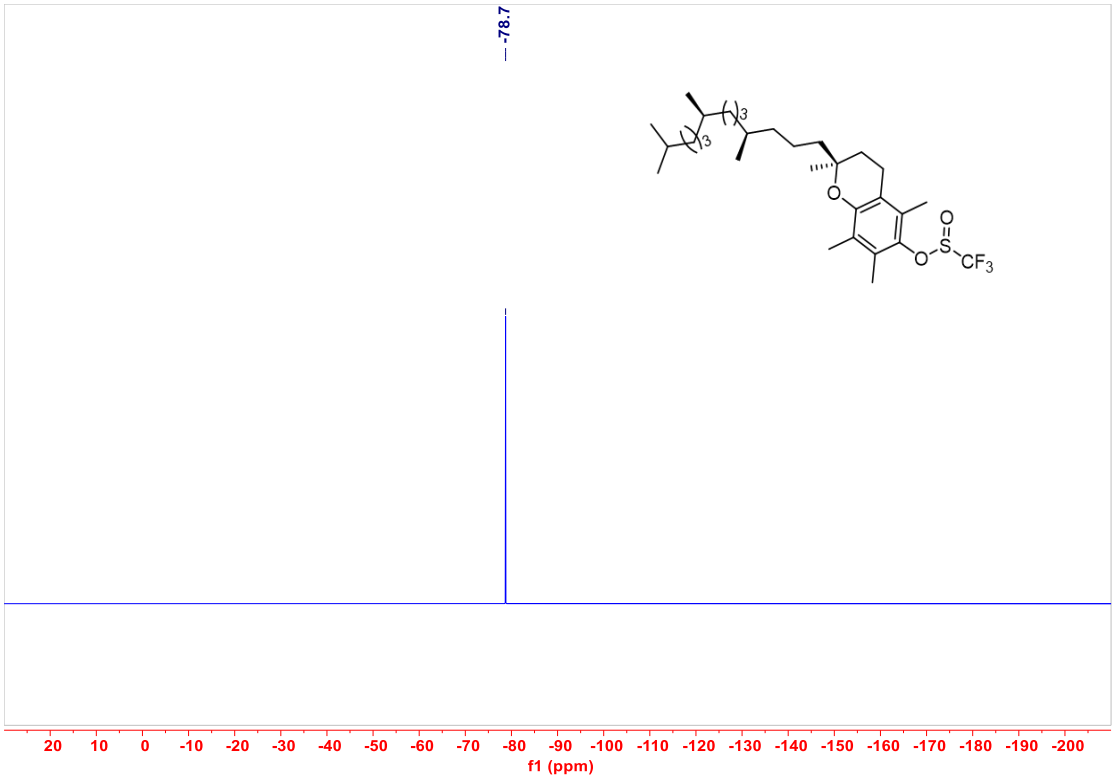
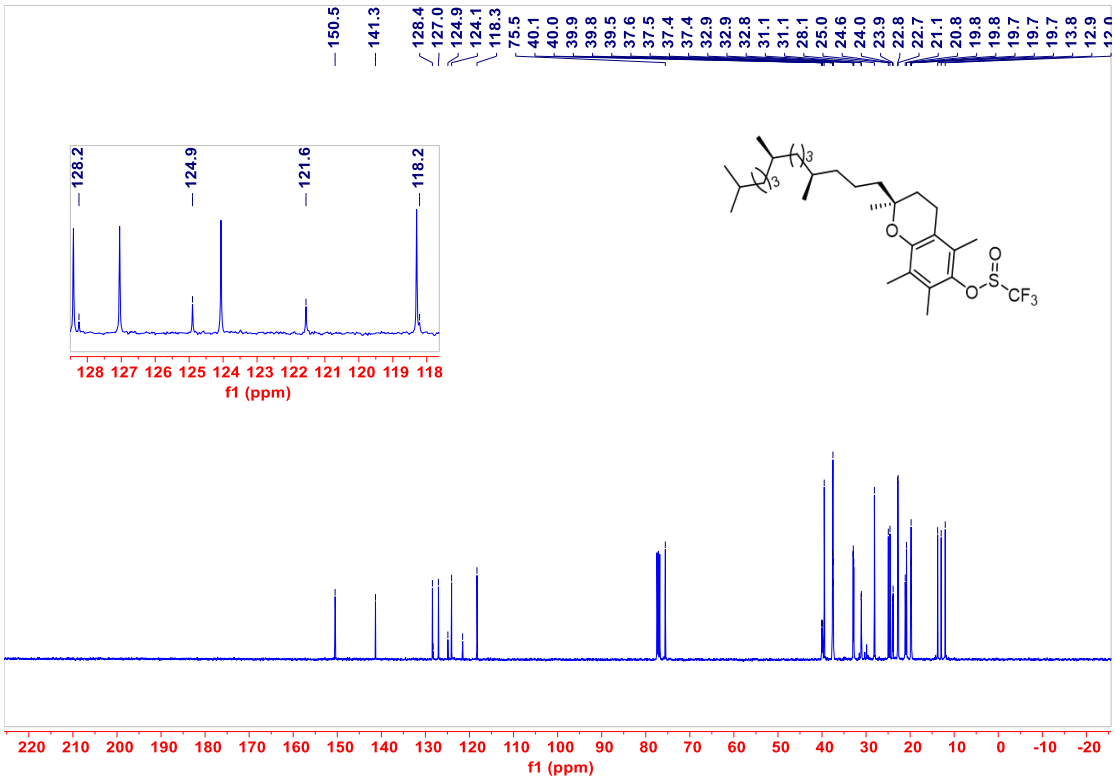
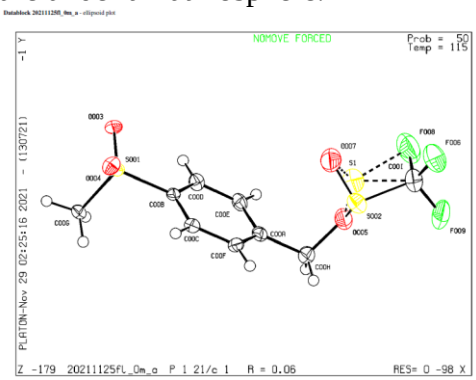
1.79
1.77
1.75
1.60
1.59
1.58
1.56
1.55
1.53
1.51
1.50
1.45
1.42
1.41
1.39
1.37
1.31
1.28
1.27
1.27
1.19
1.17
1.16
1.15
1.14
1.13
1.11
1.10
1.09
1.08
1.06
0.98
0.90
0.88
0.86
3
3
O
O
S
CF3
2.03
3.01
3.02
3.00
2.08
3.00
4.09
12.01
7.02
11.04
2.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

