Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

For

Visible Light-Mediated Atom Transfer Radical Addition of Styrene: Base Controlled Selective (Phenylsulfonyl)difluoromethylation

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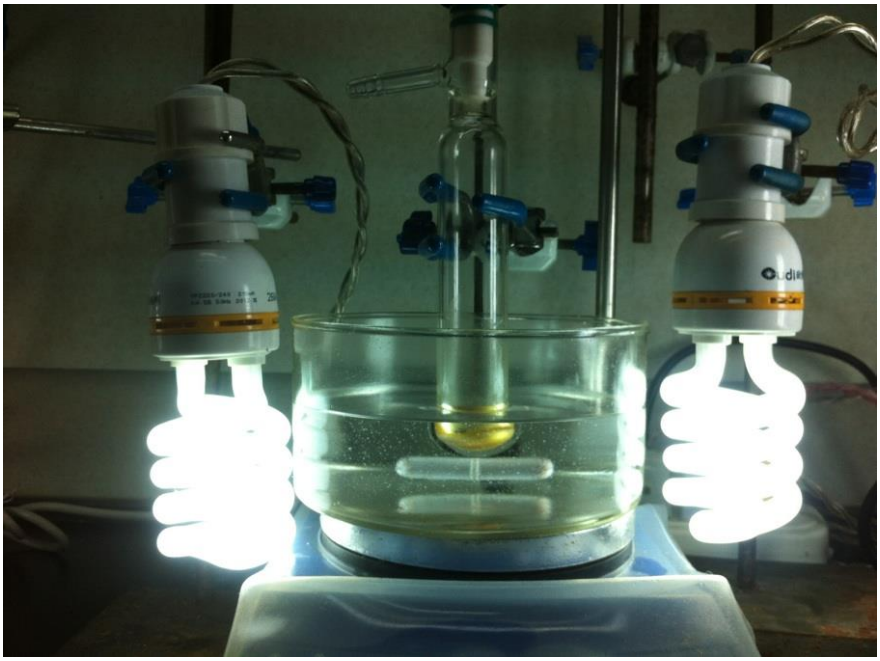
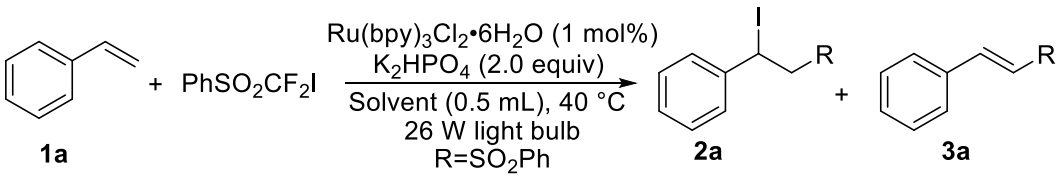
General Information:

NMR spectra were recorded on Bruker-400 (400 MHz for ^{1}H; 100 MHz for ^{13}C and 376 MHz for ^{19}F {^{1}H decoupled}) instruments internally referenced to $SiMe_4$ signal. High resolution mass spectra were recorded on P-SIMS-Gly of Bruker Daltonics Inc. using ESI-TOF (electrospray ionization-time of flight) or Micromass GCT using EI (electron impact). $Ru(bpy)_3Cl_2$[1] was were prepared according to the literature procedures and recrystallized from hot water. K_2HPO_4 were purchased from Alfa and used as received. NaOAc were purchased from Sinopharm and used as received. DABCO were purchased from Aladdin and used as received. $CHCl_3$ was distilled from CaH before use. Irradiation of visible light was performed with two 26 w compact fluorescent light bulbs, showed as below.



Tables of the Optimization of Reaction Conditions:

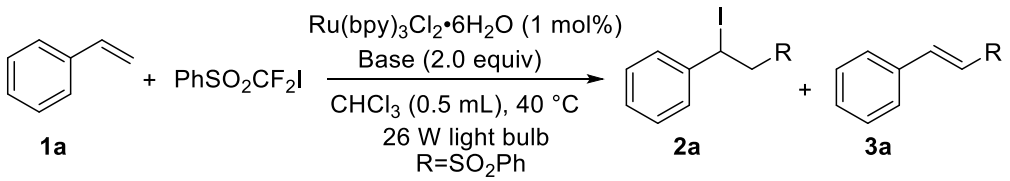
Table S1. Solvent Screening:[a]



entry	solvent	yield (2a:3a) (%)[b]	entry	solvent	yield (2a:3a) (%)[b]
1	DMF	trace/-	6	DCM	35/1
2	DMSO	trace/-	7	$CHCl_3$	42/0
3	Acetone	12/0	8	$Cl_2CHCHCl_2$	34/1
4	MeCN	trace/-	9	MeOH	0/-
5	EtOAc	12/0	10	THF	25/0

[a] **1a** (0.3 mmol, 1.5 equiv), $PhSO_2CF_2I$ (0.2 mmol, 1.0 equiv), N_2, 24 h. [b] Yield determined by ^{19}F NMR yield

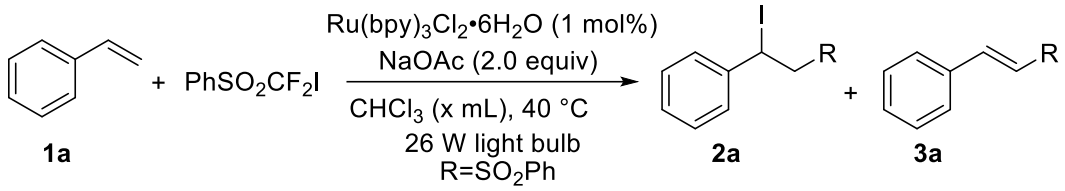
Table S2. Base Screening: [a]



entry	base	yield(**2a:3a**) (%)	entry	base	yield(**2a:3a**) (%)
1	Na_2CO_3	40/1	8	DABCO	0/92
2	Cs_2CO_3	0/-	9	none	31/2
3	NaOAc	52/0	10	K_3PO_4	33/3
4	AgOAc	trace/-	11	TsNa	45/4
5	$KHCO_3$	35/1	12	CF_3COONa	trace/-
6	$NaHCO_3$	43/3	13	NaOH	0/-
7	NEt_3	0/27			

[a] **1a** (0.3 mmol, 1.5 equiv), $PhSO_2CF_2I$ (0.2 mmol, 1.0 equiv), N_2, 24 h. [b] Yield determined by ^{19}F NMR yield

Table S3. Concentration Screening:[a]



1a **2a** **3a**

entry	$CHCl_3$ (mL)	yield (2a:3a) (%)[b]	entry	$CHCl_3$ (mL)	yield (2a:3a) (%)[b]
1	0.2	31/1	3	2	46/0
2	1	48/0	4	4	86/1

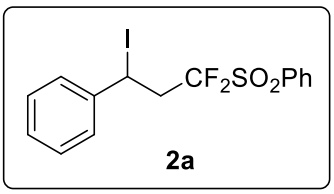
[a] **1a** (0.3 mmol, 1.5 equiv), $PhSO_2CF_2I$ (0.2 mmol, 1.0 equiv), N_2, 24 h. [b] Yield determined by ^{19}F NMR yield

Preparation of Substrates:

All the styrene derivatives **1b-s** were prepared according to the literature.[2] **4a** was purchased from Energy Chemistry and used as received. **4b**, **4e** and **4f** was were prepared according to the literature.[3] **4c** was prepared according to the literature.[4] **4d** was prepared according to the literature.[5] $PhSO_2CF_2I$ was prepared according to the literature.[6]

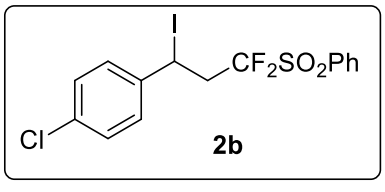
General Procedure of ATRA Reaction of Styrene:

$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **2a** as a white solid (70.0 mg, 83%). (Note: All of the reactions were very sensitive to the size of the catalyst and powdery c atalyst was needed to obtain reproducible results).



2a

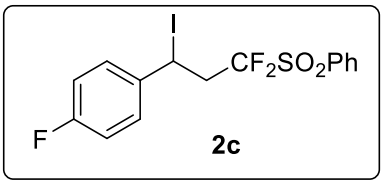
2a: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.61-7.57 (m, 2H), 7.42 (d, *J* = 7.2 Hz, 2H), 7.31-7.22 (m, 3H), 5.47 (dd, *J* = 9.2, 5.6 Hz, 1H), 3.62-3.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6, 135.7, 131.6, 130.9, 129.4, 128.9, 128.6, 126.9, 122.9 (t, *J* = 287.2 Hz), 40.6 (t, *J* = 18.6 Hz), 17.1 (t, *J* = 2.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.4 (d, *J* = 227.8 Hz), -104.4 (d, *J* = 227.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{13}O_2F_2SINa$: 444.9547, found: 444.9558.



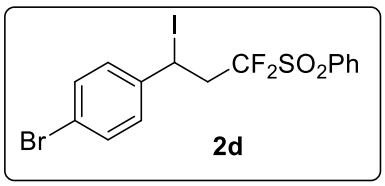
2b

2b: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.75 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.61-7.57 (m, 2H),

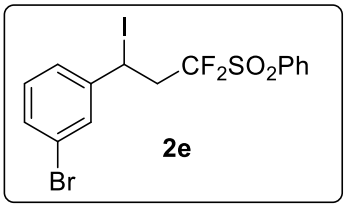
7.37-7.34 (m, 2H), 7.28-7.25 (m, 2H), 5.45-5.42 (m, 1H), 3.59-3.39 (m,2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2, 135.7, 134.2, 131.5, 130.9, 129.5, 129.1, 128.3, 122.8 (t, 288.7 Hz), 40.7 (t, *J* = 18.8 Hz), 15.7 (t, *J* = 2.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.8 (d, *J* = 228.8 Hz), -104.4 (d, *J* = 228.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_2SIClNa$: 478.9157, found: 478.9156.



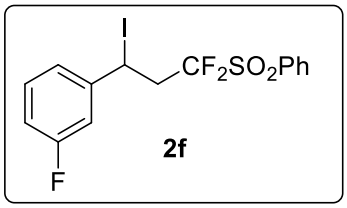
2c: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.74 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.60-7.56 (m, 2H), 7.42-7.39 (m, 2H), 6.99-6.95 (m, 2H), 5.47-5.45 (m, 1H), 3.59-3.39 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3 (d, *J* = 247.3 Hz), 138.6 (d, *J* = 3.4 Hz), 135.7, 131.5, 130.9, 129.5, 128.7 (d, *J* = 8.4 Hz), 122.9 (t, *J* = 288.8 Hz), 115.9 (d, *J* = 21.9 Hz), 40.9 (t, *J* = 18.7 Hz), 16.0 (t, *J* = 2.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.0 (d, *J* = 228.6 Hz), -104.4 (d, *J* = 228.6 Hz), -112.4. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_3SINa$: 462.9452, found: 462.9451.



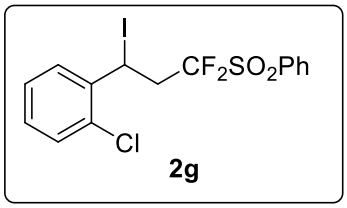
2d: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.7 Hz, 2H), 7.75 (t, *J* = 7.2 Hz, 1H), 7.62-7.56 (m, 2H), 7.43-7.41 (m, 2H), 7.33-7.27 (m, 2H), 5.44-5.40 (m, 1H), 3.58-3.38 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 135.8, 132.1, 131.5, 131.0, 129.5, 128.6, 122.8 (t, *J* = 288.4 Hz), 122.4, 40.7 (t, *J* = 18.6 Hz), 15.7 (t, *J* = 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.7 (d, *J* = 228.8 Hz), -104.3 (d, *J* = 228.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_2SBrINa$: 522.8652, found: 522.8661.



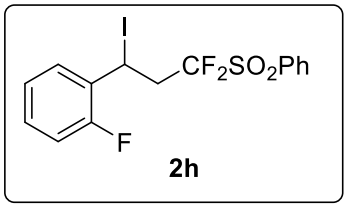
2e: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.75 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.61-7.57 (m, 2H), 7.55 (t, *J* = 2.0 Hz, 1H), 7.38-7.34 (m, 2H), 7.17 (t, *J* = 8.0 Hz, 1H), 5.40-5.36 (m, 1H), 3.57-3.38 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 135.8, 131.7, 131.5, 131.0, 130.4, 130.0, 129.5, 125.7, 122.8 (t, *J* = 288.8 Hz), 122.6, 40.6 (t, *J* = 18.8 Hz), 15.0 (t, *J* = 2.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.0 (d, *J* = 228.7 Hz), -104.3 (d, *J* = 228.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_2SBrINa$: 522.8652, found: 522.8653.



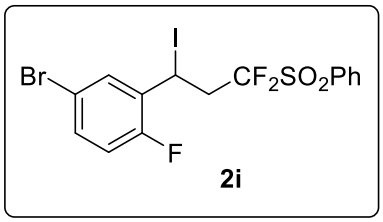
2f: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.75 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.61-7.57 (m, 2H), 7.30-7.23 (m, 1H), 7.19 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.12 (dt, *J* = 9.6, 2.0 Hz, 1H), 6.94 (tdd, *J* = 8.4, 2.4, 1.2 Hz, 1H), 5.44-5.40 (m, 1H), 3.58-3.37 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6 (d, *J* = 245.9 Hz), 144.9 (d, *J* = 7.4 Hz), 135.8, 131.6, 131.0, 130.5 (d, *J* = 8.3 Hz), 129.5, 122.8 (t, *J* = 288.7 Hz), 122.6 (d, *J* = 2.8 Hz), 115.7 (d, *J* = 21.2 Hz), 114.1 (d, *J* = 22.5 Hz). 40.5 (t, *J* = 18.8 Hz), 15.3 (q, *J* = 2.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.1 (d, *J* = 228.2 Hz), -104.4 (d, *J* = 228.6 Hz), -111.8. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_3ISNa$: 462.9452, found: 462.9460.



2g: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.6 Hz, 2H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.52-7.48 (m, 3H), 7.21-7.17 (m, 2H), 7.12-7.08 (m, 1H), 5.85-5.82 (m, 1H), 3.64-3.33 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.6, 135.7, 131.7, 131.7, 131.5, 131.0, 130.2, 129.6, 129.5, 128.8, 127.7, 122.9 (t, *J* = 288.0 Hz), 39.2 (t, *J* = 18.8 Hz), 11.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.6 (d, *J* = 227.5 Hz), -104.0 (d, *J* = 228.9 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_2IClSNa$: 478.9157, found: 478.9135.

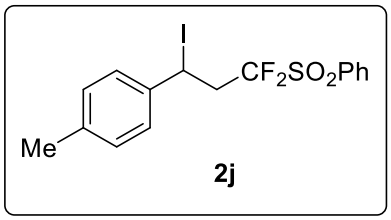


2h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.74 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.61-7.57 (m, 2H), 7.43 (td, *J* = 7.6, 1.6 Hz, 1H), 7.29-7.22 (m, 1H), 7.11 (td, *J* = 7.6, 1.0 Hz, 1H), 7.01-6.96 (m, 1H), 5.67 (dd, *J* = 10.0, 5.3 Hz, 1H), 3.70-3.39 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2 (d, *J* = 248.5 Hz), 135.7, 131.6, 131.0, 130.3 (d, *J* = 8.6 Hz,), 129.8 (d, *J* = 12.5 Hz), 129.5, 128.8 (d, *J* = 2.5 Hz), 124.7 (d, *J* = 3.6 Hz), 123.0 (t, *J* = 290.2 Hz), 116.3 (d, *J* = 21.7 Hz), 39.5 (td, *J* = 19.0, 2.2 Hz), 7.7 (q, *J* = 2.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.4 (d, *J* = 228.2 Hz), -104.7 (d, *J* = 228.2 Hz), -115.1. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{12}O_2F_3SINa$: 462.9452, found: 462.9449.



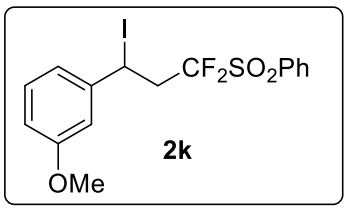
2i

2i: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.76 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.62-7.58 (m, 2H), 7.53 (dd, *J* = 6.8, 2.4 Hz, 1H), 7.35 (ddd, *J* = 8.8, 4.4, 2.8 Hz, 1H), 6.89 (dd, *J* = 10.0, 8.8 Hz, 1H), 5.56 (dd, *J* = 10.0, 5.2 Hz, 1H), 3.64-3.36 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4 (d, *J* = 249.2 Hz), 135.8, 133.2 (d, *J* = 8.6 Hz), 131.9 (d, *J* = 13.8 Hz), 131.6 (d, *J* = 2.8 Hz), 131.5,131.0, 129.5, 122.8 (t, *J* = 288.2 Hz), 118.1 (d, *J* = 23.4 Hz), 116.9 (d, *J* = 3.5 Hz), 39.4 (td, *J* = 18.8, 2.2 Hz), 6.0 (q, *J* = 2.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.0 (d, *J* = 229.1 Hz), -104.7 (d, *J* = 229.0 Hz), -116.8. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{11}O_2F_3SBrINa$: 540.8558, found: 540.8560.



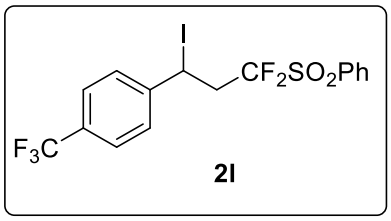
2j

2j: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.60-7.56 (m, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.47 (dd, *J* = 9.6, 5.6 Hz, 1H), 3.62-3.39 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.8, 138.6, 135.6, 131.6, 130.9, 129.6, 129.4 126.8, 123.0 (t, *J* = 289.0 Hz), 40.6 (t, *J* = 18.6 Hz), 21.3, 17.5 (t, *J* = 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.39 (d, *J* = 228.0 Hz), -104.61 (d, *J* = 228.0 Hz). RMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}O_2F_2SINa$: 458.9703, found: 458.9687.



2k

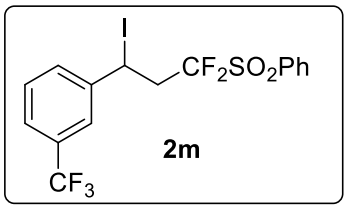
2k: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.60-7.56 (m, 2H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.94 (s, 1H), 6.78 (dd, *J* = 8.0, 2.0 Hz, 1H), 5.42 (dd, *J* = 9.6, 5.6 Hz, 1H), 3.80 (s, 3H), 3.61-3.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 144.1, 135.7, 131.6, 130.9, 129.9, 129.4, 122.9 (t, *J* = 288.9 Hz), 119.2, 114.0, 112.7, 55.4, 40.5 (t, *J* = 18.6 Hz), 16.9 (t, *J* =2.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.6 (1F, *J* = 227.8 Hz), -104.5 (1F, *J* = 227.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}O_3F_2SINa$: 474.9652, found: 474.9654.



2l

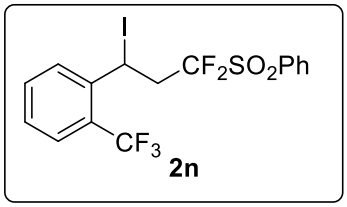
2l: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.75 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.61-7.52 (m, 6H),

5.49-5.45 (m, 1H), 3.62-3.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 135.8, 131.5, 131.0, 130.6 (q, *J* = 32.5 Hz), 129.5, 127.4, 125.9 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 270.6 Hz), 122.8 (t, *J* = 288.6 Hz), 40.6 (t, *J* = 18.9 Hz), 14.9 (t, *J* = 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.7, -100.72 (d, *J* = 229.1 Hz), -104.33 (d, *J* = 229.0 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{12}O_2F_5SINa$: 512.9421, found: 512.9426.



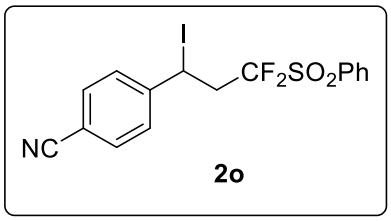
2m

2m: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.64-7.56 (m, 4H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 5.48 (dd, *J* = 9.2, 6.0 Hz, 1H), 3.62-3.41 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 135.8, 131.5, 131.3 (q, *J* = 32.4 Hz) 130.9, 130.4, 129.6, 129.5, 125.4 (q, *J* = 3.7 Hz), 123.7 (q, *J* = 270.9 Hz), 123.7 (q, *J* = 3.6 Hz), 122.8 (t, 288.4 Hz), 40.7 (t, *J* = 18.9 Hz), 14.9 (t, *J* = 2.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.73, -100.8 (d, *J* = 229.3 Hz), -104.2 (d, *J* = 229.2 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{12}O_2F_5SINa$: 512.9421, found: 512.9418.



2n

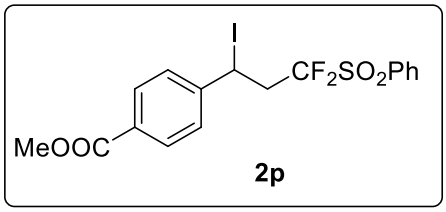
2n: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.60-7.56 (m, 3H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 5.78 (dd, *J* = 9.6, 5.2 Hz, 1H), 3.75-3.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 135.7, 132.8, 131.4, 131.0, 130.4, 129.5, 128.4, 125.9 (q, *J* = 5.8 Hz), 125.5 (q, *J* = 30.6 Hz), 124.0 (q, *J* = 272.5 Hz), 122.9 (t, *J* = 288.6 Hz), 40.4 (t, *J* = 18.7 Hz), 9.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7, -103.7 (d, *J* = 227.4 Hz), 104.6 (dq, *J* = 227.4, 4.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{12}O_2F_5SINa$: 512.9421, found: 512.9427.



2o

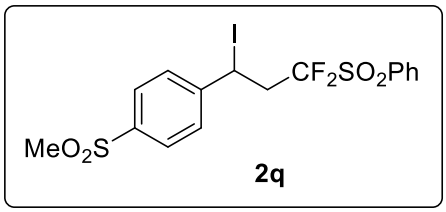
2o: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.7 Hz, 2H), 7.76 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.61-7.56 (m, 4H), 7.53-7.50 (m, 2H), 5.46-5.43 (m, 1H), 3.60-3.38 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.6, 135.9, 132.7, 131.4, 130.9, 129.5, 127.8, 122.7 (t, *J* = 288.3 Hz), 118.3, 112.3, 40.4 (t, *J* = 19.0 Hz), 14.4 (d, *J* = 2.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.43 (d, *J* = 229.5

Hz), -104.19 (d, *J* = 229.5 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{12}NO_2F_2SINa$: 469.9499, found: 469.9501.



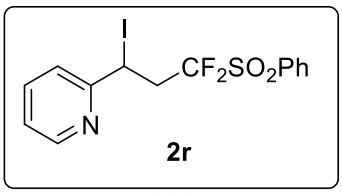
2p

2p: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.59-7.55 m, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 5.47 (dd, *J* = 9.6, 5.6 Hz, 1H), 3.89 (s, 3H), 3.62-3.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 147.4, 135.7, 131.5, 130.9, 130.2, 129.5, 127.0, 122.8 (t, *J* = 288.6 Hz), 52.3, 40.4 (t, *J* = 18.8 Hz), 15.4 (t, *J* = 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.8 (d, *J* = 228.9 Hz), -104.3 (d, *J* = 228.9 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{17}H_{15}O_4F_2SINa$: 502.9601, found: 502.9604.



2q

2q: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.89-7.86 (m, 2H), 7.76 (tt, *J* = 7.6, 1.2 Hz), 7.63-7.58 (m, 4H), 5.50-5.46 (m, 1H), 3.62-3.42 (m, 2H), 3.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.5, 140.4, 135.9, 131.3, 130.9, 129.5, 128.1, 128.0, 122.7 (t, *J* = 288.2 Hz), 44.5, 40.5 (t, *J* = 18.9 Hz), 14.2 (t, 2.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.3 (d, *J* = 228.9 Hz), -104.1 (d, *J* = 229.3 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}O_4F_2S_2INa$: 522.9322, found: 522.9319.



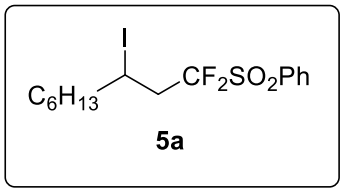
2r

2r: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (ddd, *J* = 4.8, 1.6, 0.8 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 2H), 7.73 (td, *J* = 7.6, 1.2 Hz, 1H), 7.63-7.55 (m, 3H), 7.31 (dt, *J* = 7.8, 0.8 Hz, 1H), 7.14 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 5.54 (dd, *J* = 10.0, 4.4 Hz, 1H), 4.00-3.86 (m, 1H), 3.47-3.33 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 149.7, 136.9, 135.5, 131.8, 130.8, 129.3, 123.0, 123.0 (t, *J* = 289.7 Hz), 120.9, 38.7 (t, *J* = 19.0 Hz), 17.5 (t, *J* = 9.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.23 (d, *J* = 229.6 Hz), -103.79 (d, *J* = 229.6 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{14}H_{12}NO_2F_2SINa$: 445.9499, found: 445.9498.

General Procedure of ATRA Reaction of Aliphatic Alkene:

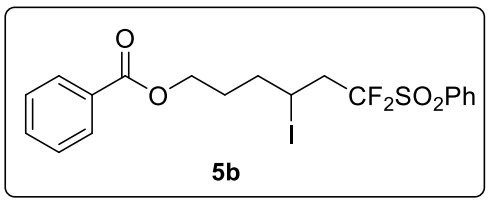
$Ru(bpy)_3Cl_2·6H_2O$ (1.5mg, 0.002 mmol), K_2CO_3 (55.2 mg, 0.4 mmol) and

$PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). 1-Octene **4a** (33.6 mg, 0.3 mmol) and $CHCl_3$ (0.5 mL) were added via syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **5a** as a pale yellow oil (75.6 mg, 88%).



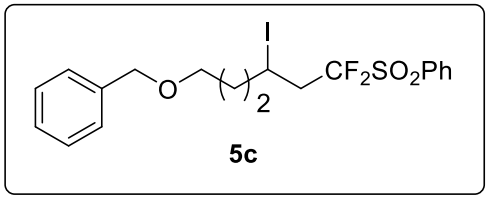
5a

5a: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.77 (td, *J* = 7.6, 1.2 Hz, 1H), 7.64-7.60 (m, 2H), 4.38-4.31 (m, 1H), 3.23-2.99 (m, 2H), 1.87-1.70 (m, 2H), 1.58-1.47 (m, 1H), 1.46-1.35 (m, 1H), 1.33-1.22 (m, 6H), 0.87 (t, *J* = 7.2 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.7, 131.8, 130.9, 129.5, 123.5 (t, *J* = 287.4 Hz), 40.3, 39.8 (t, *J* = 18.9 Hz,), 31.6, 29.4, 28.2, 22.6, 21.4 (t, *J* = 7.2 Hz), 14.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.6 (d, *J* = 227.4 Hz), -103.2 (d, *J* = 227.1 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{21}O_2F_2SINa$: 453.0173, found: 453.0171.



5b

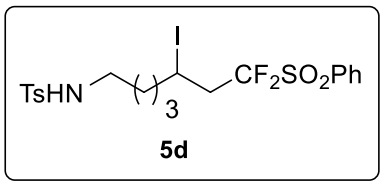
5b: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-8.01 (m, 2H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.76 (tt, *J* = 7.6, 0.8 Hz, 1H), 7.62-7.58 (m, 2H), 7.54 (tt, J = 7.2 Hz, 1.2 Hz, 1H), 7.43-7.39 (m, 2H), 4.47-4.40 (m, 1H), 4.35 (t, *J* = 6.0 Hz, 2H), 3.29-3.02 (m, 2H), 2.09-1.86 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 135.7, 133.0, 131.7, 130.9, 130.1, 129.6, 129.5, 128.4, 123.3 (t, *J* = 289.2 Hz), 63.6, 39.9 (t, *J* = 19.1 Hz), 36.8, 28.9, 20.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.1 (d, *J* = 228.4 Hz), -103.1 (d, *J* = 228.4 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{19}H_{19}O_4F_2SINa$: 530.9914, found: 530.9909.



5c

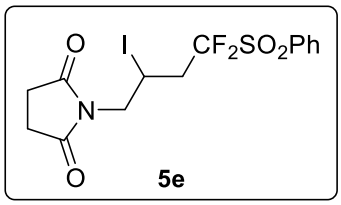
5c: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.76 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.63-7.59 (m, 2H), 7.35-7.24 (m, 5H), 4.48 (s,

2H), 4.41-4.34 (m, 1H), 3.49 (t, *J* = 5.6 Hz, 2H), 3.25-3.00 (m, 2H), 1.97-1.82 (m, 3H), 1.71-1.66 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 135.7, 131.7, 130.9, 129.5, 128.4, 127.7, 127.6, 123.4 (t, *J* = 287.5 Hz), 73.0, 68.9, 39.8 (t, *J* = 19.0 Hz), 37.3, 29.8, 20.9 (t, *J* = 1.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.6 (d, *J* = 227.4 Hz), -103.2 (d, *J* = 227.4 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{19}H_{21}O_3F_2SINa$: 517.0122, found: 517.0125.



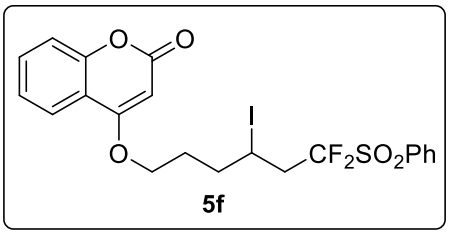
5d

5d: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.66-7.62 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.78 (t, *J* = 6.0 Hz, 1H), 4.30-4.23 (m, 1H), 3.20-2.91 (m, 4H), 2.42 (s, 3H), 1.78-1.65 (m, 2H), 1.53-1.33 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5, 136.9, 135.8, 131.7, 130.9, 129.8, 129.5, 127.2, 123.3 (t, *J* = 287.3 Hz), 42.9, 39.8 (t, *J* = 19.0 Hz), 39.5, 28.5, 26.5, 21.6, 20.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.3 (d, *J* = 227.8 Hz), -103.0 (d, *J* = 227.8 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{20}H_{24}NO_4F_2S_2INa$: 594.0057, found: 594.0050.



5e

5e: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.79 (t, *J* = 7.6 Hz, 1H), 7.65-7.61 (m, 2H), 4.71-4.64 (m, 1H), 3.99 (dd, J = 14.0, 8.0 Hz, 1H), 3.81 (dd, *J* = 13.6, 7.6 Hz, 1H), 3.23-3.04 (m, 2H), 2.76 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.7, 135.8, 131.5, 130.9, 129.5, 122.9 (t, *J* = 287.4 Hz), 46.3, 38.0 (t, *J* = 20.2 Hz), 28.2, 12.3 (t, *J* = 2.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.5 (d, *J* = 229.5 Hz), -103.7 (d, *J* = 229.5 Hz). HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{14}H_{15}NO_4IF_2S$: 457.9735, found: 457.9741.



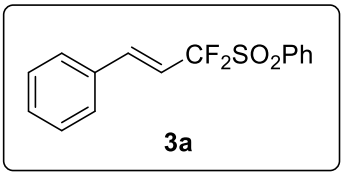
5f

5f: ^{1}H NMR (400 MHz, CDCl3) δ 7.96 (d, *J* = 7.9 Hz, 2H), 7.81-7.76 (m, 2H), 7.64 (t, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 8.4 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.25 (d, *J* = 8.8 Hz, 1H), 5.67 (s, 1H), 4.49 (s, 1H), 4.18 (s, 2H), 3.33-3.05 (m, 2H), 2.27-2.02 (m, 4H). ^{13}C NMR (101 MHz, CDCl3) δ 165.5, 162.9, 153.4, 135.8, 132.5, 131.7, 130.9, 129.5, 124.0, 123.3 (t, *J* = 289.87 Hz), 123.1, 116.9, 115.7, 90.7, 68.2, 40.1 (t, *J* = 19.2 Hz), 36.7, 28.7, 19.8 (t, *J*

= 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.72 (d, *J* = 228.9 Hz), -102.88 (d, *J* = 228.9 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{21}H_{19}O_5F_2SINa$: 570.9864, found: 570.9858.

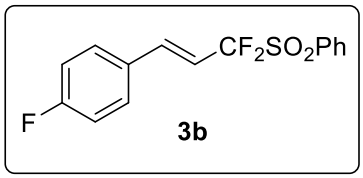
General Procedure of Heck-type Reaction of Styrene:

$Ru(bpy)_3Cl_2·6H_2O$ (1.5mg, 0.002 mmol), DABCO (44.8 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol) and $CHCl_3$ (0.5 mL) were added via syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **3a** as a white solid (54.0 mg, 92%).



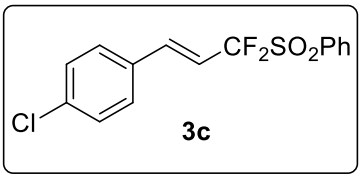
3a

3a[7]：^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.64-7.60 (m, 2H), 7.50-7.47 (m, 2H), 7.40-7.38 (m, 3H), 7.19 (dt, *J* = 16.4 Hz, 2.0 Hz, 1H), 6.39 (dt, *J* = 16.0 Hz, 12.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4 (t, *J* = 8.8 Hz), 135.4, 133.7, 133.1, 130.9, 130.5, 129.4, 129.0, 128.0, 121.6 (t, *J* = 281.7 Hz), 112.5 (t, *J* = 22.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.2.

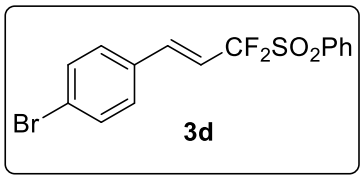


3b

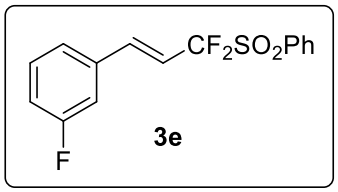
3b: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.76 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.67 -7.60 (m, 2H), 7.50-7.45 (m, 2H), 7.16 (dt, *J* = 16.4, 2.0 Hz, 1H), 7.11-7.05 (m, 2H), 6.31 (dt, *J* = 16.2, 11.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.0 (d, *J* = 250.0 Hz), 141.1 (t, *J* = 8.9 Hz), 135.4, 133.0, 130.9, 129.9, 129.9, 129.4, 121.6 (t, *J* = 281.8 Hz), 116.2 (d, *J* = 22.0 Hz), 112.2 (td, *J* = 22.5, 2.3Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.1, -109.4. HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{15}H_{12}O_2F_3S$: 313.0510, found: 313.0509.



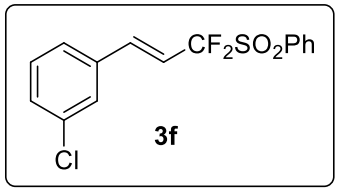
3c: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.6 Hz, 2H), 7.76 (tt, *J* = 7.2, 0.8 Hz, 1H), 7.65-7.61 (m, 2H), 7.43-7.41 (m, 2H), 7.37-7.35 (m, 2H), 7.15 (dt, *J* = 16.0, 2.0 Hz, 1H), 6.36 (dt, *J* = 16.4, 11.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1 (t, *J* = 8.9 Hz), 136.5, 135.4, 133.0, 132.2, 130.9, 129.4, 129.3, 129.2, 121.5 (t, *J* = 281.9 Hz), 113.2 (t, *J* = 22.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.3. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{11}O_2F_2SClNa$: 351.0034, found: 351.0028.



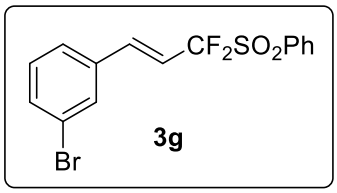
3d: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.2 Hz, 2H), 7.77 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.66-7.61 (m, 2H), 7.56-7.52 (m, 2H), 7.38-7.34 (m, 2H), 7.14 (dt, *J* = 16.0, 2.2 Hz, 1H), 6.39 (dt, *J* = 16.4, 11.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2 (t, *J* = 8.9 Hz), 135.5, 133.0, 132.6, 132.3, 130.9, 129.4, 129.4, 124.8, 121.5 (t, *J* = 281.9 Hz), 113.3 (t, *J* = 22.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.3. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{11}O_2F_2SBrNa$: 394.9529, found: 394.9527.



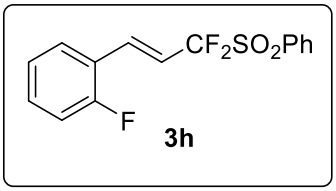
3e: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 2H), 7.78 (tt, *J* = 7.6 Hz, 1H), 7.65-7.61 (m, 2H), 7.40-7.34 (m, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.20-7.14 (m, 2H), 7.10 (td, *J* = 8.4, 2.0 Hz, 1H), 6.40 (dt, *J* = 16.0, 11.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1 (d, *J* = 245.7 Hz), 141.1 (td, *J* = 8.9, 2.6 Hz), 135.8 (d, *J* = 7.7 Hz), 135.5, 132.9, 130.9, 130.6 (d, *J* = 8.3 Hz), 129.4, 123.9 (d, *J* = 2.7 Hz), 121.4 (t, *J* = 281.9 Hz), 117.4 (d, *J* = 21.3 Hz), 114.4 (d, *J* = 22.0 Hz), 114.1 (t, *J* = 22.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.5, -112.2. HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{15}H_{12}O_2F_3S$: 313.0510, found: 313.0527.



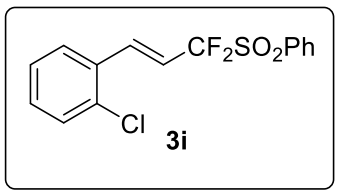
3f:[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.78 (tt, *J* = 7.6, 0.8 Hz, 1H), 7.65-7.61 (m, 2H), 7.48 (s, 1H), 7.39-7.31 (m, 3H), 7.14 (dt, *J* = 16.2, 2.1 Hz, 1H), 6.41 (dt, *J* = 16.2, 11.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9 (t, *J* = 8.9 Hz), 135.5, 135.4, 135.1, 132.9, 130.9, 130.4, 130.3, 129.4, 127.8, 126.1, 121.3 (t, *J* = 282.0 Hz), 114.2 (t, *J* = 22.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.5.



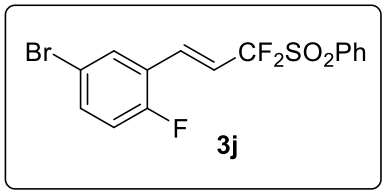
3g: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 2H), 7.77 (tt, *J* = 7.6, 0.8 Hz, 1H), 7.67 -7.60 (m, 3H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 8.0 Hz, 1H), 7.12 (tt, *J* = 16.0, 2.0 Hz, 1H), 6.40 (dt, *J* = 16.0, 11.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8 (t, *J* = 8.9 Hz), 135.7, 135.5, 133.3, 132.9, 130.9, 130.7, 130.5, 129.4, 126.6, 123.1, 119.9 (t, *J* = 281.9 Hz), 114.2 (t, *J* = 22.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.6. HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{15}H_{12}O_2F_2SBr$: 372.9709, found: 372.9699.



3h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.65-7.61 (m, 2H), 7.51 (t, *J* = 8.4 Hz, 1H), 7.40-7.35 (m, 1H), 7.32 (dt, *J* = 16.4, 2.2 Hz, 1H), 7.18 (td, *J* = 7.6, 1.2 Hz, 1H), 7.13-7.08 (m, 1H), 6.52 (dt, *J* = 16.4, 11.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2 (d, *J* = 252.3 Hz), 135.4, 135.2 (td, *J* = 9.3, 3.1 Hz), 133.0, 132.0 (d, *J* = 8.8 Hz), 130.9, 129.4, 129.1, 124.6 (d, *J* = 3.6 Hz), 121.7 (d, *J* = 11.5 Hz), 121.4 (d, *J* = 281.8 Hz), 116.3 (d, *J* = 21.8 Hz), 115.2 (td, *J* = 22.3, 7.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.7, -114.8. HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{15}H_{12}O_2F_3S$: 313.0510, found: 313.0519.

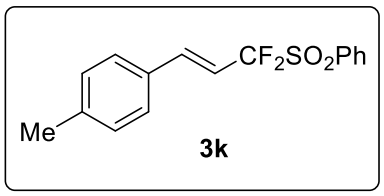


3i: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.6 Hz, 2H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.65-7.56 (m, 4H), 7.42-7.40 (m, 1H), 7.35-7.28 (m, 2H), 6.41 (dt, *J* = 16.2, 11.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4 (t, *J* = 9.1 Hz), 135.5, 134.6, 132.9, 131.93, 131.3, 130.9, 130.2, 129.4, 127.8, 127.3, 121.3 (t, *J* = 283.8 Hz), 115.3 (t, *J* = 22.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.7. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{11}O_2F_2SClNa$: 351.0034, found: 351.0036.



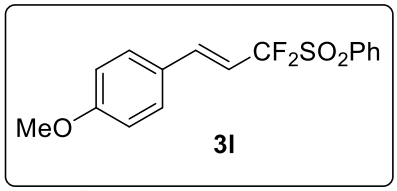
3j: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.9 Hz, 2H), 7.78 (t, *J* = 7.2 Hz, 1H), 7.65-7.61 (m, 3H), 7.49-7.45 (m, 1H), 7.23 (d, *J* = 17.2 Hz), 7.01 (t, *J* = 9.2 Hz, 1H), 6.52 (dt, *J* = 16.3, 11.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1 (d, *J* = 252.9 Hz), 135.5, 134.6 (d, *J* = 8.7 Hz), 133.8 (td, *J* = 9.4, 2.9 Hz,), 132.8, 131.6 (d, *J* = 2.7 Hz), 131.0, 129.4, 123.6 (d, *J* = 13.0 Hz), 121.1 (t, *J* = 282.4 Hz), 118.1 (d,

J = 23.5 Hz), 117.2 (d, *J* = 3.4 Hz), 116.8 (td, *J* = 22.5, 6.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.0, -116.9. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{10}O_2F_3SBrNa$: 412.9435, found: 412.9430.



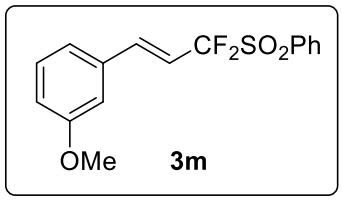
3k

3k[7]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.64-7.60 (m, 2H), 7.38 (d, *J* = 8.0 Hz), 7.20 (d, *J* = 8.0 Hz), 7.15 (d, *J* = 16.0 Hz, 1H), 6.32 (dt, *J* = 16.4, 11.6 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3 (t, *J* = 8.8 Hz), 140.9, 135.3, 133.2, 131.0, 130.9 129.7, 129.4, 128.0, 121.8 (t, *J* = 281.6 Hz), 111.2 (t, *J* = 22.3 Hz), 21.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.0.



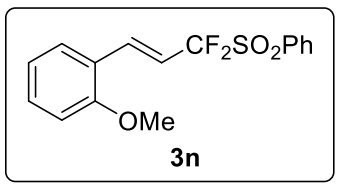
3l

3l: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.44 (d, *J* = 8.8 Hz, 2H), 7.13 (d, *J* = 16.4 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.22 (dt, *J* = 16.4, 12.0 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5, 141.9 (t, *J* = 8.9 Hz), 135.3, 133.2, 130.9, 129.6, 129.3, 126.5, 122.0 (t, *J* = 281.5 Hz), 114.4, 109.6, 22.2, 55.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.7. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{14}O_3F_2SNa$: 347.0529, found: 347.0522.



3m

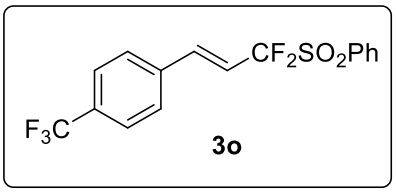
3m: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.55-7.51 (m, 2H), 7.23-6.84 (m, 5H), 6.30 (dt, *J* = 15.6, 12.0 Hz, 1H), 3.74 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 142.3 (t, *J* = 8.8 Hz), 135.4, 135.0, 133.0, 130.9, 130.0, 129.4, 121.6 (t, *J* = 281.8 Hz), 120.6, 116.4, 112.8, 112.7 (t, *J* = 22.2 Hz), 55.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.3. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{14}O_3F_2NaS$: 347.0529, found: 347.0528.



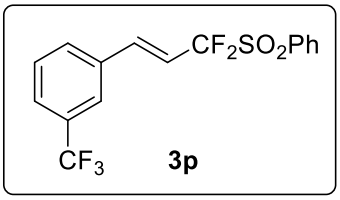
3n

3n: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 2H), 7.49-7.41 (m, 2H), 7.39-7.31 (m, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.3 Hz, 1H), 6.52 (dt, *J* = 16.3, 12.2 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 137.9 (t, *J* = 9.4 Hz), 135.2, 133.3, 131.7, 130.9, 129.3,

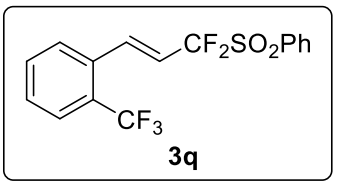
129.2, 122.6, 122.0 (t, *J* = 281.6 Hz), 120.8, 112.9 (t, *J* = 22.0 Hz), 111.2, 55.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.1. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{14}O_3F_2SNa$: 347.0529, found: 347.0514.



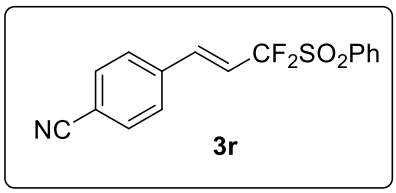
3o: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.8 Hz, 2H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.67-7.59 (m, 6H), 7.24 (d, *J* = 15.6 Hz, 2H), 6.49 (dt, *J* = 16.2, 11.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8 (t, *J* = 8.9 Hz), 137.0, 135.6, 132.8, 132.1 (q, *J* = 32.8 Hz), 130.9, 129.5, 128.2, 126.0 (q, *J* = 3.8 Hz),123.8 (q, *J* = 270.6Hz) 121.2 (t, *J* = 282.6Hz), 115.4 (t, *J* = 22.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8, -101.6. HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{16}H_{12}O_2F_5S$: 363.0478, found: 363.0488.



3p: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.7 Hz, 2H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.73 (s, 1H), 7.69-7.62 (m, 4H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.24 (dt, *J* = 16.4, 2.0 Hz, 1H), 7.22 (s, 0H), 6.48 (dt, *J* = 16.2, 11.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8 (t, *J* = 8.9 Hz), 135.5, 134.4, 132.8, 131.6 (q, *J* = 32.7 Hz), 131.0, 129.6, 129.51, 126.9 (q, *J* = 3.7 Hz), 124.7 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 270N Hz), 121.3 (t, *J* = 282.1 Hz), 114.8 (t, *J* = 22.5 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9, -101.5 (d, *J* = 1.7 Hz), -101.5 (d, *J* = 1.7 Hz). HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{16}H_{12}O_2F_5S$: 363.0478, found: 363.0487.



3q: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 2H), 7.77 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.64-7.54 (m, 4H), 7.49 (t, *J* = 7.6 Hz, 1H), 6.40 (dt, *J* = 16.0, 11.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.2 (td, *J* = 9.0, 2.1 Hz), 135.6, 132.7, 132.5, 132.4, 130.9, 129.9, 129.4, 128.7 (q, *J* = 30.4 Hz), 128.2, 126.2 (q, *J* = 5.5 Hz), 123.9 (q, *J* = 272.4 Hz), 120.9 (t, *J* = 282.3 Hz), 117.2 (t, *J* = 22.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.0, -102.2. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{11}O_2F_5SNa$: 385.0298, found: 385.0291.

