Electronic Supplementary Material (ESI) for ChemComm.

1-Bromoethene-1-Sulfonyl Fluoride (BESF) as a Connective SuFEx Hub: *In Situ* Generation and Syntheses of 3-Substituted Isoxazole-5-Sulfonyl Fluorides, 1-Substituted-1*H*-1,2,3-Triazole-4-Sulfonyl Fluorides, 2-Amino-1-Bromoethane-1-Sulfonyl Fluorides and 4-Bromo-β-Sultams

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General Methods

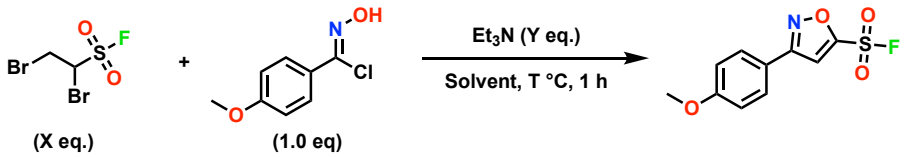
Unless otherwise stated, all reactions were performed with reagent grade solvents. All other reagents and solvents were obtained from commercial sources and used without further purification. The progress of reactions was monitored using thin layer chromatography (TLC) and visualised using UV light and stained using a basic $KMnO_4$ (potassium permanganate) solution. Flash column chromatography was performed using Biotage® SNAP cartridges with KP-Sil 50 μm as the stationary phase on a Biotage® Isolera™ One. Petrol refers to petroleum spirit (b.p. 40-60 °C).

NMR spectra (^1H and ^{13}C) were recorded on Bruker Ascend™ 400 (400 MHz) and Ultrashield™ 500 PLUS (500 MHz) spectrometers, as dilute solutions in the stipulated solvent. All chemical shifts (δ) are reported in parts per million (ppm) with 1H and 13C NMR referenced to solvent signals [^1H NMR: $CHCl_3$ (7.27); ^{13}C NMR: $CDCl_3$ (77.16)] Coupling constants (J) are reported in Hertz (Hz) and recorded after averaging. The multiplicity of the 1H NMR signals are designated by one of the following abbreviations: s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet, br=broad signal. Infra-red spectra were obtained using a Agilent Cary 660 FTIR spectrometer in ATR mode, with the peaks recorded as ν_{max}/cm^{-1}. HRMS were obtained using an Agilent 6530 accurate-mass Q-TOF LC/MS in electrospray ionisation (ESI) or a Bruker micrOTOF-Q in electron ionisation (EI) mode. Melting point data was collected using a Gallenkamp melting point apparatus.

Preparation of 1,2-dibromoethane-1-sulfonyl fluoride (1)[1]

To a solution of ethenesulfonyl fluoride (540 μL, 6.52 mmol) in $CHCl_3$ (4.5 mL) was added bromine (1.00 mL, 19.5 mmol) and the solution heated to reflux for 3 h. The reaction mixture was cooled, diluted with Et_2O (30 mL) and washed with 10% $Na_2S_2O_{3(aq)}$ until the organic fraction became clear and colourless and was then washed with H_2O (20 mL) and dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure to yield the desired 1,2-dibromoethane-1-sulfonyl fluoride (1.53 g, 87%) which was used without further purification; **^1H NMR** (500 MHz, $CDCl_3$) δ 5.23 (dd, *J* = 8.6, 4.8 Hz, 1H), 4.18 (dd, *J* = 11.9, 4.7 Hz, 1H), 3.84 (ddd, *J* = 11.9, 8.5, 1.1 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 57.51 (d, *J* = 21.2 Hz), 28.41; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 47.3; **IR** ν max (ATR)/cm^{-1}: 3029, 2973, 1410, 1215, 802.

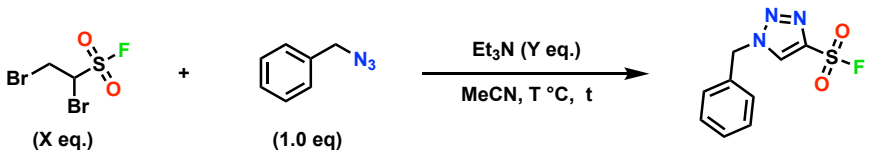
Table S-1 Optimisation of 3,5-isoxazole formation



Entry[a]	Solvent	T °C	X eq.	Y eq.	Yield (%)
1	CH_2Cl_2	0 to r.t.	1.0	3.0	53
2	EtOAc	0 to r.t.	1.0	3.0	58
3	DMF	0 to r.t.	1.0	3.0	16
4	THF	0 to r.t.	1.0	3.0	67
5	THF	-78 to r.t.	1.0	3.0	64
6	THF	0 to r.t.	1.1	3.1	96
7	THF	0 to r.t.	1.2	3.2	95[b]

[a] Isolated yields, reactions performed on 0.5 mmol and purified by column chromatography (8% EtOAc in petroleum ether); [b] Isolated without extensive chromatographic purification.

Table S-2 Optimisation of 1,4-triazole formation



Entry[a]	Solvent	T °C	t (h)	X eq.	Y eq.	Yield (%)
1	MeCN	0 to r.t.	24	1	2	-[b]
2	MeCN	0 to 50	24	1	2	-[c]
3	MeCN	0 to 90	2	1	2	18
4	MeCN	0 to 90	2	3	2	62
5	MeCN	0 to 90	3	4	3	87

[a] Isolated yields; reactions performed on 0.25 mmol; [b] No product formed.

General Reaction Procedures

General Procedure A

To a solution of 1,2-dibromoethane-1-sulfonyl fluoride (1.2 mmol) in THF (2 mL) at 0 °C was added Et_3N (3.2 mmol) and stirred for 5 min. To the mixture was then added the desired *N*-hydroxyimidoyl chloride, warming to room temperature and stirred for a further 1 h. The reaction mixture was diluted with H_2O (5 mL), extracted with EtOAc (10 mL), washed with brine (20 ml) and H_2O (20 mL), dried over anhydrous $MgSO_4$ and filtered. The solvent was removed under reduced pressure to yield the crude compound.

General Procedure B

To a solution of 1,2-dibromoethane-1-sulfonyl fluoride (0.75 mmol) in MeCN (1 mL) at 0 °C was added Et_3N (1.0 mmol) and stirred for 5 min. To the mixture was then added the desired azide (0.25 mmol) and heated to 90 °C for 3 h. After cooling to room temperature, the crude reaction mixture was extracted with EtOAc (10 mL), washed with brine (20 mL) and H_2O (20 mL), dried over anhydrous $MgSO_4$ and filtered. The solvent was removed under reduced pressure, and the crude compound purified by flash column chromatography.

General Procedure C

To a solution of 1,2-dibromoethane-1-sulfonyl fluoride (13.5 μL, 0.10 mmol) in MeCN (0.5 mL) at 0 °C was added triethylamine (13.9 μL, 0.10 mmol) and stirred for 5 min. To the mixture was added the desired amine (0.10 mmol) and the solution was warmed to room temperature and stirred for 30 min. The reaction mixture was extracted with EtOAc (10 mL), washed with H_2O (10 mL), dried over anhydrous $MgSO_4$ and filtered. The solvent was removed under reduced pressure to yield the desired compound.

General Procedure D

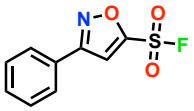
To a solution of 1,2-dibromoethane-1-sulfonyl fluoride (13.5 μL, 0.10 mmol) in MeCN (0.5 mL) at 0 °C was added triethylamine (13.9 μL, 0.10 mmol) and stirred for 5 min. To the mixture was then added the desired amine (0.10 mmol) and the solution heated to 50 °C for 30 min, followed by the addition of a solution of K_2CO_3 (14.0 mg, 0.10 mmol) in H_2O (100 μL). The solution was then stirred for a further 30 min at 50 °C and extracted into EtOAC (20 mL). The organic layer was washed with H_2O (10 mL), dried over anhydrous $MgSO_4$, filtered and the solvent removed under reduced pressure to yield the desired compound.

General Procedure E

To a solution of sulfonyl fluoride (0.10 mmol) and TBS-ether (0.10 mmol) in a solution of MeCN (0.4 mL) was added DBU (3 μL, 0.02 mmol). The reaction mixture was stirred for the required amount of time. Upon completion, the reaction mixture was extracted into EtOAc (5 mL), then washed with brine (10 mL) and H_2O (10 mL). The aqueous layer was then extracted with EtOAc (5 mL), the organic fractions combined, dried over anhydrous $MgSO_4$ and filtered. The solvent was removed under reduced pressure, and the crude compounds purified by flash column chromatography.

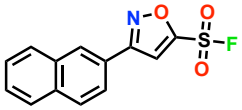
Experimental Data

3-Phenylisoxazole-5-sulfonyl fluoride (4a)[2]



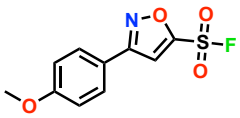
Following general procedure **A**, the crude product was filtered through a pad of silica (30% EtOAc in petrol) to obtain **4a** as a beige solid (193 mg, 85%). **m.p.** 52-53 °C (lit: 69-70 °C)[2]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.81 (m, 2H), 7.60-7.50 (m, 3H), 7.48 (d, *J* = 1.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.4, 158.9 (d, *J* = 39.0 Hz), 131.7, 129.6, 127.2, 126.5, 110.3 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.5; **HRMS** (EI^+): calculated for $C_9H_7FNO_3S$ [$M+H^+$]: m/z = 228.0131, m/z found 228.0179; **IR** ν max (ATR)/cm^{-1}: 3706, 3146, 3119, 2966, 2922, 2862, 1428, 1213, 1054, 781, 766, 684, 628.

3-(Naphthalen-2-yl)isoxazole-5-sulfonyl fluoride (4b)[2]



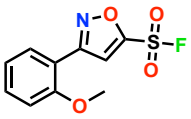
Following general procedure **A,** the crude product was filtered through a pad of silica (30% EtOAc in petrol) to obtain **4b** as a beige solid (262 mg, 95%). **m.p.** 86-88 °C (lit: 101-102 °C)[2]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.28-8.24 (m, 1H), 8.01-7.88 (m, 4H), 7.65-7.57 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.3, 158.8 (d, *J* = 38.7 Hz), 134.7, 133.1, 129.6, 128.8, 128.2, 128.1, 127.6, 127.4, 123.7, 123.4, 110.5 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.5; **HRMS** (EI^+): calculated for $C_{13}H_9FNO_3S$ [$M+H^+$]: m/z = 278.0287, m/z found 278.0327; **IR** ν max (ATR)/cm^{-1}: 3160, 2851, 1602, 1427, 1399, 1211, 901, 630.

3-(4-Methoxyphenyl)isoxazole-5-sulfonyl fluoride (4c)



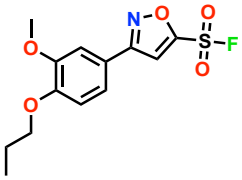
Following general procedure **A** (5.38 mmol of *N*-hydroxyimidoyl chloride used), the crude product was filtered through a pad of silica (30% EtOAc in petrol) to obtain **4c** as a colourless solid (1.31 g, 95%). **m.p.** 52-53 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79-7.74 (m, 2H), 7.41 (d, *J* = 1.4 Hz, 1H), 7.07-6.99 (m, 2H), 3.89 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.9, 162.3, 158.5 (d, *J* = 38.5 Hz), 128.7, 118.7, 115.0, 110.2 (d, *J* = 3.5 Hz), 55.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.3; **HRMS** (EI^+): calculated for $C_{10}H_9FNO_4S$ [$M+H^+$]: m/z = 258.0236, m/z found 258.0287; **IR** ν max (ATR)/cm^{-1}: 2929, 2851, 1603, 1525, 1423, 1254, 1214, 1176, 1022, 799.

3-(2-Methoxyphenyl)isoxazole-5-sulfonyl fluoride (4d)[2]



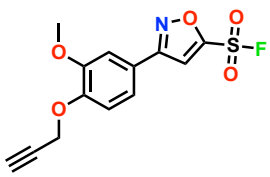
Following general procedure **A**, the crude product was purified by flash column chromatography (5% EtOAc in petroleum ether) to obtain **4d** as a beige solid (154 mg, 60%). **m.p**. 56-60 °C (lit:76-77 °C)[2]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.72 (d, *J* = 1.5 Hz, 1H), 7.52 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.13-7.08 (m, 1H), 7.08-7.04 (m, 1H), 3.96 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.9, 157.5 (d, *J* = 38.1 Hz), 157.4, 133.1, 129.5, 121.4, 115.2, 114.0 (d, *J* = 3.7 Hz), 111.7, 55.8; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.5; **HRMS** (EI^+): calculated for $C_{10}H_9FNO_4S$ [$M+H^+$]: m/z = 258.0236, m/z found 258.0299; **IR** ν̃ max (ATR)/cm^{-1}: 3182, 2929, 2841, 1602,1468, 1431, 1417, 1207, 1024, 786, 754, 626.

3-(3-Methoxy-4-propoxyphenyl)isoxazole-5-sulfonyl fluoride (4e)



Following general procedure **A**, the crude product was purified by flash column chromatography (0-20% EtOAc in petroleum ether) to obtain **4e** as a colourless solid (196 mg, 63%). **m.p.** 92-93 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 1.4 Hz, 1H), 7.41 (d, *J* = 2.1 Hz, 1H), 7.30 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 4.06 (t, *J* = 6.8 Hz, 2H), 3.96 (s, 3H), 1.97-1.87 (m, 2H), 1.08 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.0, 158.5 (d, *J* = 38.4 Hz), 151.7, 150.2, 120.7, 118.7, 112.6, 110.3 (d, *J* = 3.6 Hz), 109.7, 70.7, 56.4, 22.5, 10.6; **HRMS** (EI^+): calculated for $C_{13}H_{15}FNO_5S$ [$M+H^+$]: m/z = 316.0655, m/z found 316.0690; **IR** ν̃ max (ATR)/cm^{-1}: 3164, 2973, 2944, 2882, 1599, 1525, 1469, 1434, 1268, 1229, 1207, 1126, 1008, 791.

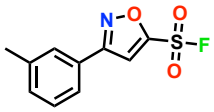
3-(3-Methoxy-4-(prop-2-yn-1-yloxy)phenyl)isoxazole-5-sulfonyl fluoride (4f)



Following general procedure **A**, the crude product was purified by flash column chromatography (0-20% EtOAc in petroleum ether) to obtain **4f** as a colourless solid (32 mg, 34%). **m.p**. 98-100 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ

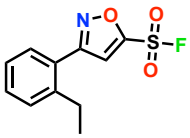
7.45-7.42 (m, 2H), 7.32 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 4.85 (d, *J* = 2.4 Hz, 2H), 3.97 (s, 3H), 2.57 (t, *J* = 2.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.8, 158.6 (d, *J* = 38.7 Hz), 150.4, 149.7, 120.2, 120.0, 114.1, 110.1 (d, *J* = 3.6 Hz), 109.9, 77.8, 76.4, 56.7, 56.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.4; **HRMS** (EI^+): calculated for $C_{13}H_{11}FNO_5S$ [$M+H^+$]: m/z = 312.0342, m/z found 312.0371; **IR** ν max (ATR)/cm^{-1}: 3306, 2972, 2886, 1602, 1471, 1429, 1208, 1058, 1016, 793.

3-(*m*-Tolyl)isoxazole-5-sulfonyl fluoride (4g)[2]



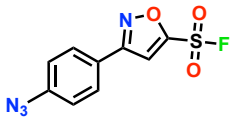
Following general procedure **A**, the crude product was purified by flash column chromatography (8% EtOAc in petroleum ether) to obtain **4g** as a colourless solid (174 mg, 72%). **m.p.** 50-52 °C (lit: 129-130 °C)[2]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69-7.65 (m, 1H), 7.64-7.59 (m, 1H), 7.46 (d, *J* = 1.4 Hz, 1H), 7.45-7.39 (m, 1H), 7.39-7.35 (m, 1H), 2.45 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.4, 158.7 (d, *J* = 38.7 Hz), 139.5, 132.5, 129.4, 127.7, 126.3, 124.3, 110.5 (d, *J* = 3.6 Hz), 21.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.4. **HRMS** (EI^+): calculated for $C_{10}H_9FNO_3S$ [$M+H^+$]: m/z = 242.0287, m/z found 242.0342; **IR** ν max (ATR)/cm^{-1}: 3706, 2966, 2922, 2864, 1436, 1219, 1054, 787, 625.

3-(2-Ethylphenyl)isoxazole-5-sulfonyl fluoride (4h)



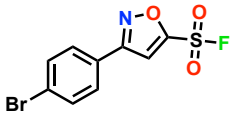
Following general procedure **A**, the crude product was filtered through a pad of silica (10% EtOAc in petrol) to obtain **4h** as a brown oil (246 mg, 96%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52-7.44 (m, 2H), 7.43-7.39 (m, 1H), 7.37-7.31 (m, 2H), 2.83 (q, *J* = 7.5 Hz, 2H), 1.24 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.8, 158.2 (d, *J* = 38.7 Hz), 143.6, 131.3, 130.0, 130.0, 126.6, 125.4, 112.9 (d, *J* = 3.6 Hz), 27.0, 15.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.6; **HRMS** (EI^+): calculated for $C_{11}H_{11}FNO_3S$ [$M+H^+$]: m/z = 256.0444, m/z found 256.0500; **IR** ν max (ATR)/cm^{-1}: 3155, 2973, 2936, 2876, 1438, 1215, 791, 762.

3-(4-Azidophenyl)isoxazole-5-sulfonyl fluoride (4i)



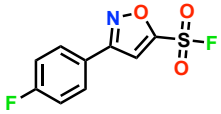
Following general procedure **A**, the crude product was purified by flash column chromatography (10% EtOAc in petroleum ether) to obtain **4i** as an orange solid (267 mg, 99%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.80 (m, 2H), 7.45 (d, *J* = 1.4 Hz, 1H), 7.21-7.14 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 158.9 (d, *J* = 38.8 Hz), 143.7, 128.7, 122.9, 120.1, 110.2 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.5; **IR** ν max (ATR)/cm^{-1}: 2923, 2127, 2092, 1600, 1423, 1283, 1215, 1123, 801.

3-(4-Bromophenyl)isoxazole-5-sulfonyl fluoride (4j)[2]



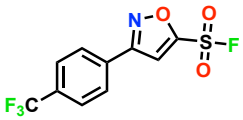
Following general procedure **A**, the crude product was purified by flash column chromatography (10% EtOAc in petroleum ether) to obtain **4j** a colourless solid (218 mg, 71%). **m.p.** 90-91 °C (lit: 96-97°C)[2]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77-7.66 (m, 4H), 7.46 (d, *J* = 1.4 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 159.2 (d, *J* = 38.9 Hz), 132.9, 128.6, 126.4, 125.3, 110.2 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.6; **HRMS** (EI^+): calculated for $C_9H_6BrFNO_3S$ [$M+H^+$]: m/z = 305.9236, m/z found 305.9263; **IR** ν max (ATR)/cm^{-1}: 3098, 2918, 2851, 1592, 1432, 1418, 1213, 804, 783, 624.

3-(4-Fluorophenyl)isoxazole-5-sulfonyl fluoride (4k)



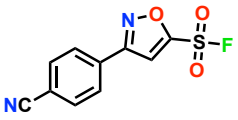
Following general procedure **A**, **4k** was isolated as an orange solid (232 mg, 95%). **m.p.** 61-64 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88-7.80 (m, 2H), 7.45 (d, *J* = 1.4 Hz, 1H), 7.29-7.19 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.9 (d, *J* = 253 Hz), 162.4, 159.1 (d, *J* = 39.0 Hz), 129.3 (d, *J* = 8.8 Hz), 122.7 (d, *J* = 3.6 Hz), 116.9 (d, *J* = 22.2 Hz), 110.2 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.5, -107.4; **HRMS** (EI^+): calculated for $C_9H_6F_2NO_3S$ [$M+H^+$]: m/z = 246.0036, m/z found 246.0098; **IR** ν max (ATR)/cm^{-1}: 3417, 3110, 1602, 1425, 1235, 1216, 1330, 838, 788, 636.

3-(4-(Trifluoromethyl)phenyl)isoxazole-5-sulfonyl fluoride (4l)



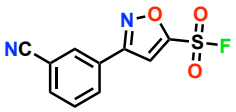
Following general procedure **A**, the crude product was purified by flash column chromatography (8% EtOAc in petroleum ether) to obtain **4l** as a colourless solid (222 mg, 75%). **m.p.** 80-82 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01-7.94 (m, 2H), 7.84-7.79 (m, 2H), 7.52 (d, *J* = 1.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.2, 159.5 (d, *J* = 39.3 Hz), 133.6 (q, *J* = 33.1 Hz), 129.8, 127.6, 126.6 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 272.6 Hz), 110.3 (d, *J* = 3.6 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.74, -63.14; **HRMS** (EI^+): calculated for $C_{10}H_6F_4NO_3S$ [$M+H^+$]: m/z = 296.0005, m/z found 296.0057; **IR** ν max (ATR)/cm^{-1}:3707, 2966, 2922, 2864, 2845, 1439, 1322, 1114, 1064, 1053, 798, 626.

3-(4-Cyanophenyl)isoxazole-5-sulfonyl fluoride (4m)



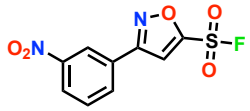
Following general procedure **A**, the crude product was purified by flash column chromatography (8% EtOAc in petroleum ether) to obtain **4m** as a yellow solid (170 mg, 67%). **m.p.** 116-119 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01-7.95 (m, 2H), 7.91-7.81 (m, 2H), 7.52 (d, *J* = 1.3 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.9, 159.7 (d, *J* = 39.6 Hz), 133.3, 130.5, 127.8, 117.8, 115.5, 110.2 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.8; **HRMS** (EI^+): calculated for $C_{10}H_6FN_2O_3S$ [$M+H^+$]: m/z = 253.0083, m/z found 253.0131; **IR** ν max (ATR)/cm^{-1}: 2958, 2920, 2851, 2229, 1423, 1216, 630.

3-(3-Cyanophenyl)isoxazole-5-sulfonyl fluoride (4n)



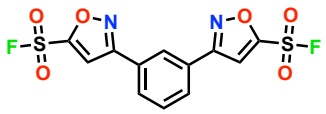
Following general procedure **A**, **4n** was isolated as a beige solid (245 mg, 97%). **m.p.** 113-116 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19-8.13 (m, 1H), 8.10 (ddd, *J* = 7.9, 1.8, 1.1 Hz, 1H), 7.90-7.82 (m, 1H), 7.73-7.67 (m, 1H), 7.52 (d, *J* = 1.4 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.6, 159.7 (d, *J* = 39.5 Hz), 134.9, 131.2, 130.6, 130.6, 127.9, 117.6, 114.2, 110.0 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.9; **HRMS** (EI^+): calculated for $C_{10}H_6FN_2O_3S$ [$M+H^+$]: m/z = 253.0083, m/z found 253.0141; **IR** ν max (ATR)/cm^{-1}: 3141, 3111, 3086, 2926, 2234, 1720, 1432, 1417, 1218, 909, 808, 729, 626.

3-(3-Nitrophenyl)isoxazole-5-sulfonyl fluoride (4o)[2]



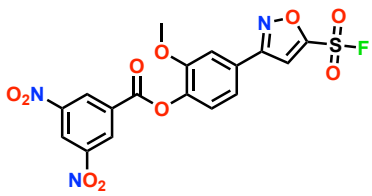
Following general procedure **A**, the crude product was purified by flash column chromatography (0-20% EtOAc in petroleum ether) to obtain **4o** as a yellow solid (177 mg, 65%). **m.p**. 64-66 °C (lit: 67-68 °C); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.72-8.67 (m, 1H), 8.44 (ddd, *J* = 8.3, 2.2, 1.0 Hz, 1H), 8.23 (ddd, *J* = 7.8, 1.7, 1.1 Hz, 1H), 7.80-7.76 (m, 1H), 7.59 (d, *J* = 1.3 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.6, 159.9 (d, *J* = 39.7 Hz), 149.0, 132.7, 130.9, 128.2, 126.3, 122.3, 110.1 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.9; **HRMS** (EI^+): calculated for $C_9H_6FN_2O_5S$ [$M+H^+$]: m/z = 272.9981, m/z found 273.0036; **IR** ν max (ATR)/cm^{-1}: 2961, 1928, 2851, 1528, 1438, 1349, 1255, 1216, 796.

3-(3-(5-(Fluorosulfonyl)isoxazol-3-yl)phenyl)isoxazole-5-sulfonyl fluoride (4p)



Following a modified version of general procedure **A**, where 1,2-dibromoethane-1-sulfonyl fluoride (2.4 mmol) and Et_3N (6.4 mmol) were used, the crude product was purified by flash column chromatography (10% EtOAc in petroleum ether) to obtain **4p** as a colourless solid (240 mg, 64%). **m.p.** 96-98 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37-8.32 (m, 1H), 8.03 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.74 (t, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 1.3 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.3, 159.4 (d, *J* = 39.4 Hz), 130.8, 130.0, 127.9, 125.6, 110.3 (d, *J* = 3.4 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.8; **HRMS** (EI^+): calculated for $C_{12}H_6F_2N_2O_6S_2$ [$M+H^+$]: m/z = 376.9714, m/z found 376.9744; **IR** ν max (ATR)/cm^{-1}: 3152, 2956, 2923, 2852, 1439, 1420, 1396, 1246, 1212, 1311, 786, 744, 614.

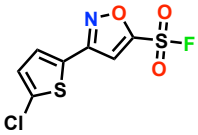
4-(5-(Fluorosulfonyl)isoxazol-3-yl)-2-methoxyphenyl 3,5-dinitrobenzoate (4q)



Following general procedure **A**, the crude product was purified by flash column chromatography (0-20% EtOAc in petroleum ether) to obtain **4q** as a beige solid (416 mg, 89%). **m.p.** 122-124 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.36-9.35 (m, 2H), 9.34-9.33 (m, 1H), 7.60 (d, *J* = 1.9 Hz, 1H), 7.51 (d, *J* = 1.3 Hz, 1H), 7.44 (dd, *J* = 8.2, 1.9 Hz, 1H), 7.38 (d, *J* = 8.2 Hz, 1H), 3.94 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 160.5, 159.2 (d, *J* = 39.0 Hz), 151.8, 149.0,

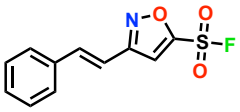
141.8, 132.8, 130.2, 126.2, 123.7, 123.2, 120.2, 111.0, 110.4 (d, *J* = 3.5 Hz), 56.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.7; **IR** ν̃ max (ATR)/cm^{-1}: 3111, 1742; 1548, 1437, 1345, 1283, 1213,1174, 1149, 797, 717.

3-(5-Chlorothiophen-2-yl)isoxazole-5-sulfonyl fluoride (4r)



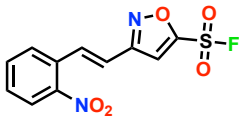
Following general procedure **A**, the crude product was filtered through a pad of silica (10% EtOAc in petroleum ether) to obtain **4r** as a brown amorphous solid (202 mg, 76%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36-7.33 (m, 2H), 7.02 (d, *J* = 4.0 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.0 (d, *J* = 39.4 Hz), 157.8, 135.5, 129.1, 127.4, 126.1, 109.7 (d, *J* = 3.6 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.7; **HRMS** (EI^+): calculated for $C_7H_4ClFN_3O_2S_2$ [M+H^+]: m/z = 267.9305, m/z found 267.9367; **IR** ν̃ max (ATR)/cm^{-1}: 3105, 1711, 1579, 1434, 1415, 1211, 794.

(*E*)-3-Styrylisoxazole-5-sulfonyl fluoride (4s)[2]



Following general procedure **A**, the crude product was purified by flash column chromatography (10% EtOAc in petroleum ether) to obtain **4s** as a beige solid (176 mg, 70%). **m.p.** 92-93 °C (lit: 94-95 °C)[2]; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58-7.54 (m, 2H), 7.47-7.39 (m, 4H), 7.30 (d, *J* = 16.6 Hz, 1H), 7.15 (d, *J* = 16.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.4, 158.2 (d, *J* = 38.7 Hz), 139.4, 134.8, 130.2, 129.2, 127.5, 113.4, 109.6 (d, *J* = 3.5 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.3; **HRMS** (EI^+): calculated for $C_{11}H_9FNO_3S$ [M+H^+]: m/z = 254.0287, m/z found 254.0341; **IR** ν̃ max (ATR)/cm^{-1}: 3703, 3136, 3093, 2971, 2923, 1639, 1430, 1208, 967, 898, 813, 787.

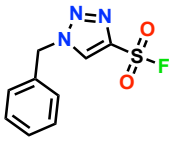
(*E*)-3-(2-Nitrostyryl)isoxazole-5-sulfonyl fluoride (4t)



Following general procedure **A**, the crude product was purified by flash column chromatography (10% EtOAc in petroleum ether) to obtain **4t** as a colourless solid (136 mg, 46%). **m.p.** 109-111°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.84 (d, *J* = 16.4 Hz, 1H), 7.78-7.70 (m, 2H), 7.62-7.56 (m, 1H), 7.47 (d, *J* = 1.3 Hz, 1H), 7.13 (d, *J* = 16.4 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.9, 158.8 (d, *J* = 39.2 Hz), 148.1, 134.9, 134.0, 130.8,

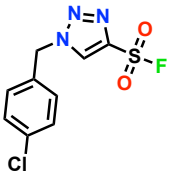
130.4, 128.9, 125.3, 118.4, 109.7 (d, *J* = 3.4 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 64.6; **HRMS** (EI^+): calculated for $C_{11}H_8FN_2O_5S$ [$M+H^+$]: m/z = 299.0138, m/z found 299.0166; **IR** ν max (ATR)/cm^{-1}: 3706, 3155, 2967, 2922, 2865, 2844, 2360, 2341, 1524, 1435, 1348, 1209, 1055, 1014, 743, 621.

1-Benzyl-1*H*-1,2,3-triazole-4-sulfonyl fluoride (6a)



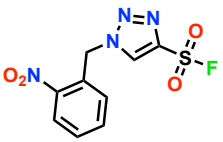
Following general procedure **B**, the crude product was purified by flash column chromatography (30-60% Et_2O in petroleum ether) to obtain **6a** as a beige solid (52 mg, 87%). m.p. 76-77 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 1.1 Hz, 1H), 7.49-7.43 (m, 3H), 7.40-7.32 (m, 2H), 5.65 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.5 (d, *J* = 36.7 Hz), 132.4, 130.0, 129.8, 128.8, 128.1 (d, *J* = 3.1 Hz), 55.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 66.4; **HRMS** (ESI^+): calculated for $C_9H_8FN_3O_2SNa$ [$M+Na^+$]: m/z =264.0219, m/z found 264.0014; **IR** ν max (ATR)/cm^{-1}: 3112, 2923, 2852, 1423, 1402, 1203, 1102, 1047, 774, 716, 700.

1-(4-Chlorobenzyl)-1*H*-1,2,3-triazole-4-sulfonyl fluoride (6b)



Following general procedure **B**, the crude product was purified by flash column chromatography (30-60% Et_2O in petroleum ether) to obtain **6b** as a beige solid (40 mg, 58%). **m.p.** 88-90 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 1.2 Hz, 1H), 7.48-7.42 (m, 2H), 7.32-7.28 (m, 2H), 5.62 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 140.6 (only observed by HMBC), 136.3, 130.9, 130.1, 130.1, 128.0 (d, *J* = 2.8 Hz), 54.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 66.4; **HRMS** (ESI^+): calculated for $C_9H_7ClFN_3O_2SNa$ [$M+Na^+$]: m/z = 297.9829, m/z found 297.9820; **IR** ν max (ATR)/cm^{-1}: 3115, 1494, 1417, 1203, 1090, 804, 743.

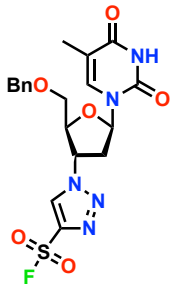
1-(2-Nitrobenzyl)-1*H*-1,2,3-triazole-4-sulfonyl fluoride (6c)



Following general procedure **B**, the crude product was purified by flash column chromatography (30-60% Et_2O in petroleum ether) to obtain **6c** as a beige solid (40 mg, 56%). **m.p.** 122-124 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.51

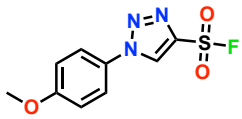
(d, *J* = 1.2 Hz, 1H), 8.22 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.76 (td, *J* = 7.6, 1.4 Hz, 1H), 7.67 (td, *J* = 8.1, 7.5, 1.5 Hz, 1H), 7.54-7.49 (m, 1H), 6.00 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.9, 140.6 (d, *J* = 37.1 Hz), 135.0, 132.5, 131.3, 129.2 (d, *J* = 3.0 Hz), 128.0, 126.1, 52.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 66.5; **HRMS** (ESI^+): calculated for $C_9H_7FN_4O_4SNa$ [$M+Na^+$]: m/z = 309.0070, m/z found 309.0085; **IR** ν max (ATR)/cm^{-1}: 3126, 2923, 2853, 1519, 1417, 1341, 1206, 788, 728.

1-((2*S*,3*S*,5*R*)-2-((Benzyloxy)methyl)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)tetrahydrofuran-3-yl)-1*H*-1,2,3-triazole-4-sulfonyl fluoride (6d)



Following general procedure **B** heating at 90 °C for 6 h, the crude product was purified by flash column chromatography (0-40% EtOAc in petroleum ether) to obtain **6d** as a grey solid (39 mg, 34%). **m.p.** 109-112 **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 1.1 Hz, 1H), 7.51-7.46 (m, 2H), 7.35-7.28 (m, 3H), 7.26-7.24 (m, 1H), 6.12 (dd, *J* = 7.3, 6.0 Hz, 1H), 5.64 (dt, *J* = 8.9, 5.6 Hz, 1H), 5.13 (s, 2H), 4.51-4.47 (m, 1H), 4.05 (dd, *J* = 12.3, 2.7 Hz, 1H), 3.83-3.75 (m, 1H), 3.19-3.09 (m, 1H), 3.07-2.98 (m, 1H), 1.98 (d, *J* = 1.3 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.2, 151.1, 140.8 (only observed by HMBC), 136.6, 136.2, 129.4, 128.7 (d, *J* = 2.9 Hz), 128.6, 128.0, 111.2, 90.6, 85.1, 61.9, 61.0, 44.7, 37.5, 13.4; **^{19}F NMR** (376 MHz,$CDCl_3$) δ 66.5; **HRMS** (ESI^+): calculated for $C_{19}H_{20}FN_5O_6SNa$ [$M+Na^+$]: m/z = 488.1016, m/z found 488.0936; **IR** ν max (ATR)/cm^{-1}: 3471 3060, 2927, 2852, 1698, 1664, 1633, 1488, 1413, 1212, 1094, 800.

1-(4-Methoxyphenyl)-1*H*-1,2,3-triazole-4-sulfonyl fluoride (6e)



Following general procedure **B** heating at 90 °C for 6 h, the crude product was purified by flash column chromatography (15% EtOAc in petroleum ether) to obtain **6e** as a yellow solid (40 mg, 63%). **m.p.** 94-97 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 1.2 Hz, 1H), 7.70-7.63 (m, 2H), 7.12-7.07 (m, 2H), 3.91 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.3, 140.7 (d, *J* = 37.0 Hz) 128.9, 126.5 (d, *J* = 3.0 Hz), 123.0, 115.4, 55.9; **^{19}F NMR** (376 MHz,

$CDCl_3$) δ 66.6; **HRMS** (ESI^+): calculated for $C_9H_8FN_3O_3SNa$ [M+Na^+]: m/z = 280.0168, m/z found 280.0022; **IR** ν max (ATR)/cm^{-1}: 3134, 2918, 2850, 1611, 1517, 1420, 1252, 1213, 1030, 778.

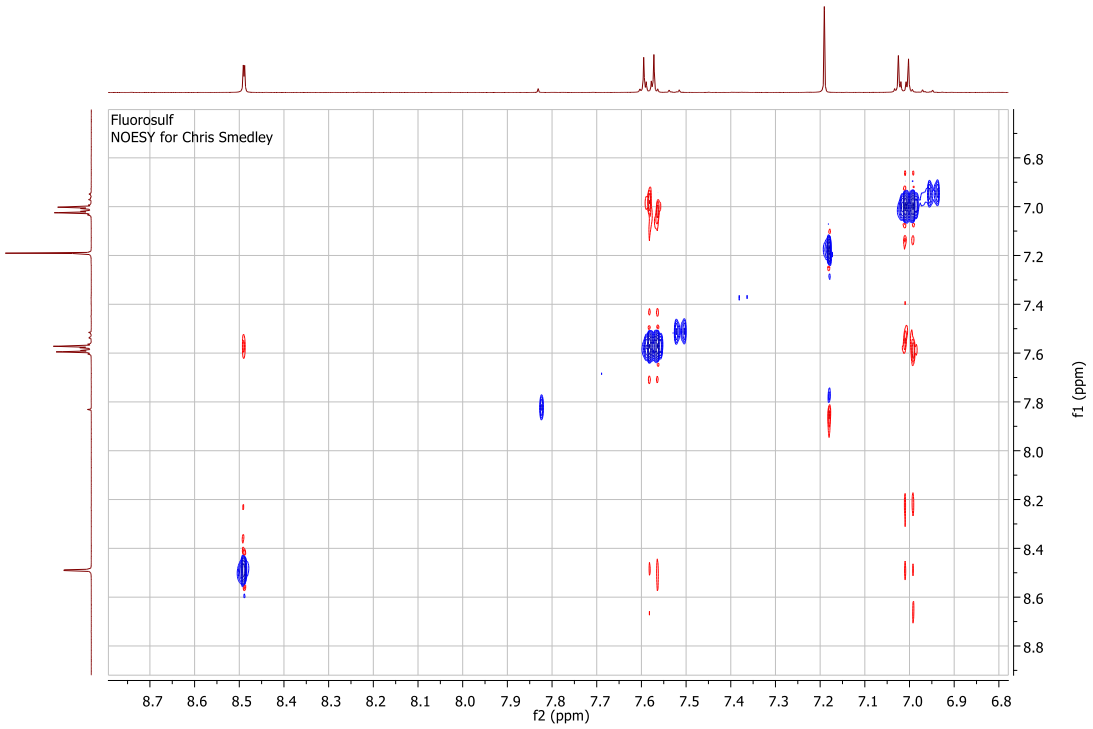
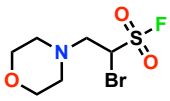


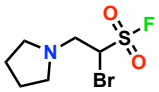
Figure S-1 Regiochemistry of 1-(4-methoxyphenyl)-1*H*-1,2,3-triazole-4-sulfonyl fluoride 6e was determined by NOE correlation spectroscopy to show the 1,4-regioisomer and can been seen in the above spectra.

1-Bromo-2-morpholinoethane-1-sulfonyl fluoride (7a)



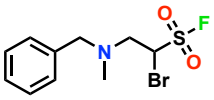
Following general procedure **C** (1.00 mmol of morpholine), **7a** was isolated as a brown oil (259 mg, 94%).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.17-5.08 (m, 1H), 3.76-3.70 (m, 4H), 3.35-3.27 (m, 1H), 3.18-3.09 (m, 1H), 2.67-2.61 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 66.9, 60.8, 56.0 (d, *J* = 15.2 Hz), 53.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 50.1; **HRMS** (ESI^+): calculated for $C_6H_{11}BrFNO_3S$ [M+H^+]: m/z = 275.9700, m/z found 275.9702; **IR** ν max (ATR)/cm^{-1}: 2958,2858, 2818, 1419, 1205, 1112.

1-Bromo-2-(pyrrolidin-1-yl)ethane-1-sulfonyl fluoride (7b)



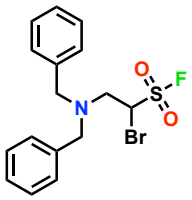
Following general procedure **C**, **7b** was isolated as a yellow oil (22 mg, 85%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.07 (dd, *J* = 7.9, 5.4 Hz, 1H), 3.41 (ddd, *J* = 13.8, 5.5, 0.8 Hz, 1H), 3.28 (ddd, *J* = 13.8, 7.9, 2.9 Hz, 1H), 2.74-2.66 (m, 4H), 1.87-1.79 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 58.5, 57.6 (d, *J* = 15.6 Hz), 54.3, 24.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 48.8; **HRMS** (ESI^+): calculated for $C_6H_{11}BrFNO_2S$ [M+H$^+$]: m/z = 259.9751, m/z found 275.9747; **IR** ν max (ATR)/cm^{-1}: 2972, 2806, 1415, 1207.

2-(Benzyl(methyl)amino)-1-bromoethane-1-sulfonyl fluoride (7c)



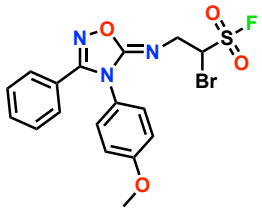
Following general procedure **C** (1.00 mmol of *N*-benzylamine), **7c** was isolated as a brown oil (303 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.27 (m, 5H), 4.97 (dd, *J* = 7.6, 5.9 Hz, 1H), 3.74-3.63 (m, 2H), 3.40 (dd, *J* = 14.3, 5.9 Hz, 1H), 3.19 (ddd, *J* = 14.3, 7.6, 3.1 Hz, 1H), 2.37 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.6, 129.1, 128.6, 127.8, 62.5, 60.0, 57.0 (d, *J* = 14.9 Hz), 42.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 49.3; **HRMS** (ESI^+): calculated for $C_{10}H_{13}BrFNO_2S$ [M+H$^+$]: m/z = 309.9907, m/z found 309.9798. **IR** ν max (ATR)/cm^{-1}: 2954, 2802, 1454, 1410, 1206.

1-Bromo-2-(dibenzylamino)ethane-1-sulfonyl fluoride (7d)



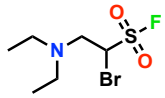
Following a modified general procedure **C** (reaction heated from 0 to 50 °C), **7d** was isolated as a yellow oil (36 mg, 92%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42-7.28 (m, 10H), 4.59 (dd, *J* = 8.0, 5.5 Hz, 1H), 3.81-3.69 (m, 4H), 3.53 (dd, *J* = 14.6, 5.5 Hz, 1H), 3.26 (ddd, *J* = 14.6, 8.0, 2.6 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.8, 129.2, 128.8, 127.9, 59.7, 57.7, 57.5 (d, *J* = 14.8 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ 48.3. **HRMS** (ESI^+): calculated for $C_{16}H_{17}BrFNO_2S$ [M+H$^+$]: m/z = 386.0220, m/z found 386.0119; **IR** ν max (ATR)/cm^{-1}: 3064, 3030, 2807, 1453, 1415, 1208.

(*E*)-1-Bromo-2-((4-(4-methoxyphenyl)-3-phenyl-1,2,4-oxadiazol-5(4*H*)-ylidene)amino)ethane-1-sulfonyl fluoride (7e)



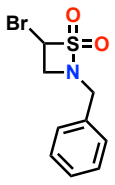
Following general procedure **C**, the crude product was purified by flash column chromatography (15-70% EtOAc in petrol) to obtain **7e** as a colorless amorphous solid (32 mg, 71%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50-7.44 (m, 1H), 7.37 -7.33 (m, 4H), 7.17-7.11 (m, 2H), 6.94-6.90 (m, 2H), 5.24-5.21 (m, 1H), 4.27 (ddd, *J* = 14.3, 5.9, 0.8 Hz, 1H), 4.13 (ddd, *J* = 14.3, 7.0, 2.0 Hz, 1H), 3.82 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.2, 157.9, 156.5, 132.0, 129.0, 129.0, 128.6, 125.1, 122.7, 115.1, 58.6 (d, *J* = 17.3 Hz), 55.7, 49.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 48.4; **HRMS** (ESI^+): calculated for $C_{17}H_{15}BrFN_3O_4S$ [M+H^+]: m/z = 380.0162, m/z found 380.0164; **IR** ν max (ATR)/cm^{-1}: 3062, 2906, 2839, 1698, 1513, 1410.

1-Bromo-2-(diethylamino)ethane-1-sulfonyl fluoride (7f)



Following general procedure **C**, **7f** was isolated as a yellow oil (21 mg, 81%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.98 (dd, *J* = 7.4, 5.8 Hz, 1H), 3.41 (dd, *J* = 14.7, 5.8 Hz, 1H), 3.15 (ddd, *J* = 14.7, 7.4, 3.4 Hz, 1H), 2.66 (q, *J* = 7.2 Hz, 4H), 1.06 (t, *J* = 7.2 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$ δ 58.0 (d, *J* = 12.7 Hz), 57.1, 47.8, 12.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ 49.5.; **HRMS** (ESI^+): calculated for $C_6H_{13}BrFNOS$ [M+H^+]: m/z = 261.9907, m/z found 261.9773. **IR** ν max (ATR)/cm^{-1}: 2972, 2819, 2469, 1412, 1204.

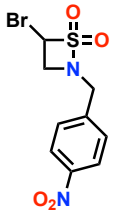
2-Benzyl-4-bromo-1,2-thiazetidine 1,1-dioxide (8a)[1]



Following general procedure **D**, **8a** was isolated as a yellow oil (22 mg, 79%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42-7.31 (m, 5H), 5.65 (dd, *J* = 7.1, 4.7 Hz, 1H), 4.36-4.22 (m, 2H), 3.68 (dd, *J* = 7.1, 7.1 Hz, 1H), 3.17 (dd, *J* = 7.1, 4.7 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 133.6, 129.1, 128.8, 128.6, 60.3, 50.9, 47.1; **HRMS** (EI^+): calculated for

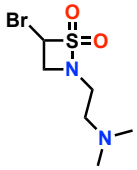
$C_9H_{11}BrNO_2S$ [M+H$^+$]: m/z = 275.9688, m/z found 275.9747; **IR** ν max (ATR)/cm^{-1}: 3031, 2925, 2855, 1445, 1334, 1178.

4-Bromo-2-(4-nitrobenzyl)-1,2-thiazetidine 1,1-dioxide (8b)



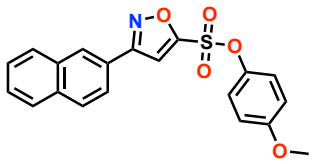
Following general procedure **D** (HCl salt of amine used with 1.0 equivalent extra of Et_3N), **8b** was isolated as a yellow amorphous solid (21 mg, 67%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.29-8.18 (m, 2H), 7.62-7.52 (m, 2H), 5.72 (dd, *J* = 7.2, 4.7 Hz, 1H), 4.38 (s, 2H), 3.79 (dd, *J* = 7.2, 7.2 Hz, 1H), 3.27 (dd, *J* = 7.2, 4.7 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.1, 141.3, 129.3, 124.3, 60.7, 50.5, 47.7; **HRMS** (EI$^+$): calculated for $C_9H_9BrN_2O_4SNa$ [M+Na$^+$]: m/z = 342.9359, m/z found 342.9633; **IR** ν max (ATR)/cm^{-1}: 2924, 2853, 1604, 1518, 1343.

4-Bromo-2-(2-(dimethylamino)ethyl)-1,2-thiazetidine 1,1-dioxide (8c)



Following general procedure **D** (HCl salt of amine used with 1.0 equivalent extra of Et_3N), **8c** was isolated as a yellow oil (15 mg, 58%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.63 (dd, *J* = 7.2, 4.9 Hz, 1H), 3.88 (dd, *J* = 7.2, 7.2 Hz, 1H), 3.31-3.14 (m, 3H), 2.57 (t, *J* = 6.2 Hz, 2H), 2.31 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 60.5, 57.2, 48.0, 45.5, 45.3; **IR** ν max (ATR)/cm^{-1}: 2823, 2773, 1619, 1462, 1328, 1172. **HRMS** (ESI$^+$): calculated for $C_6H_{13}BrN_2O_2S$ [M+H$^+$]: m/z = 256.9954, m/z found 256.9954; **IR** ν max (ATR)/cm^{-1}: 2947, 2823, 2773, 1619, 1328, 1172.

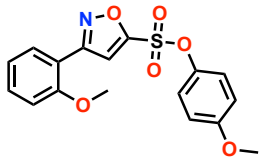
4-Methoxyphenyl 3-(naphthalen-2-yl)isoxazole-5-sulfonate (16a)



Following general procedure **E** stirring for 1 h, the crude product was purified by flash column chromatography (0-20% EtOAc in petroleum ether) to obtain **16a** as a colourless solid (28 mg, 74%). **m.p.** 80-81 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25-8.20 (m, 1H), 7.99-7.87 (m, 4H), 7.64-7.54 (m, 2H), 7.31 (s, 1H), 7.15-7.09 (m, 2H), 6.91-6.84 (m, 2H), 3.79 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.8, 161.8, 158.9, 142.6, 134.5, 133.0, 129.3, 128.6, 127.9,

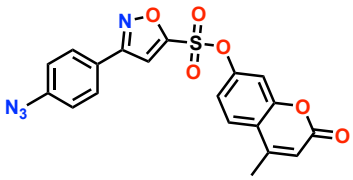
127.8, 127.3, 127.2, 124.1, 123.3, 123.0, 115.0, 109.4, 55.6; **HRMS** (ESI$^+$): calculated for $C_{20}H_{15}NO_5SNa$ [M+Na$^+$]: m/z = 404.0569, m/z found 404.0511; **IR** ν max (ATR)/cm^{-1}: 2922, 1500, 1251, 1198, 1167, 1056, 1029, 879, 833.

4-Methoxyphenyl 3-(2-methoxyphenyl)isoxazole-5-sulfonate (16b)



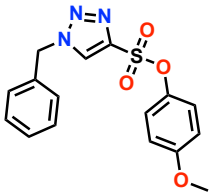
Following general procedure **E** stirring for 2 h, the crude product was purified by flash column chromatography (0-25% EtOAc in petroleum ether) to obtain **16b** as a colourless gum (32 mg, 89%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 7.7, 1.8, 1H), 7.49 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.41 (s, 1H), 7.12-7.05 (m, 3H), 7.02 (dd, *J* = 8.4, 1.0 Hz, 1H), 6.89-6.84 (m, 2H), 3.89 (s, 3H), 3.79 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.5, 160.5, 159.0, 157.4, 142.8, 132.7, 129.5, 123.2, 121.3, 115.8, 115.1, 113.0, 111.7, 55.8, 55.7; **HRMS** (ESI$^+$): calculated for $C_{17}H_{15}NO_6SNa$ [M+Na$^+$]: m/z = 384.0518, m/z found 384.0558; **IR** ν max (ATR)/cm^{-1}: 2932, 2842, 1603, 1499, 1469, 1396, 1250, 1196, 1166, 1106, 1022, 871, 834.

4-Methyl-2-oxo-2*H*-chromen-7-yl 3-(4-azidophenyl)isoxazole-5-sulfonate (16c)



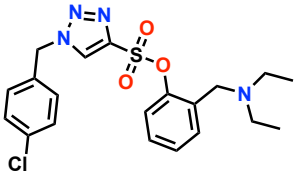
Following general procedure **E** stirring for 1 h, the crude product was purified by flash column chromatography (30% EtOAc in petroleum ether) to obtain **16c** as a yellow solid (33 mg, 79%). **m.p.** 118-120; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83-7.78 (m, 2H), 7.67-7.62 (m, 1H), 7.25 (s, 1H), 7.21-7.18 (m, 2H), 7.17-7.13 (m, 2H), 6.40-6.30 (m, 1H), 2.44 (d, *J* = 1.3 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.2, 161.6, 159.8, 154.2, 151.5, 150.8, 143.4, 128.7, 126.4, 123.2, 120.0, 119.9, 118.2, 115.8, 111.0, 109.3, 18.9; **HRMS** (ESI$^+$): calculated for $C_{19}H_{12}N_4O_6SNa$ [M+Na$^+$]: m/z = 447.0375, m/z found 447.0286; **IR** ν max (ATR)/cm^{-1}: 2922, 2863, 2128, 1739, 1605, 1403, 1280, 1194, 1056, 1013.

4-Methoxyphenyl 1-benzyl-1*H*-1,2,3-triazole-4-sulfonate (16d)



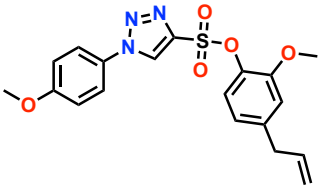
Following general procedure **E** stirring for 1 h, the crude product was purified by flash column chromatography (0-25% EtOAc in petroleum ether) to obtain **16d** as a yellow gum (26 mg, 74%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.48-7.36 (m, 3H), 7.26-7.20 (m, 2H), 7.06-6.96 (m, 2H), 6.86-6.71 (m, 2H), 5.57 (s, 2H), 3.77 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.6, 143.0, 143.0, 133.1, 129.6, 129.6, 128.4, 127.9, 123.4, 114.8, 55.7, 55.1; **HRMS** (ESI^+): calculated for $C_{16}H_{15}N_3O_4SNa$ [M+Na^+]: m/z = 368.0681, m/z found 368.0697; **IR** ν max (ATR)/cm^{-1}: 3136, 2924, 2853, 1499, 1382, 1251, 1192, 1167, 1139, 1029, 868, 836, 797, 718.

2-((Diethylamino)methyl)phenyl 1-(4-chlorobenzyl)-1*H*-1,2,3-triazole-4-sulfonate (16e)



Following general procedure **E** stirring for 3 h before the addition of an extra 20 mol% DBU and stirred for a further 3 h. The crude product was purified by flash column chromatography (0-30% EtOAc in petroleum ether) to obtain **16e** as a colourless solid (24 mg, 55%). **m.p.** 74-75 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.59-7.56 (m, 1H), 7.42-7.38 (m, 2H), 7.26-7.23 (m, 1H), 7.22-7.14 (m, 4H), 5.56 (s, 2H), 3.53 (s, 2H), 2.47 (q, *J* = 7.1 Hz, 4H), 1.00 (t, *J* = 7.1 Hz, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.2, 143.9, 135.9, 134.1, 131.5, 131.1, 129.9, 129.8, 127.8, 127.6, 127.5, 121.9, 54.4, 51.3, 47.3, 12.0; **HRMS** (ESI^+): calculated for $C_{20}H_{24}ClN_4O_3S$ [M+H^+]: m/z = 435.1258, m/z found 435.1196; **IR** ν max (ATR)/cm^{-1}: 3141, 2964, 2924, 2855, 1494, 1450, 1379, 1184, 1137, 1089, 879, 772.

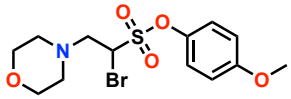
4-Allyl-2-methoxyphenyl 1-(4-methoxyphenyl)-1*H*-1,2,3-triazole-4-sulfonate (16f)



Following general procedure **E** stirring for 1 h, the crude product was purified by flash column chromatography (0-30% EtOAc in petroleum ether) to obtain **16f** as a colourless solid (31 mg, 78%). **m.p.** 74-75 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.66-7.60 (m, 2H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.09-7.04 (m, 2H), 6.79-6.74 (m, 1H), 6.75-6.71 (m, 1H), 5.99-5.87 (m, 1H), 5.13-5.07 (m, 2H), 3.89 (s, 3H), 3.67 (s, 3H), 3.38-3.34 (m, 2H); **^{13}C NMR** (101

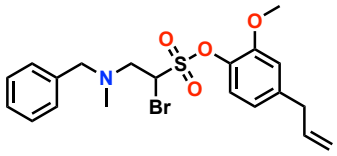
MHz, $CDCl_3$) δ 160.9, 151.6, 144.3, 141.1, 136.8, 136.7, 129.3, 125.5, 124.0, 122.7, 121.0, 116.7, 115.3, 113.3, 55.9, 55.9, 40.2; **HRMS** (ESI^+): calculated for $C_{19}H_{19}N_3O_5SNa$ [$M+Na^+$]: m/z = 424.0943, m/z found 424.0933; **IR** ν max (ATR)/cm^{-1}: 3153, 2941, 1598, 1520, 1383, 1248, 1196, 1113, 1030, 867, 828.

4-Methoxyphenyl 1-bromo-2-morpholinoethane-1-sulfonate (16g)



Following general procedure **E** stirring for 1 h, the crude product was purified by flash column chromatography (0-60% EtOAc in petrol) to obtain **16g** as a clear oil (25 mg, 66%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30-7.26 (m, 2H), 6.93-6.89 (m, 2H), 5.03-4.94 (m, 1H), 3.81 (s, 3H), 3.77-3.68 (m, 4H), 3.37 (dd, *J* = 14.2, 3.8 Hz, 1H), 3.14 (dd, *J* = 14.3, 8.8 Hz, 1H), 2.63 (d, *J* = 5.3 Hz, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.8, 142.8, 123.1, 115.1, 66.9, 60.6, 56.6, 55.8, 53.7; **HRMS** (ESI^+): calculated for $C_{13}H_{18}BrNO_5S$ [$M+H^+$]: m/z = 380.0162, m/z found 380.0164; **IR** ν max (ATR)/cm^{-1}: 2965, 2817, 1719, 1607, 1502.

4-Allyl-2-methoxyphenyl 2-(benzyl(methyl)amino)-1-bromoethane-1-sulfonate (16h)



Following general procedure **E** stirring for 1 h, the crude product was purified by flash column chromatography (0-40% EtOAc in petrol) to obtain **16h** as a clear oil (33 mg, 73%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40-7.26 (m, 5H), 7.19 (d, *J* = 8.1 Hz, 1H), 6.81-6.75 (m, 2H), 6.00-5.87 (m, 1H), 5.18 (dd, *J* = 9.7, 3.3 Hz, 1H), 5.15-5.07 (m, 2H), 3.84 (s, 3H), 3.78-3.63 (m, 2H), 3.50 (dd, *J* = 14.1, 3.4 Hz, 1H), 3.38 (dt, *J* = 6.7, 1.5 Hz, 2H), 3.33-3.22 (m, 1H), 2.35 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.3, 140.9, 138.2, 137.1, 136.7, 129.1, 128.6, 127.5, 123.8, 121.2, 116.7, 113.4, 62.4, 59.8, 59.6, 56.1, 42.4, 40.2; **HRMS** (ESI^+): calculated for $C_{20}H_{25}BrNO_4S$ [$M+H^+$]: m/z = 454.0682, m/z found 454.0672; **IR** ν max (ATR)/cm^{-1}: 3233, 2361, 1708, 1611, 1567.

Theoretical Calculations

All calculations were performed using Gaussian 16[3] revision A.03 unless noted. Geometry optimisations were performed using the M06-2X density functional[4] and the def2-TZVP basis set.[5] Harmonic vibrational frequencies were computed at the same level of theory in order to characterise the stationary points as minima, representing equilibrium structures, or transition states (TSs). For all TSs, intrinsic reaction coordinate (IRC) calculations[6] were carried out to ensure the connectivity between the local minima along the reaction path. Vibrational frequencies were also utilised to determine corresponding thermochemical data (within the harmonic limit and determined at 1 atm and 298 K). In order to provide more accurate energetics, single-point calculations at the optimised geometries were performed at the MP2 level of theory[7] with a def2-TZVPP basis set,[5] inclusive of solvent effects using the polarisable continuum model (IEF-PCM) with Truhlar's SMD model[8] with parameters for THF (ε = 7.4257). Reported free energies were determined by adding the thermal corrections determined at the M06-2X/def2-TZVP level of theory (gas phase) to the MP2/def2-TZVPP solvent-corrected single point energies, which is labelled MP2/def2-TZVPP (SMD, THF)//M06-2X/def2-TZVP.

For the reaction of DBESF to BESF (Table **S1**), additional density functional theory (DFT), double-hybrid DSDPBEP86, spin-scaled MP2 and G2(MP2) calculations were carried out within Gaussian 16. DLPNO-CCSD(T)/cc-pVTZ[9] calculations were carried out within ORCA.[10] All calculations were carried out at the M06-2X/def2-TZVP geometries. All results consistently indicate that Δ*G* for the reaction of DBESF to form BESF + HBr is exergonic.

Table S-3: Relative energies (Δ*G*, kJ mol^{-1}) for the formation of BESF from DBESF at various methods and basis sets.