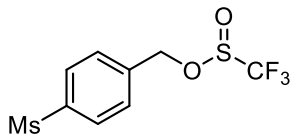

-78.7
f1 (ppm)


150.5
141.3
128.4
127.0
124.9
124.1
118.3
75.5
128.2
124.9
121.6
118.2
f1 (ppm)

6. X-ray structure

X-Ray crystallography data for **12ae** (**CCDC 2125051**): A colorless crystal suitable for X-ray crystallography was obtained from a *n*-hexane/DCM solution at room temperature under air atmosphere.





12ae

The ORTEP drawing (50% probability for thermal ellipsoids) of **12ae**

Identification code	**12ae**
Empirical formula	$C_9H_9F_3O_4S_2$
Formula weight	302.28
Temperature	115(2) K
Wavelength	1.34138 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a= 24.794(10) Å = 90° . b= 5.2770(9) Å = 92.193(16)° c= 9.1654(12) Å = 90°
Volume	1198.3(5) $Å^3$
Z, Calculated density	4, 1.676 Mg/m^3
Absorption coefficient	2.949 mm^{-1}
F(000)	616
Theta range for data collection	3.104 to 55.029°.
Limiting indices	-30<=h<=30, -6<=k<=5, -11<=l<=11
Absorption correction	MULTI-SCAN
Completeness to theta = 55.029	99.0%
Data / restraints / parameters	2264 / 138 / 174
Goodness-of-fit on F^2	1.089
R indices (all data)	R1= 0.069622, wR2 = 0.174528
Largest diff. peak and hole	1.301 and -0.882 e.$Å^{-3}$