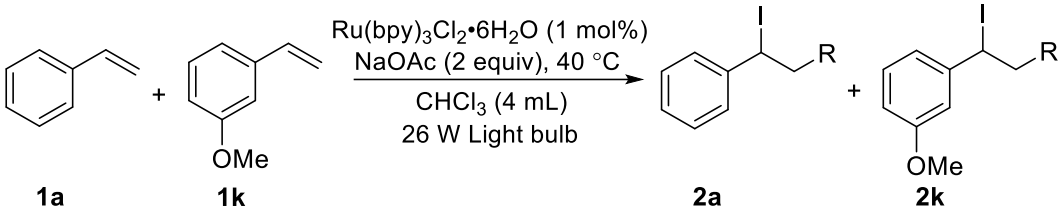


3r: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 2H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.72-7.57 (m, 6H), 7.22

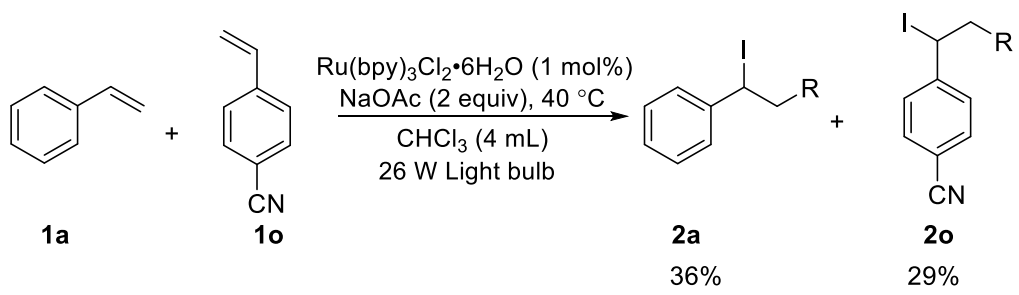
(dt, *J* = 16.4, 2.0 Hz, 1H), 6.51 (dt, *J* = 16.2, 11.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.3 (t, *J* = 8.9 Hz), 137.8, 135.6, 132.8, 132.6, 130.9, 129.5, 128.4, 121.0 (t, *J* = 282.4 Hz), 118.3, 116.5 (t, *J* = 22.6 Hz), 113.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.7. HRMS ESI (*m/z*): $[M+H]^+$ calcd. for $C_{16}H_{12}NO_2F_2S$: 320.0557, found: 320.0550.

Mechanistic Investigation:

Competition Studies:

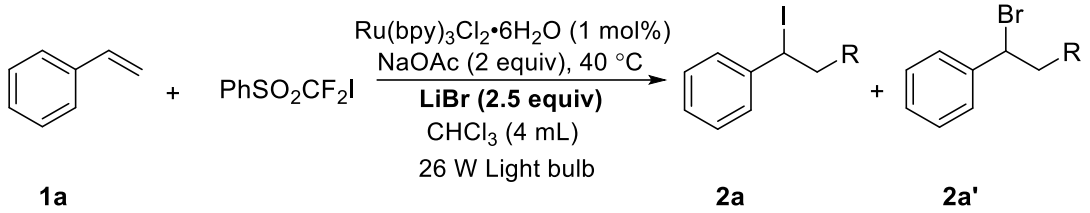


$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol), **1k** (40.2 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **2a** (20.2 mg, 24%) and **2k** (25.3 mg, 28%).

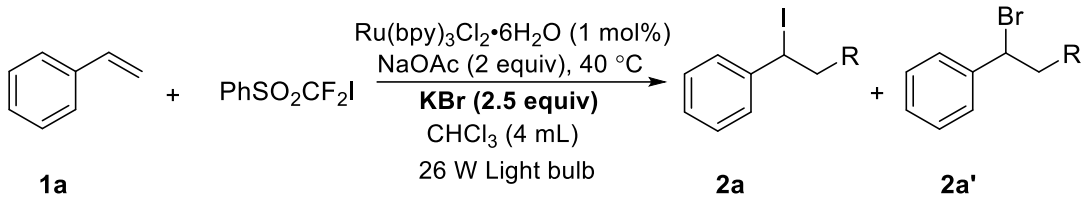


$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol), **1o** (38.7 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **2a** (30.4 mg, 36%) and **2o** (25.9 mg, 29%).

Carbocation Trapping Experiment:



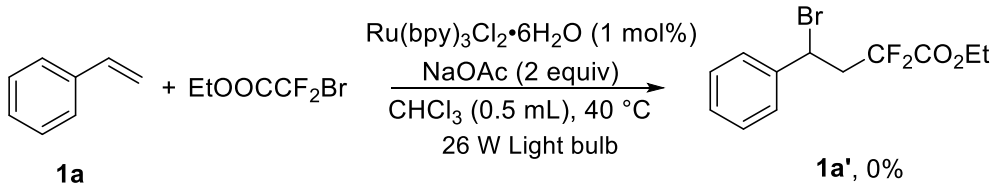
$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol), LiBr (43.4, 0.5 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and $PhCF_3$ (29.2 mg, 0.2 mmol) was added. None of **2a'** was detected by ^1H NMR and ^{19}F NMR of the crude material. **2a** was obtained with a low yield (10%, ^{19}F yield).



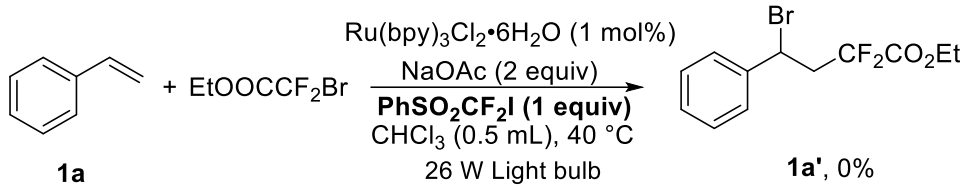
$Ru(bpy)_3Cl_2 \cdot 6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol), KBr (59.5, 0.5 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and $PhCF_3$ (29.2 mg, 0.2 mmol) was added. None of **2a'** was detected by ^1H NMR and ^{19}F NMR of the crude material. **2a** was obtained with a moderate yield (42%, ^{19}F yield).

Propagation Experiments:

In Stephenson's investigation,[8] ethyl bromoacetate which was inert to ATRA reaction with the optimized reaction conditions can undergo ATRA reaction when another atom transfer agent (ethyl bromomalonate or ethyl bromofluoroacetate) known to undergo ATRA reaction efficiently was added. It meaned that a propagation mechanism was operative. Here in we applied the same strategy to investigate the propagation mechanism. In our standard conditions $PhSO_2CF_2I$ was a good substrate for the ATRA reaction while ethyl bromodifluoroacetate can not achieve the transformation at all. We mixed them in the same reaction to test if ethyl bromodifluoroacetate can be initiated to undergo ATRA reaction.



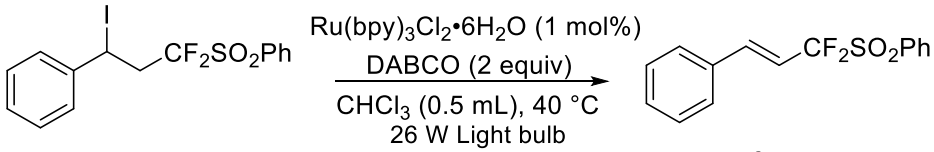
$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol) and NaOAc (33 mg, 0.4 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol), $EtOOCCF_2Br$ (40.6 mg, 0.2 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. None of the product **1a'** was detected by ^{19}F NMR.



1a **1a'**, 0%

$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (31.2 mg, 0.3 mmol), $EtOOCCF_2Br$ (81.2 mg, 0.4 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. None of the product **1a'** was detected by ^{19}F NMR and **2a** was obtained with good yield (83%, isolated yield). *This result revealed that a propagation mechanism may not be operative.*

General Procedure for Transformation of 2a to 3a:

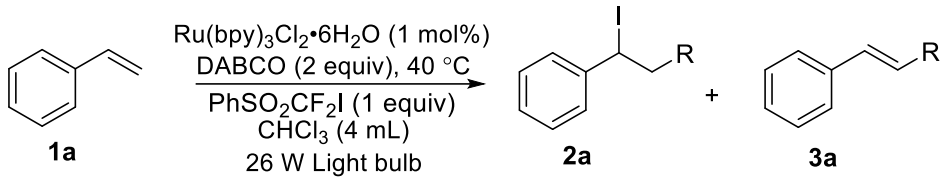


2a **3a,** 93%

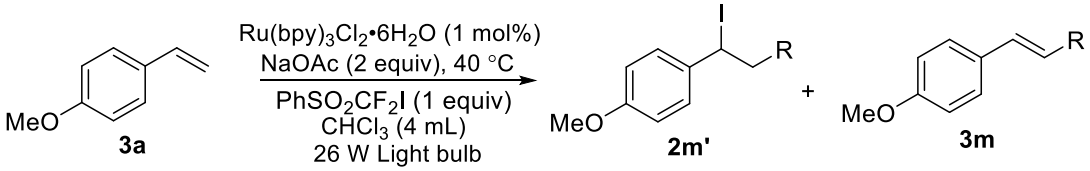
$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and **2a** (84.4 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial

approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **3a** as a white solid (54.7 mg, 93%).

Capature of Intermediate (2a and 2m'):

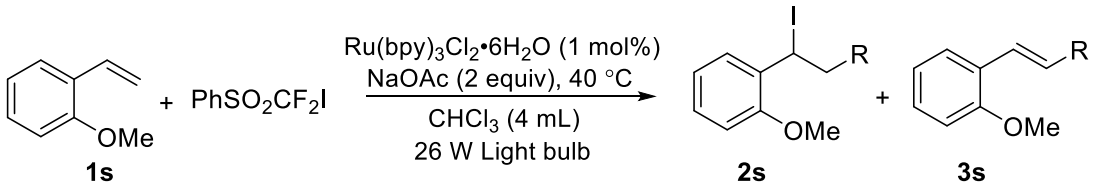


time	2a	3a
4 h	0	20%
8 h	0	73%



time	2m'	2m
4 h	0	30%
8 h	0	66%

General Procedure for Transformation of 2s to 3s:

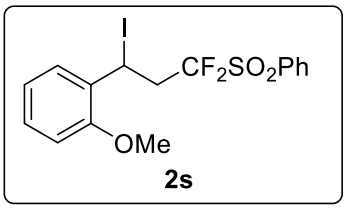


time	2s	3s
24 h	60%	23%
48 h	45%	43%

$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). 2-Methoxystyrene **1s** (40.2 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of

the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **2s** (54.2 mg, 60%) and **3s** (14.9 mg, 23%).

$Ru(bpy)_3Cl_2·6H_2O$ (1.5 mg, 0.002 mmol), NaOAc (33 mg, 0.4 mmol) and $PhSO_2CF_2I$ (63.6 mg, 0.2 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). 2-Methoxystyrene **1s** (40.2 mg, 0.3 mmol) and $CHCl_3$ (4.0 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 48 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **2s** (40.7 mg, 45%) and **3s** (27.8 mg, 43%). *This revealed that the heck-type product can be obtained from the ATRA product in the reaction.*

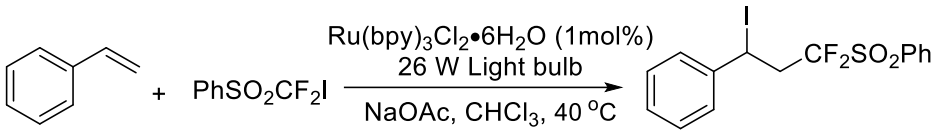


2s

2s: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.73 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.60-7.56 (m, 2H), 7.36 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.27-7.23 (m, 1H), 6.90 (td, *J* = 7.6, 0.8 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 5.81 (dd, *J* = 9.6, 5.2 Hz, 1H), 3.90 (s, 3H), 3.78-3.36 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 135.6, 131.8, 130.9, 130.4, 129.9, 129.4, 128.0, 123.3 (t, *J* = 288.3 Hz), 120.8, 115.4, 55.7, 38.8 (t, *J* = 18.6 Hz), 11.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.9 (d, *J* = 227.1 Hz, 1F), -104.6 (d, *J* = 227.1 Hz, 1F). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{16}H_{15}O_3F_2SINa$: 474.9652, found: 474.9659.

General Procedure for Derivatization of Product:

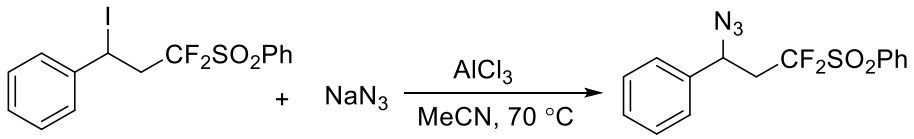
Gram-scale reaction:



1a, 4.5mmol **2a**, 78%, 1.47g

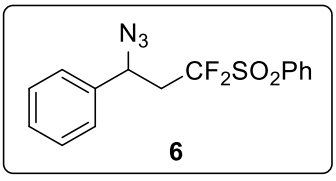
$Ru(bpy)_3Cl_2 \cdot 6H_2O$ (22.5 mg, 0.030 mmol), NaOAc (495 mg, 6 mmol) and $PhSO_2CF_2I$ (954 mg, 3 mmol) were combined in an oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Styrene **1a** (468 mg, 4.5 mmol) and $CHCl_3$ (60 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 40 °C with two 26 W compact fluorescent light bulbs (one on either side of the vial approximately 5 cm away) for 24 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **2a** as a white solid (1.47 g, 78%).

Reaction of 2a with NaN_3:



2a **6**, 74%

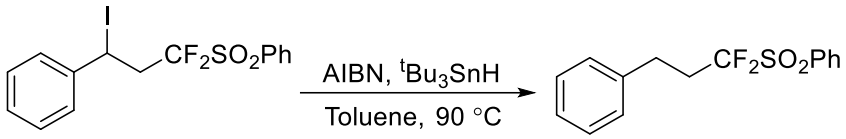
2a (21 mg, 0.05 mmol), NaN_3 (10 mg, 0.15 mmol) and $AlCl_3$ (3.5 mg, 0.025 mmol) were combined in a 5 mL oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). MeCN (0.5 mL) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 70 °C for 16 h. The mixture was then cooled to room temperature, filtered through a plug of silica and washed with EtOAc. The filtrate was concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **6** as a colorless oil (12.5 mg, 74%).



6: ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.77 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.64-7.60 (m, 2H), 7.44-7.34 (m, 5H), 4.97-4.94 (m, 1H), 2.94-2.73 (m, 2H).

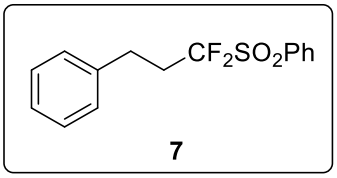
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.1, 135.7, 131.8, 131.0, 129.5, 129.3, 129.1, 126.8, 123.0 (t, *J* = 286.6 Hz), 59.6 (t, J = 2.4 Hz), 35.9 (t, *J* = 19.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.4 (d, *J* = 229.7 Hz), -103.3 (d, *J* = 229.7 Hz). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{13}N_3O_2F_2SNa$: 360.0594, found: 360.0590.

Reductive De-iodination of 2a:



2a **7**, quant

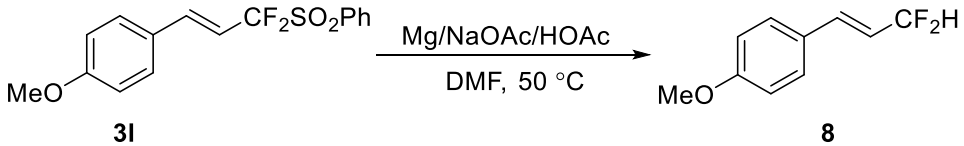
2a (21 mg, 0.05 mmol) and AIBN (24.6 mg, 0.15 mmol) were combined in a 5 mL oven-dried sealing tube. The vessel was evacuated and backfilled with N_2 (repeated for 3 times). Toluene (0.5 mL) and ^{t}Bu$_3$SnH (43.6 mg, 0.15 mmol) were added *via* syringe. The tube was sealed with a Teflon lined cap and the reaction mixture was placed into a preheated oil bath at 90 °C for 3 h. The mixture was then cooled to room temperature, concentrated under vacuum and purified by preparatory thin layer chromatography (PE:EA = 30:1) to give product **7** as a colorless oil (quant yield was obtained).



7

7: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.64-7.60 (m, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.24-7.20 (m, 3H), 2.97-2.93 (m, 2H), 2.72-2.58 (m, 2H). 139.2, 135.4, 132.5, 130.9, 129.4, 128.8, 128.4, 126.8, 124.2 (t, *J* = 284.5 Hz), 31.3 (t, *J* = 20.0 Hz), 27.2 (t, *J* = 3.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.7. HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{15}H_{14}O_2F_2SNa$: 319.0580, found: 319.0568.

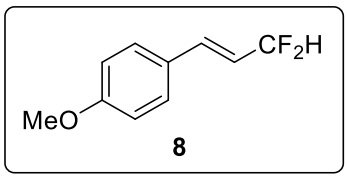
Reductive Desulfonylation:



3l **8**

Into a 10 mL flask containing compound **3l** (32.4 mg, 0.1 mmol) in DMF (1 mL) at room temperature was added HOAc/NaOAc (1:1) buffer solution (8 mol/L, 1 mL).

Magnesium turnings (36 mg, 1.5 mmol) were added in portions. The reaction was stirred at 50 °C until the material was consumed as determined by TLC and quenched with water. The mixture was extracted with Et_2O, and the combined organic layer was washed with water and brine, dried over Na_2SO_4, filtrated and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (PE:EA = 10:1) to give product **8** as a white solid (16.6 mg, 90%).



8

8: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.8 Hz, 2H), 6.91-6.87 (m, 2H), 6.84-6.78 (m, 1H), 6.22 (td, *J* = 56.0, 6.0 Hz, 1H), 6.17-6.07 (m, 1H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.73, 136.8 (t, *J* = 12.2 Hz), 128.8, 127.2, 118.8 (t, *J* = 23.8 Hz), 115.9 (t, *J* = 231.7 Hz), 114.3, 55.4. ^{19}F NMR (376 MHz, $CDCl_3$). HRMS ESI (*m/z*): $[M+Na]^+$ calcd. for $C_{10}H_{10}OF_2Na$: 207.0597, found: 207.0597.

References:

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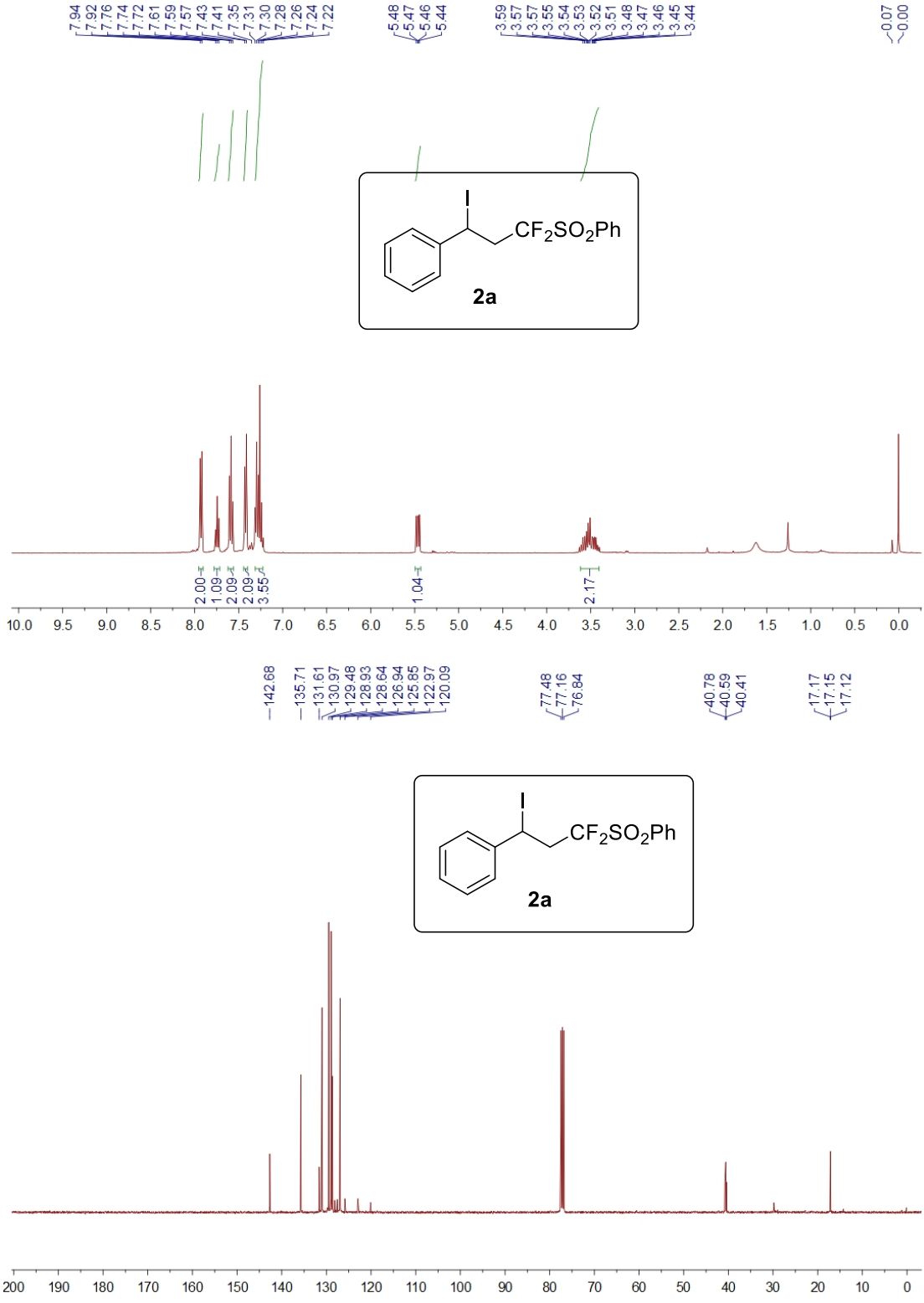
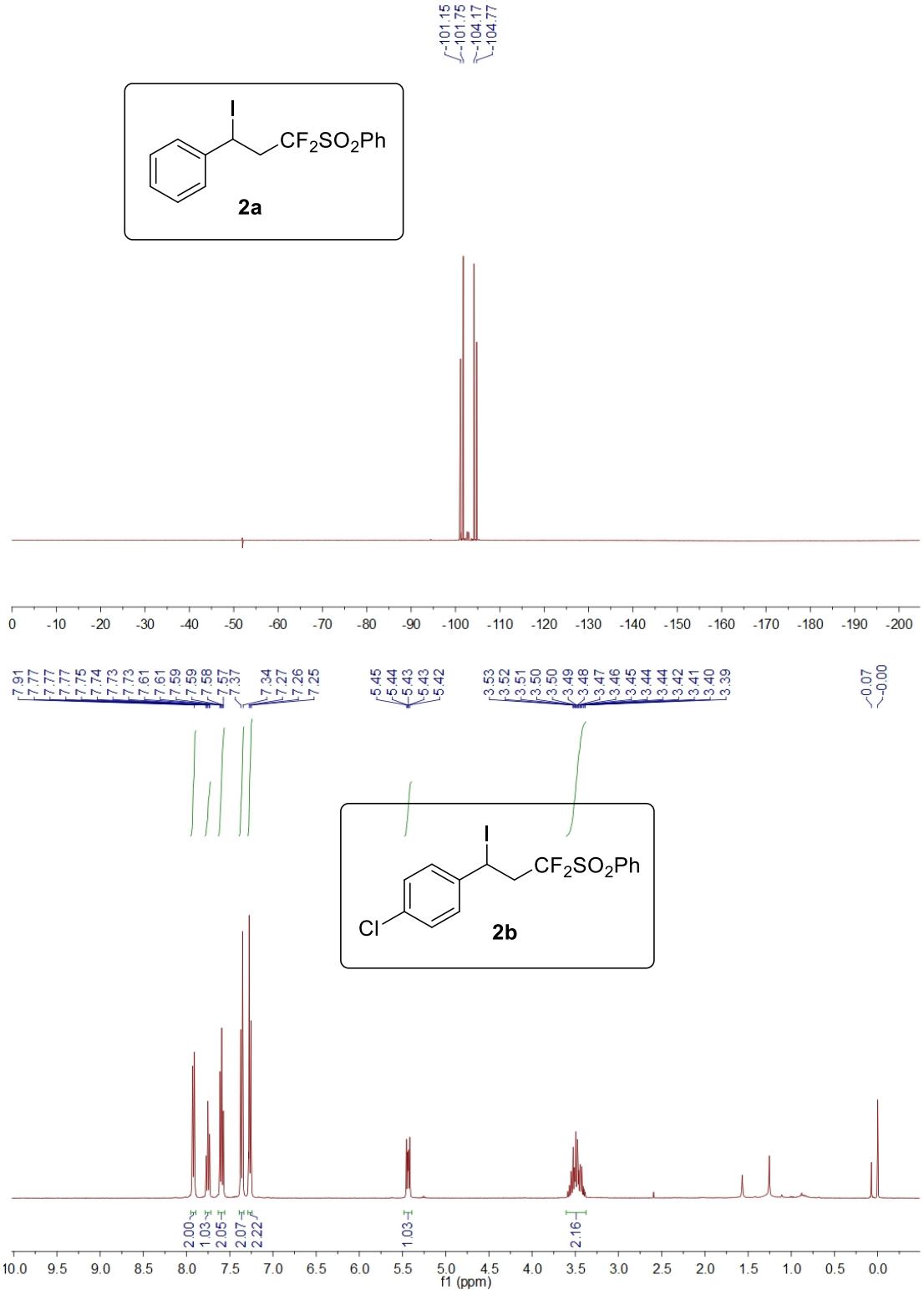
Copies of ^{1}H, ^{13}C and ^{19}F NMR Spectra




-101.15
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-104.17
-104.77
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CF2SO2Ph
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7.74
7.73
7.73
7.61
7.61
7.59
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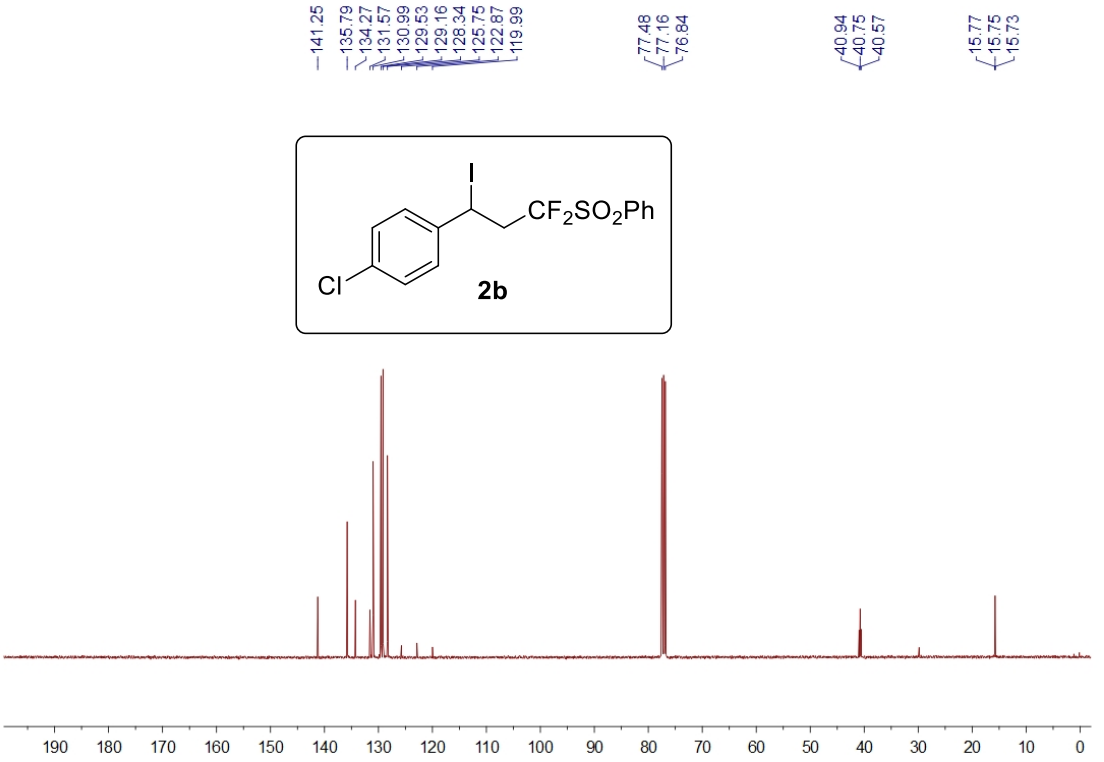
1.03
2.16
f1 (ppm)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128.34
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122.87
119.99
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77.16
76.84
40.94
40.75
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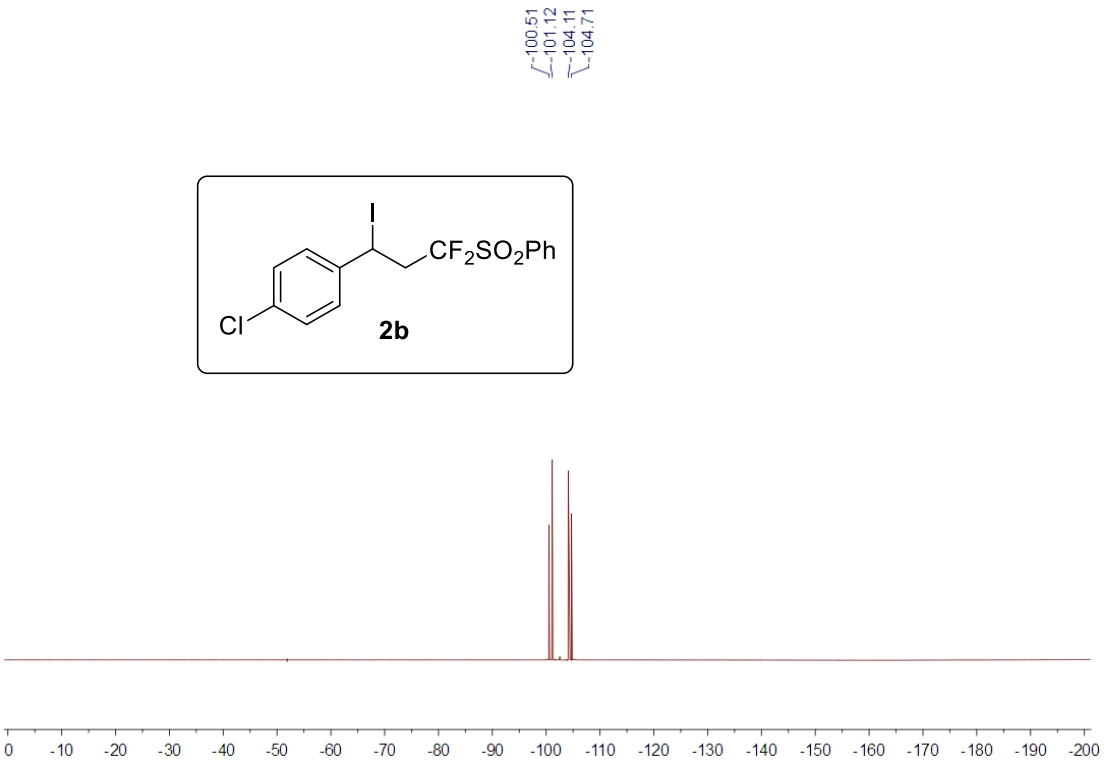
15.75
15.73
I
CF2SO2Ph
Cl
2b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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101.12
104.11
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Cl
2b
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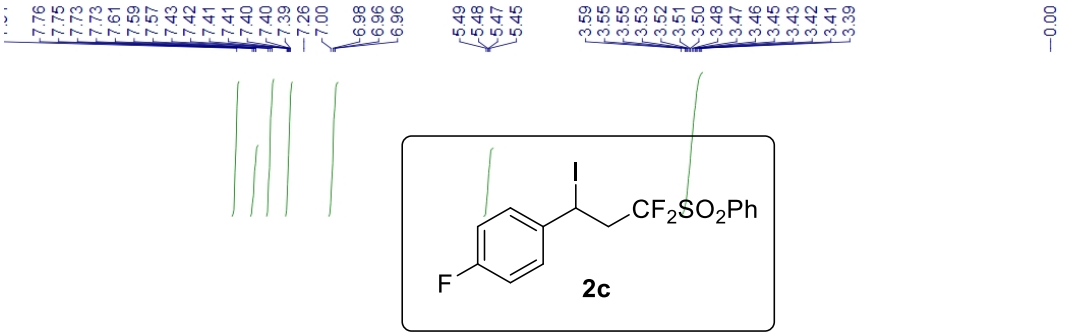
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7.41
7.40
7.40
7.39
7.26
7.00
6.98
6.96
6.96
5.49
5.48
5.47
5.45
3.59
3.55
3.55
3.53
3.52
3.51
3.50
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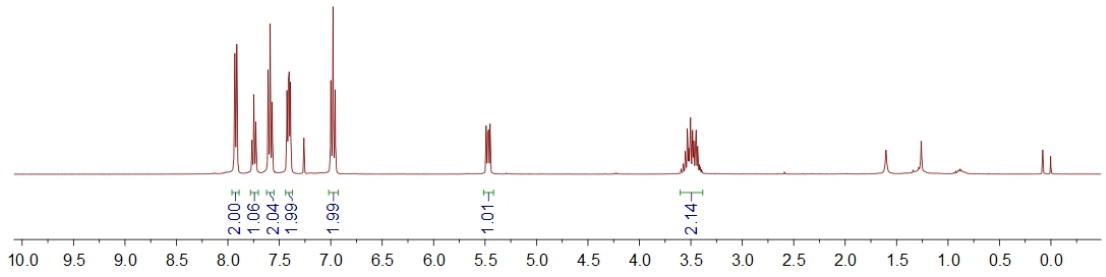
3.45
3.43
3.42
3.41
3.39
0.00
I
CF2SO2Ph
F
2c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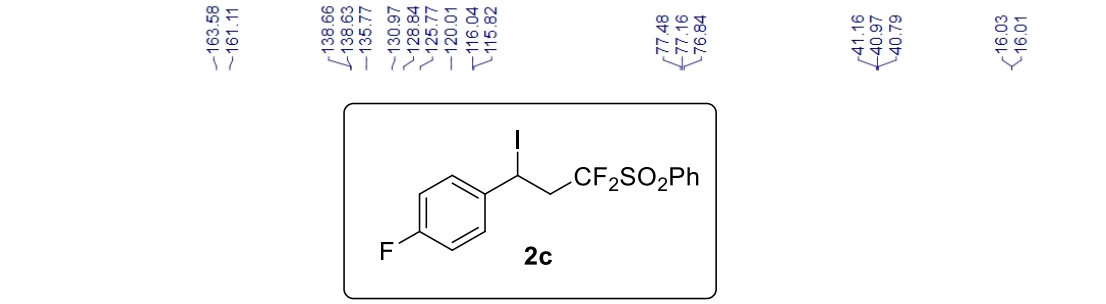
1.06
2.04
1.99
1.99
1.01
2.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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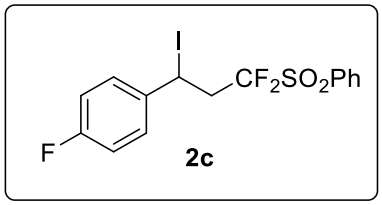
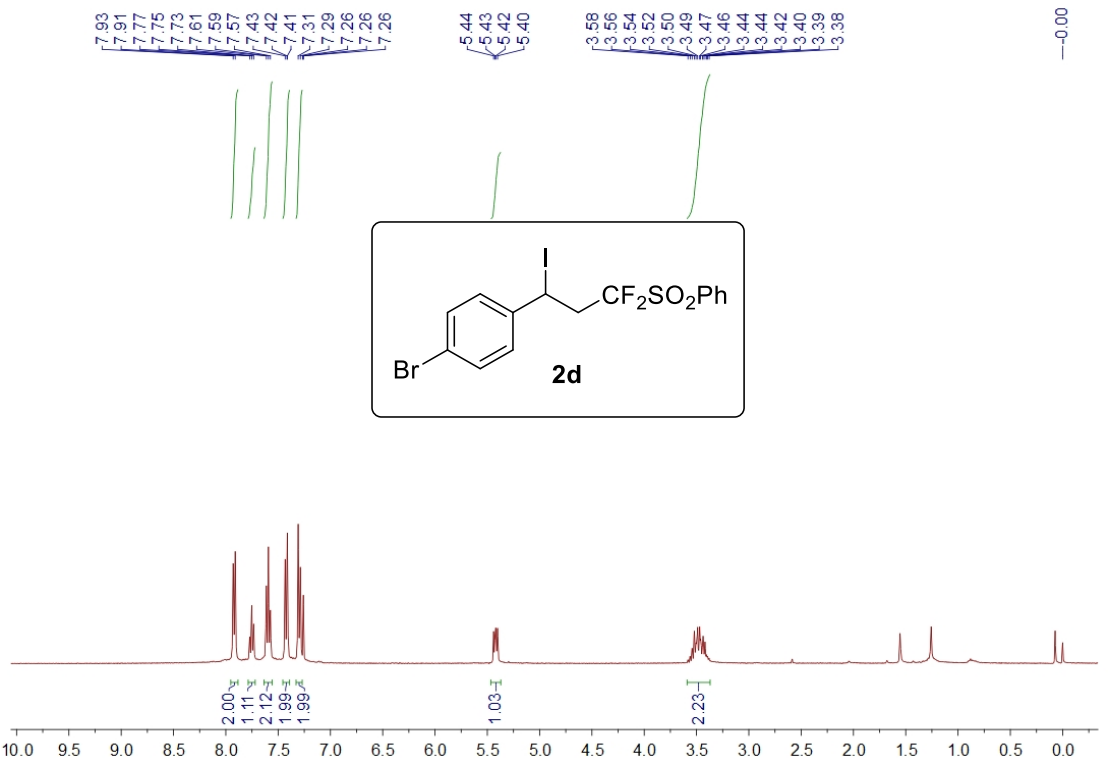
138.66
138.63
135.77
130.97
128.84
125.77
120.01
116.04
115.82
77.48
77.16
76.84
41.16
40.97
40.79
16.03
16.01
I
CF2SO2Ph
F
2c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


I
CF2SO2Ph
F
2c

-100.72
-101.33
-104.18
-104.79
-112.42
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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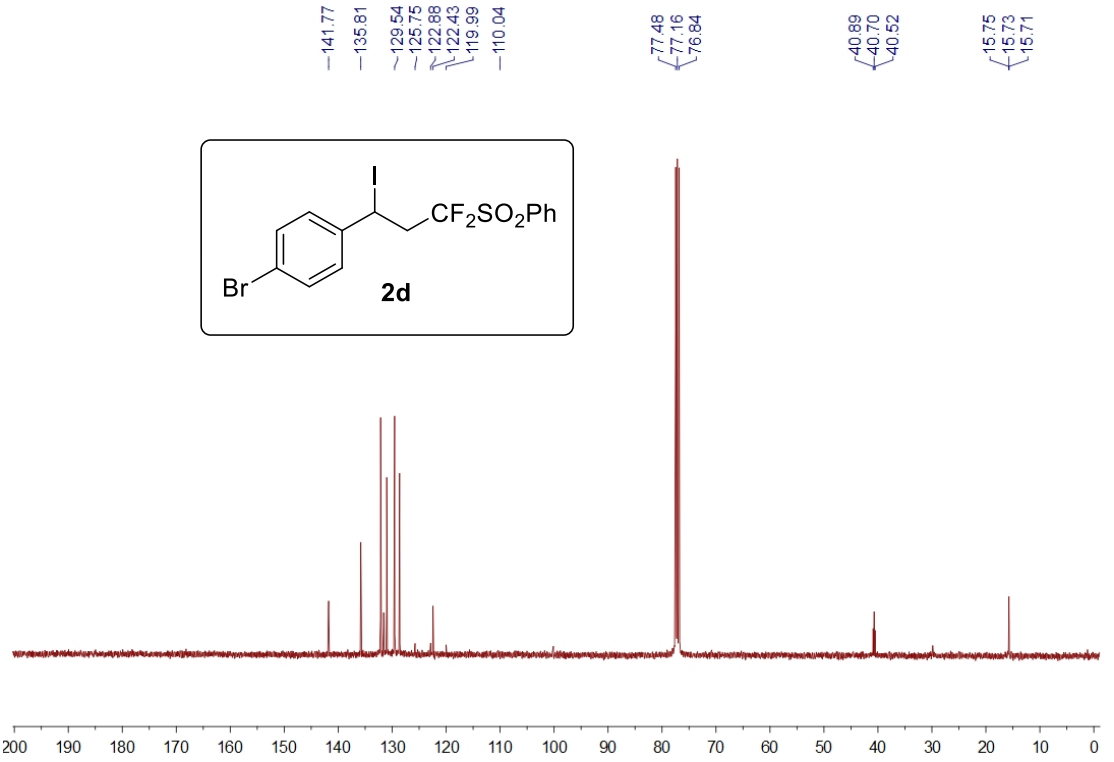
7.61
7.59
7.57
7.43
7.42
7.41
7.31
7.29
7.26
7.26
7.26
5.44
5.43
5.42
5.40
3.58
3.56
3.54
3.52
3.50
3.49
3.47
3.46
3.44
3.44
3.42
3.40
3.39
3.38
0.00
I
CF2SO2Ph
Br
2d
2.00
1.11
2.12
1.99
1.99
1.03
2.23
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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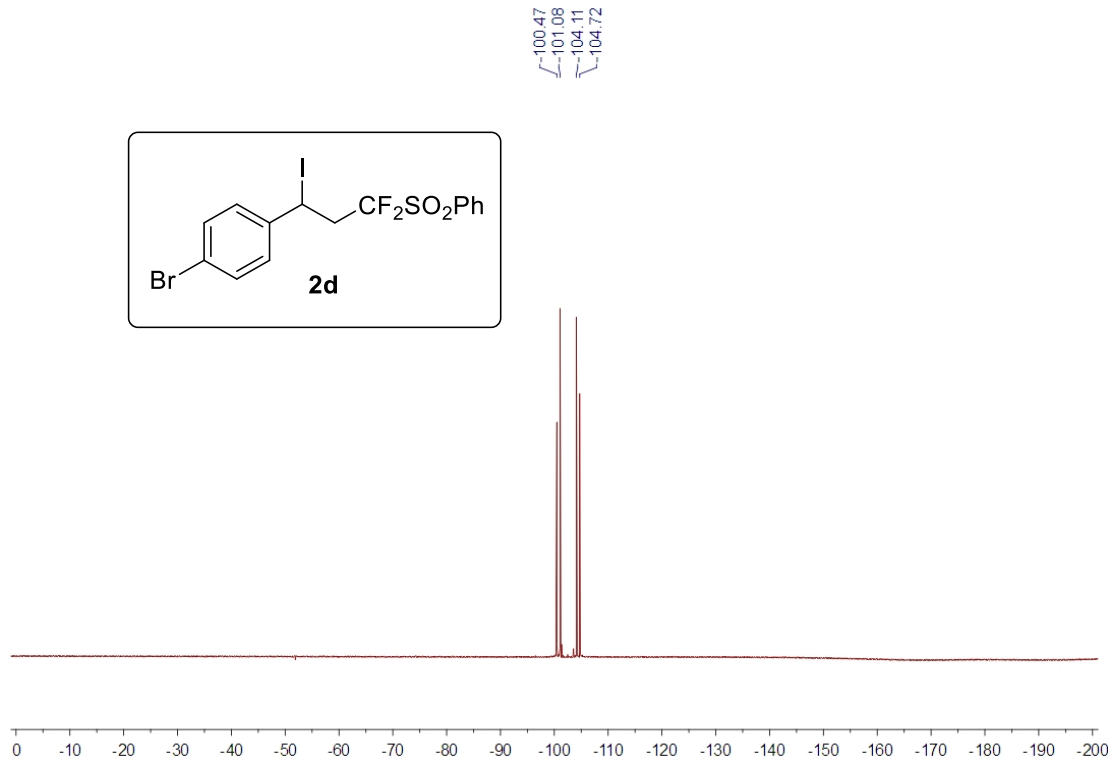
122.43
119.99
110.04
77.48
77.16
76.84
40.89
40.70
40.52
15.75
15.73
15.71
I
CF2SO2Ph
Br
2d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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104.11
104.72
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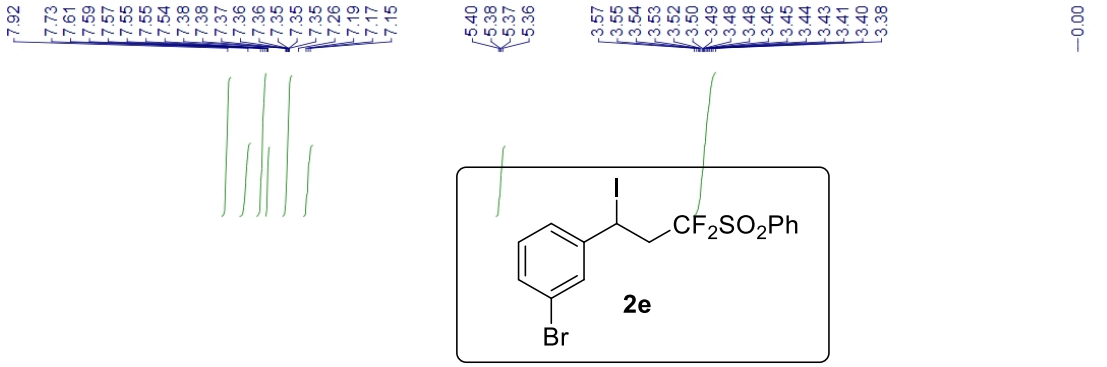
CF2SO2Ph
Br
2d
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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7.73
7.61
7.59
7.57
7.55
7.55
7.54
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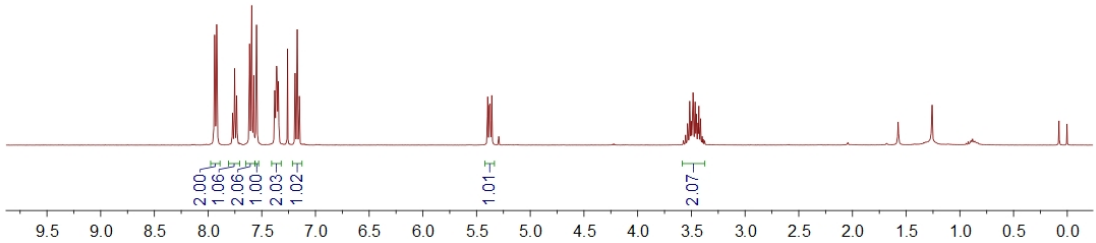
7.38
7.37
7.36
7.36
7.35
7.35
7.35
7.26
7.19
7.17
7.15
5.40
5.38
5.37
5.36
3.57
3.55
3.54
3.53
3.52
3.50
3.49
3.48
3.48
3.46
3.45
3.44
3.43
3.41
3.40
3.38
0.00
I
CF2SO2Ph
2e
Br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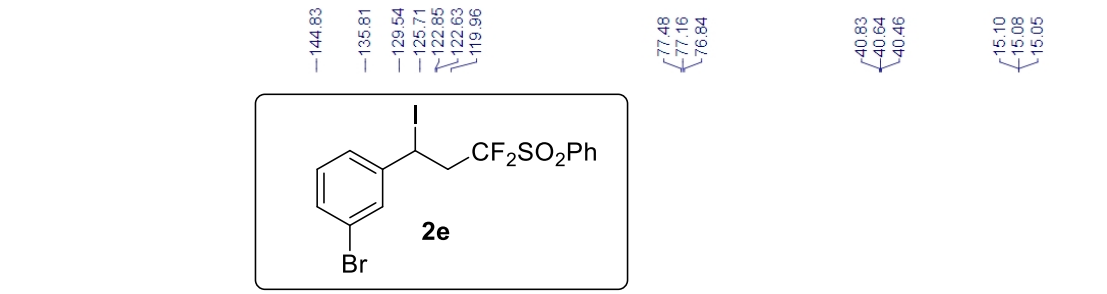
1.06
2.06
1.00
2.03
1.02
1.01
2.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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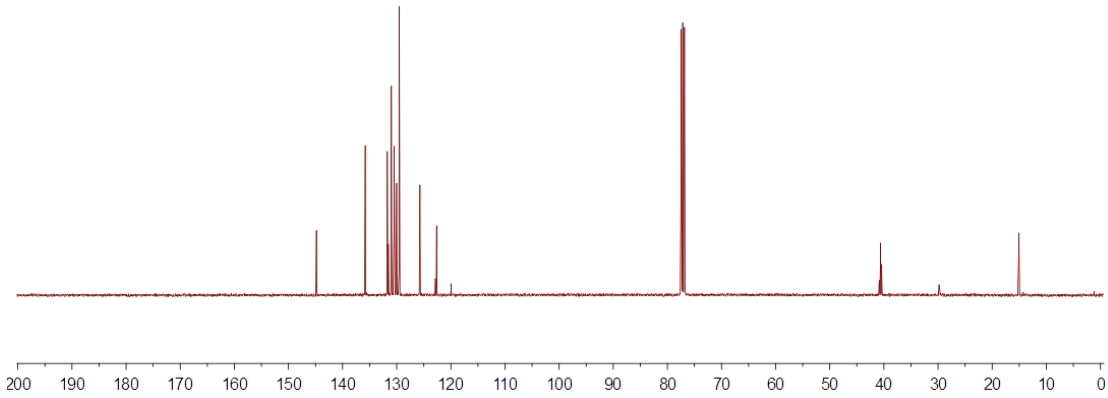
135.81
129.54
125.71
122.85
122.63
119.96
77.48
77.16
76.84
40.83
40.64
40.46
15.10
15.08
15.05
I
CF2SO2Ph
2e
Br