Method/Basis Set	Δ*G* (kJ mol^{-1})
M06-2X/def2-TZVP	28.7
MP2/def2-TZVPP	38.2
SCS-MP2/def2-TZVPP	27.9
SOS-MP2/def2-TZVPP	22.8
PBE0/def2-TZVPP	25.0
DLPNP-CCSD(T)/cc-pVTZ	21.8
DSDPBEP86/def2-TZVPP	17.5
B3LYP-D3/6-311+G(d)	32.5
B3LYP/6-311+G(d)	17.4
G2(MP2)	25.5

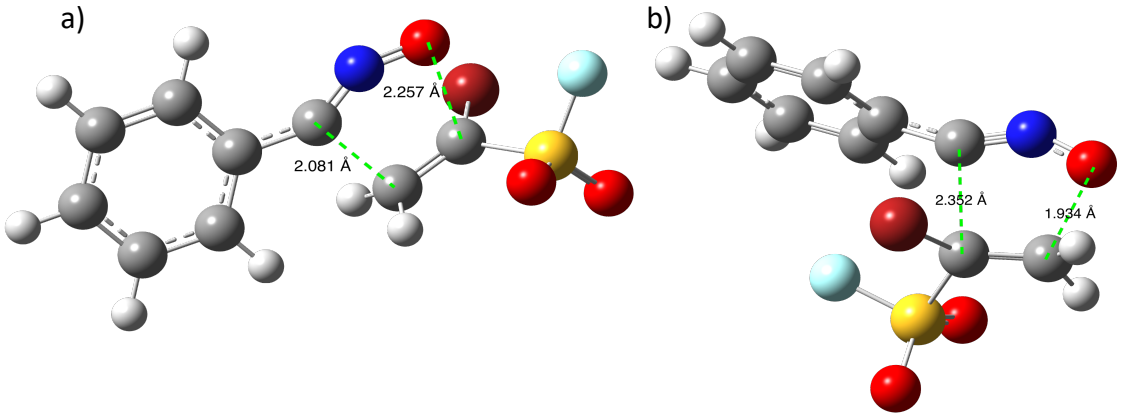


Figure S-2: Computed transition state interatomic distances (Å) for the formation of a) 3-phenylisoxazole-5-sulfonyl fluoride and b) 3-phenylisoxazole-4-sulfonyl fluoride.

Cartesian coordinates of M06-2X/def2-TZVP Optimised Geometries.

HBr

E_e = -2573.00544477 (Hartrees)

0 1

35	0.000000	0.000000	0.039484
1	0.000000	0.000000	-1.381934

BESF

E_e = -5869.13992592 (Hartrees)

0 1

6	-0.746818	-0.922727	0.453062
1	-0.652337	-0.694092	1.510484
1	-0.598496	-1.984803	0.278282
16	1.902720	-0.775707	-0.15454
8	1.844168	-2.181664	-0.322058
8	2.858135	0.024705	-0.816396
6	0.242623	-0.122752	-0.371136
1	0.061380	-0.239321	-1.439675
35	-2.565799	-0.517346	-0.068563
35	0.209518	1.761844	0.021675
9	2.069168	-0.522151	1.375630

DBESF

E_e = -3296.11326837 (Hartrees)

0 1

6	-0.746818	-0.922727	0.453062
1	-0.652337	-0.694092	1.510484
1	-0.598496	-1.984803	0.278282
16	1.902720	-0.775707	-0.15454
8	1.844168	-2.181664	-0.322058
8	2.858135	0.024705	-0.816396
6	0.242623	-0.122752	-0.371136
1	0.061380	-0.239321	-1.439675
35	-2.565799	-0.517346	-0.068563
35	0.209518	1.761844	0.021675
9	2.069168	-0.522151	1.375630

Ph-CNO

E_e = -397.355596546 (Hartrees)

0 1

6	-1.471362	0.000324	-0.000241
7	-2.623216	-0.000005	0.000094
8	-3.825673	-0.000115	0.000154
6	-0.040002	0.000274	-0.000187
6	0.658459	1.209236	-0.000106
6	0.657992	-1.208982	-0.000056
6	2.043048	1.202531	0.000074
1	0.110231	2.141371	-0.000122
6	2.042606	-1.202835	0.000031
1	0.109422	-2.140922	-0.000112
6	2.736991	-0.000293	0.000126
1	2.581874	2.140598	0.000140

1	2.581063	-2.141118	0.000102
1	3.818911	-0.000500	0.000251

TS1 - 3,5-isoxazole formation

E_e = -3693.39889214 (Hartrees)

0 1

16	-2.316881	1.273205	-0.179143
8	-3.370576	1.189813	-1.121381
8	-1.534324	2.446826	-0.036392
35	-2.027649	-1.800712	-0.247203
9	-2.966525	0.981949	1.198693
6	-1.235455	-0.101007	-0.351285
6	-0.039193	0.108124	-0.978831
1	0.193725	1.116465	-1.30031
1	0.415358	-0.714397	-1.515626
6	1.392117	0.106015	0.531340
7	0.652127	0.099780	1.470520
8	-0.515176	0.073772	1.780617
6	2.792393	0.084369	0.174366
6	3.196967	0.373416	-1.126464
6	3.744311	-0.233541	1.147497
6	4.544403	0.346161	-1.451474
1	2.464196	0.625216	-1.880531
6	5.085778	-0.254129	0.812819
1	3.420614	-0.458834	2.154676
6	5.489283	0.033568	-0.485866
1	4.854353	0.572911	-2.46267
1	5.820400	-0.498516	1.568462
1	6.539967	0.013646	-0.742828

TS1 – 3,4-isoxazole formation

E_e = -3693.40417618 (Hartrees)

0 1

16	1.097146	-1.467942	0.636897
8	2.017691	-1.696954	1.688164
8	0.764482	-2.490783	-0.292088
35	1.449581	1.584351	0.801129
9	-0.236438	-1.067163	1.348104
6	1.452270	-0.003664	-0.241018
6	2.289350	-0.132325	-1.326838
1	2.537237	-1.128415	-1.669531
1	2.993740	0.654078	-1.553658
6	-0.545305	0.215845	-1.463893
7	0.078629	0.307337	-2.465525
8	1.234286	0.263334	-2.898159
6	-1.787237	0.201141	-0.747247
6	-2.222067	1.351592	-0.088937
6	-2.520047	-0.984949	-0.673829
6	-3.405218	1.314843	0.629097
1	-1.631151	2.255334	-0.145899
6	-3.702421	-1.006410	0.043133
1	-2.145611	-1.873551	-1.164493
6	-4.143218	0.140131	0.693629
1	-3.750845	2.202876	1.140635
1	-4.277761	-1.920275	0.102557

1	-5.066044	0.115848	1.258346

Intermediate - 3,5-isoxazole formation

E_e = -3693.53045347 (Hartrees)

0 1

6	1.073205	0.023859	0.126892
6	-1.214135	-0.115030	0.348562
6	-0.164179	-0.260015	-0.719884
1	-0.165886	-1.282672	-1.107799
1	-0.273286	0.435700	-1.546476
8	0.672238	-0.090624	1.447729
7	-0.727458	-0.040747	1.520960
6	-2.659348	-0.101917	0.102118
6	-3.555165	0.094627	1.155306
6	-3.145640	-0.294960	-1.188019
6	-4.915763	0.094824	0.912150
1	-3.170159	0.245735	2.154832
6	-4.512769	-0.295351	-1.426663
1	-2.460461	-0.450595	-2.012010
6	-5.397987	-0.100165	-0.378463
1	-5.606793	0.248241	1.730374
1	-4.883155	-0.447901	-2.431535
1	-6.464108	-0.098544	-0.563549
35	1.816483	1.800779	-0.215558
16	2.349595	-1.227608	-0.177977
8	1.819122	-2.489173	0.180960
8	2.967187	-0.997695	-1.428159
9	3.358661	-0.822844	0.925040

Int1 – 3,4-isoxazole formation

E_e = -3693.51029983 (Hartrees)

0 1

6	1.767144	1.425471	-0.953191
6	-0.450387	0.995346	-0.339706
6	0.908584	0.311008	-0.339936
8	0.946452	2.588230	-0.90532
7	-0.341202	2.228135	-0.647837
6	-1.767441	0.400722	-0.054692
6	-2.911837	1.163106	-0.31231
6	-1.908091	-0.884665	0.462175
6	-4.166237	0.647601	-0.049566
1	-2.801888	2.159057	-0.718335
6	-3.172602	-1.395734	0.723496
1	-1.043456	-1.494552	0.675722
6	-4.301714	-0.635577	0.469737
1	-5.043867	1.247022	-0.25243
1	-3.267533	-2.394013	1.129324
1	-5.285417	-1.038068	0.673134
35	0.988915	-1.332774	-1.361181
16	1.463027	-0.010100	1.358682

8	1.506154	1.233167	2.032109
8	0.879112	-1.164632	1.926669
9	2.943598	-0.388851	1.028725
1	2.682516	1.623507	-0.400244
1	1.996963	1.190652	-1.99213

Product – 3,4-isoxazole

E_e = -1120.53827903 (Hartrees)

0 1

6	0.124713	1.091793	-0.171459
6	-1.987414	1.721331	-0.153041
6	-1.225443	0.602797	-0.105623
1	-3.054451	1.870304	-0.118668
8	-1.213909	2.782873	-0.252686
7	0.105281	2.392674	-0.259573
16	-1.928116	-0.967872	0.042032
8	-1.500707	-1.842397	-0.985187
8	-3.297927	-0.813665	0.363495
9	-1.209812	-1.451440	1.337055
6	1.411981	0.381842	-0.100136
6	1.568121	-0.892703	-0.637751
6	2.496235	1.017962	0.504994
6	2.801065	-1.524691	-0.566671
1	0.738762	-1.386070	-1.124976
6	3.723165	0.380910	0.571740
1	2.363894	2.007223	0.921978
6	3.877348	-0.892240	0.037483
1	2.918163	-2.513852	-0.98876
1	4.836479	-1.390295	0.093521
1	4.560077	0.876392	1.045723

Product – 3,5-isoxazole

E_e = -1120.53131731 (Hartrees)

0 1

6	-0.759251	-0.321781	-0.015544
6	1.399185	-0.162877	0.033827
6	0.309022	0.622762	0.100590
1	0.280922	1.689976	0.226061
8	1.073858	-1.445761	-0.106417
7	-0.287976	-1.535220	-0.141374
16	3.088764	0.265256	0.145039
8	3.785015	-0.669366	0.938377
8	3.164801	1.662552	0.336742
9	3.506254	-0.009392	-1.327655
6	-2.206765	-0.066154	-0.002043
6	-2.688241	1.236994	-0.084149
6	-3.106011	-1.127936	0.090658
6	-4.053686	1.479208	-0.074487
1	-1.998936	2.067793	-0.164583
6	-4.467981	-0.882028	0.099098
1	-2.726945	-2.138869	0.157842
6	-4.945142	0.420748	0.017210
1	-4.419710	2.495123	-0.140294
1	-6.010640	0.609137	0.025737
1	-5.161528	-1.709200	0.172560

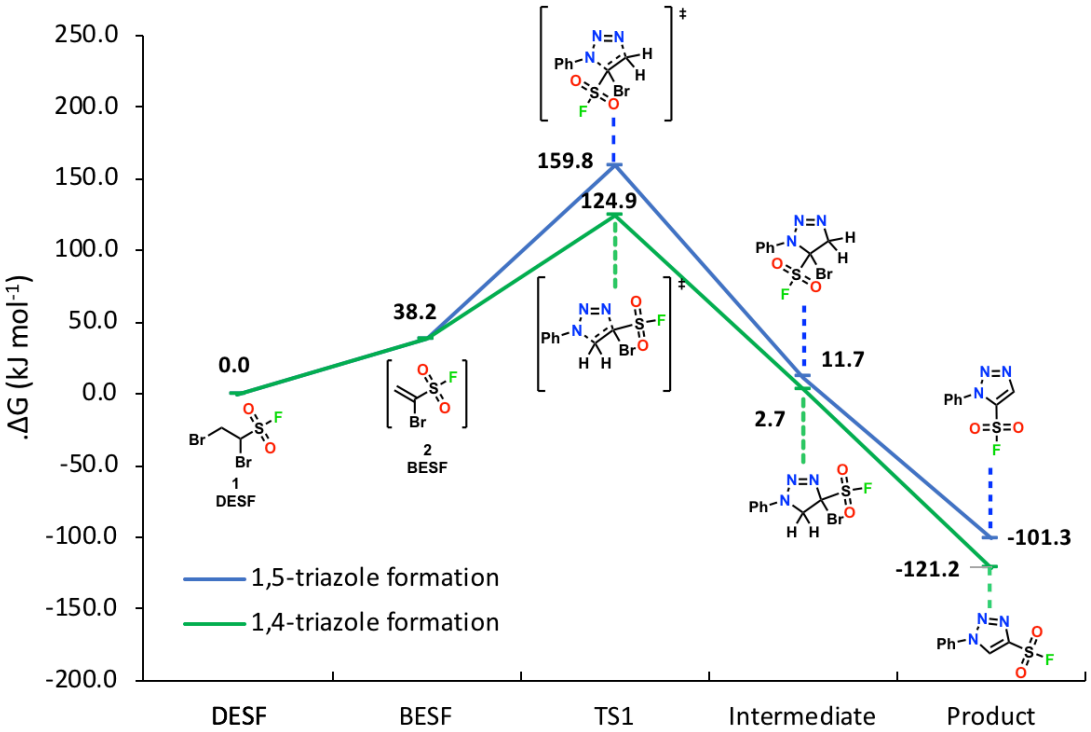


Figure S-3 Calculated free energy profile (ΔG, kJ mol^{-1}) of 1,4- and 1,5-triazole formation reactions at the MP2/def2-TZVPP(SMD,THF)//M06-2X/def2-TZVP level of theory.

Ph-N_3

E_e = -393.538879144 (Hartrees)

0 1

6	-0.000017023	-0.000011691	0.000002436
6	0.000002137	-0.000005381	-0.000004962
6	0.000001058	0.000003564	0.000001671
6	0.000004746	0.000004976	0.000002014
6	-0.000002286	-0.000001896	0.00000051
6	0.000010585	0.000008745	-0.000004406
1	0.000001689	0.000001753	0.000000898
1	-0.000001279	-0.000001751	-0.00000052
1	0.000000167	-0.000005342	-0.000004872
1	0.000003364	-0.000001244	-0.000002888
1	0.000002719	0.000000859	-0.000000335
7	-0.000007659	-0.000003679	-0.000002812
7	0.000016948	-0.000003220	-0.000002576
7	-0.000015165	0.000014306	0.000015844

TS1 – 1,5-triazole

E_e = -3689.53345805 (Hartrees)

0 1

16	1.090523	1.394180	0.84128
8	2.250638	2.250415	0.650849

8	0.316040	1.426965	2.07156
35	2.157953	-0.489018	-1.360928
9	0.070483	1.823809	-0.358723
6	1.444997	-0.292919	0.388444
6	1.790355	-1.167805	1.419379
1	1.722090	-0.815040	2.44508
1	2.579013	-1.891121	1.230584
7	-0.465577	-2.099121	0.86604
6	-1.954518	-0.608103	-0.14495
6	-2.200254	0.019499	-1.374764
6	-2.938470	-0.628794	0.858000
6	-3.437946	0.619748	-1.603526
1	-1.426624	0.026034	-2.136361
6	-4.174384	-0.033357	0.612026
1	-2.737235	-1.116339	1.808186
6	-4.427517	0.593561	-0.614738
1	-3.630805	1.104050	-2.556996
1	-4.941815	-0.057346	1.381285
1	-5.393158	1.056930	-0.798618
1	-0.674320	-1.182346	0.029404
7	0.435679	-2.481782	1.53439

TS1 – 1,4-triazole

E_e = -3689.58601579 (Hartrees)

0 1

16	0.000002398	-0.000001474	-0.000000547
8	-0.000000582	0.000000707	-0.000001911
8	-0.000000913	0.000001086	0.000000781
35	0.000001506	-0.000003219	-0.000002899
9	-0.000001485	-0.000002833	-0.000000829
6	-0.000002004	0.000000747	-0.000008014
6	-0.000011055	0.000000966	-0.000004738
1	0.000001554	0.000003286	0.000002555
1	0.000001643	0.000003259	-0.00000167
7	-0.000032664	-0.000003358	0.000006502
6	0.000006606	0.000004756	0.000002640
6	-0.000000225	0.000002153	0.000002232
6	0.000000083	-0.000002388	0.000000085
6	0.000000214	0.000002252	0.000001464
1	-0.000000445	0.000003091	0.000002602
6	-0.000001023	-0.000002180	-0.000001032
1	-0.000000265	-0.000004257	-0.000000348
6	0.000000551	0.000000700	0.000000625
1	0.000001105	0.000004610	0.000002458
1	-0.000000724	-0.000002741	-0.000000931
1	0.000000397	0.000001644	0.000000508
7	0.000024446	0.000000566	-0.000006901

7	0.000010882	-0.000007371	0.000007370

Intermediate – 1,4-triazole

E_e = -3689.67910183 (Hartrees)

0 1

6	-1.062653	0.060684	0.112845
6	0.185869	-0.147027	-0.745664
7	1.196490	0.055889	0.279134
7	0.661094	0.058032	1.495406
7	-0.584181	0.035920	1.498297
16	-2.222144	-1.296119	-0.143285
8	-2.847896	-1.171085	-1.405004
8	-1.585367	-2.492456	0.264215
9	-3.271002	-0.940045	0.935385
1	0.264214	0.576661	-1.55208
6	2.584973	-0.009046	0.081566
6	3.079403	-0.213894	-1.202373
6	3.459259	0.140276	1.157246
6	4.451129	-0.270076	-1.407639
1	2.406751	-0.332276	-2.041044
6	4.822404	0.077441	0.933123
1	3.064773	0.300194	2.149769
6	5.328219	-0.126260	-0.345841
1	4.828593	-0.430130	-2.40887
1	5.498388	0.191439	1.770329
1	6.396081	-0.171720	-0.509506
1	0.247033	-1.163464	-1.147054
35	-1.950053	1.754699	-0.219159

Intermediate – 1,5-triazole

E_e = -3689.66879331 (Hartrees)

0 1

6	-1.751806	1.692886	-0.276135
6	-0.894267	0.427683	-0.128876
7	0.397006	0.980657	-0.107134
7	0.355798	2.297552	-0.560128
7	-0.789605	2.712339	-0.685735
16	-1.393008	-0.484734	1.361635
8	-2.806313	-0.494903	1.414682
8	-0.617416	-1.642084	1.586434
9	-0.915915	0.582610	2.396639
6	1.671449	0.354790	-0.031658
6	1.817957	-1.024952	-0.102447
6	2.790527	1.171344	0.128851
6	3.088031	-1.579268	-0.019919
1	0.964889	-1.674193	-0.209209

6	4.048727	0.601080	0.199682
1	2.668932	2.242020	0.192331
6	4.206673	-0.776521	0.125870
1	3.192170	-2.654797	-0.072309
1	4.911451	1.242498	0.321847
1	5.192103	-1.217928	0.187601
1	-2.180765	2.003681	0.679504
1	-2.553226	1.588081	-1.000121
35	-1.253729	-0.830209	-1.63902

Product – 1,4-triazole

E_e = -1116.71302651 (Hartrees)

0 1

6	-1.393815	-0.224597	-0.121266
6	-0.284372	0.544743	0.100404
7	0.731761	-0.306599	-0.118112
7	0.266889	-1.526928	-0.44797
7	-1.013808	-1.481023	-0.45297
16	-3.044673	0.294409	-0.022232
8	-3.044067	1.682916	0.258441
8	-3.827338	-0.281613	-1.044561
9	-3.466068	-0.417055	1.299482
1	-0.166153	1.570440	0.399143
6	2.132578	-0.060263	-0.040046
6	2.618428	1.211937	-0.301772
6	2.981352	-1.104534	0.296101
6	3.981947	1.444326	-0.207389
1	1.945931	2.006259	-0.597425
6	4.342875	-0.859637	0.373771
1	2.571075	-2.085443	0.488671
6	4.845186	0.411533	0.12898
1	4.368614	2.433796	-0.410605
1	5.013308	-1.667544	0.634158
1	5.908874	0.595838	0.196059

Product – 1,5-triazole

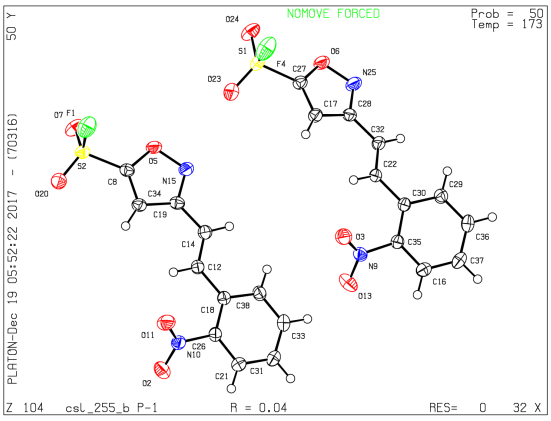
E_e = -1116.69660986 (Hartrees)

0 1

6	-2.082869	1.702300	-0.18734
6	-1.264692	0.605307	-0.122549
7	-0.003209	1.100545	-0.211541
7	-0.059184	2.425148	-0.315516
7	-1.298062	2.793003	-0.310748

16	-1.759016	-1.043740	0.076869
8	-3.130862	-1.040085	0.411737
8	-1.230698	-1.882514	-0.9314
9	-0.970871	-1.388858	1.375139
6	1.266654	0.445042	-0.128462
6	1.568905	-0.599046	-0.987398
6	2.177840	0.909107	0.808490
6	2.812286	-1.205504	-0.884431
1	0.848358	-0.927727	-1.722073
6	3.419653	0.301225	0.891141
1	1.907757	1.735123	1.451817
6	3.734709	-0.758490	0.050440
1	3.060328	-2.023756	-1.546665
1	4.139674	0.653265	1.617393
1	4.703756	-1.234131	0.122161
1	-3.157022	1.747067	-0.146183

Table S-4 X-ray data of structure 4t (CCDC 1839108)[11]



Datablock: csl_255_b

Bond precision: C-C = 0.0024 A Wavelength=1.54184

Cell:	a=8.2004(16)	b=11.919(2)	c=12.400(3)
	alpha=93.86(3)	beta=93.52(3)	gamma=95.79(3)
Temperature:	173 K		
	Calculated		Reported
Volume	1200.2(4)		1200.2(4)
Spaces group	P -1		P-1
Hall group	-P 1		?
Moiety formula	C11 H7 F N2 O5 S		?
Sum formula	C11 H7 F N2 O5 S		C11 H7 F N2 O5 S
Mr	298.25		298.25
Dx, g cm^{-3}	1.651		1.651
Z	4		4
Mu (mm^{-1})	2.775		2.775
F000	608.0		608.0
F000’	611.57		
H, k, lmax	9, 14, 15		9, 14, 15
Nref	4548		4544
Tmin, Tmax	0.505, 0.717		0,433, 0.732
Tmin’	0.361		

Correction method= # Reported T Limits: Tmin=0.443 Tmax=0.732
AbsCorr = MULTI-SCAN
Data completeness= 0.999 Theta(max)= 70.070

R(reflections)= 0.0363(4121) wR2(reflections)= 0.112(4554)