200
190
180
170
160
150
140
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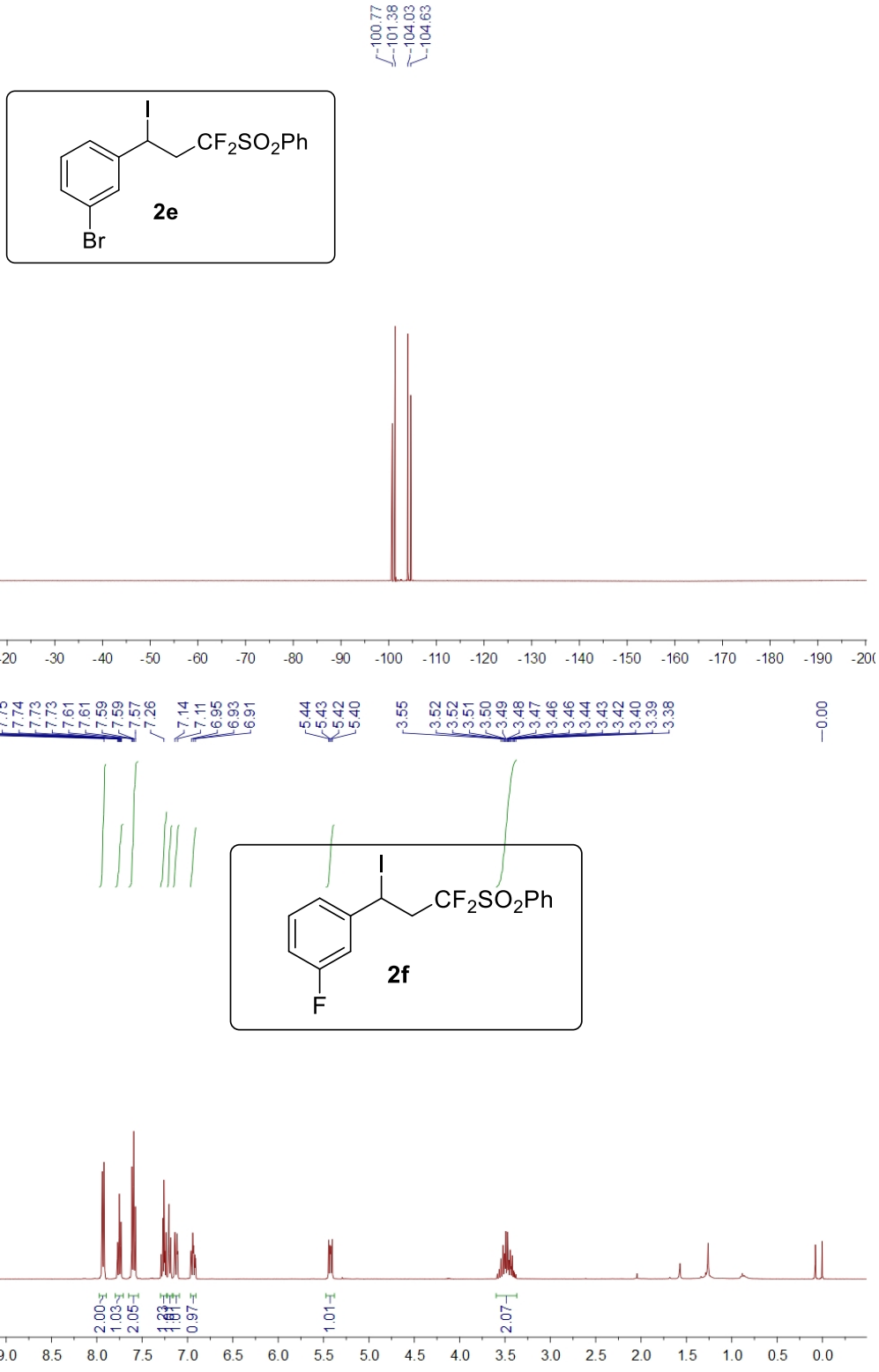
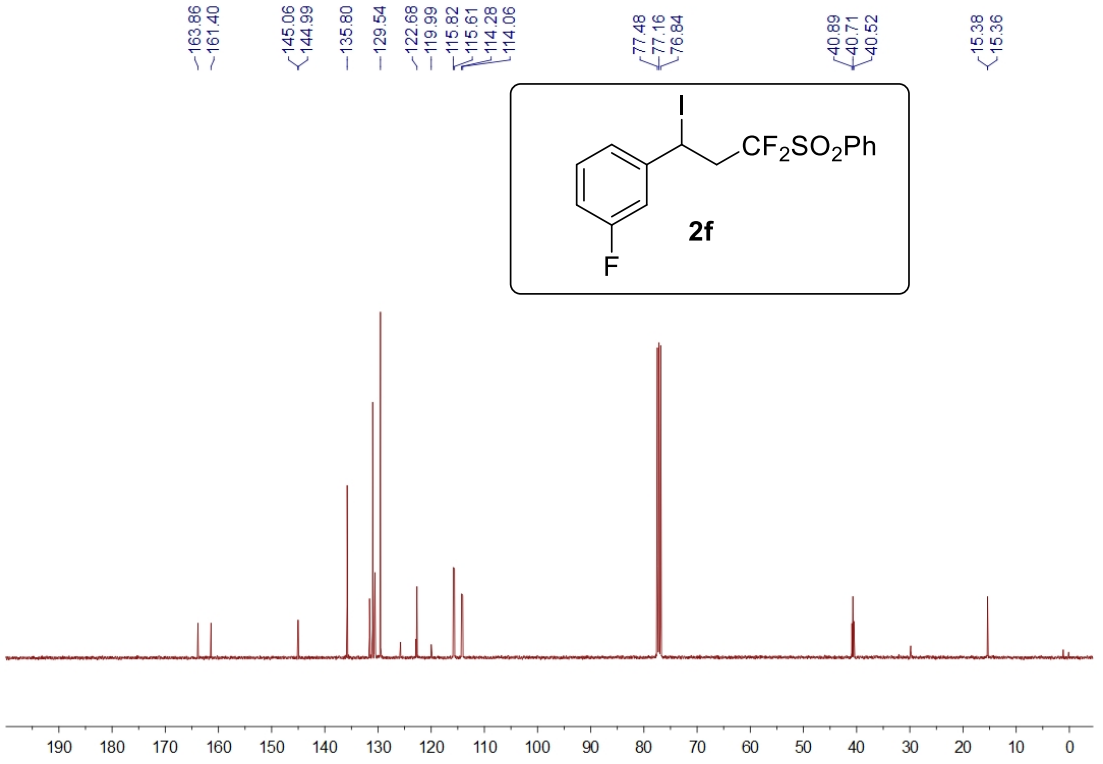
120
110
100
90
80
70
60
50
40
30
20
10
0


100.77
101.38
104.03
104.63
I
CF2SO2Ph
2e
Br
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
7.77
7.77
7.76
7.75
7.75
7.74
7.73
7.73
7.61
7.61
7.59
7.59
7.57
7.26
7.14
7.11
6.95
6.93
6.91
5.44
5.43
5.42
5.40
3.55
3.52
3.52
3.51
3.50
3.49
3.48
3.47
3.46
3.46
3.44
3.43
3.42
3.40
3.39
3.38
0.00
I
CF2SO2Ph
2f
F
2.00
1.03
2.05
1.01
0.97
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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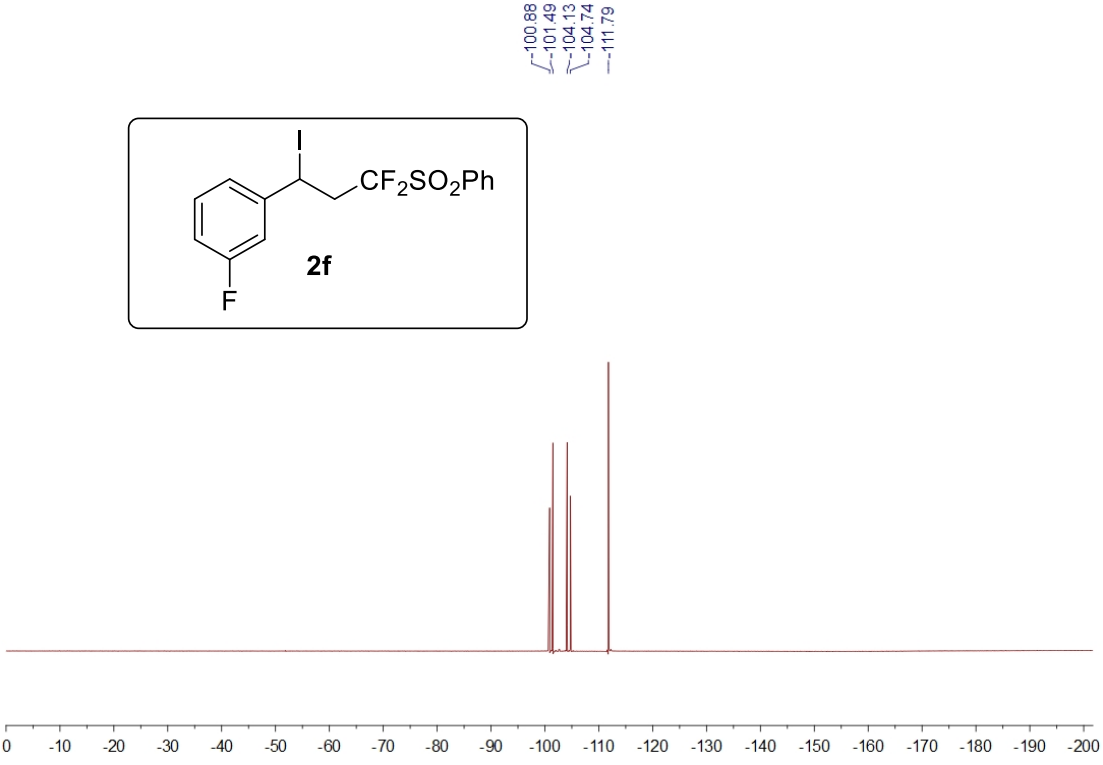
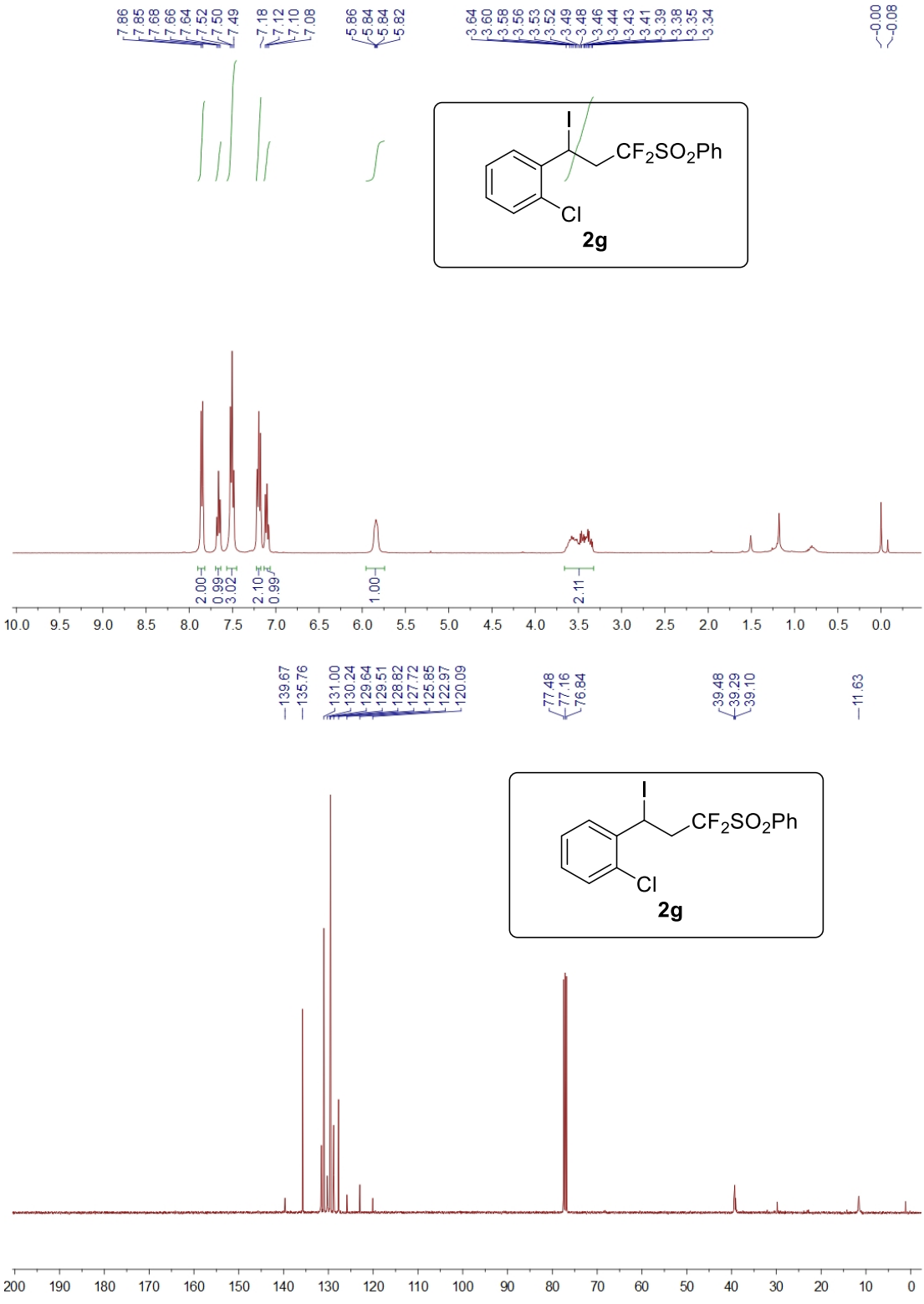
122.68
119.99
115.82
115.61
114.28
114.06
77.48
77.16
76.84
40.89
40.71
40.52
15.38
15.36
I
CF2SO2Ph
2f
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


100.88
101.49
104.13
104.74
111.79
I
CF2SO2Ph
2f
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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7.68
7.66
7.64
7.52
7.50
7.49
7.18
7.12
7.10
7.08
5.86
5.84
5.84
5.82
3.64
3.60
3.58
3.56
3.53
3.52
3.49
3.48
3.46
3.44
3.43
3.41
3.39
3.38
3.35
3.34
0.00
0.08
I
CF2SO2Ph
Cl
2g
2.00
0.99
3.02
2.10
0.99
1.00
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
139.67
135.76
131.00
130.24
129.64
129.51
128.82
127.72
125.85
122.97
120.09
77.48
77.16
76.84
39.48
39.29
39.10
11.63
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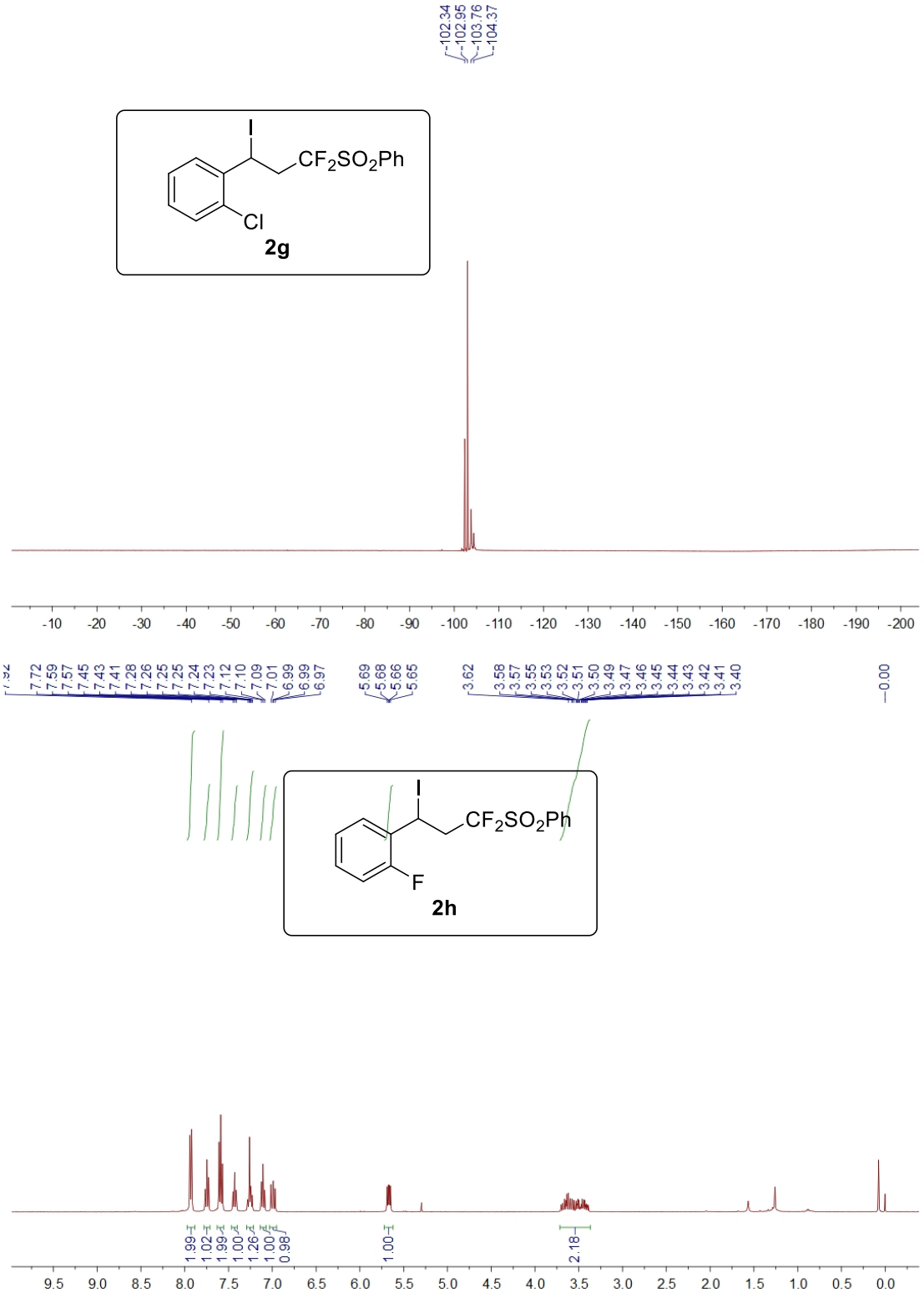
CF2SO2Ph
Cl
2g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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102.95
103.76
104.37
I
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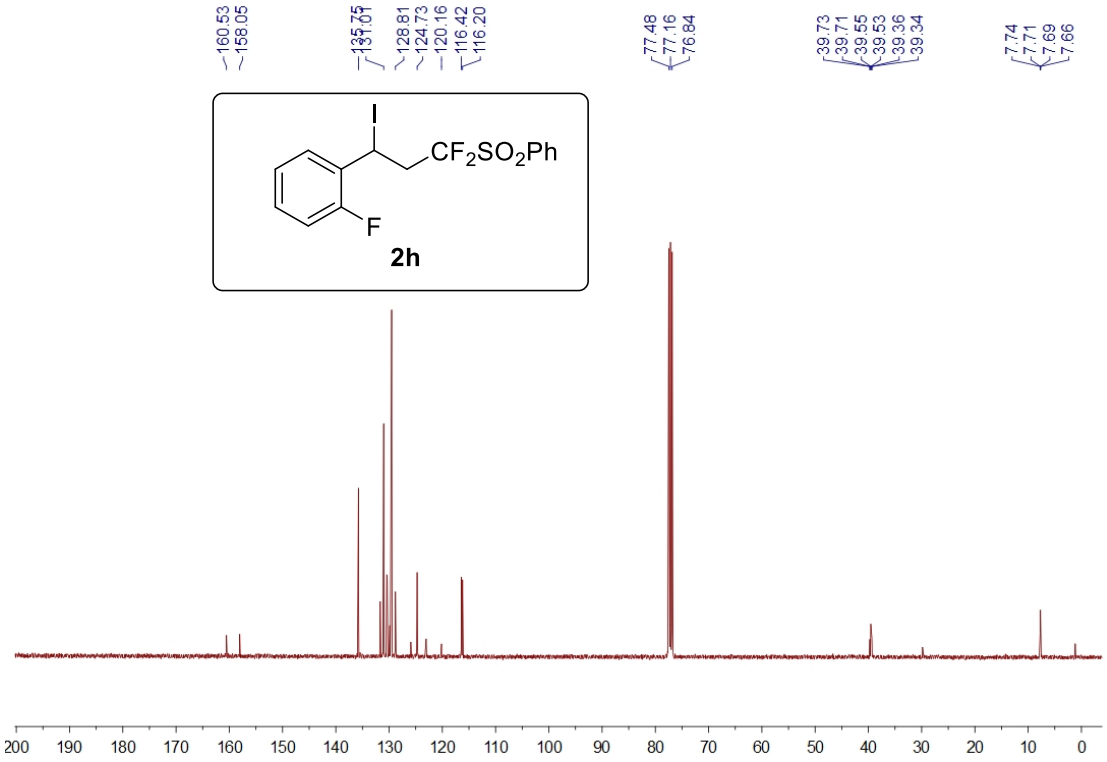
Cl
2g
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
7.72 7.59 7.57 7.45 7.43 7.41 7.28 7.26 7.25 7.25 7.24 7.23 7.12 7.10 7.09 7.01 6.99 6.99 6.97
5.69 5.68 5.66 5.65
3.62 3.58 3.57 3.55 3.53 3.52 3.51 3.50 3.49 3.47 3.46 3.45 3.44 3.43 3.42 3.41 3.40
0.00
I
CF2SO2Ph
F
2h
1.99 1.02 1.99 1.00 1.26 1.00 0.98
1.00
2.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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120.16
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77.48
77.16
76.84
39.73
39.71
39.55
39.53
39.36
39.34
7.74
7.71
7.69
7.66
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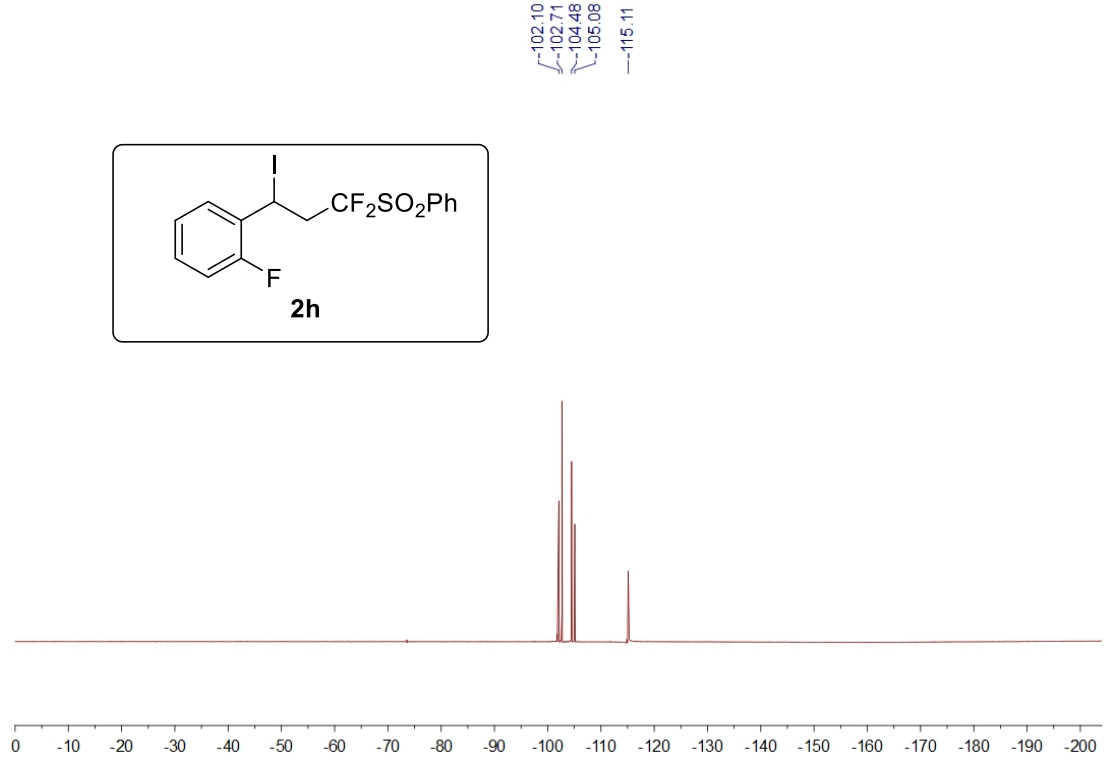
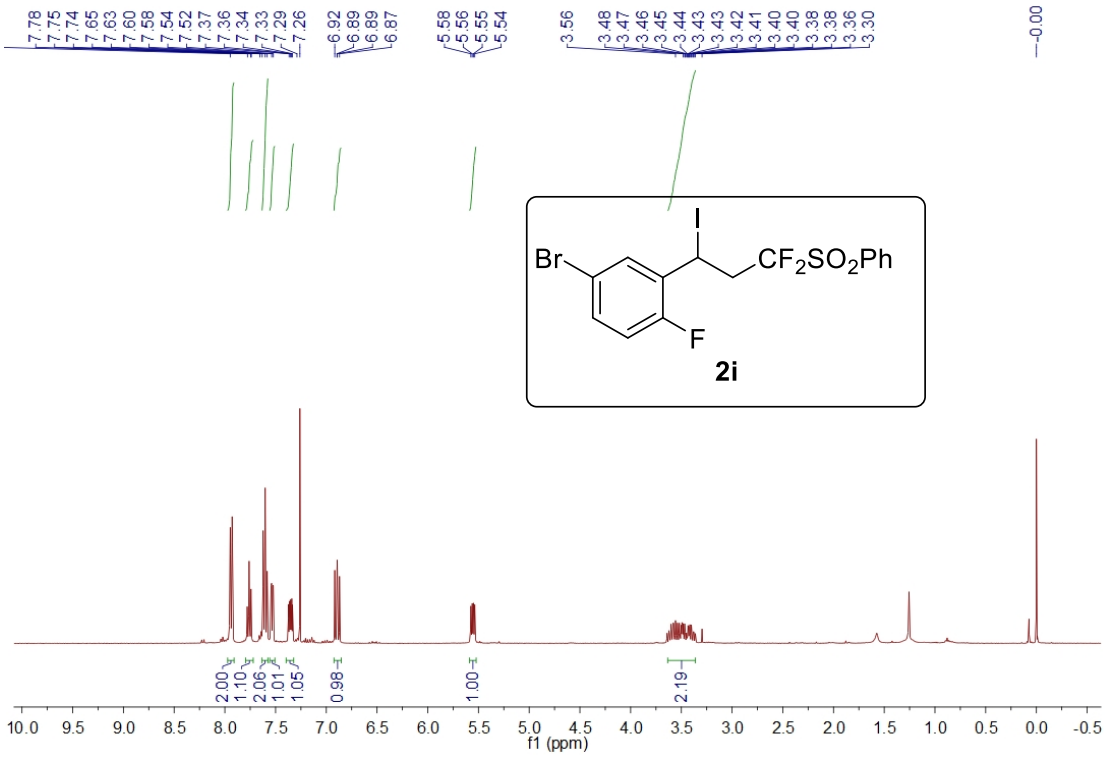
CF2SO2Ph
F
2h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


-102.10
-102.71
-104.48
-105.08
-115.11
I
CF2SO2Ph
F
2h
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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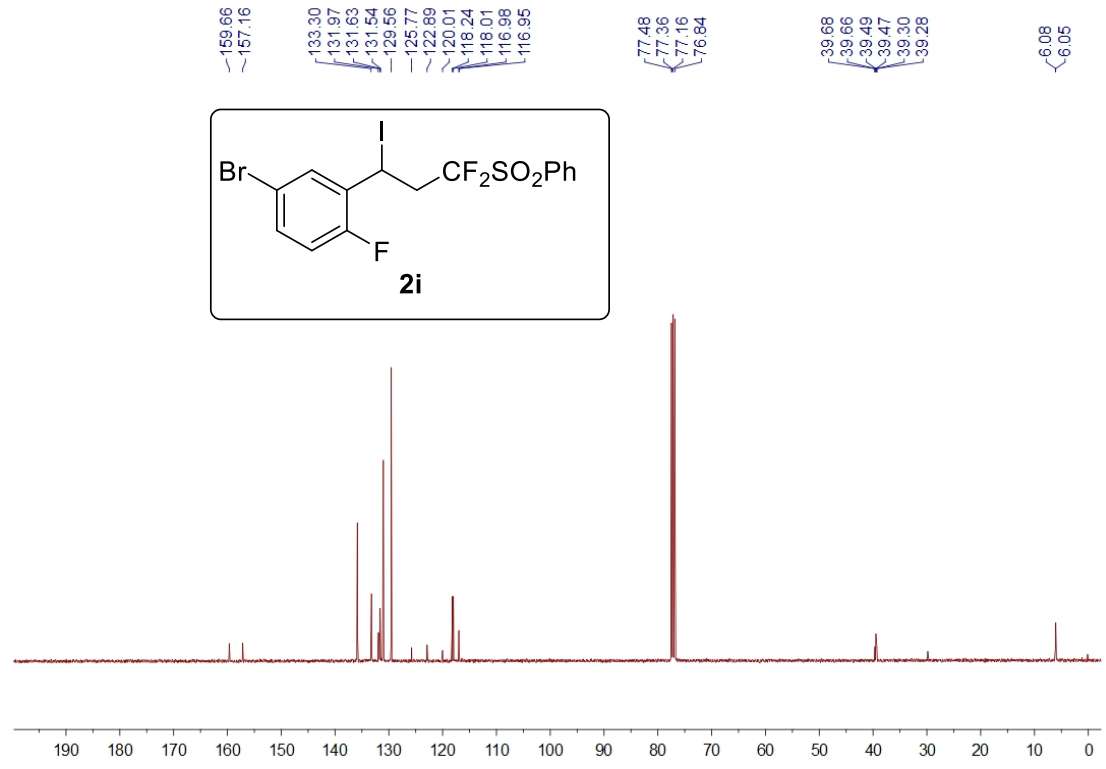
7.60
7.58
7.54
7.52
7.37
7.36
7.34
7.33
7.29
7.26
6.92
6.89
6.89
6.87
5.58
5.56
5.55
5.54
3.56
3.48
3.47
3.46
3.45
3.44
3.43
3.43
3.42
3.41
3.40
3.40
3.38
3.36
3.30
0.00
Br
I
CF2SO2Ph
F
2i
2.00
1.10
2.06
1.01
1.05
0.98
1.00
2.19
f1 (ppm)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157.16
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131.63
131.54
129.56
125.77
122.89
120.01
118.24
118.01
116.98
116.95
77.48
77.36
77.16
76.84
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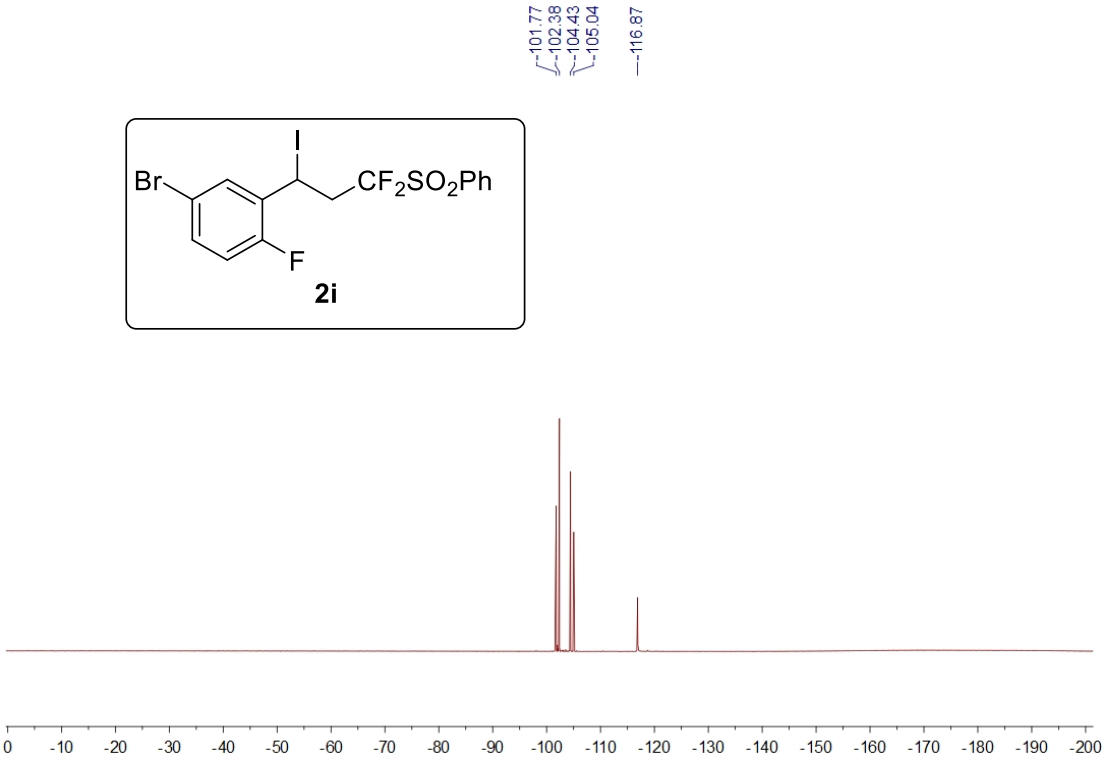
6.08
6.05
Br
I
CF2SO2Ph
F
2i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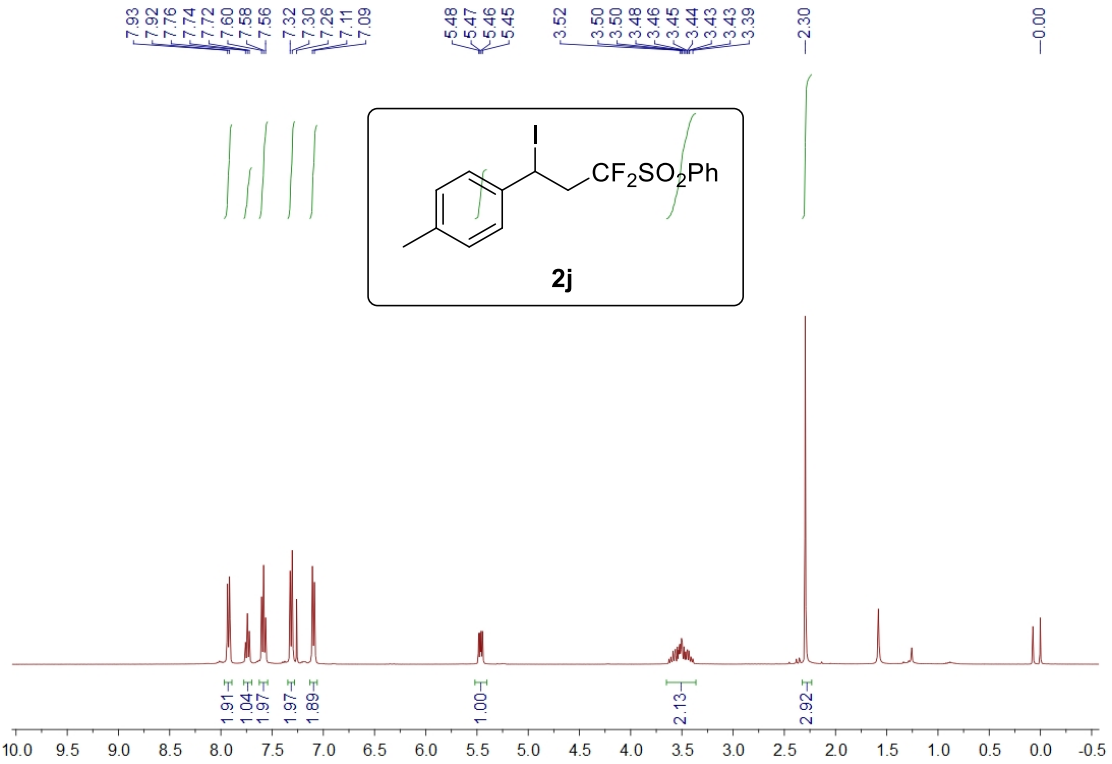
-104.43
-105.04
-116.87
I
Br
CF2SO2Ph
F
2i
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200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7.92
7.76
7.74
7.72
7.60
7.58
7.56
7.32
7.30
7.26
7.11
7.09
5.48
5.47
5.46
5.45
3.52
3.50
3.50
3.48
3.46
3.45
3.44
3.43
3.43
3.39
2.30
0.00
I
CF2SO2Ph
2j
1.91
1.04
1.97
1.97
1.89
1.00
2.13
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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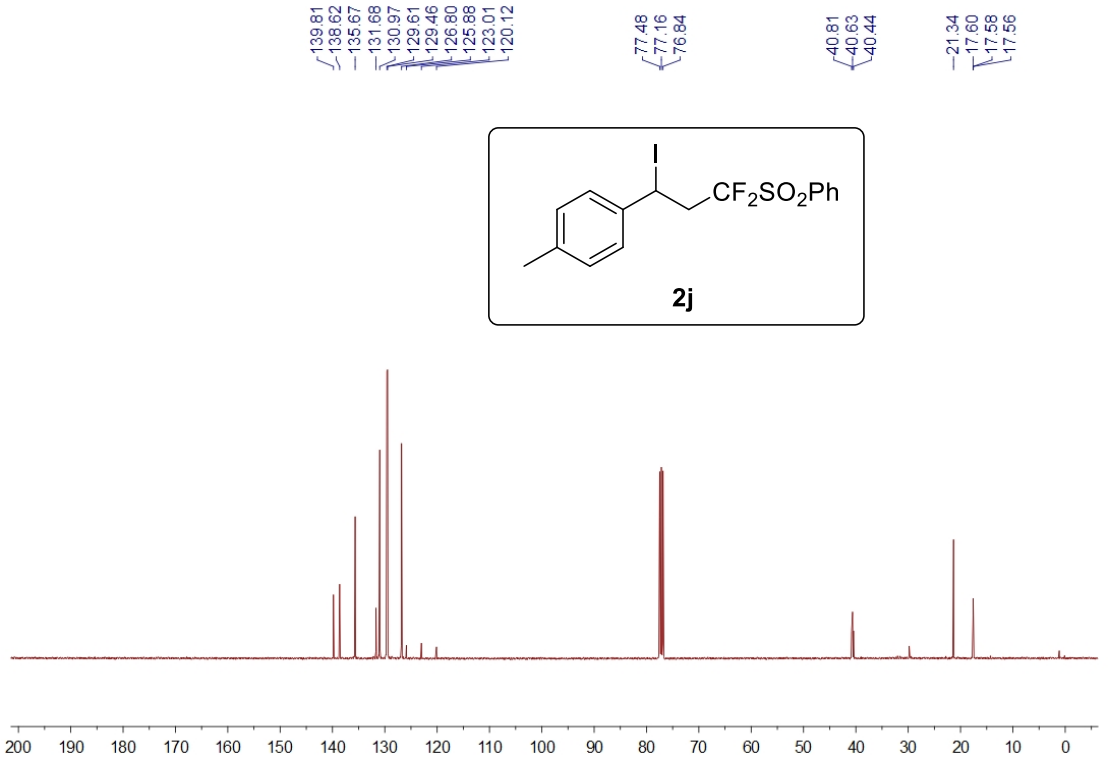
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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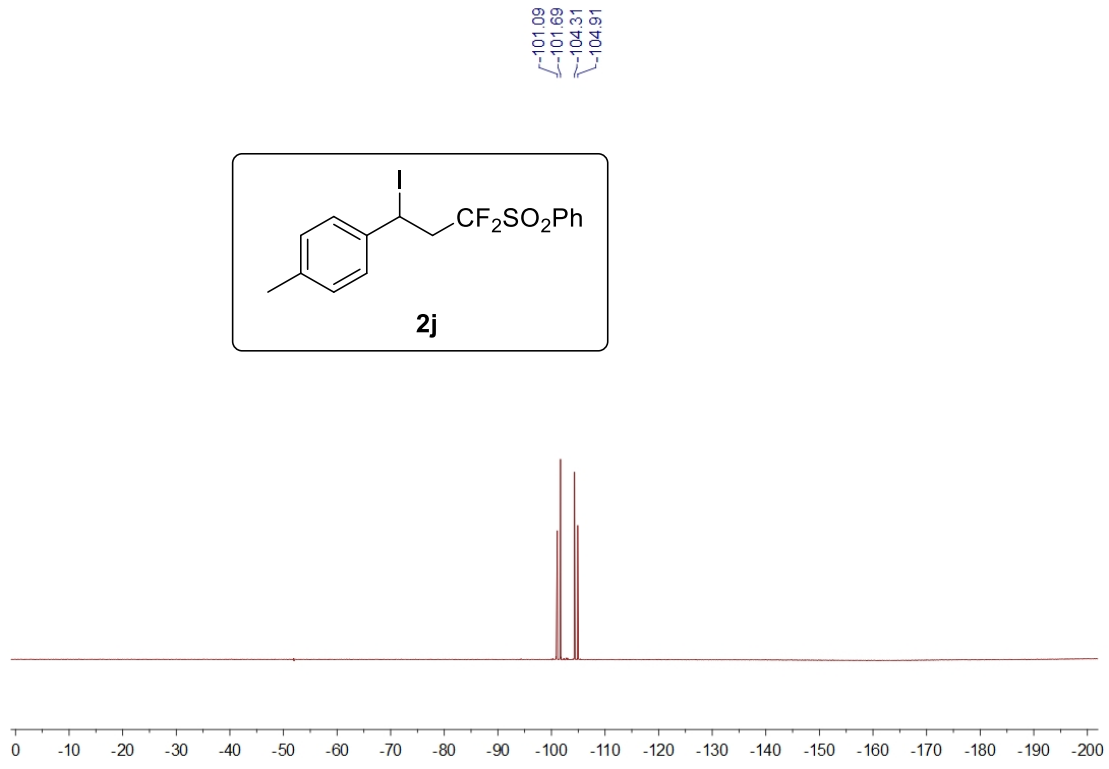
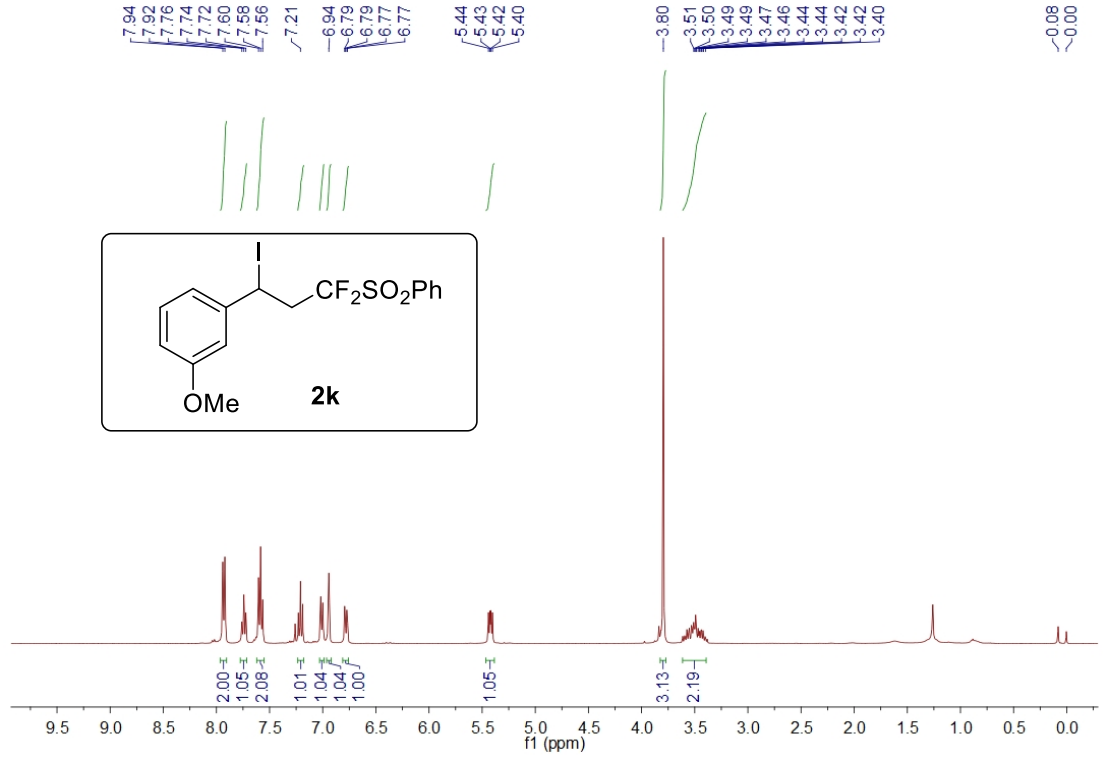
138.62
135.67
131.68
130.97
129.61
129.46
126.80
125.88
123.01
120.12
77.48
77.16
76.84
40.81
40.63
40.44
21.34
17.60
17.58
17.56
I
CF2SO2Ph
2j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