S = 1.095 Npar= 361

References

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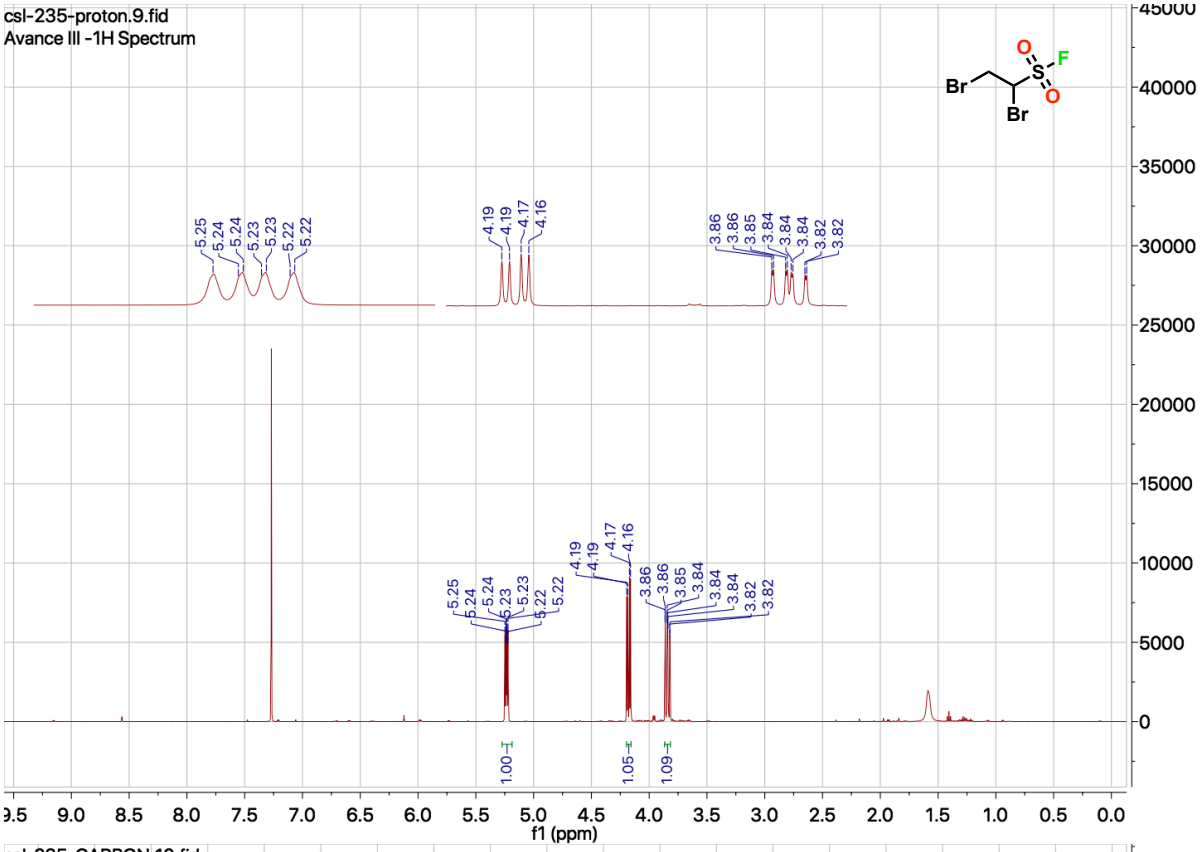
NMR Spectra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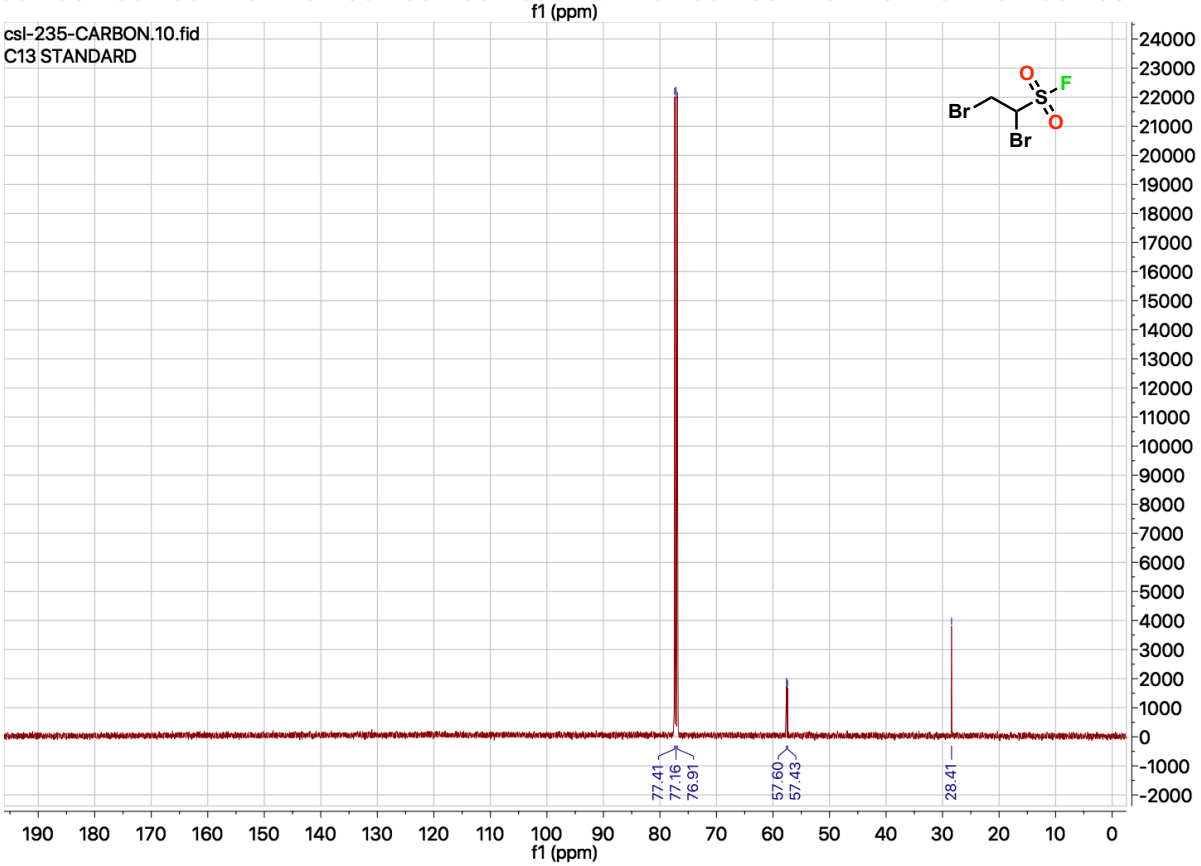
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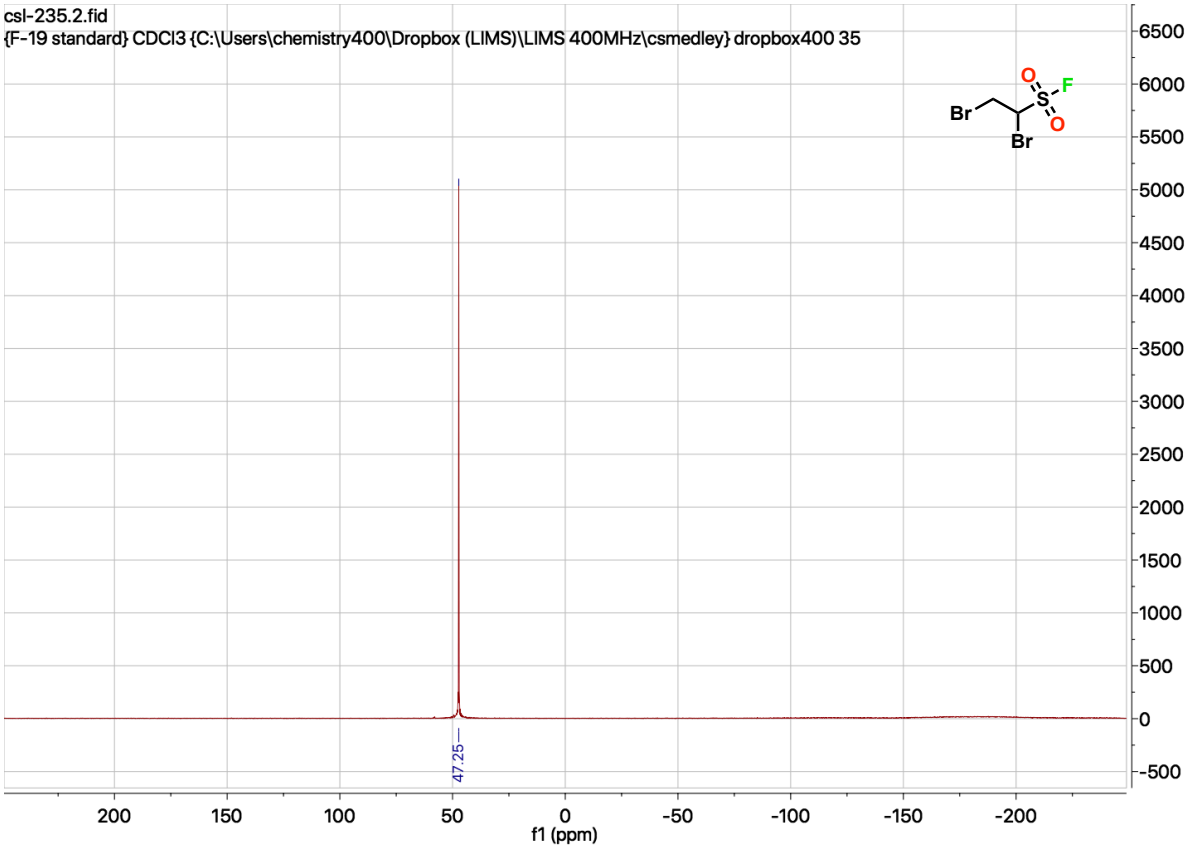
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6000
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4500
4000
3500
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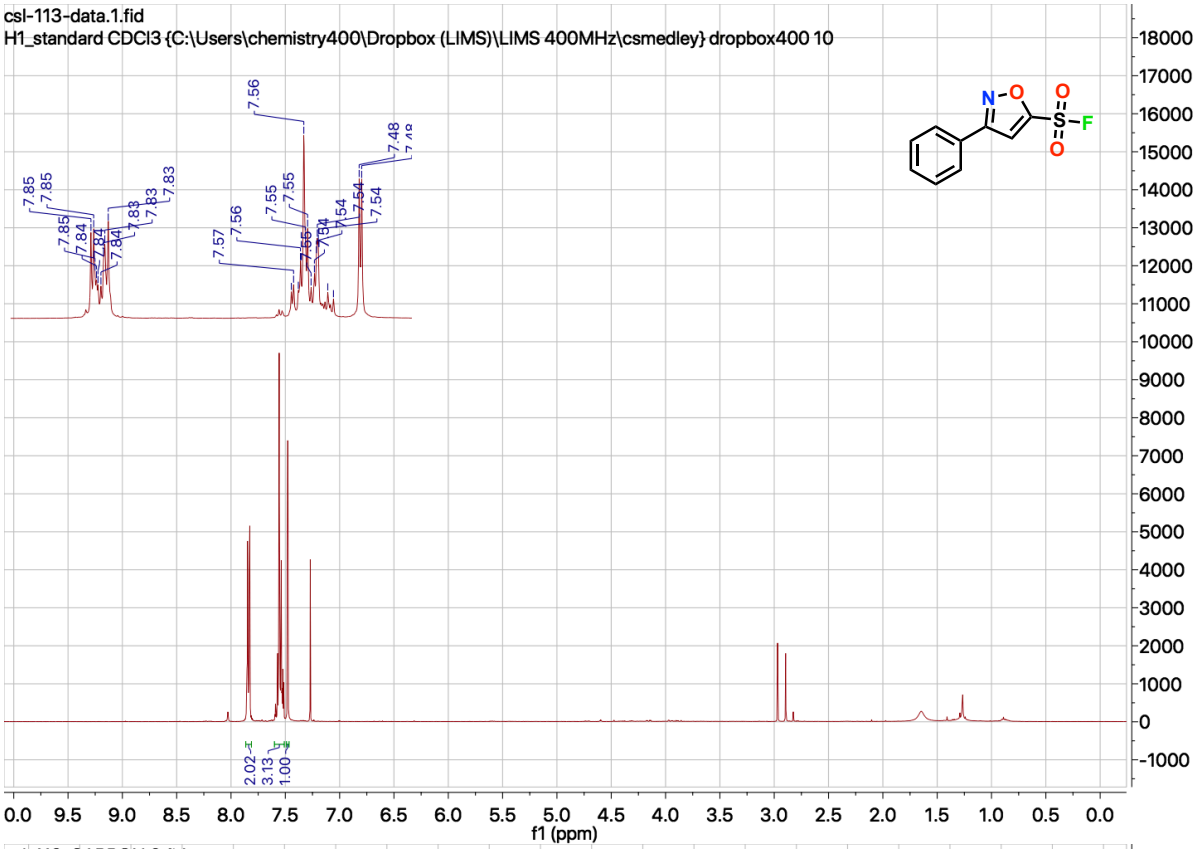
-200
f1 (ppm)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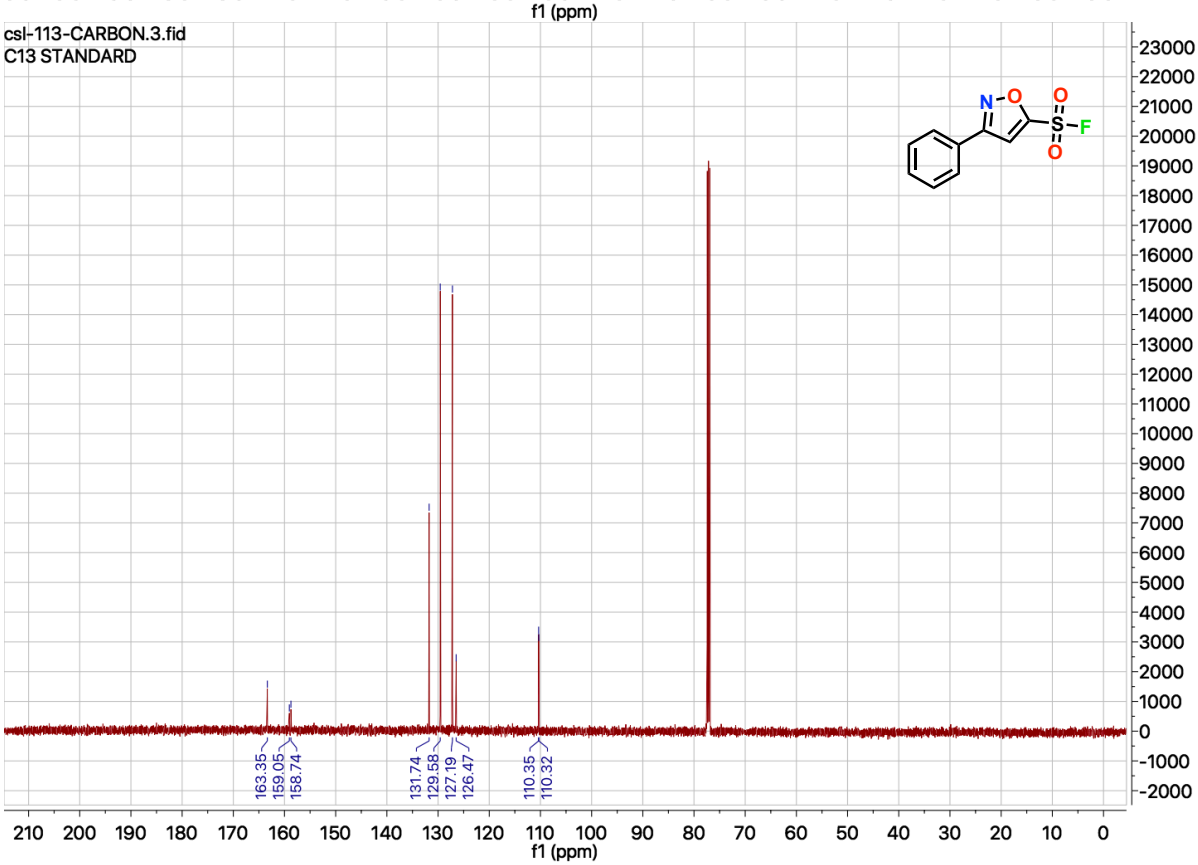
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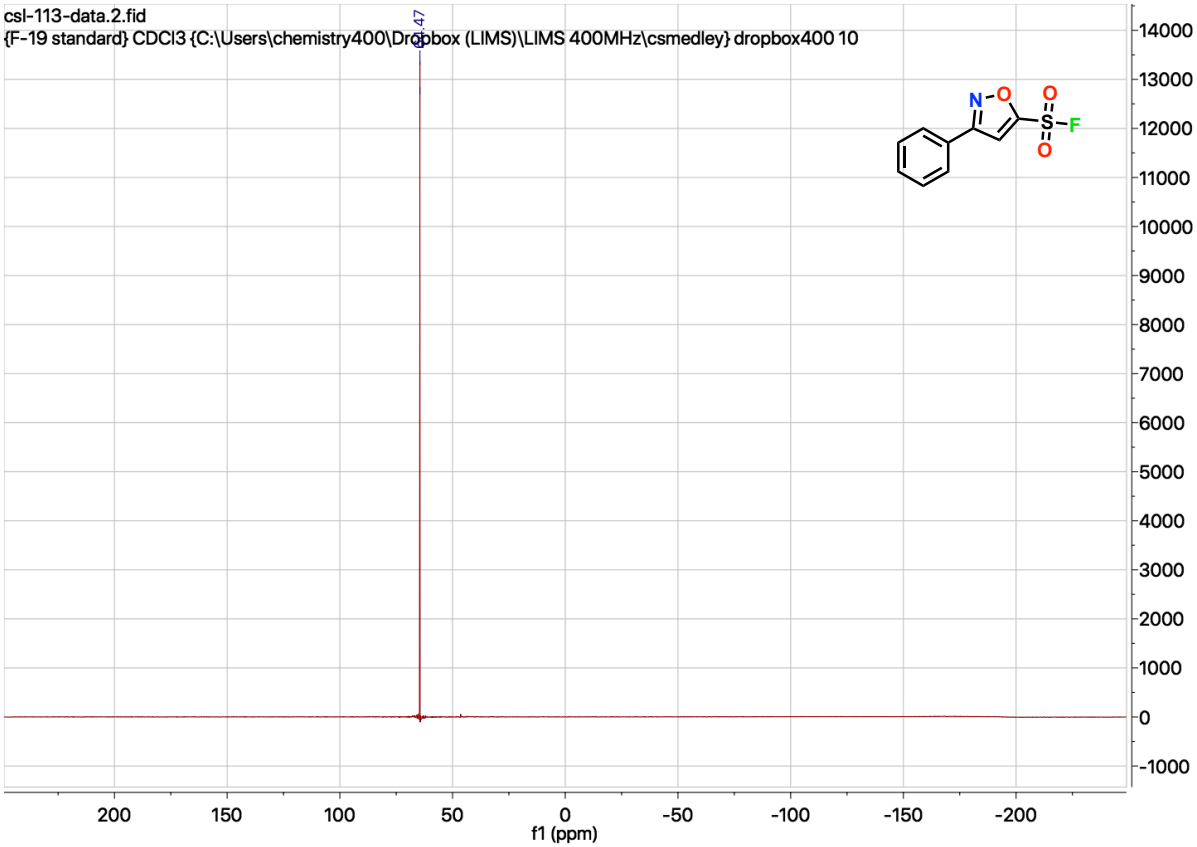
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S
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12000
11000
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9000
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7000
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-100
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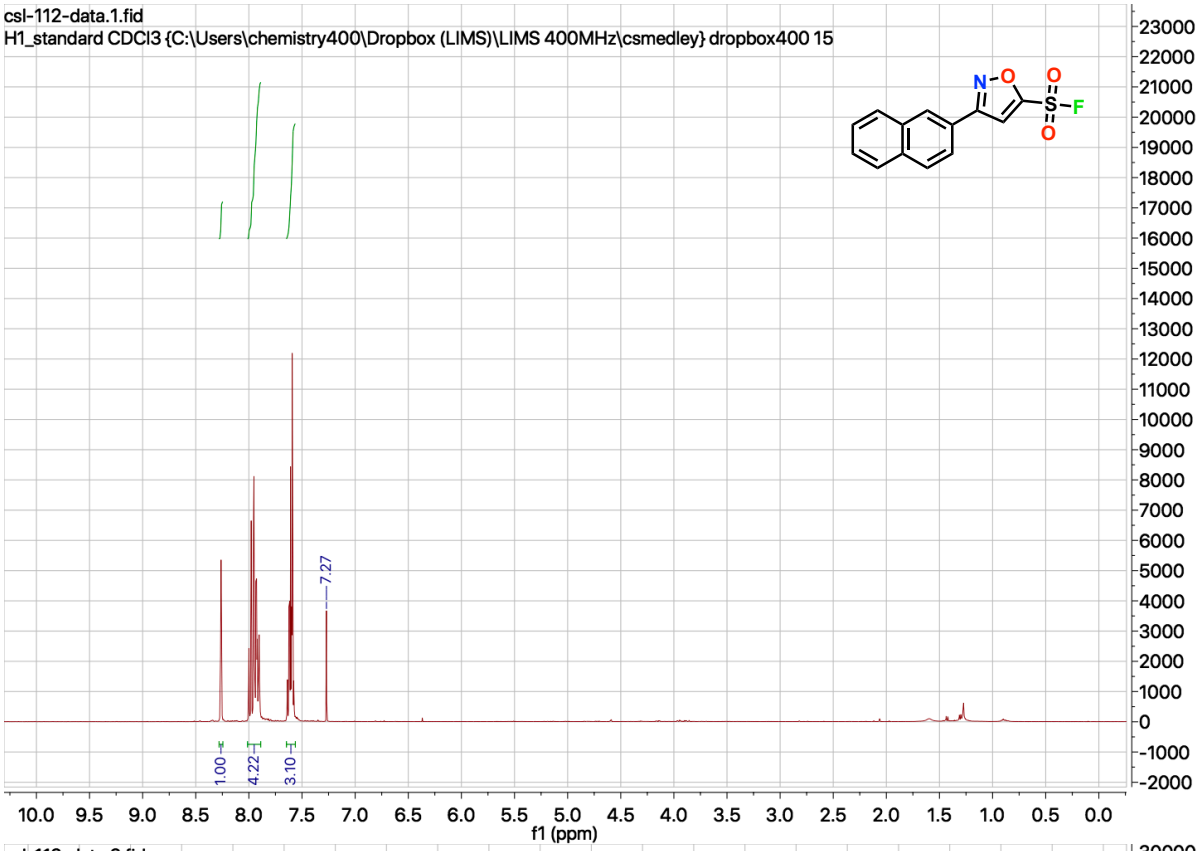
-200
f1 (ppm)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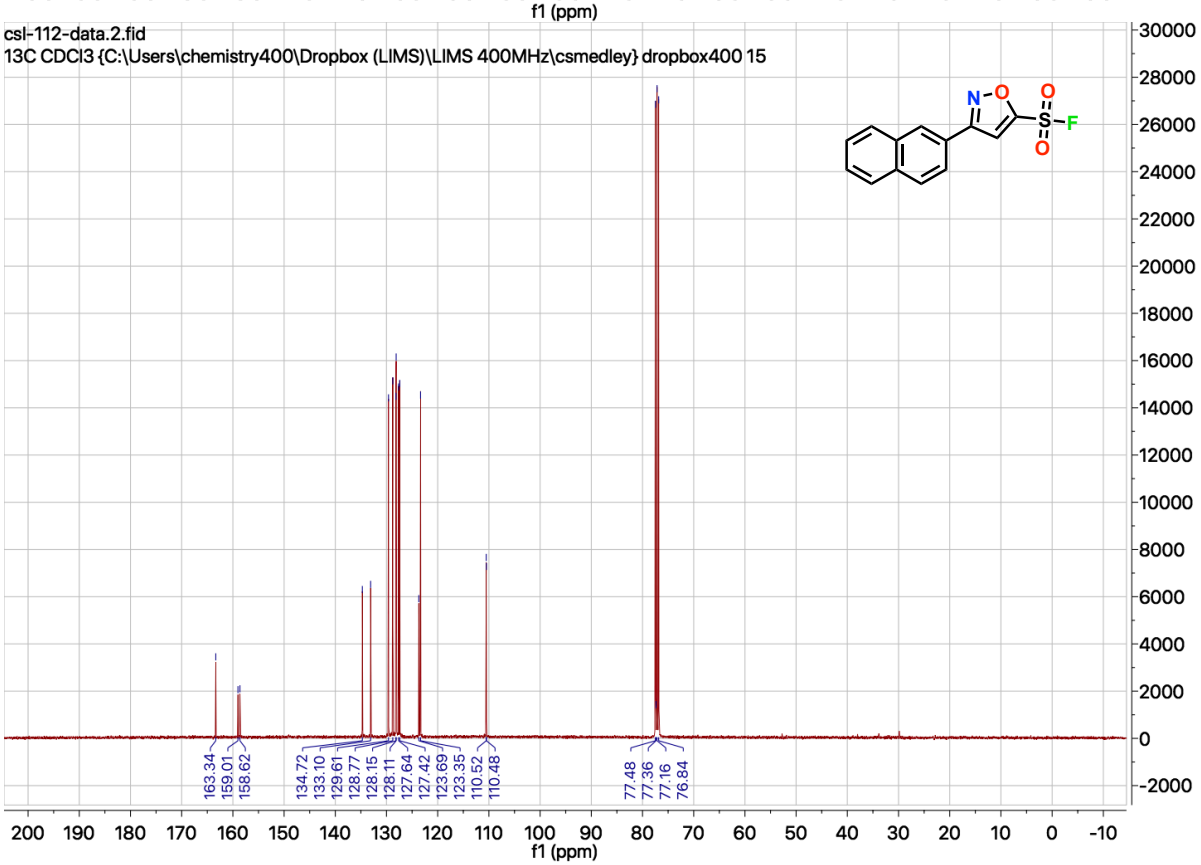
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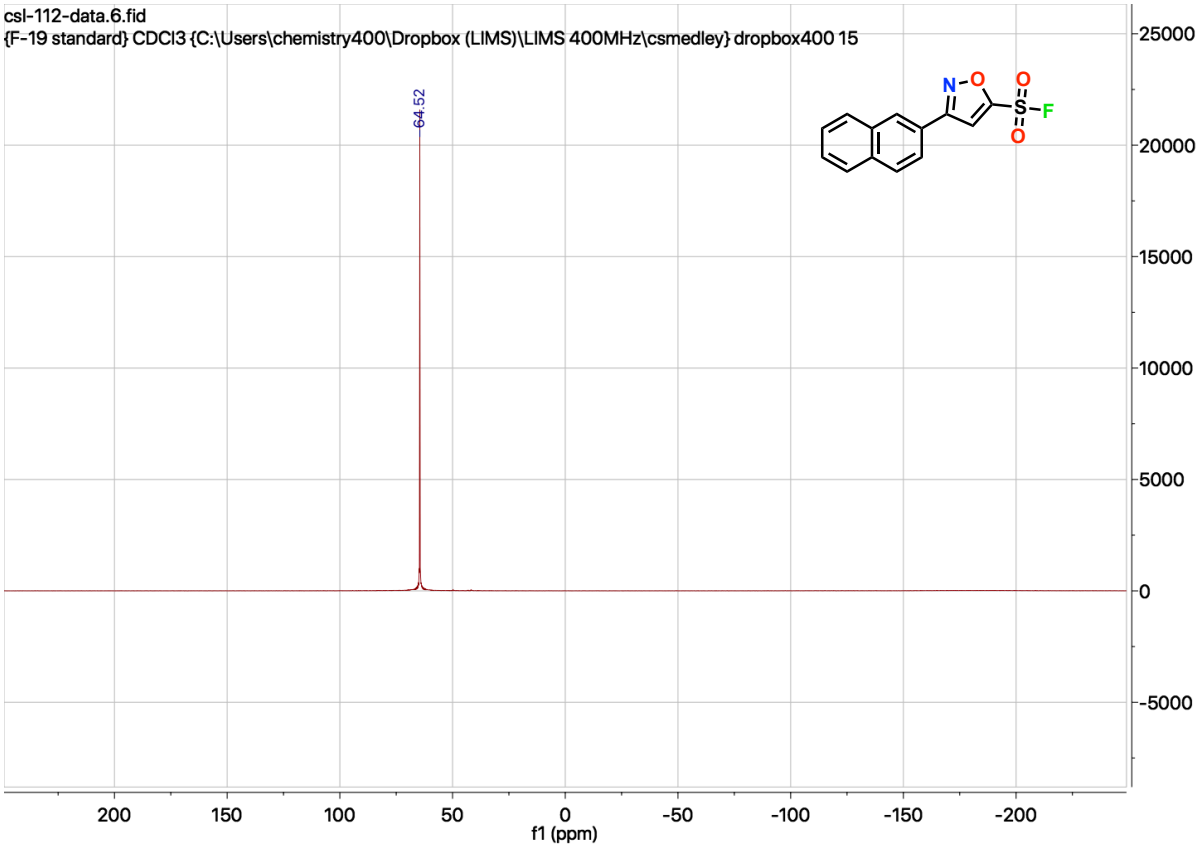
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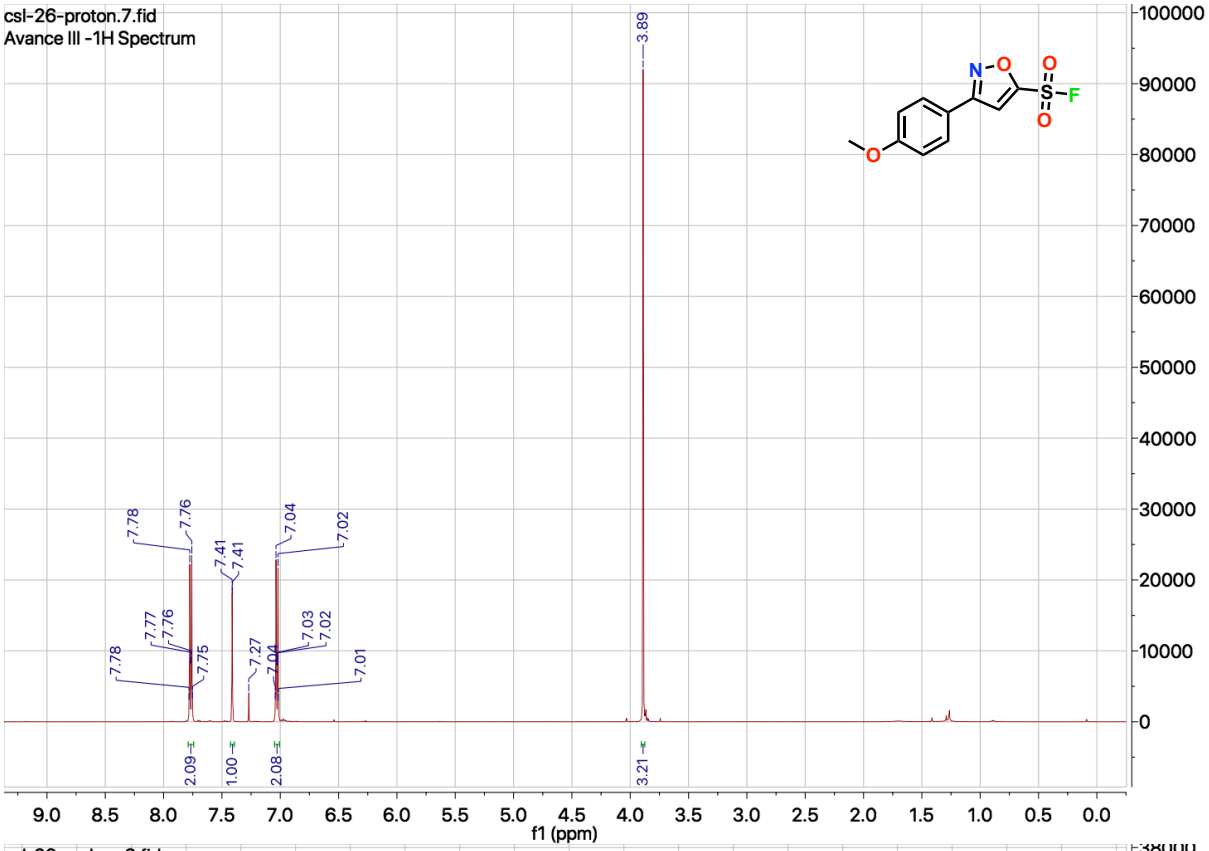
f1 (ppm)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1.00
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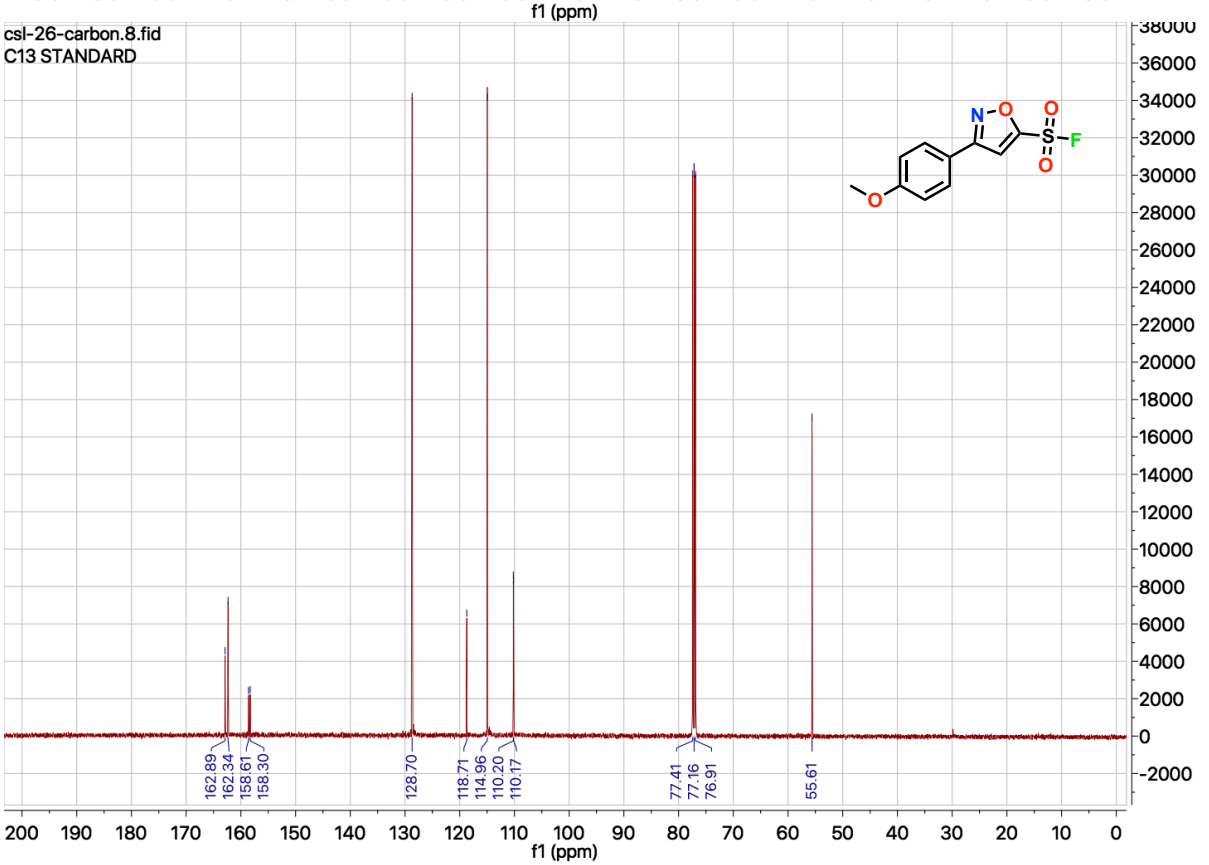
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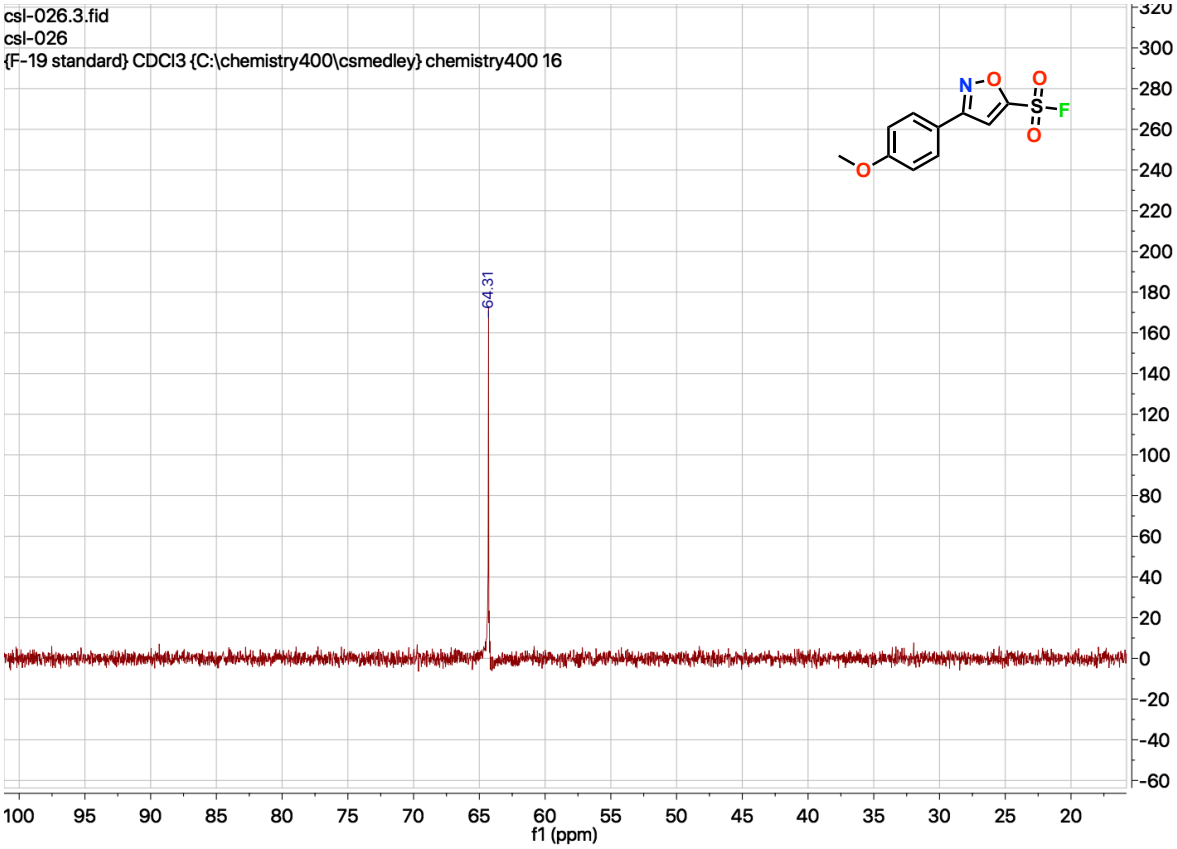
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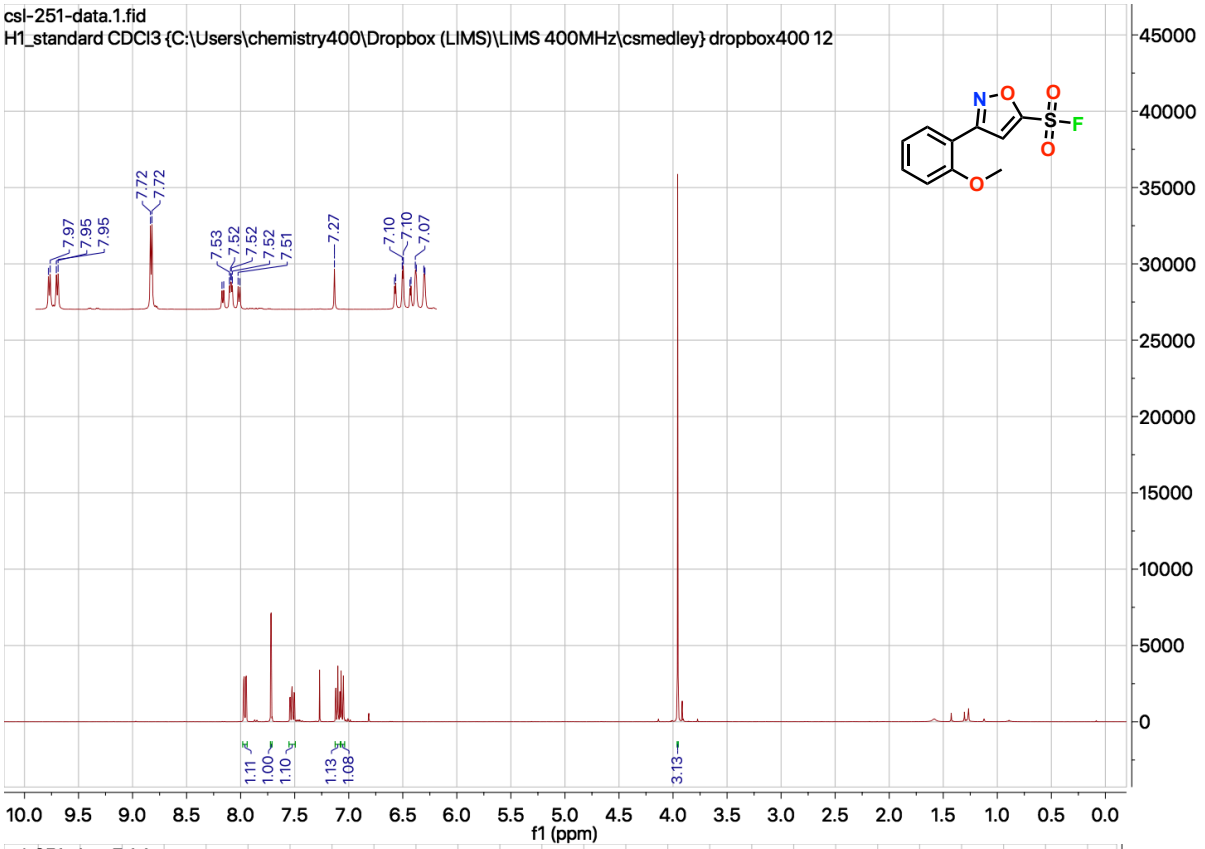
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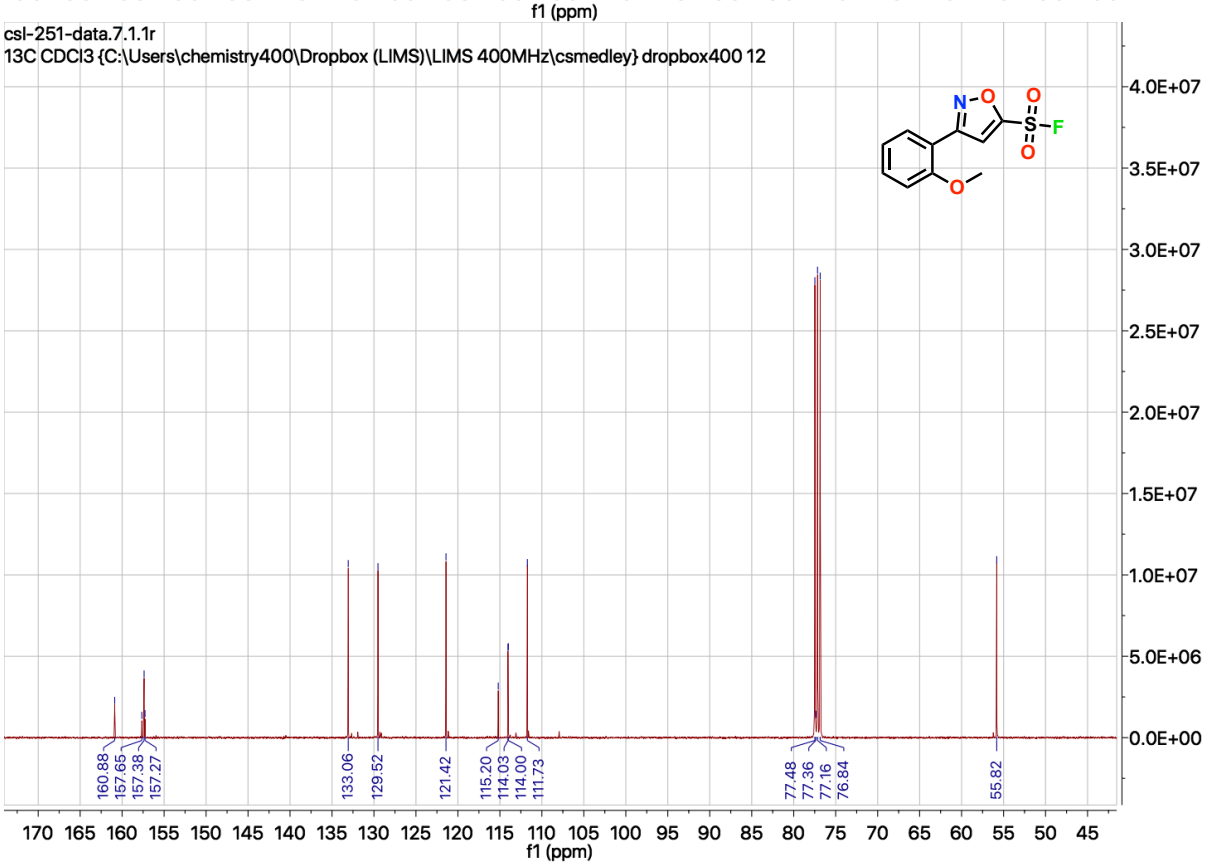
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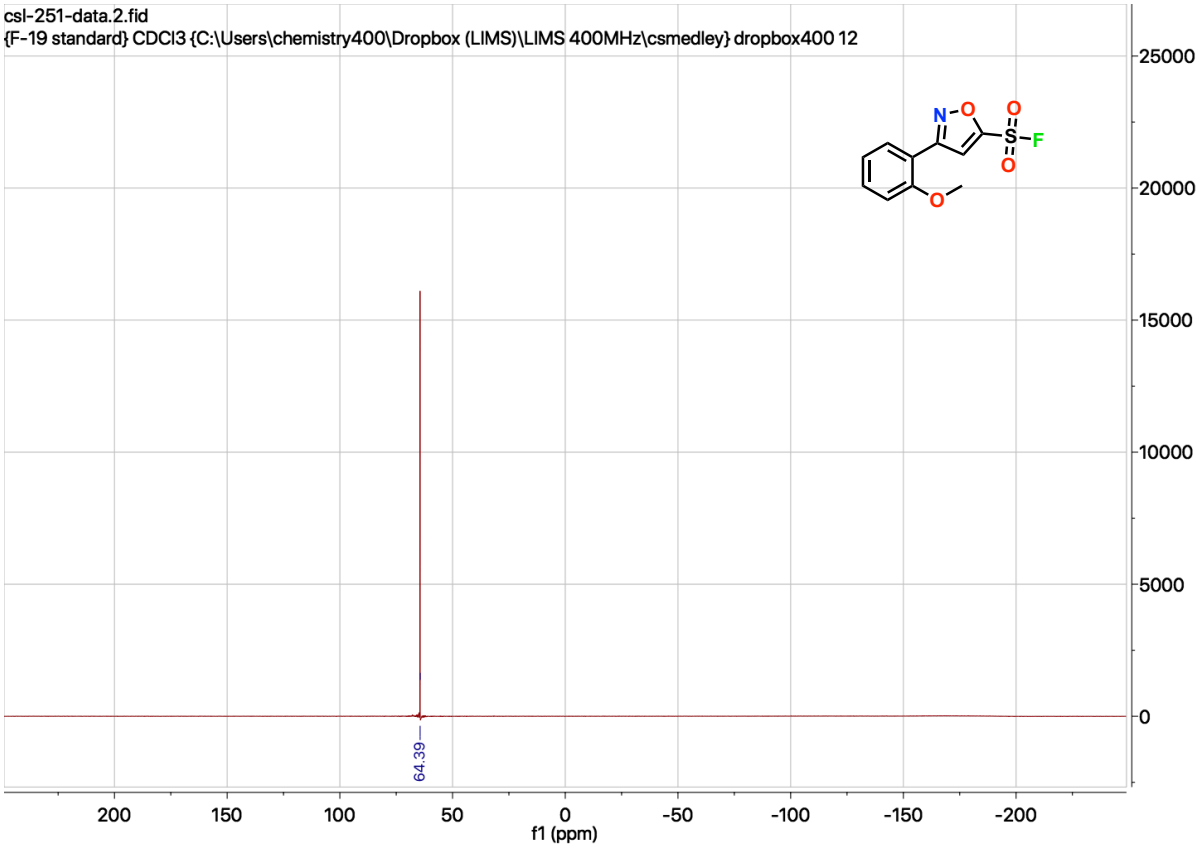
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50
0
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-100
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f1 (ppm)
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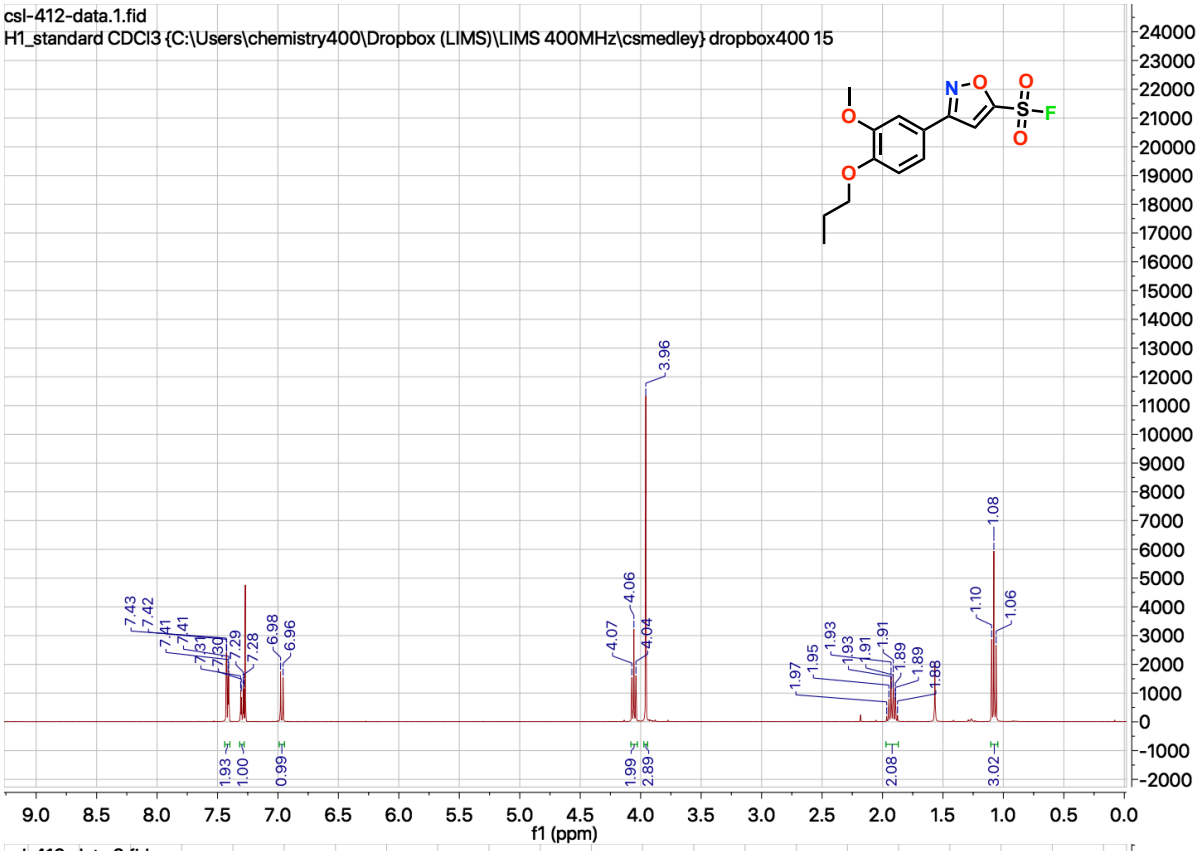
O
O
S
F
O
O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1.95
1.93
1.93
1.91
1.91
1.89
1.89
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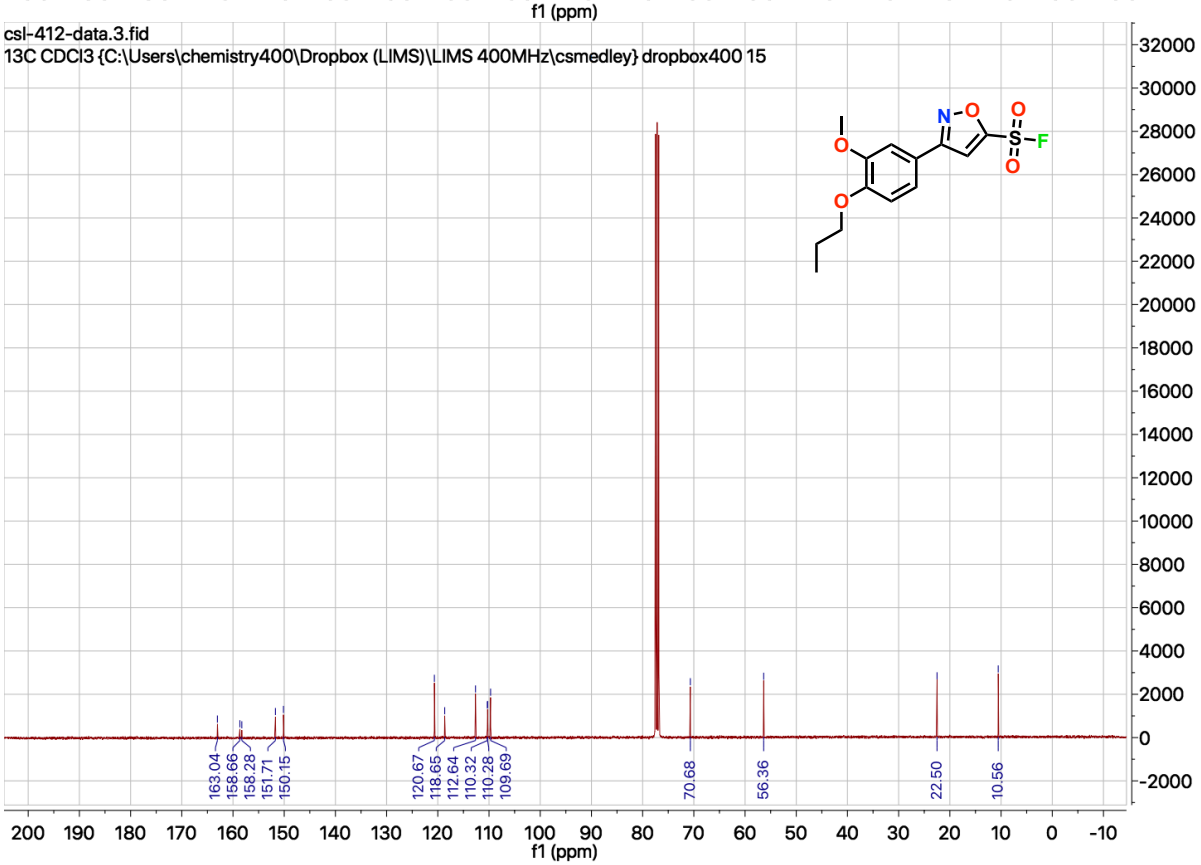
f1 (ppm)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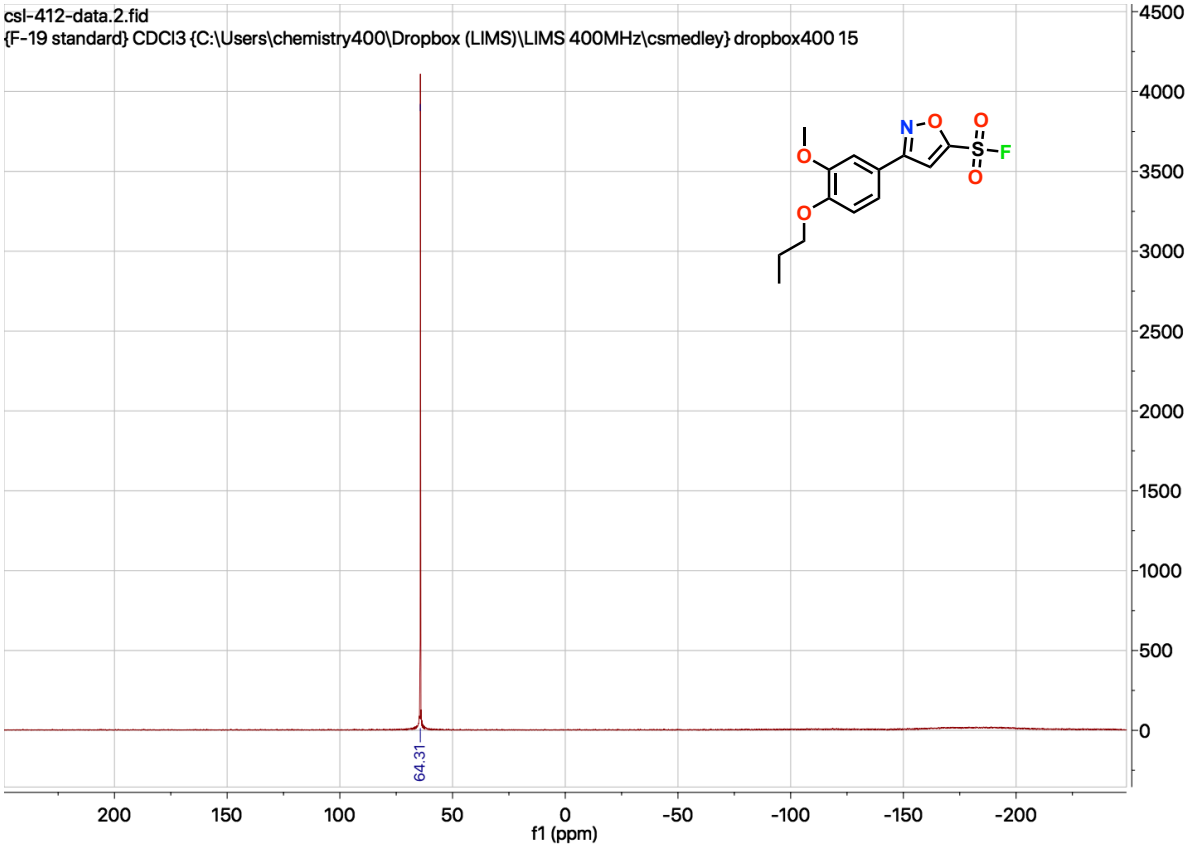
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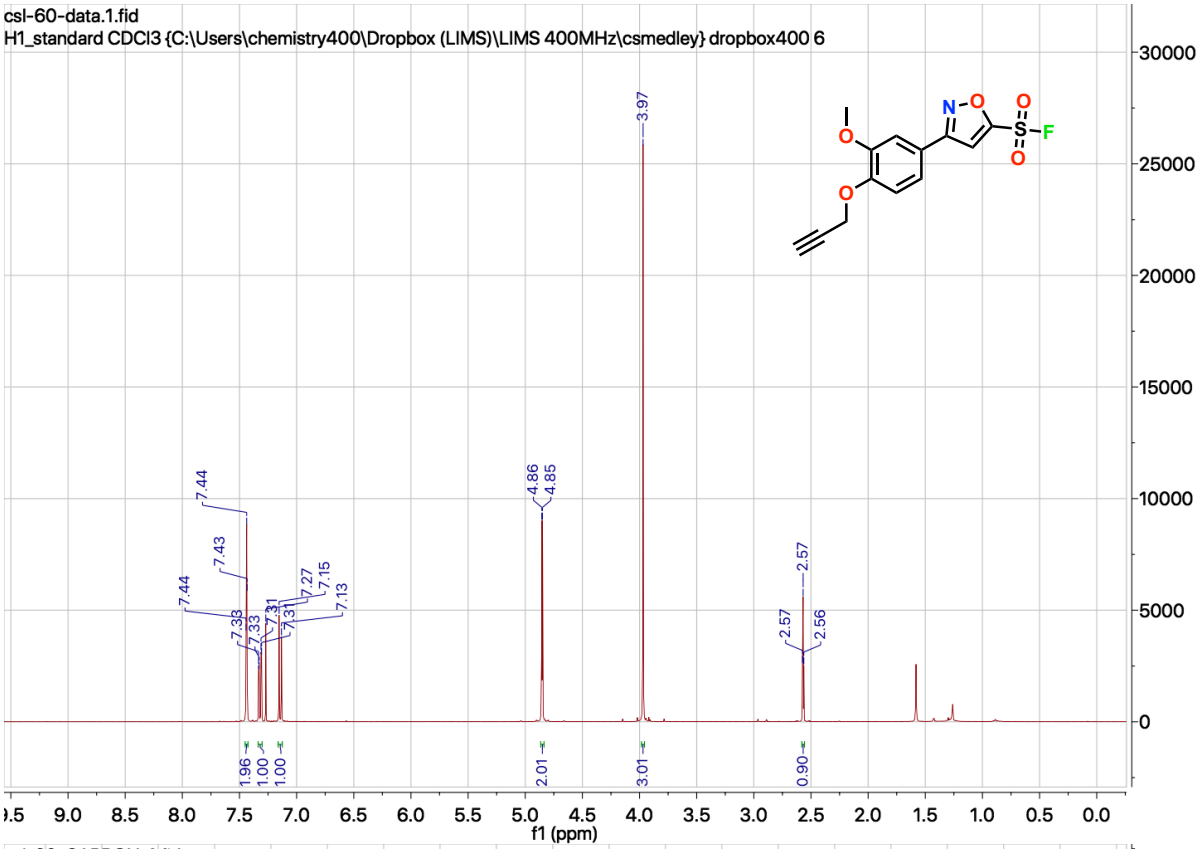
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7.31
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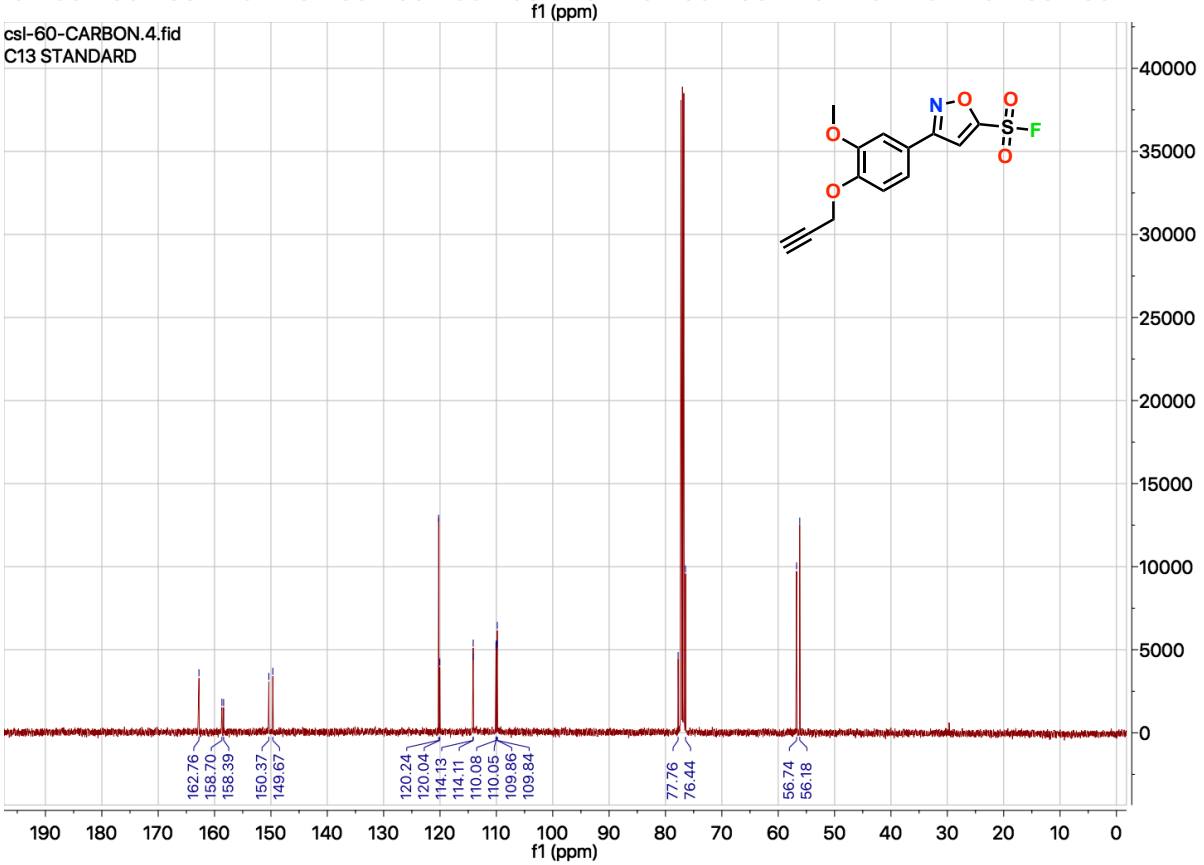
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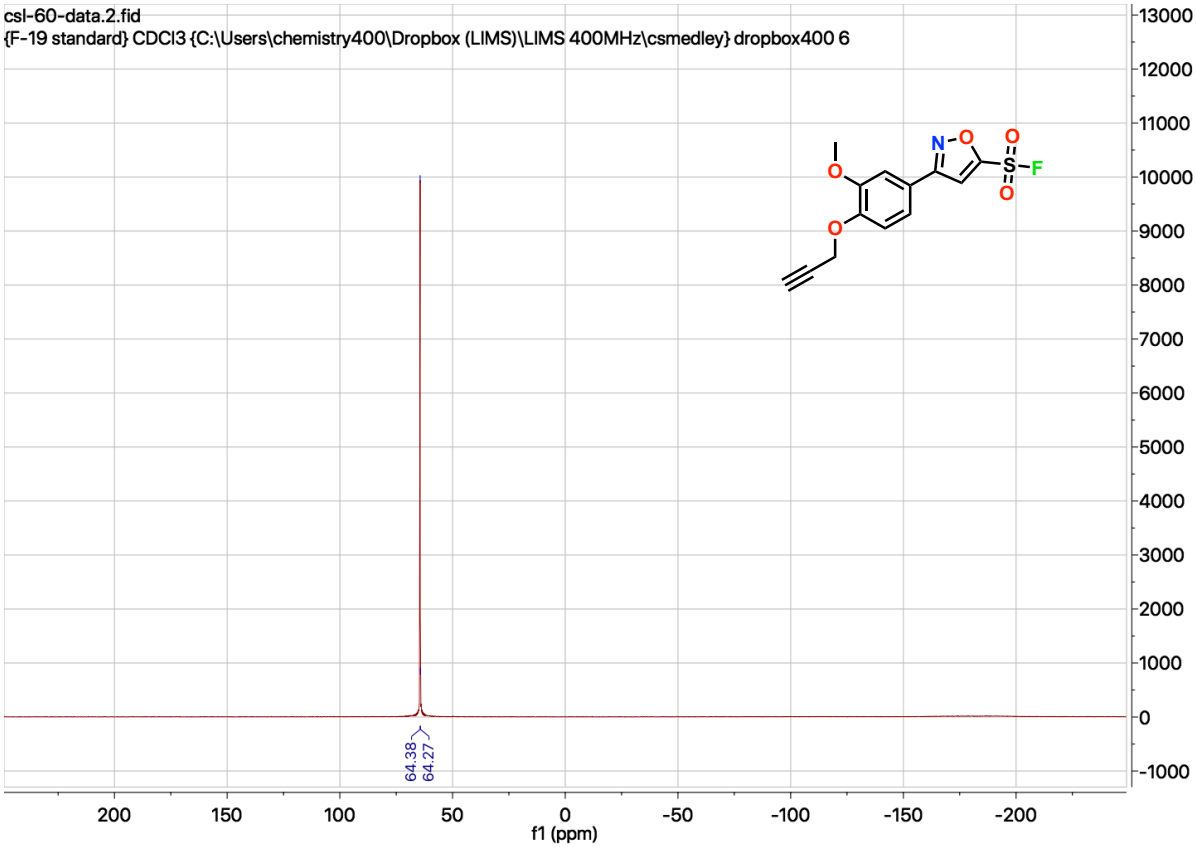
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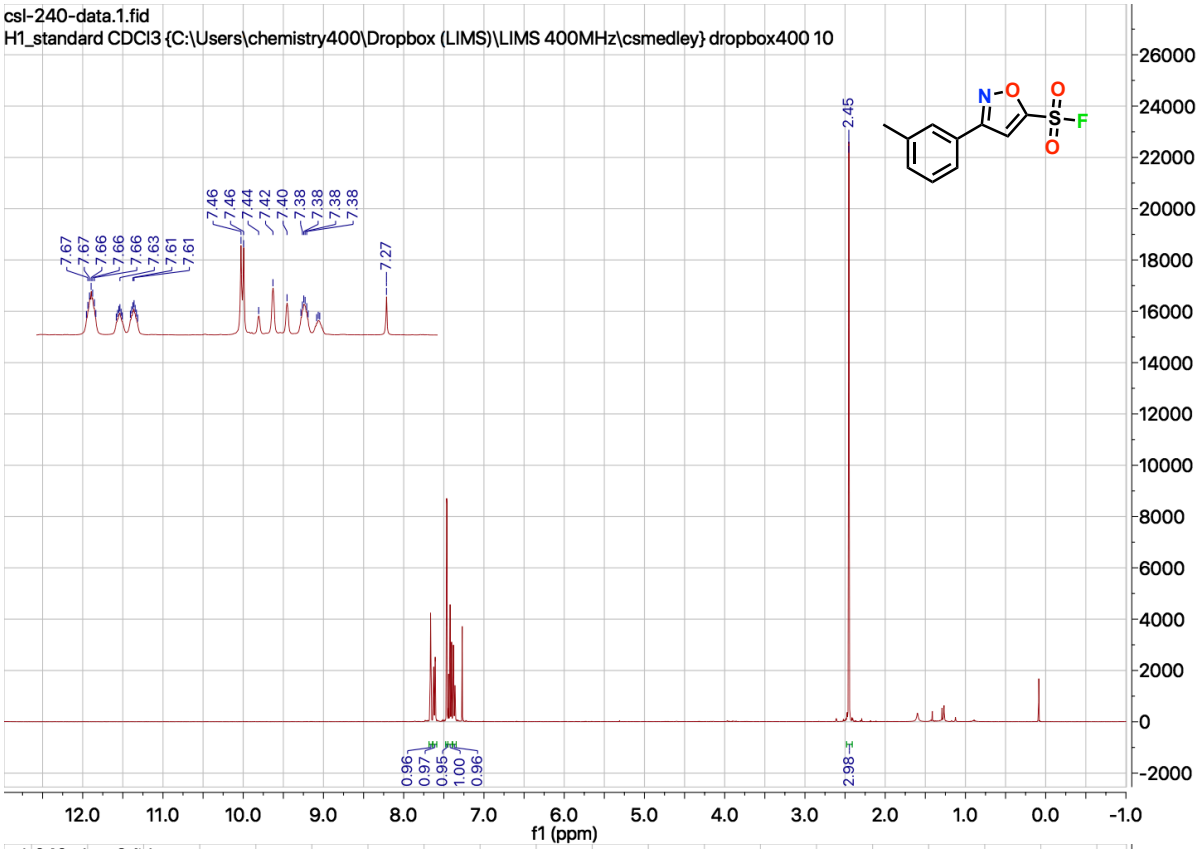
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7.44
7.42
7.40
7.38
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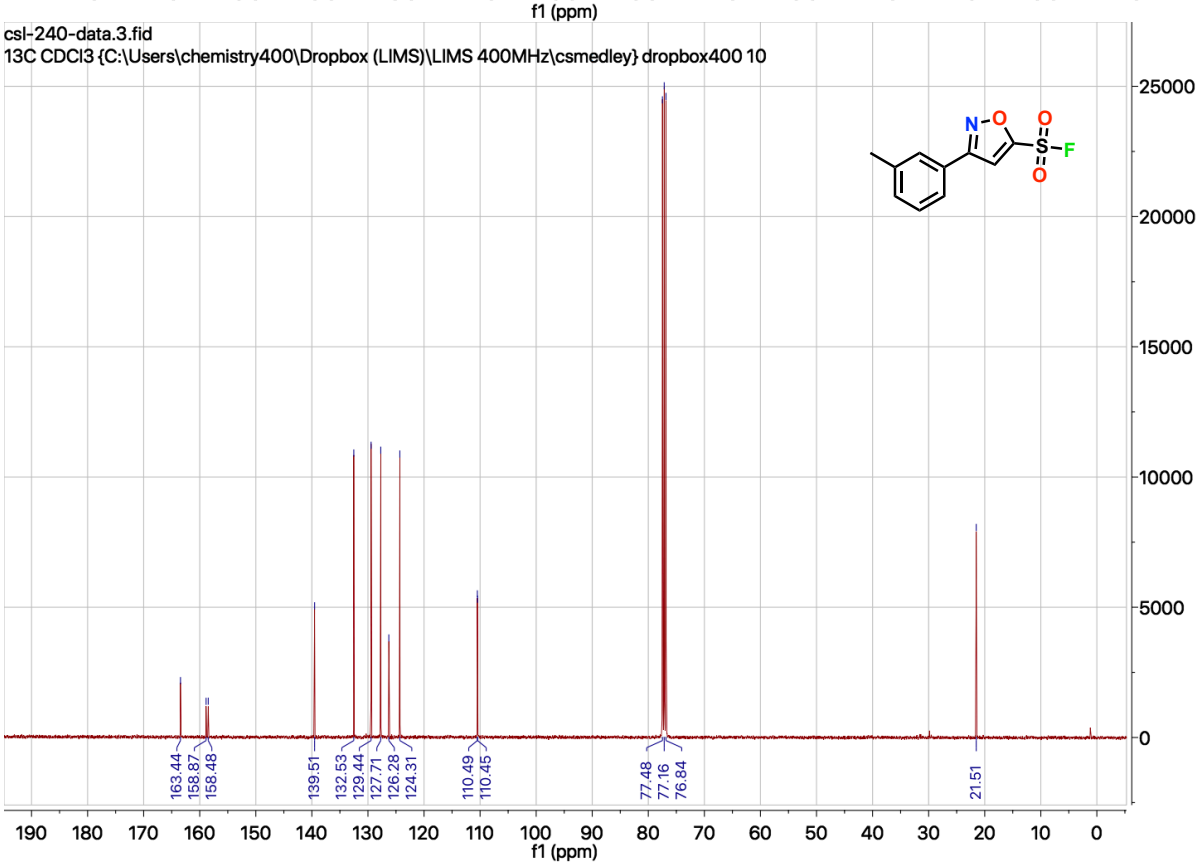
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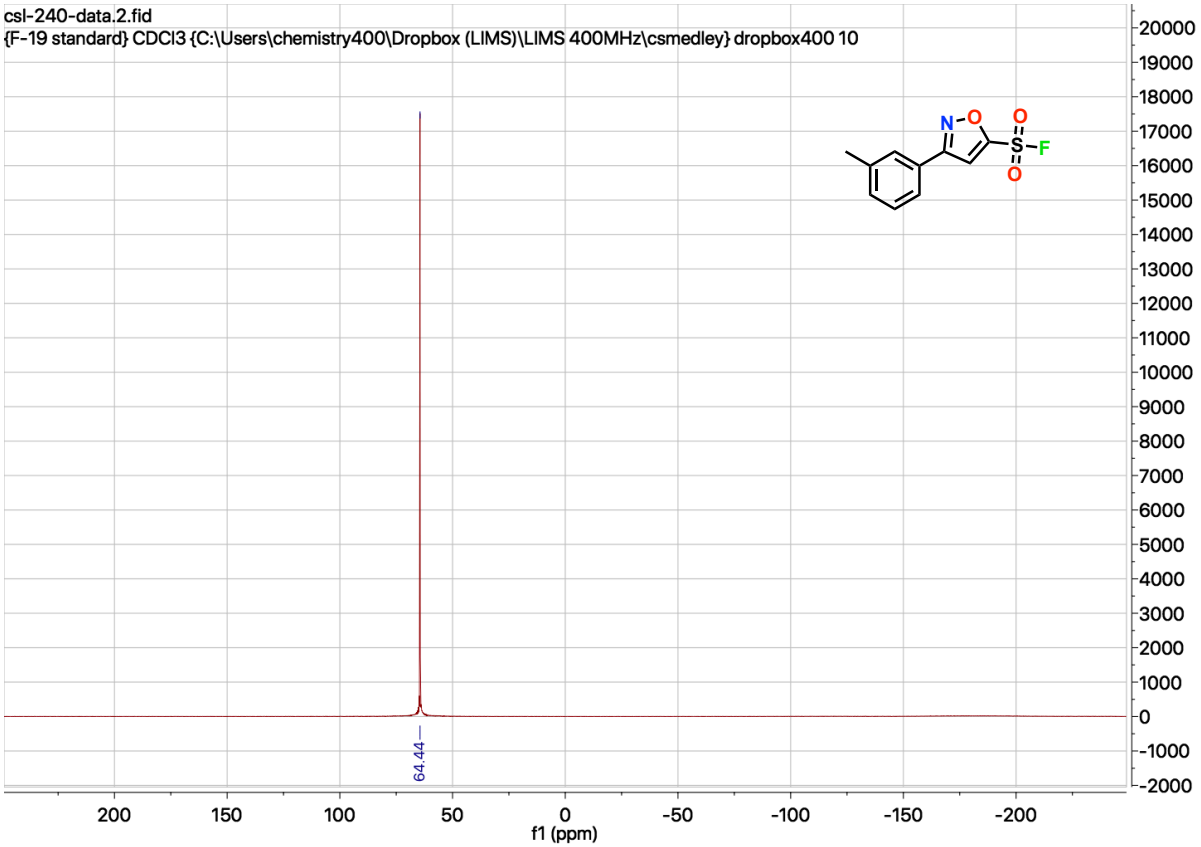
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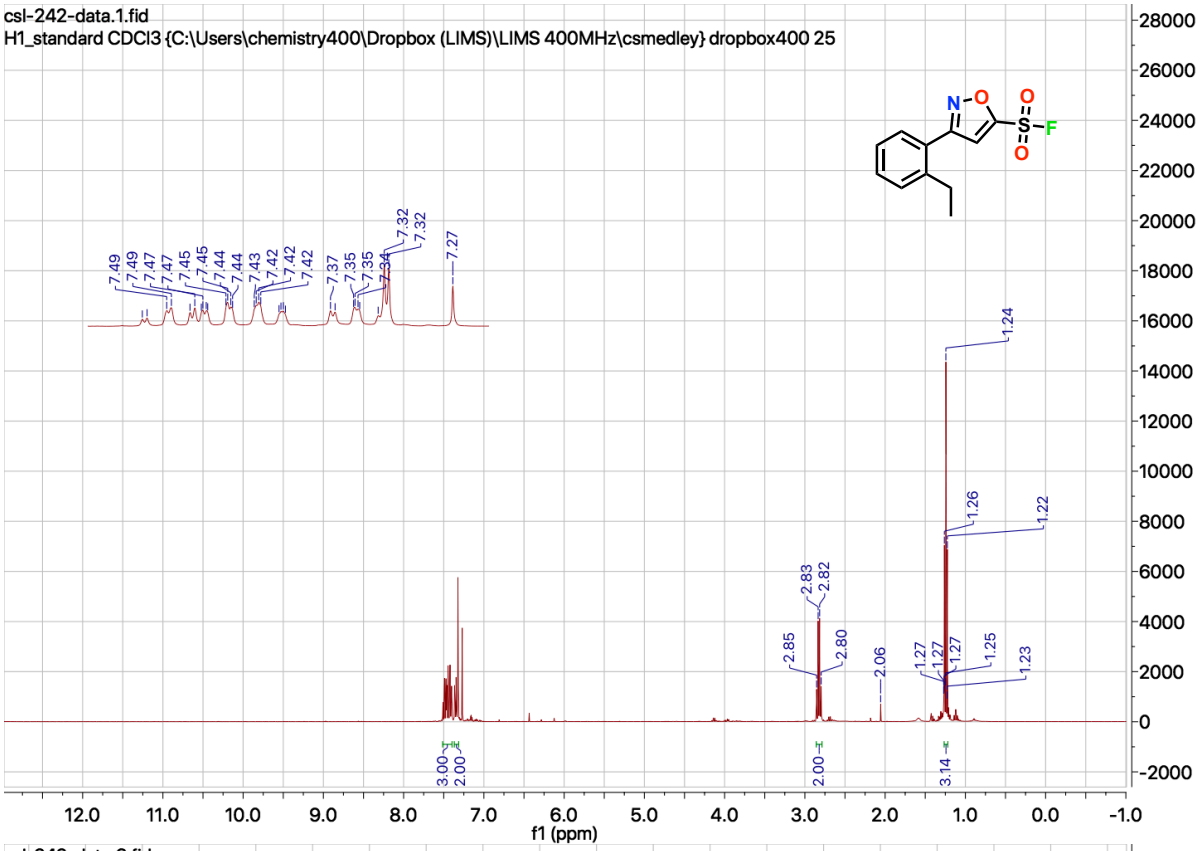
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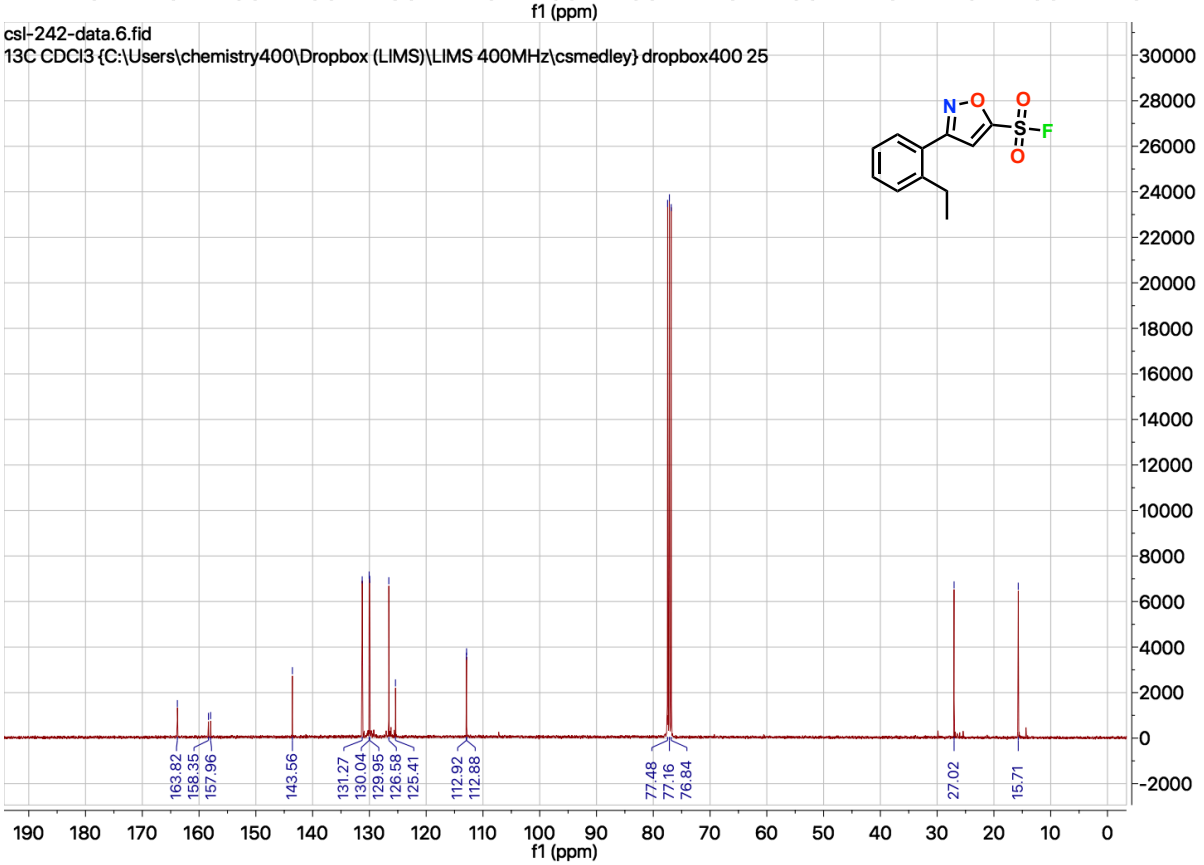
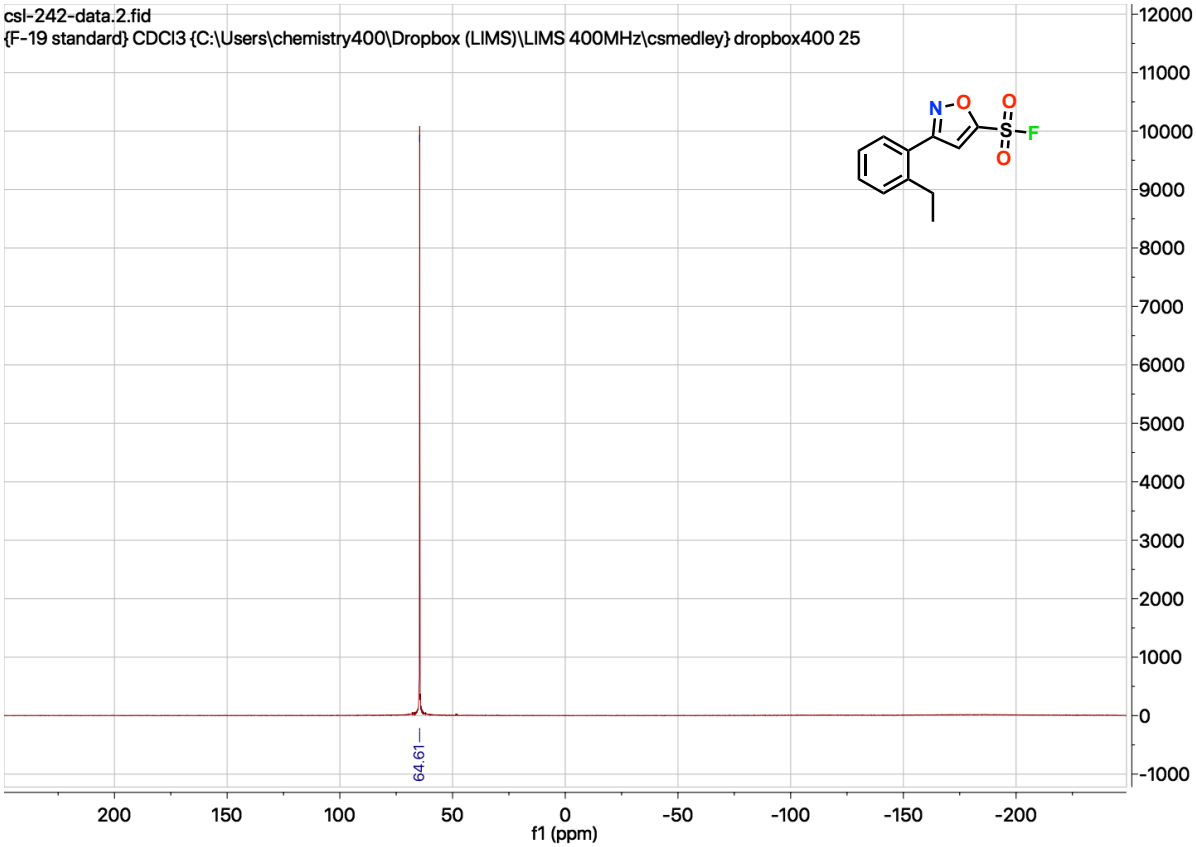
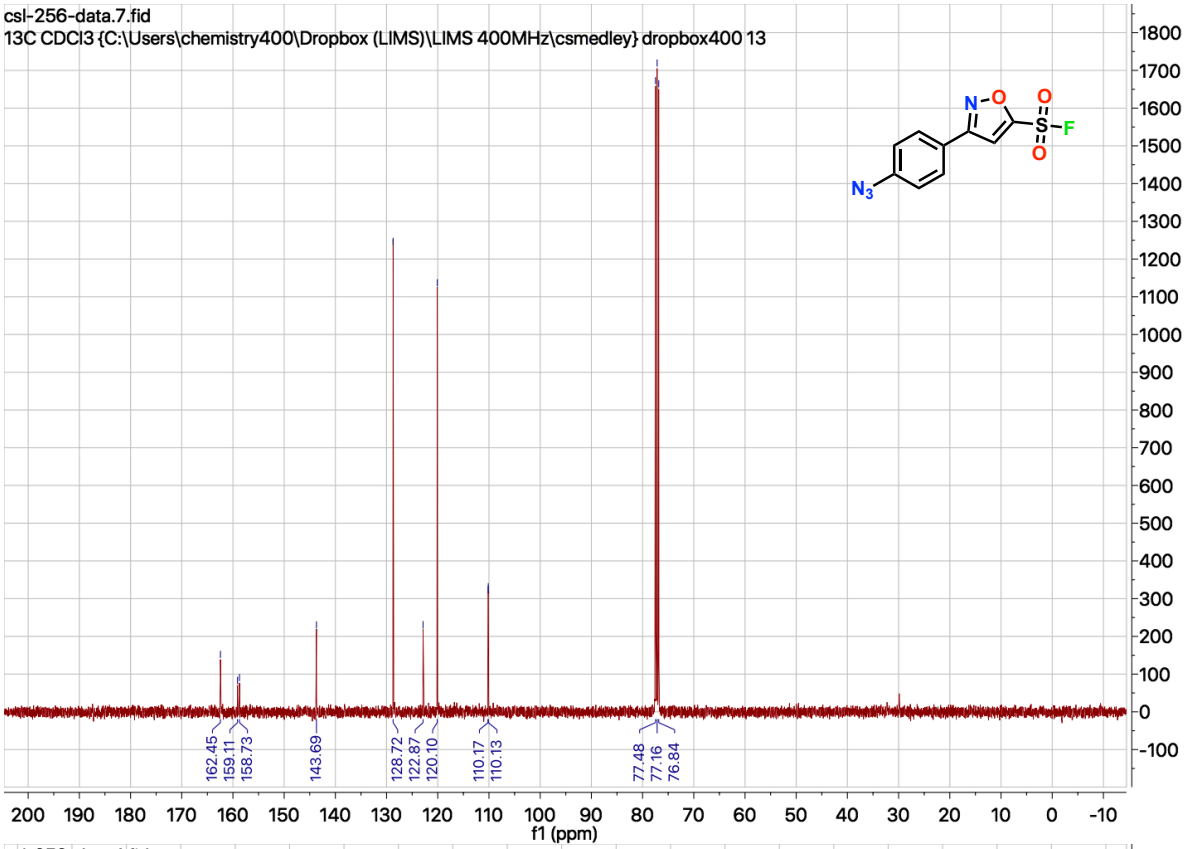
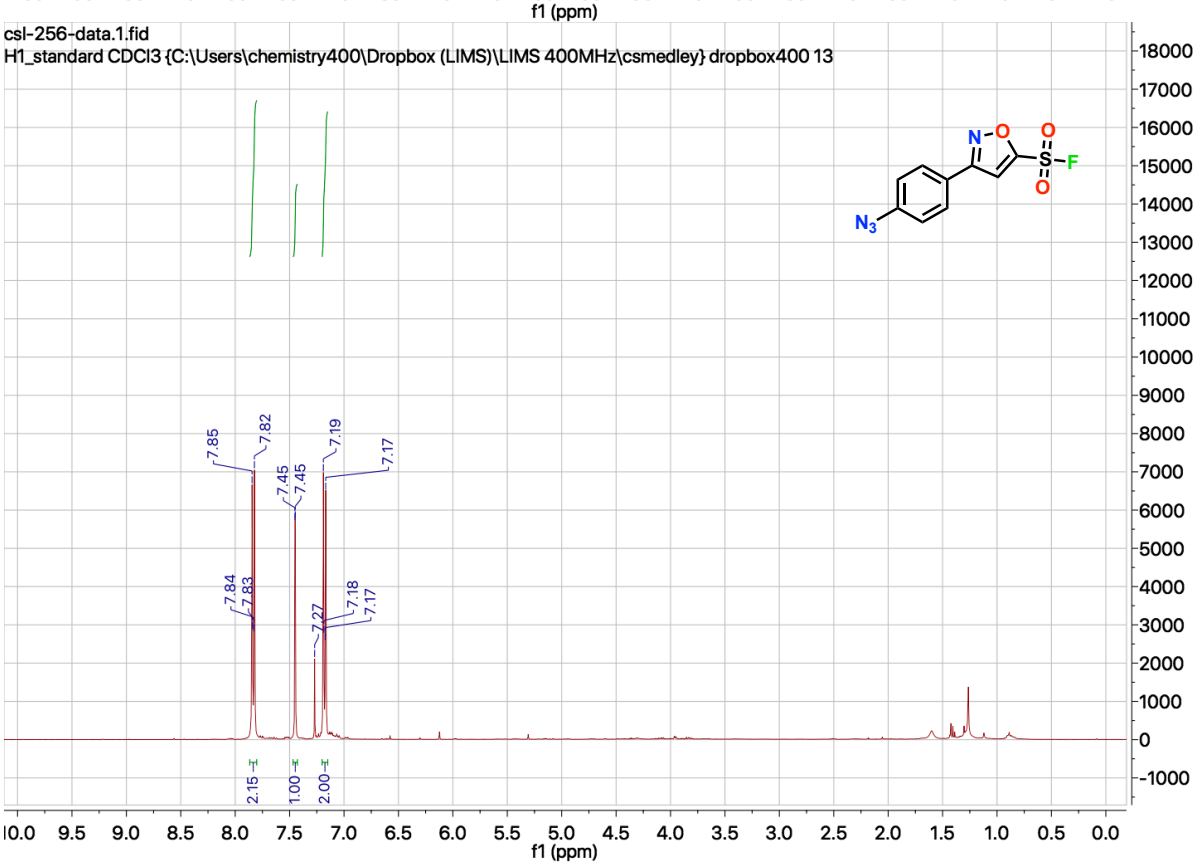
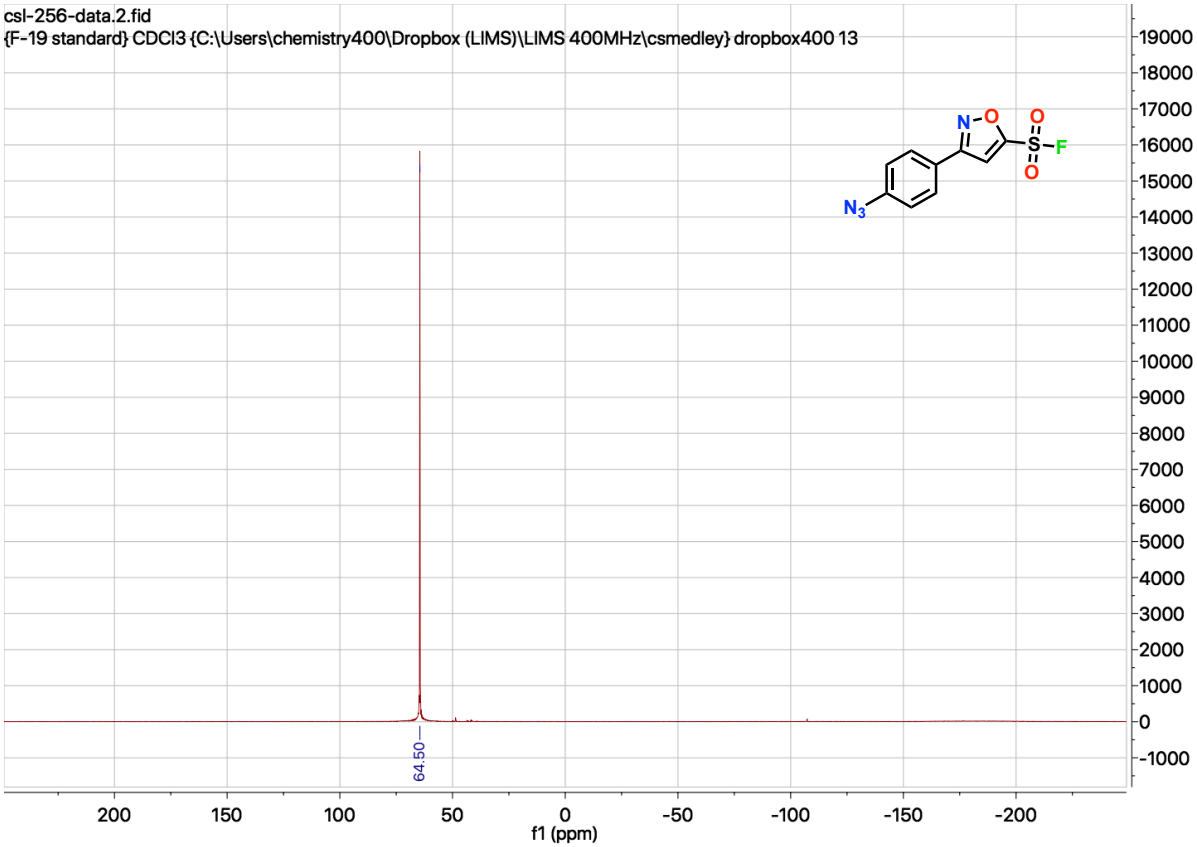
7.49
7.49
7.47
7.47
7.45
7.45
7.44
7.44
7.43
7.42
7.42
7.42
7.37
7.35
7.35
7.34
7.32
7.32
7.27
2.85
2.83
2.82
2.80
2.06
1.27
1.27
1.27
1.26
1.25
1.24
1.23
1.22
3.00
2.00
2.00
3.14
f1 (ppm)

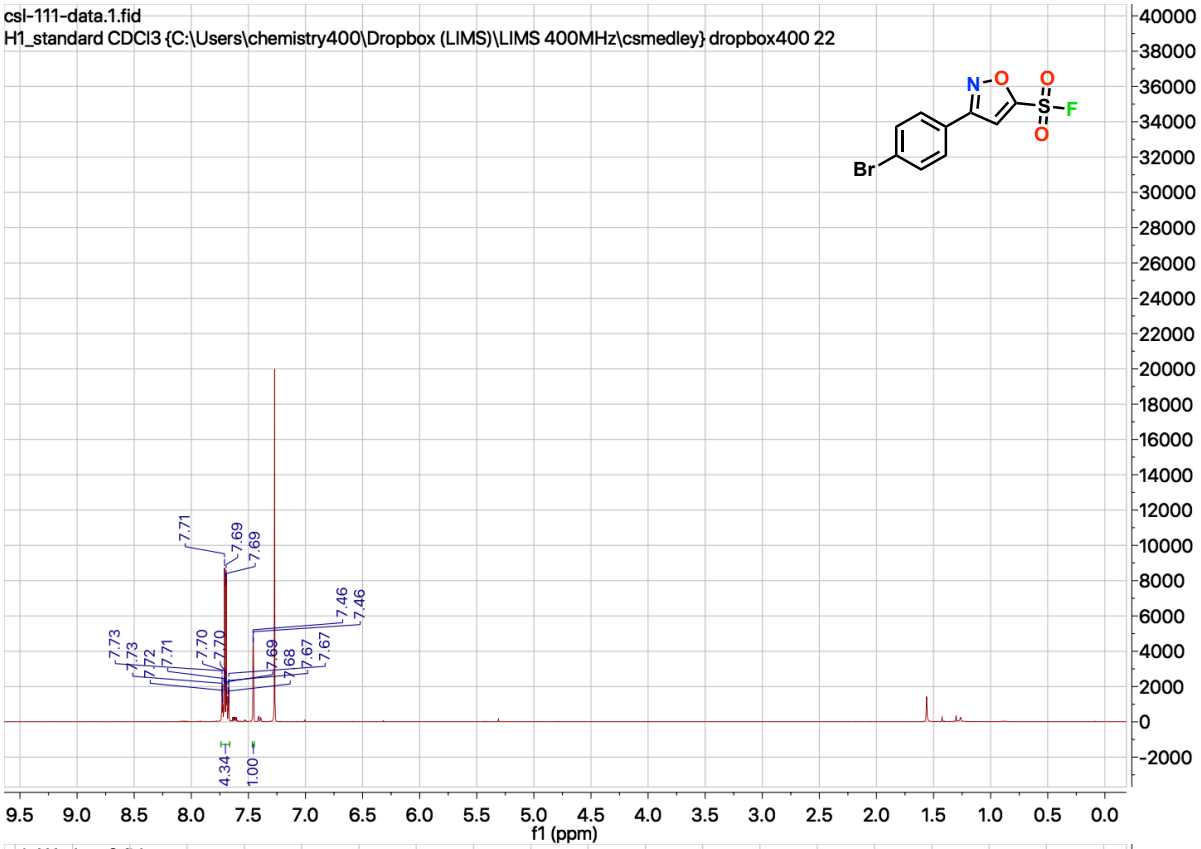

csl-242-data.6.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 25
163.82
158.35
157.96
143.56
131.27
130.04
129.95
126.58
125.41
112.92
112.88
77.48
77.16
76.84
27.02
15.71
f1 (ppm)

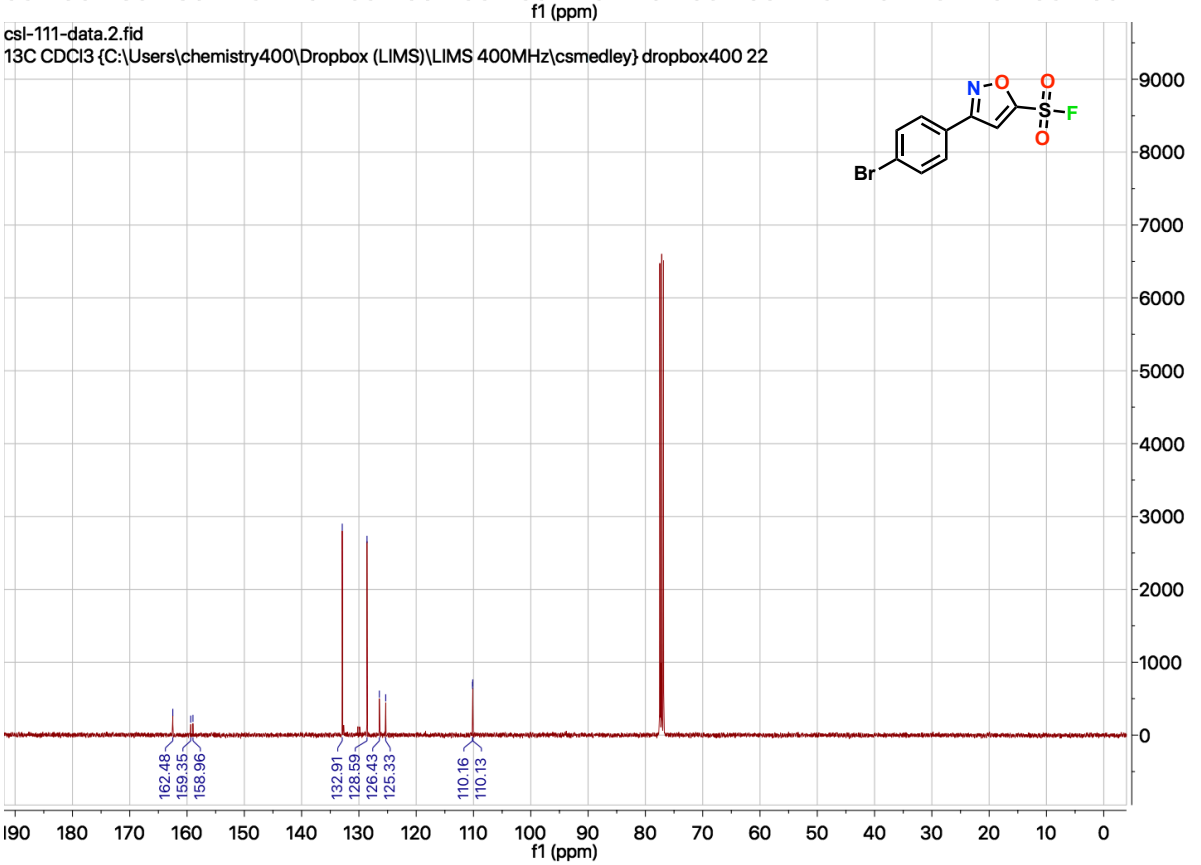

csl-242-data.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 25
64.61
f1 (ppm)

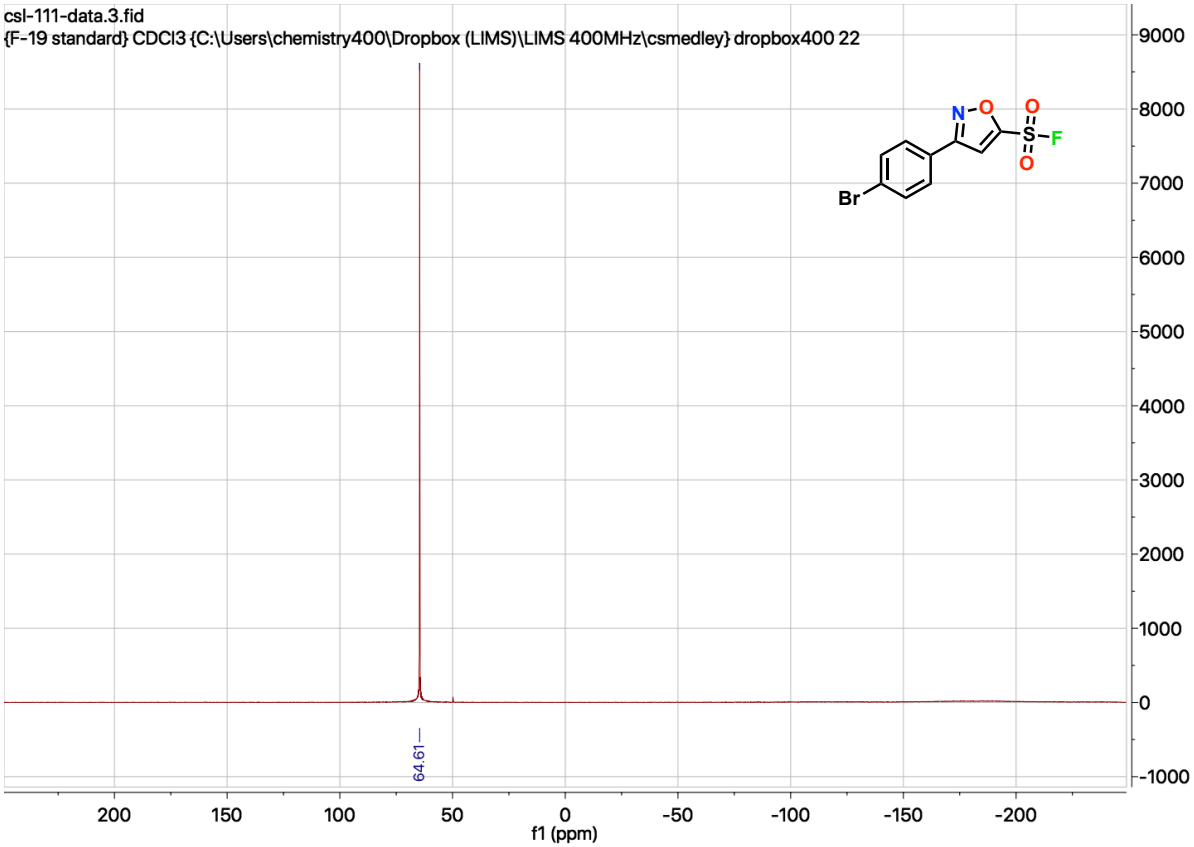

csl-256-data.7.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 13
162.45
159.11
158.73
143.69
128.72
122.87
120.10
110.17
110.13
77.48
77.16
76.84
f1 (ppm)

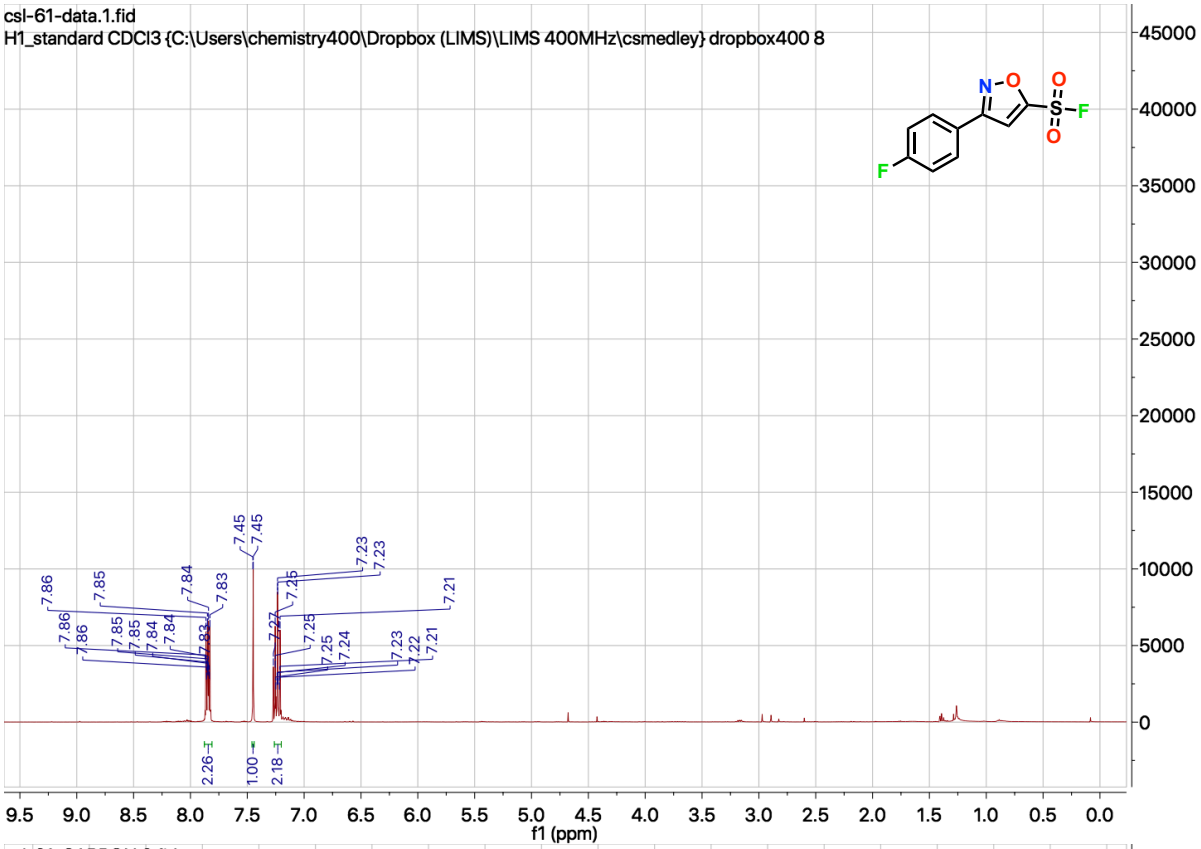

csl-256-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 13
7.85
7.82
7.45
7.45
7.19
7.17
7.84
7.83
7.27
7.18
7.17
2.15
1.00
2.00
f1 (ppm)

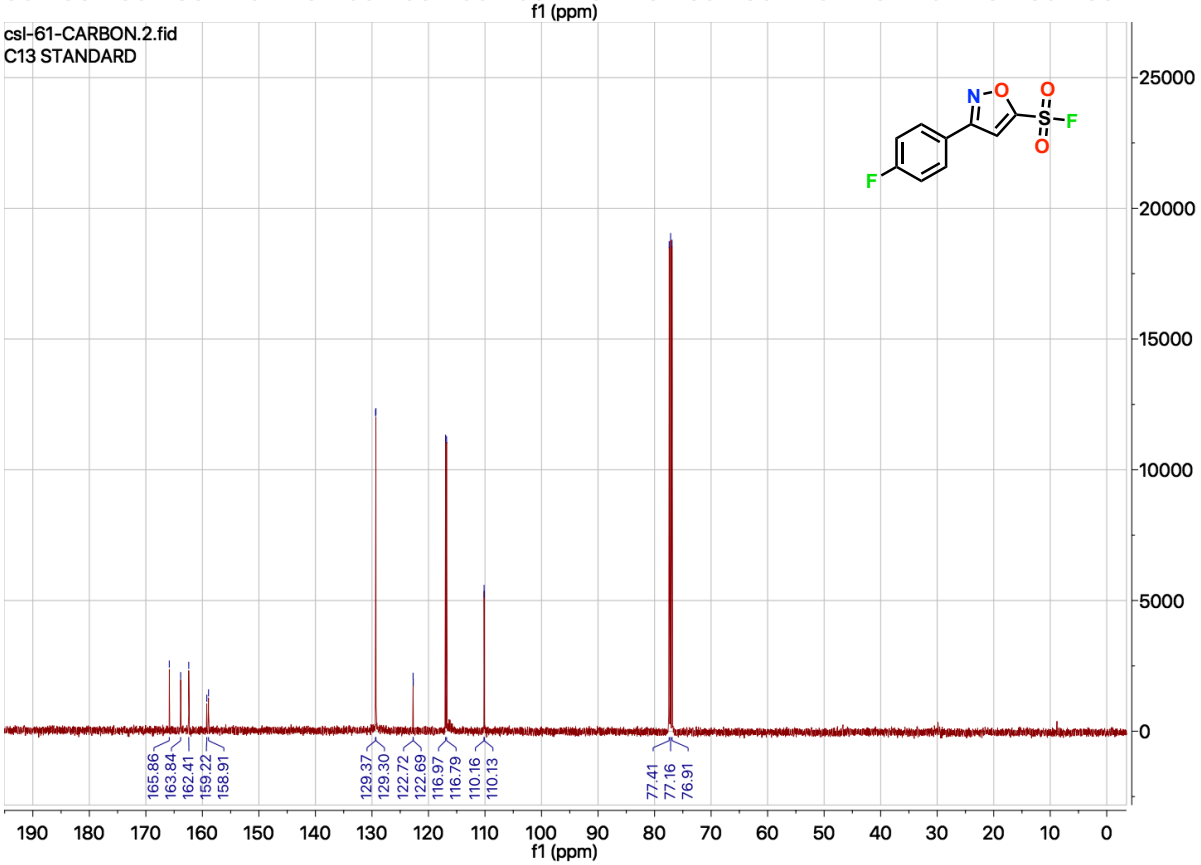

csl-256-data.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 13
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
64.50
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
N
O
O
S
F
O
N3

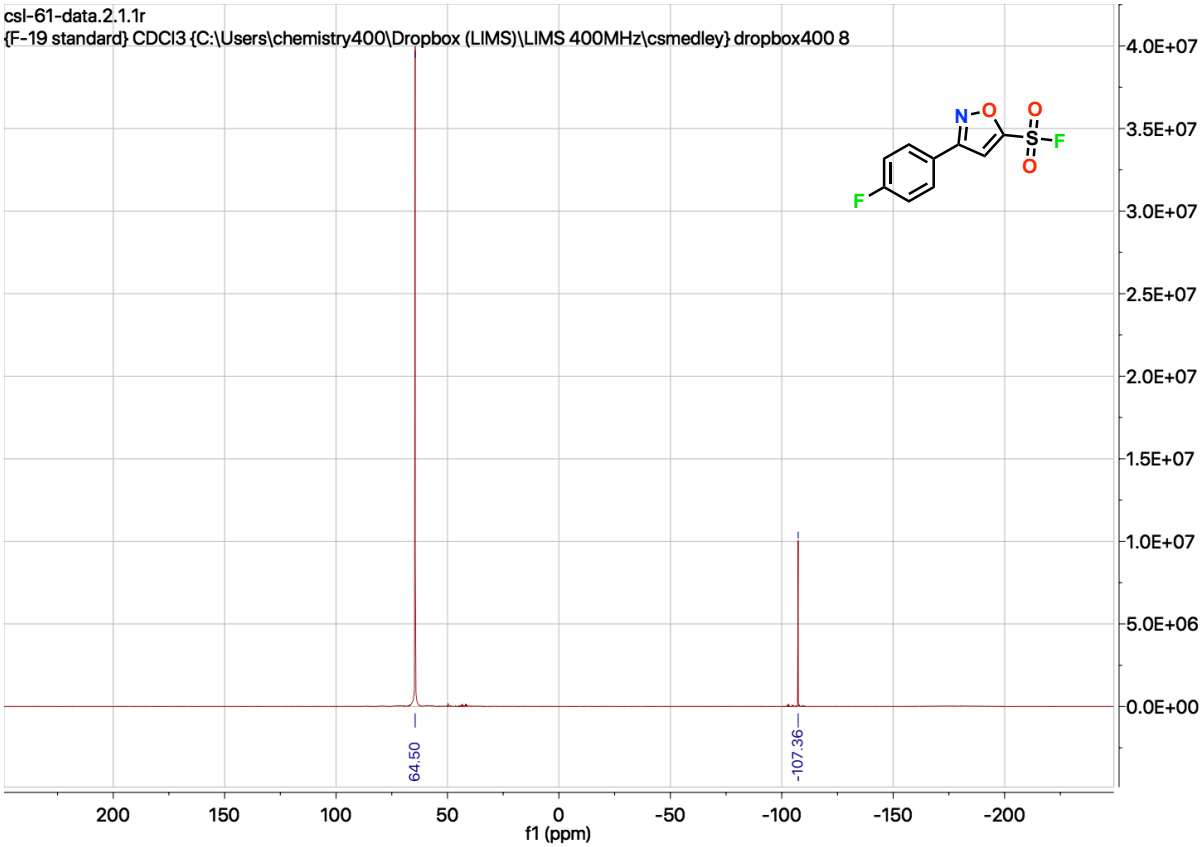

csl-111-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 22
Br
N
O
S
F
7.71
7.69
7.69
7.46
7.46
7.73
7.73
7.72
7.71
7.70
7.70
7.69
7.68
7.67
7.67
4.34
1.00
f1 (ppm)

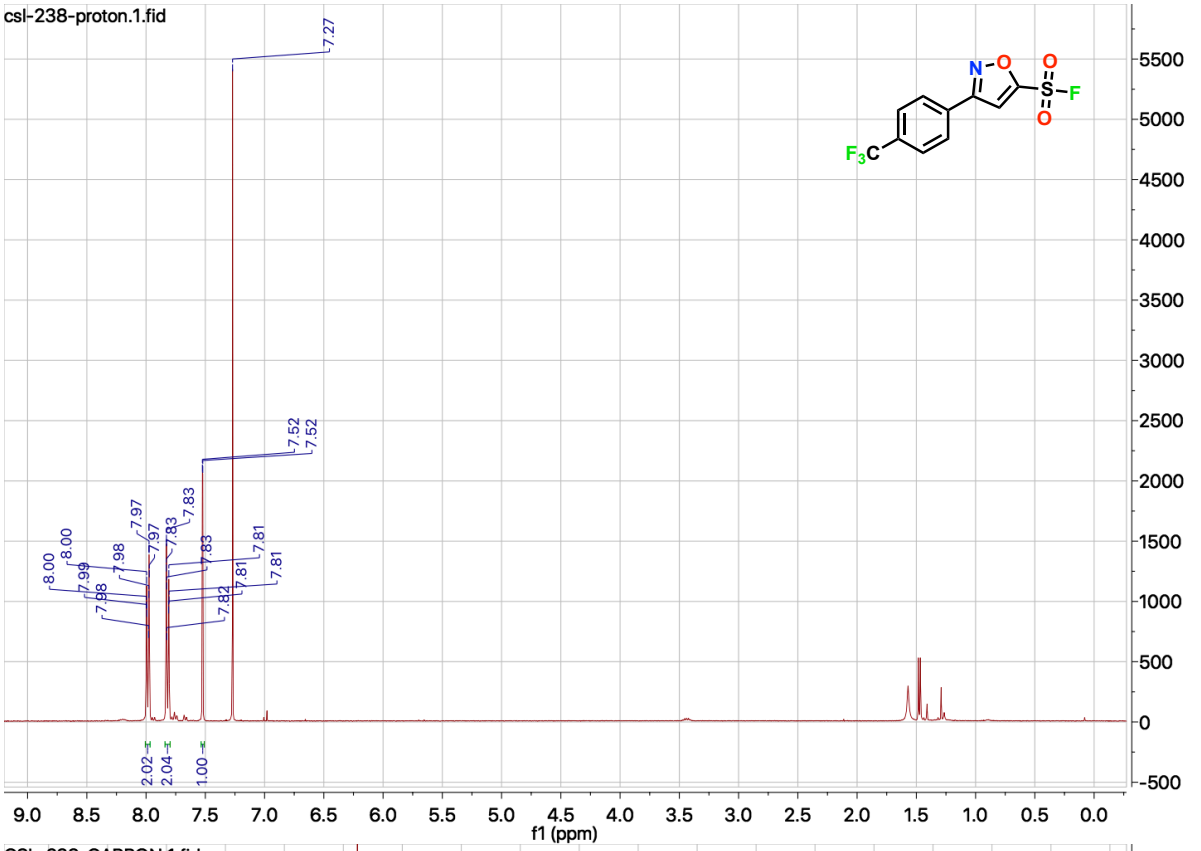

csl-111-data.2.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 22
Br
N
O
S
F
162.48
159.35
158.96
132.91
128.59
126.43
125.33
110.16
110.13
f1 (ppm)

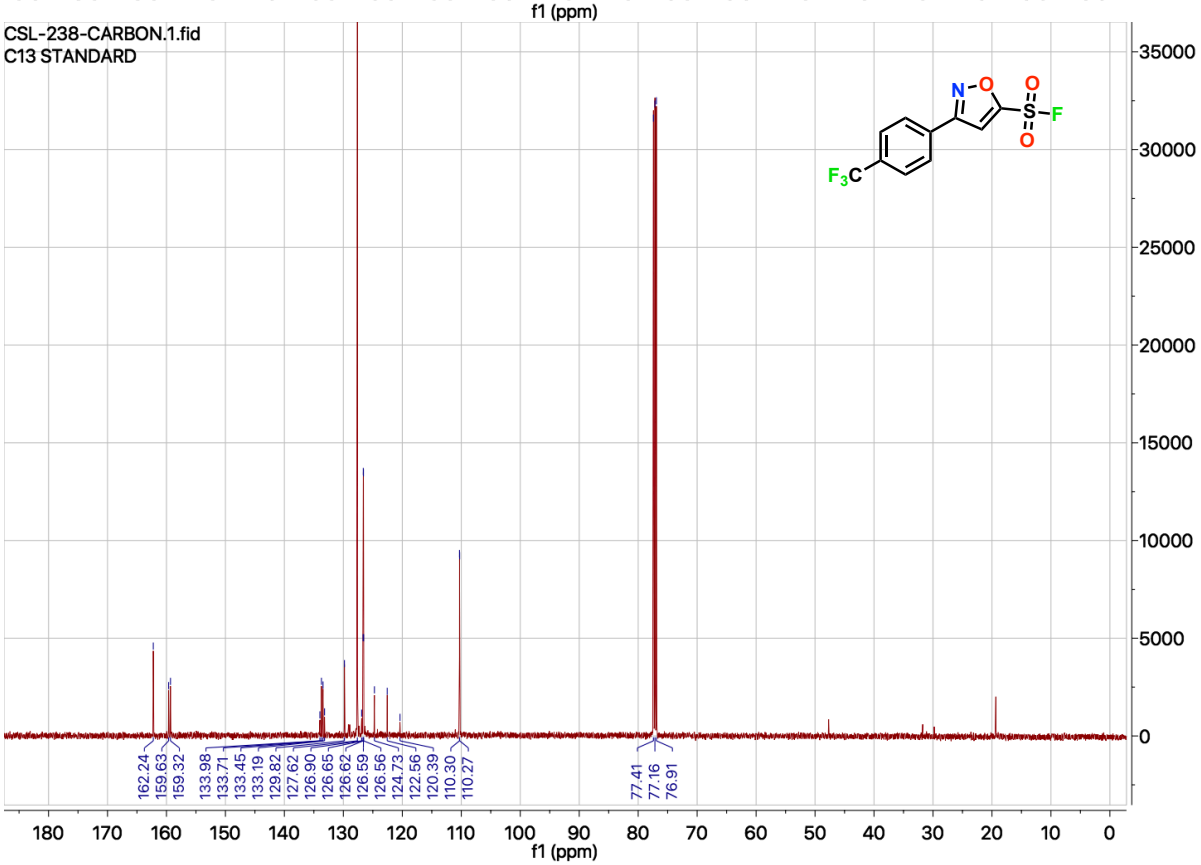

csl-111-data.3.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 22
N
O
O
S
F
O
Br
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
64.61
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)

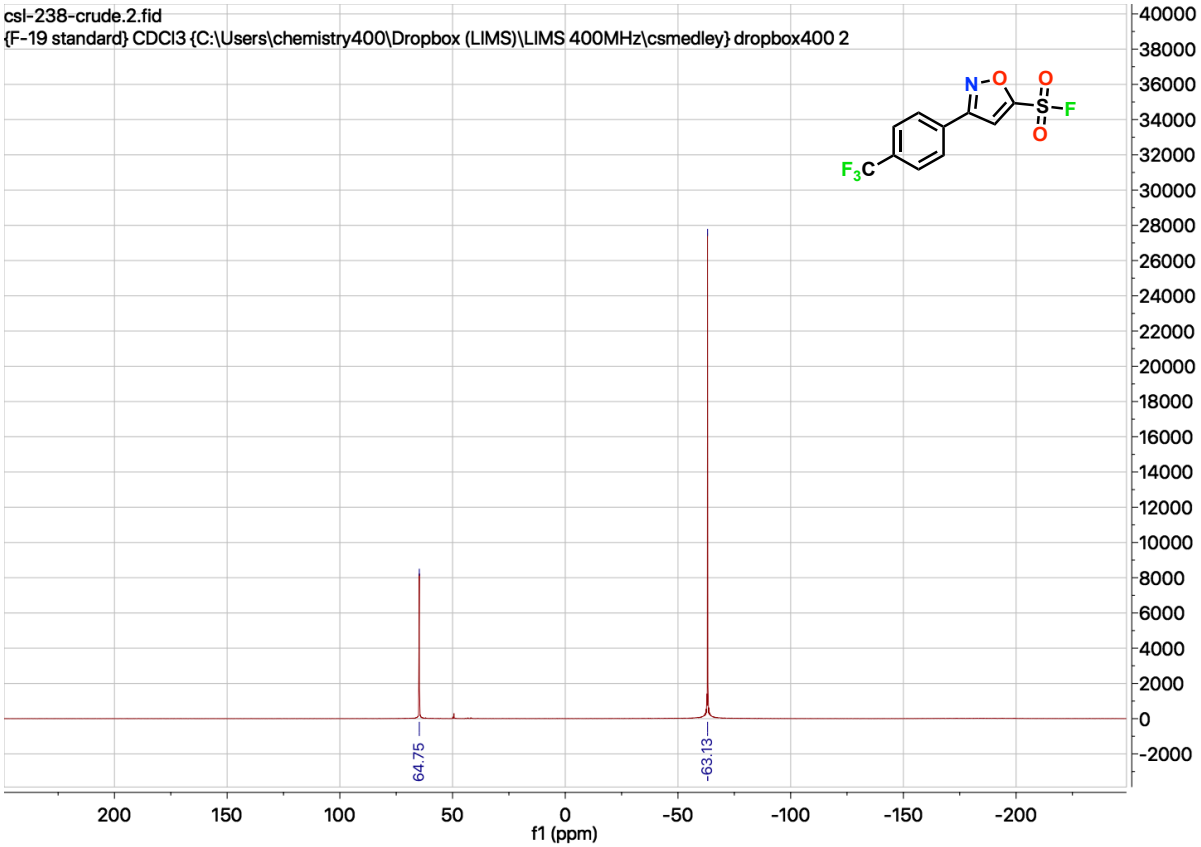

csl-61-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 8
f1 (ppm)

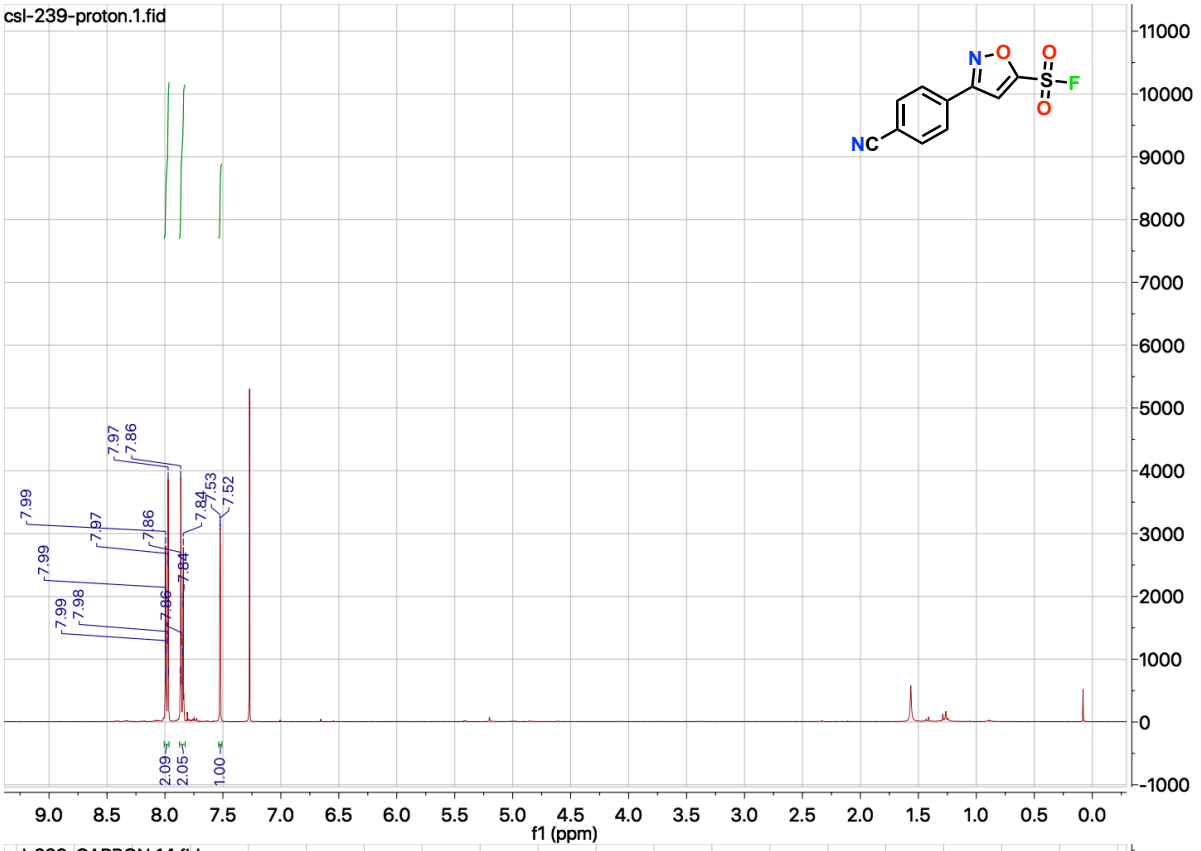

csl-61-CARBON.2.fid
C13 STANDARD
f1 (ppm)

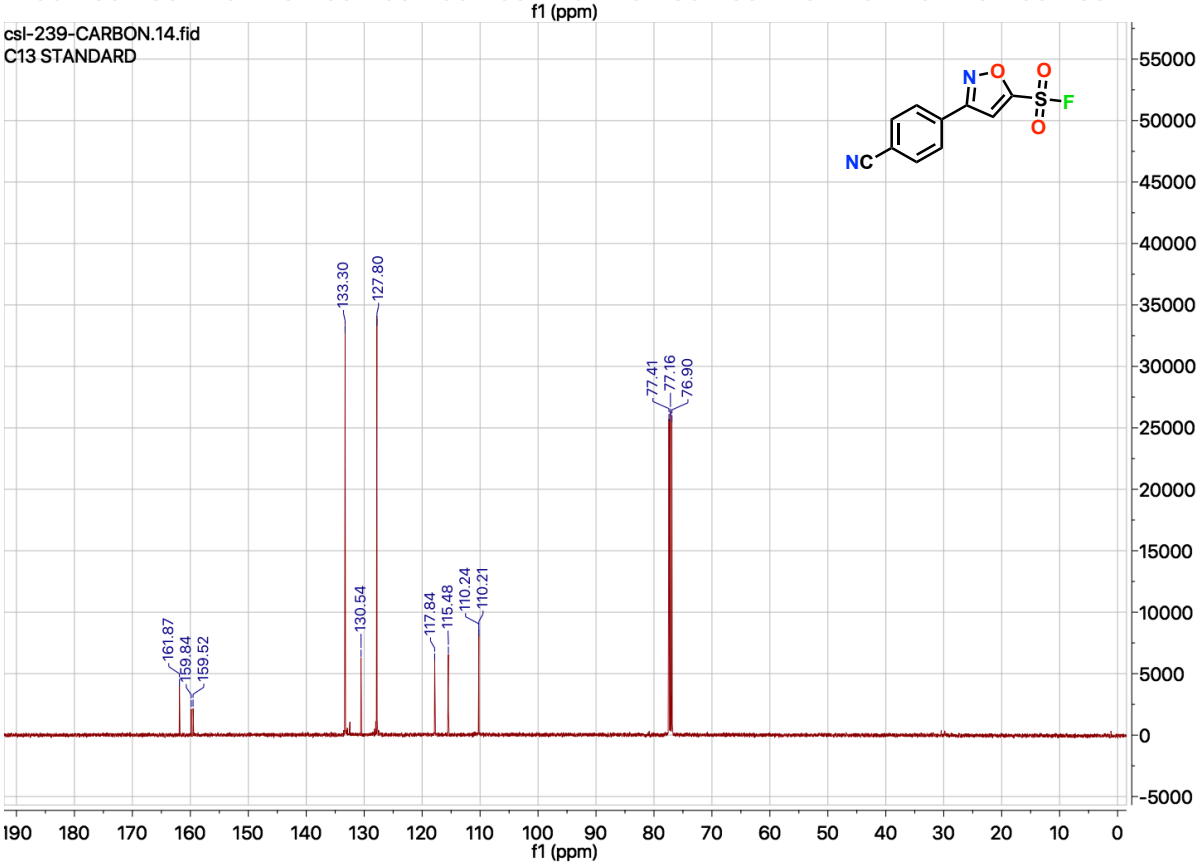

csl-61-data.2.1.1r
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 8
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
64.50
-107.36
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
N
O
O
S
F
O
F

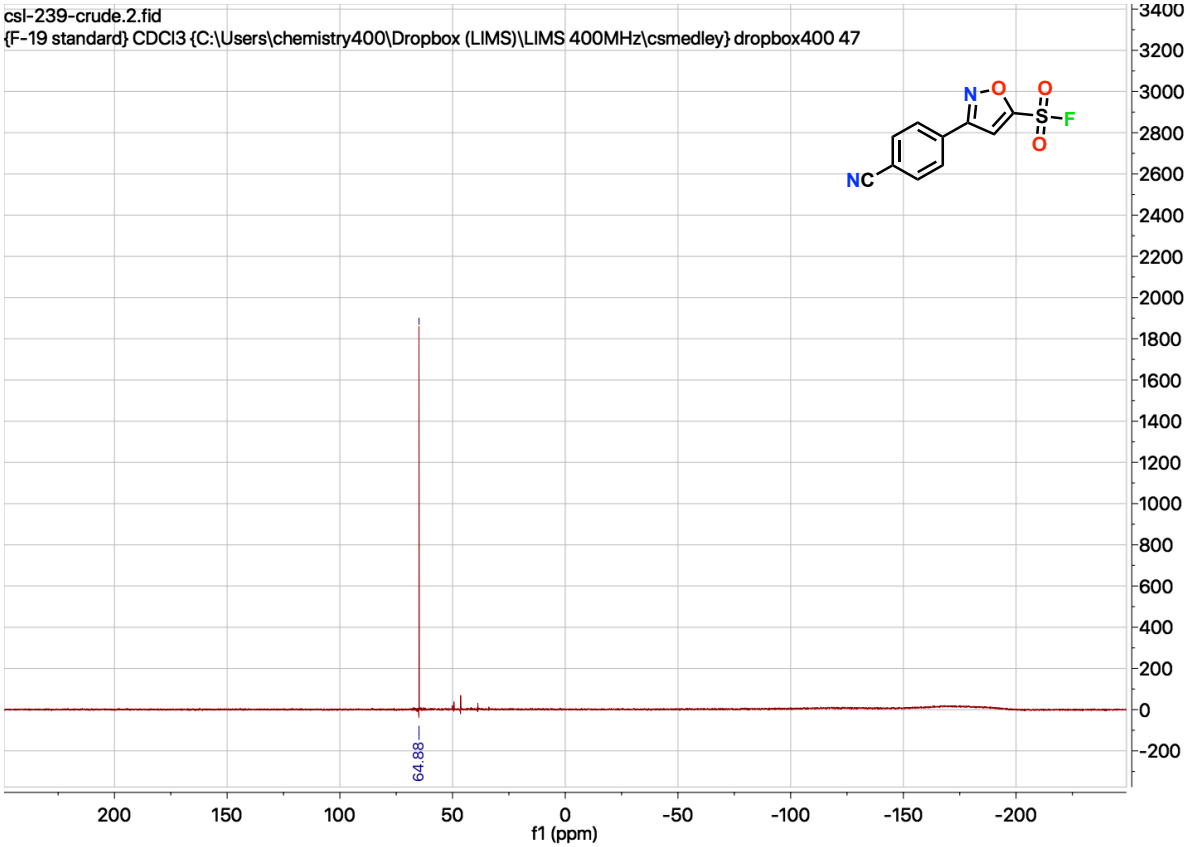

csl-238-proton.1.fid
7.27
7.52
7.52
7.97
7.97
7.83
7.83
7.83
7.81
7.81
7.81
7.82
8.00
8.00
7.99
7.98
7.98
2.02
2.04
1.00
f1 (ppm)

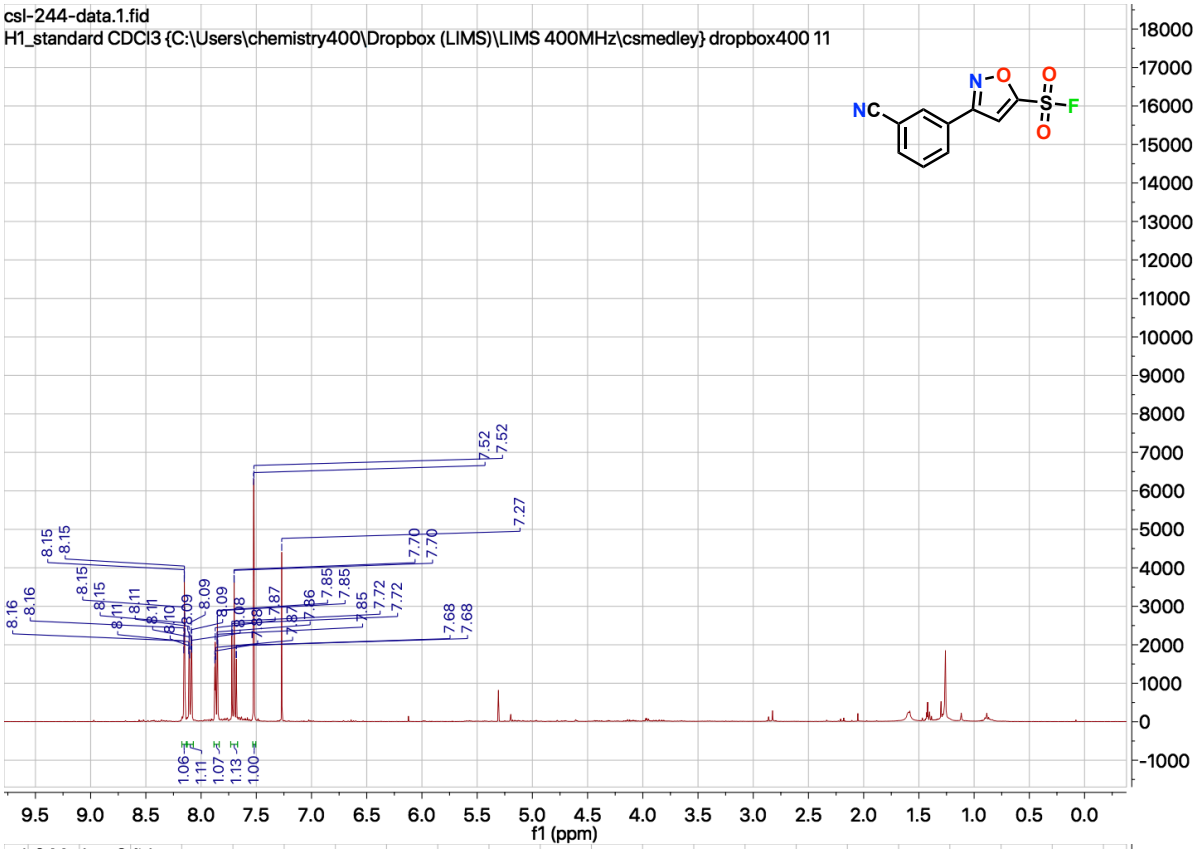

CSL-238-CARBON.1.fid
C13 STANDARD
162.24
159.63
159.32
133.98
133.71
133.45
133.19
129.82
127.62
126.90
126.65
126.62
126.59
126.56
124.73
122.56
120.39
110.30
110.27
77.41
77.16
76.91
f1 (ppm)

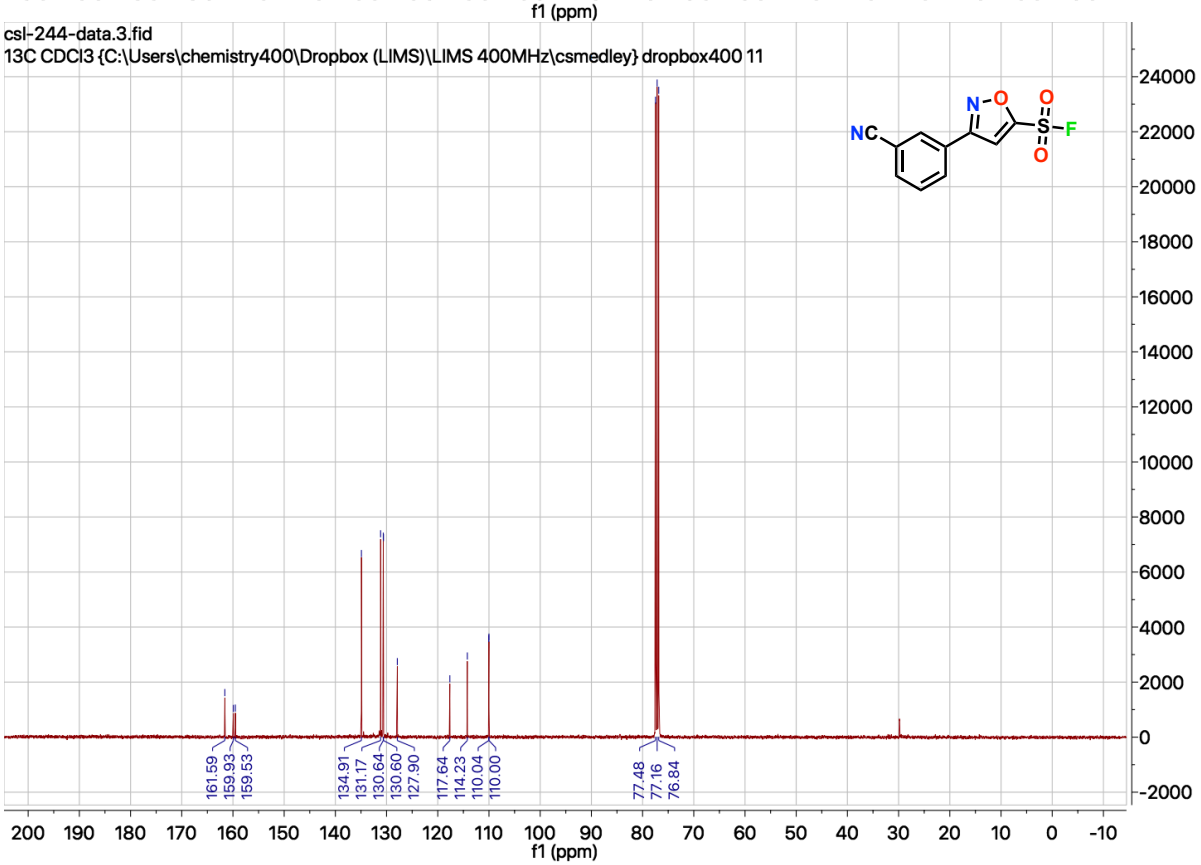

csl-238-crude.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 2
64.75
-63.13
f1 (ppm)

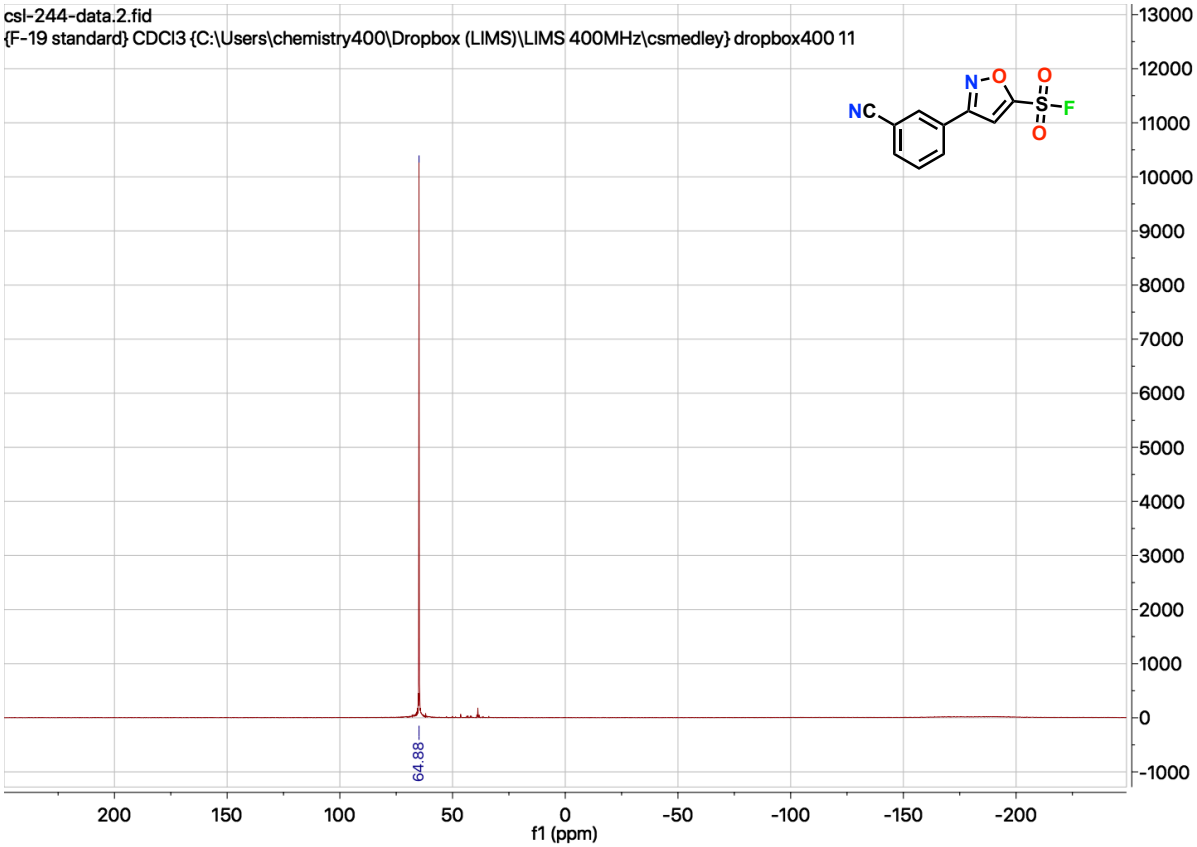

csl-239-proton.1.fid
7.99
7.97
7.86
7.84
7.53
7.52
2.09
2.05
1.00
f1 (ppm)

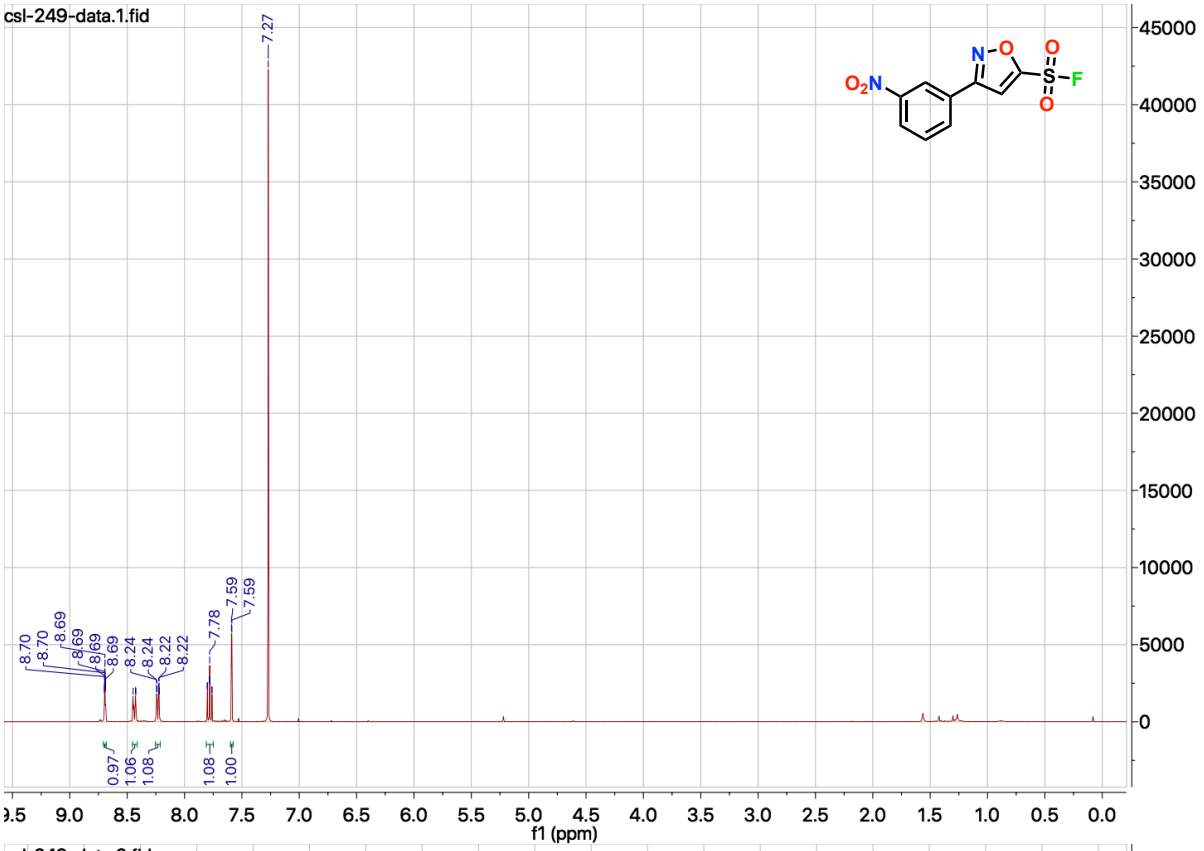

csl-239-CARBON.14.fid
C13 STANDARD
133.30
127.80
130.54
161.87
159.84
159.52
117.84
115.48
110.24
110.21
77.41
77.16
76.90
f1 (ppm)

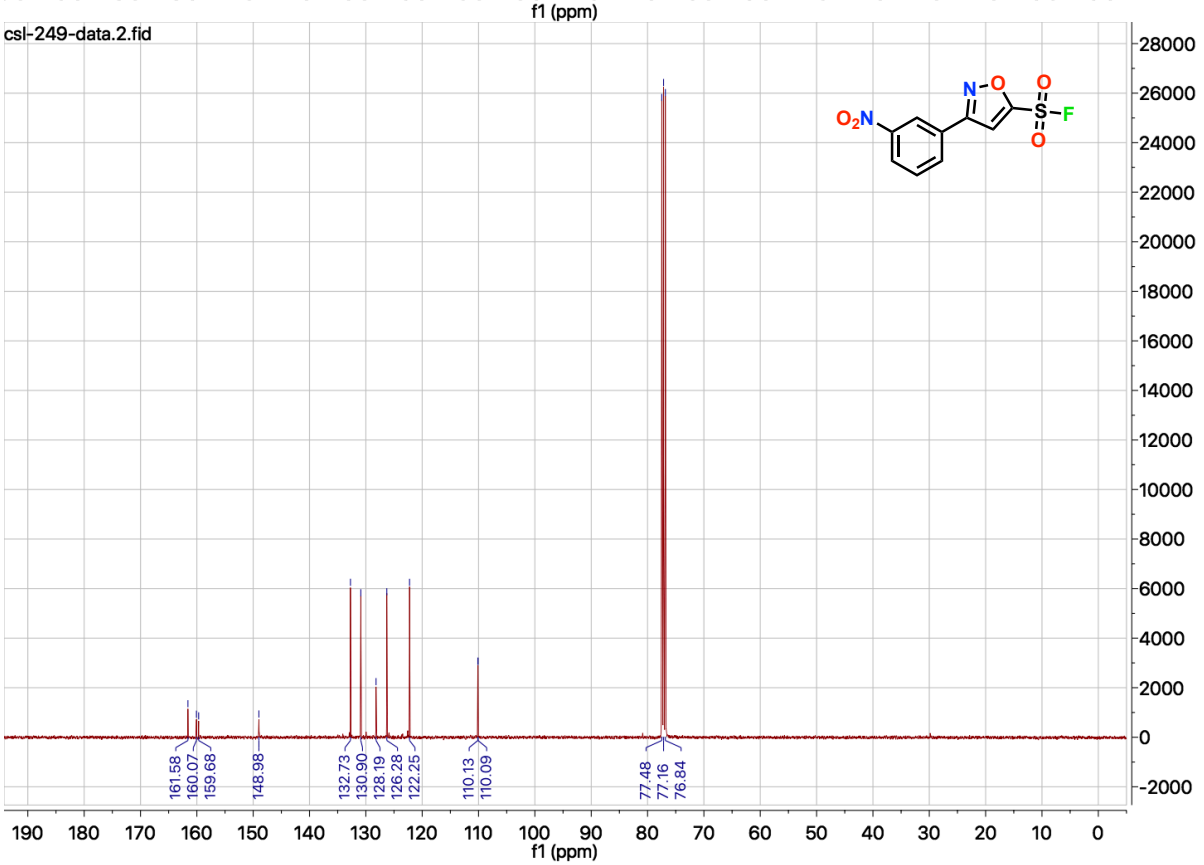

csl-239-crude.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 47
N
O
O
S
F
O
NC
64.88
f1 (ppm)

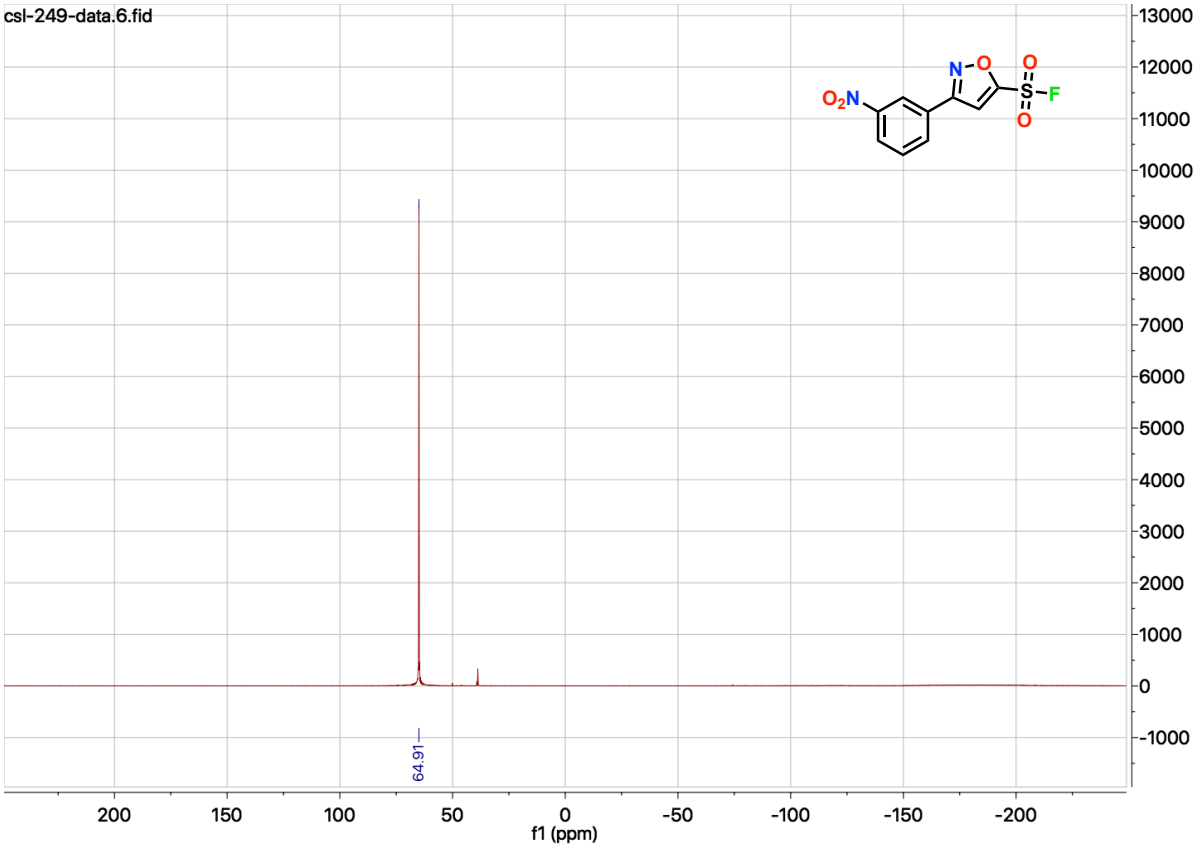

csl-244-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 11
f1 (ppm)