-101.09
-101.69
-104.31
-104.91
I
CF2SO2Ph
2j
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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7.60
7.58
7.56
7.21
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6.79
6.79
6.77
6.77
5.44
5.43
5.42
5.40
3.80
3.51
3.50
3.49
3.49
3.47
3.46
3.44
3.44
3.42
3.42
3.40
0.08
0.00
CF2SO2Ph
OMe
2k
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2.08
1.01
1.04
1.04
1.00
1.05
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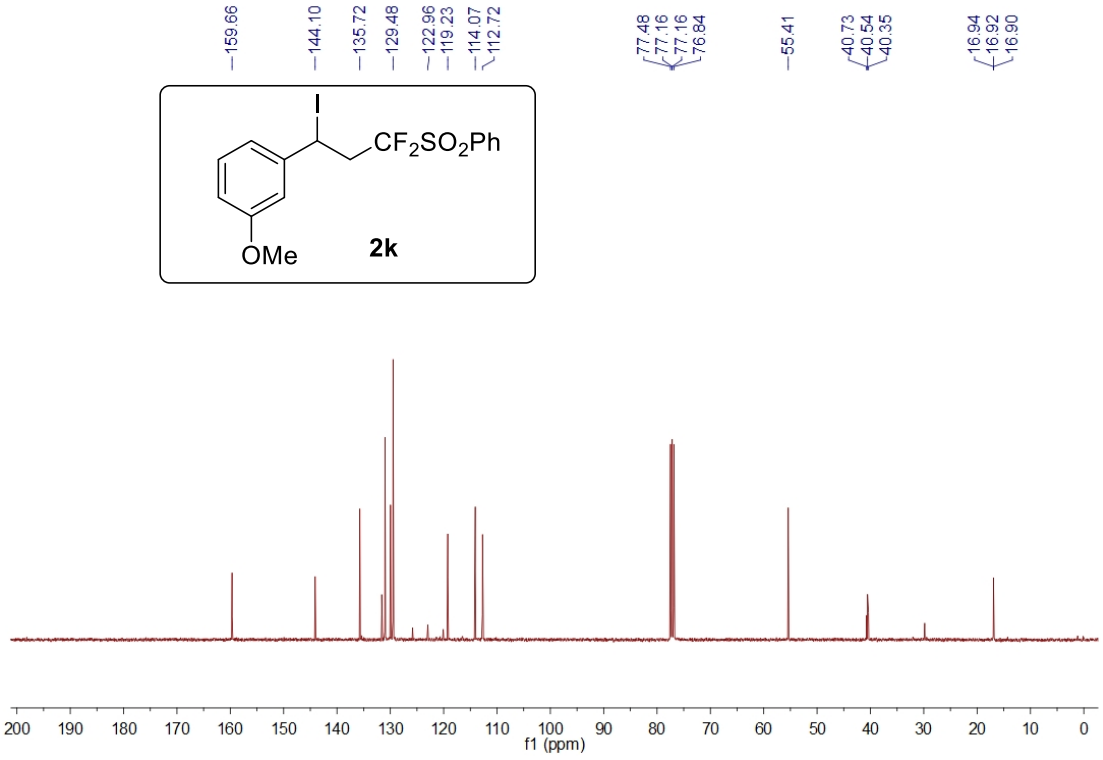
f1 (ppm)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112.72
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77.16
77.16
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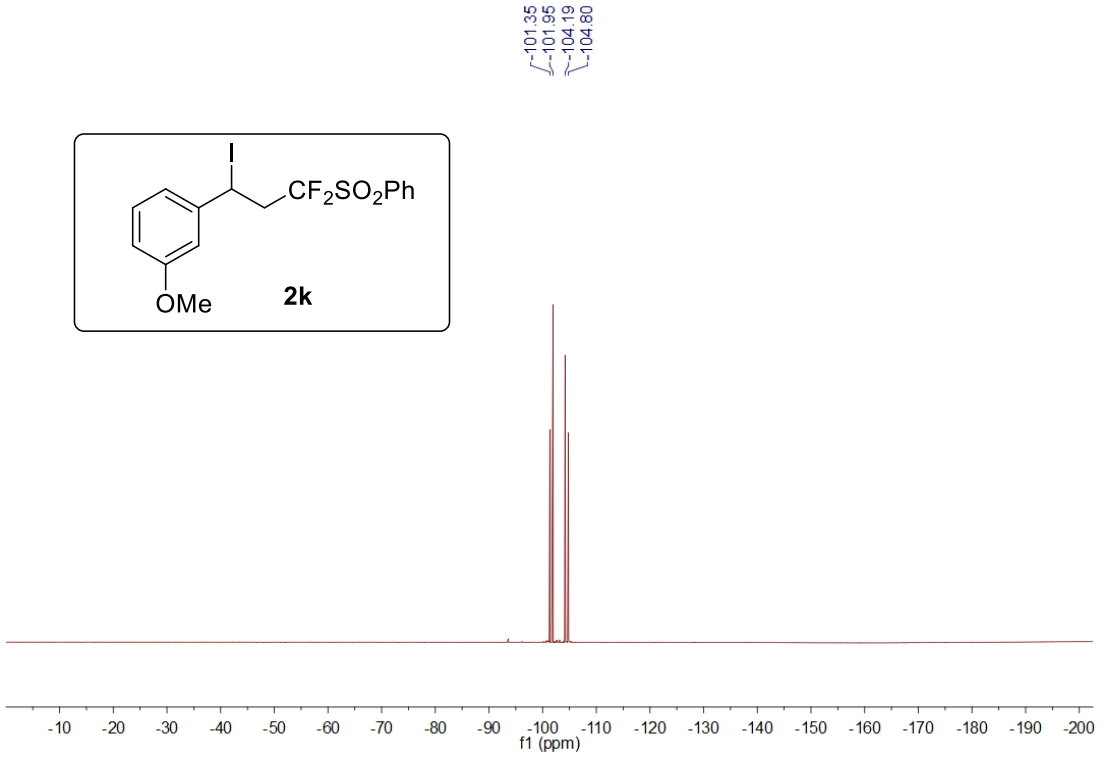
40.54
40.35
16.94
16.92
16.90
CF2SO2Ph
OMe
2k
f1 (ppm)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-104.80
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OMe
2k
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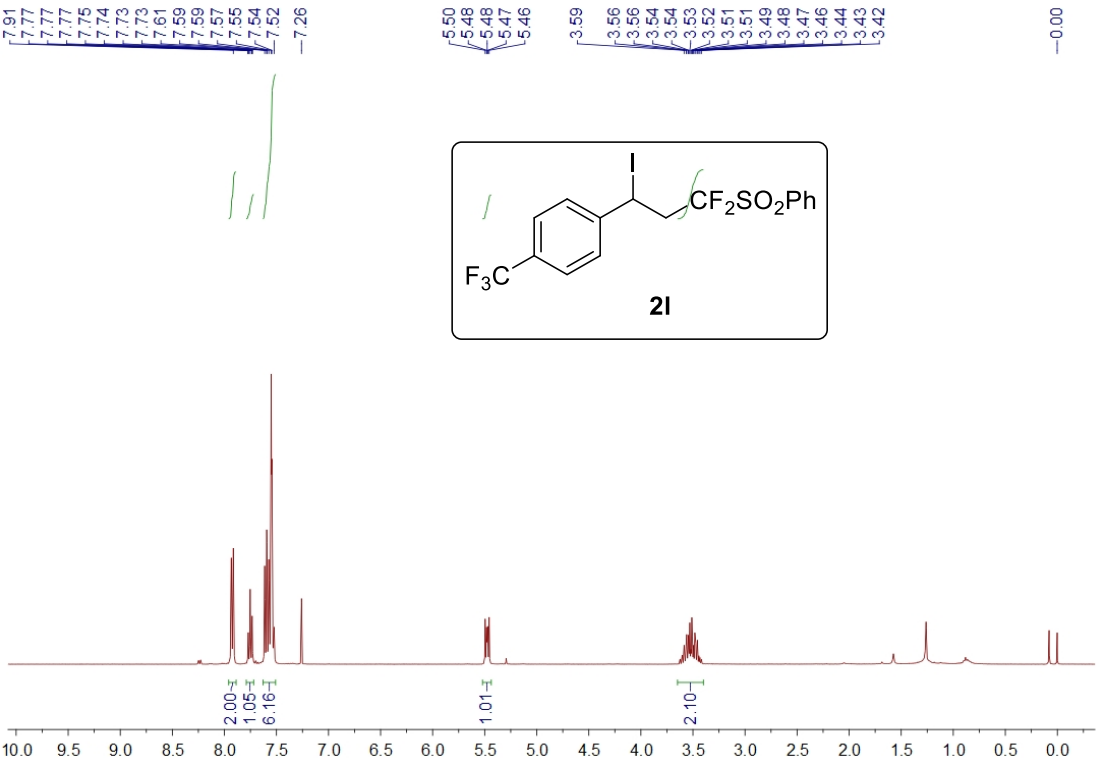
f1 (ppm)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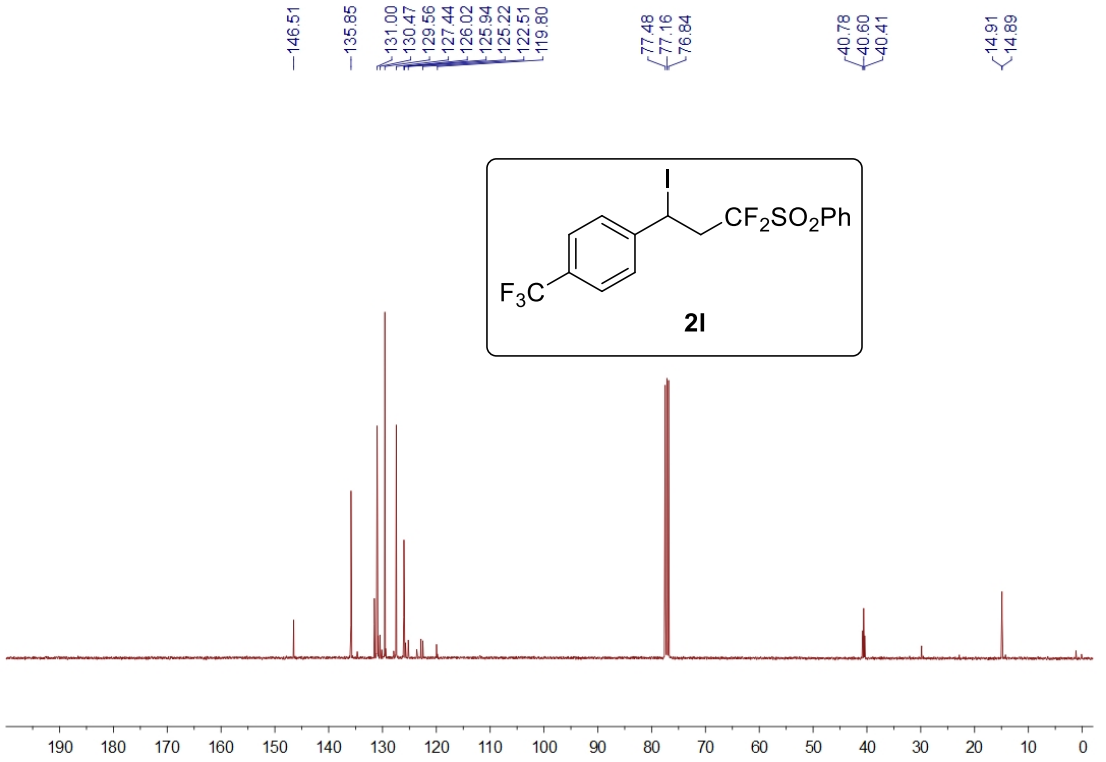
5.50 5.48 5.48 5.47 5.46
3.59 3.56 3.56 3.54 3.54 3.53 3.52 3.51 3.51 3.49 3.48 3.47 3.46 3.44 3.43 3.42
0.00
I
CF2SO2Ph
F3C
2l
2.00 1.05 6.16 1.01 2.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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125.94
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122.51
119.80
77.48
77.16
76.84
40.78
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14.89
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F3C
2l
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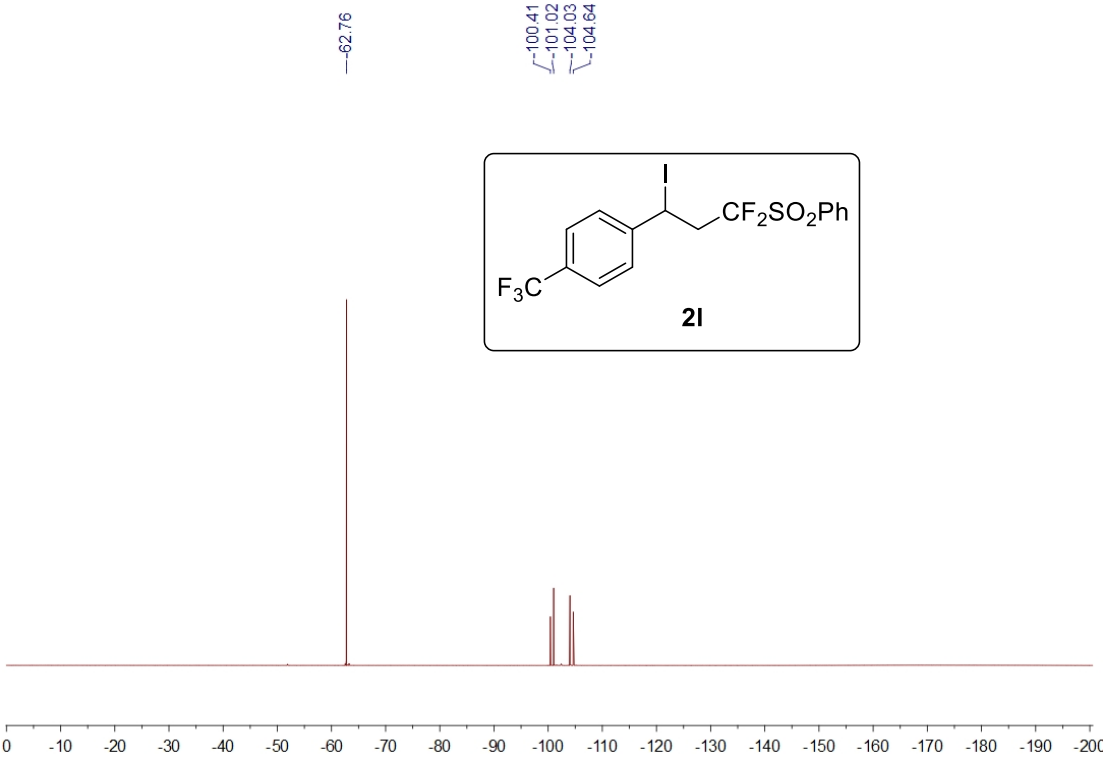
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101.02
104.03
104.64
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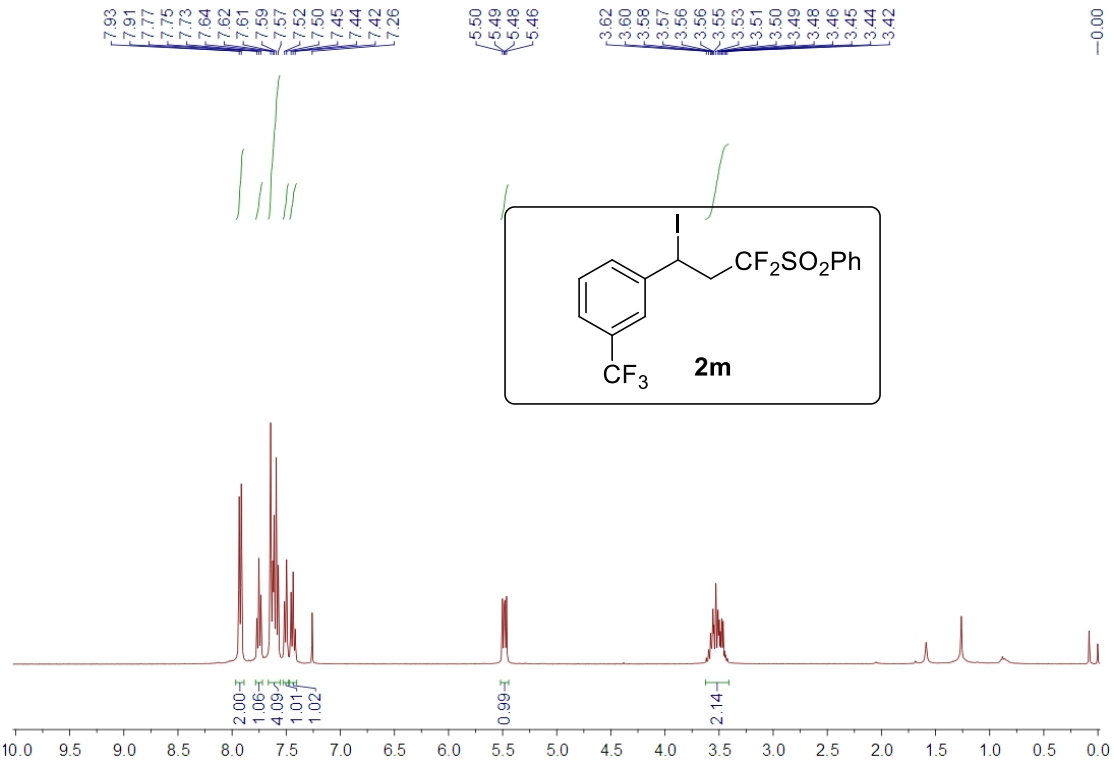
CF2SO2Ph
F3C
2l
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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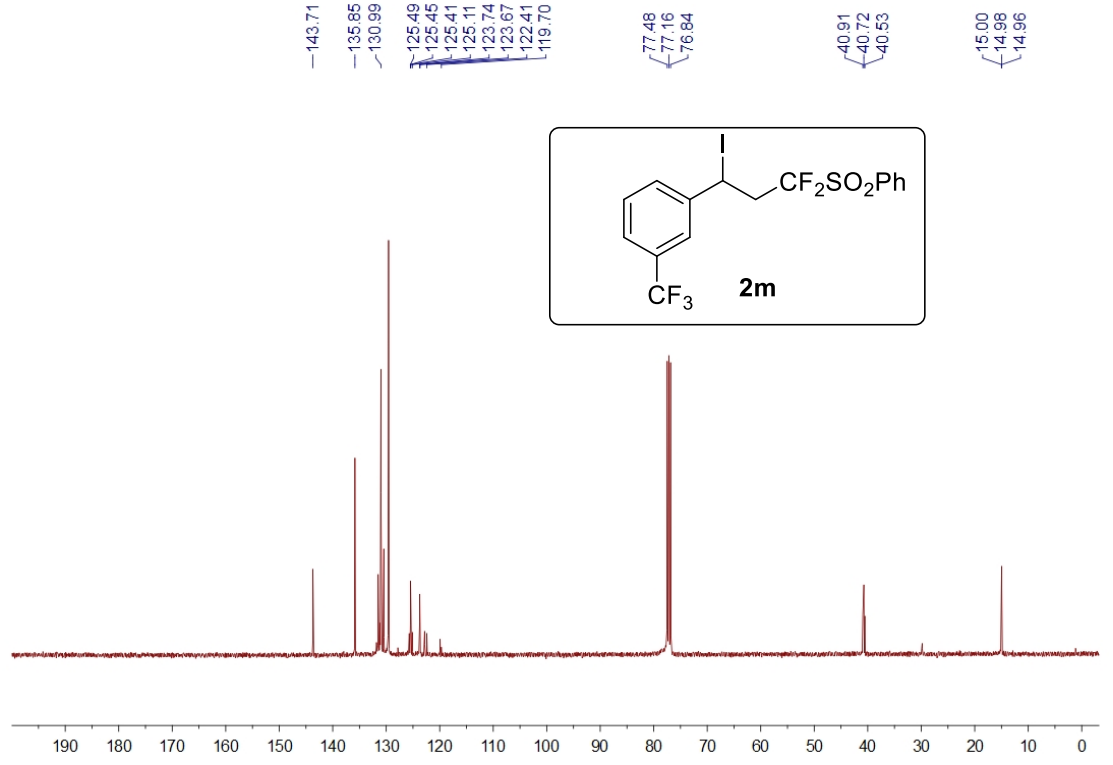
7.44
7.42
7.26
5.50
5.49
5.48
5.46
3.62
3.60
3.58
3.57
3.56
3.56
3.55
3.53
3.51
3.50
3.49
3.48
3.46
3.45
3.44
3.42
0.00
I
CF2SO2Ph
CF3
2m
2.00
1.06
4.09
1.01
1.02
0.99
2.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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122.41
119.70
77.48
77.16
76.84
40.91
40.72
40.53
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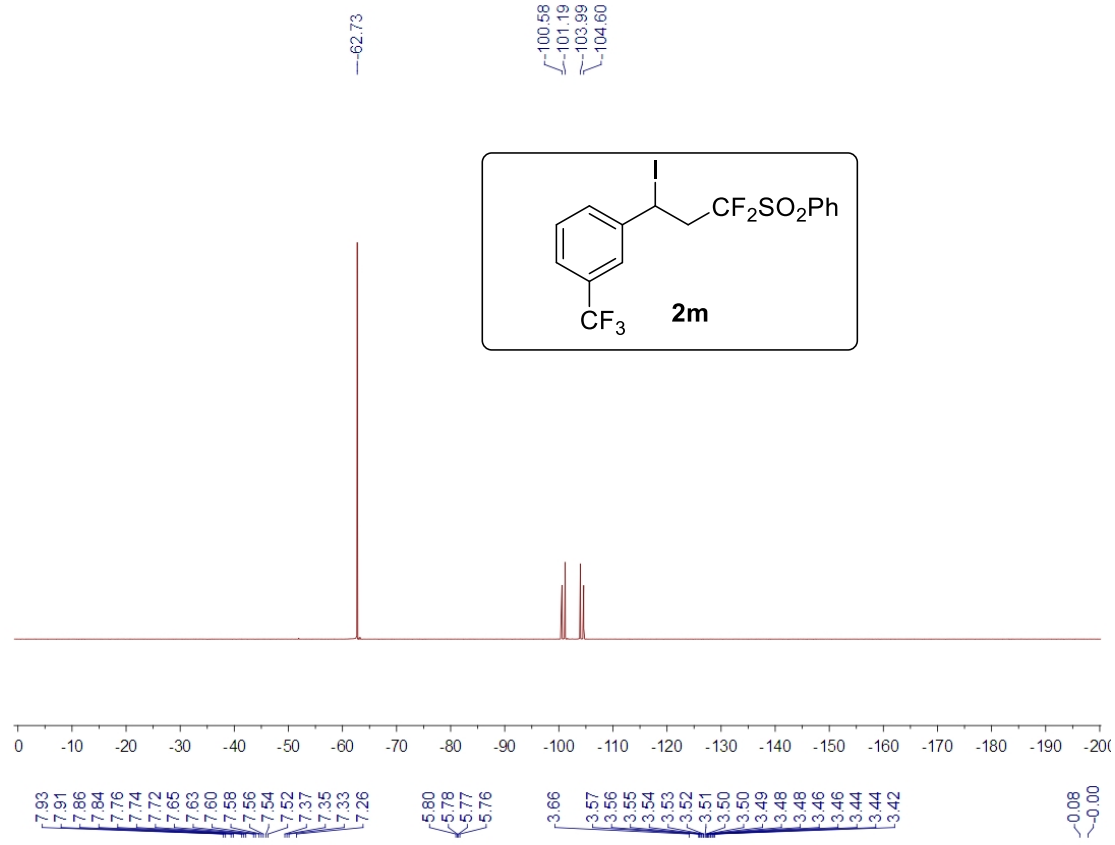
14.96
I
CF2SO2Ph
CF3
2m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

C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-103.99
-104.60
I
CF2SO2Ph
CF3
2m
7.93
7.91
7.86
7.84
7.76
7.74
7.72
7.65
7.63
7.60
7.58
7.56
7.54
7.52
7.37
7.35
7.33
7.26
5.80
5.78
5.77
5.76
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3.56
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3.51
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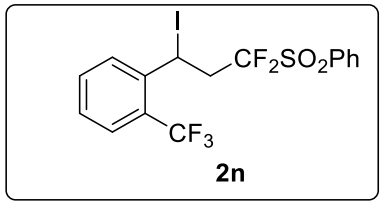
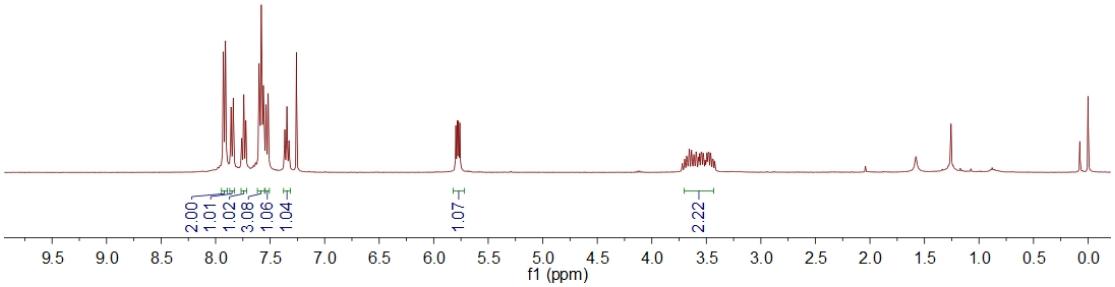
3.46
3.44
3.44
3.42
0.08
0.00


I
CF2SO2Ph
CF3
2n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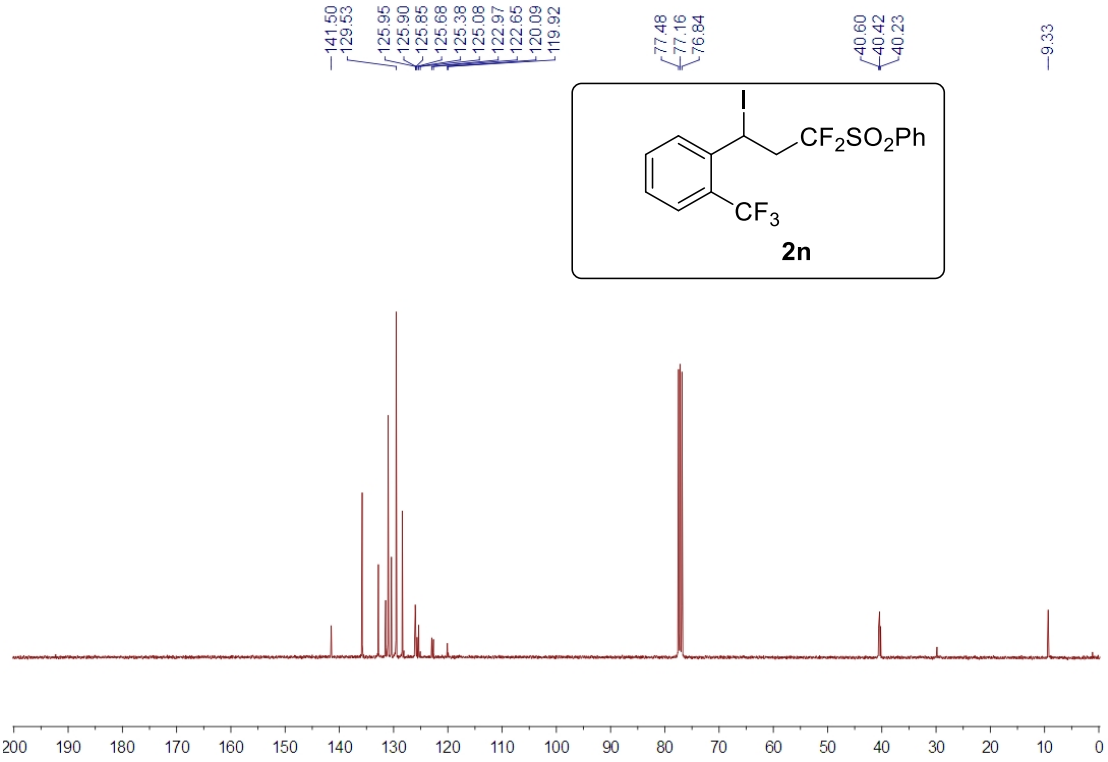
1.01
1.02
3.08
1.06
1.04
1.07
2.22
f1 (ppm)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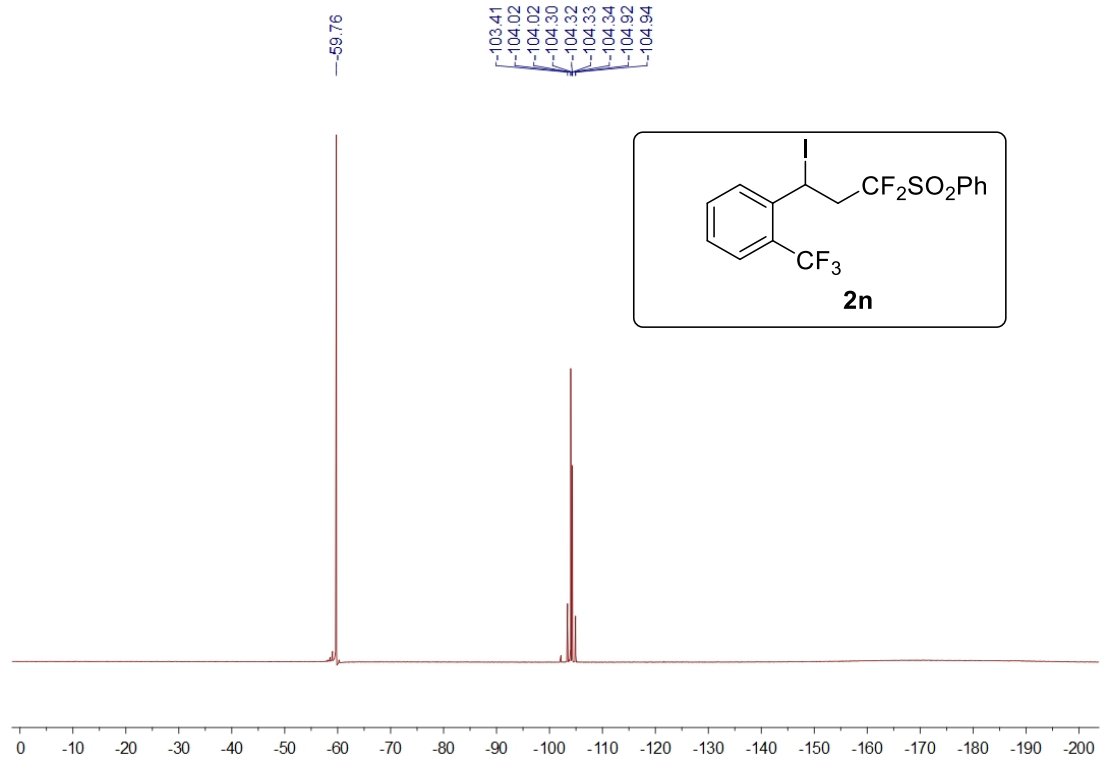
125.95
125.90
125.85
125.68
125.38
125.08
122.97
122.65
120.09
119.92
77.48
77.16
76.84
40.60
40.42
40.23
9.33
I
CF2SO2Ph
CF3
2n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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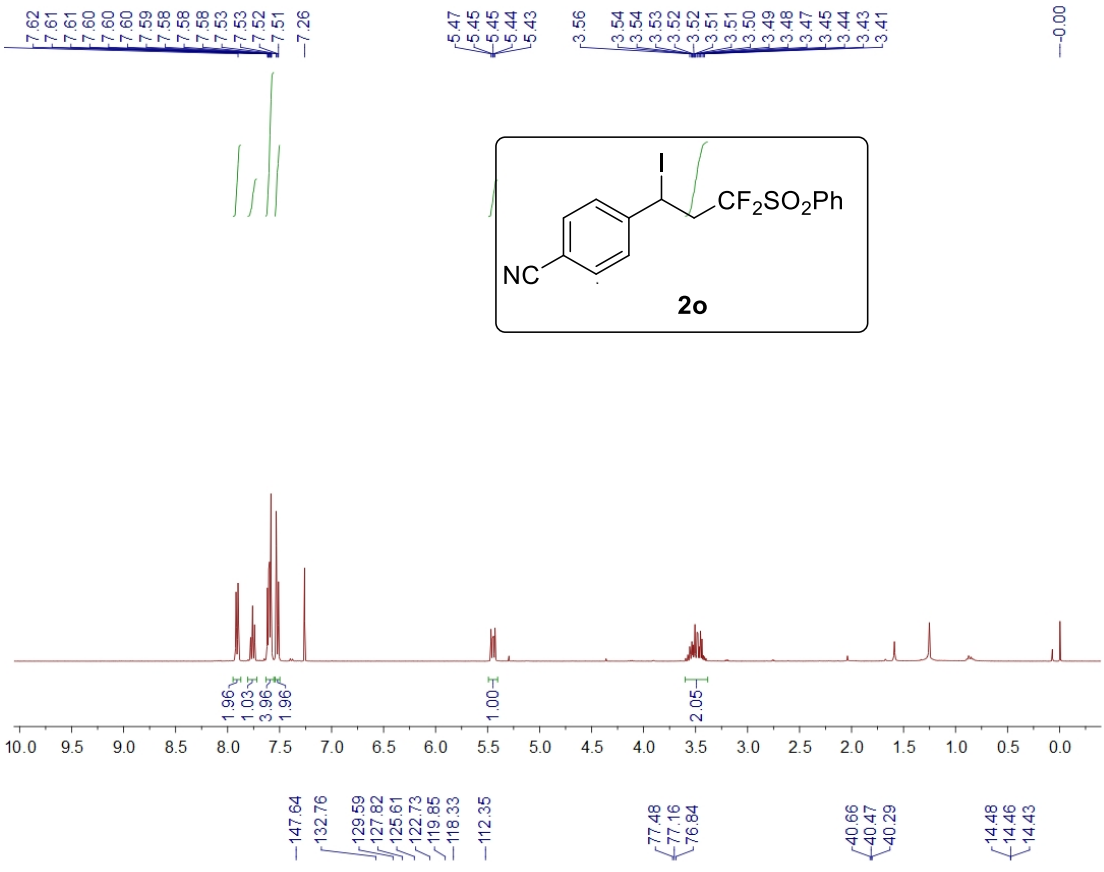
103.41
104.02
104.02
104.30
104.32
104.33
104.34
104.92
104.94
I
CF2SO2Ph
CF3
2n
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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7.60
7.59
7.58
7.58
7.58
7.53
7.52
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5.45
5.45
5.44
5.43
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3.54
3.53
3.52
3.52
3.51
3.51
3.50
3.49
3.48
3.47
3.45
3.44
3.43
3.41
0.00
I
CF2SO2Ph
NC
2o
1.96
1.03
3.96
1.96
1.00
2.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
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2.0
1.5
1.0
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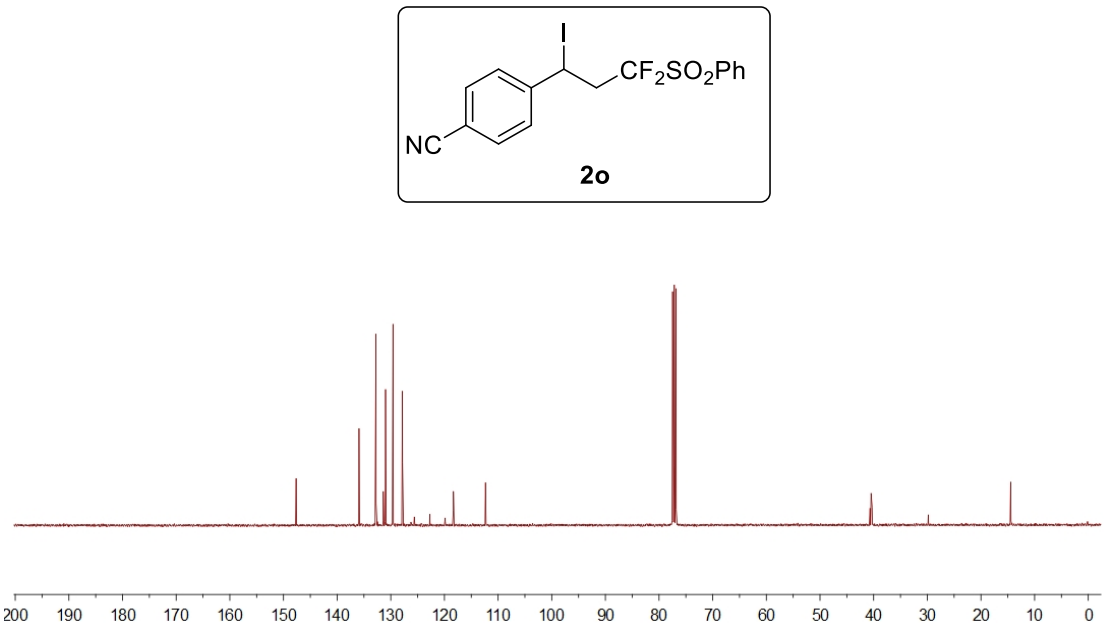
0.0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112.35
77.48
77.16
76.84
40.66
40.47
40.29
14.48
14.46
14.43
I
CF2SO2Ph
NC
2o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


-100.12
-100.73
-103.88
-104.49
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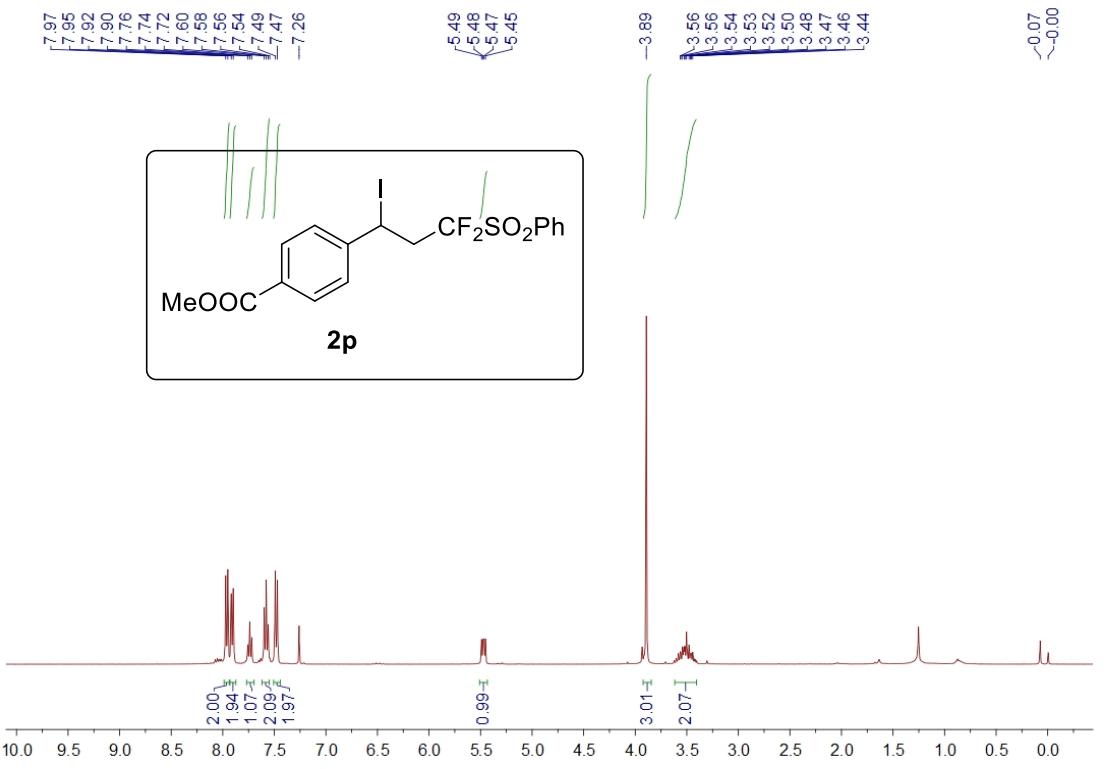
NC
2o
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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7.72
7.60
7.58
7.56
7.54
7.49
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7.26
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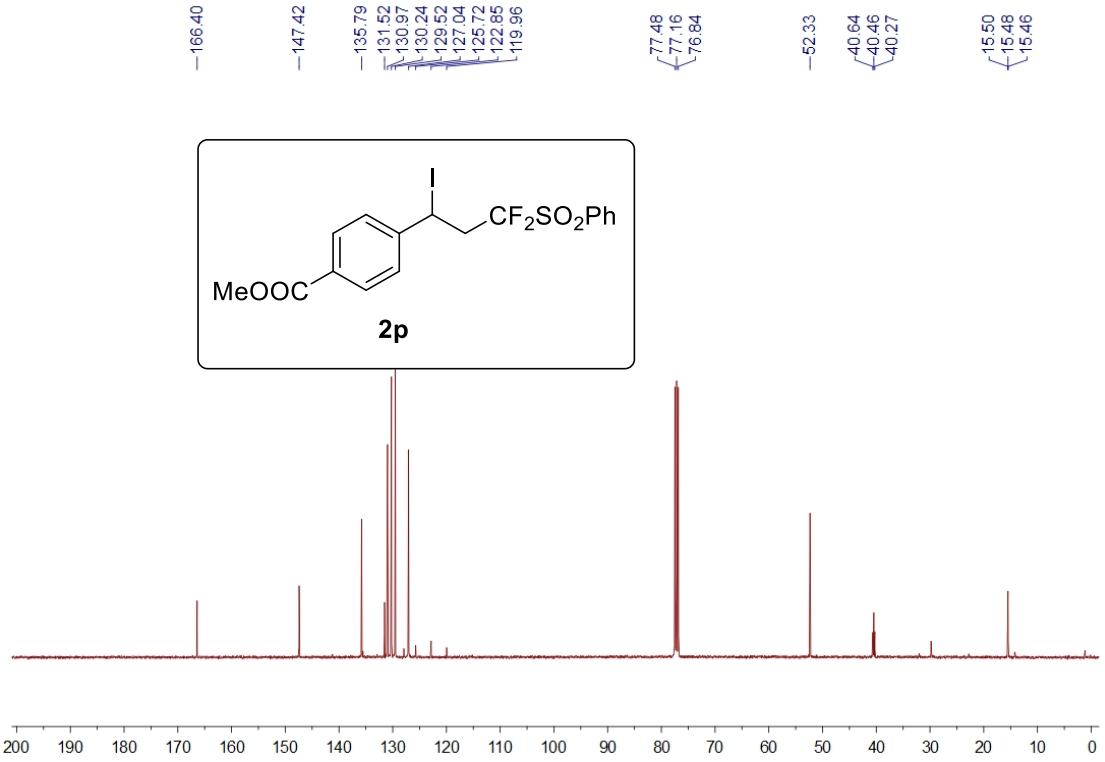
5.48
5.47
5.45
3.89
3.56
3.56
3.54
3.53
3.52
3.50
3.48
3.47
3.46
3.44
0.07
0.00
I
CF2SO2Ph
MeOOC
2p
2.00
1.94
1.07
2.09
1.97
0.99
3.01
2.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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127.04
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77.48
77.16
76.84
52.33
40.64
40.46
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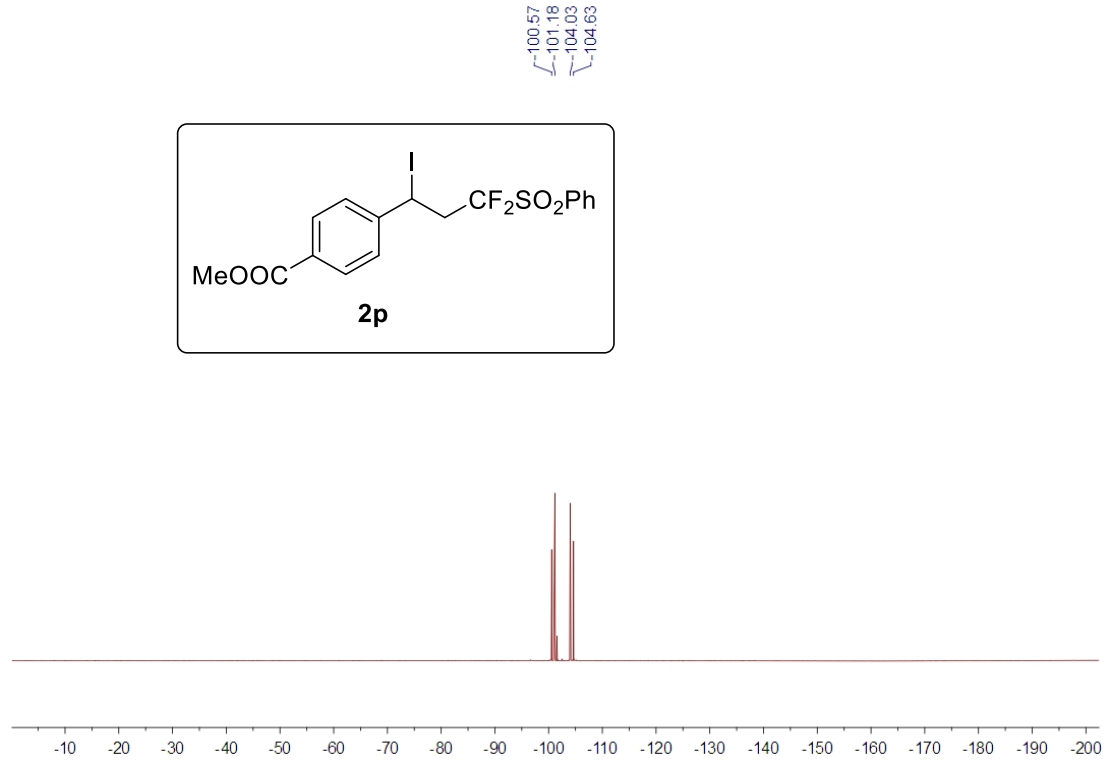
15.46
I
CF2SO2Ph
MeOOC
2p
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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MeOOC
2p
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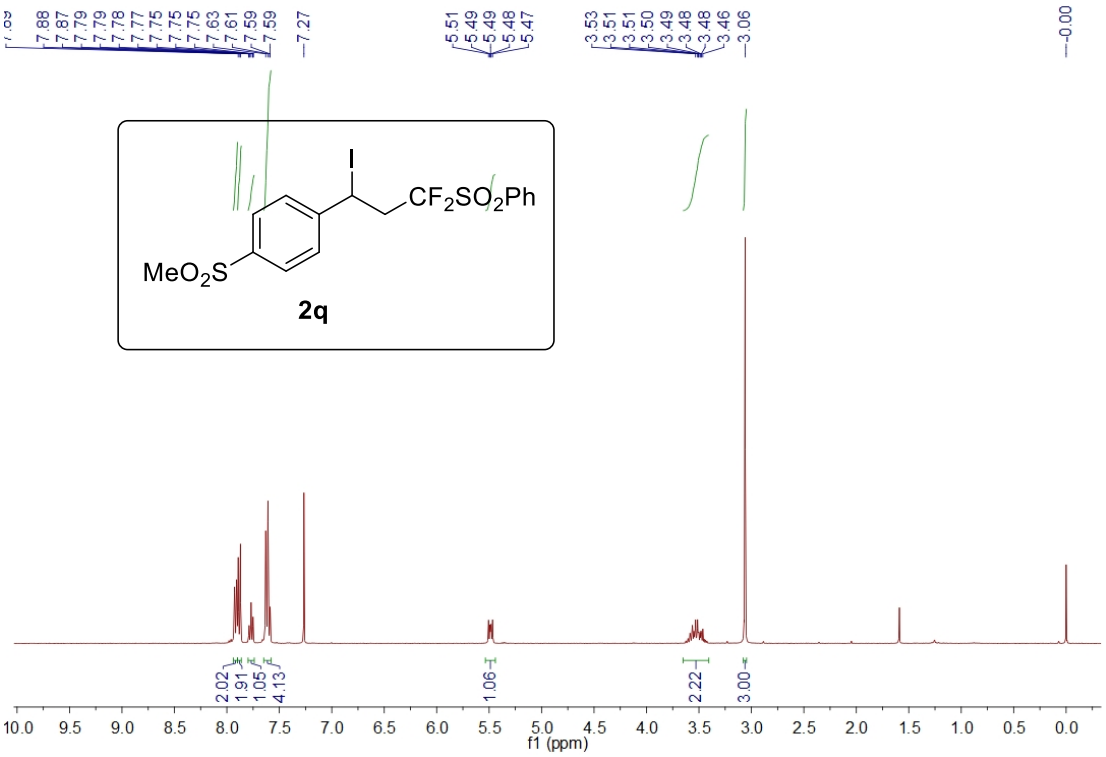
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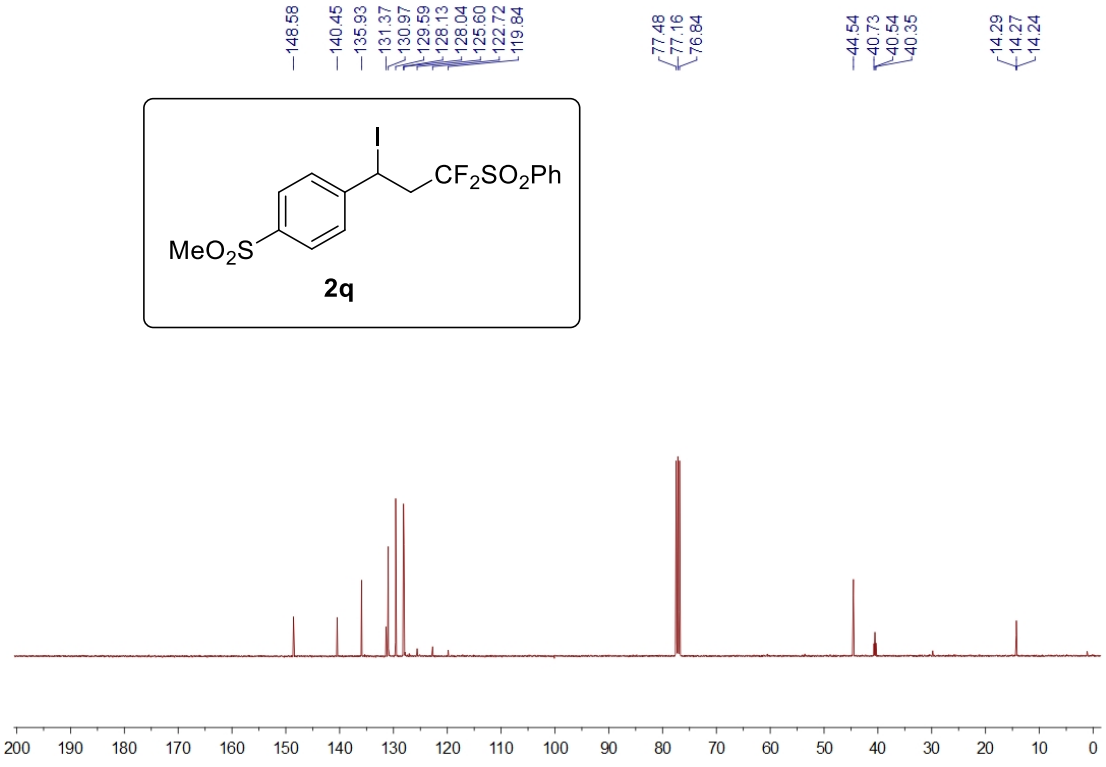
7.59
7.27
5.51
5.49
5.49
5.48
5.47
3.53
3.51
3.51
3.50
3.49
3.48
3.48
3.46
3.06
0.00
I
CF2SO2Ph
MeO2S
2q
2.02
1.91
1.05
4.13
1.06
2.22
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.04
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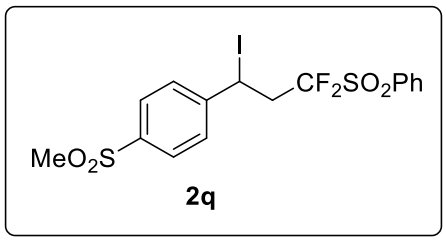
122.72
119.84
77.48
77.16
76.84
44.54
40.73
40.54
40.35
14.29
14.27
14.24
I
CF2SO2Ph
MeO2S
2q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