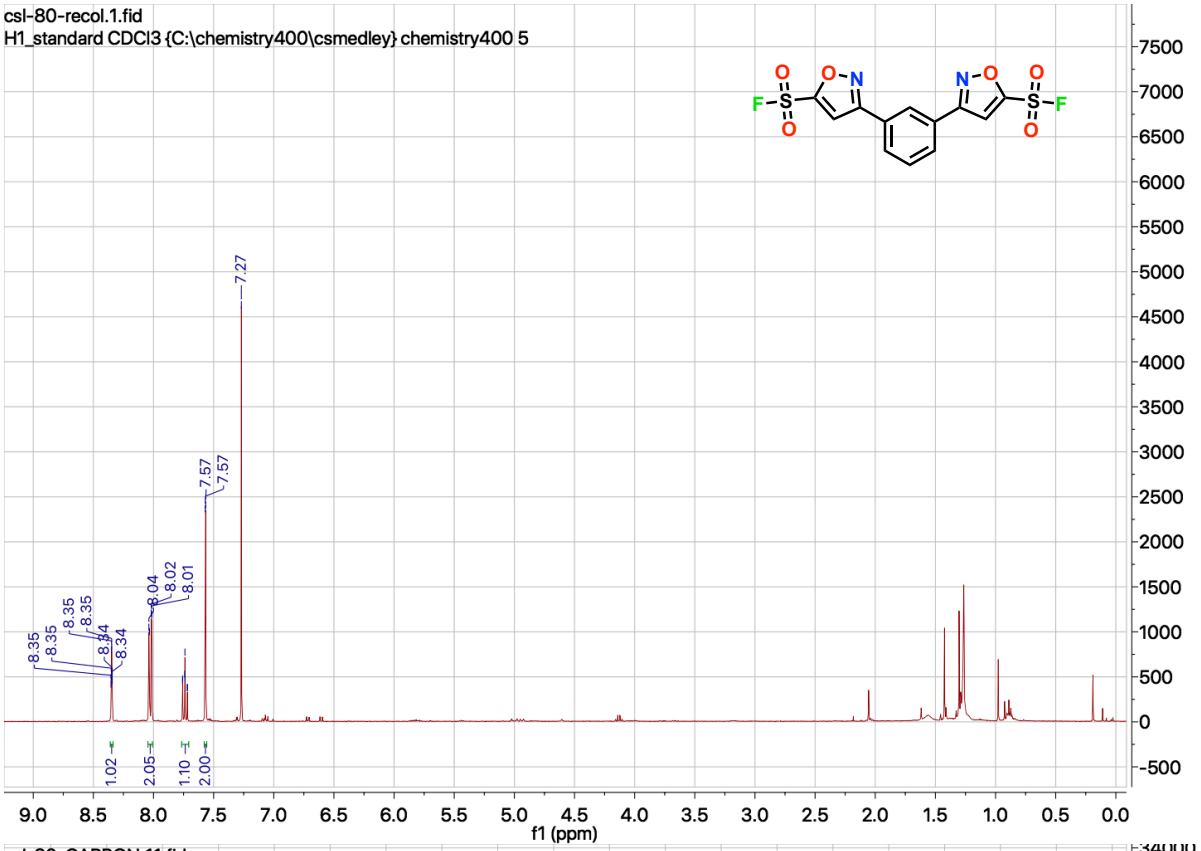

csl-244-data.3.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 11
f1 (ppm)

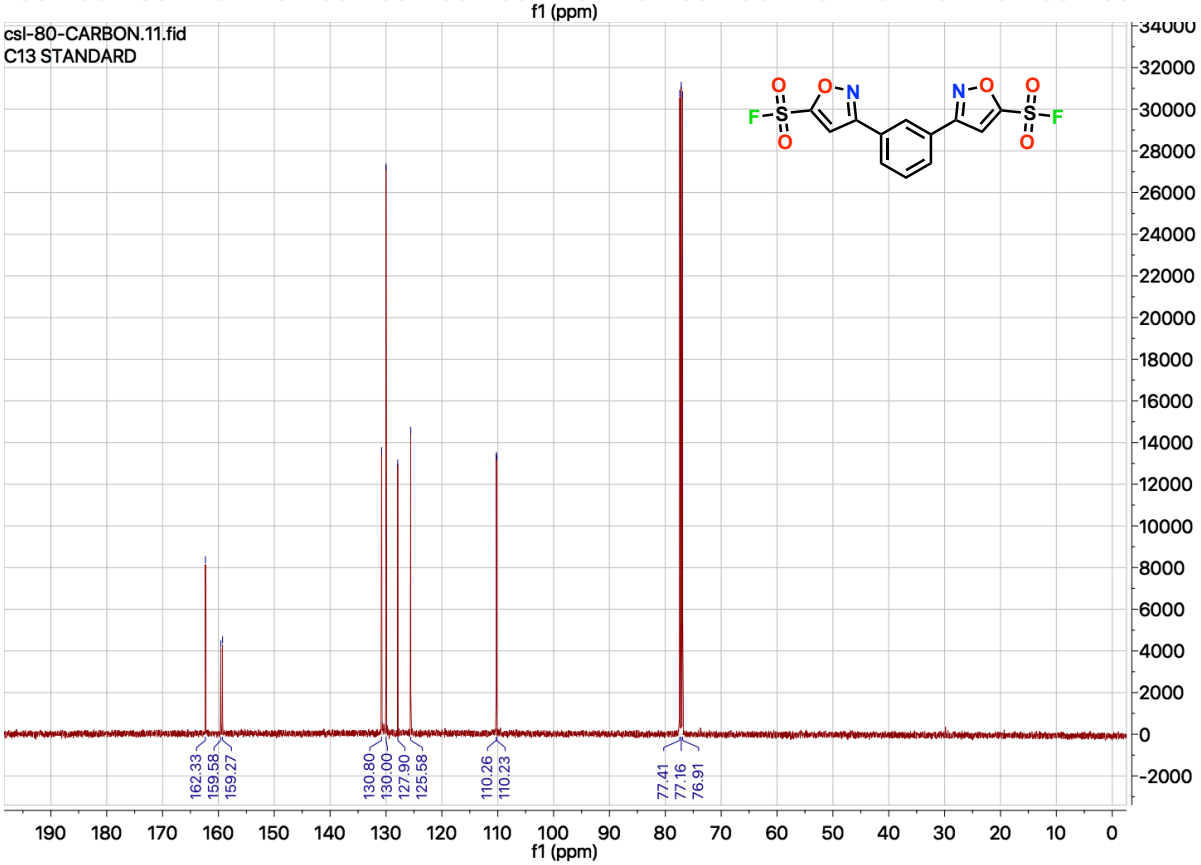

csl-244-data.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 11
NC
N
O
O
S
F
O
64.88
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)

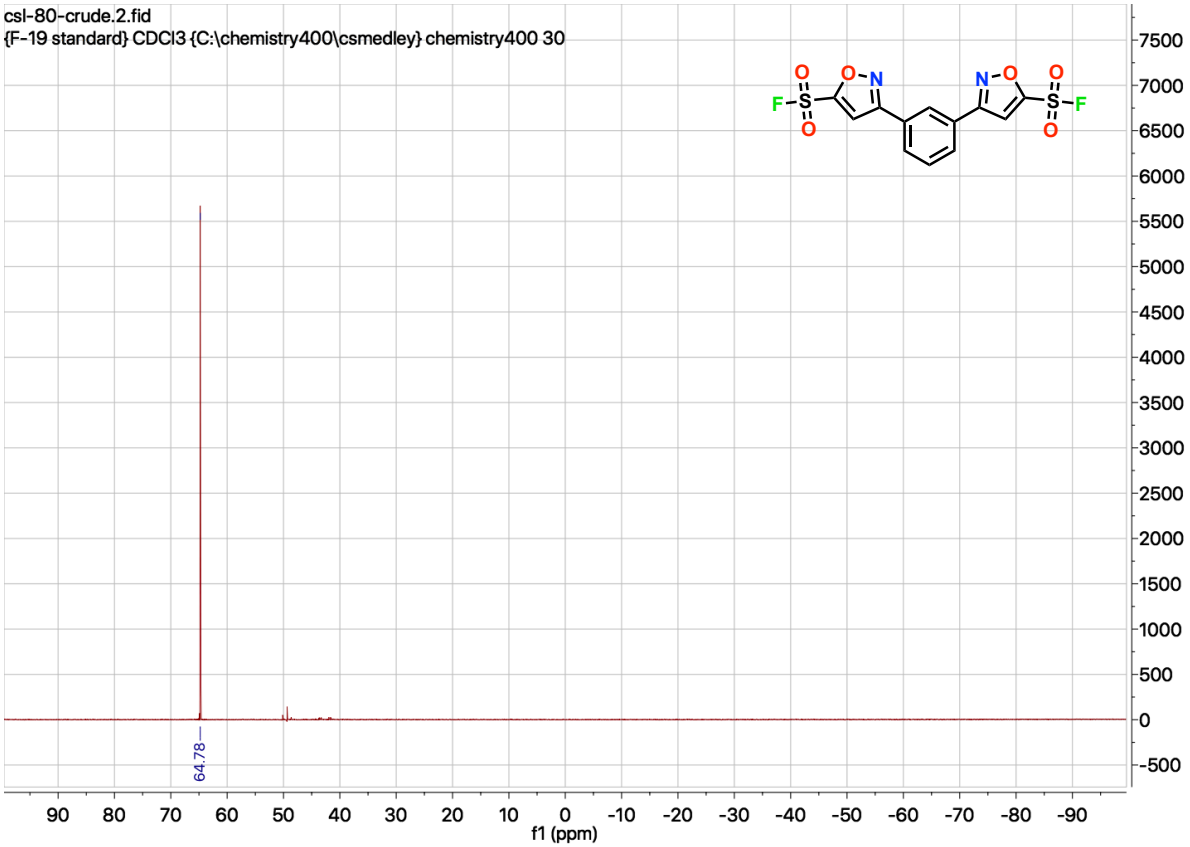

csl-249-data.1.fid
7.27
8.70
8.70
8.69
8.69
8.69
8.69
8.24
8.24
8.22
8.22
7.78
7.59
7.59
0.97
1.06
1.08
1.08
1.00
f1 (ppm)

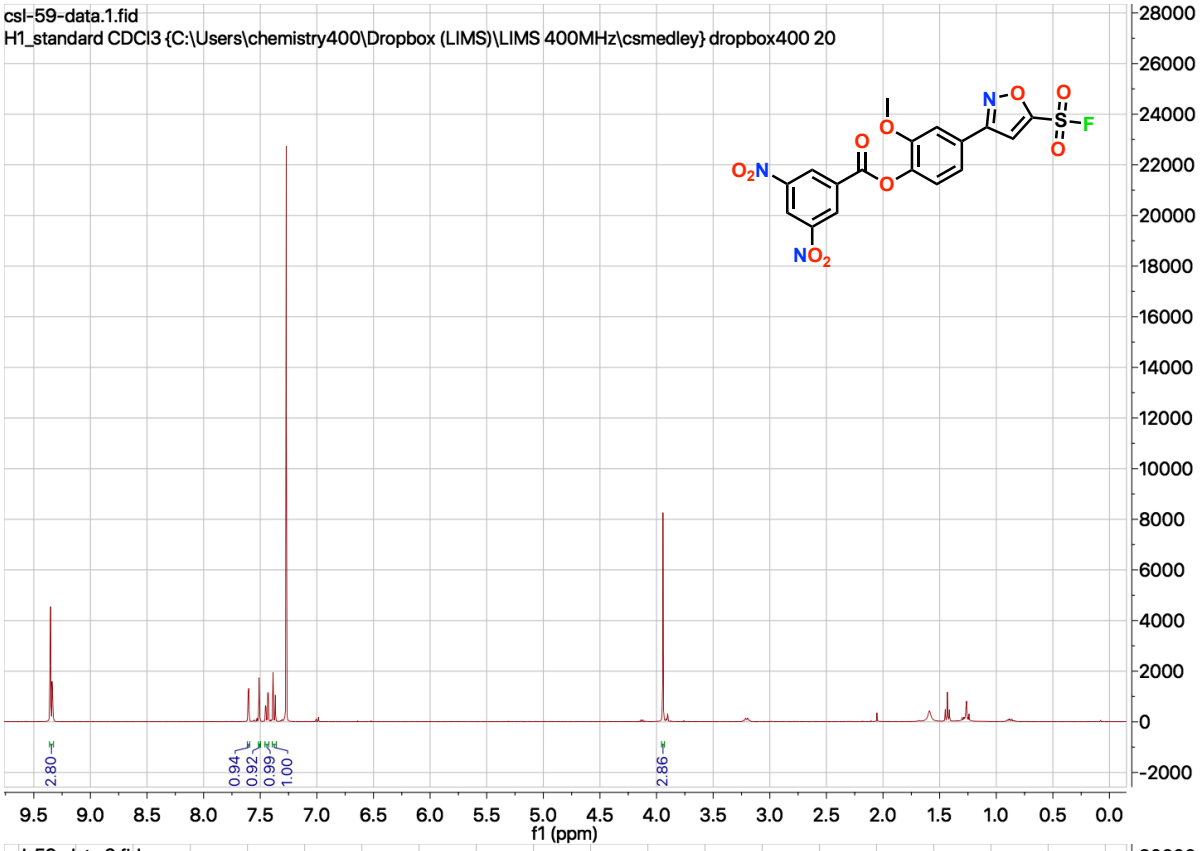

csl-249-data.2.fid
161.58
160.07
159.68
148.98
132.73
130.90
128.19
126.28
122.25
110.13
110.09
77.48
77.16
76.84
f1 (ppm)

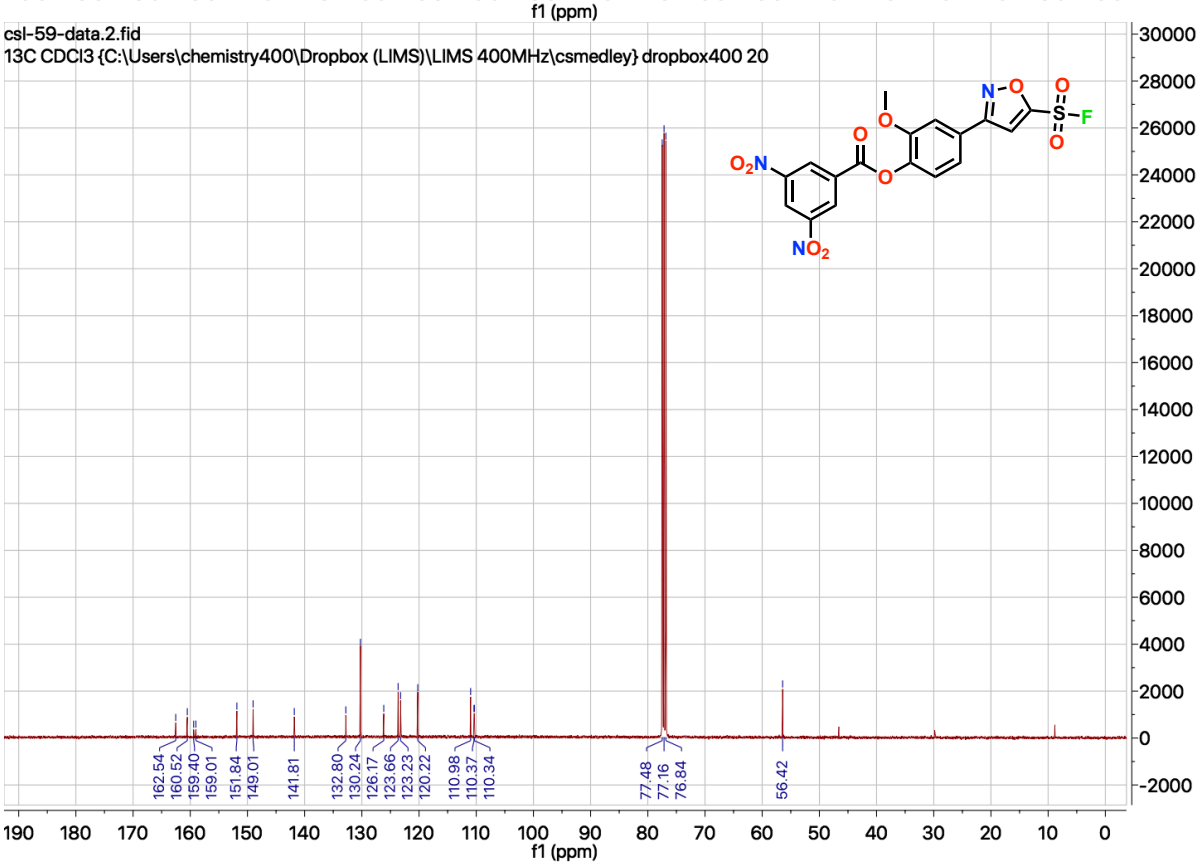

csl-249-data.6.fid
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
64.91
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
O2N
N
O
O
S
F
O

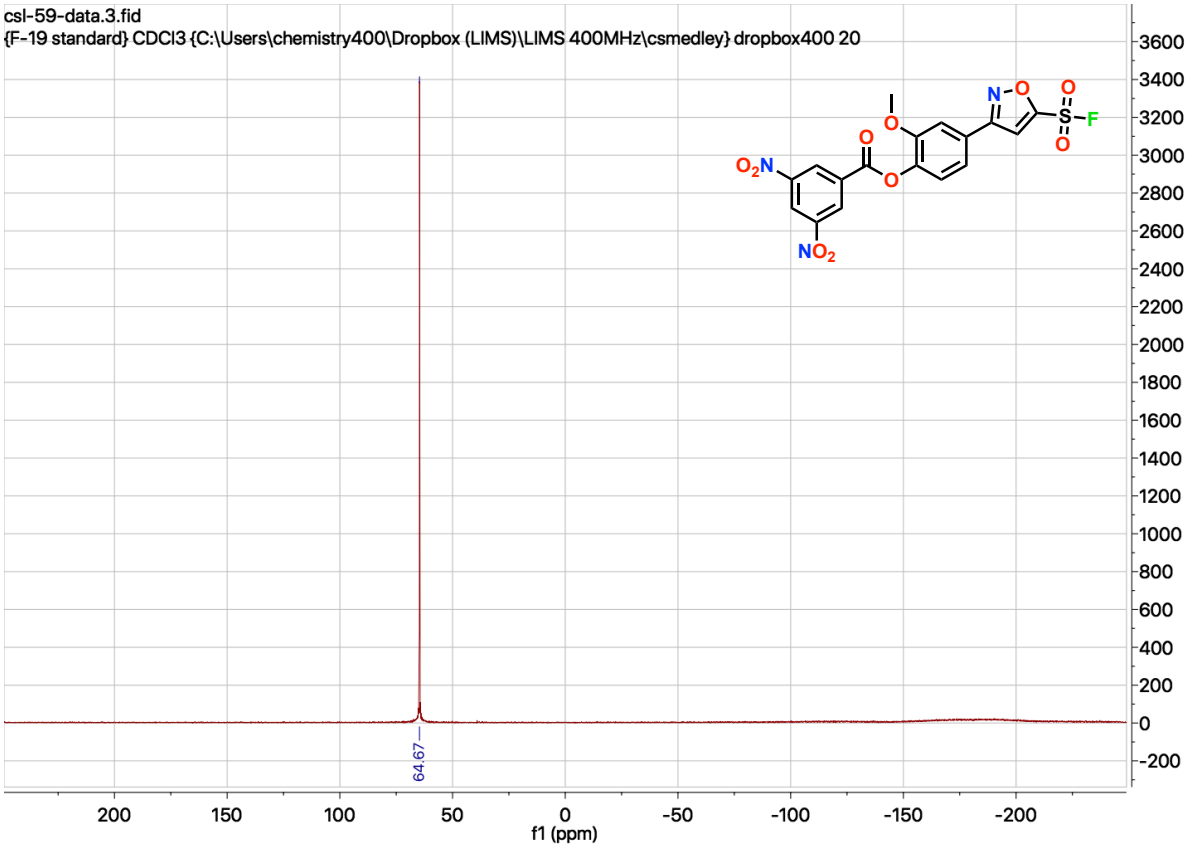

csl-80-recol.1.fid
H1_standard CDCl3 {C:\chemistry400\csmedley} chemistry400 5
7.27
7.57
7.57
8.04
8.02
8.01
8.35
8.35
8.35
8.34
8.34
1.02
2.05
1.10
2.00
f1 (ppm)

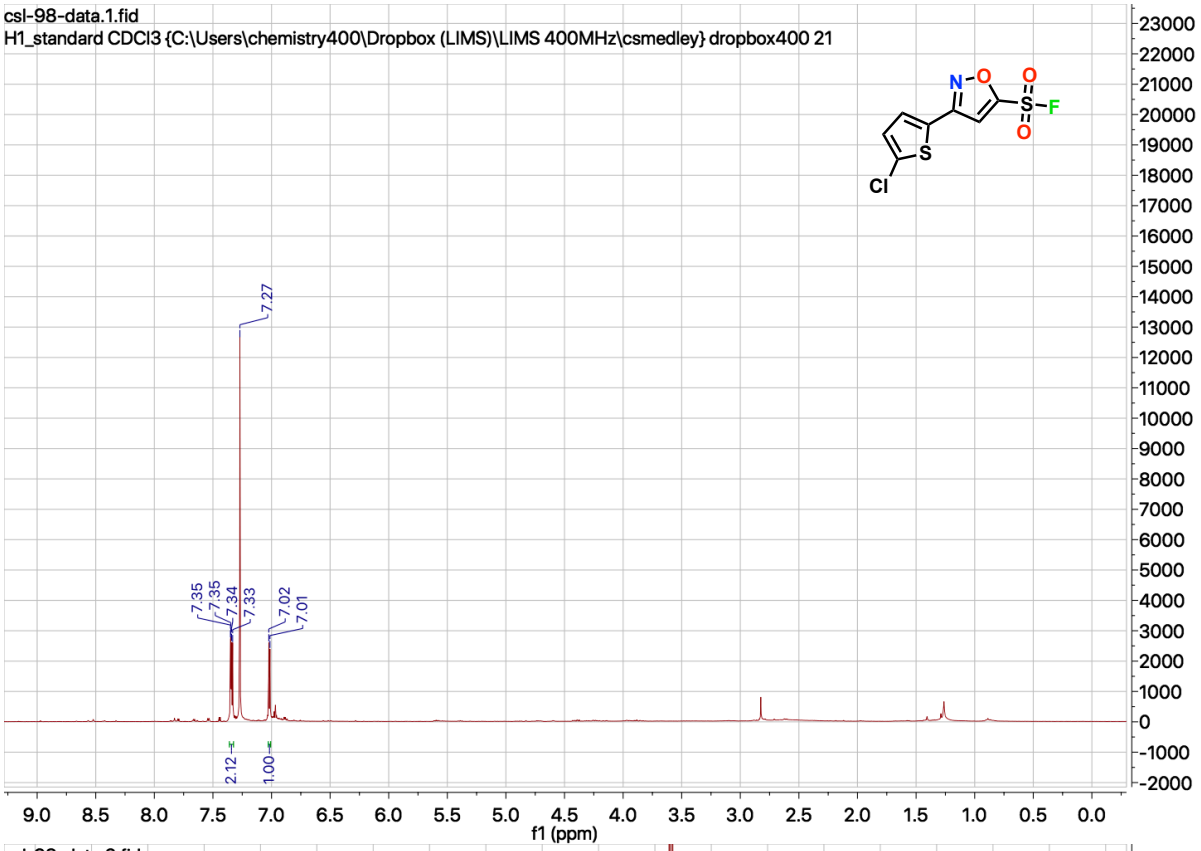

csl-80-CARBON.11.fid
C13 STANDARD
162.33
159.58
159.27
130.80
130.00
127.90
125.58
110.26
110.23
77.41
77.16
76.91
f1 (ppm)

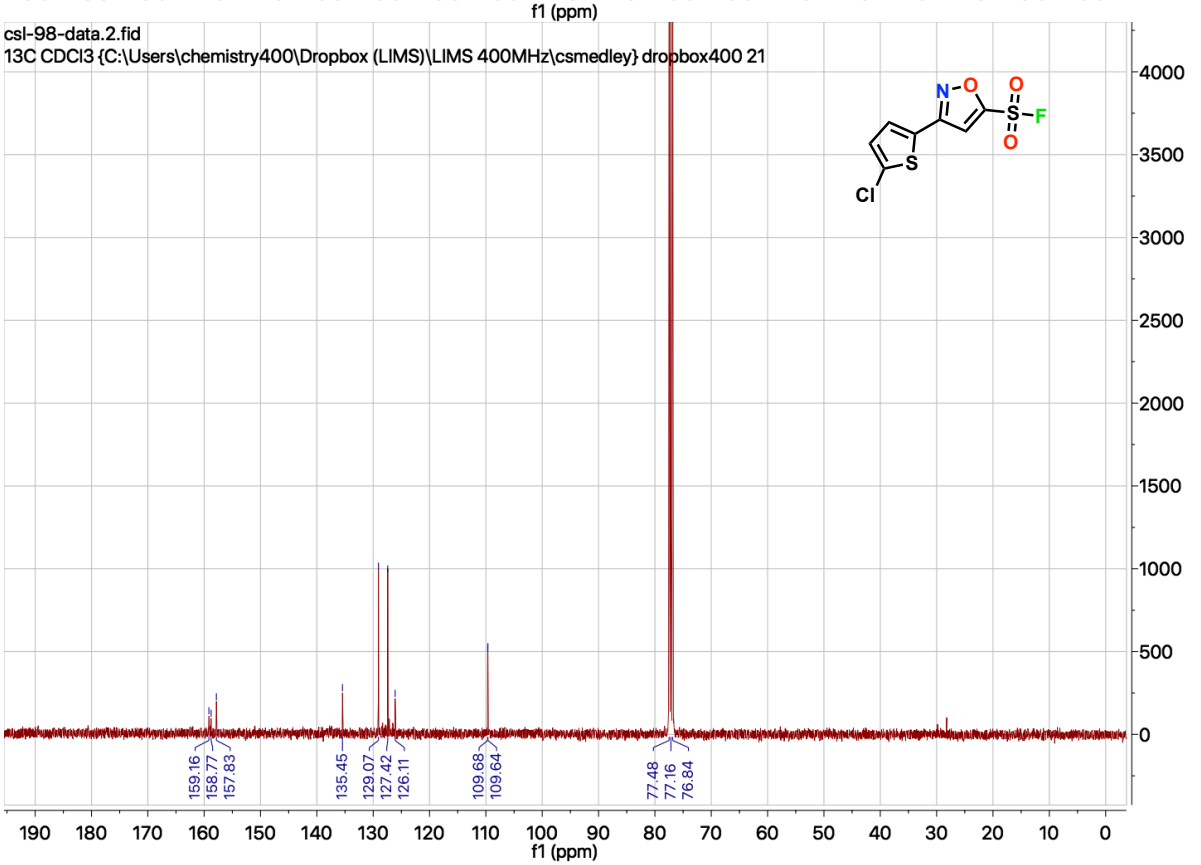

csl-80-crude.2.fid
{F-19 standard} CDCl3 {C:\chemistry400\csmedley} chemistry400 30
64.78
f1 (ppm)

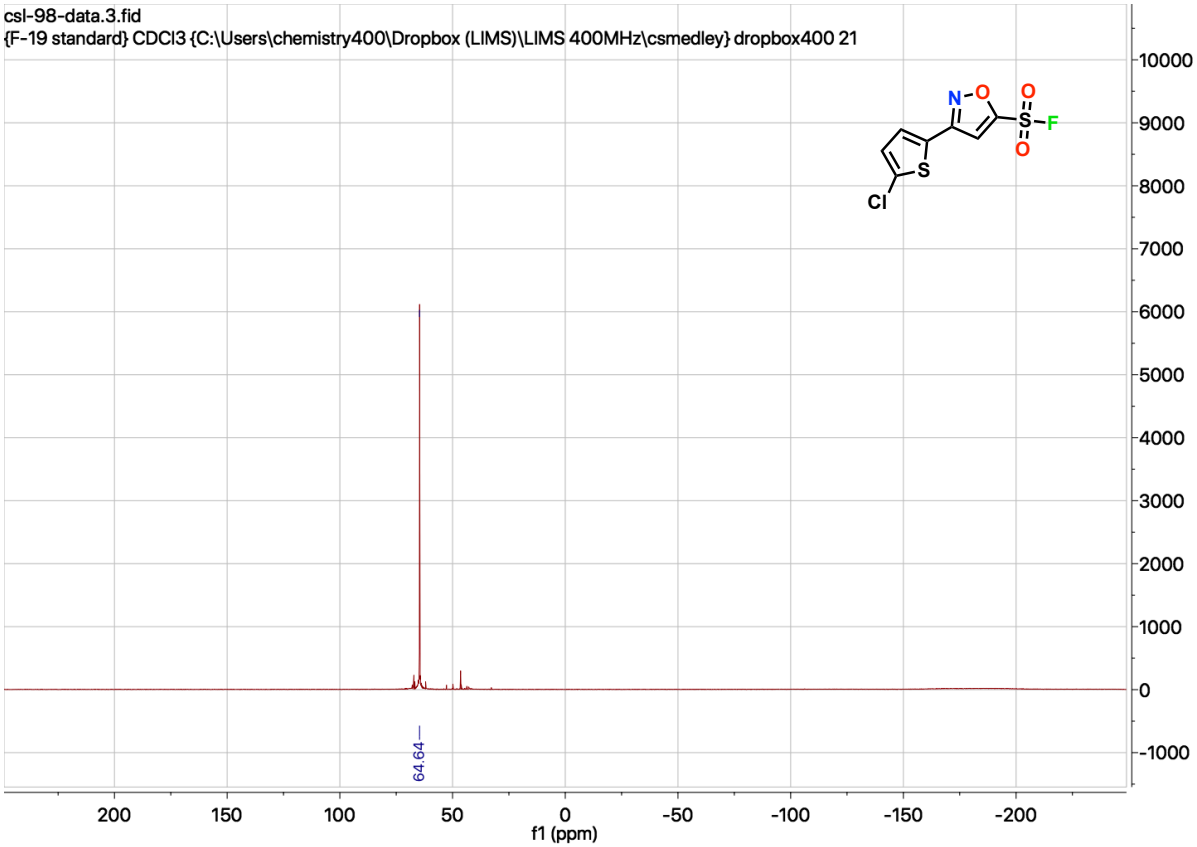

csl-59-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 20
2.80
0.94
0.92
0.99
1.00
2.86
f1 (ppm)

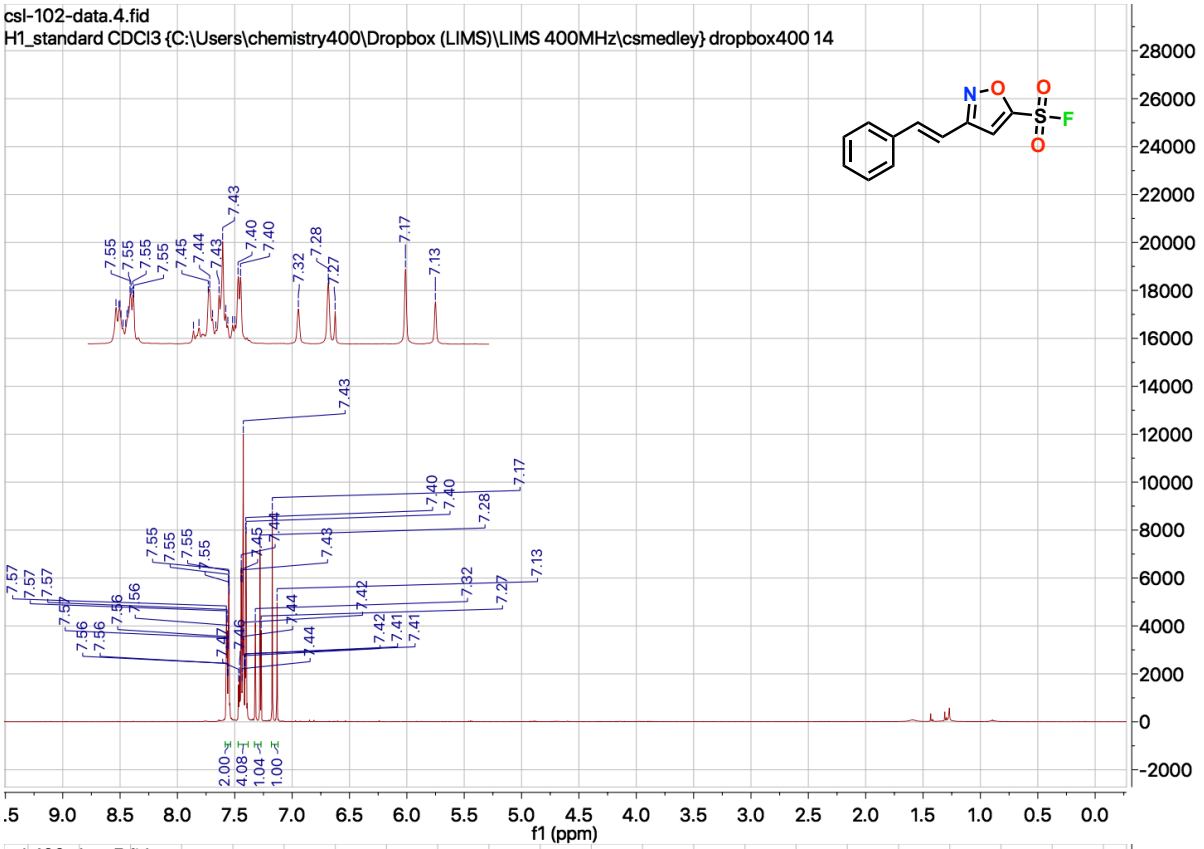

csl-59-data.2.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 20
162.54
160.52
159.40
159.01
151.84
149.01
141.81
132.80
130.24
126.17
123.66
123.23
120.22
110.98
110.37
110.34
77.48
77.16
76.84
56.42
f1 (ppm)

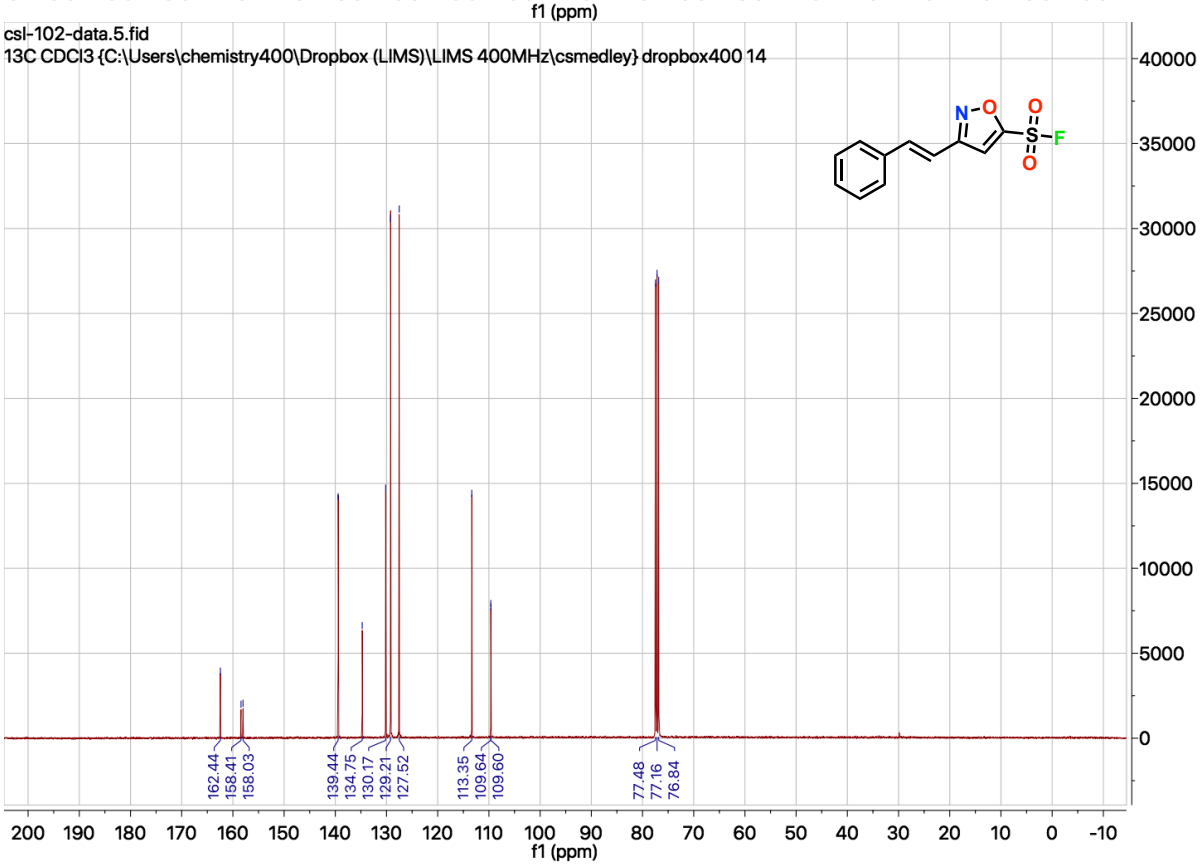

csl-59-data.3.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 20
64.67
f1 (ppm)

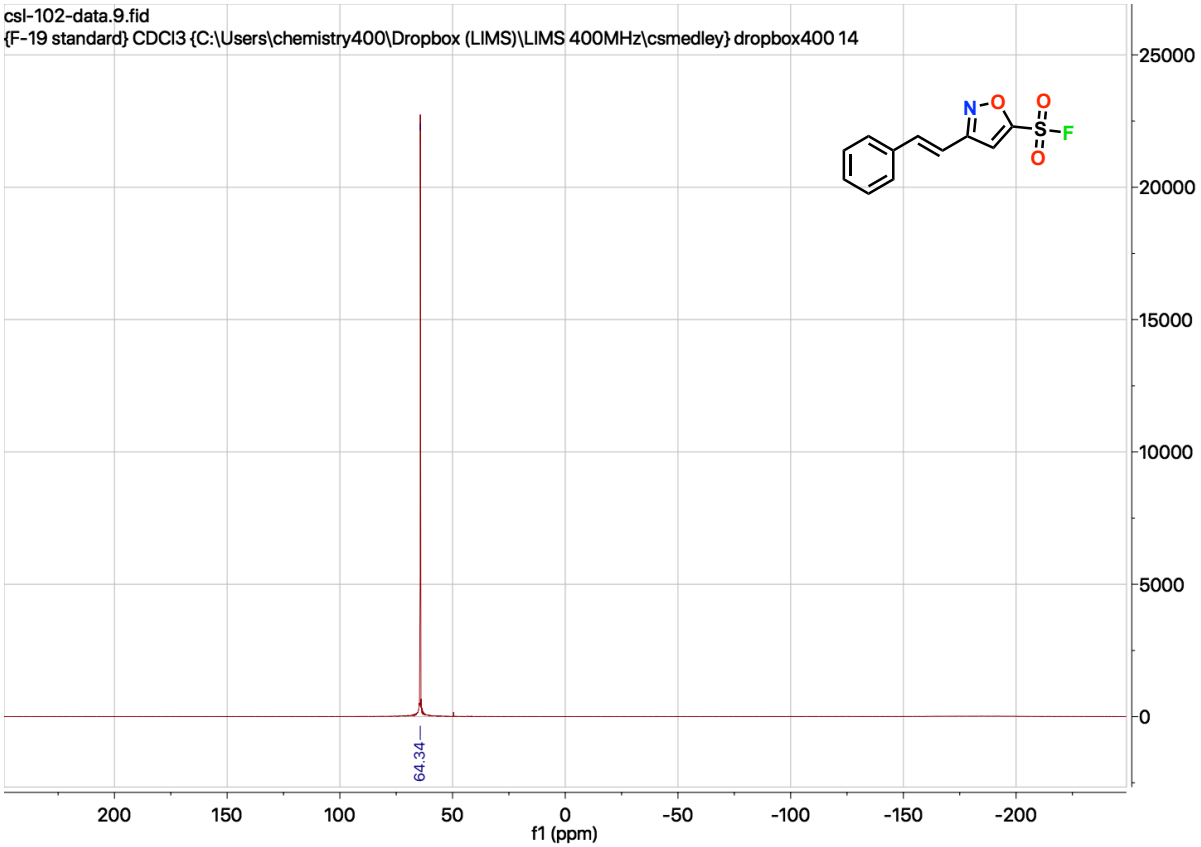

csl-98-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 21
7.27
7.35
7.35
7.34
7.33
7.02
7.01
2.12
1.00
f1 (ppm)

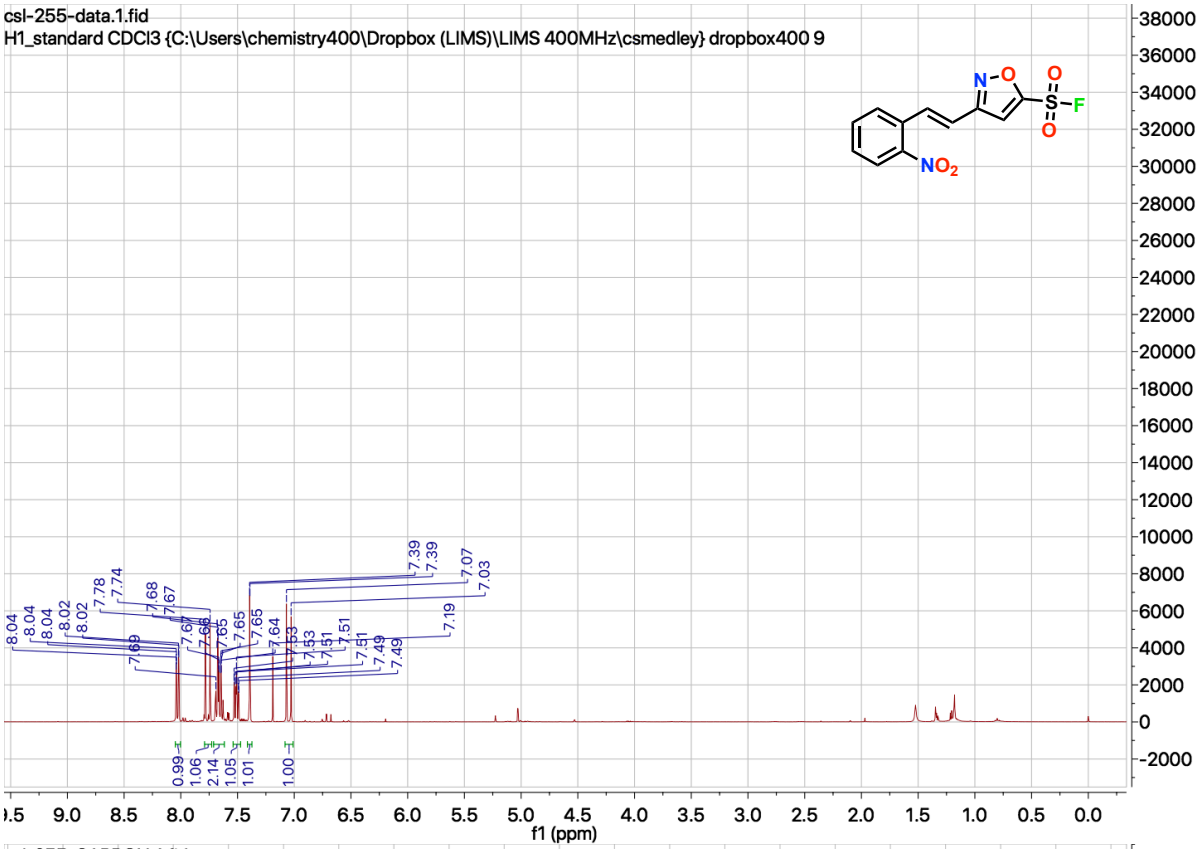

csl-98-data.2.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 21
159.16
158.77
157.83
135.45
129.07
127.42
126.11
109.68
109.64
77.48
77.16
76.84
f1 (ppm)

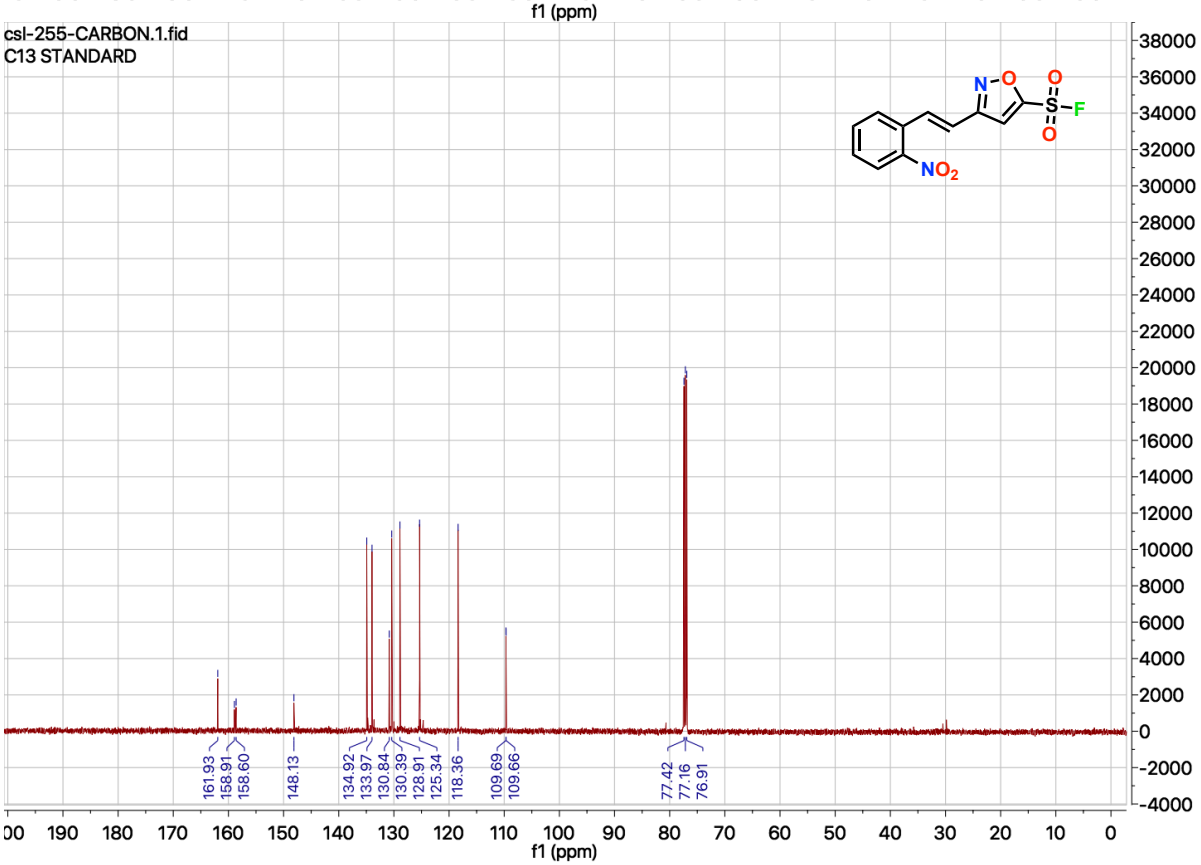

csl-98-data.3.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 21
N
O
O
S
F
O
S
Cl
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
64.64
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)

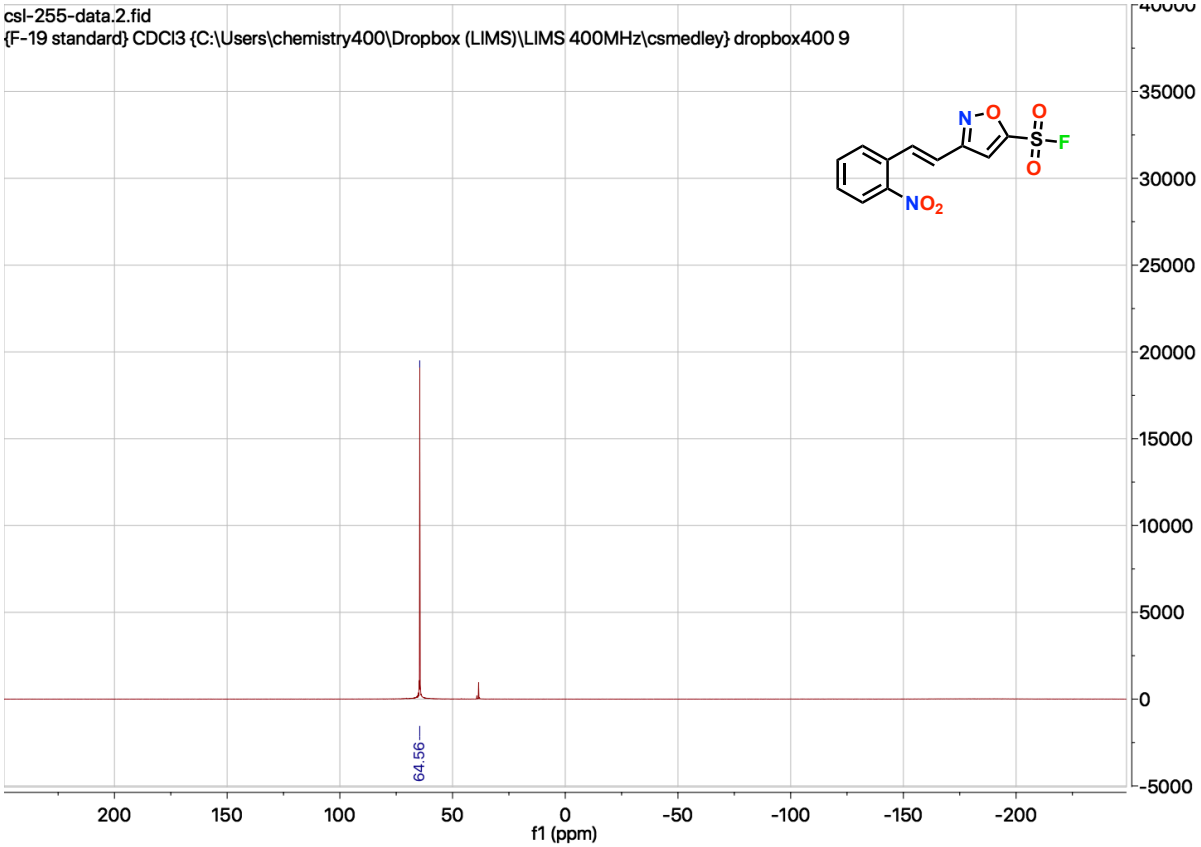

csl-102-data.4.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 14
f1 (ppm)

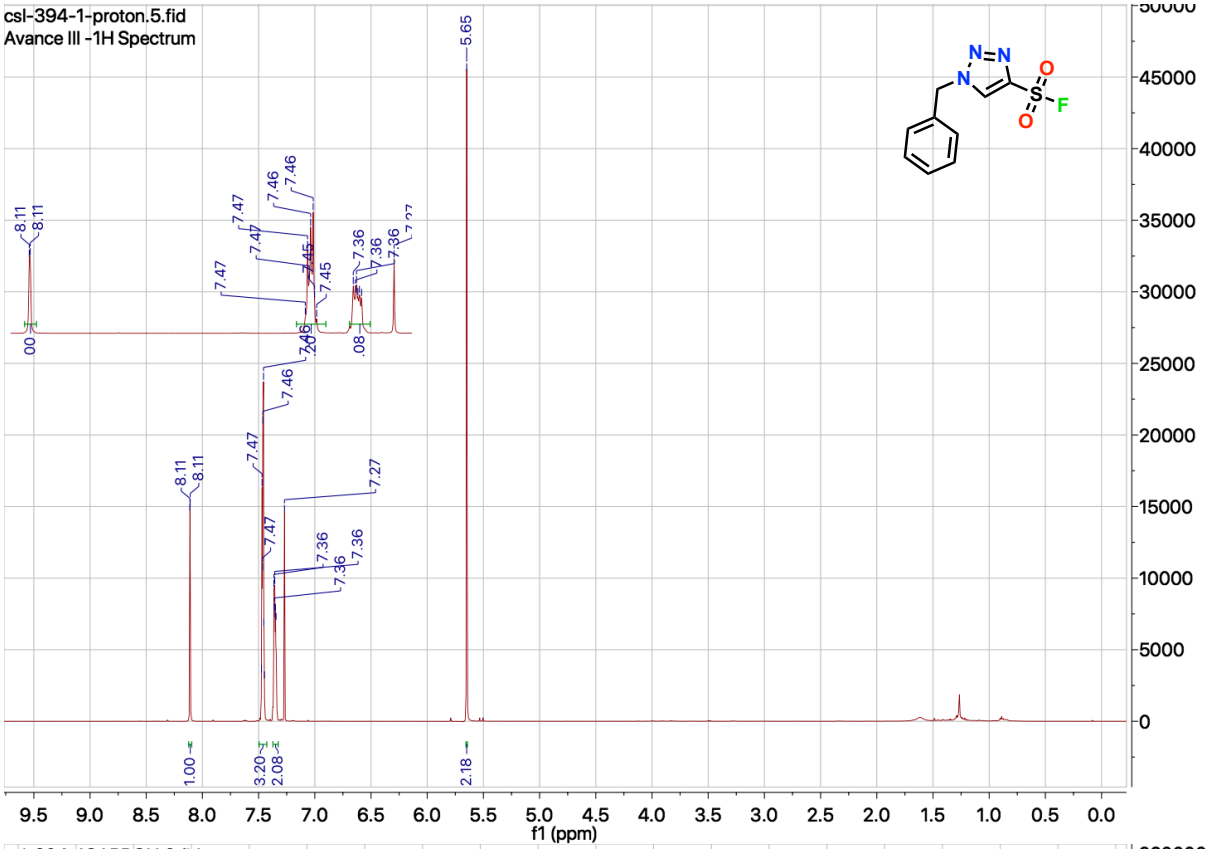

csl-102-data.5.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 14
f1 (ppm)

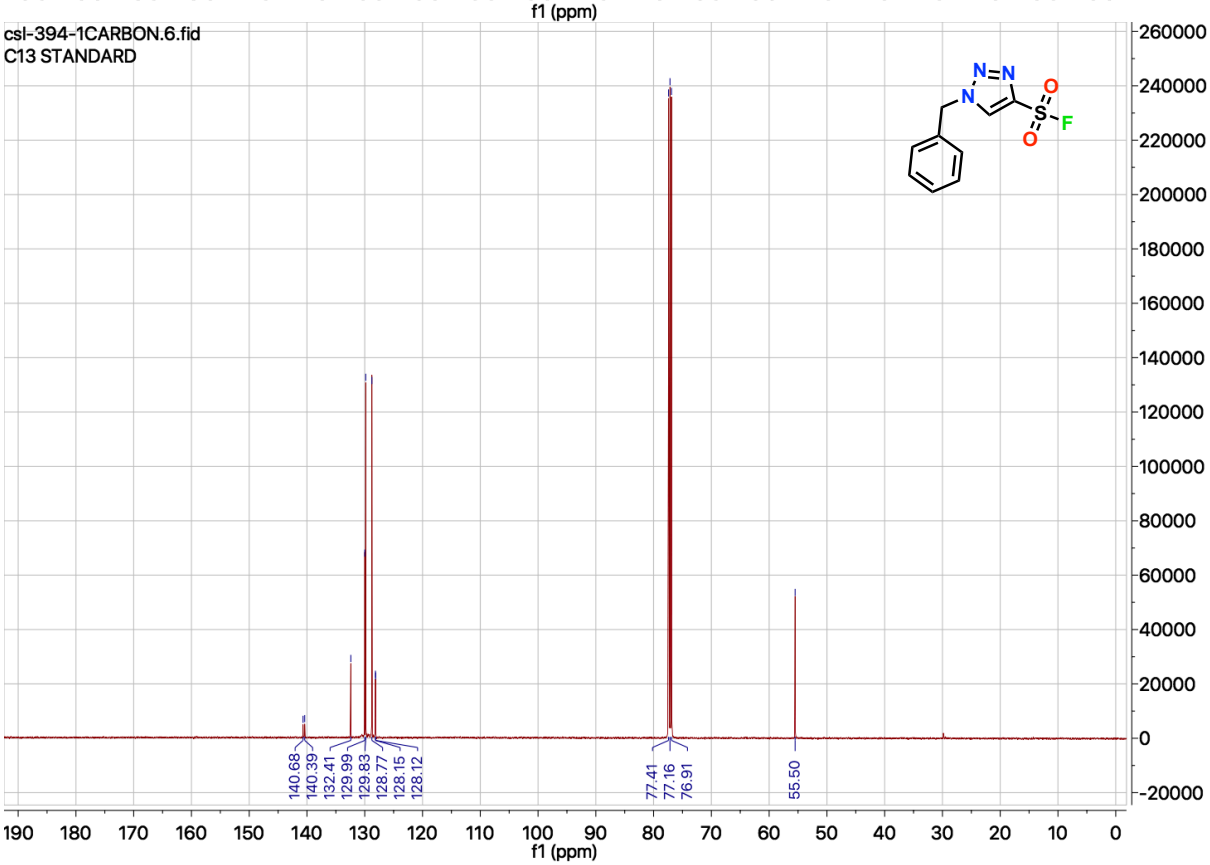

csl-102-data.9.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 14
25000
20000
15000
10000
5000
0
64.34
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
N
O
O
S
F
O

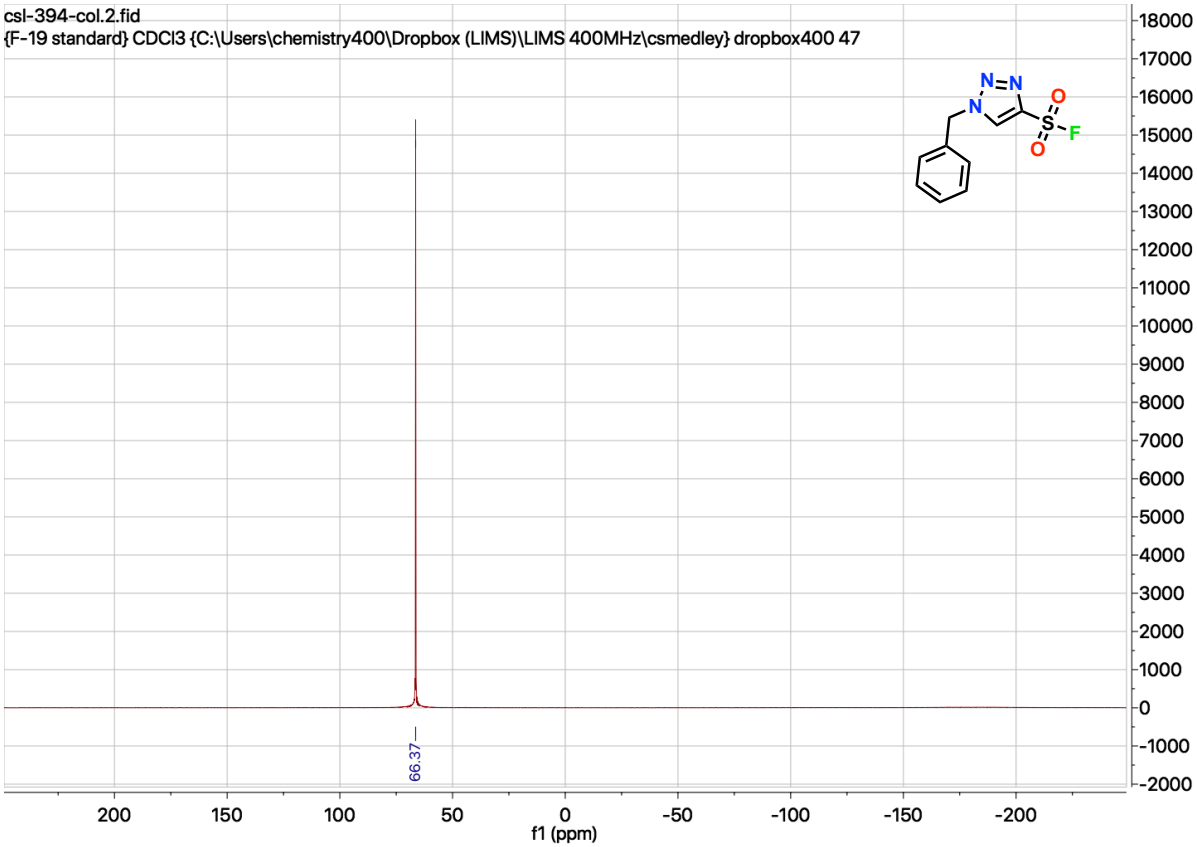

csl-255-data.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 9
f1 (ppm)

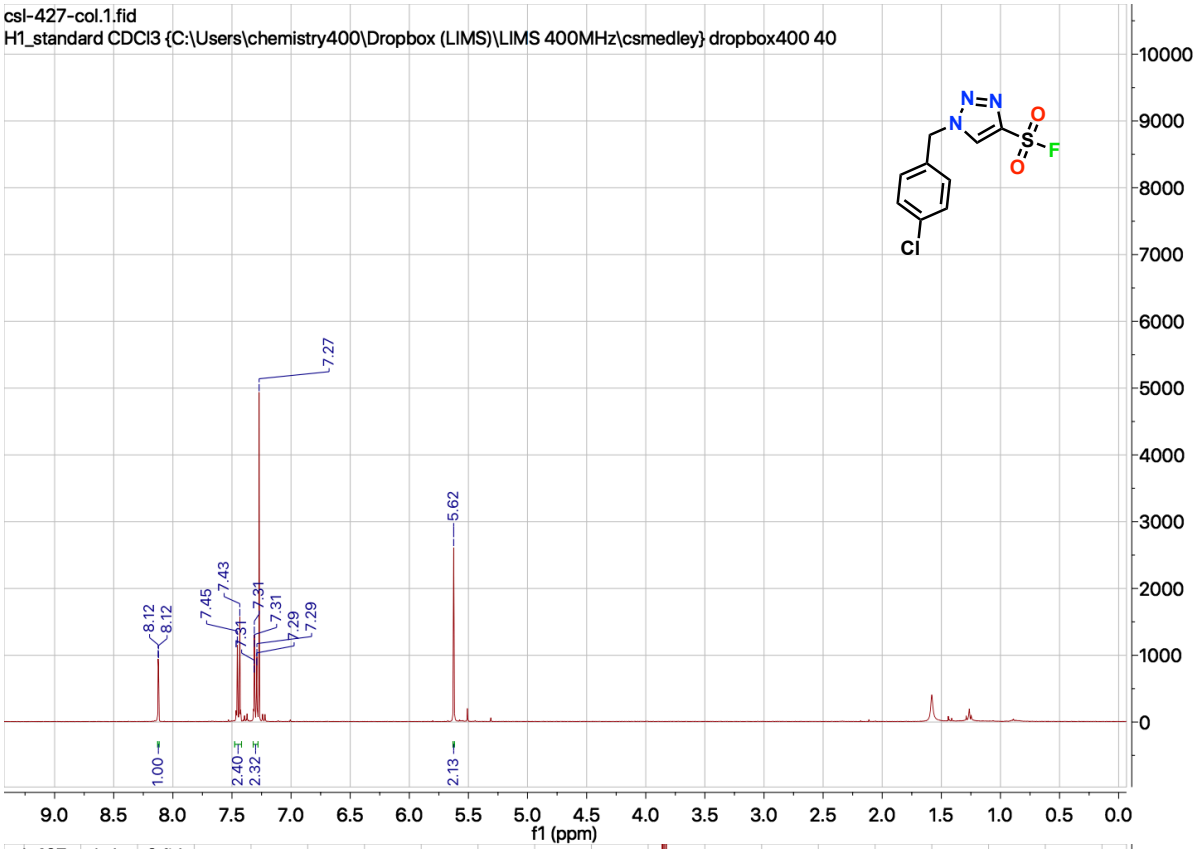

csl-255-CARBON.1.fid
C13 STANDARD
f1 (ppm)

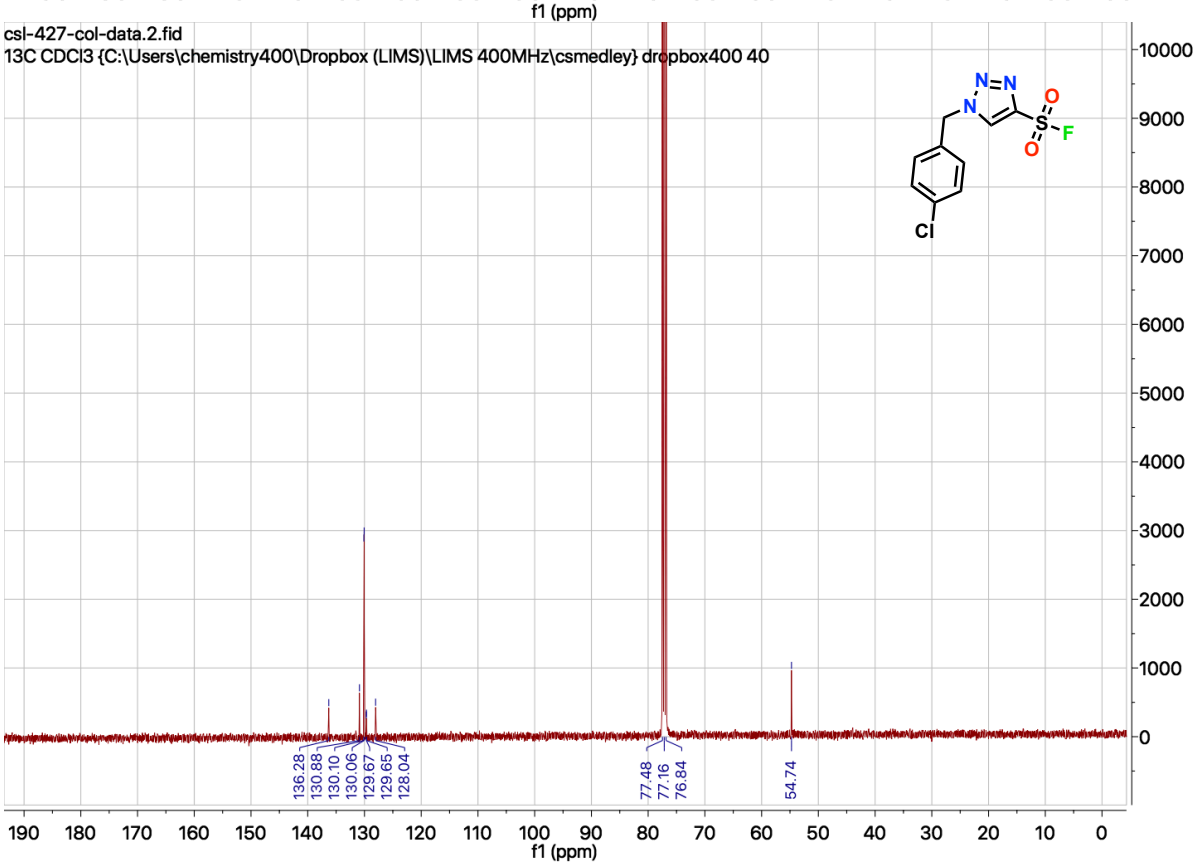

csl-255-data.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 9
35000
30000
25000
20000
15000
10000
5000
0
-5000
64.56
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
N
O
O
S
F
O
NO2

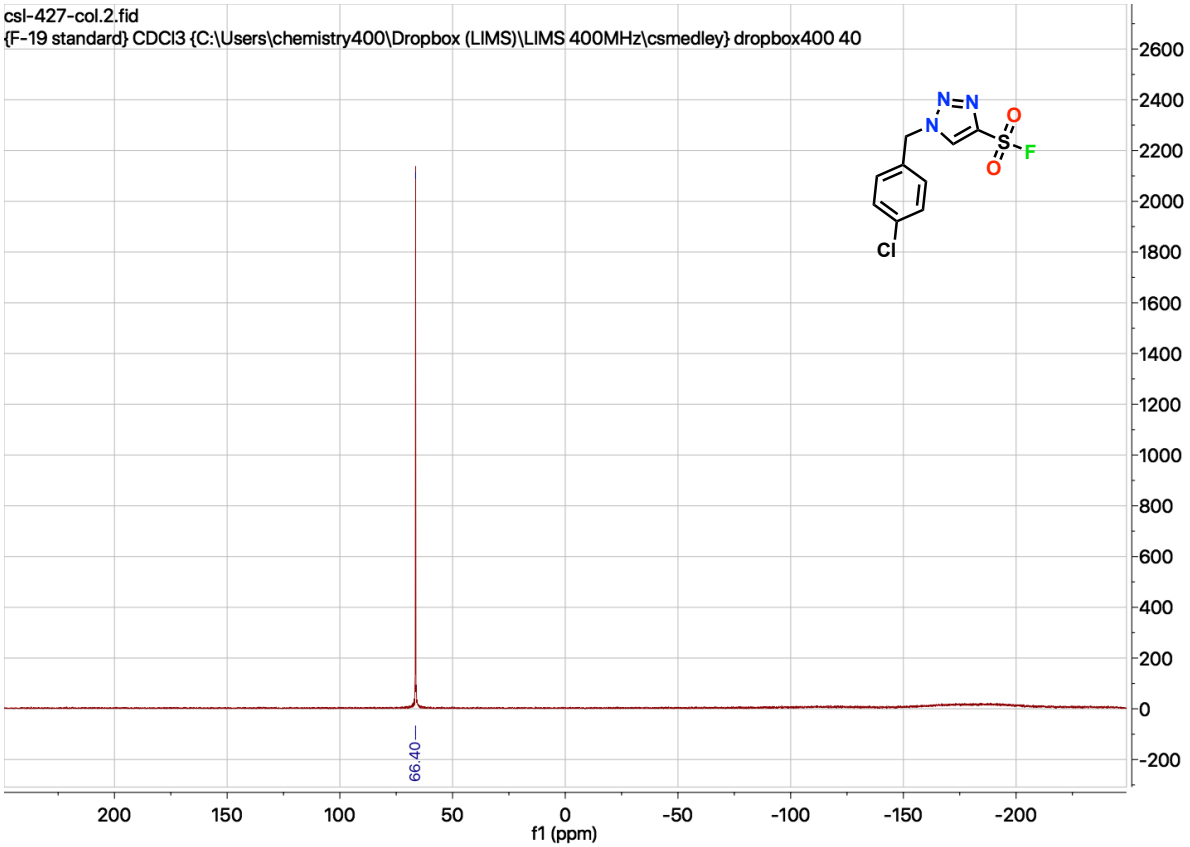

csl-394-1-proton.5.fid
Avance III -1H Spectrum
f1 (ppm)

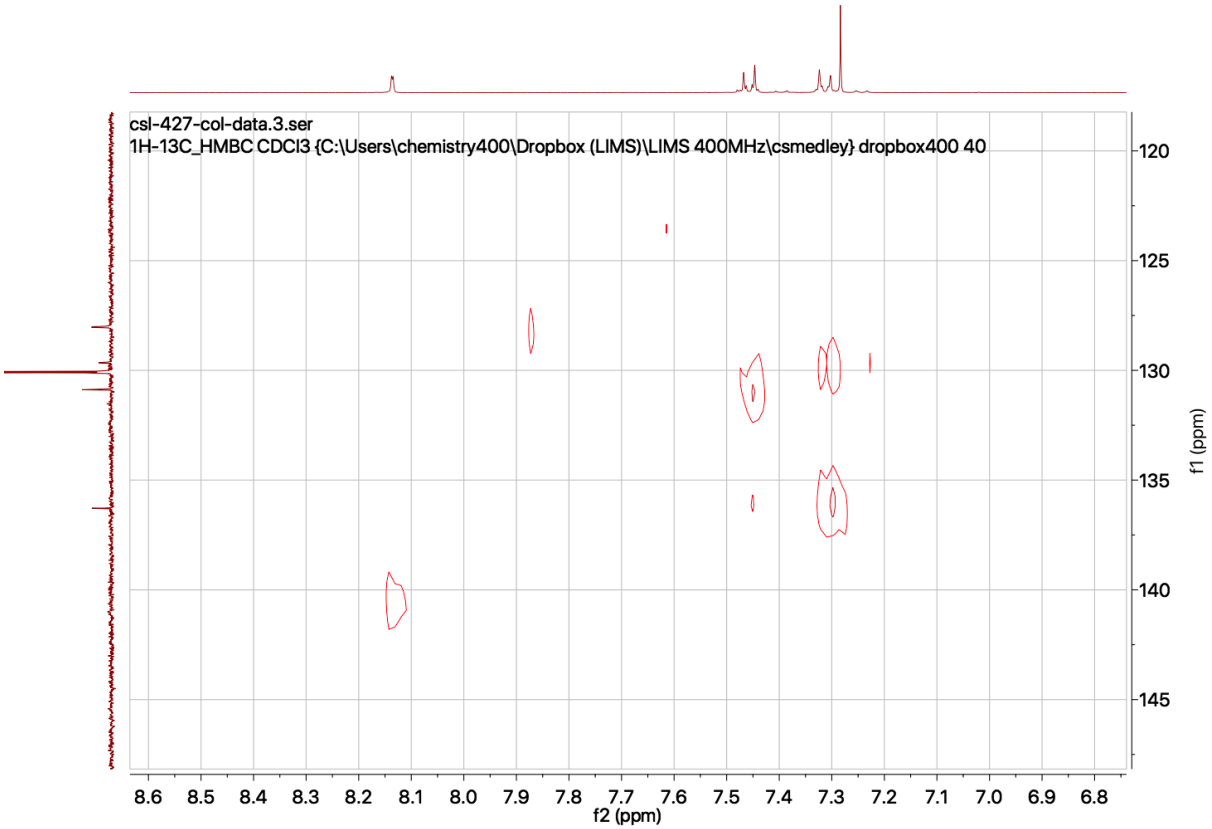

csl-394-1CARBON.6.fid
C13 STANDARD
f1 (ppm)

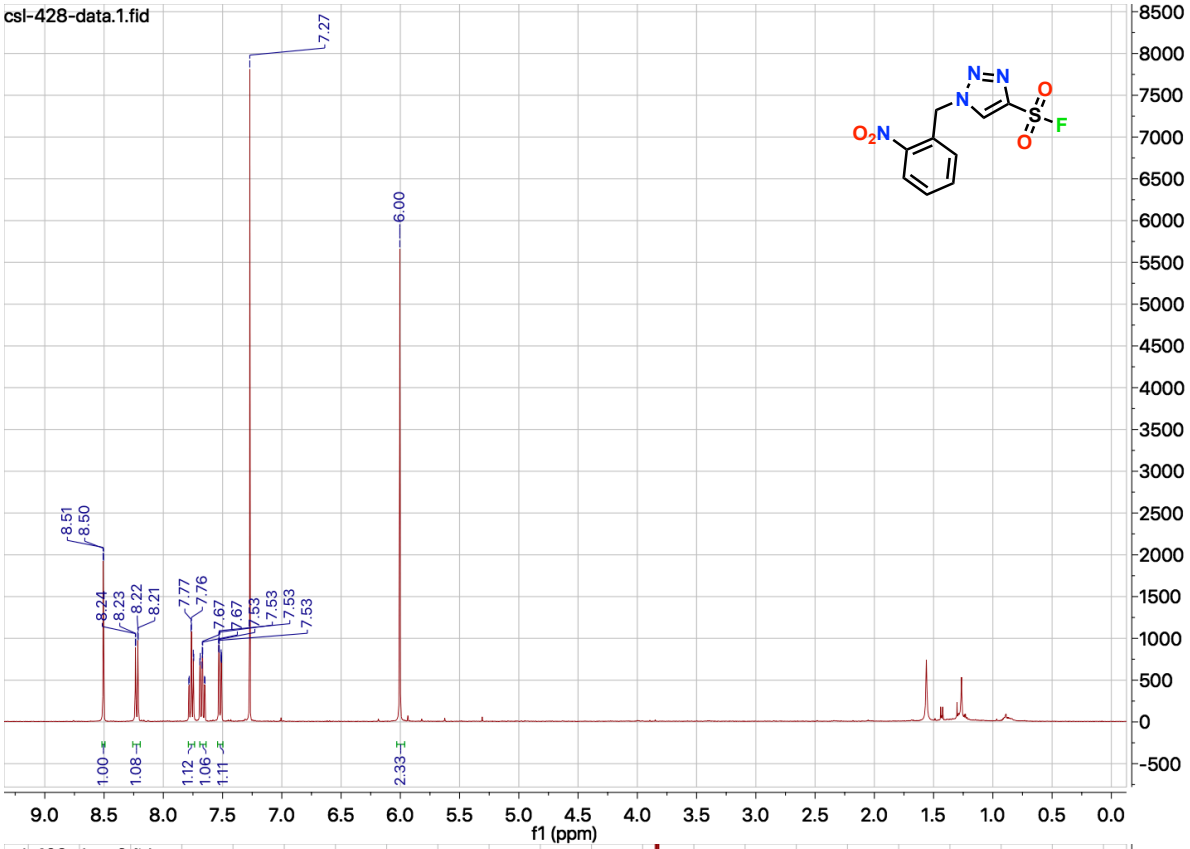

csl-394-col.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 47
66.37
f1 (ppm)

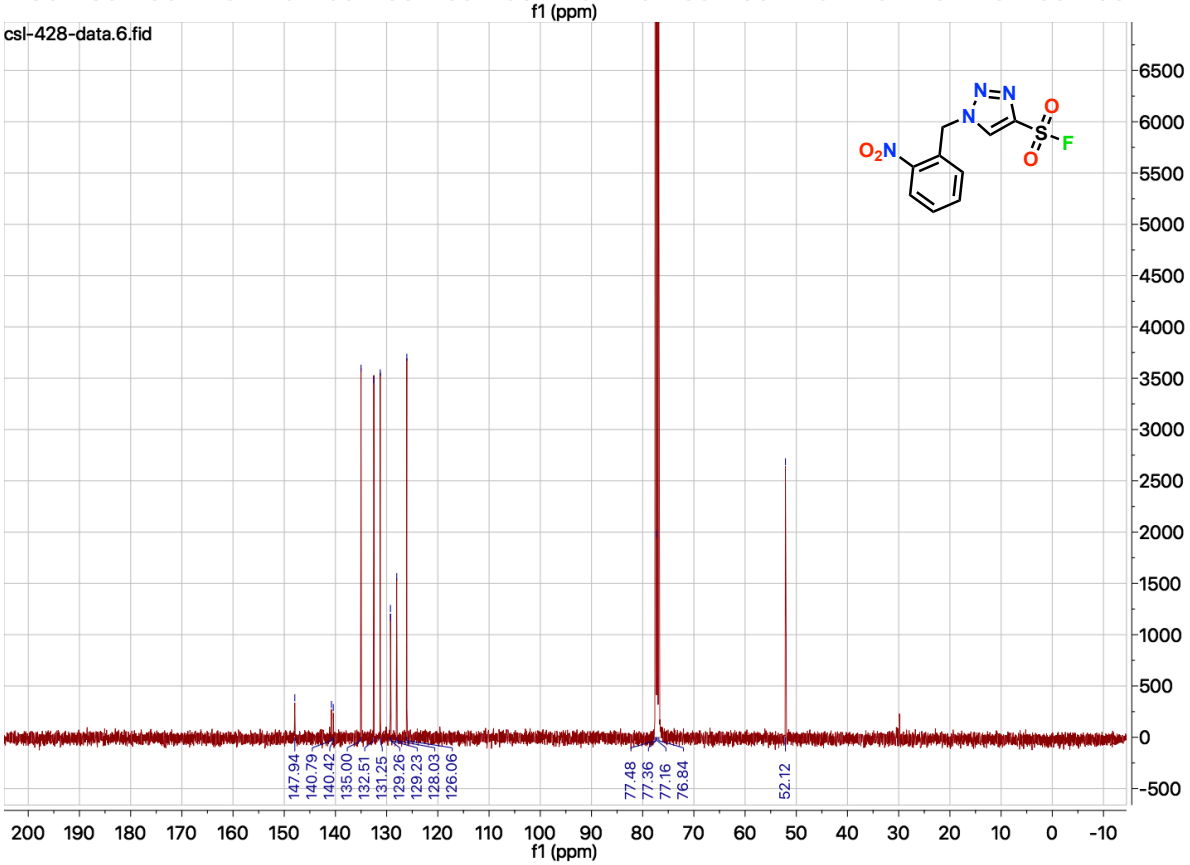

csl-427-col.1.fid
H1_standard CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 40
7.27
5.62
8.12
8.12
7.45
7.43
7.31
7.31
7.31
7.29
7.29
1.00
2.40
2.32
2.13
f1 (ppm)

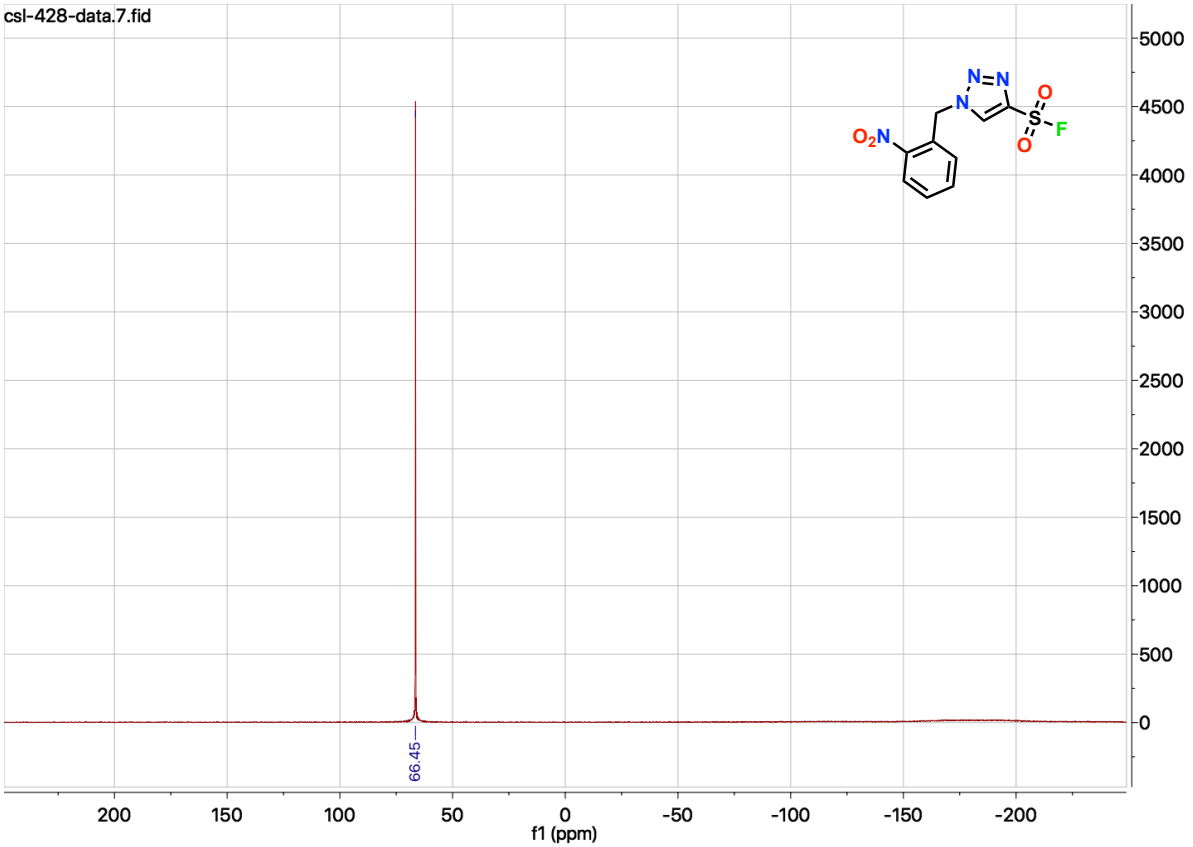

csl-427-col-data.2.fid
13C CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 40
136.28
130.88
130.10
130.06
129.67
129.65
128.04
77.48
77.16
76.84
54.74
f1 (ppm)

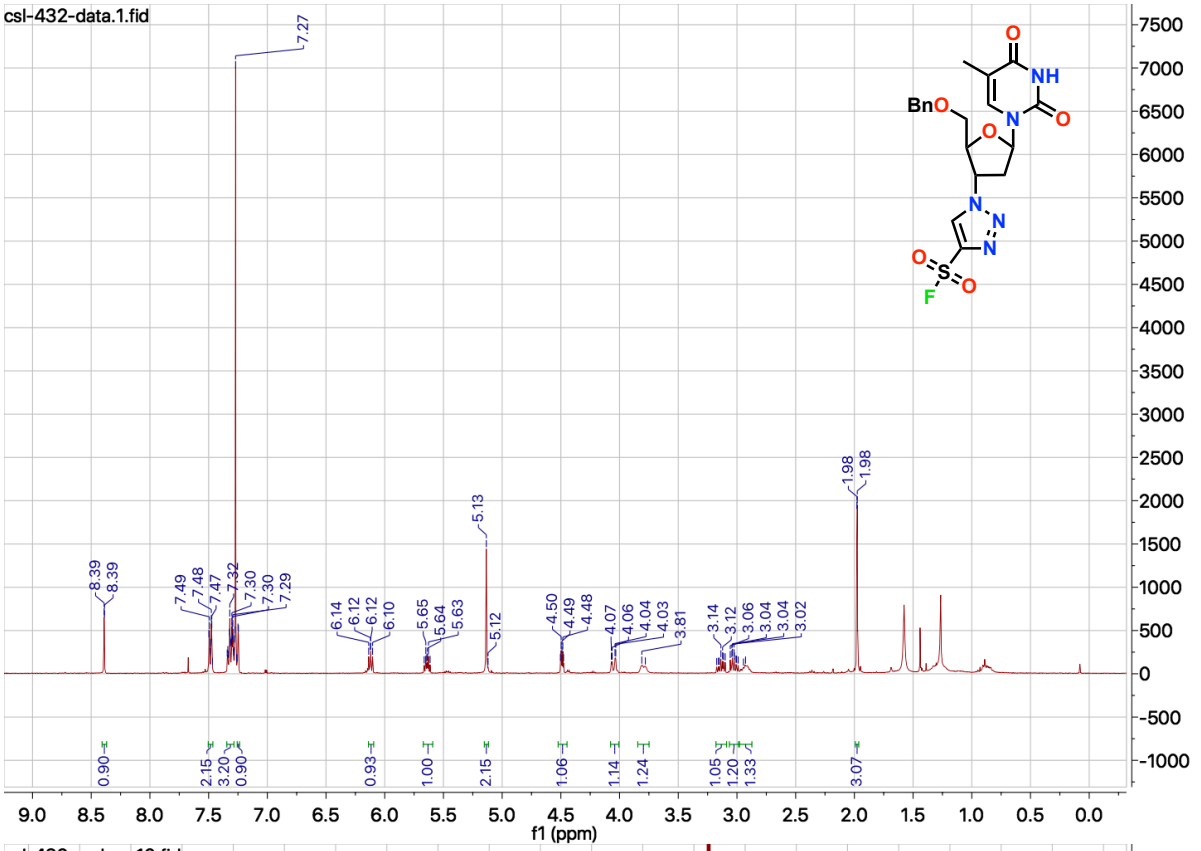

csl-427-col.2.fid
{F-19 standard} CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 40
N=N
N
O
S
F
O
Cl
66.40
f1 (ppm)

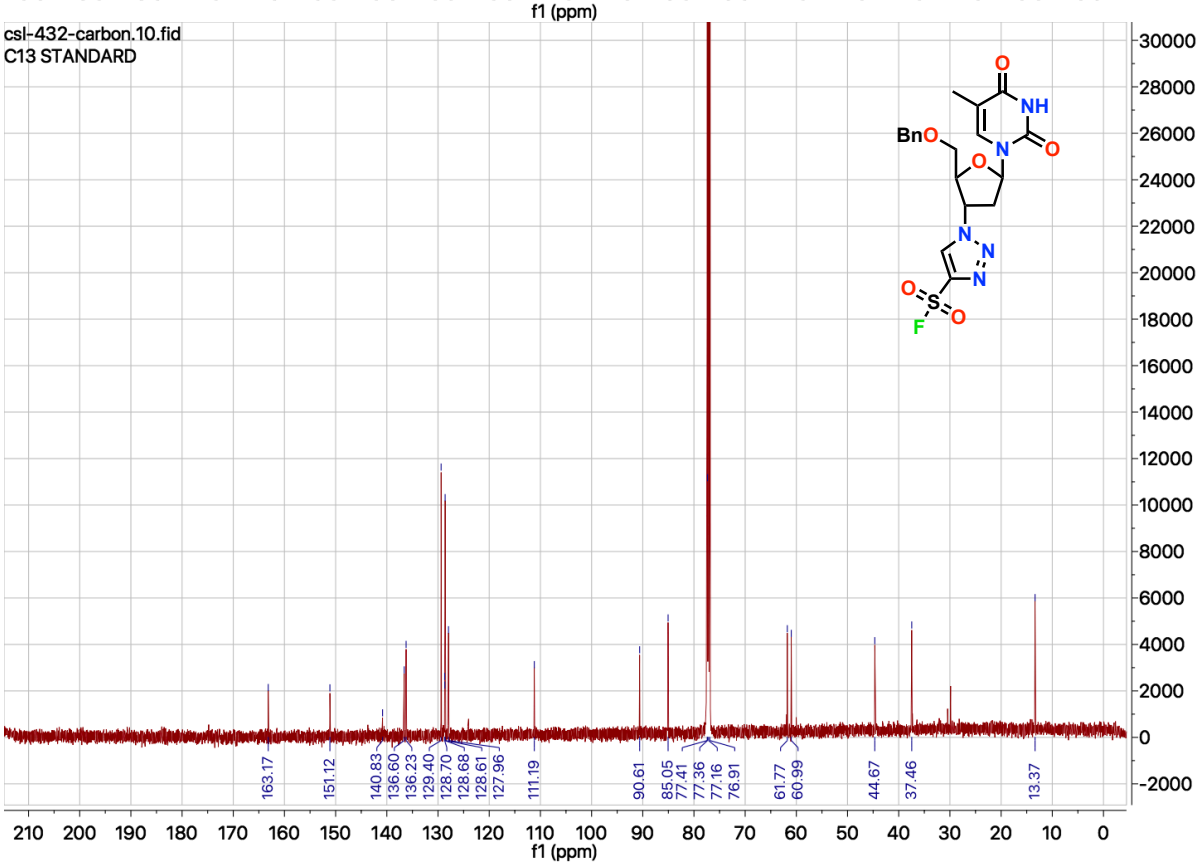

csl-427-col-data.3.ser
1H-13C_HMBC CDCl3 {C:\Users\chemistry400\Dropbox (LIMS)\LIMS 400MHz\csmedley} dropbox400 40
f2 (ppm)
f1 (ppm)

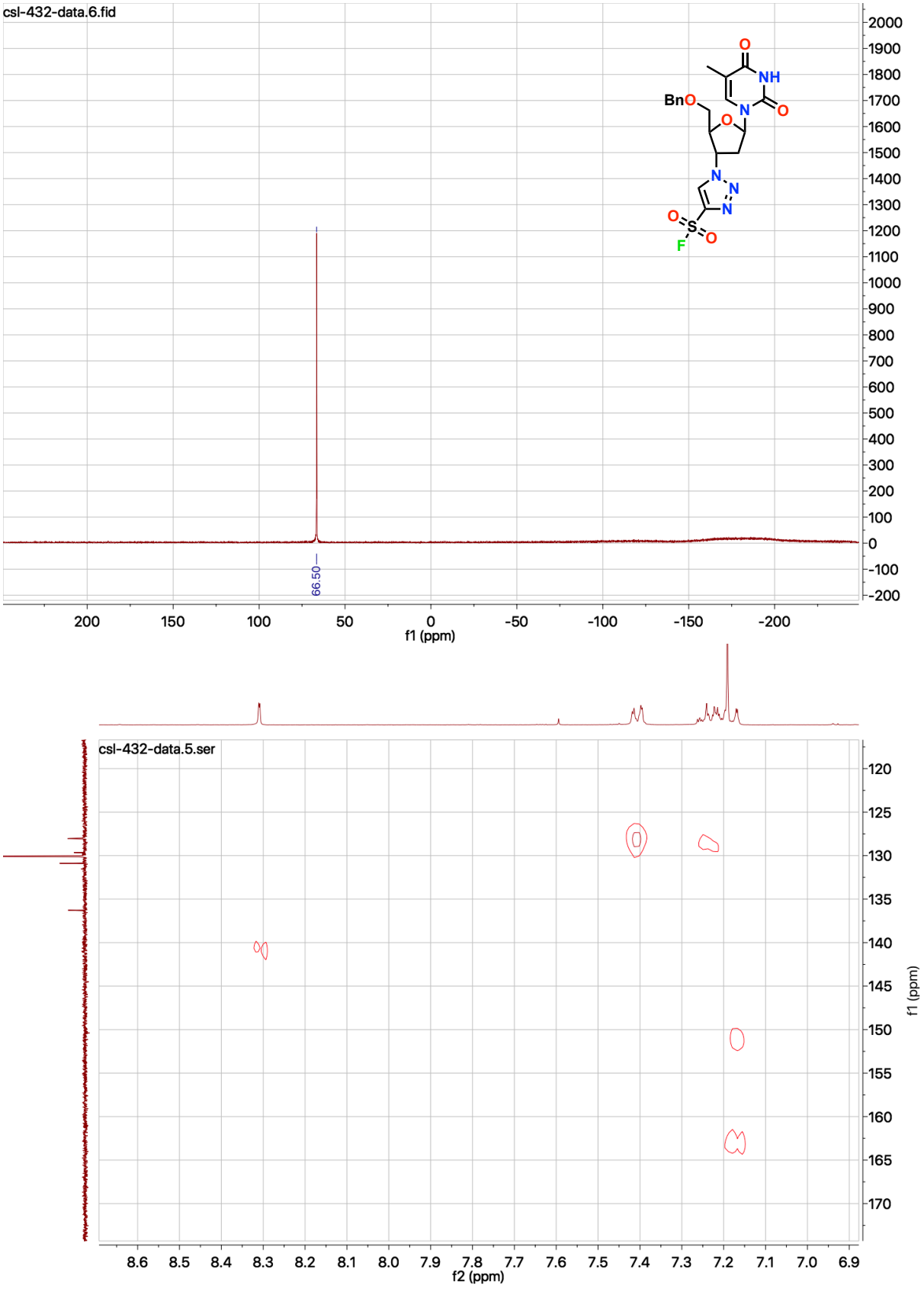

csl-428-data.1.fid
7.27
6.00
8.51
8.50
8.24
8.23
8.22
8.21
7.77
7.76
7.67
7.67
7.53
7.53
7.53
1.00
1.08
1.12
1.06
1.11
2.33
f1 (ppm)

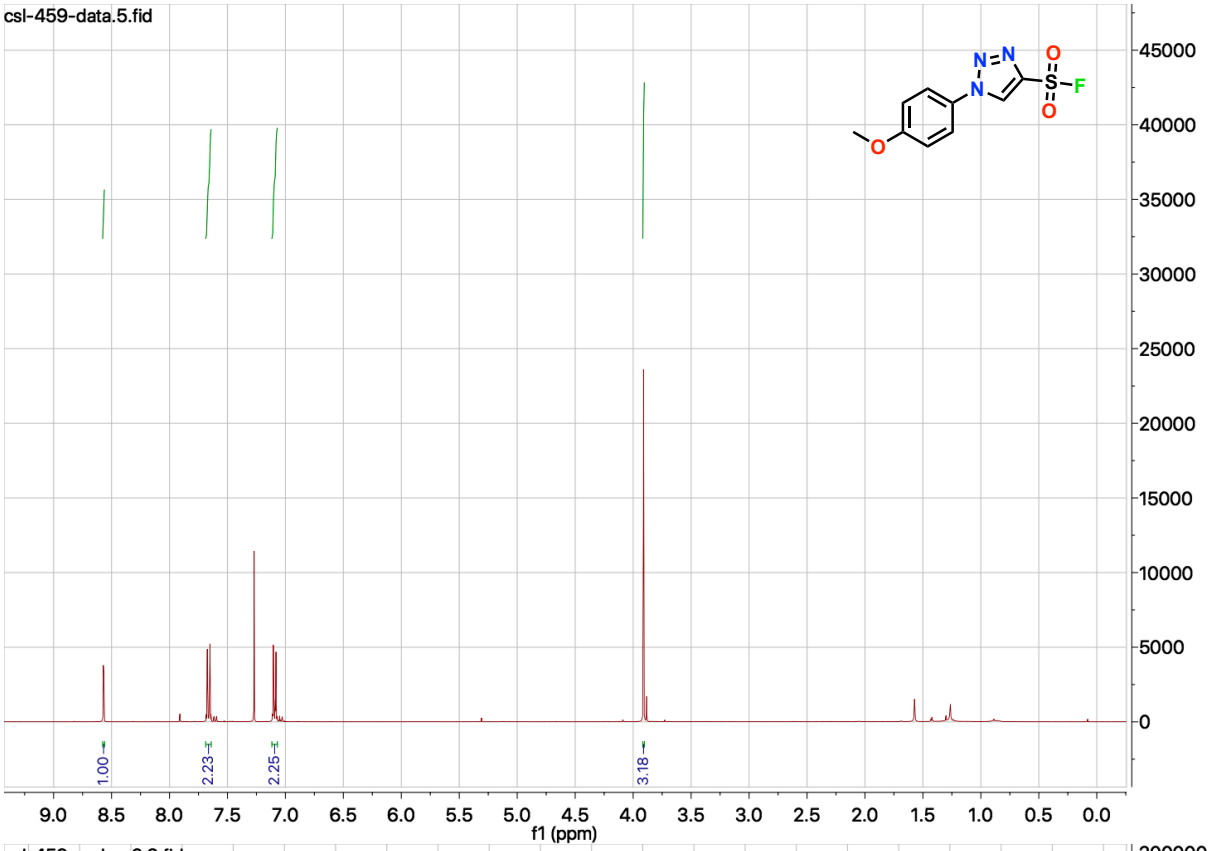

csl-428-data.6.fid
147.94
140.79
140.42
135.00
132.51
131.25
129.26
129.23
128.03
126.06
77.48
77.36
77.16
76.84
52.12
f1 (ppm)

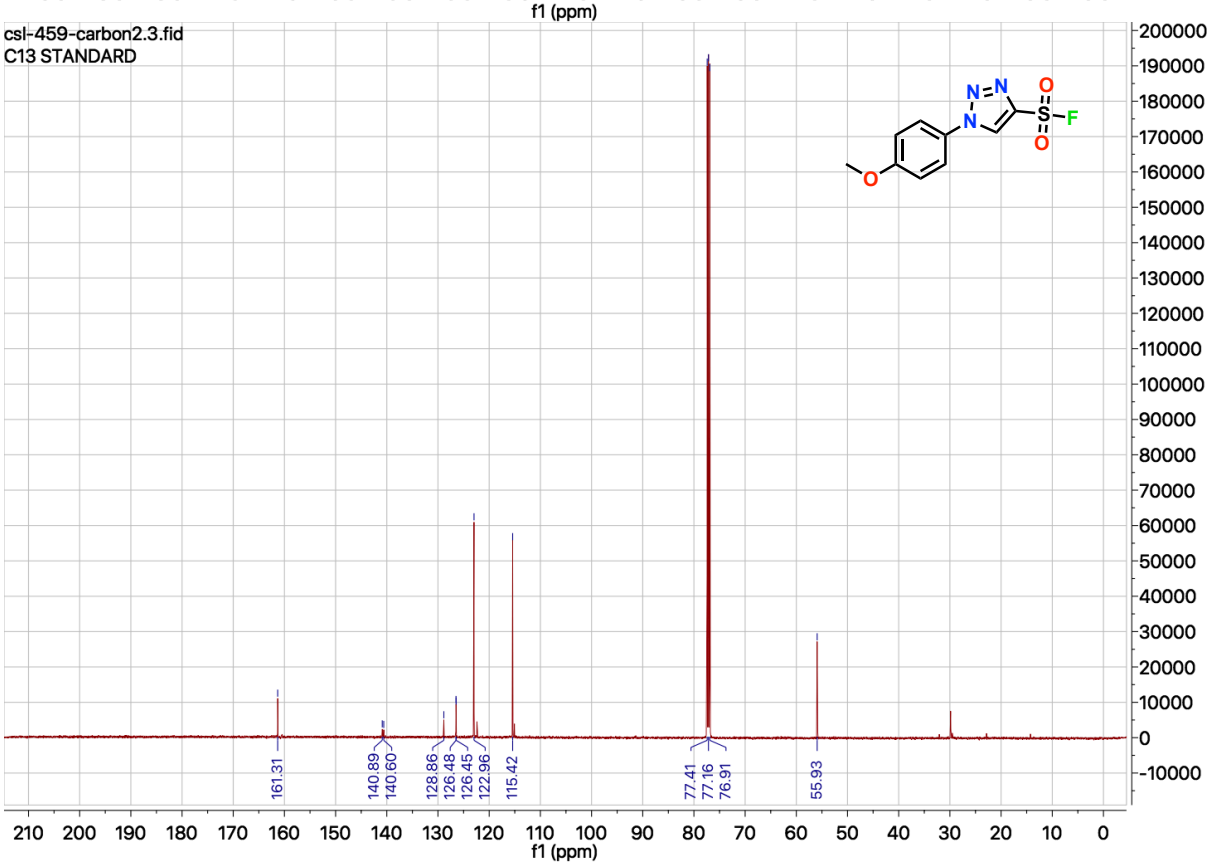

csl-428-data.7.fid
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
66.45
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
N=N
N
O
S
F
O
O2N

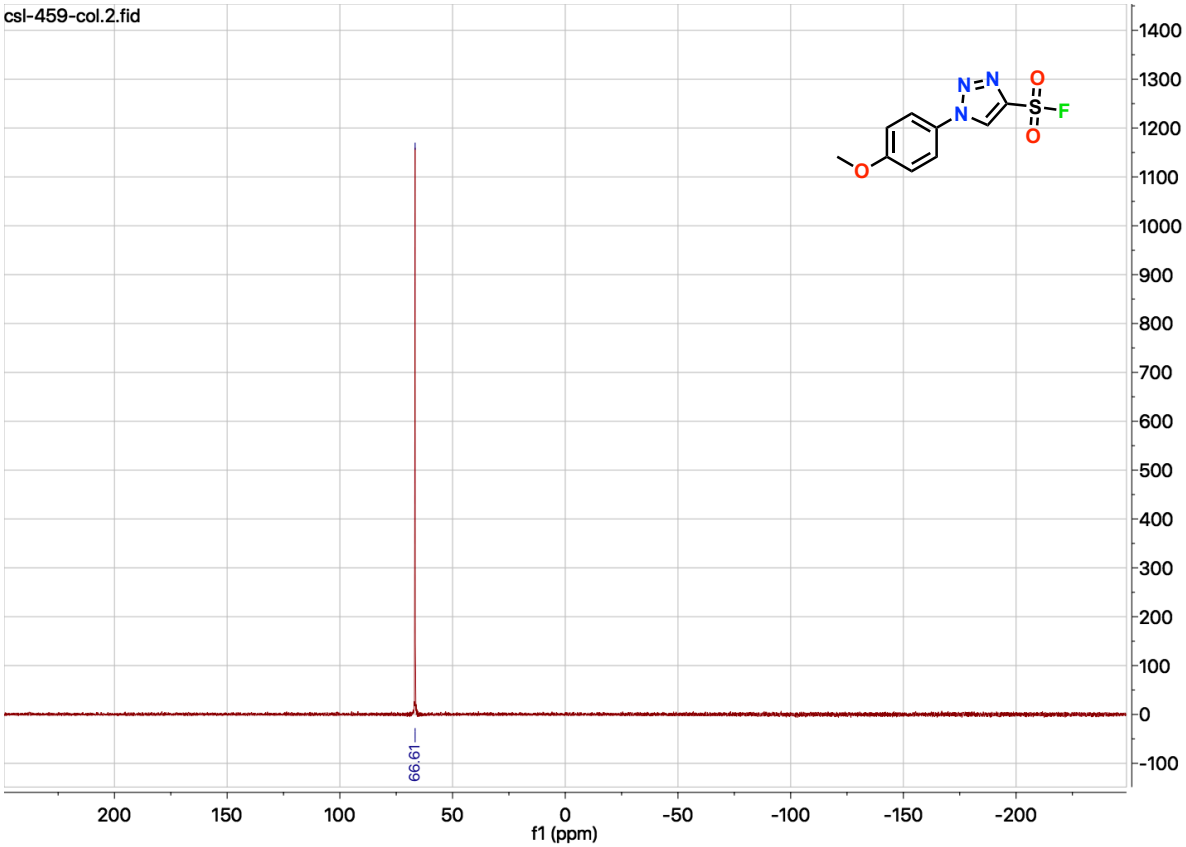

csl-432-data.1.fid
f1 (ppm)

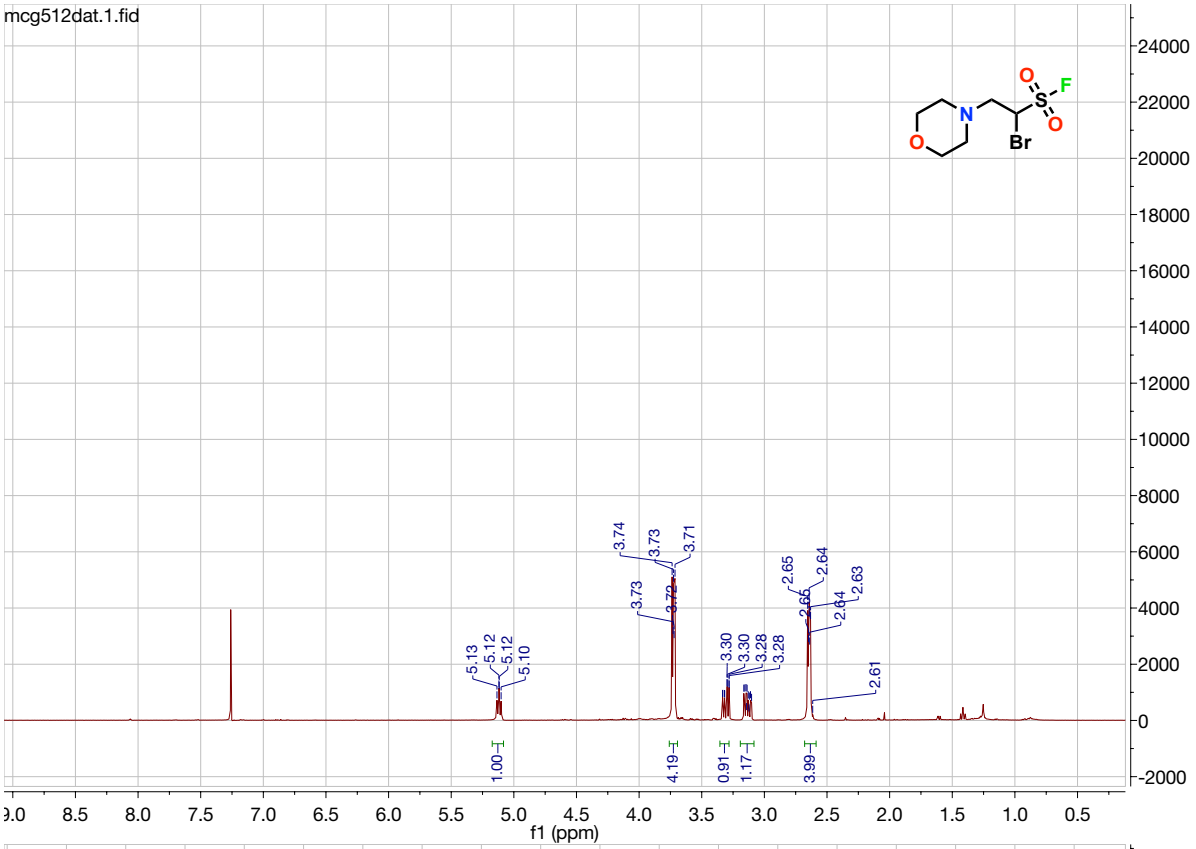

csl-432-carbon.10.fid
C13 STANDARD
f1 (ppm)

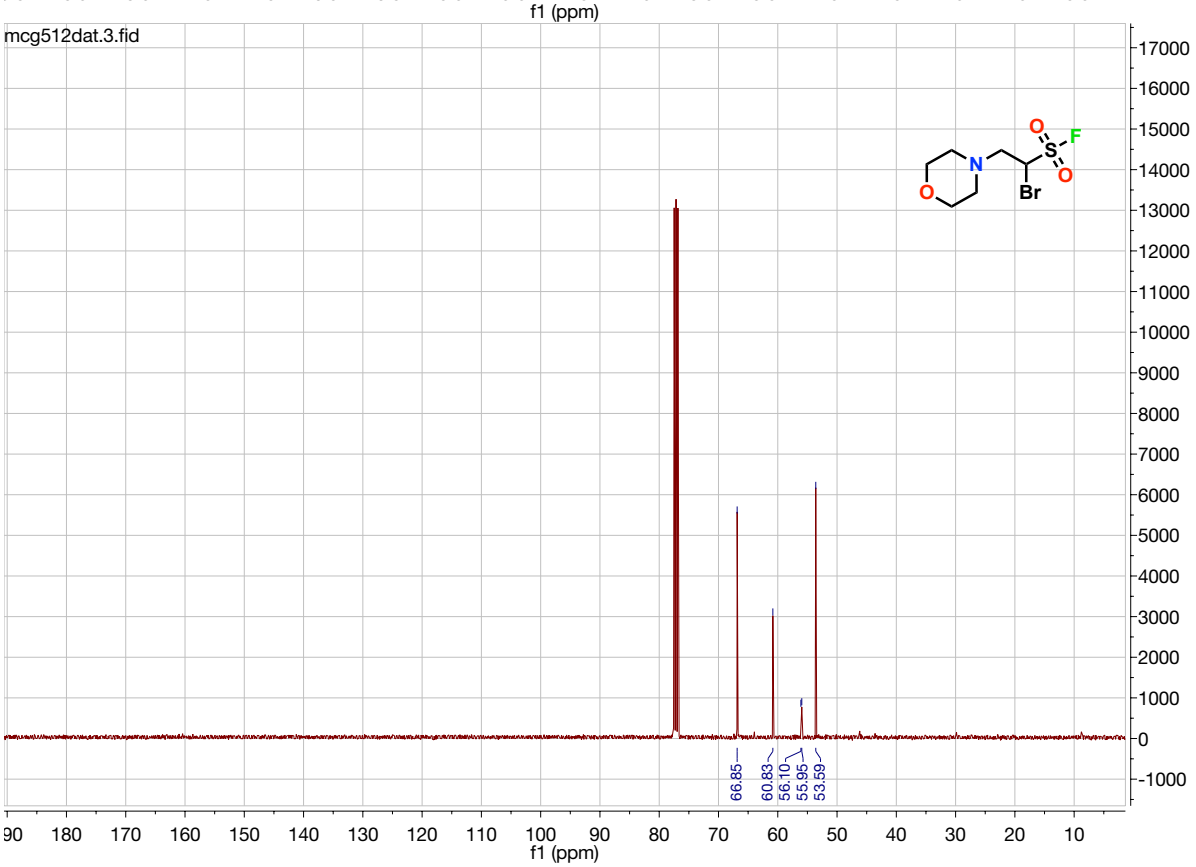

csl-432-data.6.fid
66.50
f1 (ppm)
csl-432-data.5.ser
f2 (ppm)
f1 (ppm)

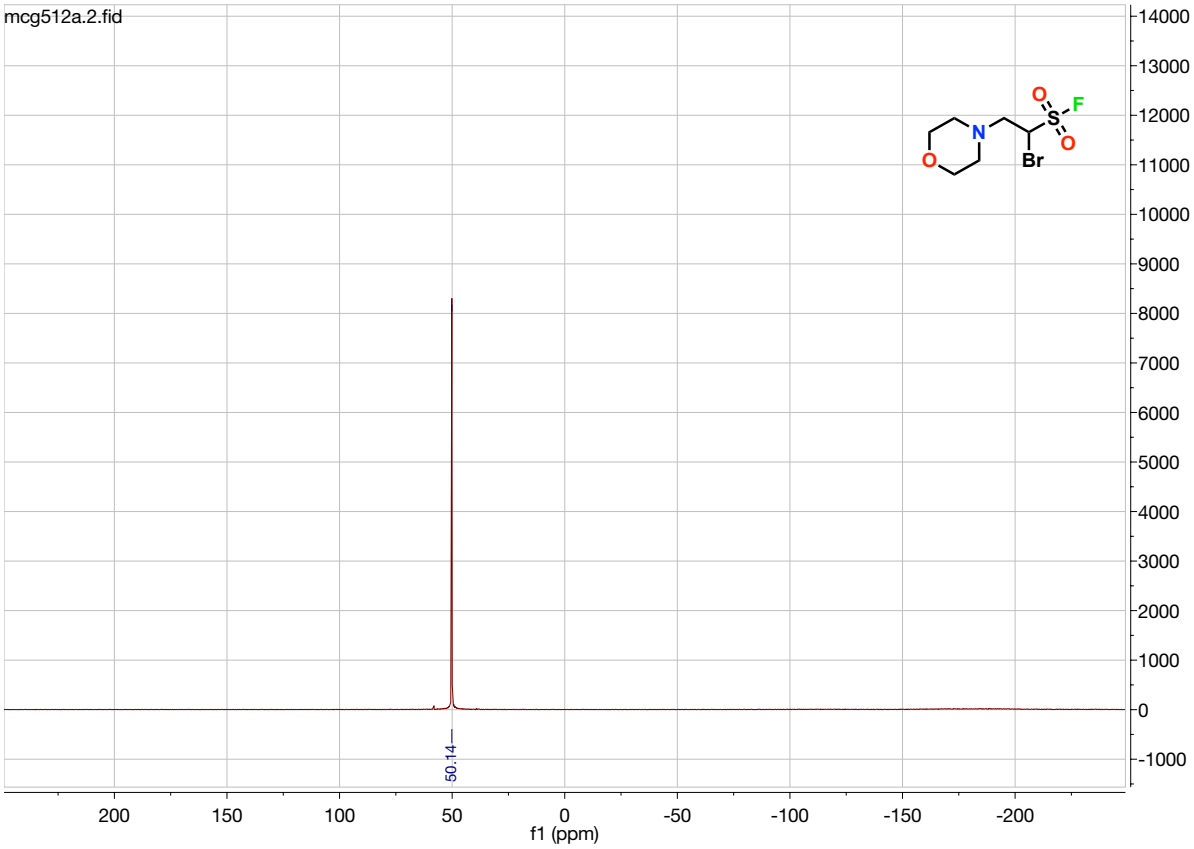

csl-459-data.5.fid
1.00
2.23
2.25
3.18
f1 (ppm)

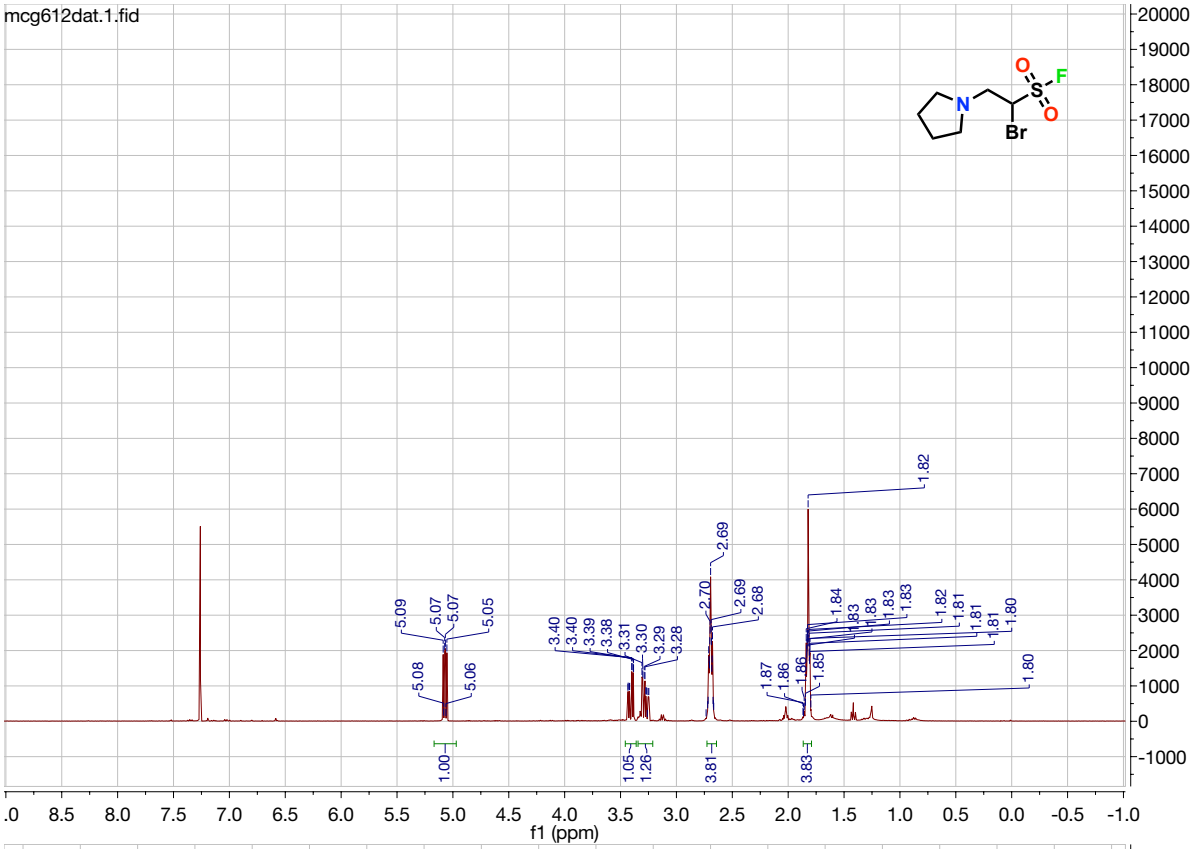

csl-459-carbon2.3.fid
C13 STANDARD
161.31
140.89
140.60
128.86
126.48
126.45
122.96
115.42
77.41
77.16
76.91
55.93
f1 (ppm)

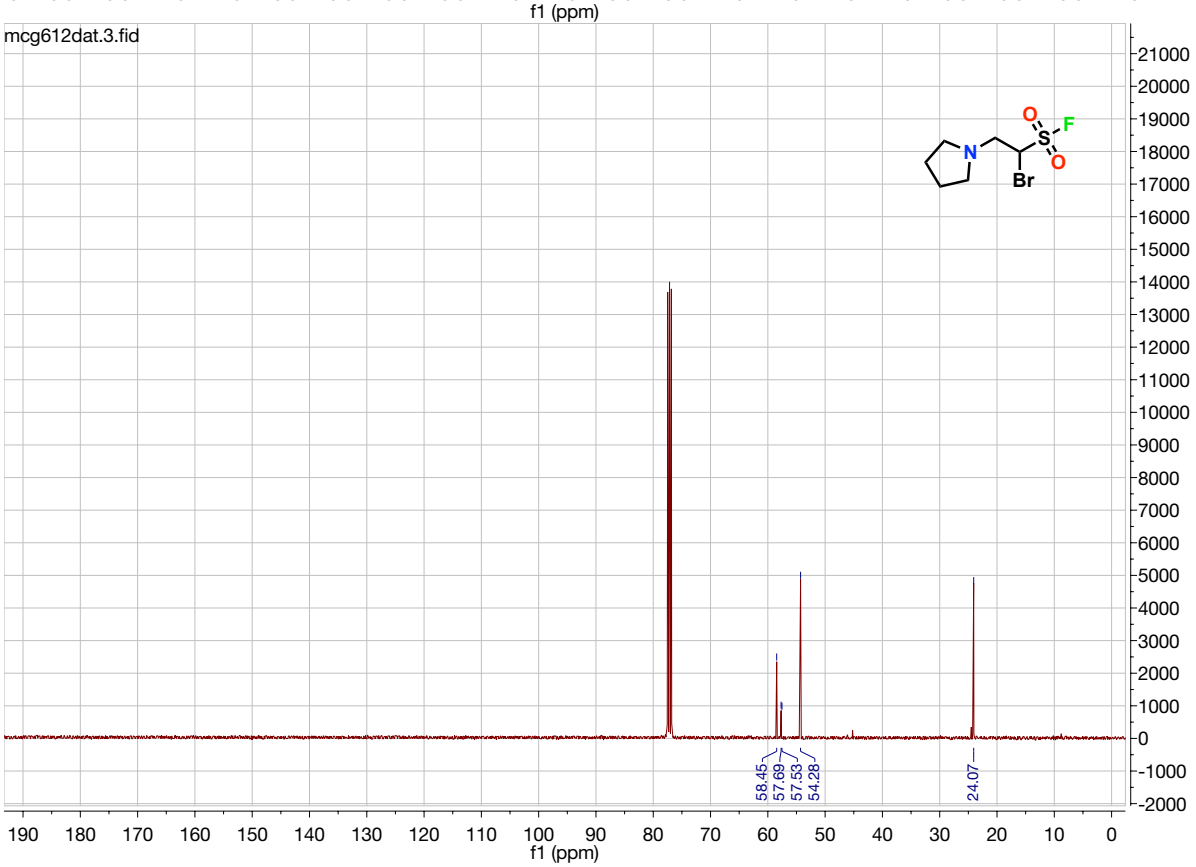

csl-459-col.2.fid
66.61
f1 (ppm)