I
CF2SO2Ph
MeO2S

2q

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8.58
8.57
8.57
8.57
8.56
8.56
8.56
7.75
7.72
7.59
7.56
7.31
7.29
7.16
7.14
7.13
5.55
5.54
5.53
5.52
3.97
3.95
3.94
3.93
3.91
3.89
3.43
3.42
3.41
3.40
3.40
3.39
3.38
3.37
3.36
3.34
3.33
-0.01
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0.99
0.99
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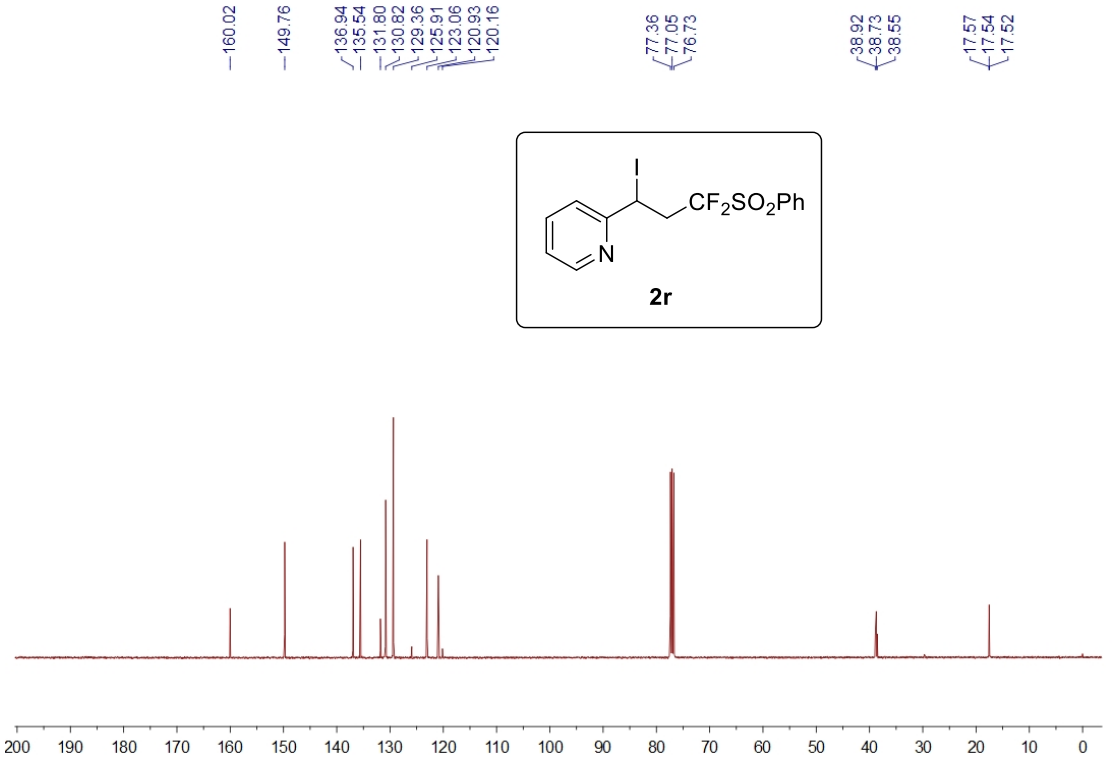
1.07
1.06

2r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125.91
123.06
120.93
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77.05
76.73
38.92
38.73
38.55
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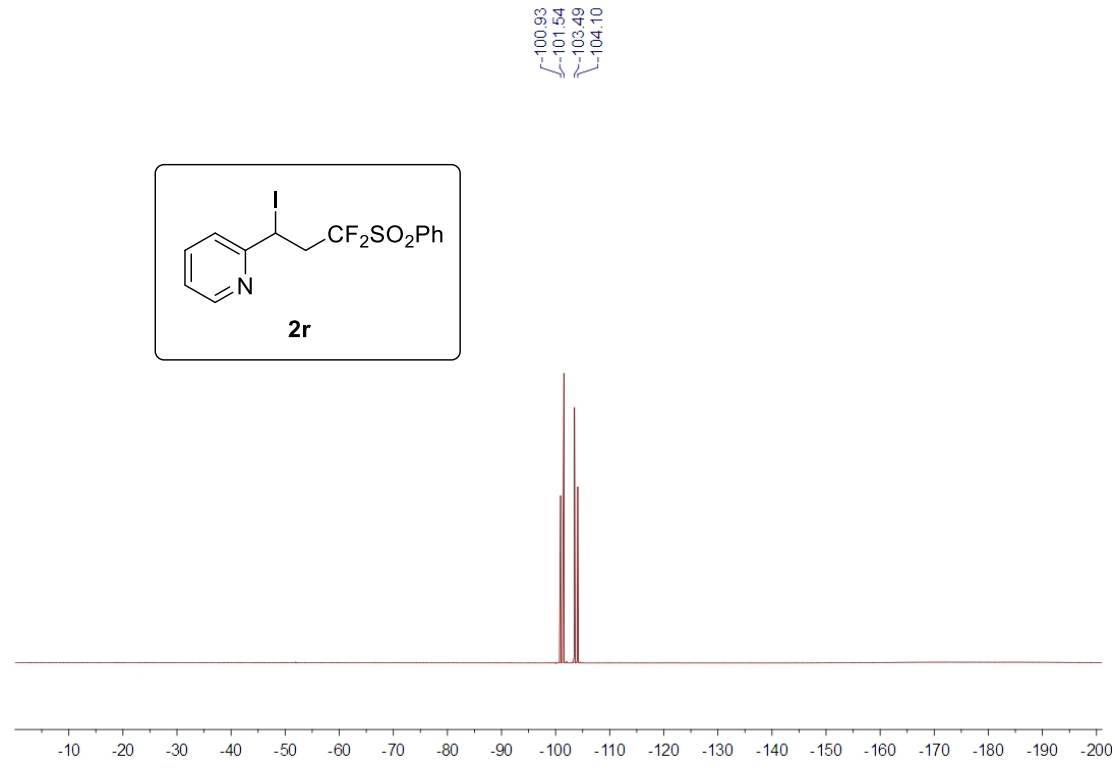
17.54
17.52
I
CF2SO2Ph
N
2r
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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101.54
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104.10
I
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N
2r
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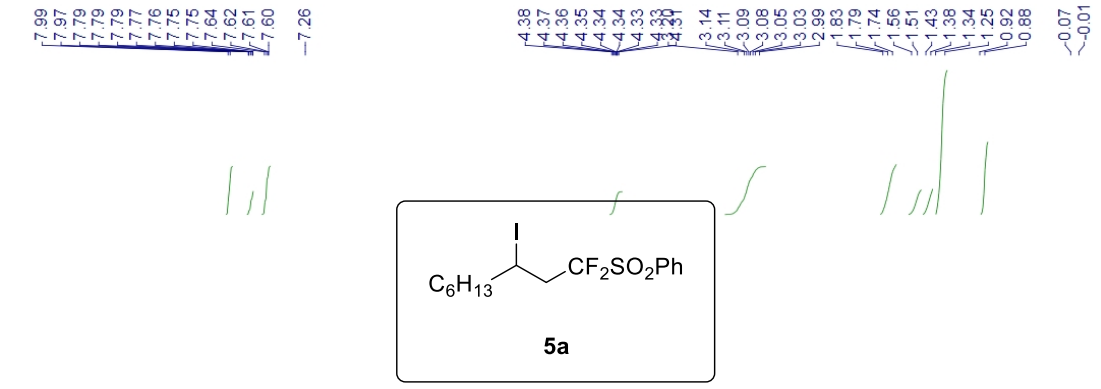
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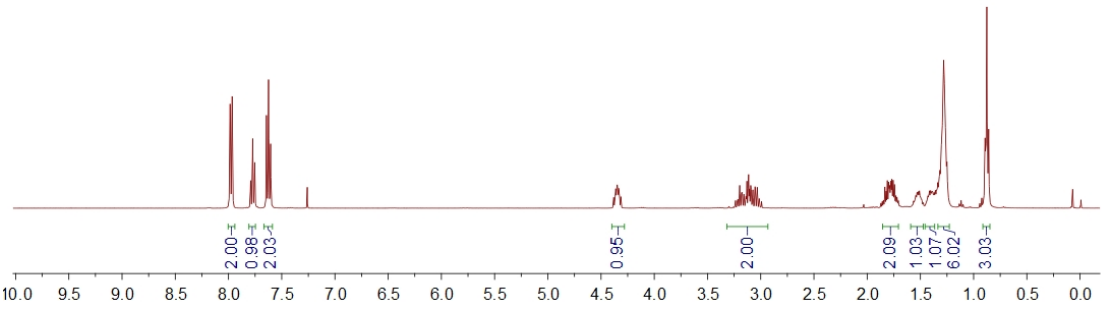
7.61
7.60
7.26
4.38
4.37
4.36
4.35
4.34
4.34
4.33
4.31
3.14
3.11
3.09
3.08
3.05
3.03
2.99
1.83
1.79
1.74
1.56
1.51
1.43
1.38
1.34
1.25
0.92
0.88
0.07
-0.01

I
C6H13
CF2SO2Ph

5a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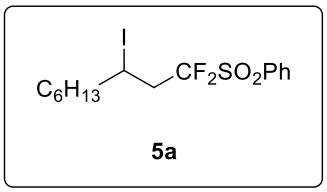
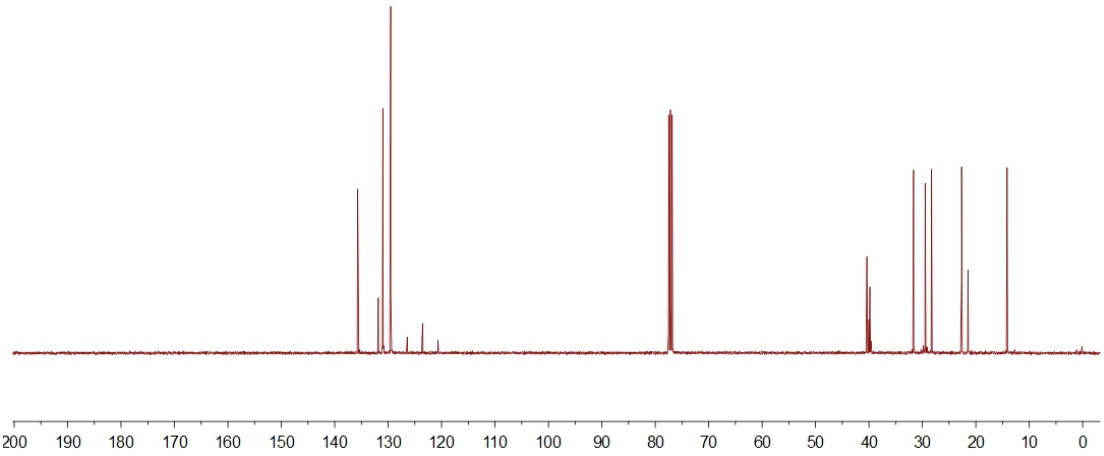
2.09
1.03
1.07
6.02
3.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


135.71
131.84
130.99
129.52
126.42
123.54
120.67
77.48
77.16
76.84
40.39
40.01
39.82
39.63
31.66
29.49
28.29
21.49
21.45
14.15