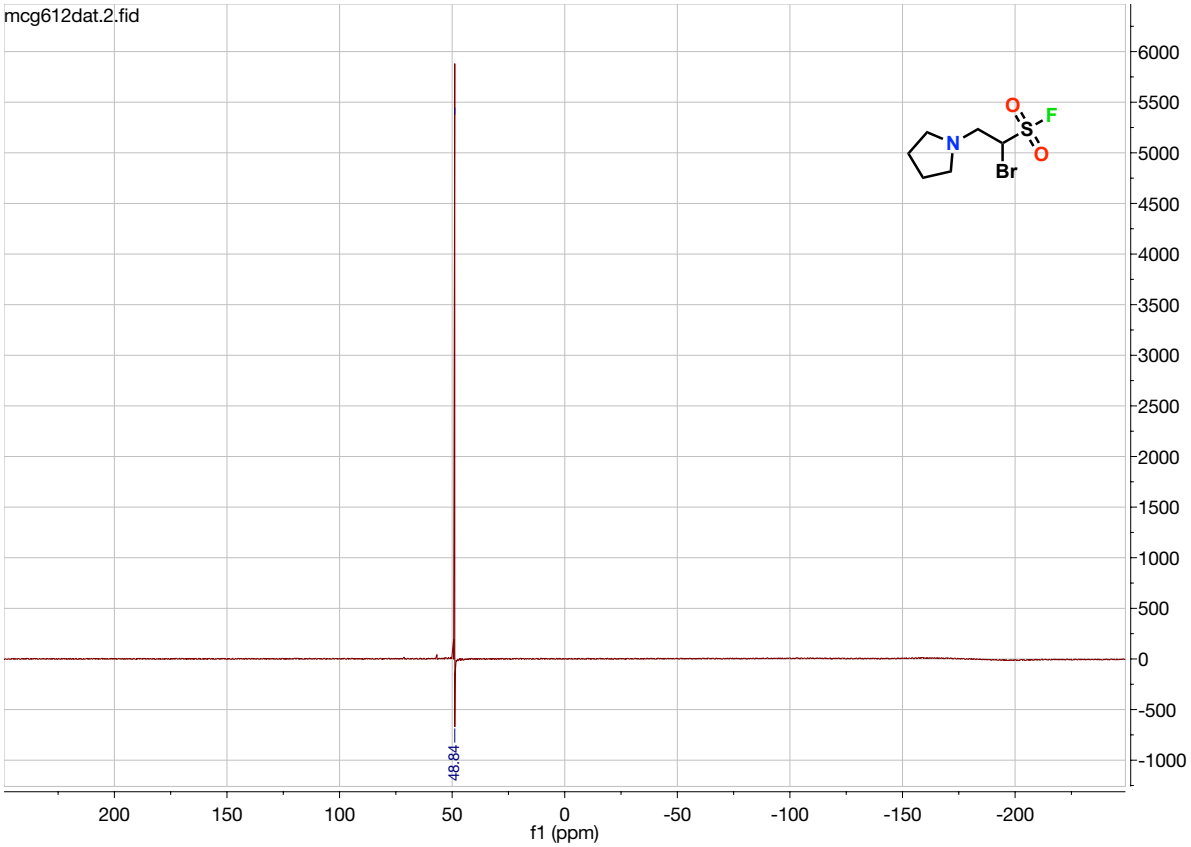

mcg512dat.1.fid
O
S
F
O
N
O
Br
3.74
3.73
3.71
3.73
3.72
2.65
2.64
2.63
2.65
2.64
5.13
5.12
5.12
5.10
3.30
3.30
3.28
3.28
2.61
1.00
4.19
0.91
1.17
3.99
f1 (ppm)

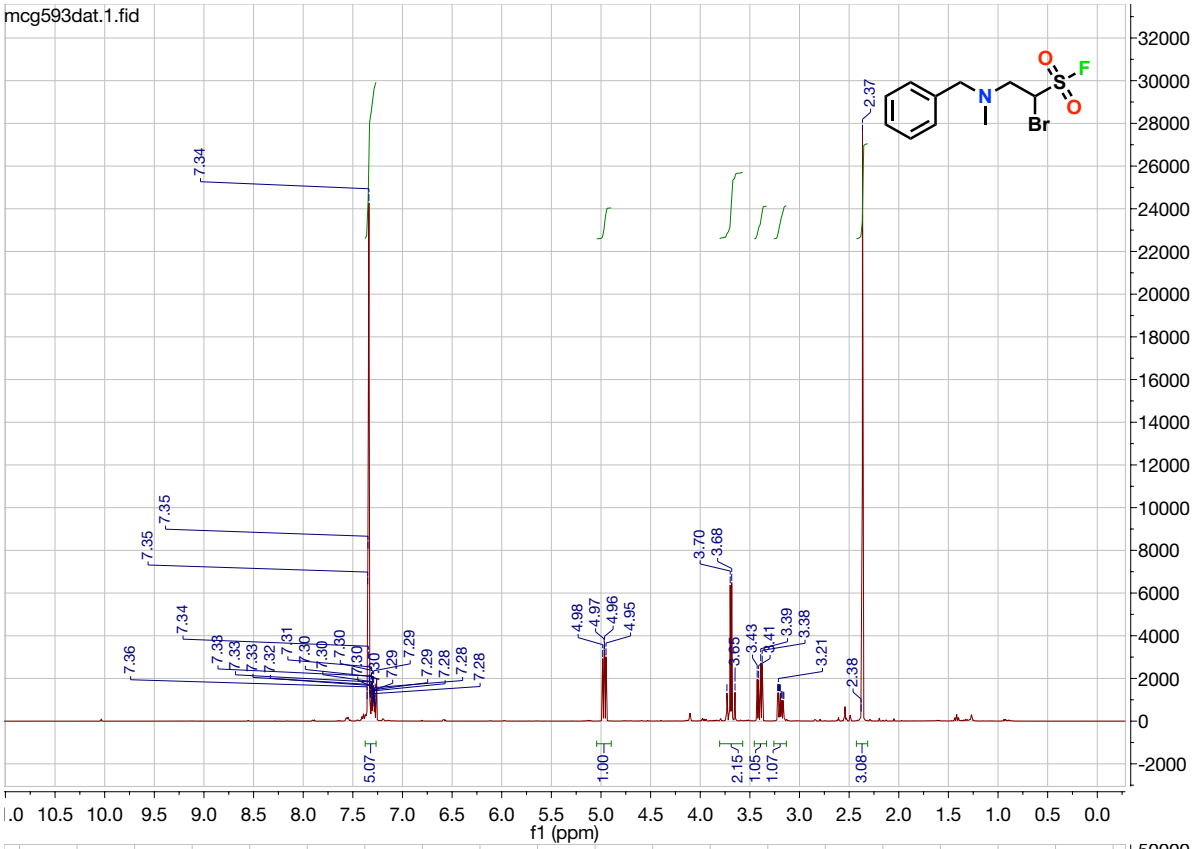

mcg512dat.3.fid
O
S
F
O
N
O
Br
66.85
60.83
56.10
55.95
53.59
f1 (ppm)

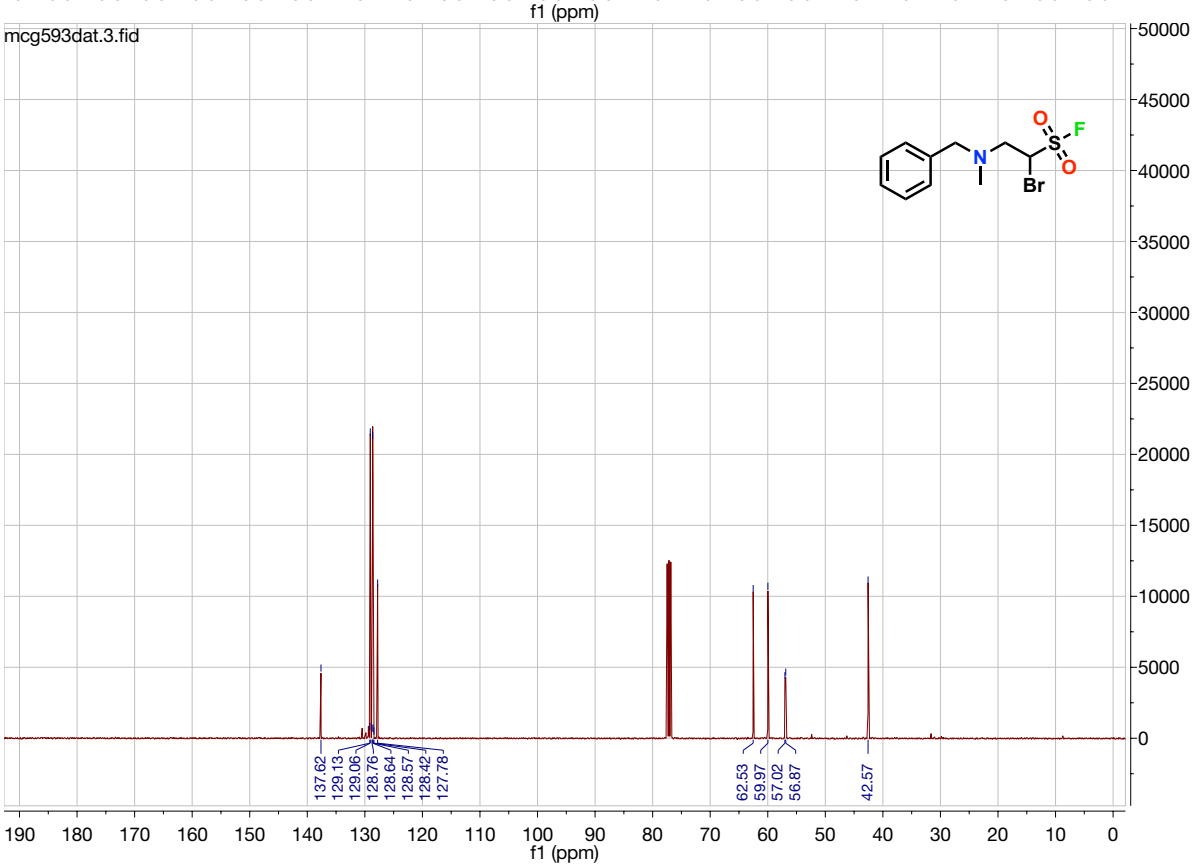

mcg512a.2.fid
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
50.14
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
O
S
F
O
N
O
Br

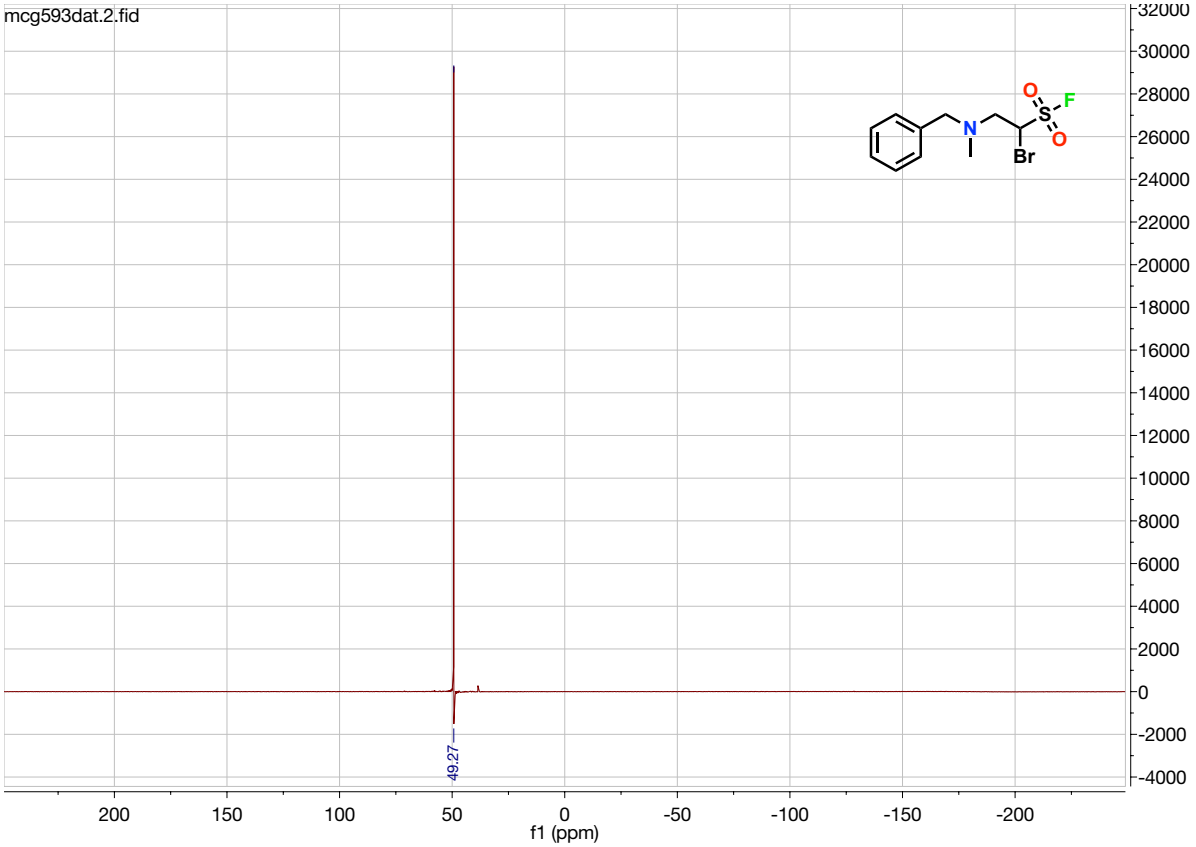

mcg612dat.1.fid
f1 (ppm)

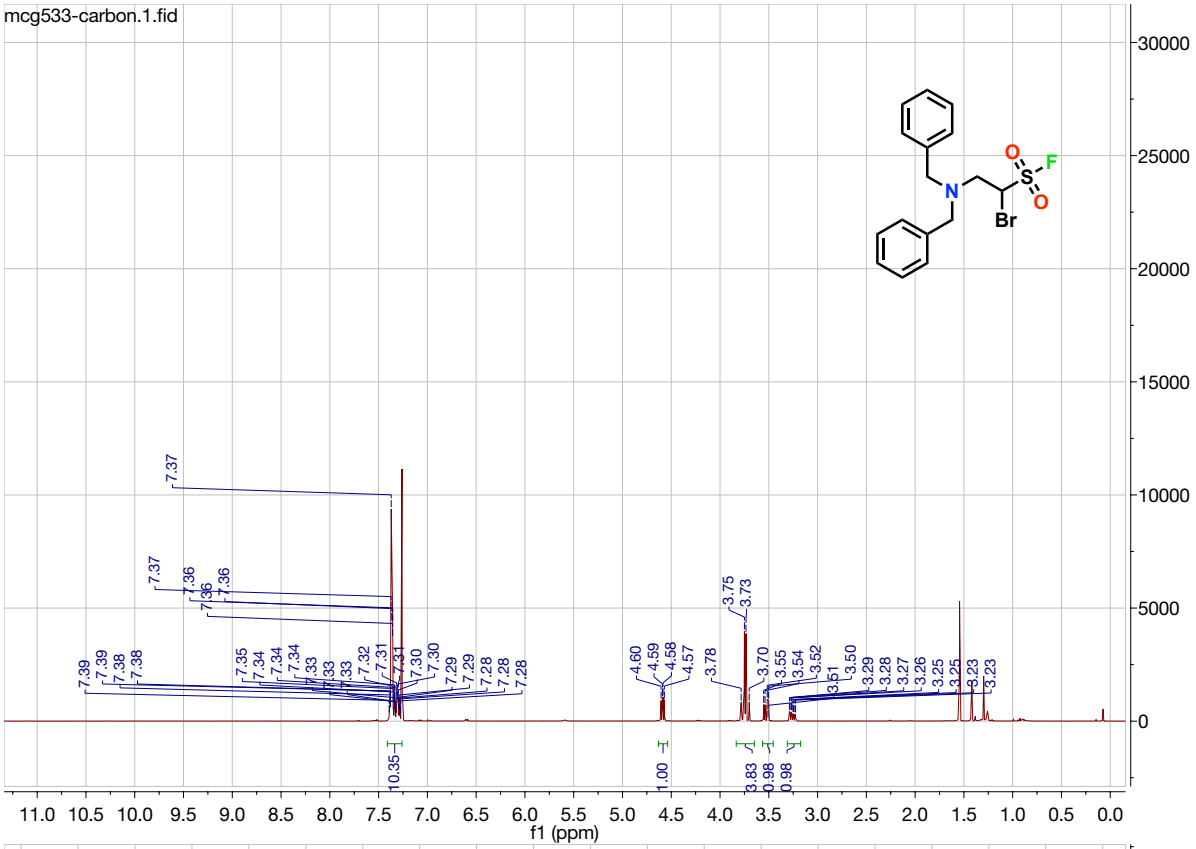

mcg612dat.3.fid
f1 (ppm)

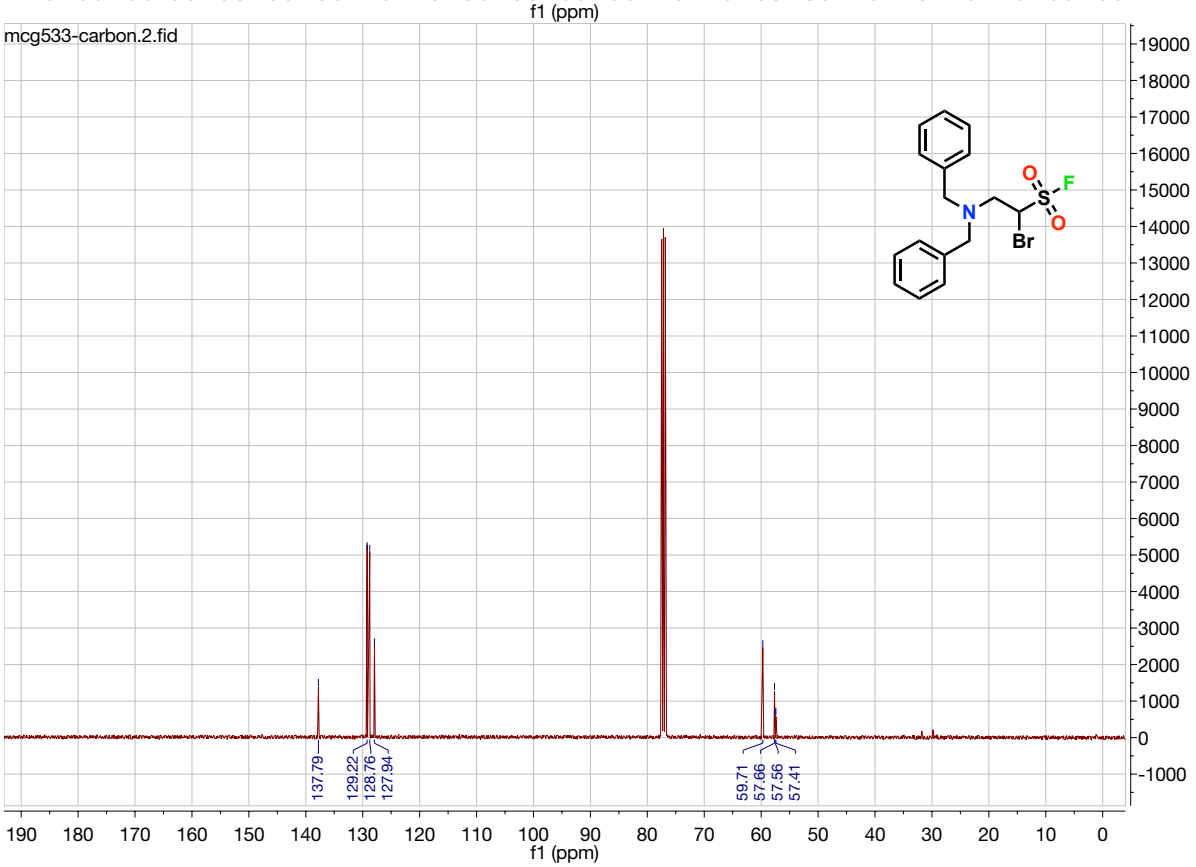

mcg612dat.2.fid
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
48.84
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
O
F
S
N
O
Br

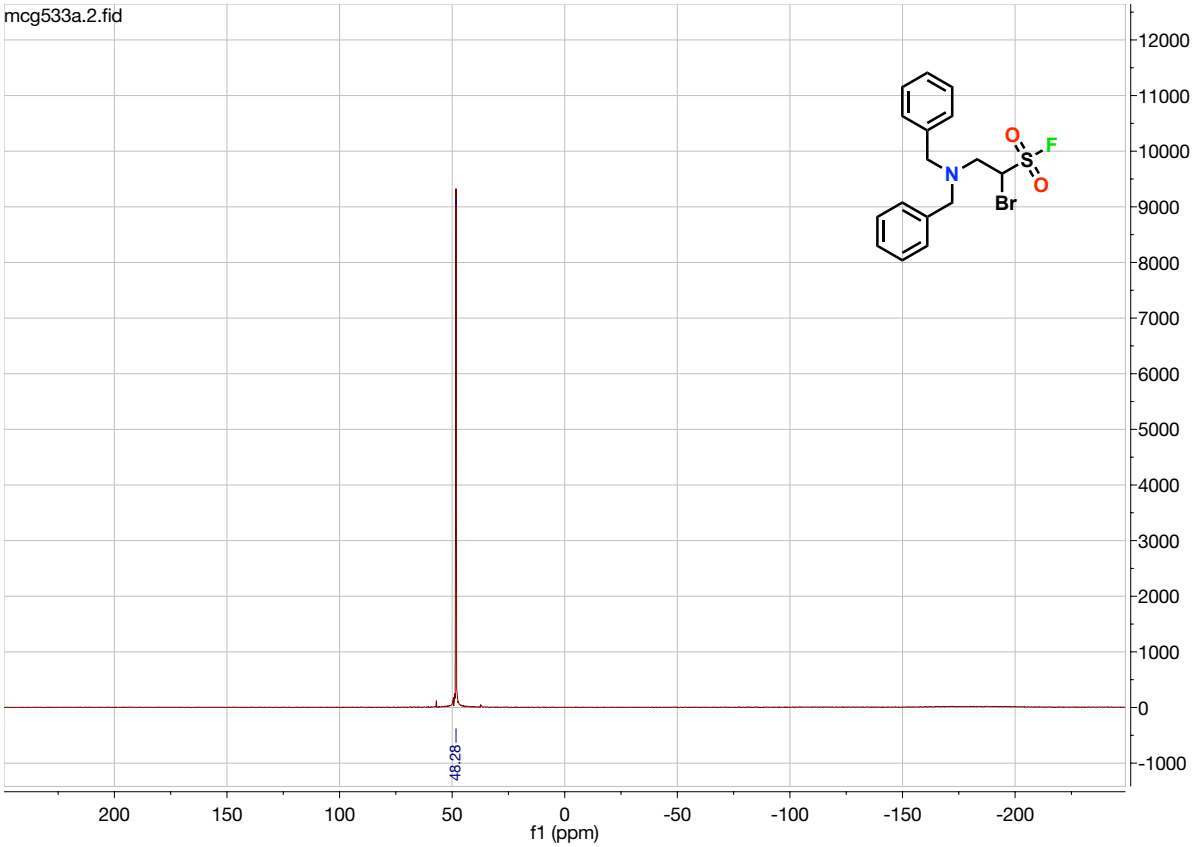

mcg593dat.1.fid
7.34
7.35
7.35
7.34
7.36
7.38
7.33
7.33
7.32
7.31
7.30
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.28
4.98
4.97
4.96
4.95
3.70
3.68
3.65
3.43
3.41
3.39
3.38
3.21
2.38
2.37
5.07
1.00
2.15
1.05
1.07
3.08
f1 (ppm)

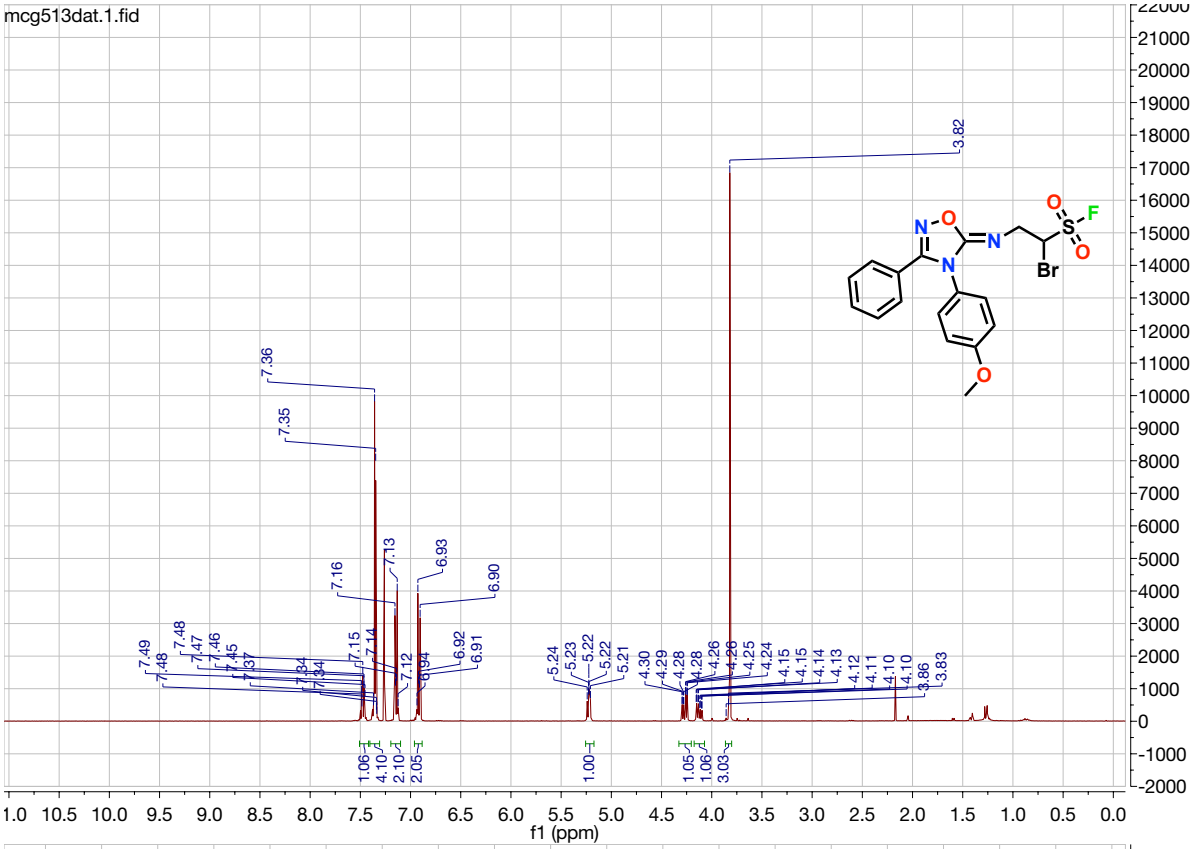

mcg593dat.3.fid
137.62
129.13
129.06
128.76
128.64
128.57
128.42
127.78
62.53
59.97
57.02
56.87
42.57
f1 (ppm)

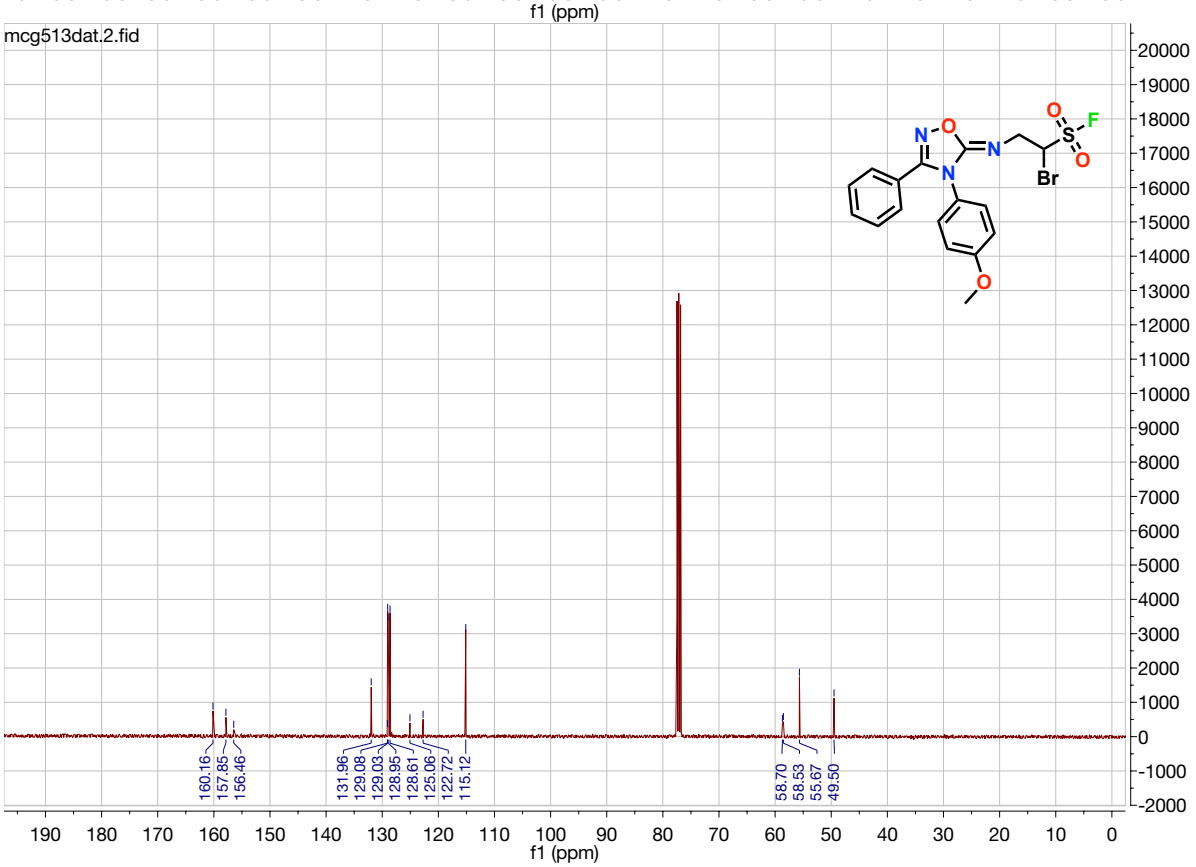

mcg593dat.2.fid
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-4000
49.27
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
O
F
S
O
N
Br

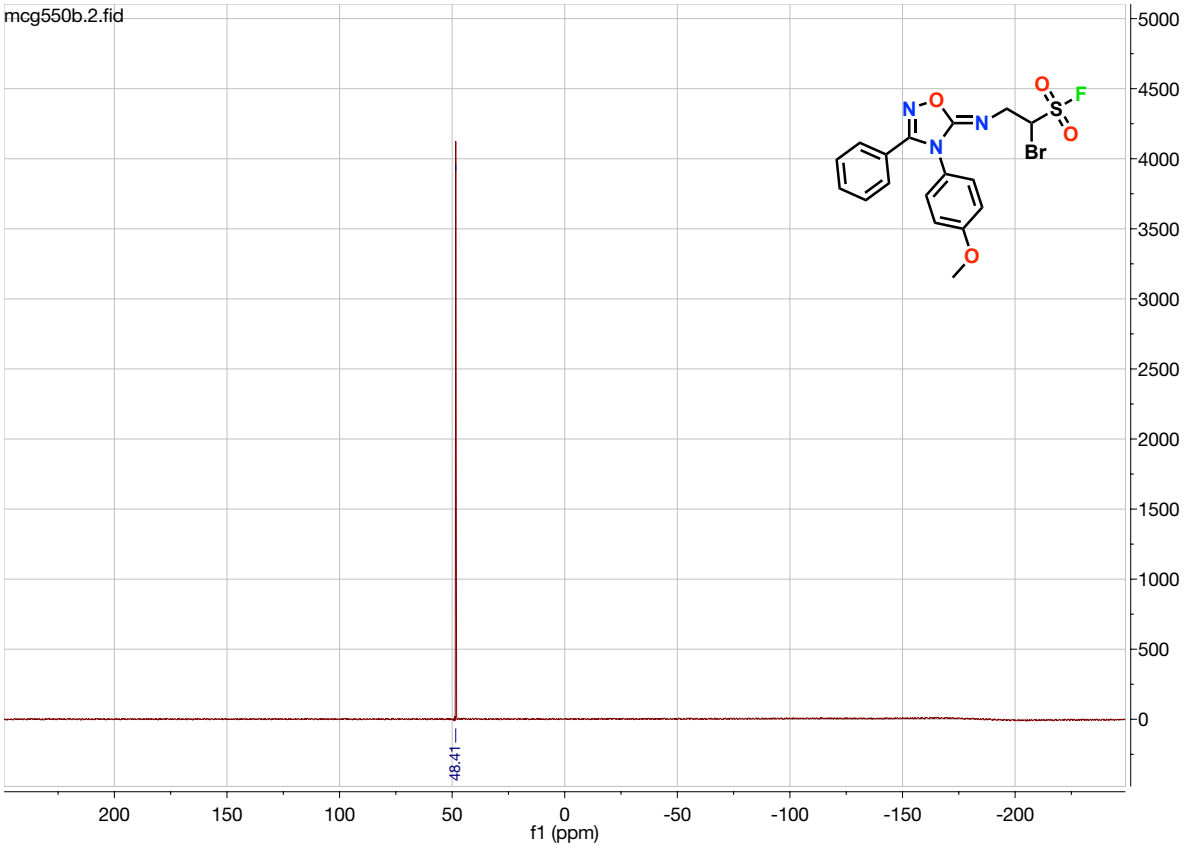

mcg533-carbon.1.fid
f1 (ppm)

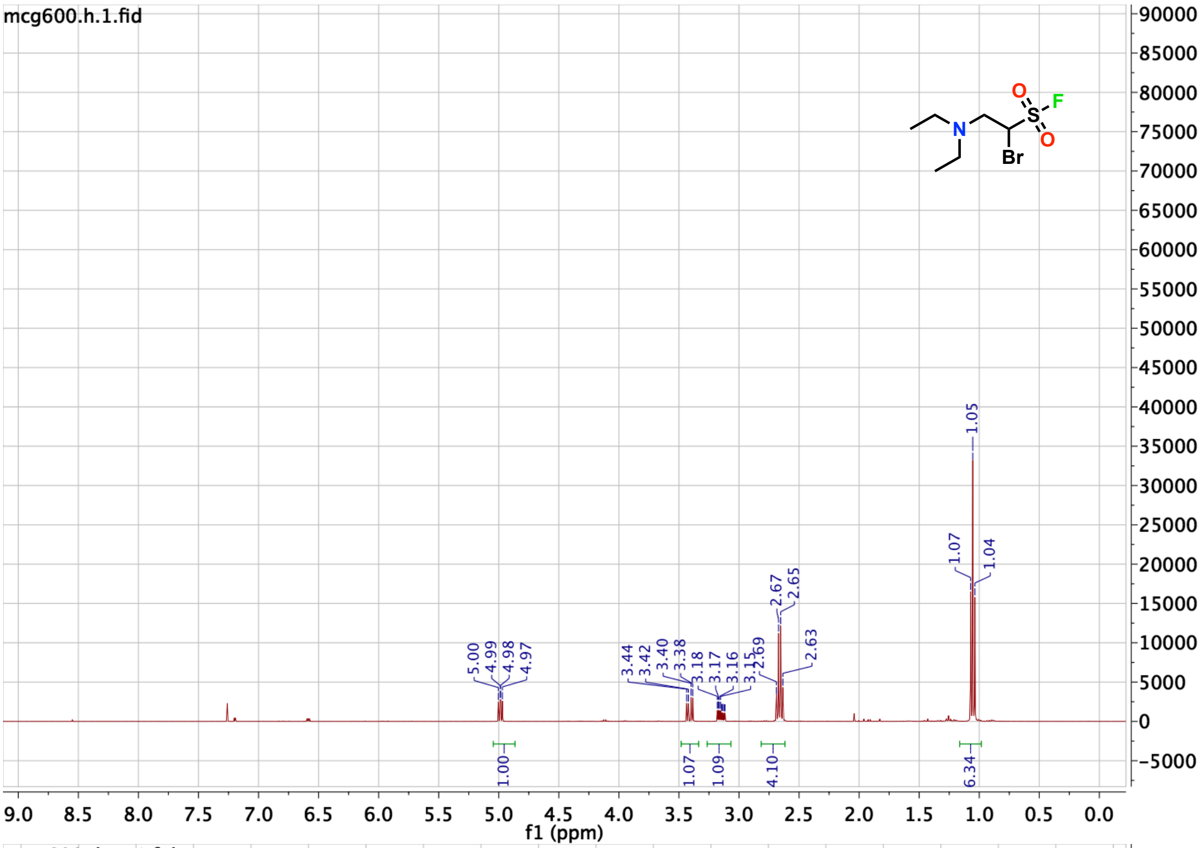

mcg533-carbon.2.fid
f1 (ppm)

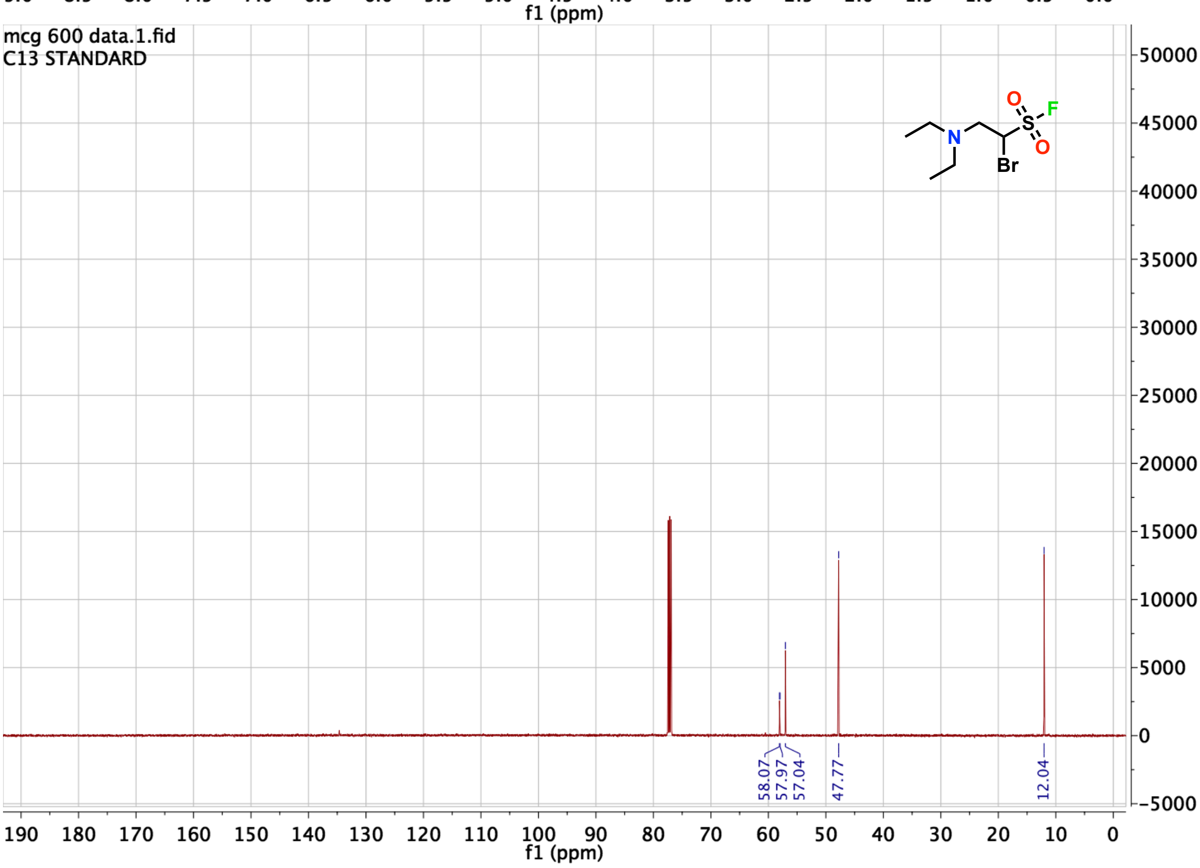

mcg533a.2.fid
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
48.28
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
O
F
S
O
N
Br

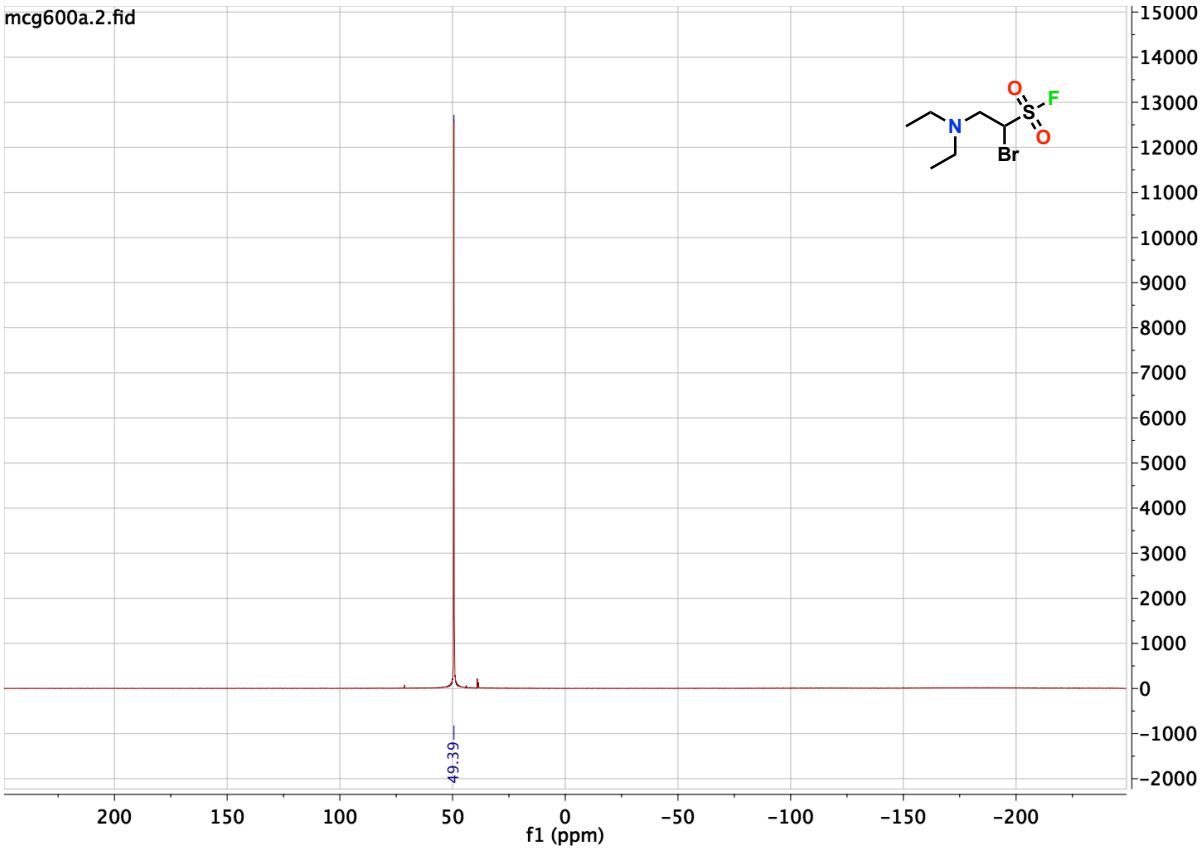

mcg513dat.1.fid
f1 (ppm)

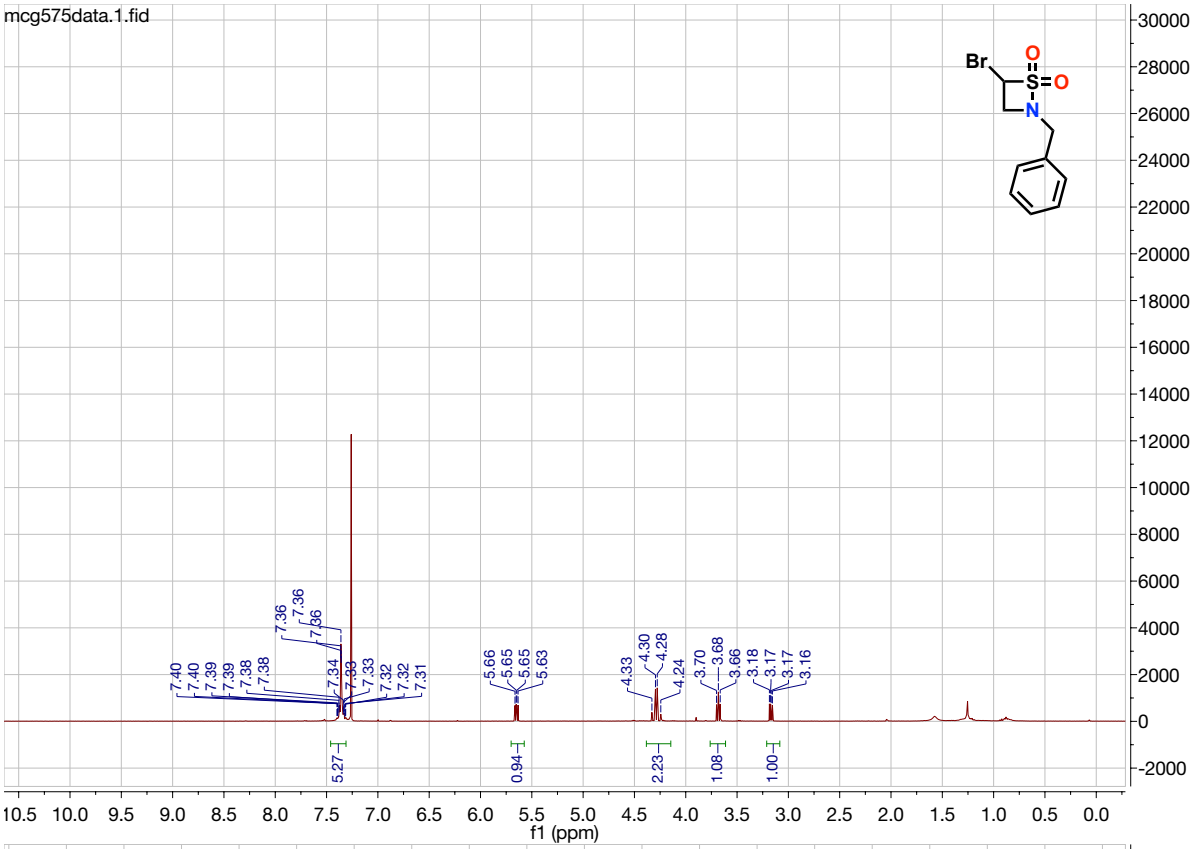

mcg513dat.2.fid
f1 (ppm)

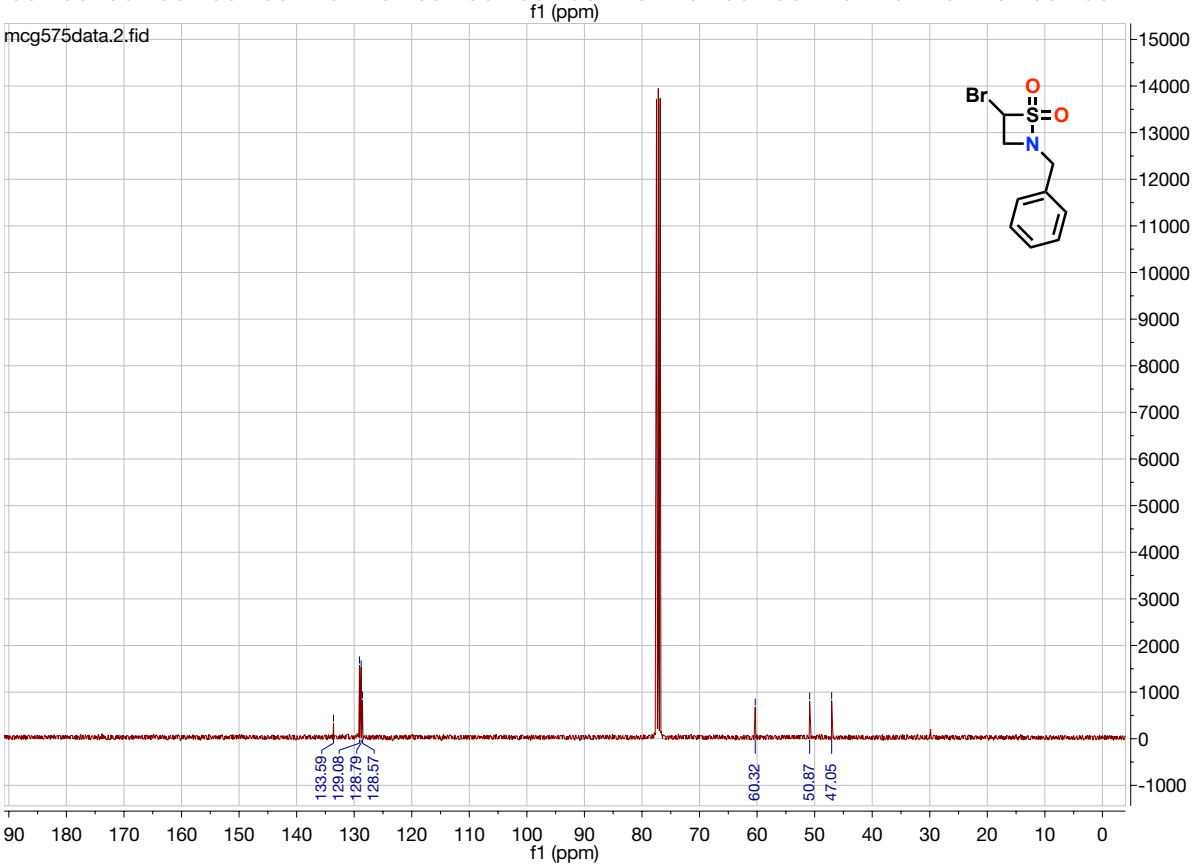

mcg550b.2.fid
48.41
f1 (ppm)
200
150
100
50
0
-50
-100
-150
-200
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
N
O
N
N
O
F
S
O
Br
O

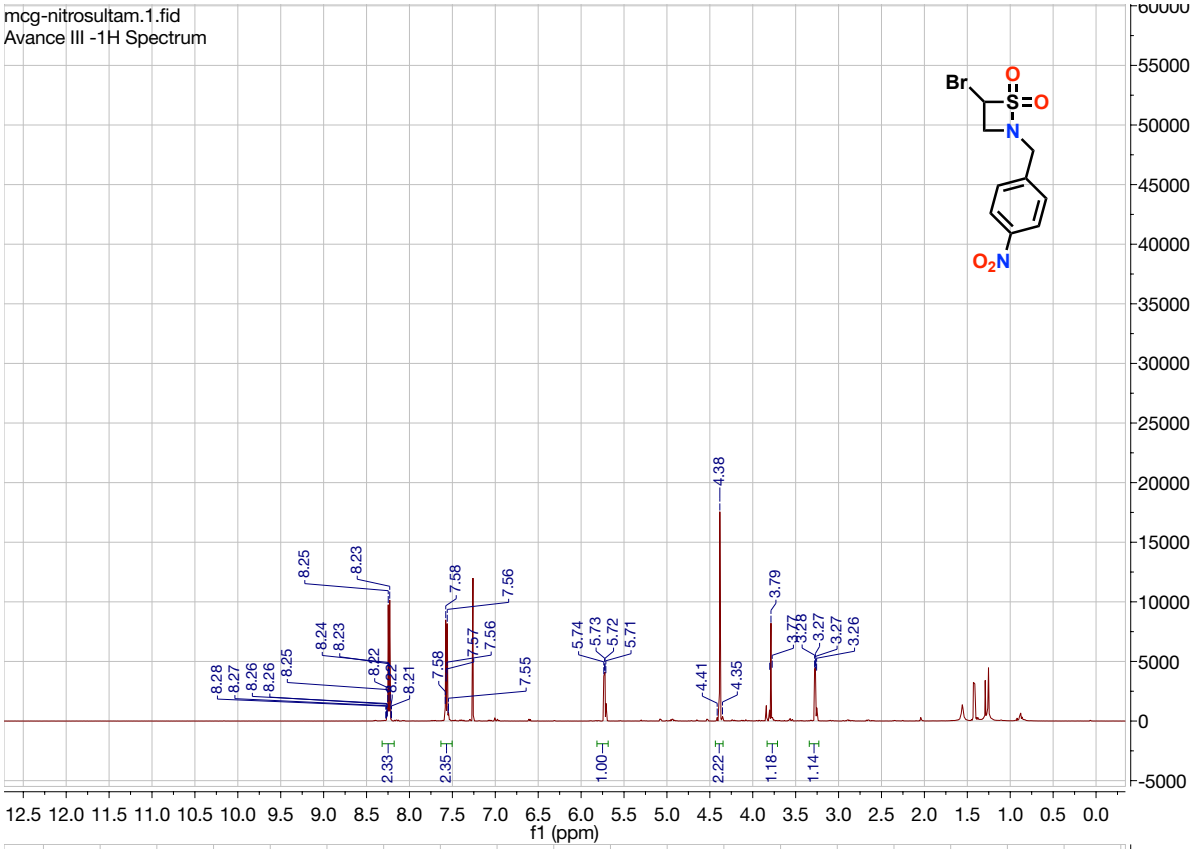

mcg600.h.1.fid
5.00
4.99
4.98
4.97
3.44
3.42
3.40
3.38
3.18
3.17
3.16
3.15
2.69
2.67
2.65
2.63
1.07
1.05
1.04
1.00
1.07
1.09
4.10
6.34
f1 (ppm)
N
O
S
F
O
Br

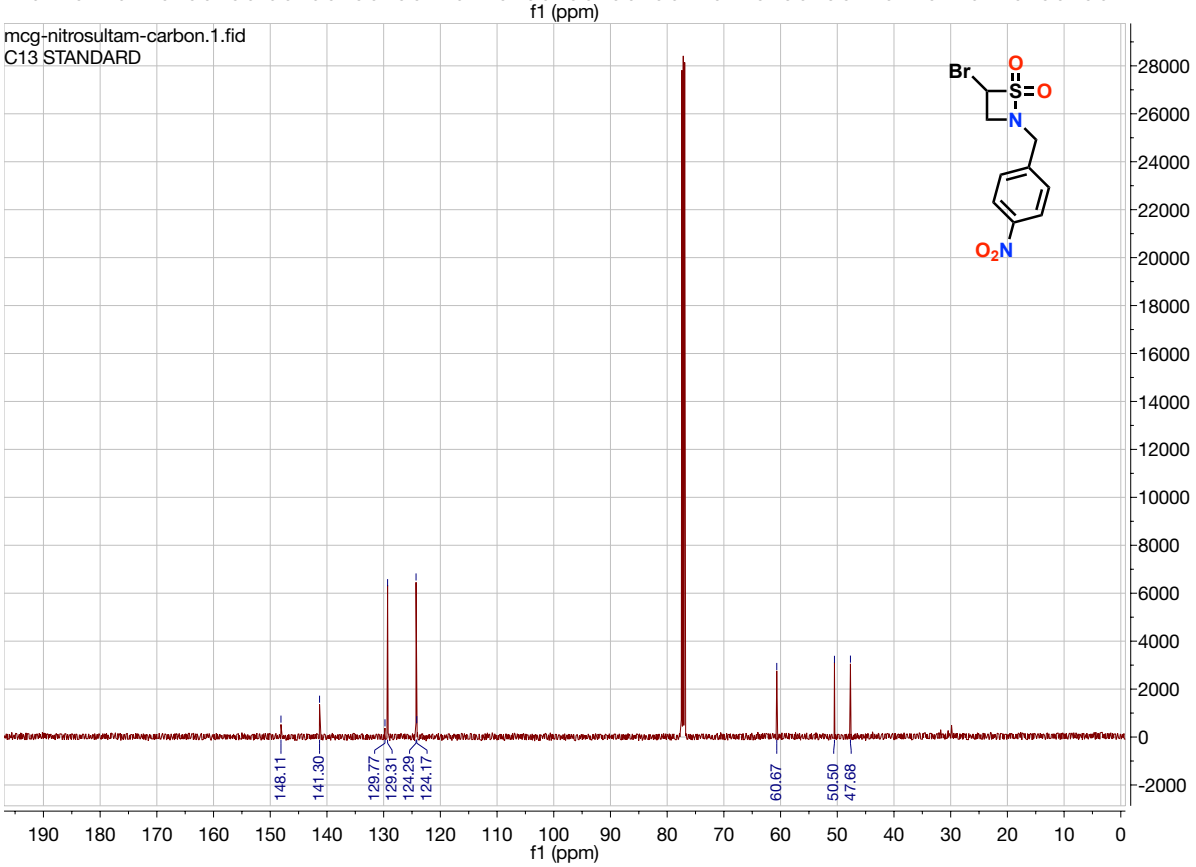

mcg 600 data.1.fid
C13 STANDARD
58.07
57.97
57.04
47.77
12.04
f1 (ppm)
N
O
S
F
O
Br

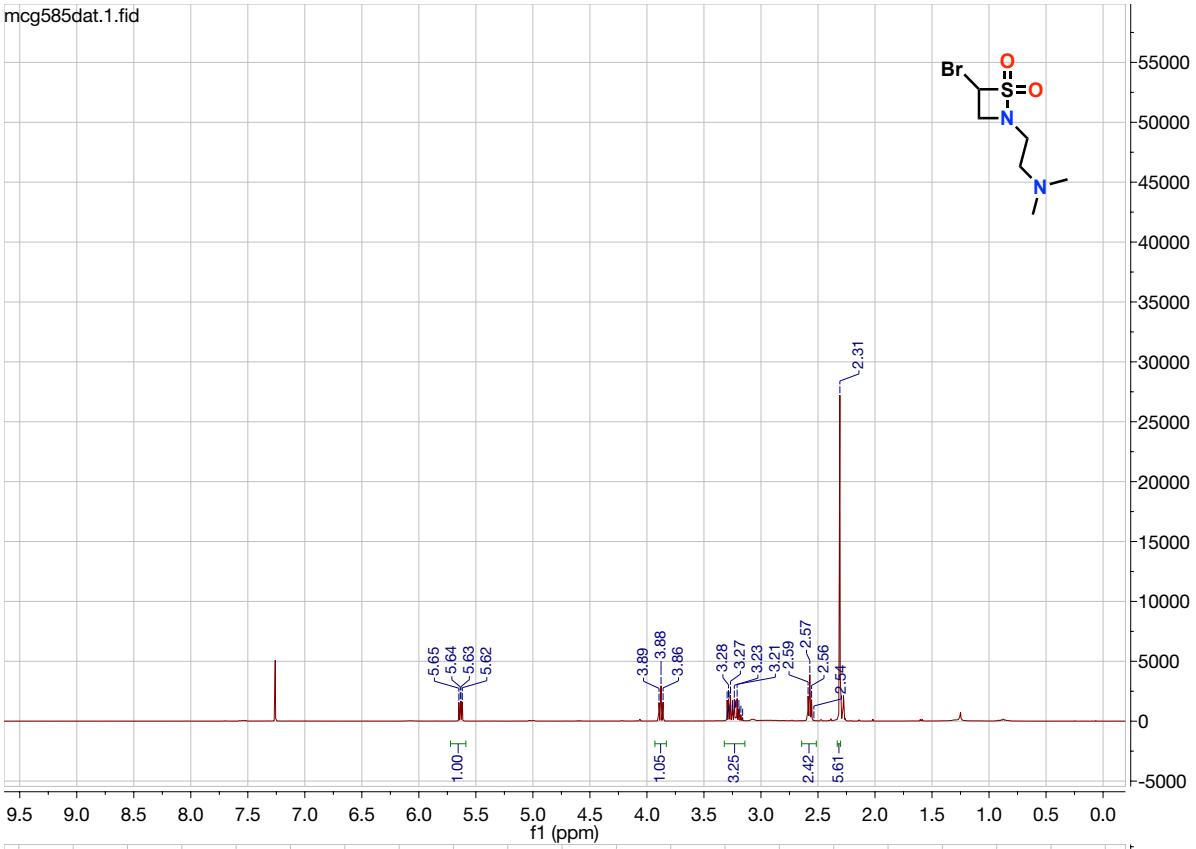

mcg600a.2.fid
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
49.39
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)
O
F
S
O
N
Br

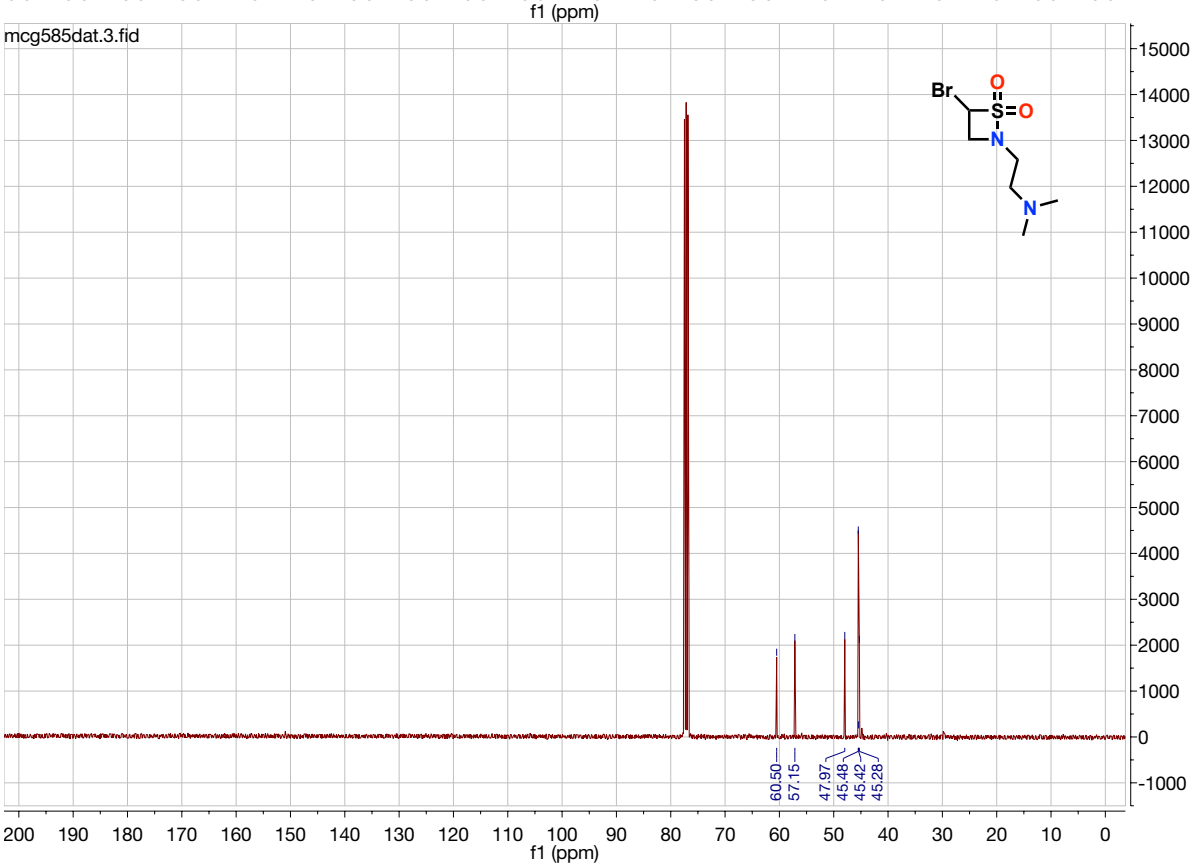

mcg575data.1.fid
Br
O
S
O
N
7.40
7.40
7.39
7.39
7.38
7.38
7.36
7.36
7.36
7.34
7.33
7.33
7.32
7.32
7.31
5.66
5.65
5.65
5.63
4.33
4.30
4.28
4.24
3.70
3.68
3.66
3.18
3.17
3.17
3.16
5.27
0.94
2.23
1.08
1.00
f1 (ppm)

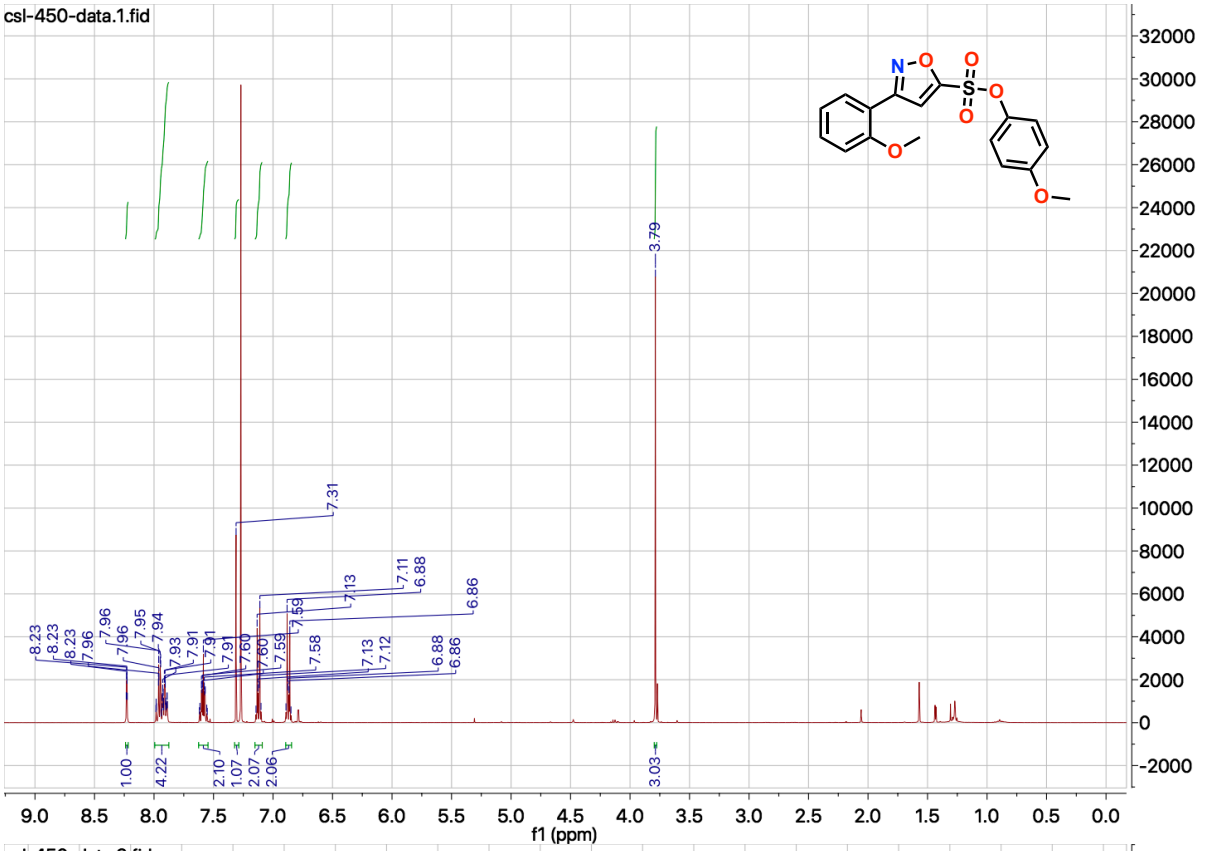

mcg575data.2.fid
Br
O
S
O
N
133.59
129.08
128.79
128.57
60.32
50.87
47.05
f1 (ppm)

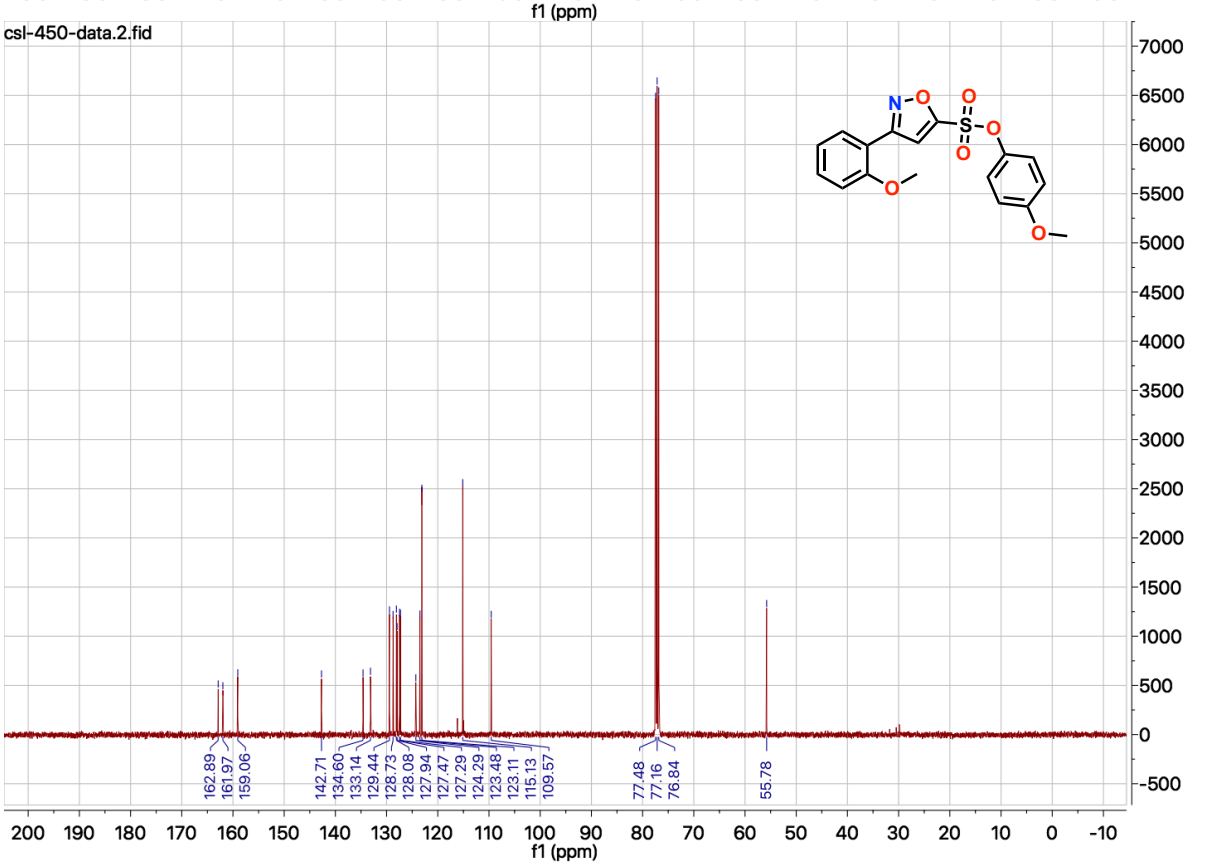

mcg-nitrosultam.1.fid
Avance III -1H Spectrum
Br
O
S=O
N
O2N
8.25
8.23
7.58
7.56
4.38
3.79
8.24
8.23
8.22
8.21
7.57
7.56
5.74
5.73
5.72
5.71
3.77
3.28
3.27
3.27
3.26
8.28
8.27
8.26
8.26
8.25
7.58
7.55
4.41
4.35
2.33
2.35
1.00
2.22
1.18
1.14
f1 (ppm)

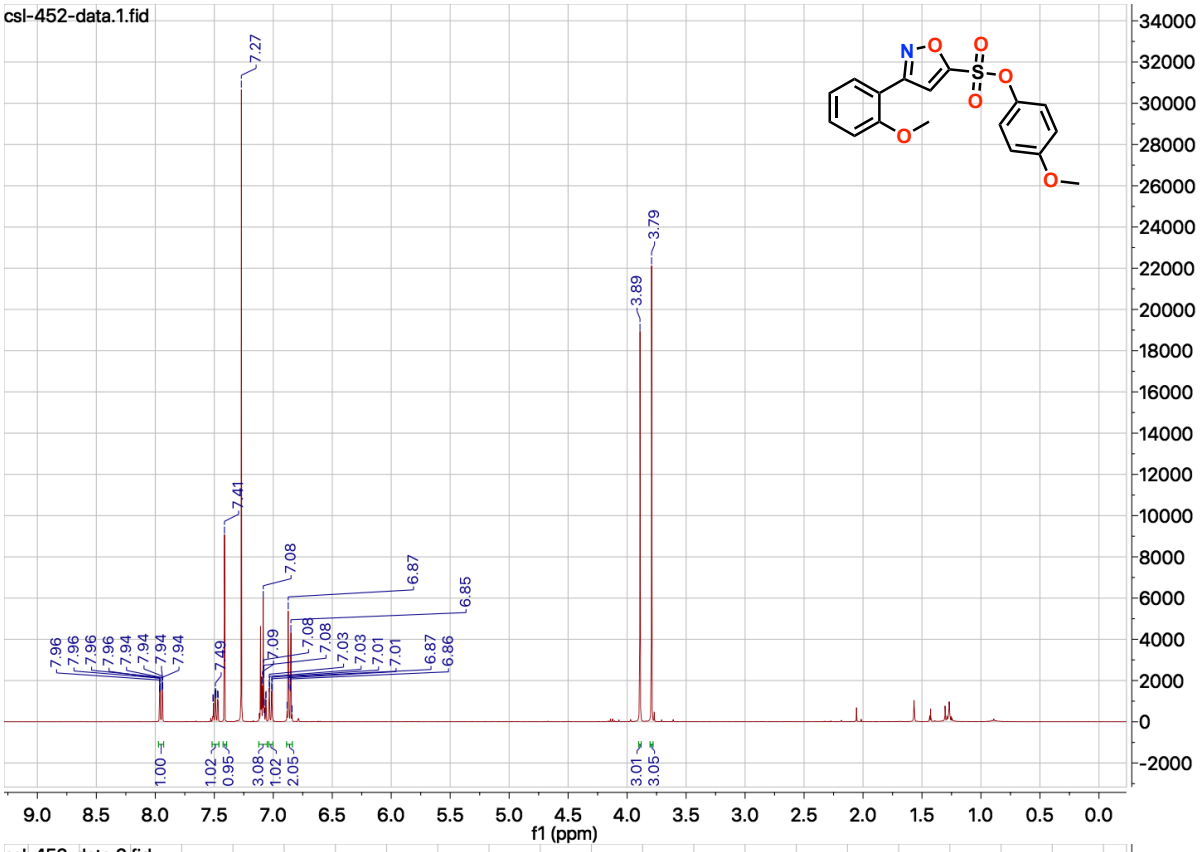

mcg-nitrosultam-carbon.1.fid
C13 STANDARD
Br
O
S=O
N
O2N
148.11
141.30
129.77
129.31
124.29
124.17
60.67
50.50
47.68
f1 (ppm)

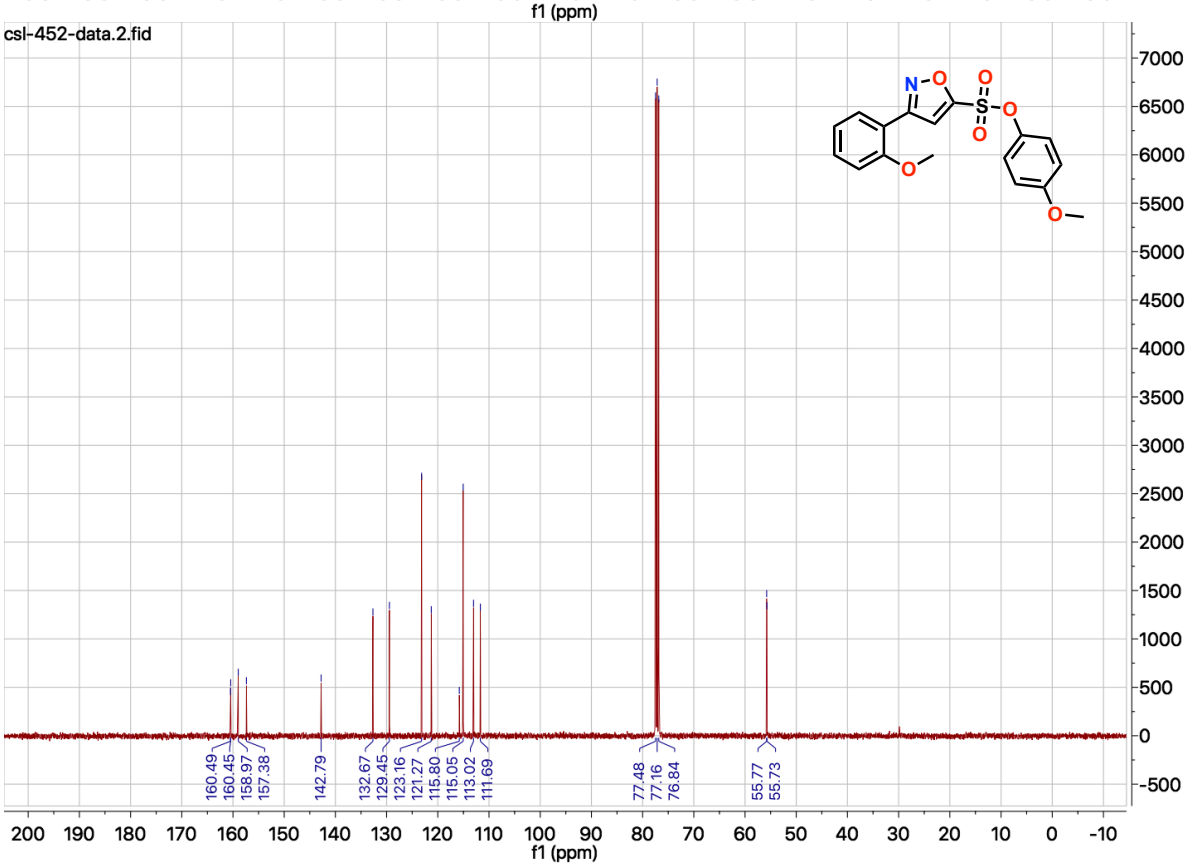

mcg585dat.1.fid
Br
O
S=O
N
N
5.65
5.64
5.63
5.62
3.89
3.88
3.86
3.28
3.27
3.23
3.21
2.59
2.57
2.56
2.54
2.31
1.00
1.05
3.25
2.42
5.61
f1 (ppm)

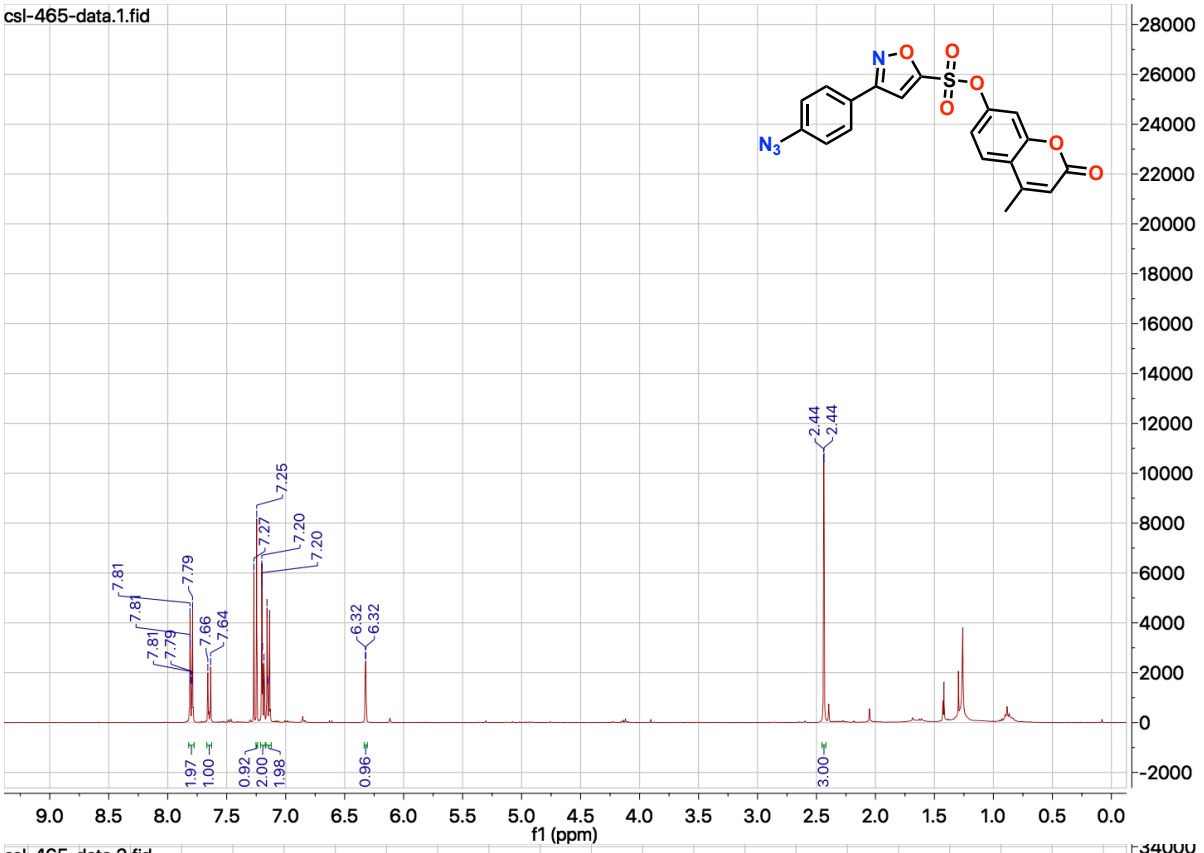

mcg585dat.3.fid
Br
O
S=O
N
N
60.50
57.15
47.97
45.48
45.42
45.28
f1 (ppm)

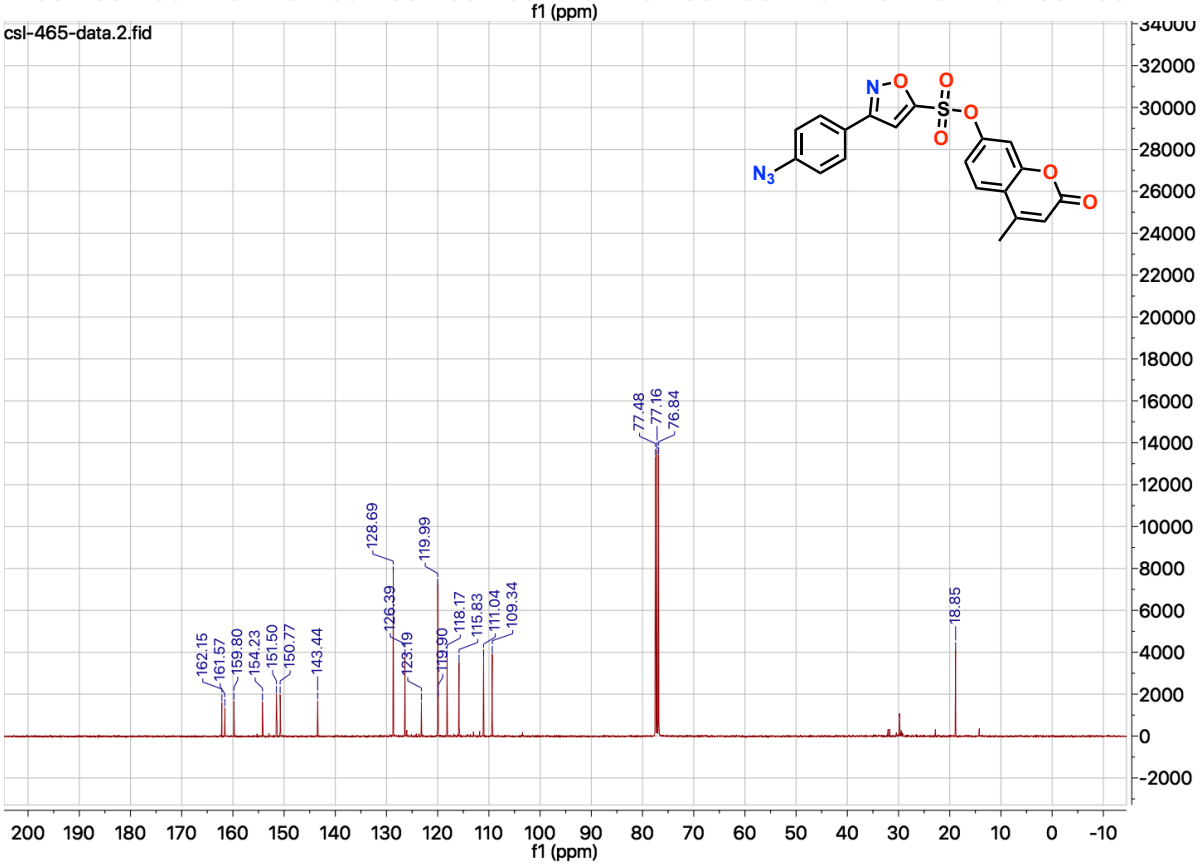

csl-450-data.1.fid
8.23
8.23
8.23
7.96
7.96
7.96
7.95
7.94
7.93
7.91
7.91
7.91
7.91
7.60
7.60
7.59
7.59
7.58
7.31
7.13
7.13
7.12
7.11
6.88
6.88
6.86
6.86
3.79
1.00
4.22
2.10
1.07
2.07
2.06
3.03
f1 (ppm)

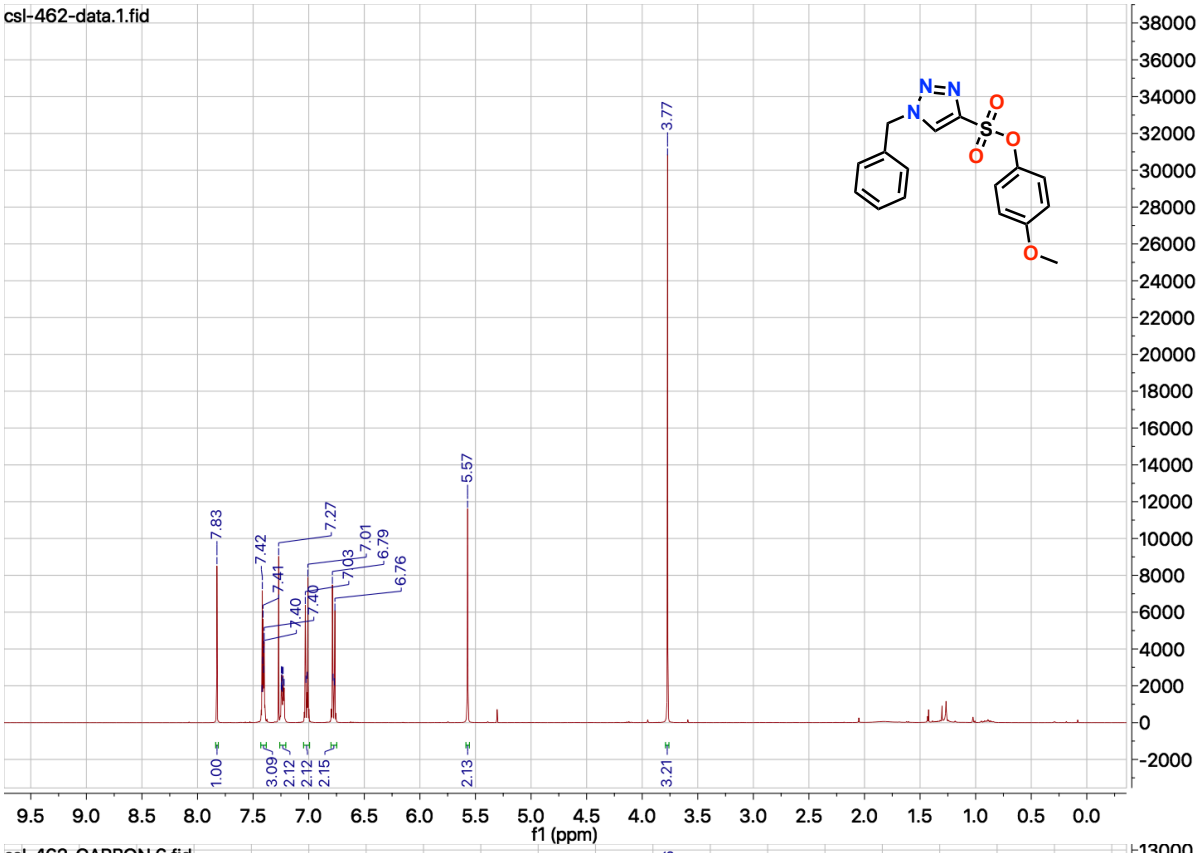

csl-450-data.2.fid
162.89
161.97
159.06
142.71
134.60
133.14
129.44
128.73
128.08
127.94
127.47
127.29
124.29
123.48
123.11
115.13
109.57
77.48
77.16
76.84
55.78
f1 (ppm)

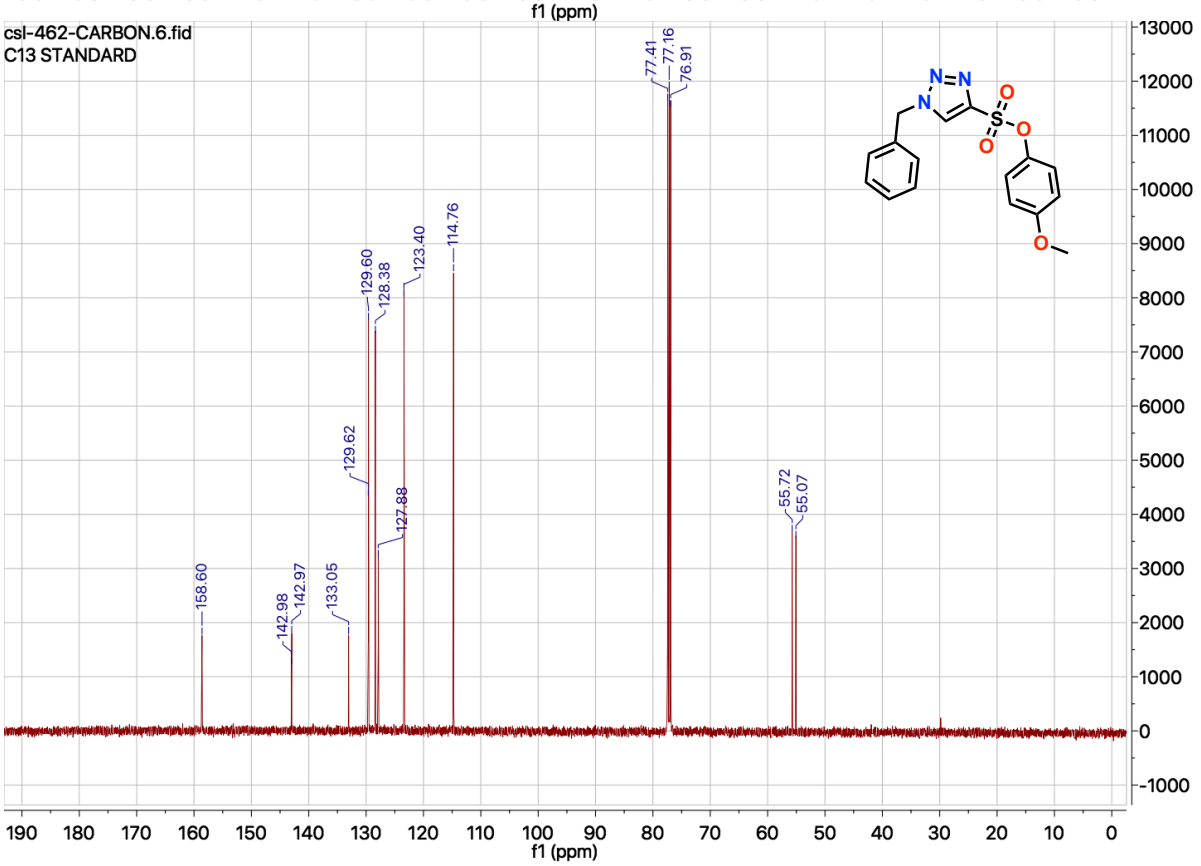

csl-452-data.1.fid
7.27
7.41
7.08
6.87
6.85
3.89
3.79
f1 (ppm)

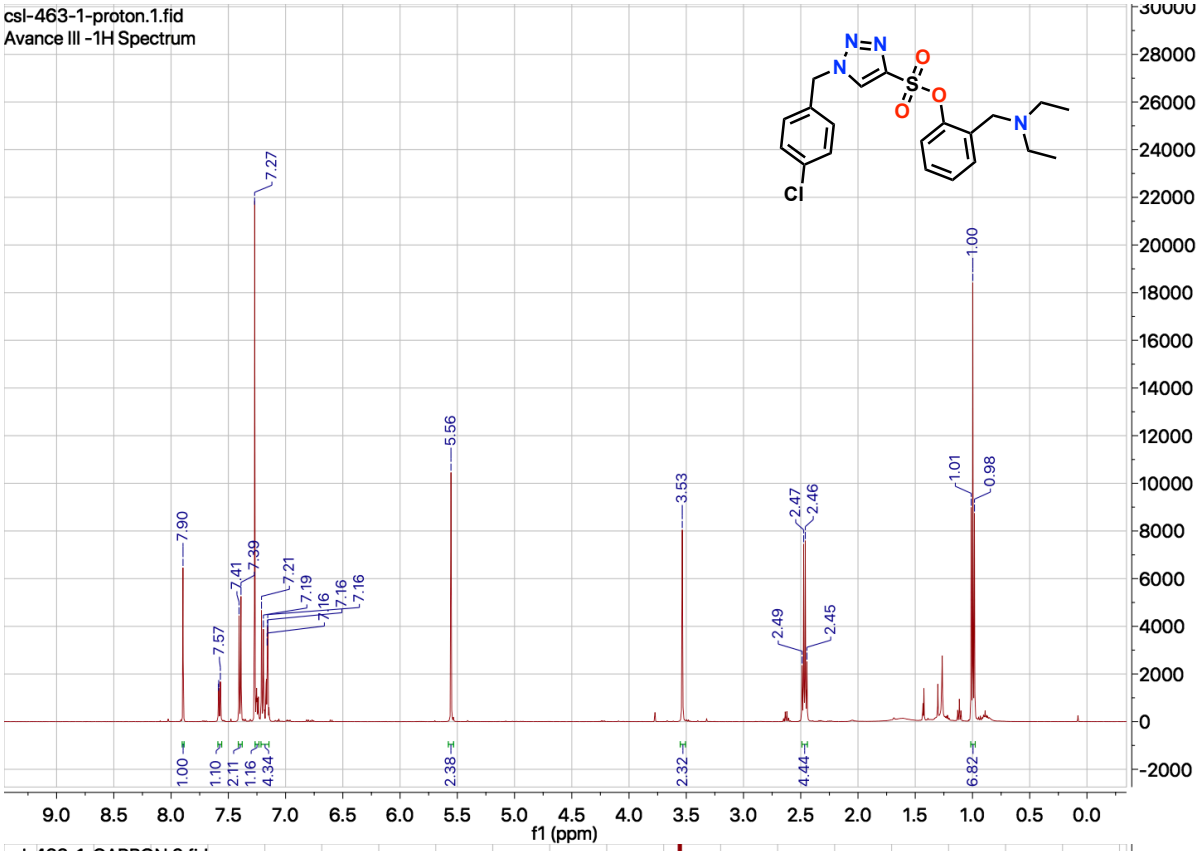

csl-452-data.2.fid
160.49
160.45
158.97
157.38
142.79
132.67
129.45
123.16
121.27
115.80
115.05
113.02
111.69
77.48
77.16
76.84
55.77
55.73
f1 (ppm)

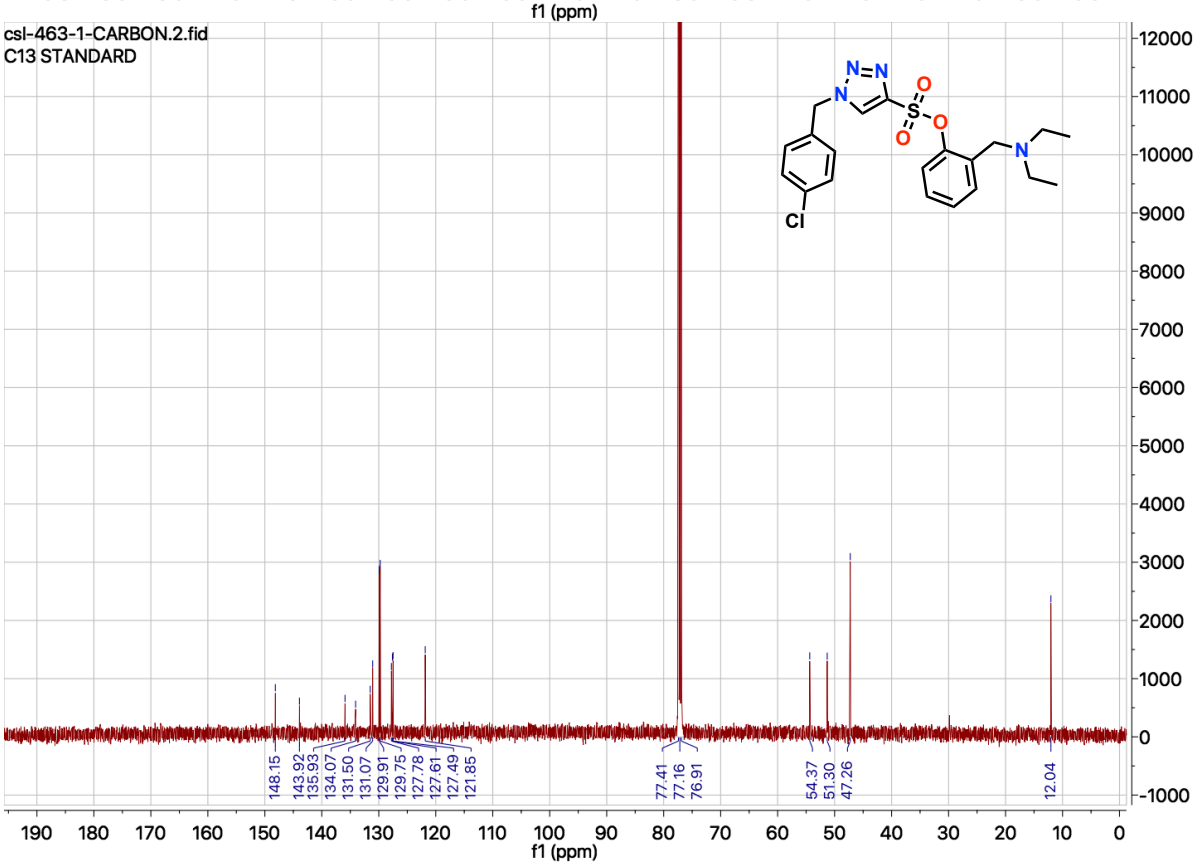

csl-465-data.1.fid
7.81
7.81
7.81
7.79
7.79
7.66
7.64
7.27
7.25
7.20
7.20
6.32
6.32
2.44
2.44
1.97
1.00
0.92
2.00
1.98
0.96
3.00
f1 (ppm)

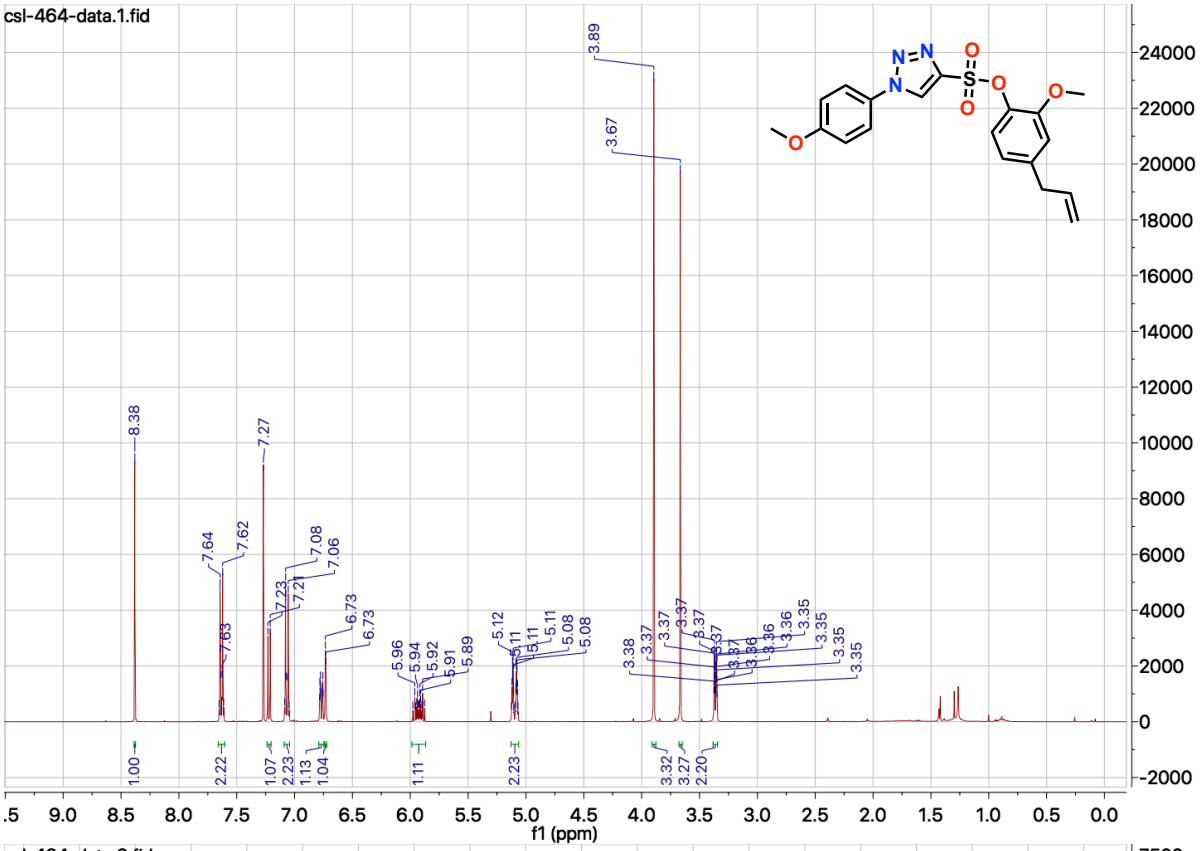

csl-465-data.2.fid
162.15
161.57
159.80
154.23
151.50
150.77
143.44
128.69
126.39
123.19
119.99
119.90
118.17
115.83
111.04
109.34
77.48
77.16
76.84
18.85
f1 (ppm)

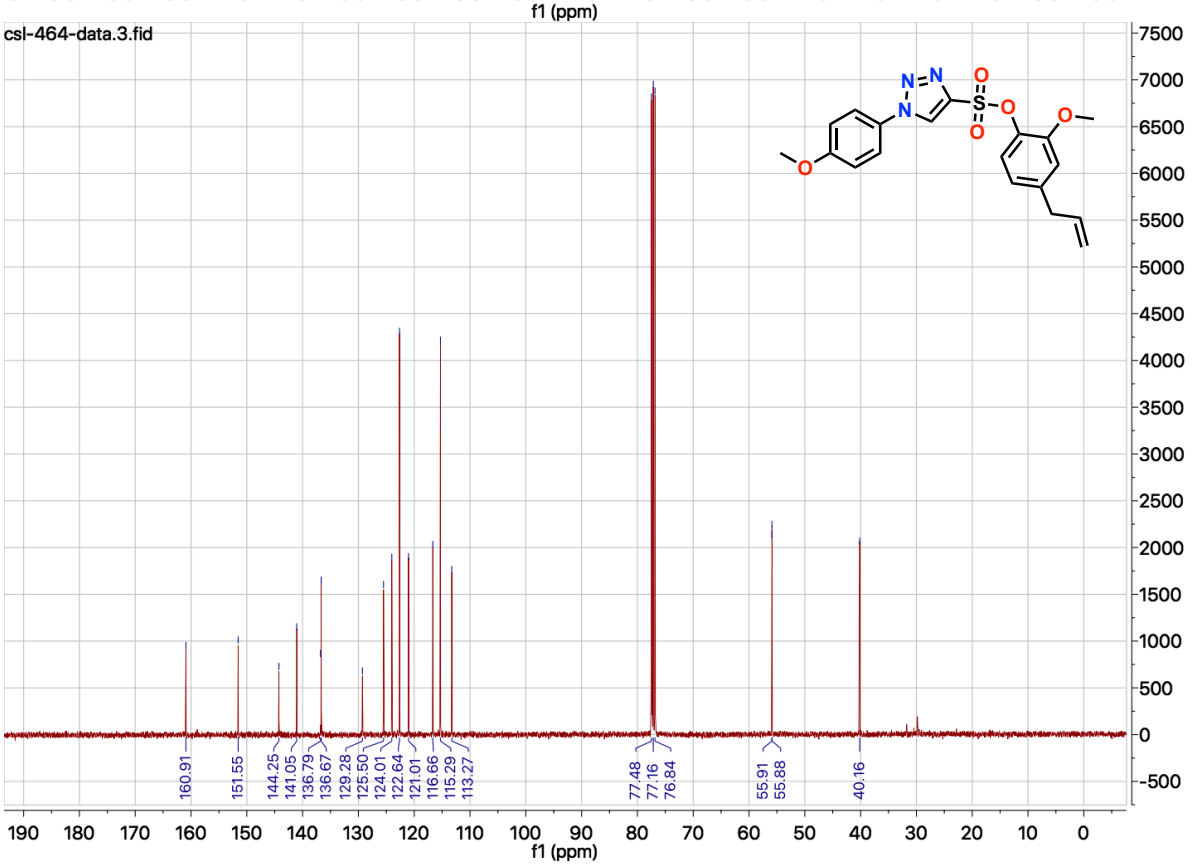

csl-462-data.1.fid
7.83
7.42
7.41
7.40
7.27
7.03
7.01
6.79
6.76
5.57
3.77
1.00
3.09
2.12
2.12
2.15
2.13
3.21
f1 (ppm)

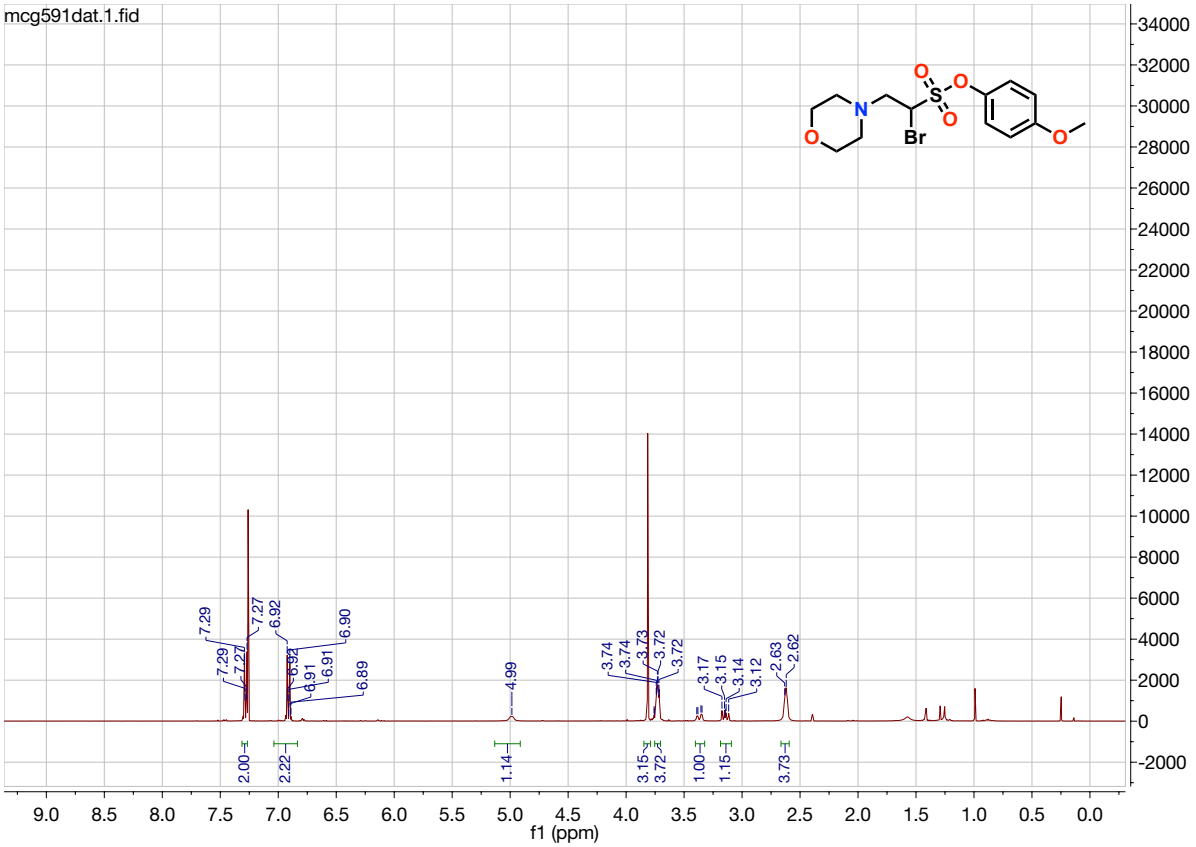

csl-462-CARBON.6.fid
C13 STANDARD
77.41
77.16
76.91
158.60
142.98
142.97
133.05
129.62
129.60
128.38
127.88
123.40
114.76
55.72
55.07
f1 (ppm)

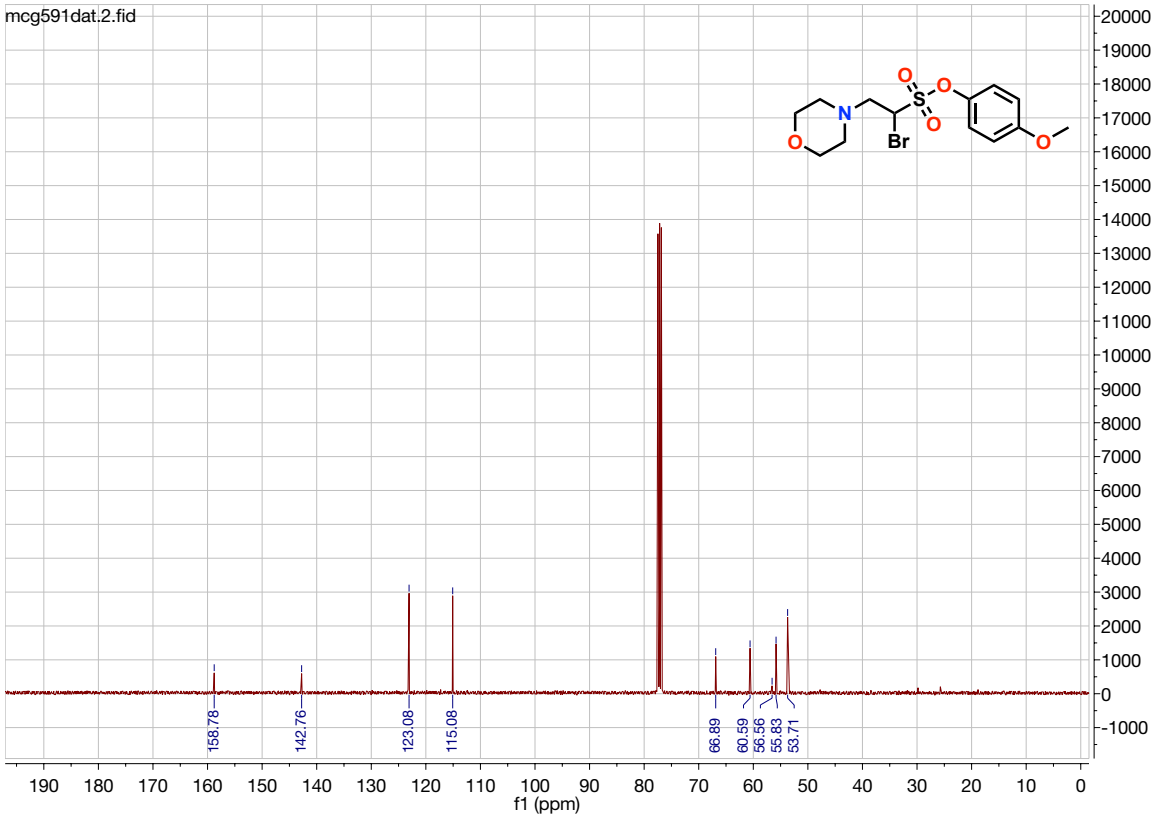

csl-463-1-proton.1.fid
Avance III -1H Spectrum
7.90
7.57
7.41
7.39
7.27
7.21
7.19
7.16
7.16
7.16
5.56
3.53
2.49
2.47
2.46
2.45
1.01
1.00
0.98
1.00
1.10
2.11
1.16
4.34
2.38
2.32
4.44
6.82
f1 (ppm)

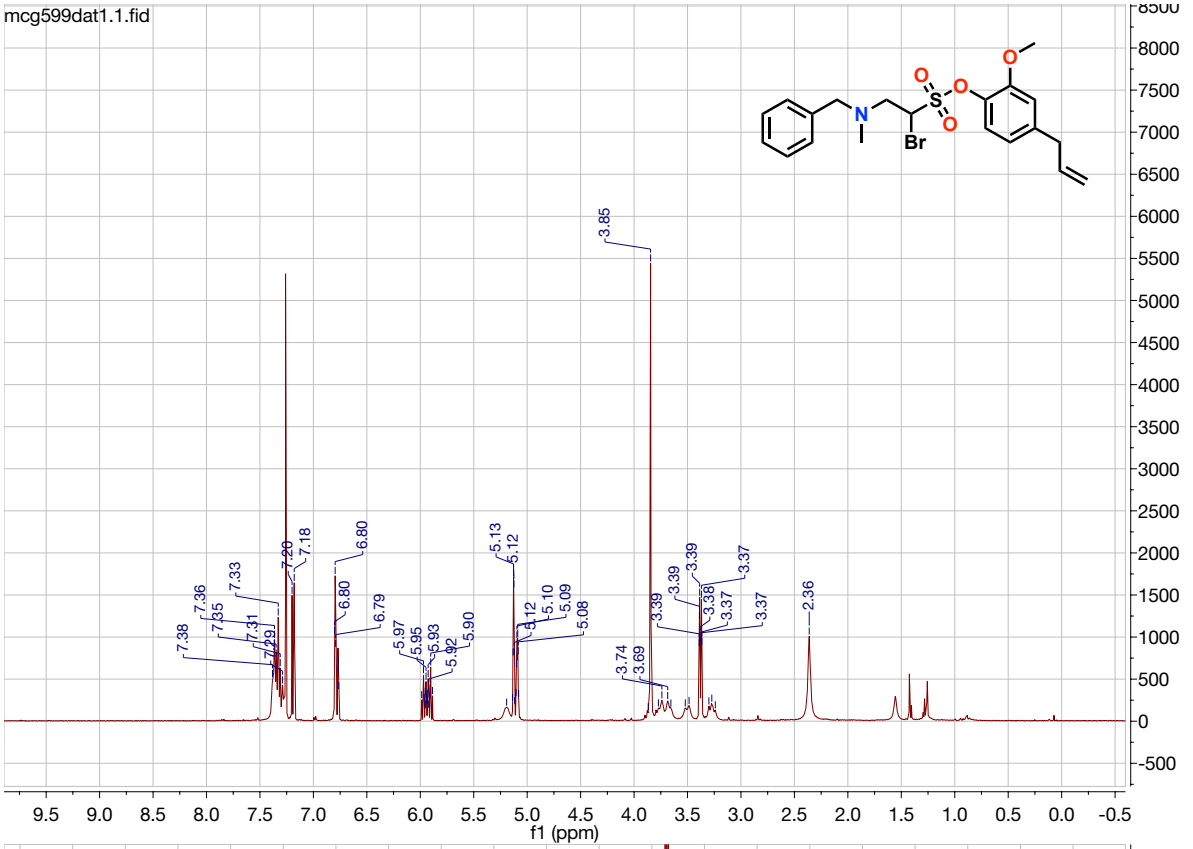

csl-463-1-CARBON.2.fid
C13 STANDARD
148.15
143.92
135.93
134.07
131.50
131.07
129.91
129.75
127.78
127.61
127.49
121.85
77.41
77.16
76.91
54.37
51.30
47.26
12.04
f1 (ppm)

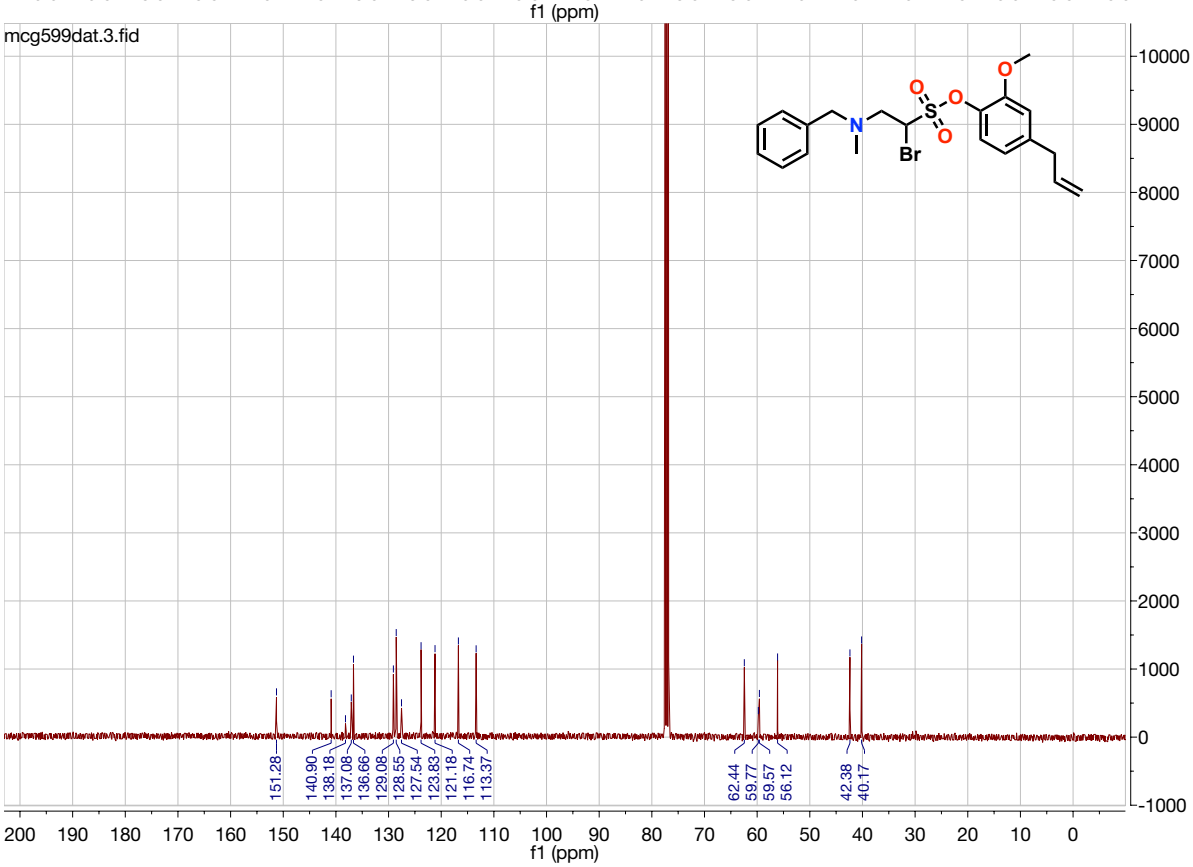

csl-464-data.1.fid
f1 (ppm)


csl-464-data.3.fid
f1 (ppm)


mcg591dat.1.fid
7.29
7.27
6.92
6.90
6.91
6.89
4.99
3.74
3.73
3.72
3.17
3.15
3.14
3.12
2.63
2.62
2.00
2.22
1.14
3.15
3.72
1.00
1.15
3.73
f1 (ppm)


mcg591dat.2.fid
158.78
142.76
123.08
115.08
66.89
60.59
56.56
55.83
53.71
f1 (ppm)


mcg599dat1.1.fid
7.38
7.36
7.35
7.33
7.31
7.29
7.20
7.18
6.80
6.80
6.79
5.97
5.95
5.93
5.92
5.90
5.13
5.12
5.12
5.10
5.09
5.08
3.85
3.74
3.69
3.39
3.39
3.39
3.38
3.37
3.37
3.37
2.36
f1 (ppm)


mcg599dat.3.fid
151.28
140.90
138.18
137.08
136.66
129.08
128.55
127.54
123.83
121.18
116.74
113.37
62.44
59.77
59.57
56.12
42.38
40.17
f1 (ppm)