I
C6H13
CF2SO2Ph

5a


200
190
180
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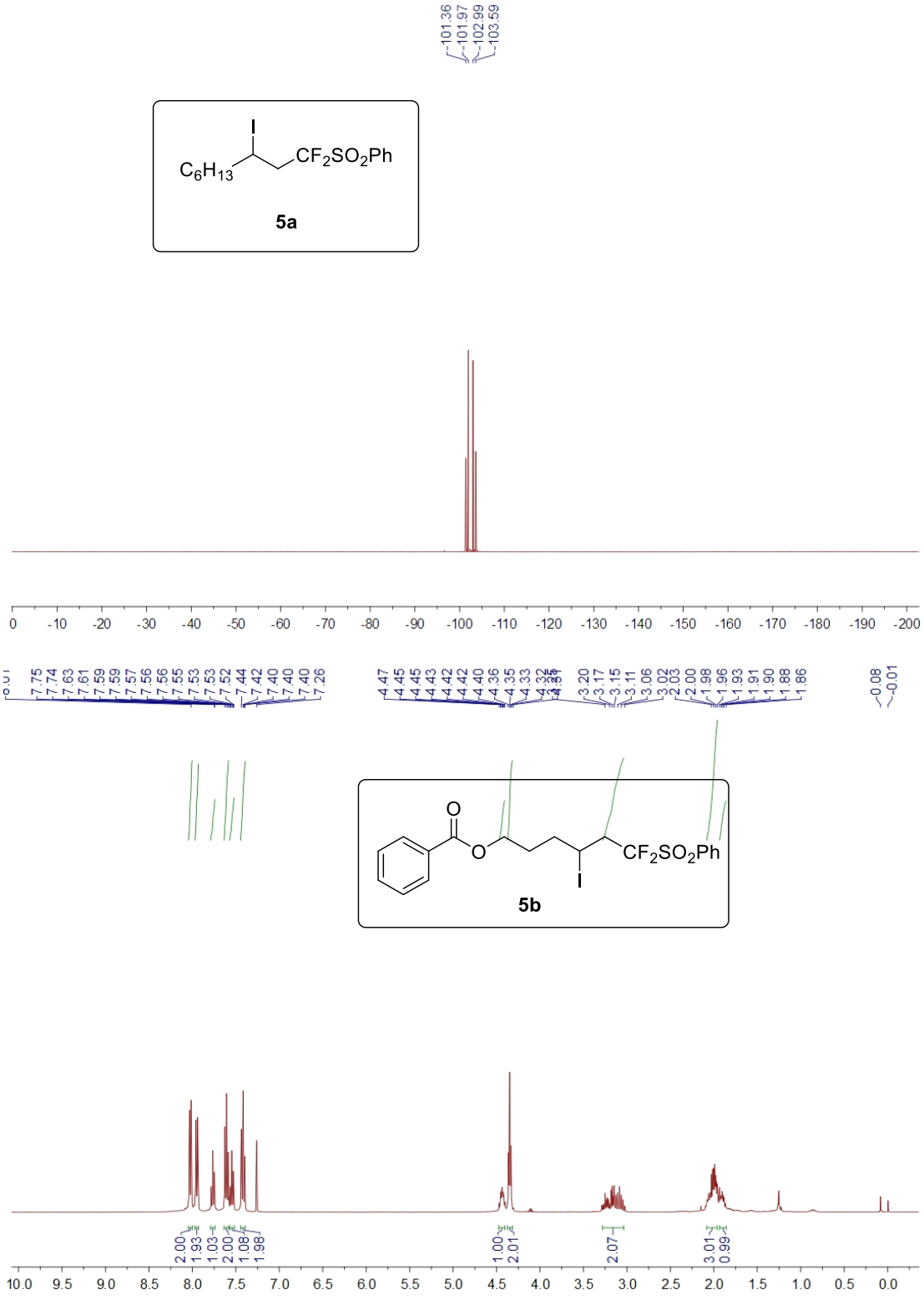
120
110
100
90
80
70
60
50
40
30
20
10
0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-101.97
-102.99
-103.59
I
C6H13
CF2SO2Ph
5a
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7.74
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3.17
3.15
3.11
3.06
3.02
2.03
2.00
1.98
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1.91
1.90
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O
CF2SO2Ph
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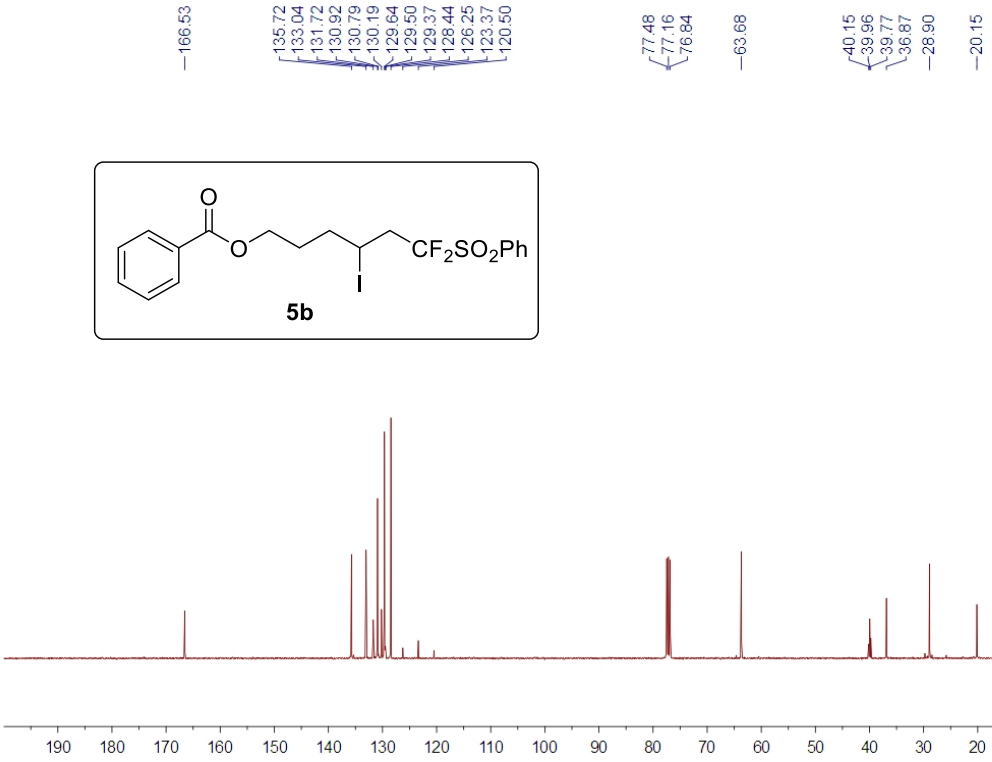
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77.16
76.84
63.68
40.15
39.96
39.77
36.87
28.90
20.15
O
O
CF2SO2Ph
I
5b
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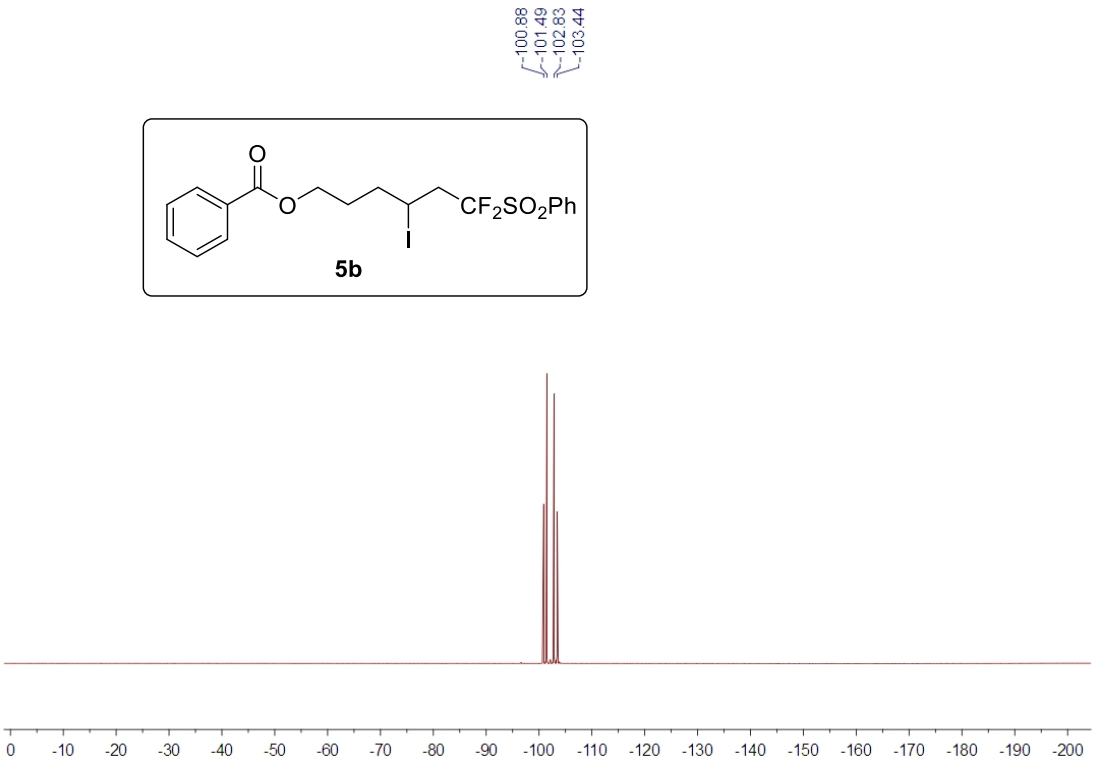
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5b
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-180
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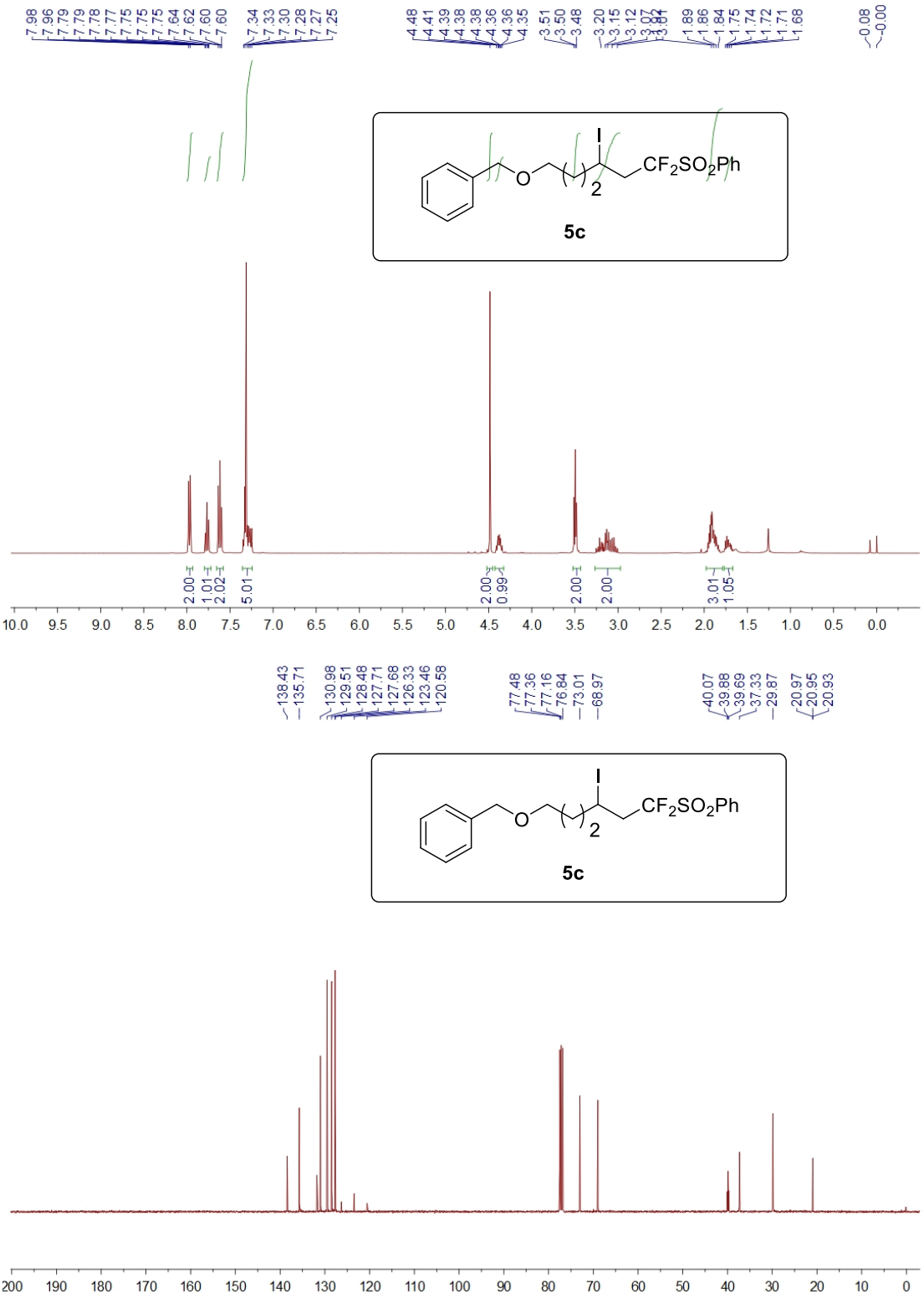
-200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7.60
7.34
7.33
7.30
7.28
7.27
7.25
4.48
4.41
4.39
4.38
4.38
4.36
4.36
4.35
3.51
3.50
3.48
3.20
3.15
3.12
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1.86
1.84
1.75
1.74
1.72
1.71
1.68
0.08
-0.00
I
O
2
CF2SO2Ph
5c
2.00
1.01
2.02
5.01
2.00
0.99
2.00
2.00
3.01
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
138.43
135.71
130.98
129.51
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126.33
123.46
120.58
77.48
77.36
77.16
76.84
73.01
68.97
40.07
39.88
39.69
37.33
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2
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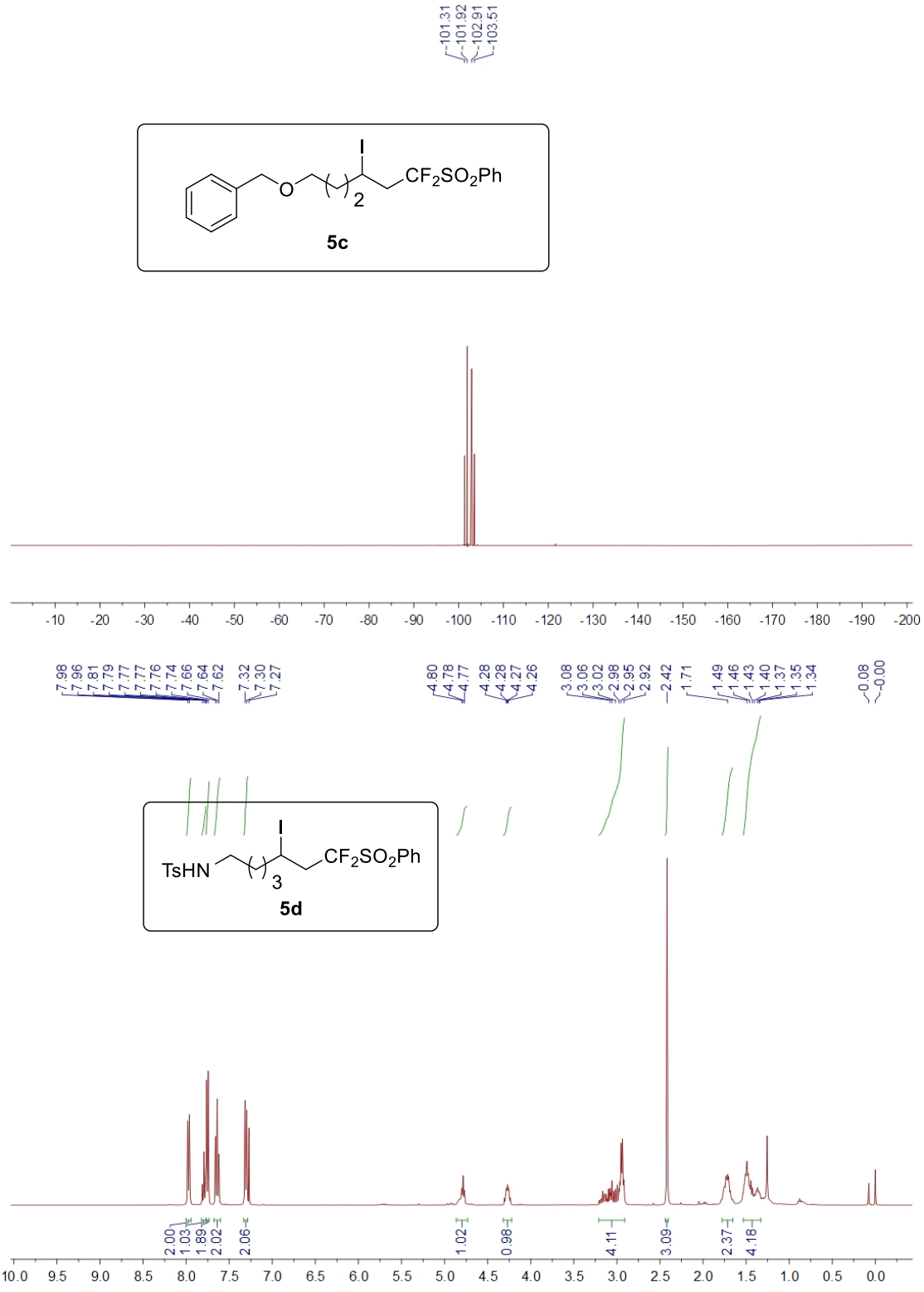
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5c
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7.96
7.81
7.79
7.77
7.77
7.76
7.74
7.66
7.64
7.62
7.32
7.30
7.27
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4.78
4.77
4.28
4.28
4.27
4.26
3.08
3.06
3.02
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2.92
2.42
1.71
1.49
1.46
1.43
1.40
1.37
1.35
1.34
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0.00
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TsHN
3
CF2SO2Ph
5d
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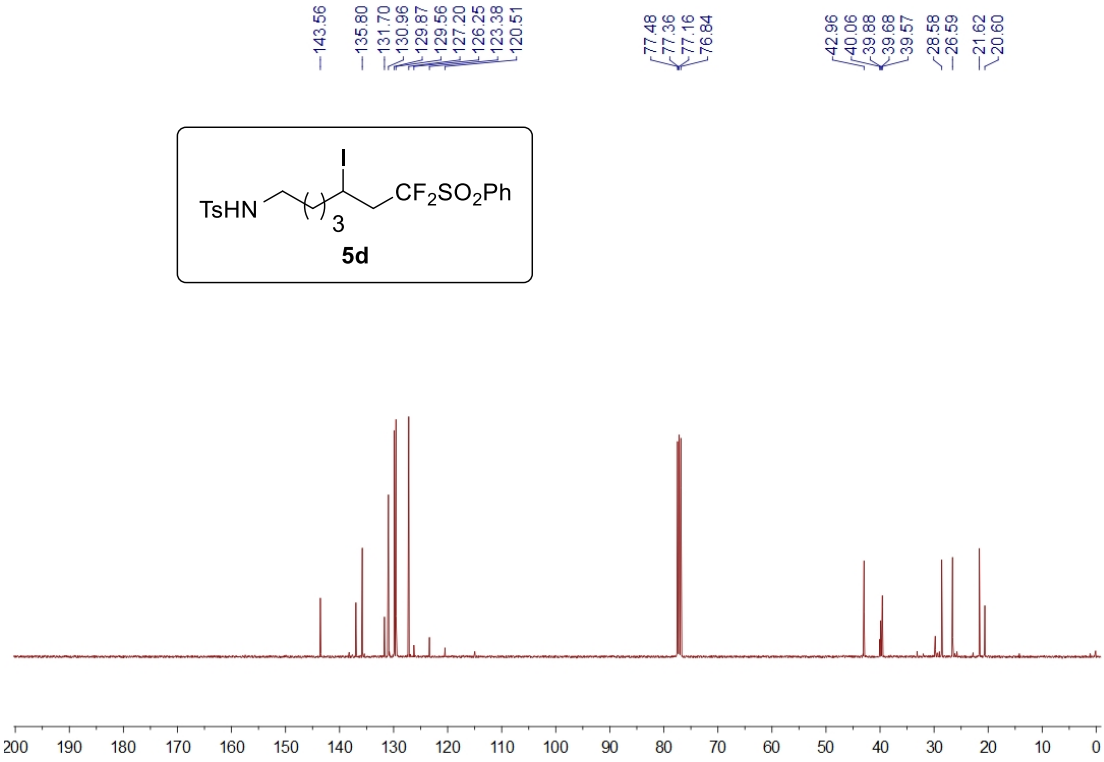
1.89
2.02
2.06
1.02
0.98
4.11
3.09
2.37
4.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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77.16
76.84
42.96
40.06
39.88
39.68
39.57
28.58
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TsHN
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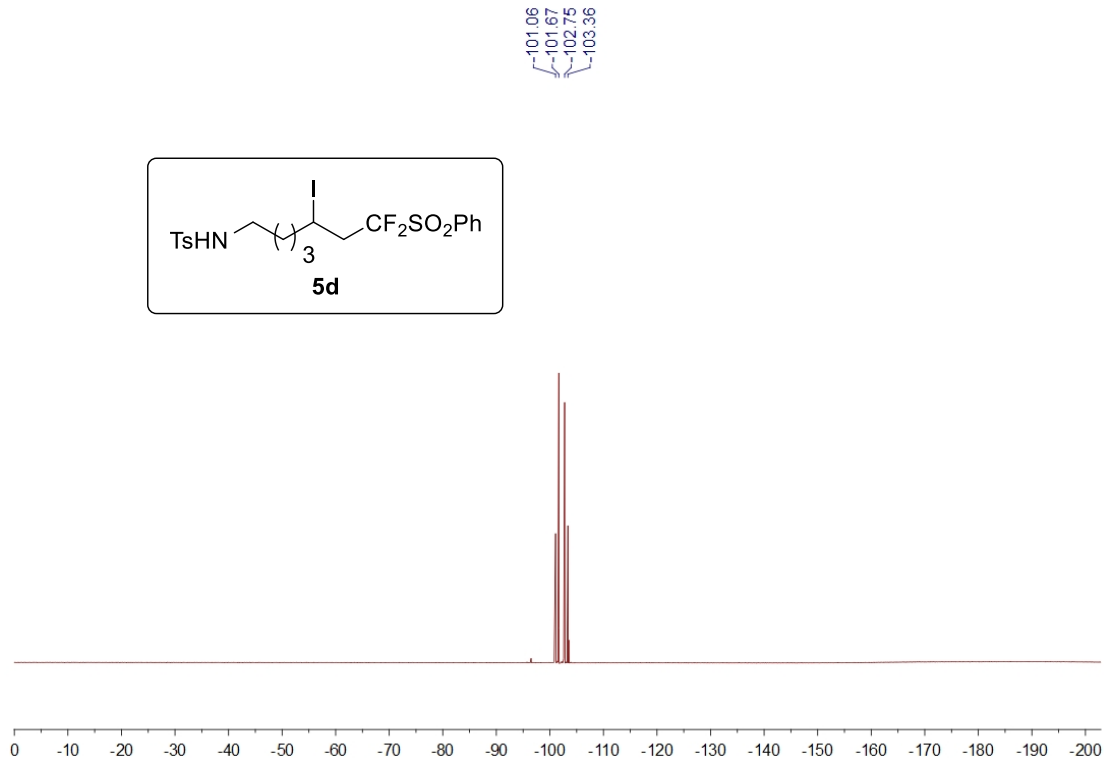
I
CF2SO2Ph
5d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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101.67
102.75
103.36
TsHN
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I
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5d
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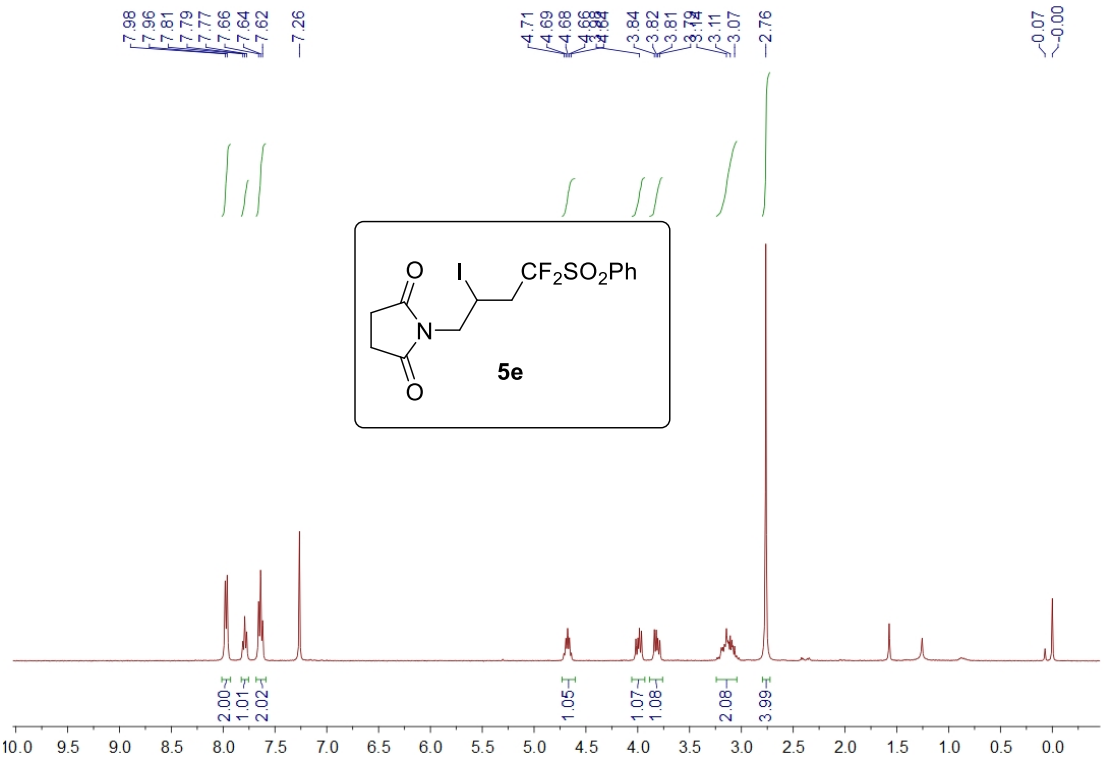
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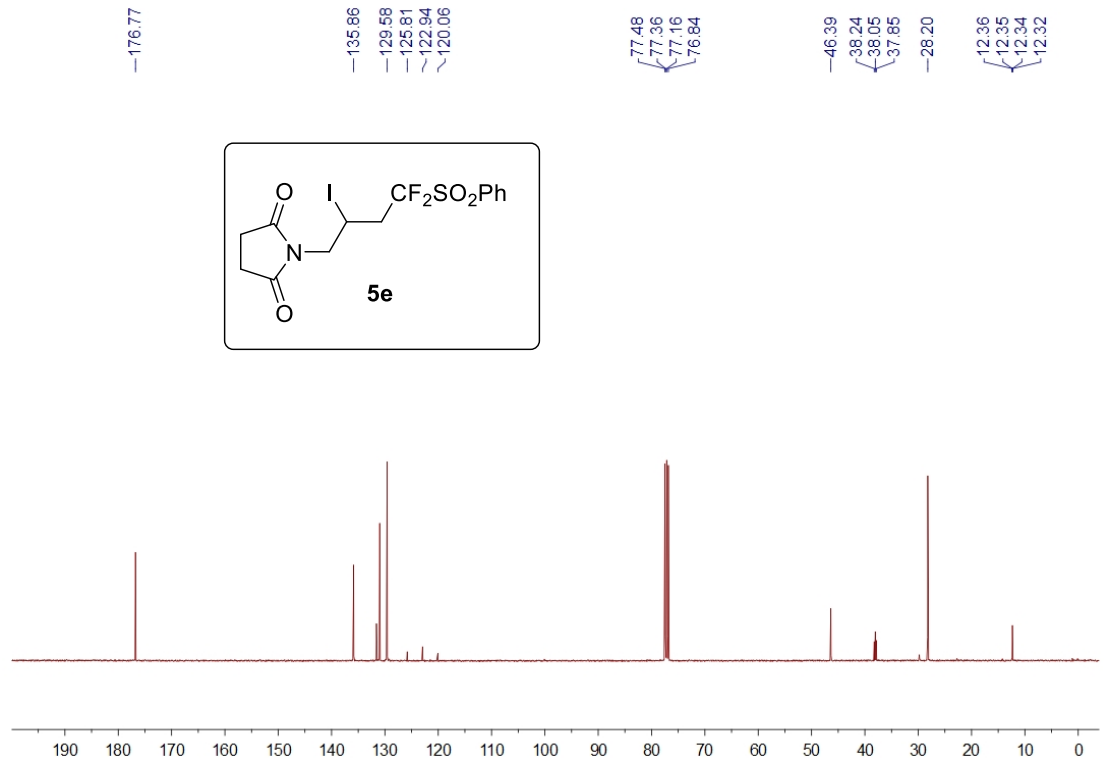
3.82
3.81
3.11
3.07
2.76
0.07
0.00
O
I
CF2SO2Ph
N
O
5e
2.00
1.01
2.02
1.05
1.07
1.08
2.08
3.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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46.39
38.24
38.05
37.85
28.20
12.36
12.35
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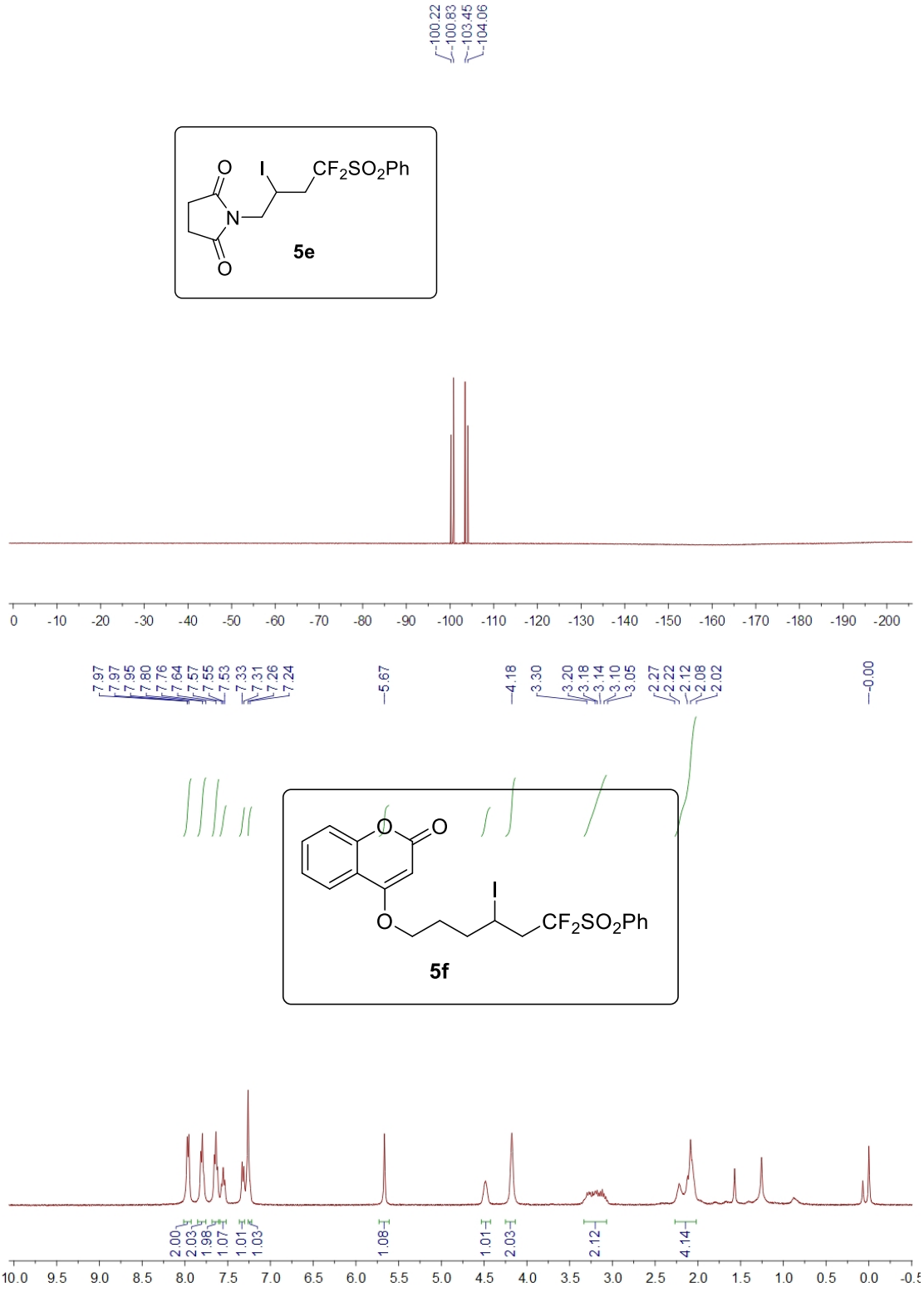
12.32
O
I
CF2SO2Ph
N
O
5e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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I
CF2SO2Ph
N
O
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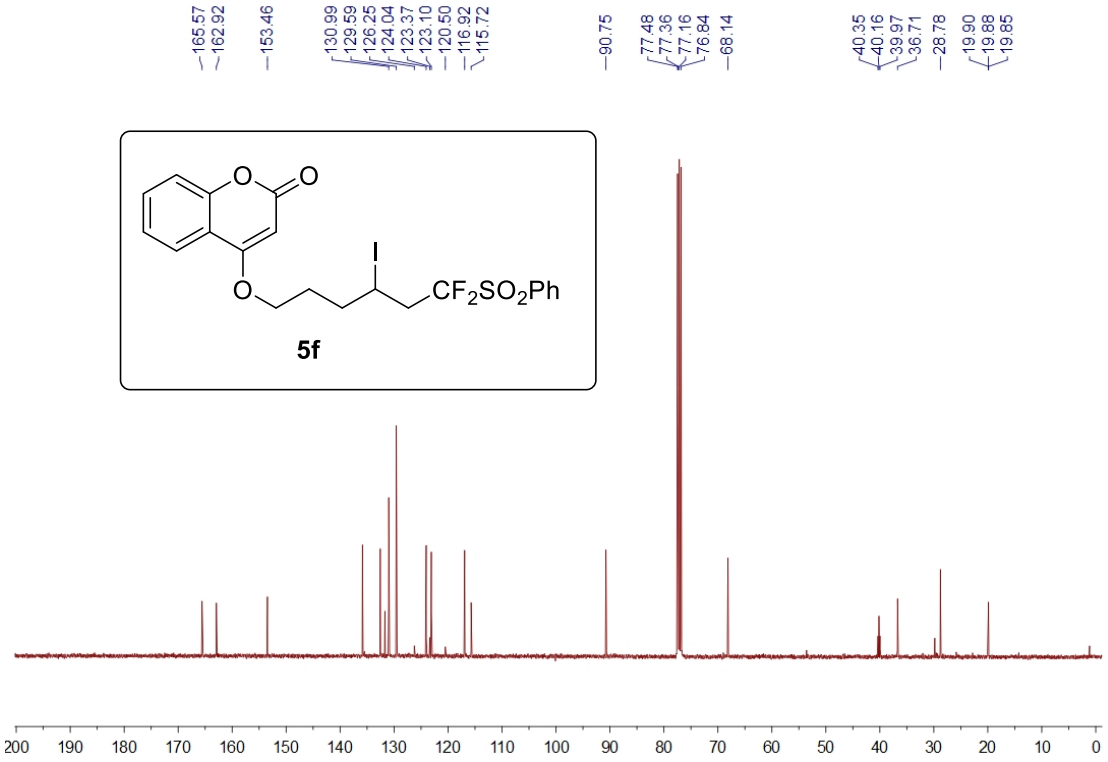
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
7.97
7.97
7.95
7.80
7.76
7.64
7.57
7.55
7.53
7.33
7.31
7.26
7.24
5.67
4.18
3.30
3.20
3.18
3.14
3.10
3.05
2.27
2.22
2.12
2.08
2.02
0.00
O
O
O
I
CF2SO2Ph
5f
2.00
2.03
1.98
1.07
1.01
1.03
1.08
1.01
2.03
2.12
4.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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120.50
116.92
115.72
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77.36
77.16
76.84
68.14
40.35
40.16
39.97
36.71
28.78
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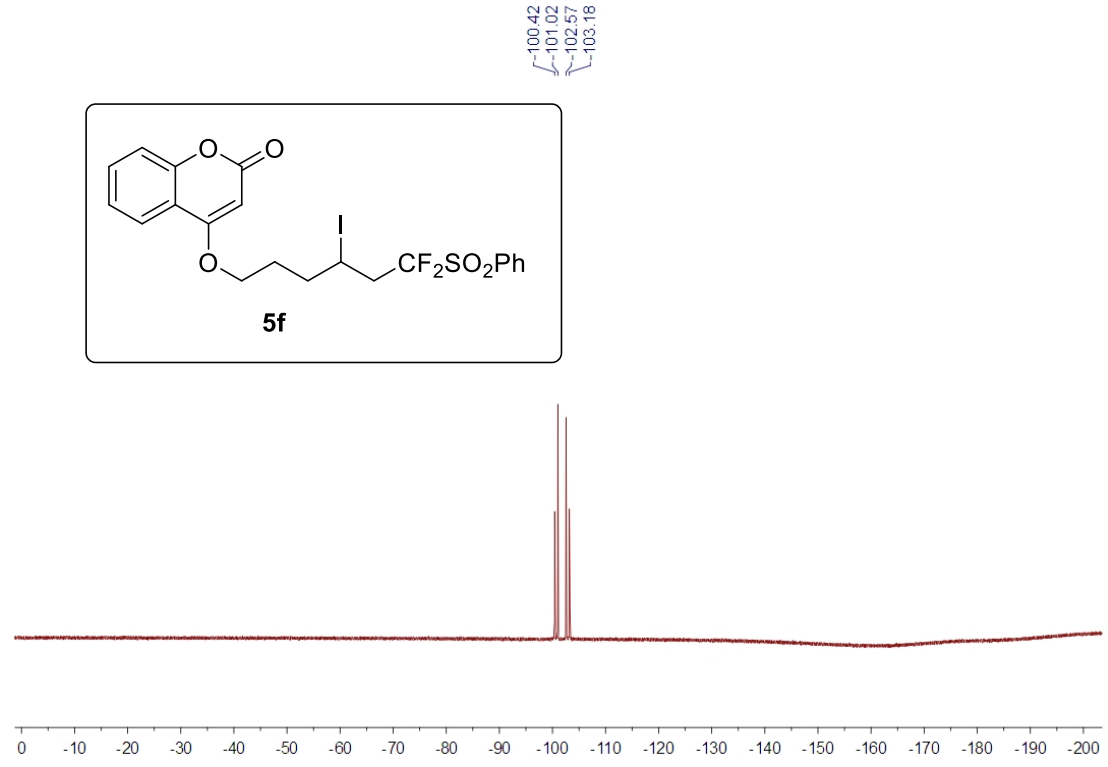
19.85
O
O
O
I
CF2SO2Ph
5f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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O
O
I
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5f
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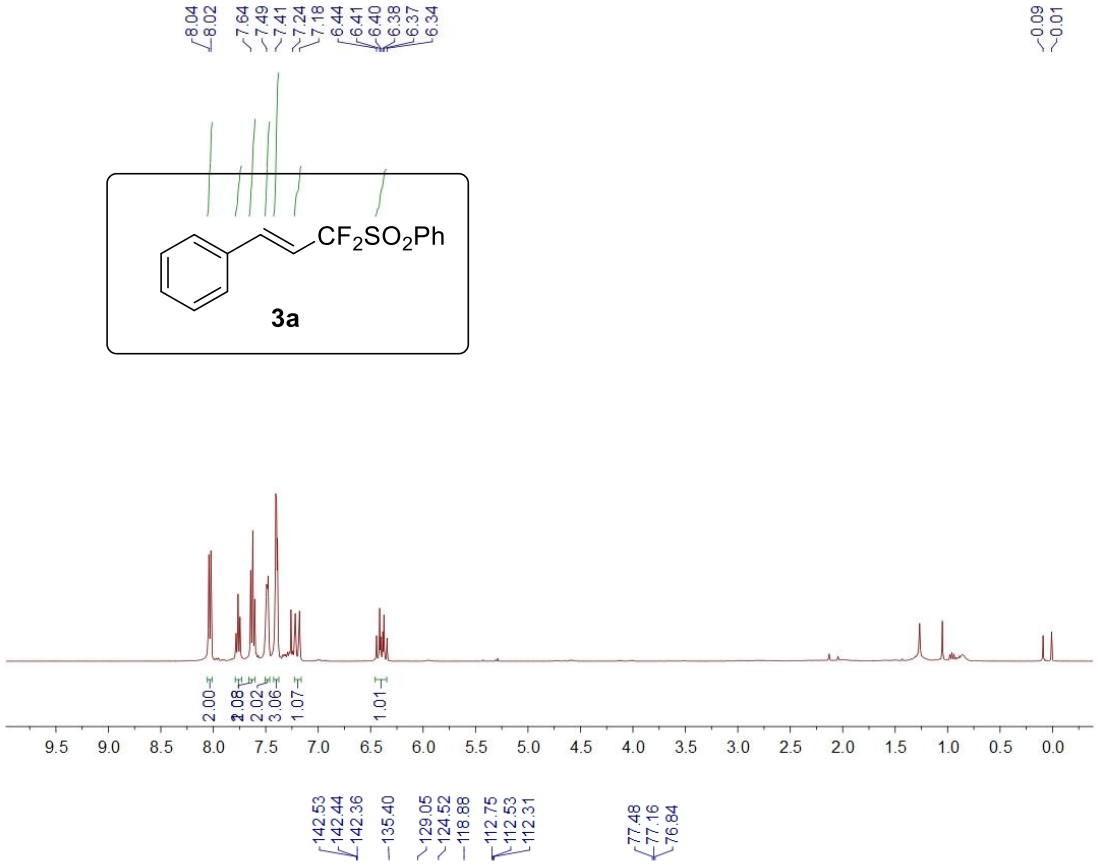
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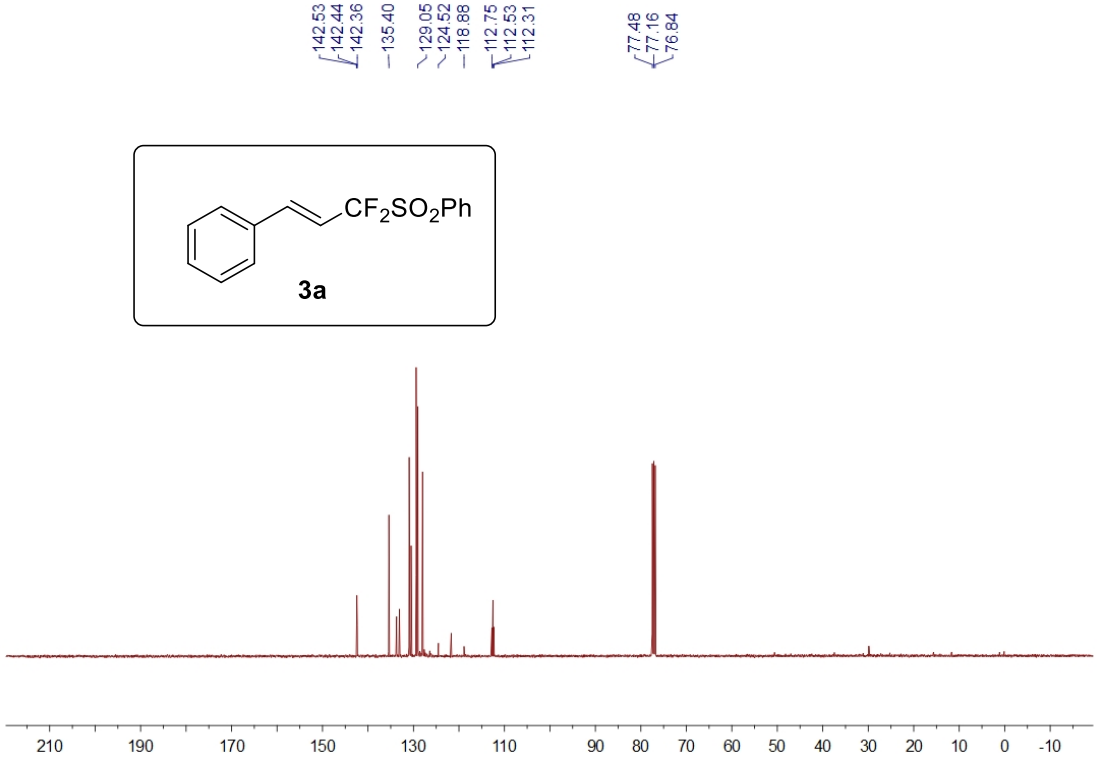
6.41
6.40
6.38
6.37
6.34
0.09
0.01
CF2SO2Ph
3a
2.00
2.08
2.02
3.06
1.07
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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77.48
77.16
76.84
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3a
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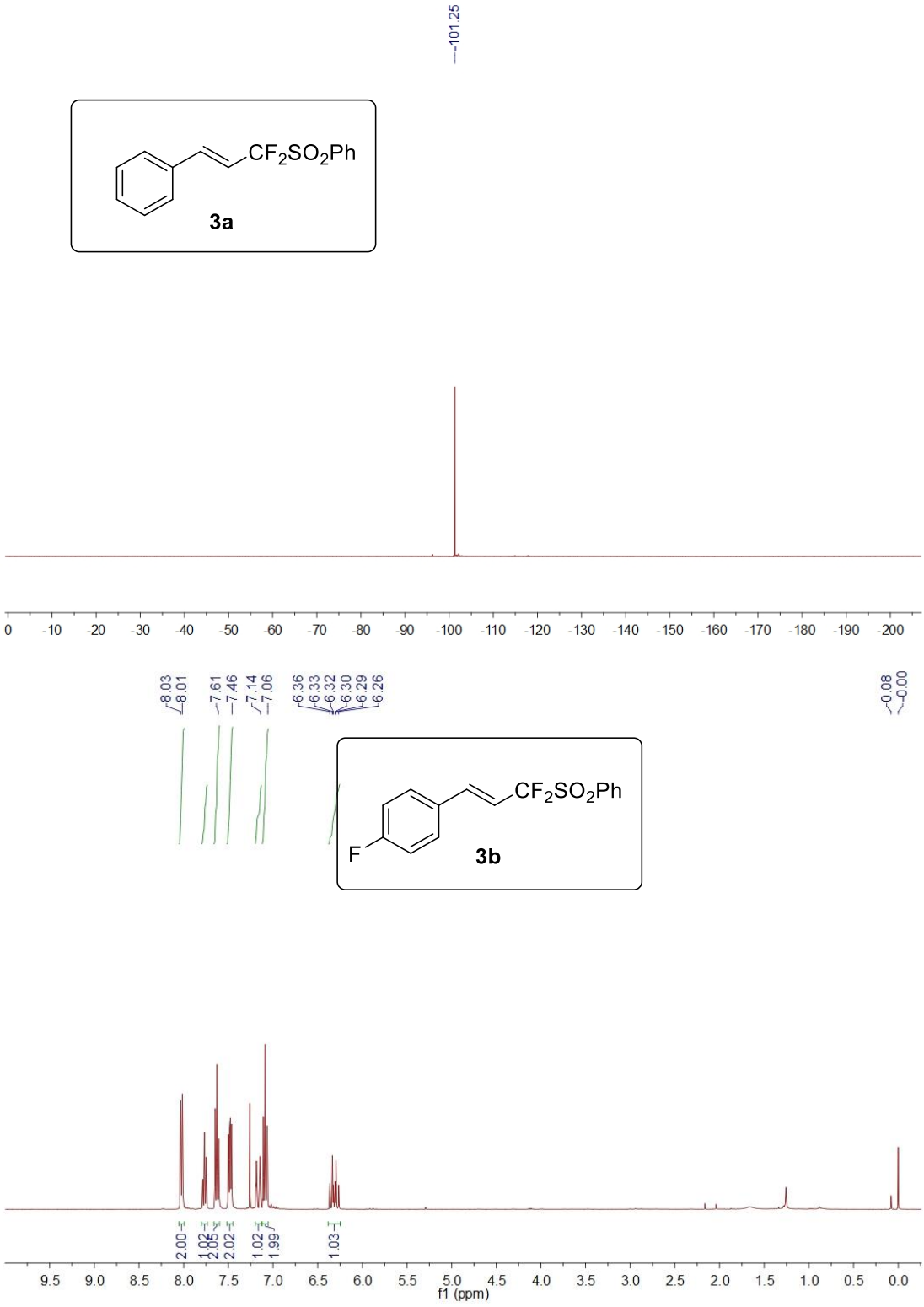
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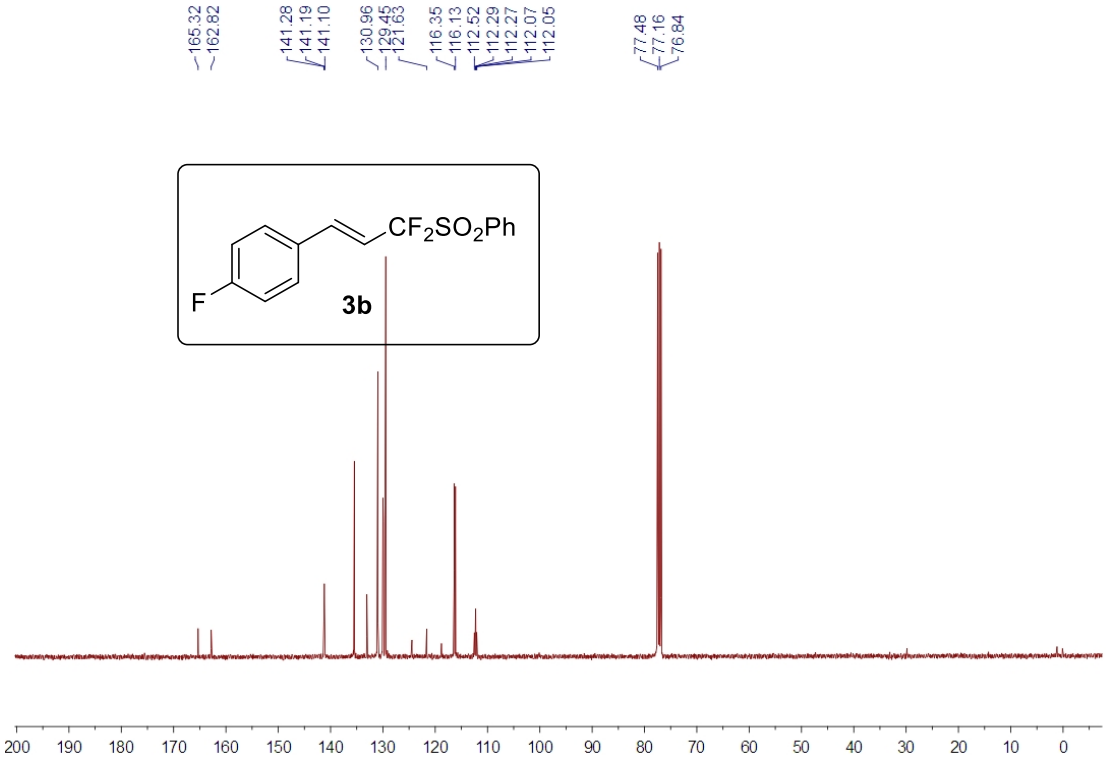
8.01
7.61
7.46
7.14
7.06
6.36
6.33
6.32
6.30
6.29
6.26
0.08
0.00
CF2SO2Ph
F
3b
2.00
1.02
1.05
2.02
1.02
1.99
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.16
76.84
CF2SO2Ph
F
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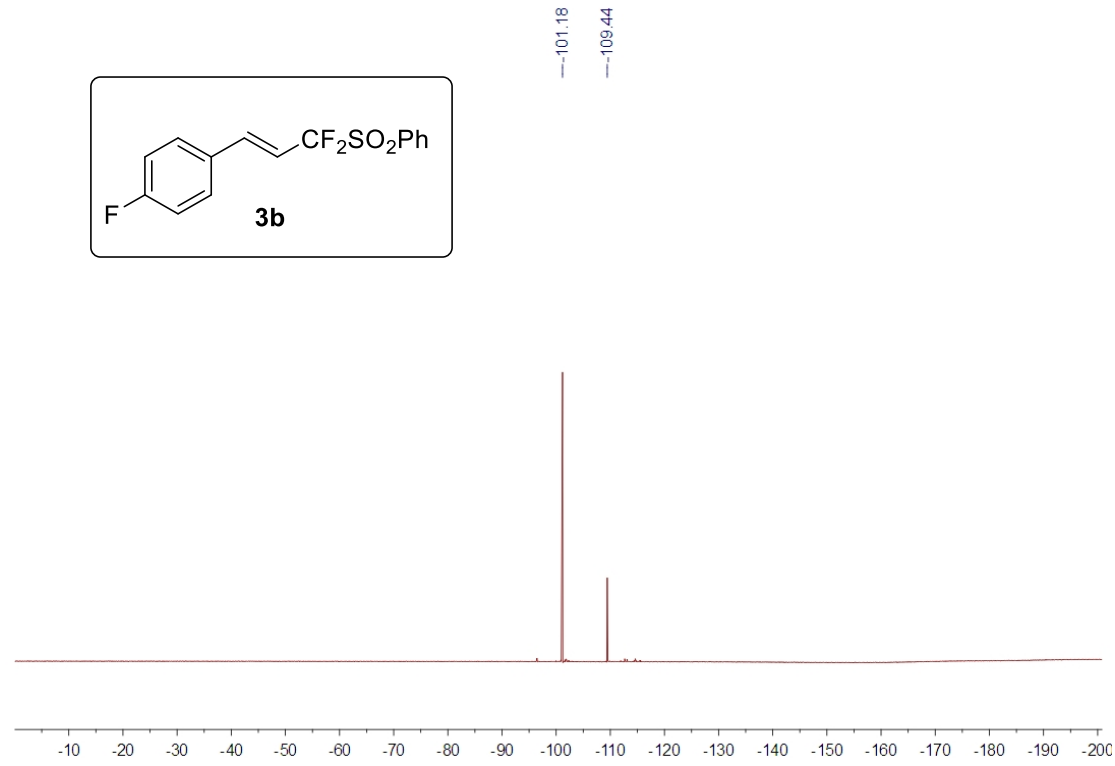
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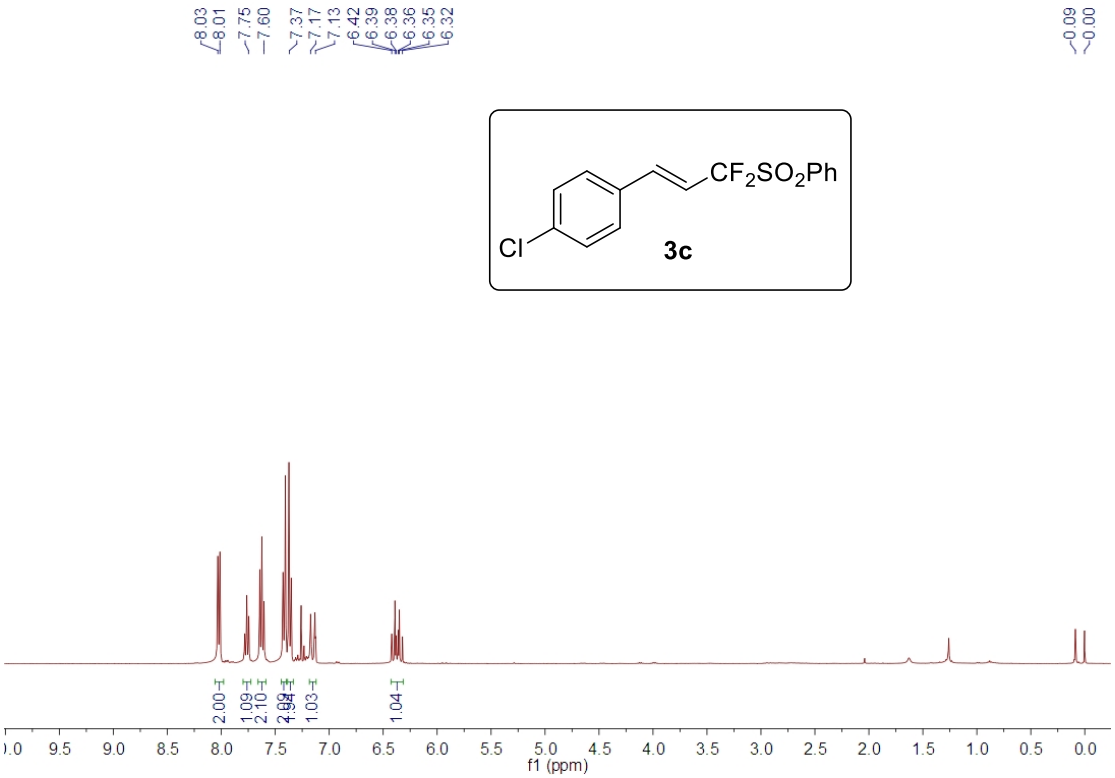
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7.17
7.13
6.42
6.39
6.38
6.36
6.35
6.32
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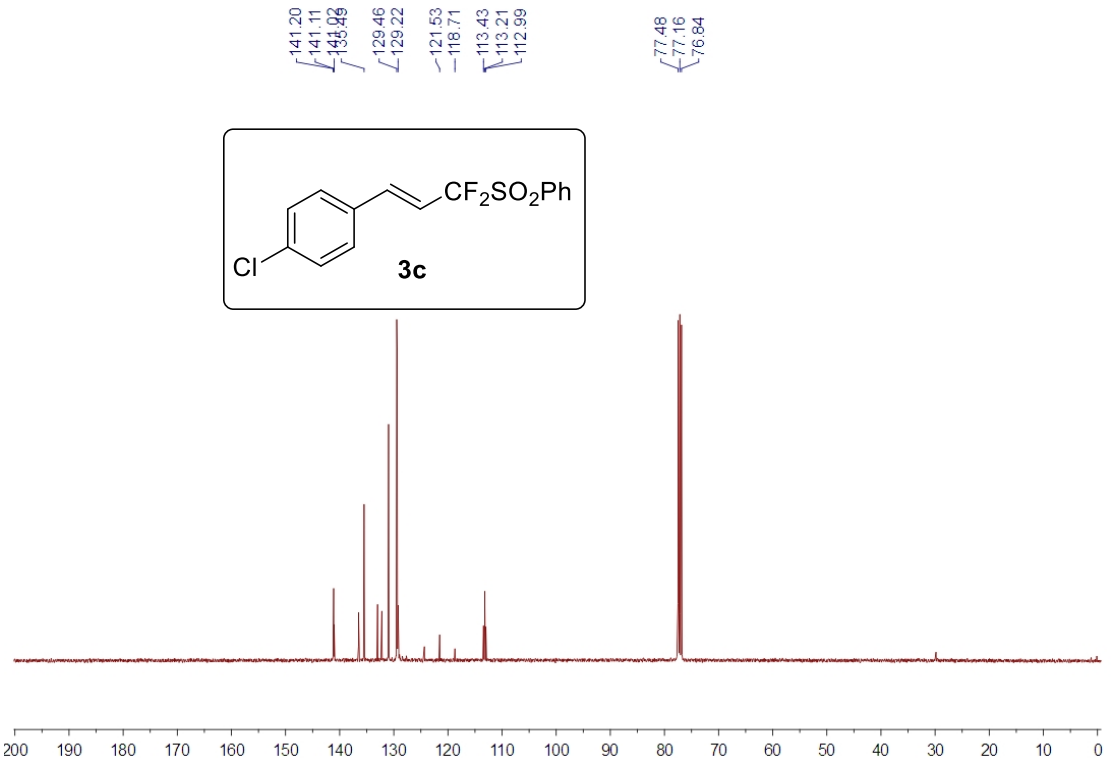
0.00
CF2SO2Ph
Cl
3c
2.00
1.09
2.10
1.03
1.04
f1 (ppm)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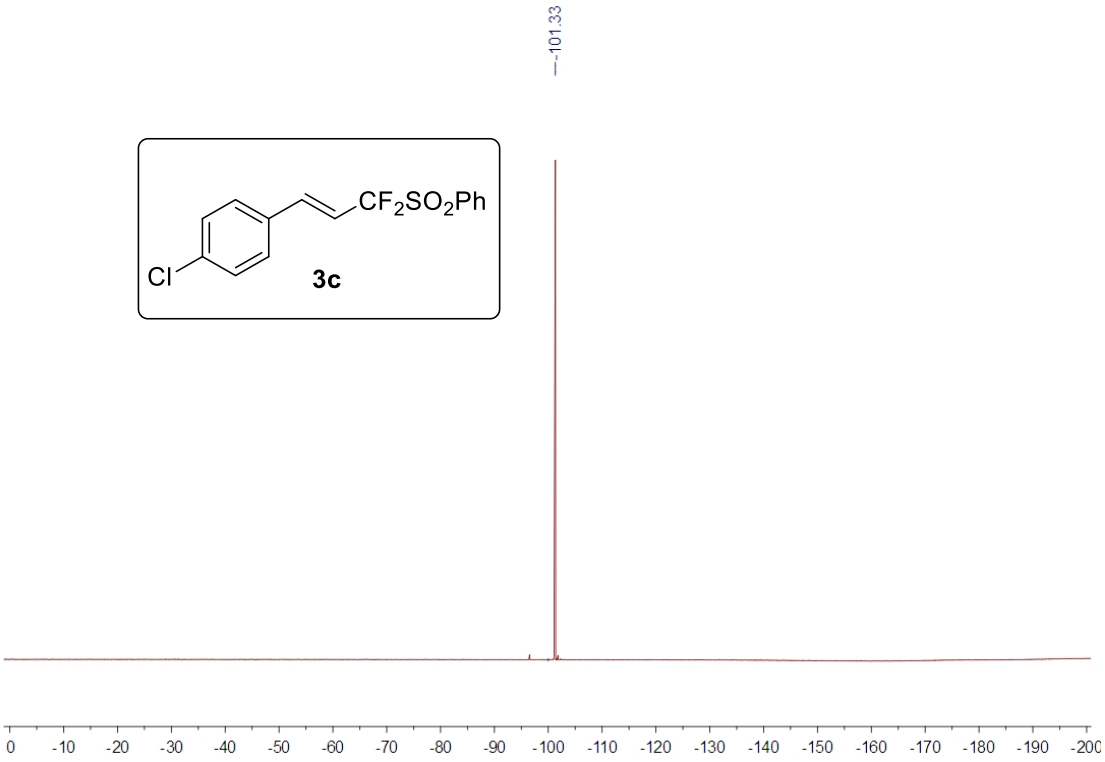
77.16
76.84
CF2SO2Ph
Cl
3c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CF2SO2Ph
Cl
3c
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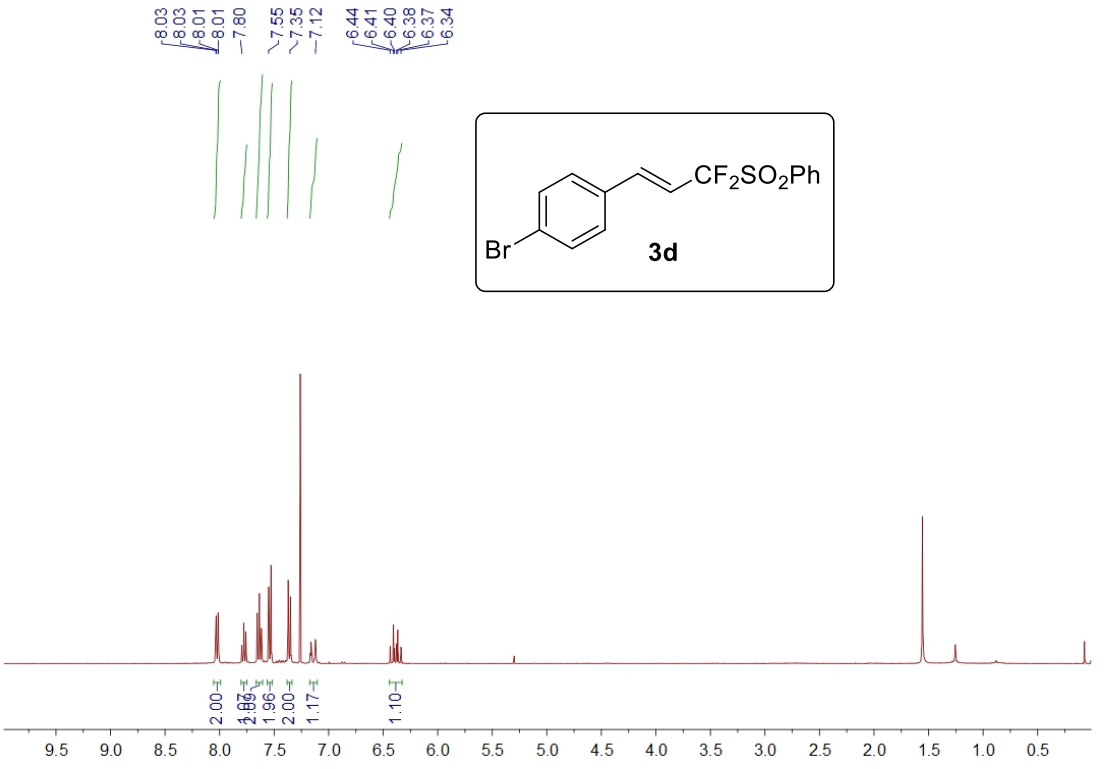
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8.01
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7.12
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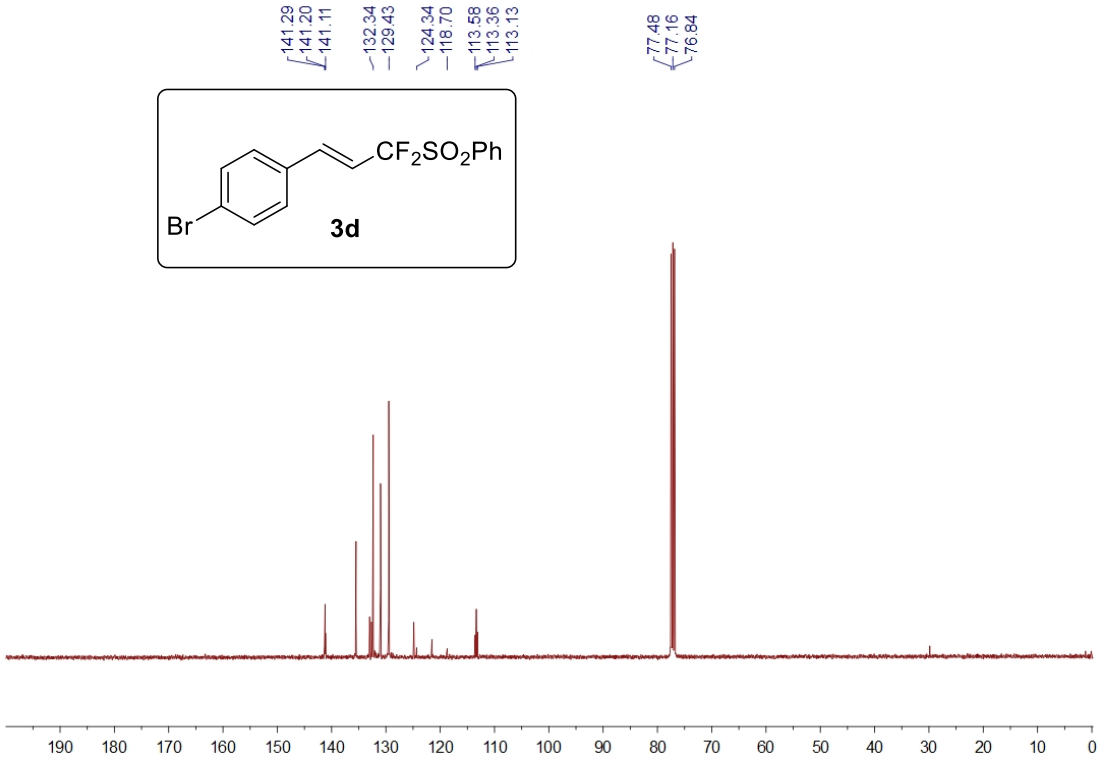
6.41
6.40
6.38
6.37
6.34
CF2SO2Ph
Br
3d
2.00
1.96
2.00
1.17
1.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5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113.58
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77.16
76.84
CF2SO2Ph
Br
3d
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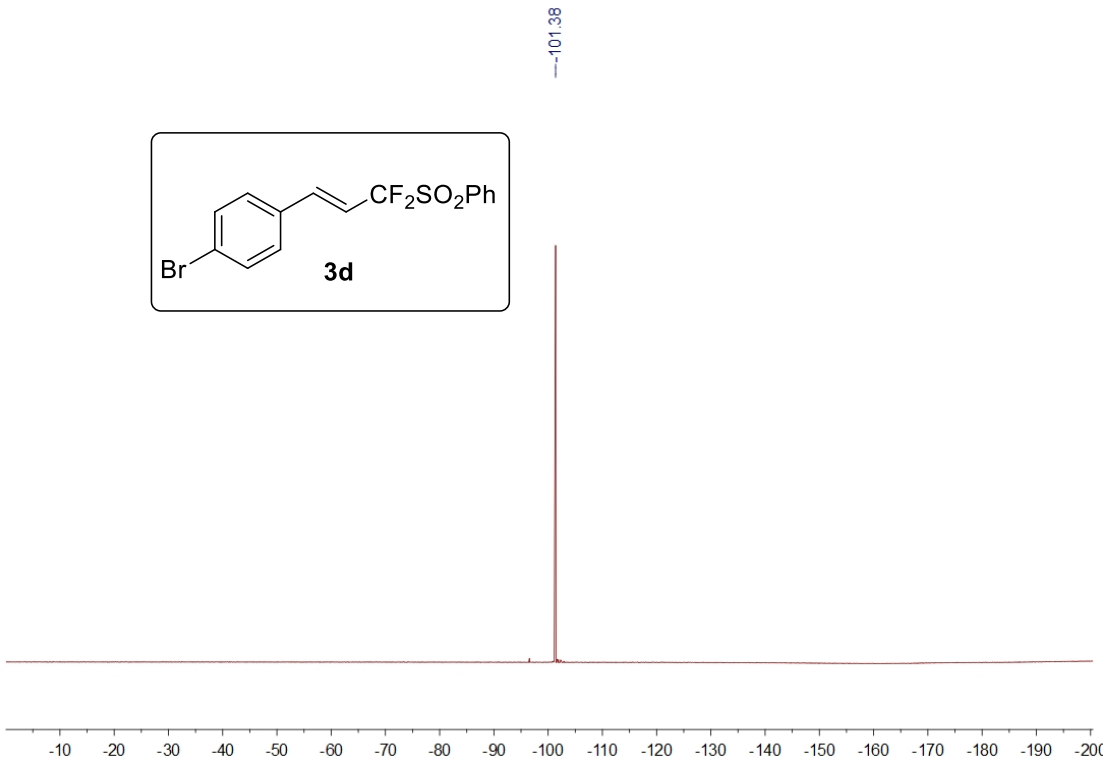
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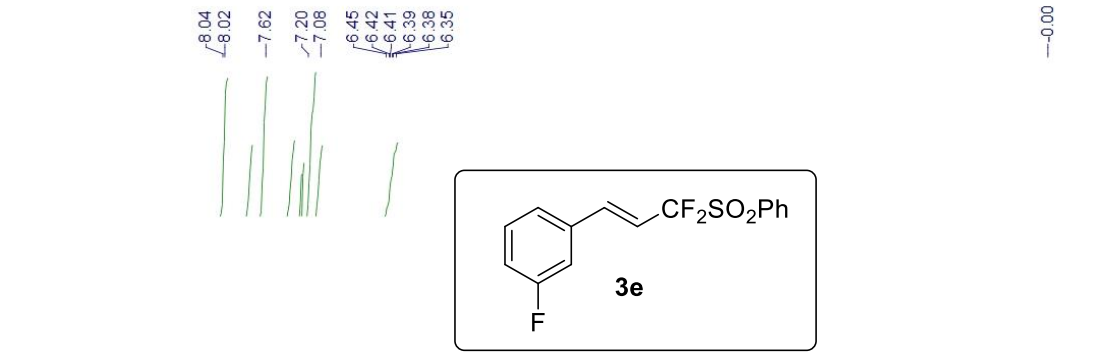
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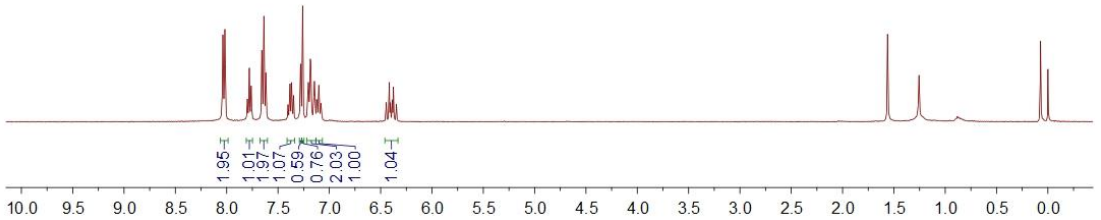
6.41
6.39
6.38
6.35
0.00
CF2SO2Ph
3e
F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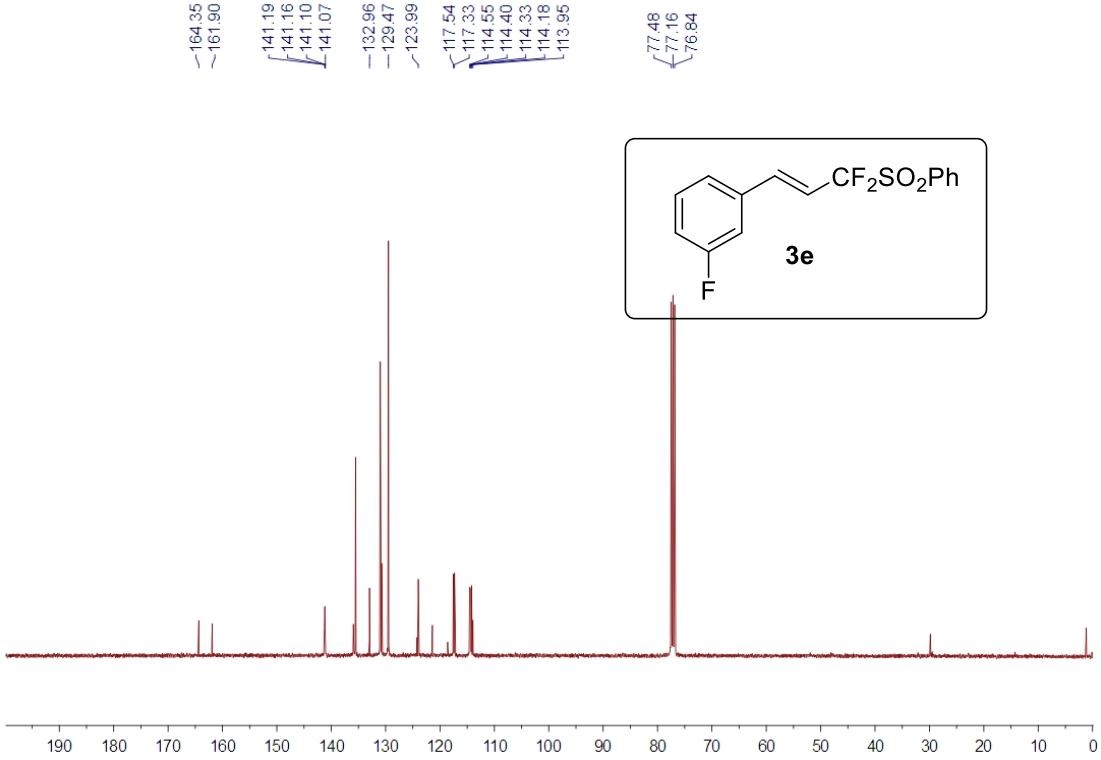
1.97
1.07
0.59
0.76
2.03
1.00
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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114.40
114.33
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77.16
76.84
CF2SO2Ph
3e
F
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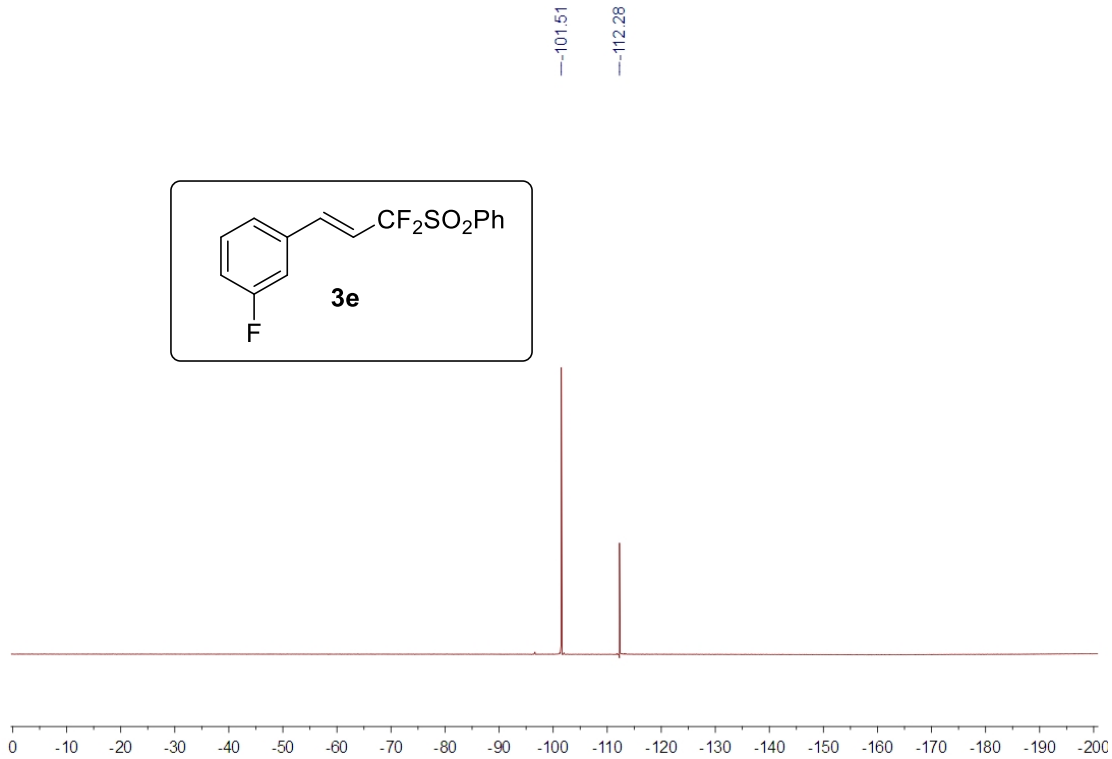
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-150
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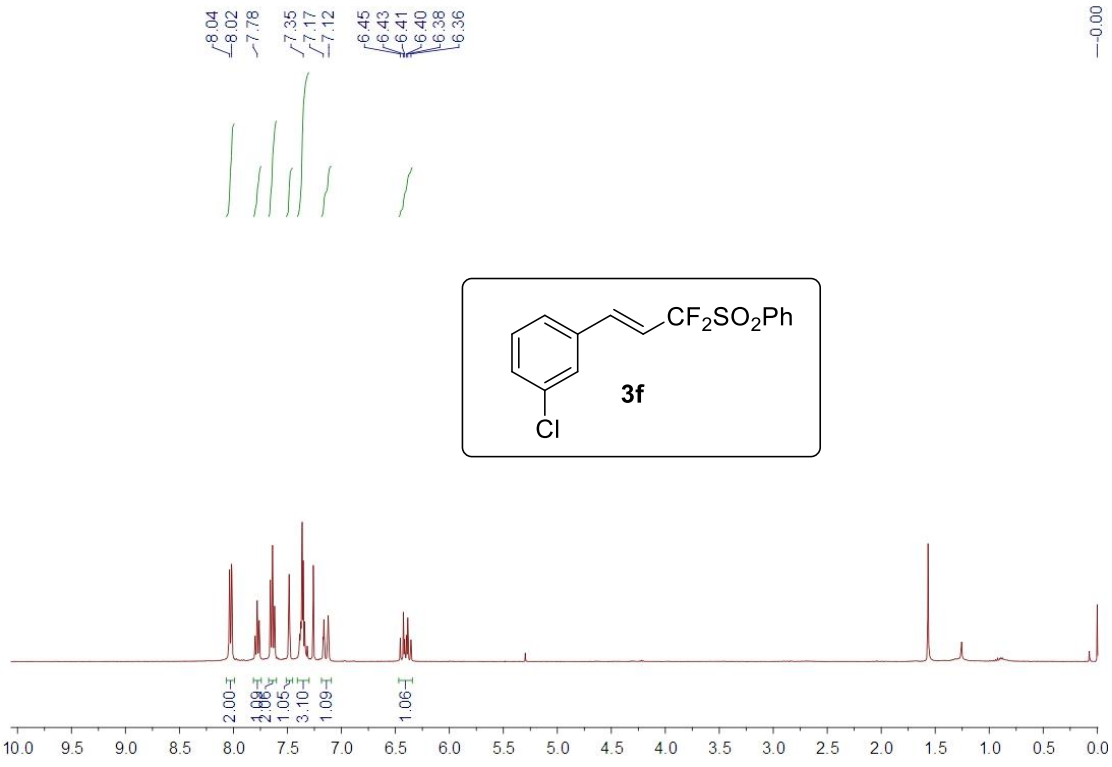
-200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6.38
6.36
0.00
CF2SO2Ph
3f
Cl
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2.08
2.05
1.05
3.10
1.09
1.06
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6.0
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3.5
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2.5
2.0
1.5
1.0
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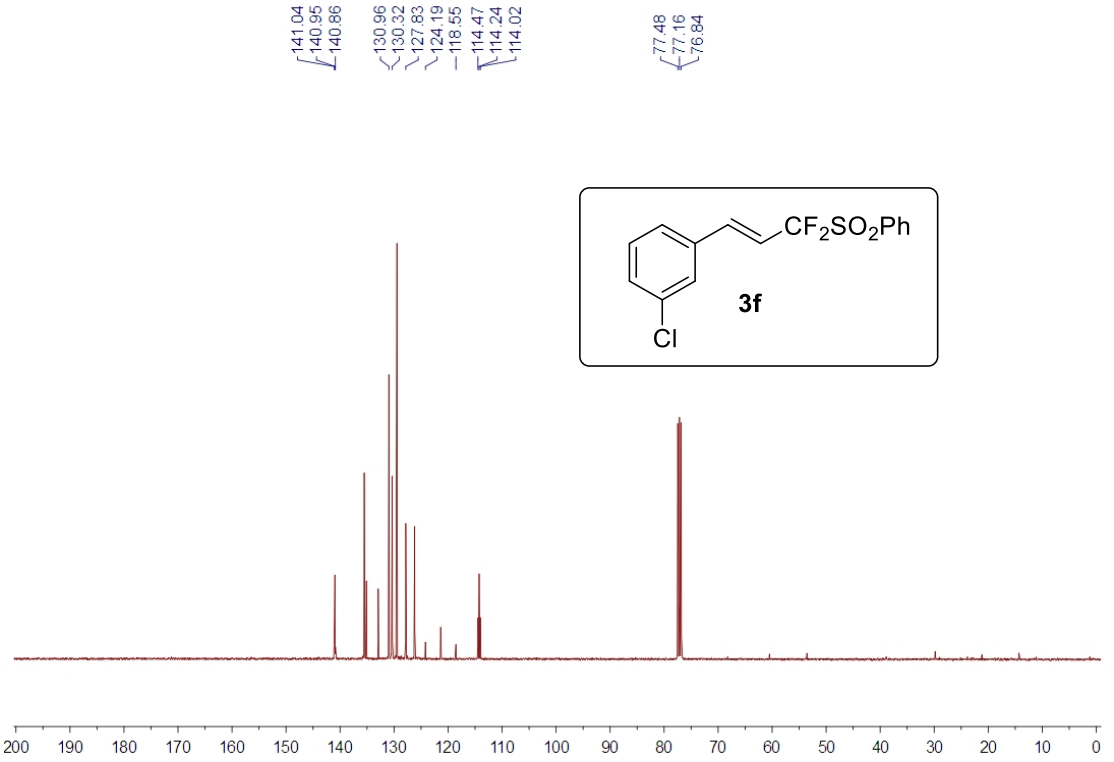
0.0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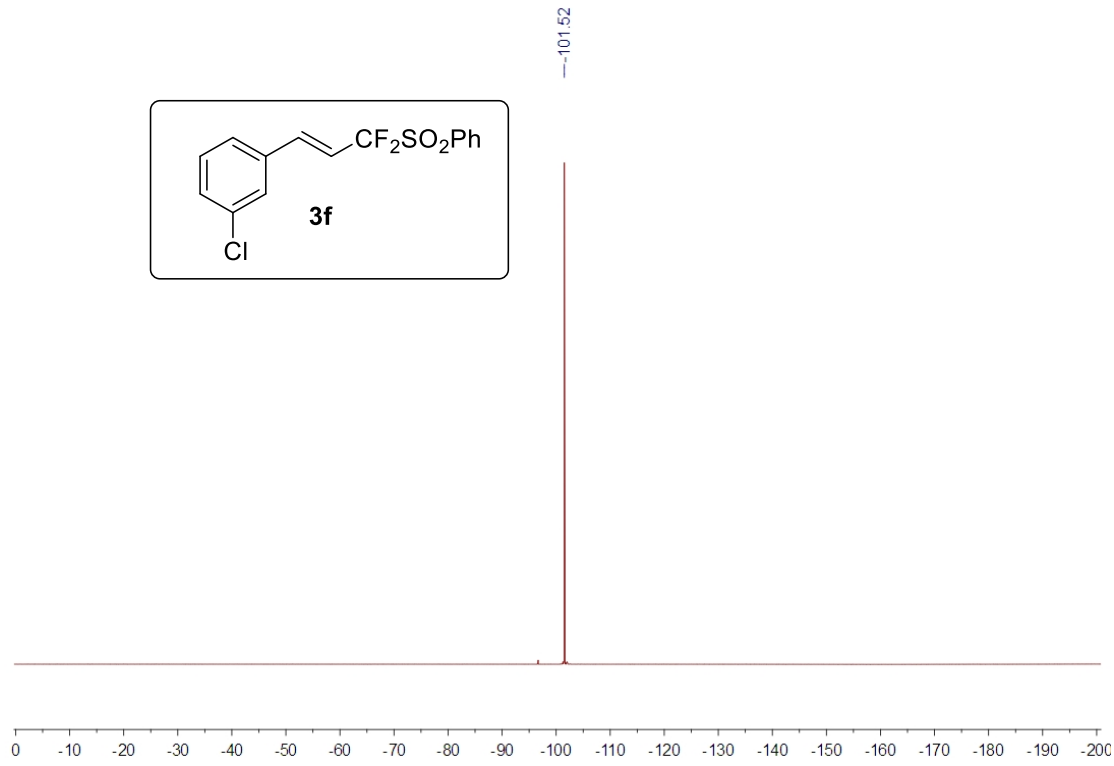
130.32
127.83
124.19
118.55
114.47
114.24
114.02
77.48
77.16
76.84
CF2SO2Ph
3f
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


101.52
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3f
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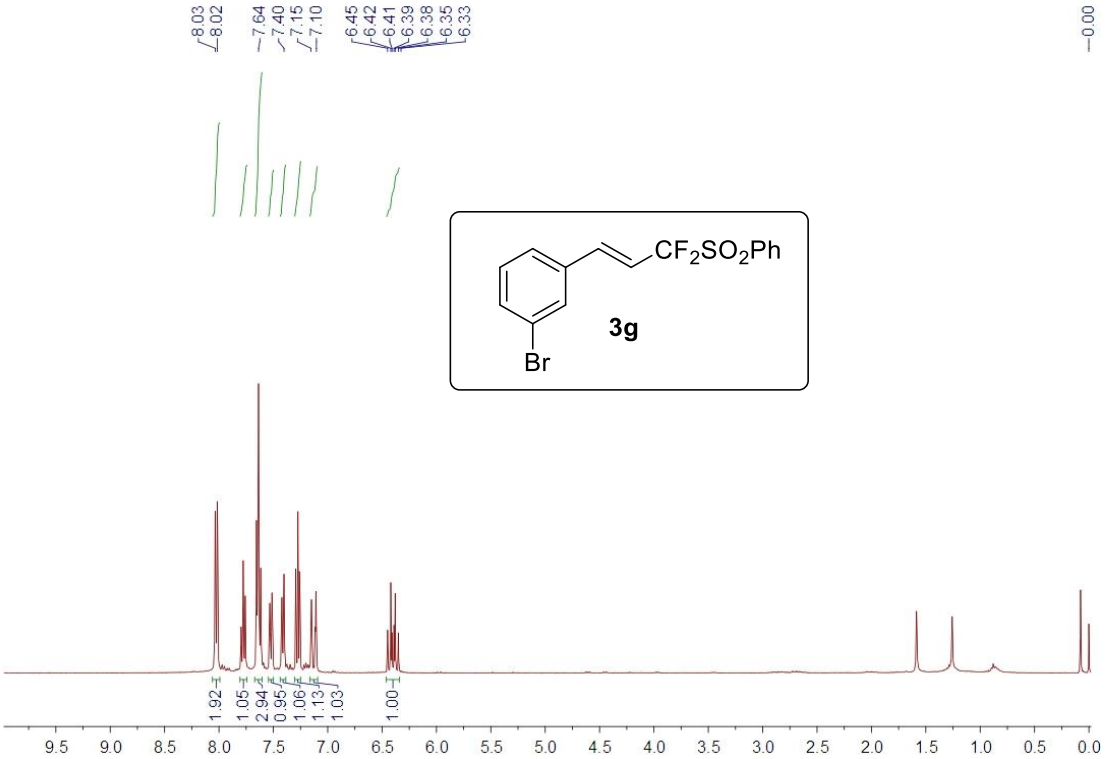
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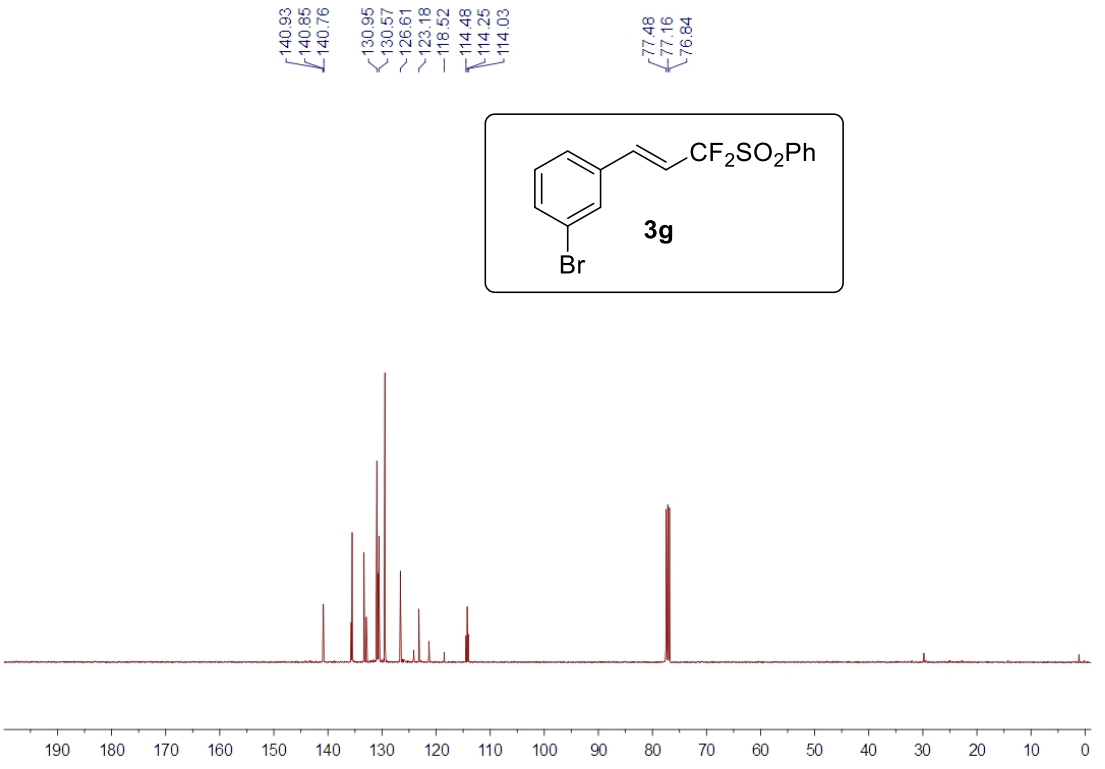
8.02
7.64
7.40
7.15
7.10
6.45
6.42
6.41
6.39
6.38
6.35
6.33
0.00
CF2SO2Ph
3g
Br
1.92
1.05
2.94
0.95
1.06
1.13
1.03
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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123.18
118.52
114.48
114.25
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77.16
76.84
CF2SO2Ph
3g
Br
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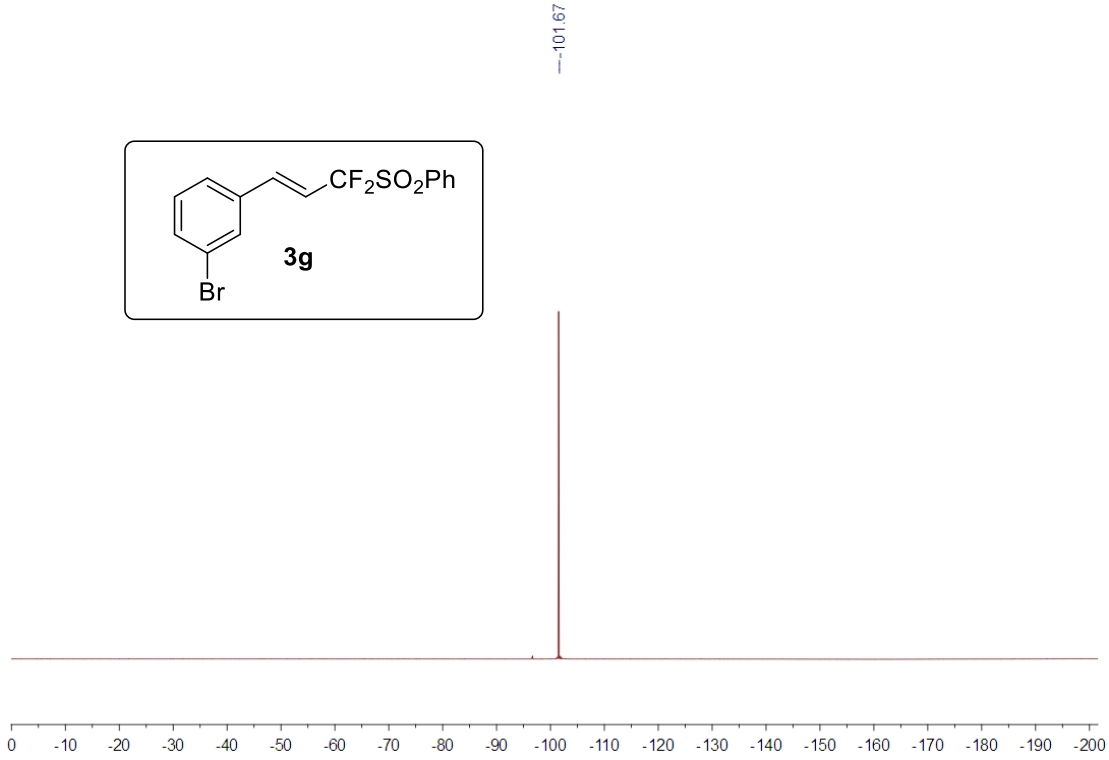
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-40
-50
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-90
-100
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-120
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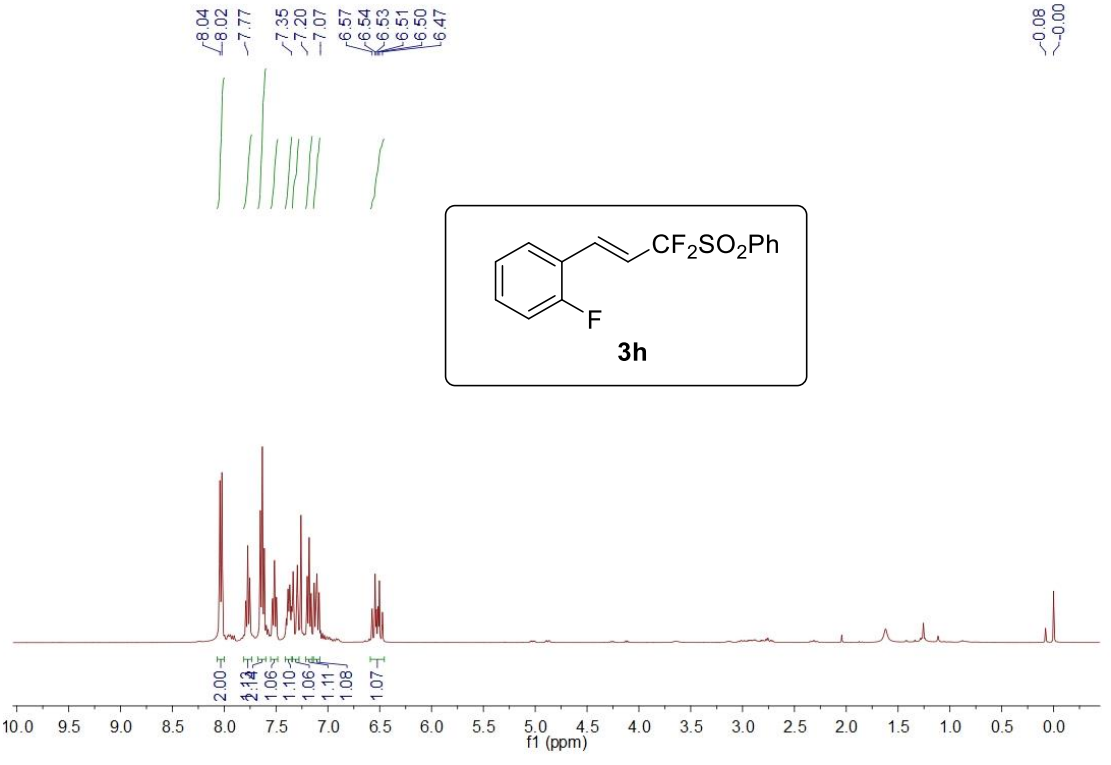
-140
-150
-160
-170
-180
-190
-200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8.02
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7.35
7.20
7.07
6.57
6.54
6.53
6.51
6.50
6.47
0.08
0.00
CF2SO2Ph
F
3h
2.00
2.13
1.06
1.10
1.06
1.11
1.08
1.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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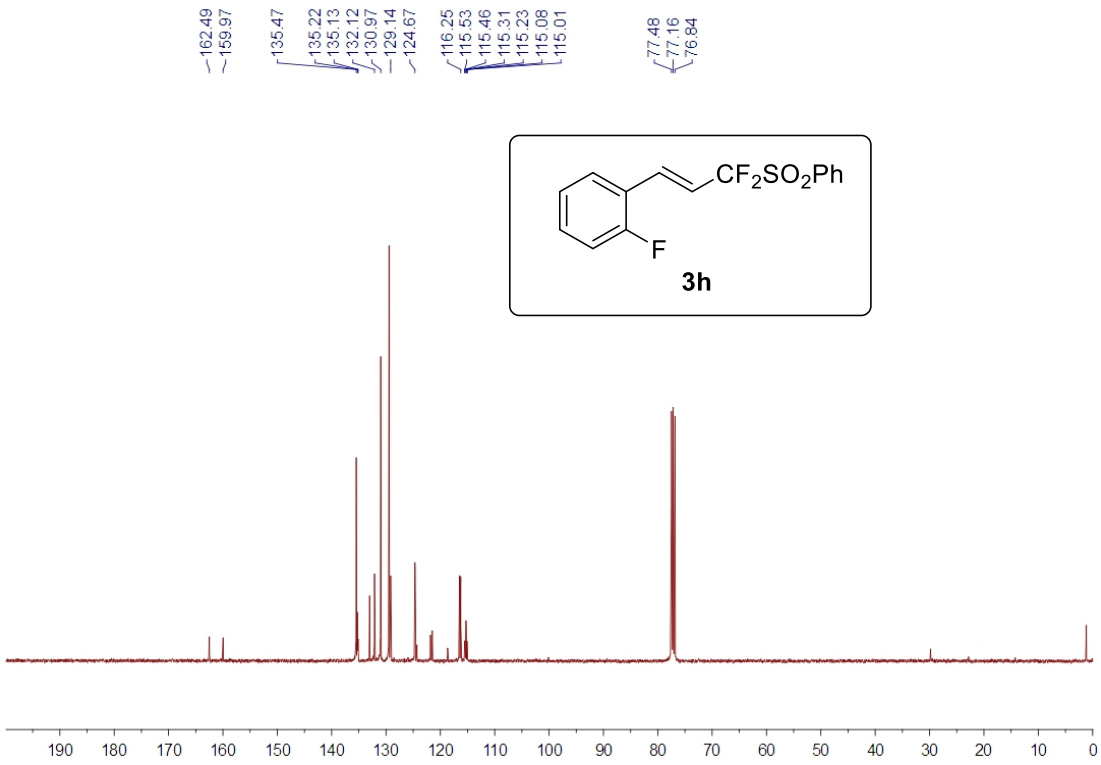
0.0
f1 (ppm)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132.12
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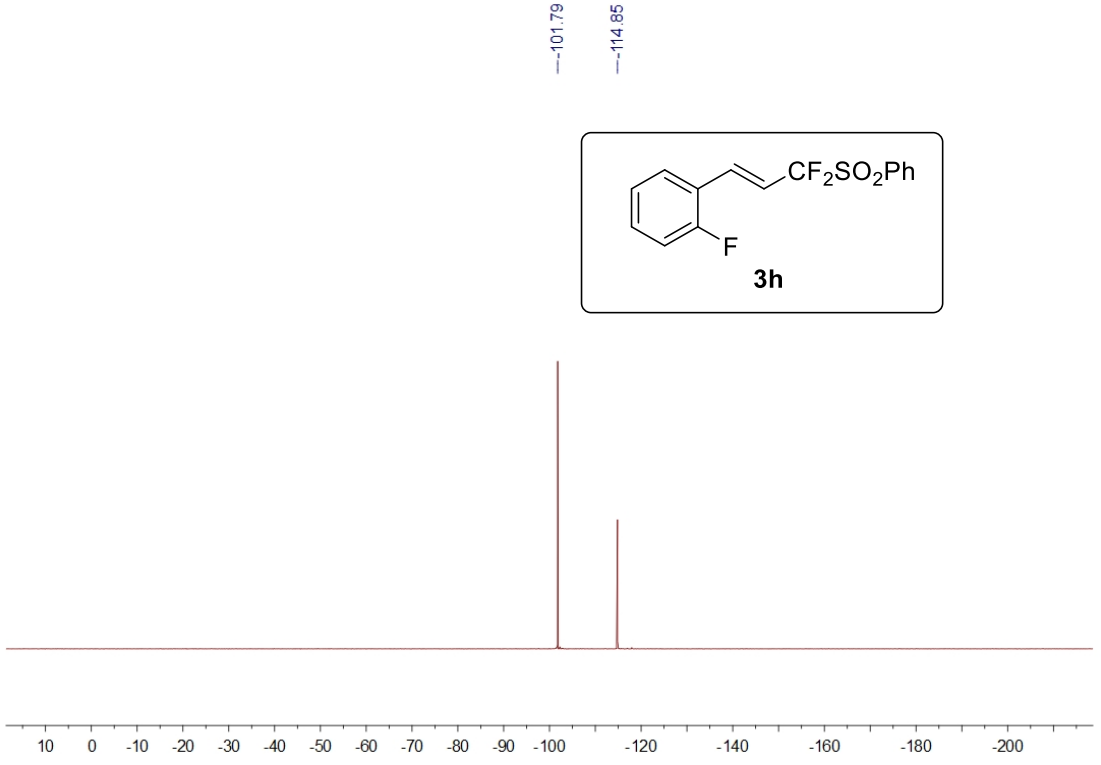
129.14
124.67
116.25
115.53
115.46
115.31
115.23
115.08
115.01
77.48
77.16
76.84
CF2SO2Ph
F
3h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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F
3h
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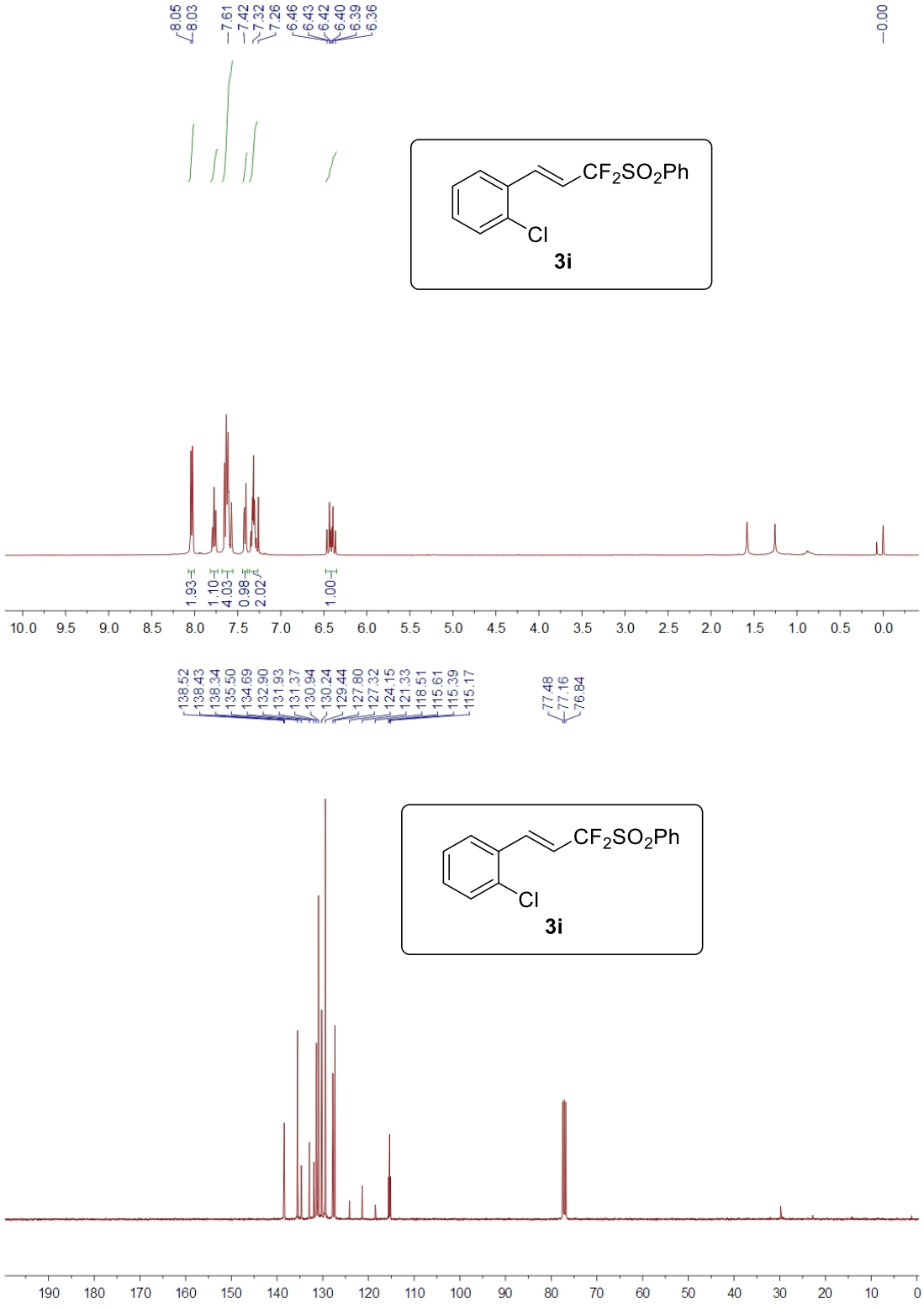
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7.61
7.42
7.32
7.26
6.46
6.43
6.42
6.40
6.39
6.36
0.00
CF2SO2Ph
Cl
3i
1.93
1.10
4.03
0.98
2.02
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
138.52
138.43
138.34
135.50
134.69
132.90
131.93
131.37
130.94
130.24
129.44
127.80
127.32
124.15
121.33
118.51
115.61
115.39
115.17
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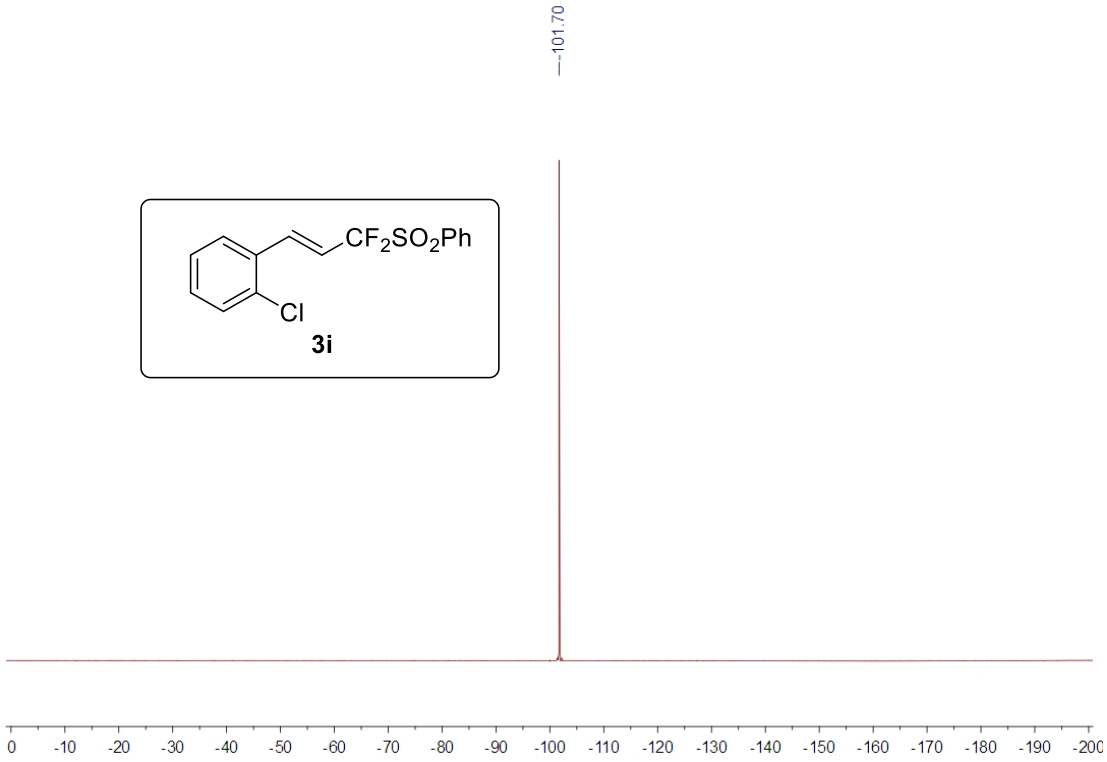
77.16
76.84
CF2SO2Ph
Cl
3i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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Cl
3i
0
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-20
-30
-40
-50
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-70
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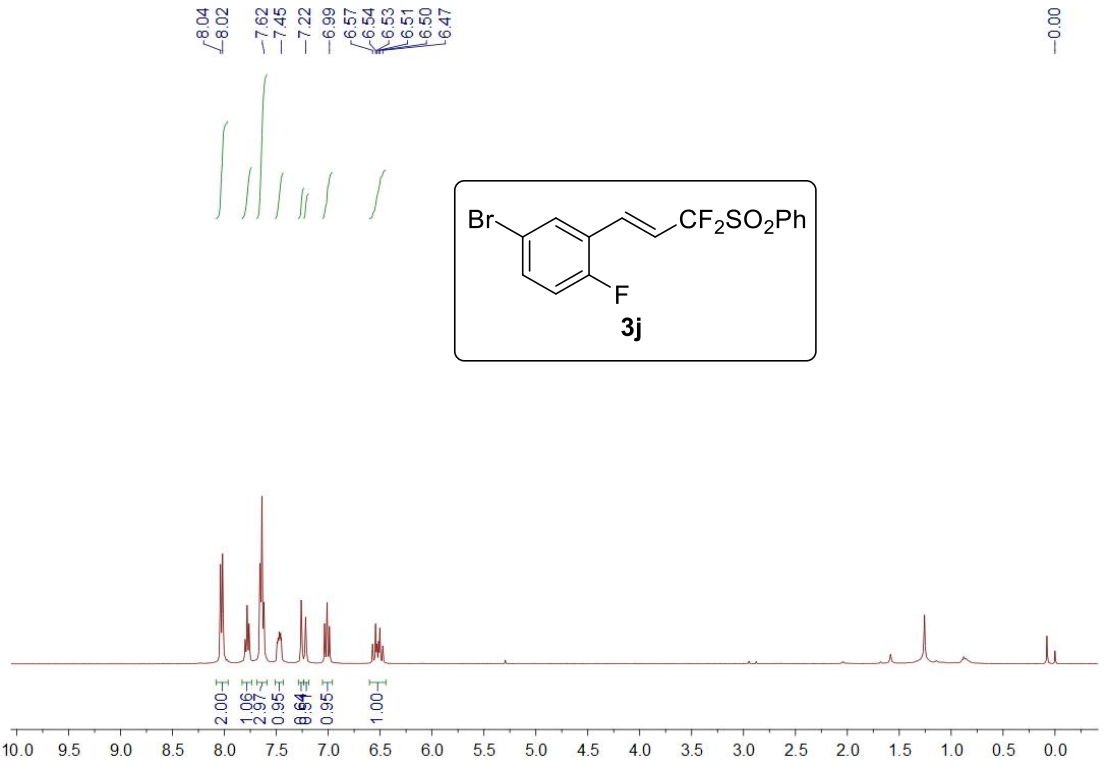
-120
-130
-140
-150
-160
-170
-180
-190
-200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8.02
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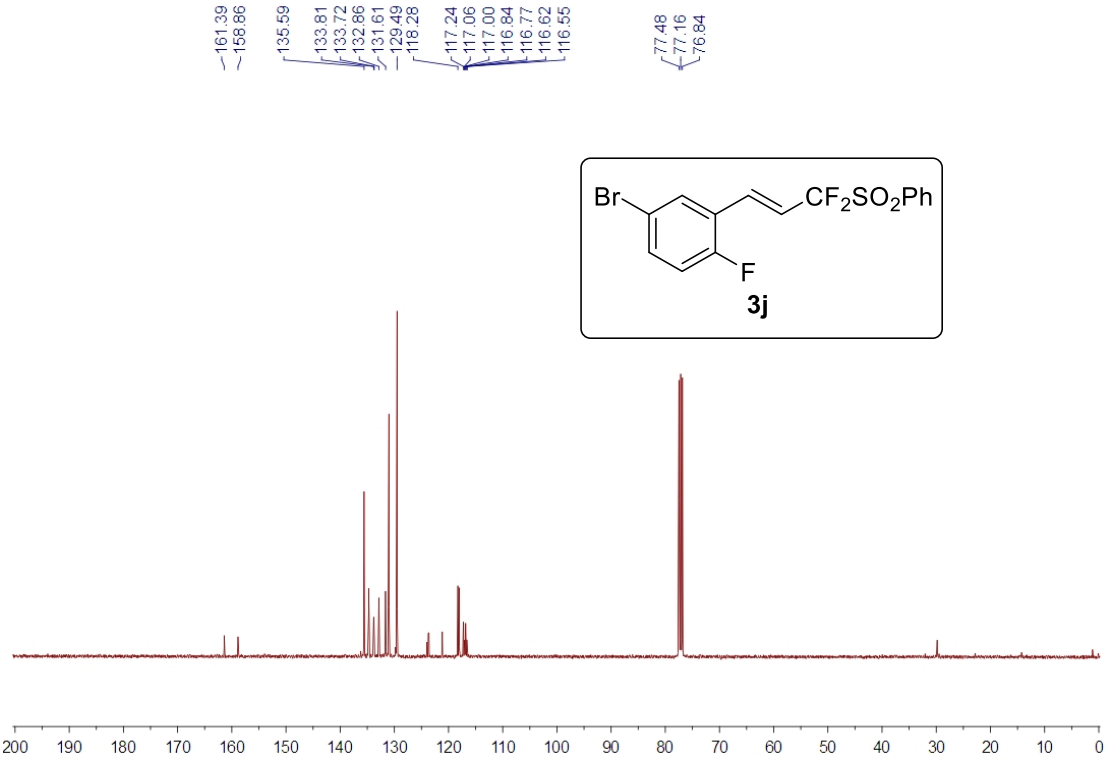
7.45
7.22
6.99
6.57
6.54
6.53
6.51
6.50
6.47
0.00
Br
CF2SO2Ph
F
3j
2.00
1.06
2.97
0.95
0.95
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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158.86
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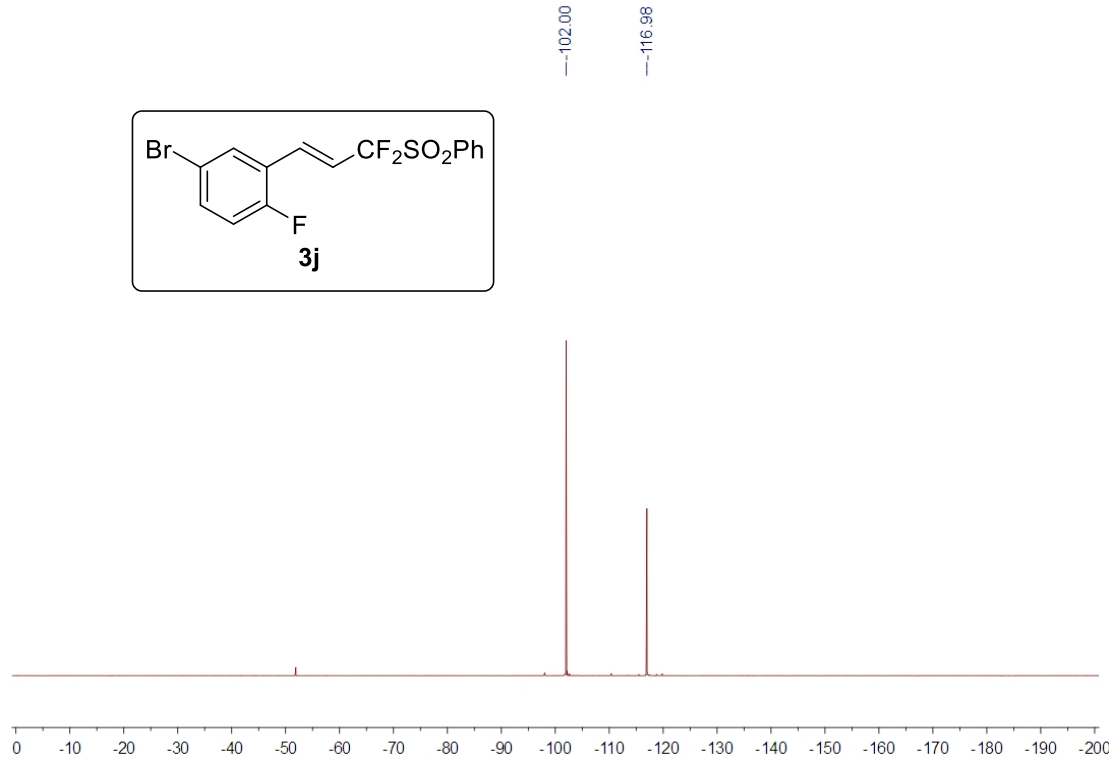
131.61
129.49
118.28
117.24
117.06
117.00
116.84
116.77
116.62
116.55
77.48
77.16
76.84
Br
CF2SO2Ph
F
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


102.00
116.98
Br
CF2SO2Ph
F
3j
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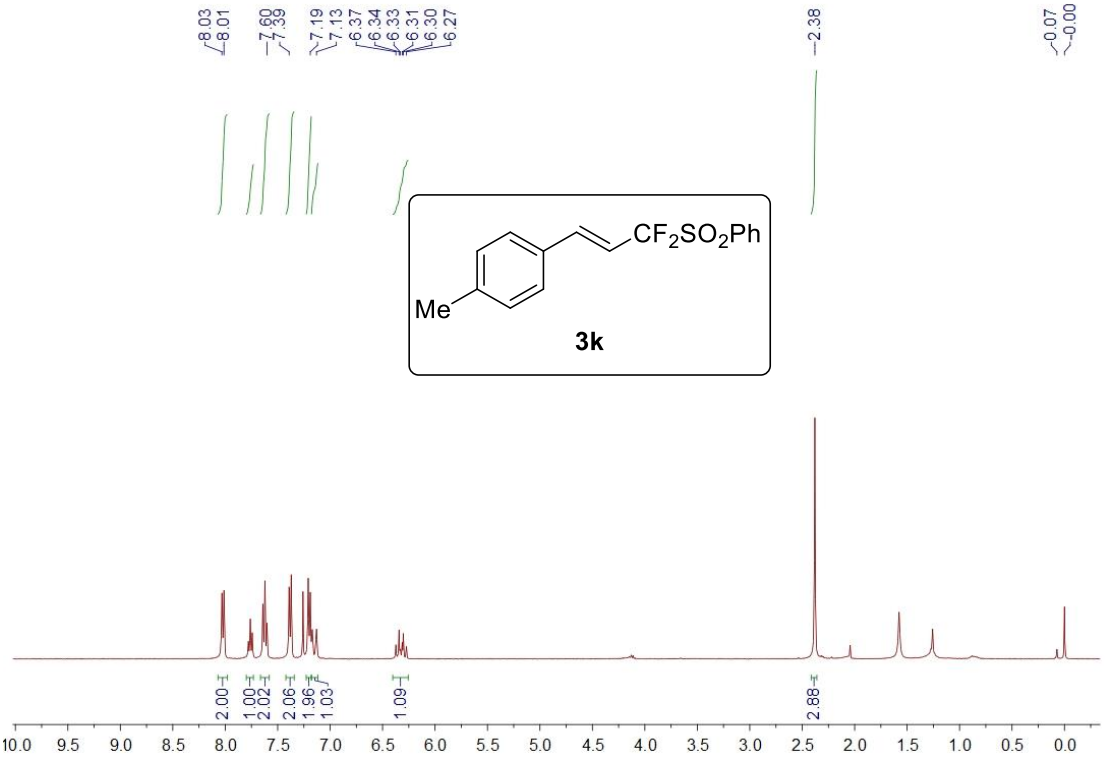
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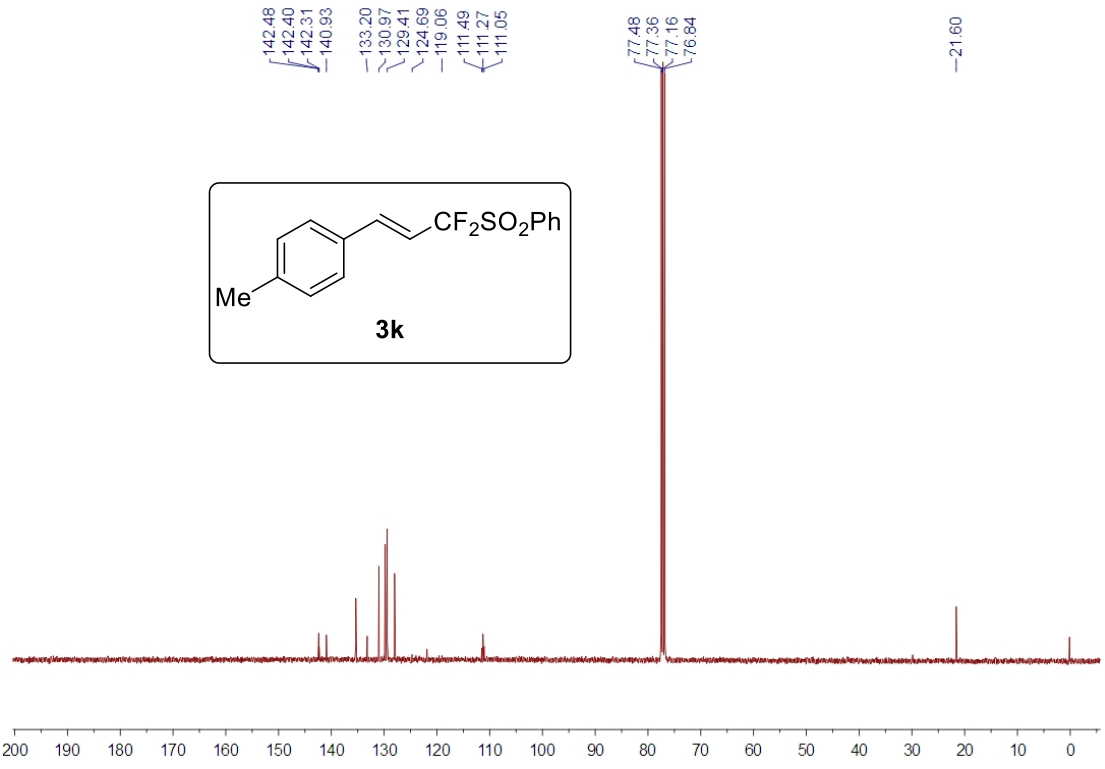
8.01
7.60
7.59
7.19
7.13
6.37
6.34
6.33
6.31
6.30
6.27
2.38
0.07
0.00
CF2SO2Ph
Me
3k
2.00
1.00
2.02
2.06
1.96
1.03
1.09
2.88
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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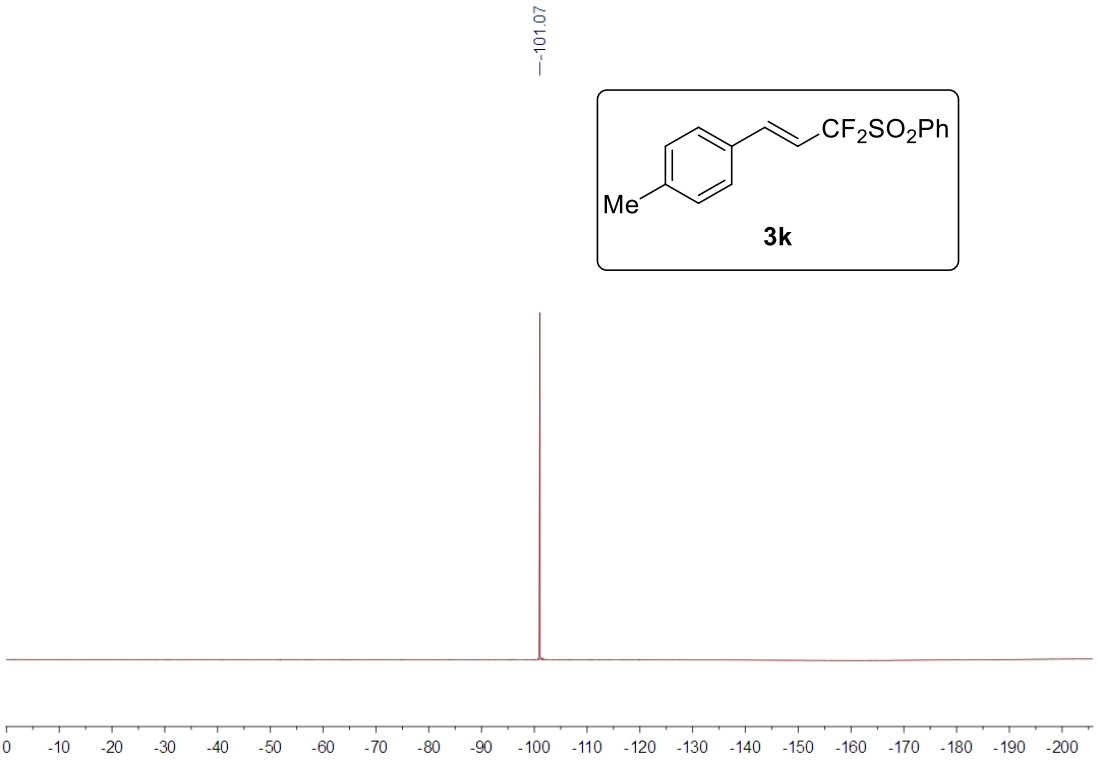
130.97
129.41
124.69
119.06
111.49
111.27
111.05
77.48
77.36
77.16
76.84
21.60
CF2SO2Ph
Me
3k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


-101.07
CF2SO2Ph
Me
3k
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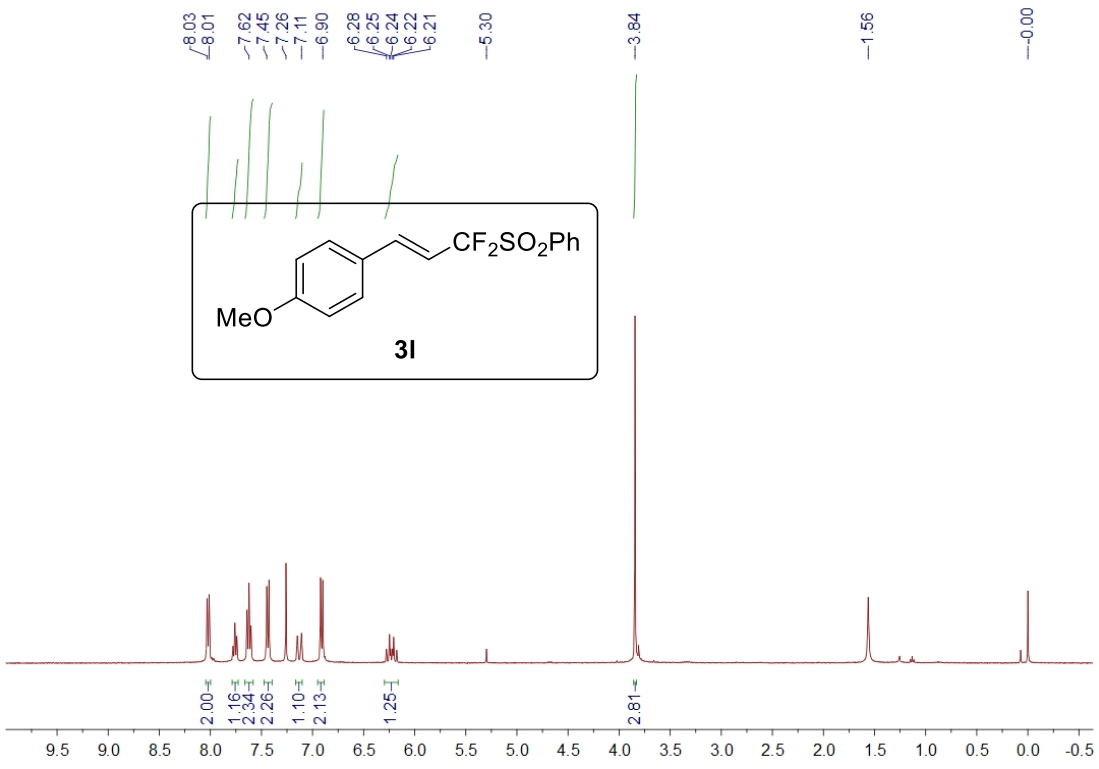
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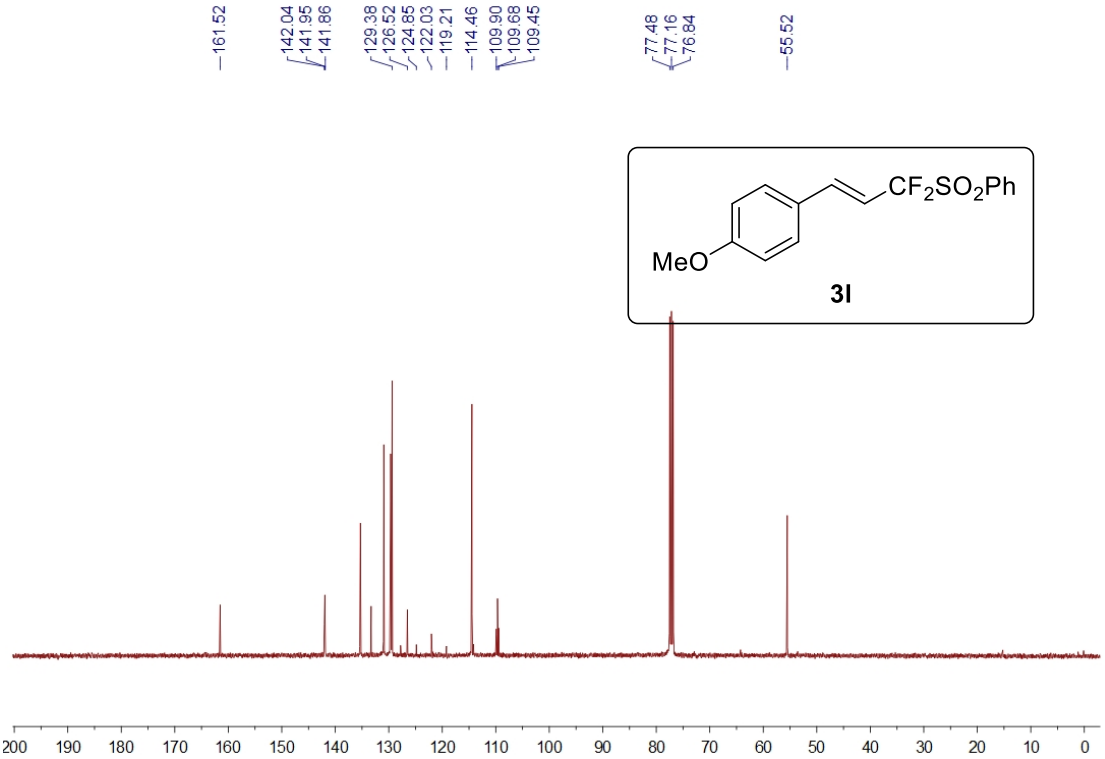
8.01
7.62
7.45
7.26
7.11
6.90
6.28
6.25
6.24
6.22
6.21
5.30
3.84
1.56
0.00
CF2SO2Ph
MeO
3l
2.00
1.16
2.34
2.26
1.10
2.13
1.25
2.81
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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141.86
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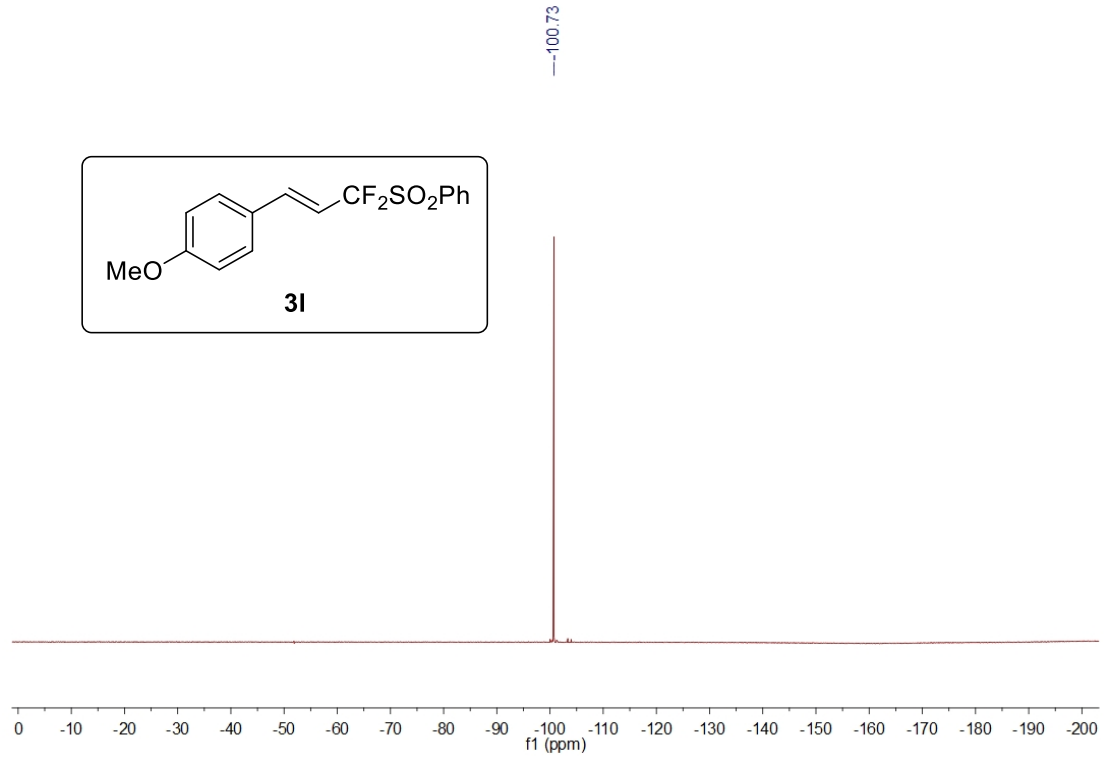
126.52
124.85
122.03
119.21
114.46
109.90
109.68
109.45
77.48
77.16
76.84
55.52
CF2SO2Ph
MeO
3l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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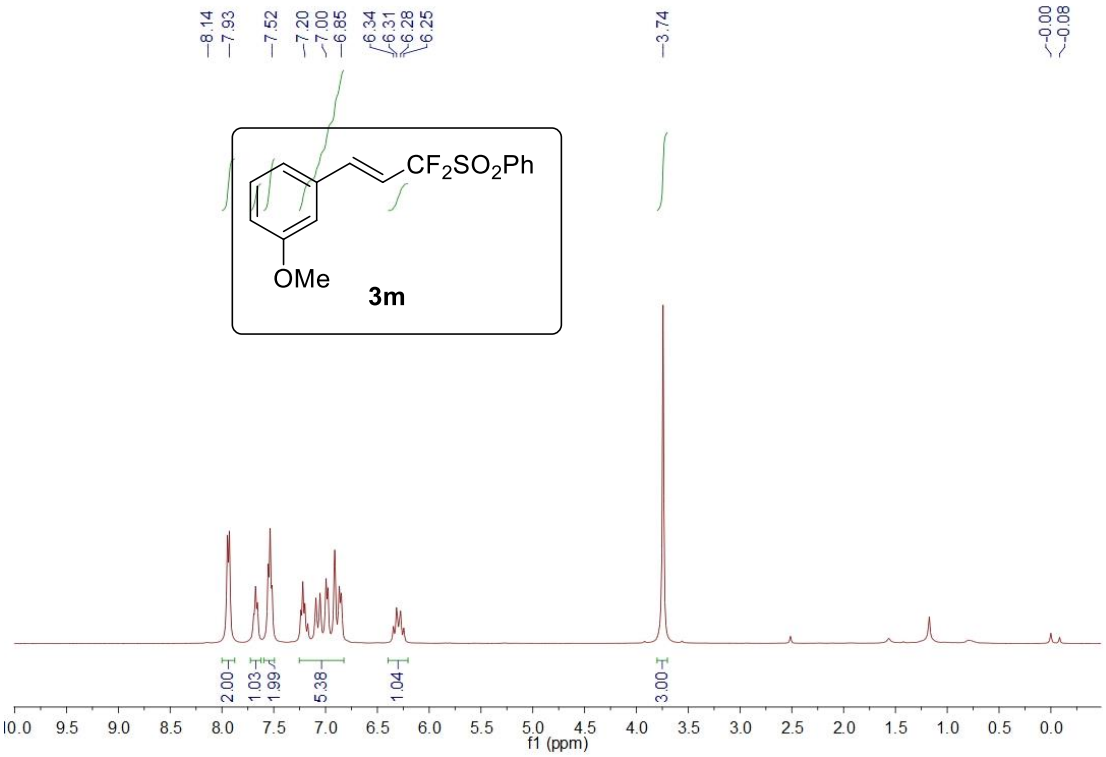
MeO
3l
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)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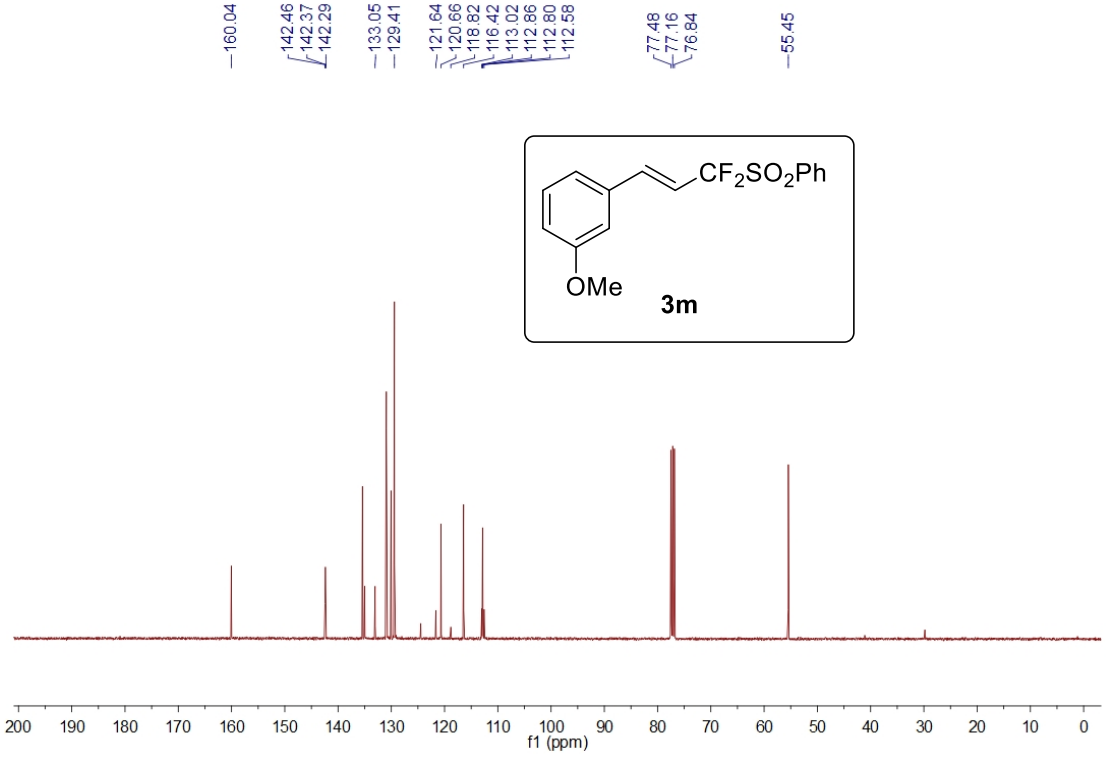
7.93
7.52
7.20
7.00
6.85
6.34
6.31
6.28
6.25
3.74
0.00
-0.08
CF2SO2Ph
OMe
3m
2.00
1.03
1.99
5.38
1.04
3.00
f1 (ppm)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142.46
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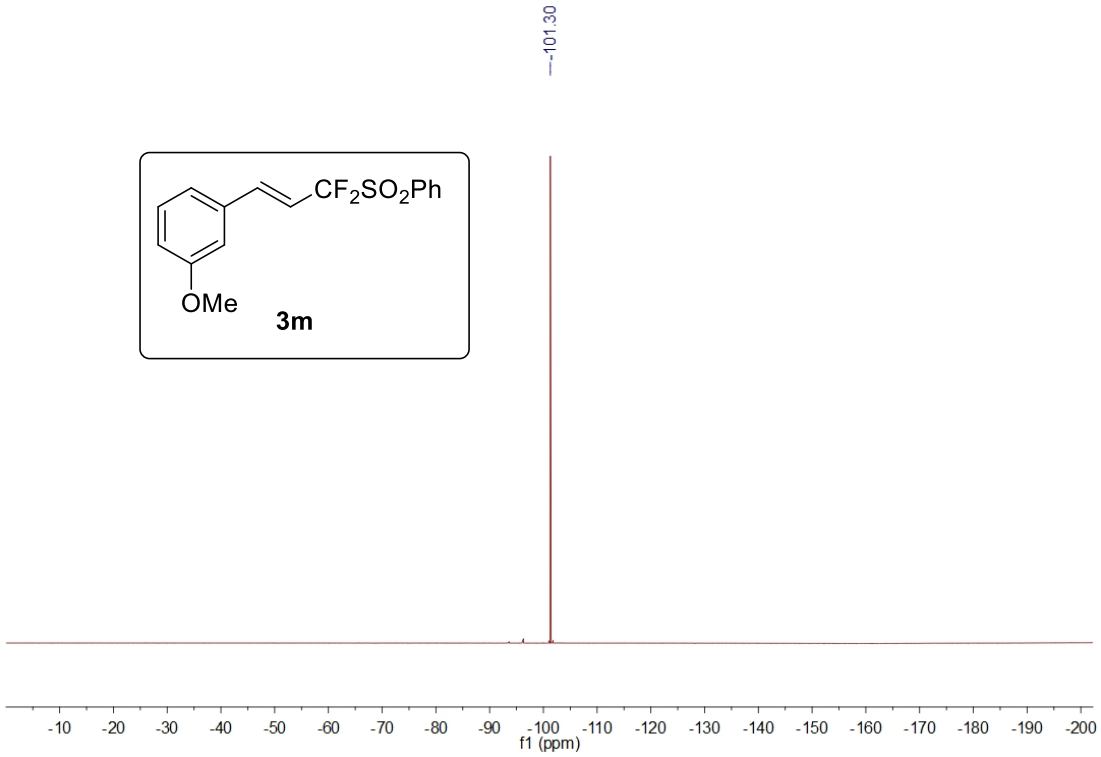
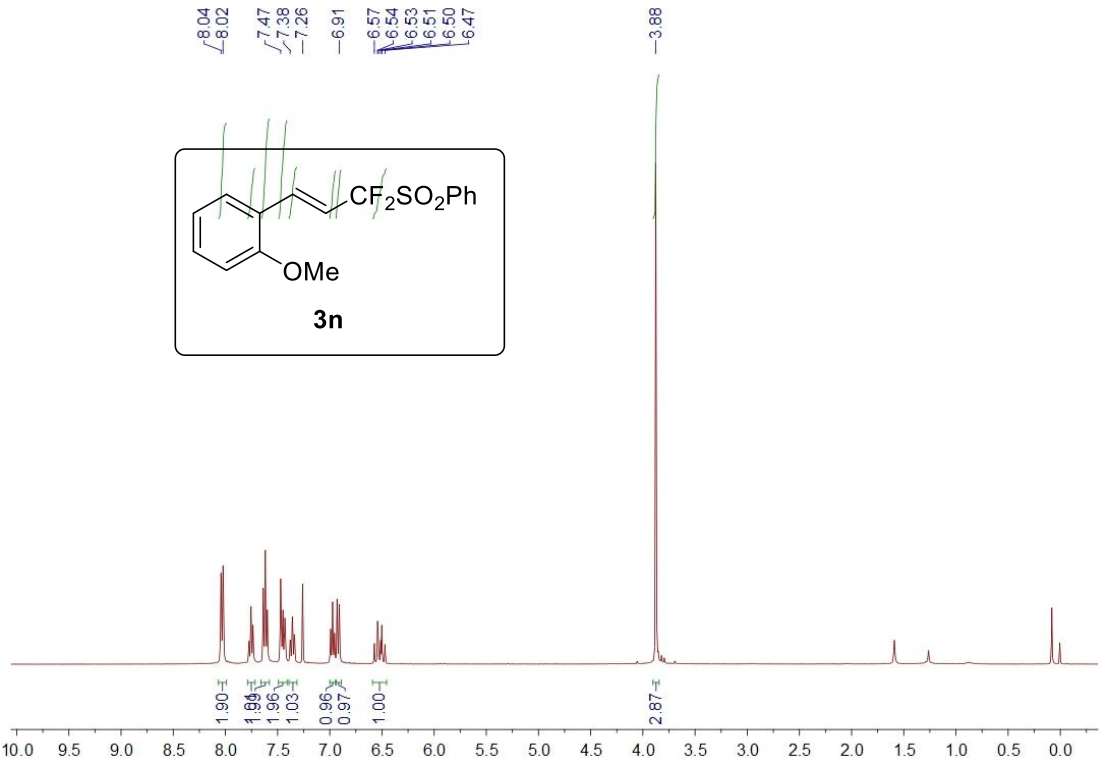
142.29
133.05
129.41
121.64
120.66
118.82
116.42
113.02
112.86
112.80
112.58
77.48
77.16
76.84
55.45
CF2SO2Ph
OMe
3m
f1 (ppm)


-101.30
CF2SO2Ph
OMe
3m
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)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8.02
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7.38
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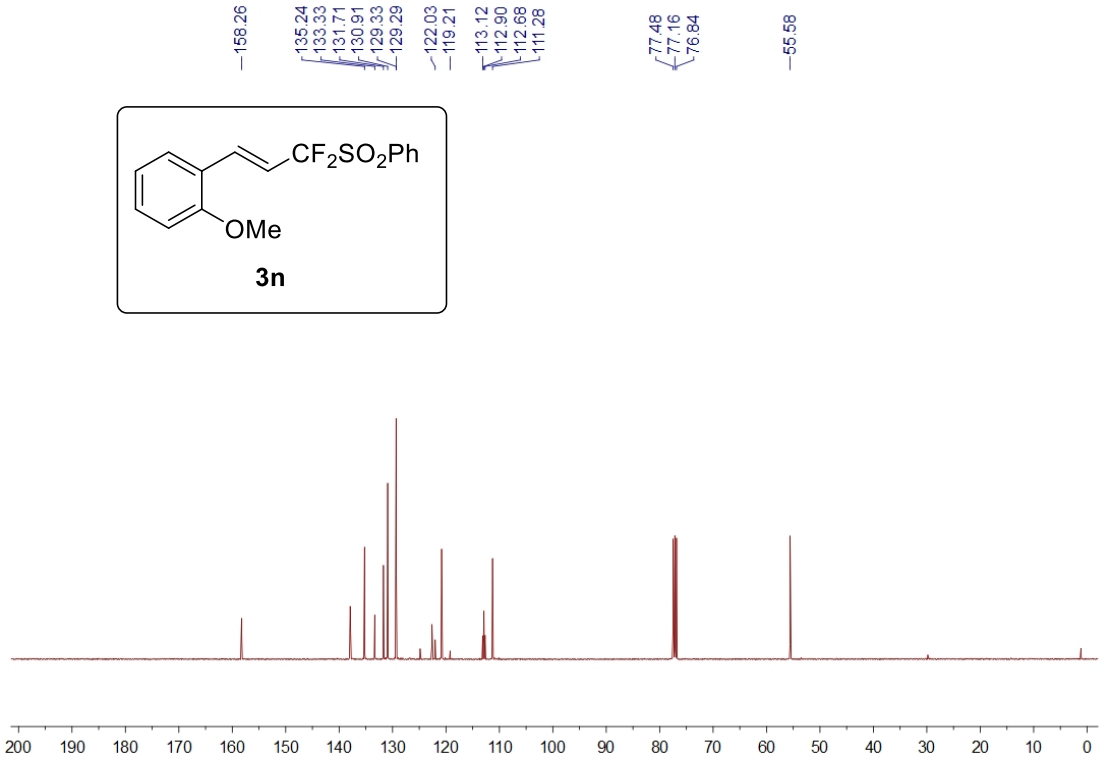
6.91
6.57
6.54
6.53
6.51
6.50
6.47
3.88
CF2SO2Ph
OMe
3n
1.90
1.84
1.96
1.03
0.96
0.97
1.00
2.87
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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135.24
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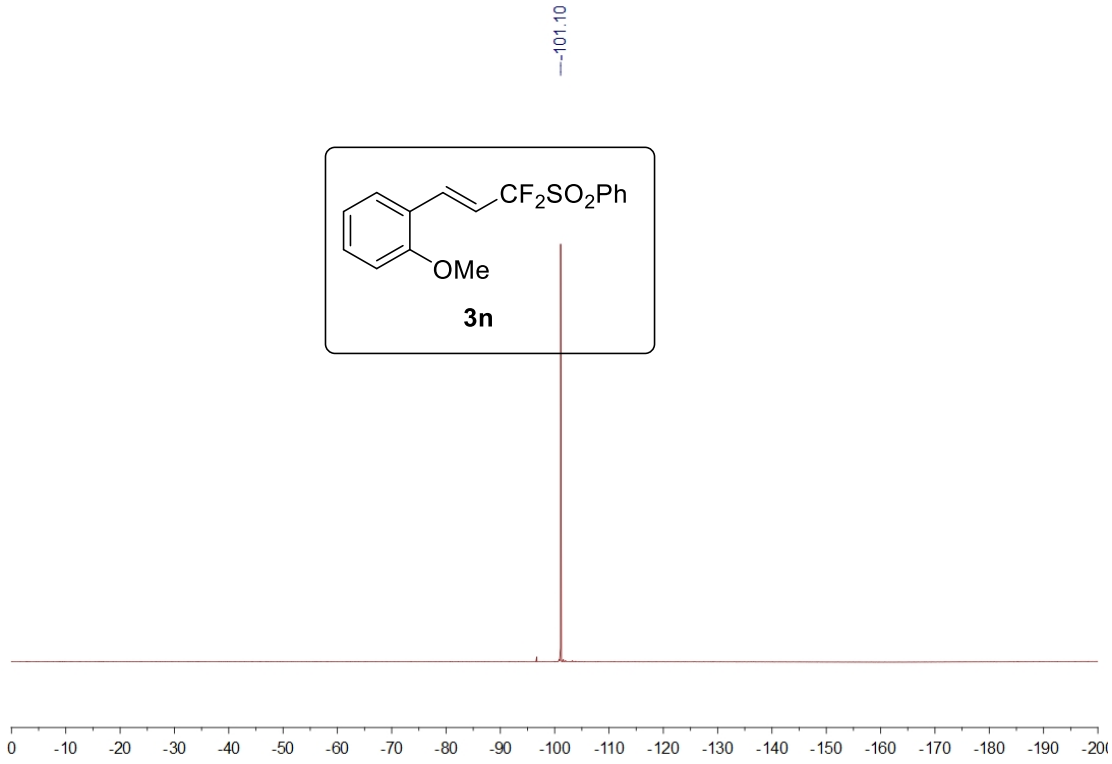
131.71
130.91
129.33
129.29
122.03
119.21
113.12
112.90
112.68
111.28
77.48
77.16
76.84
55.58
CF2SO2Ph
OMe
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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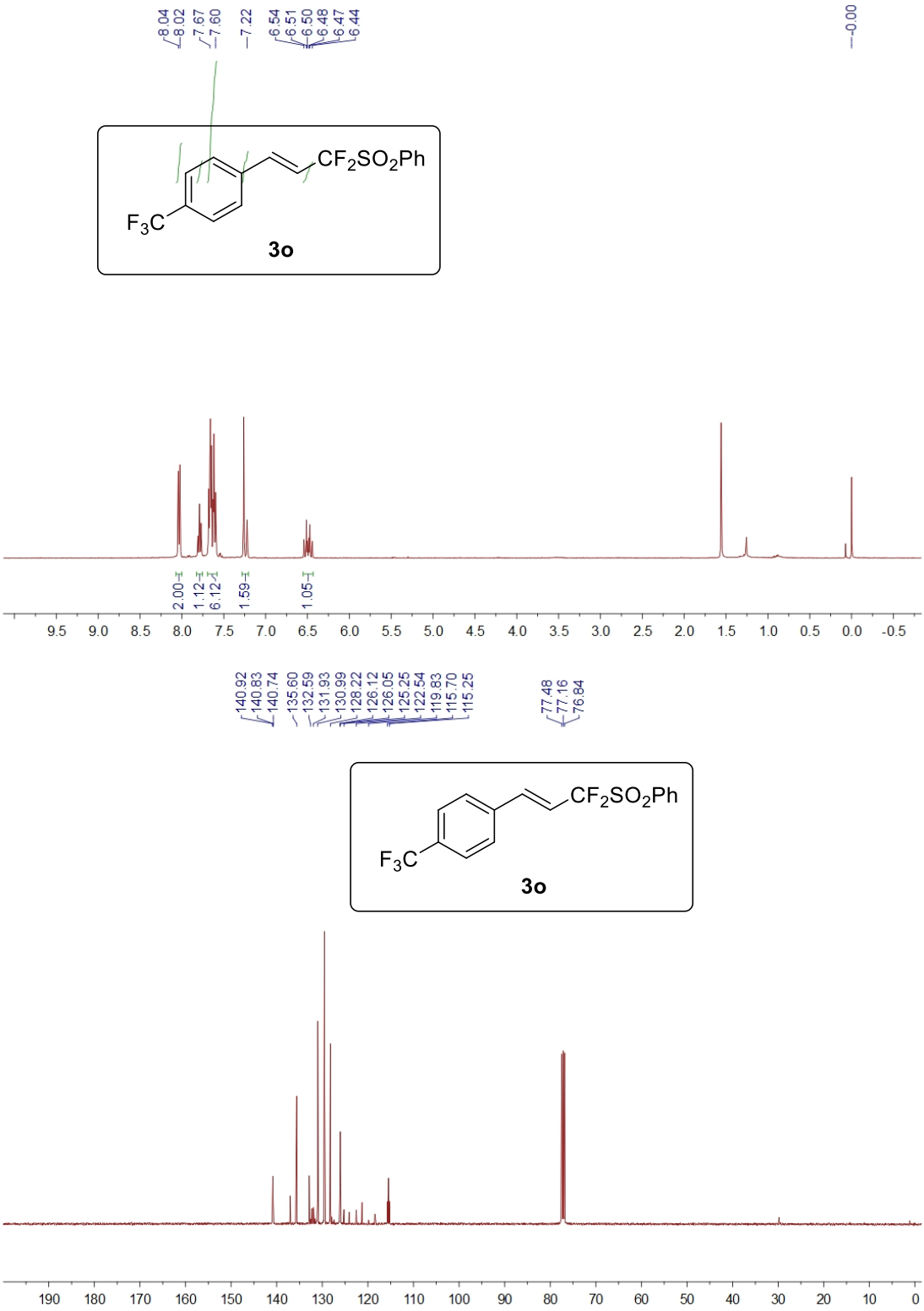
CF2SO2Ph
OMe
3n
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190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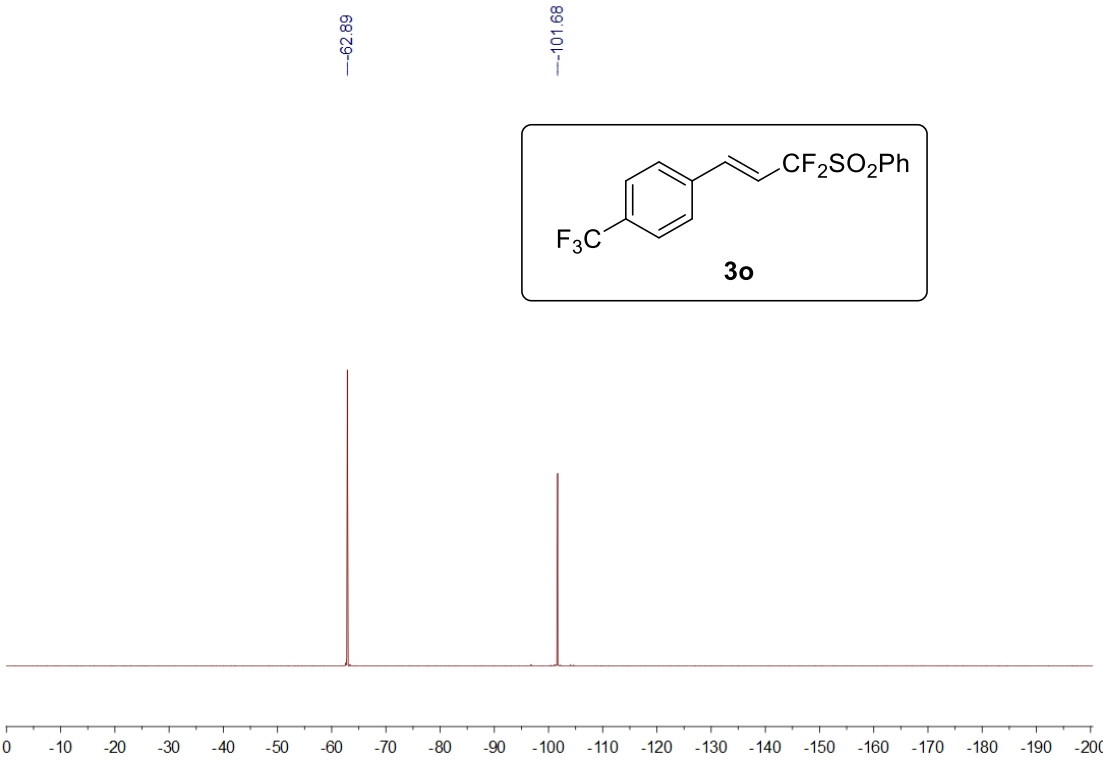
7.60
7.22
6.54
6.51
6.50
6.48
6.47
6.44
0.00
CF2SO2Ph
F3C
3o
2.00
1.12
6.12
1.59
1.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
140.92
140.83
140.74
135.60
132.59
131.93
130.99
128.22
126.12
126.05
125.25
122.54
119.83
115.70
115.25
77.48
77.16
76.84
CF2SO2Ph
F3C
3o
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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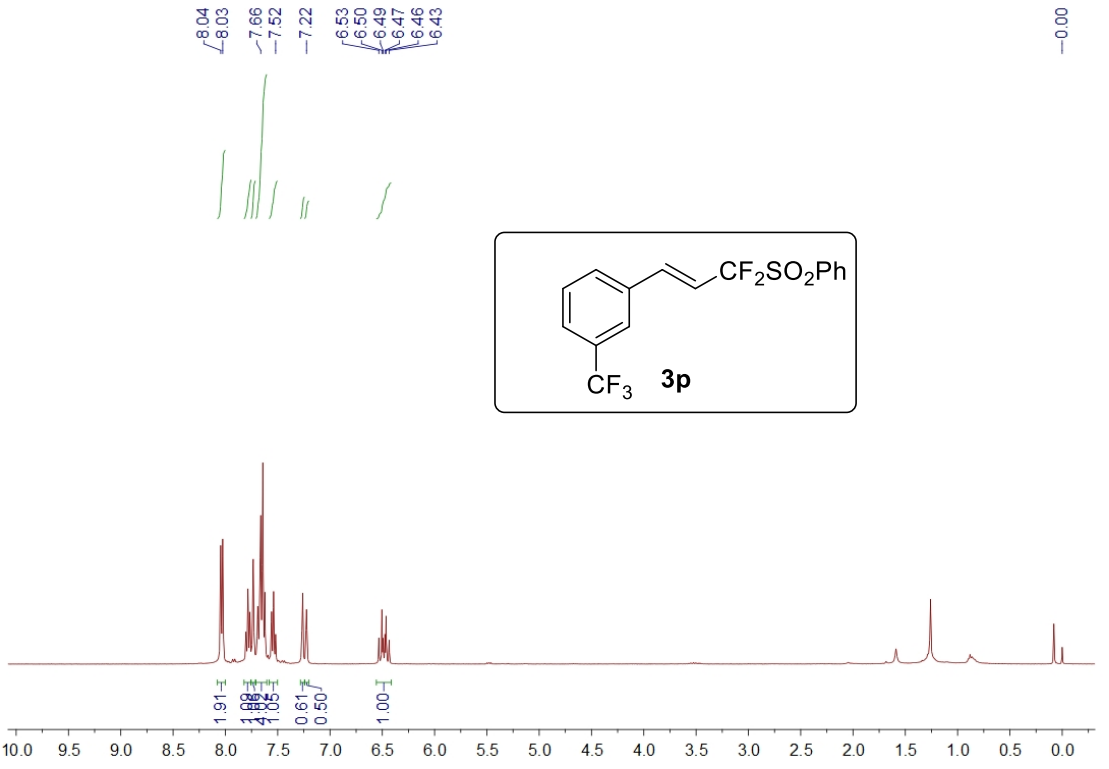
-101.68
CF_2SO_2Ph
F_3C
3o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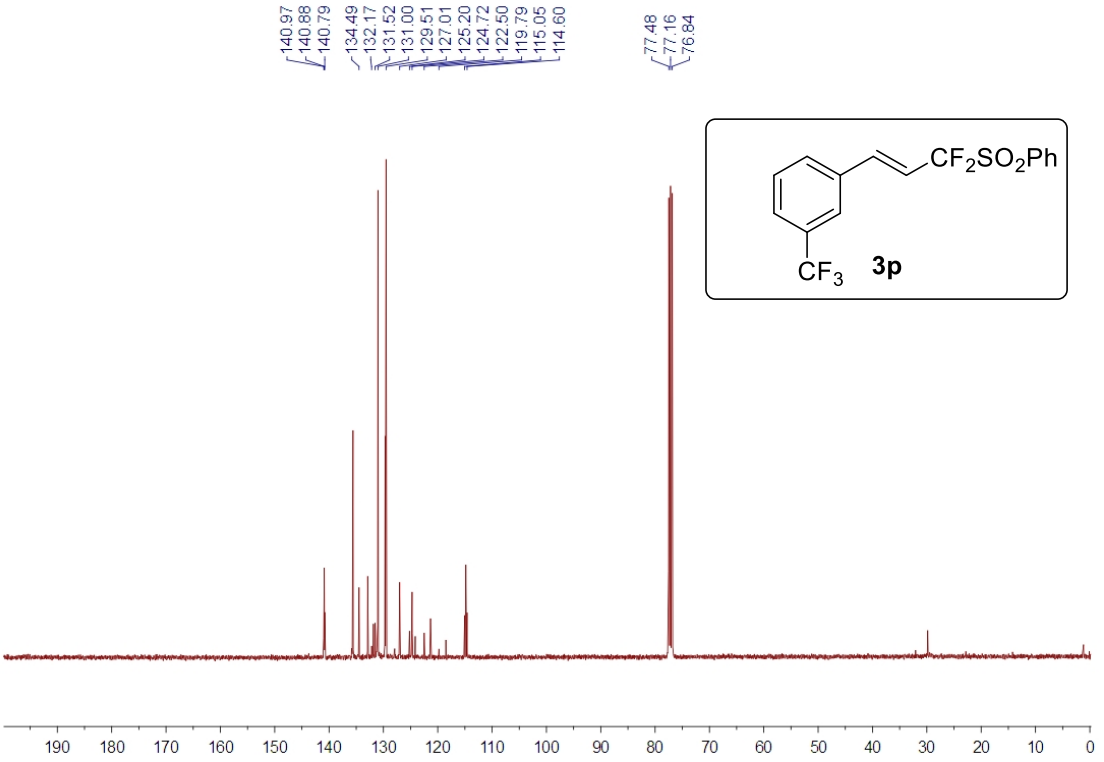
8.03
7.66
7.52
7.22
6.53
6.50
6.49
6.47
6.46
6.43
0.00
CF_2SO_2Ph
CF_3
3p
1.91
0.61
0.50
1.00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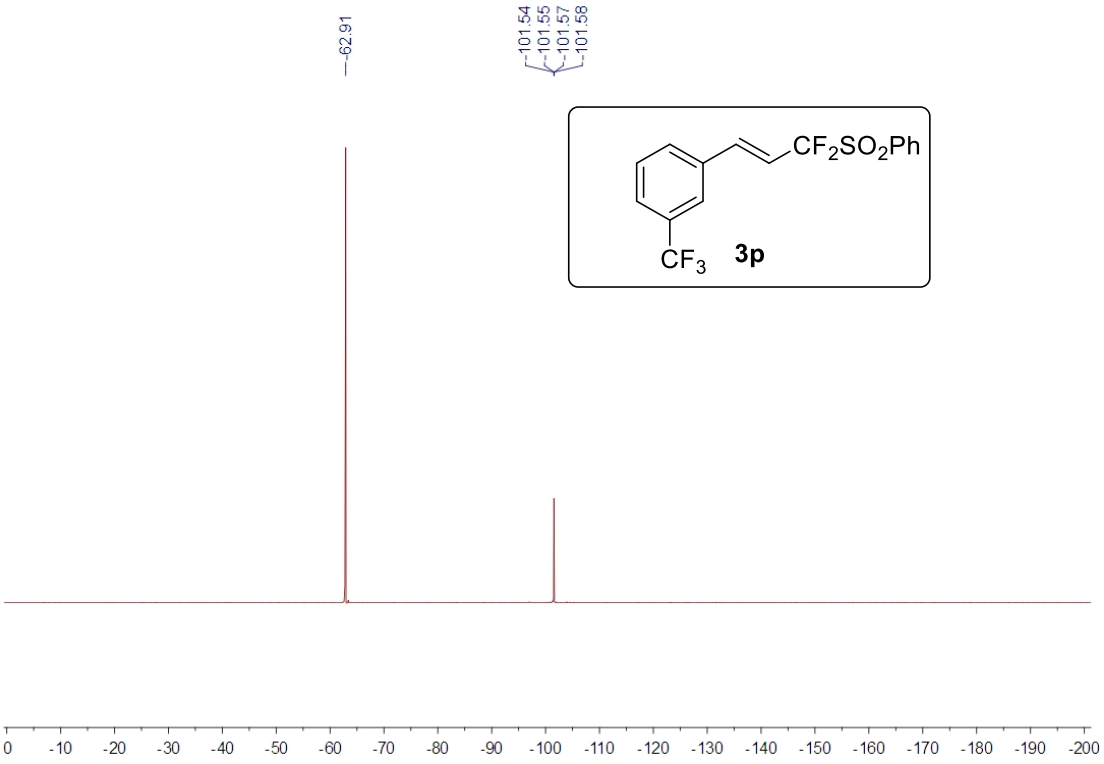
134.49
132.17
131.52
131.00
129.51
127.01
125.20
124.72
122.50
119.79
115.05
114.60
77.48
77.16
76.84
CF2SO2Ph
CF3
3p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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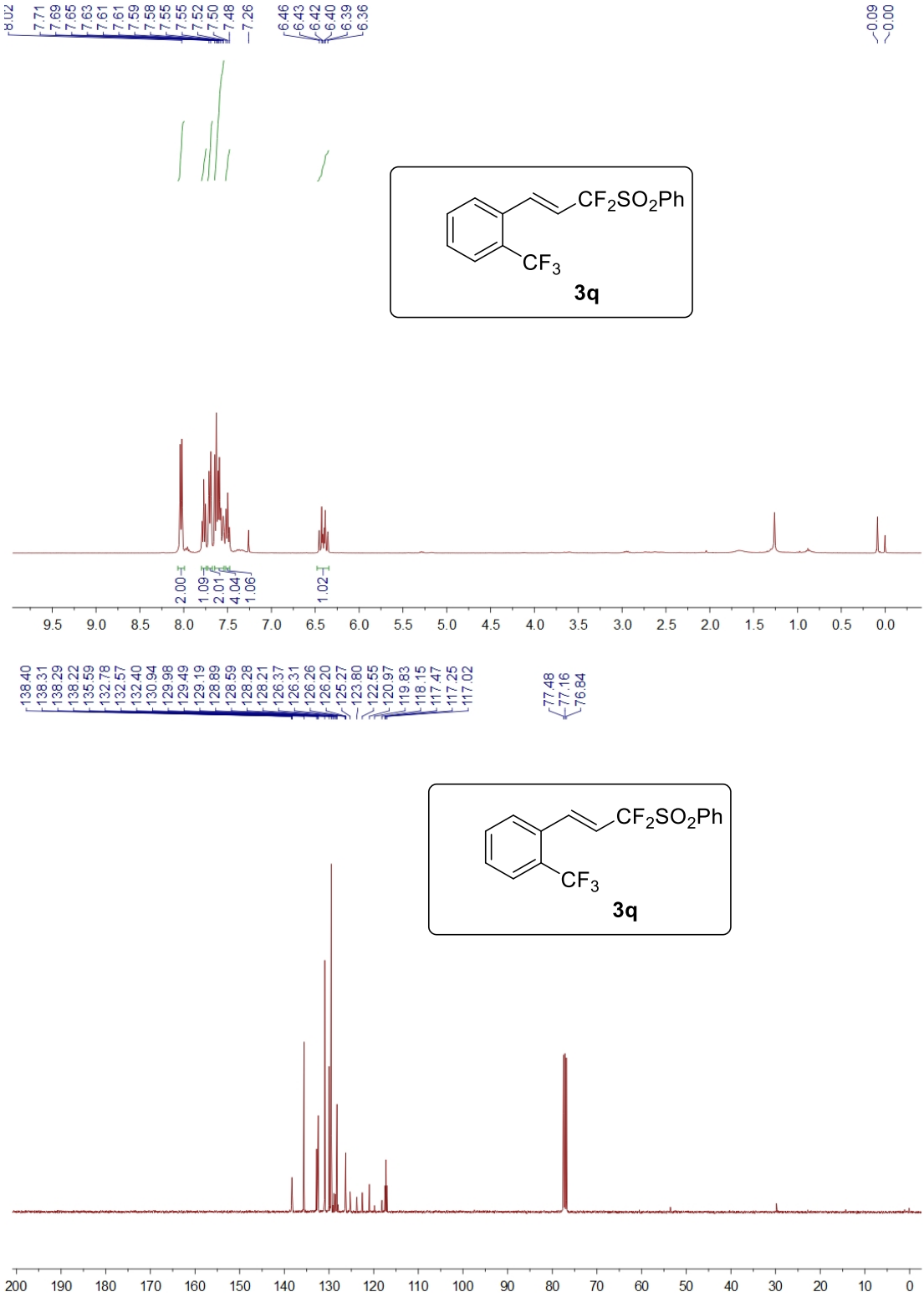
-101.54
-101.55
-101.57
-101.58
CF2SO2Ph
CF3
3p
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200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7.65
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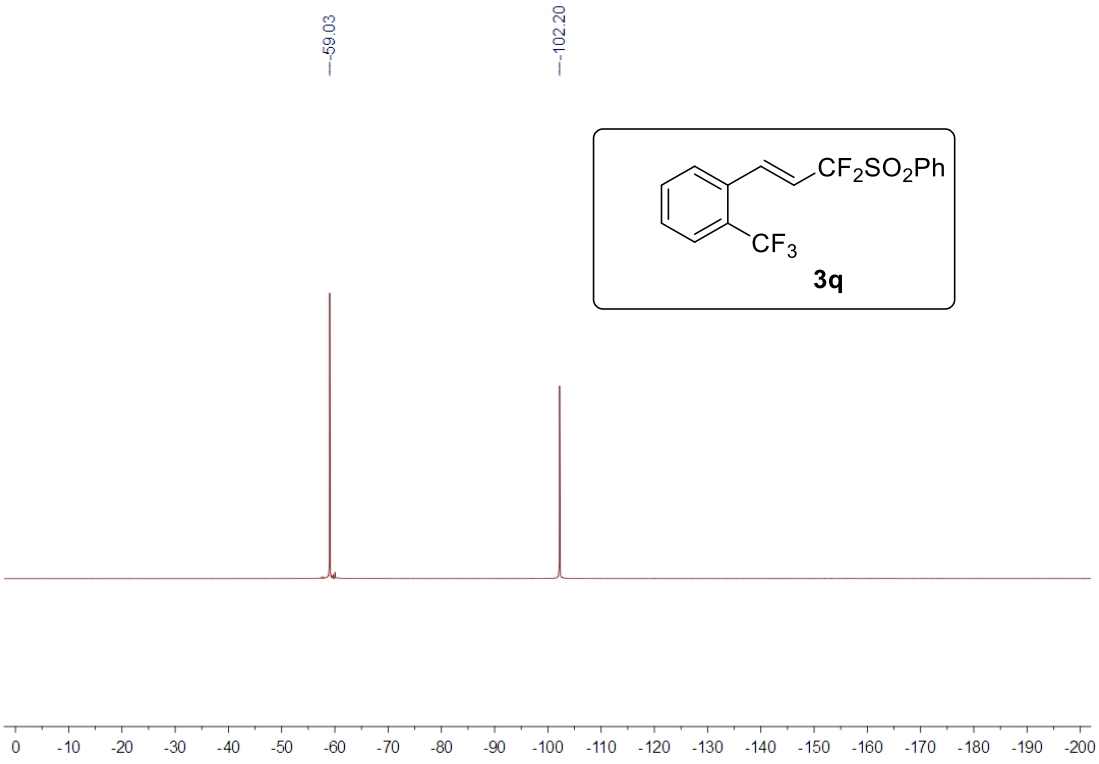
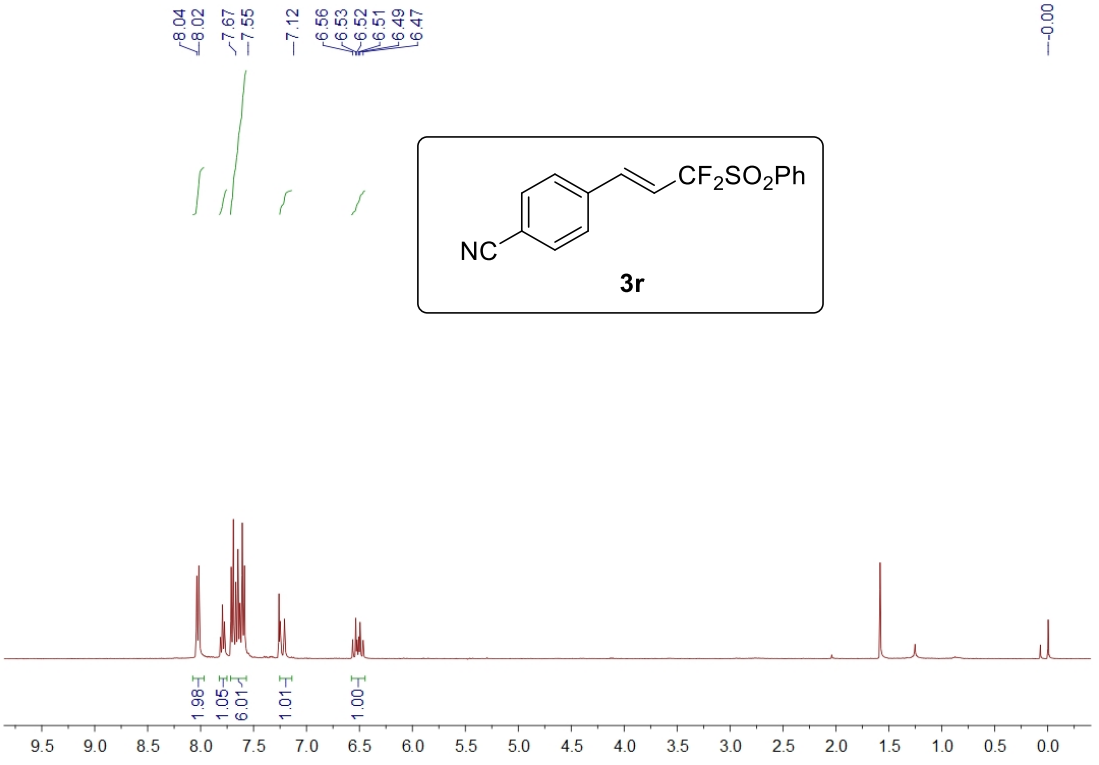
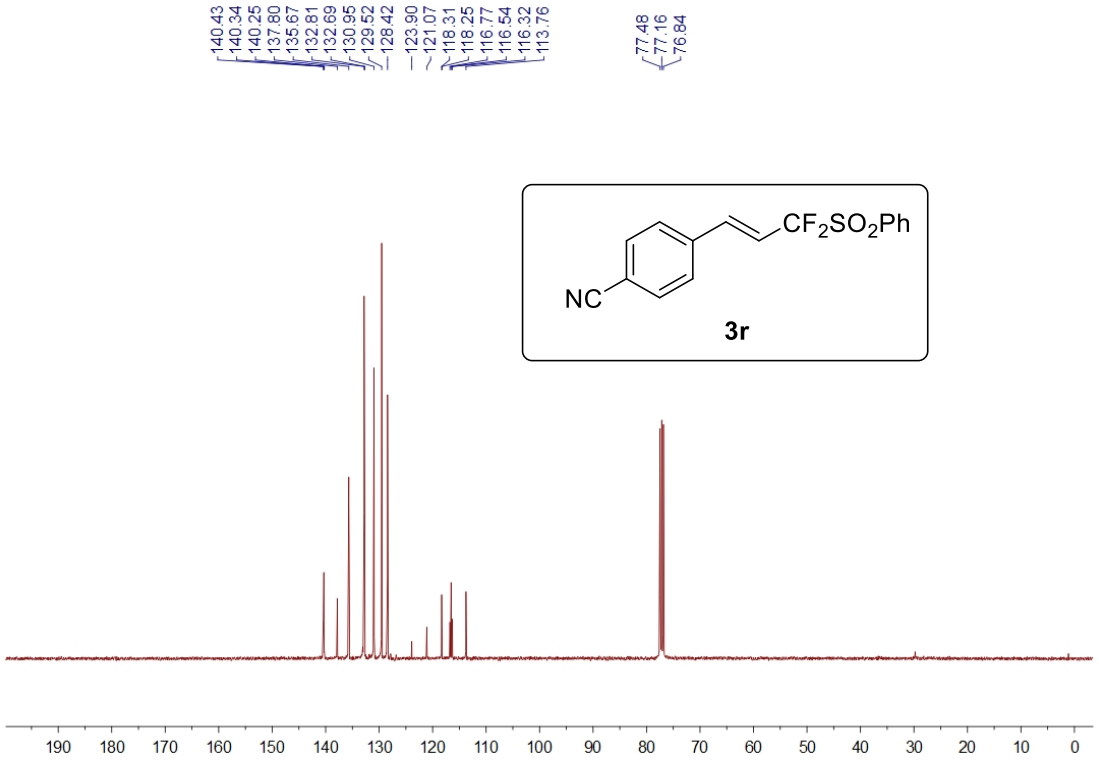
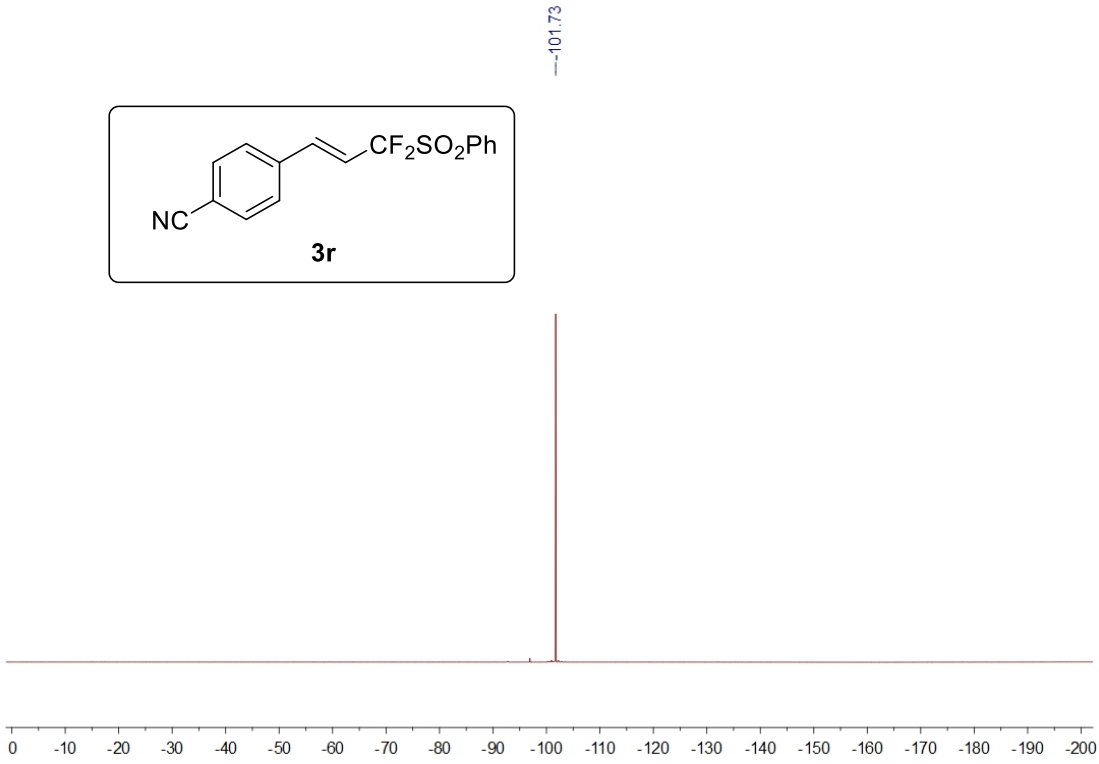
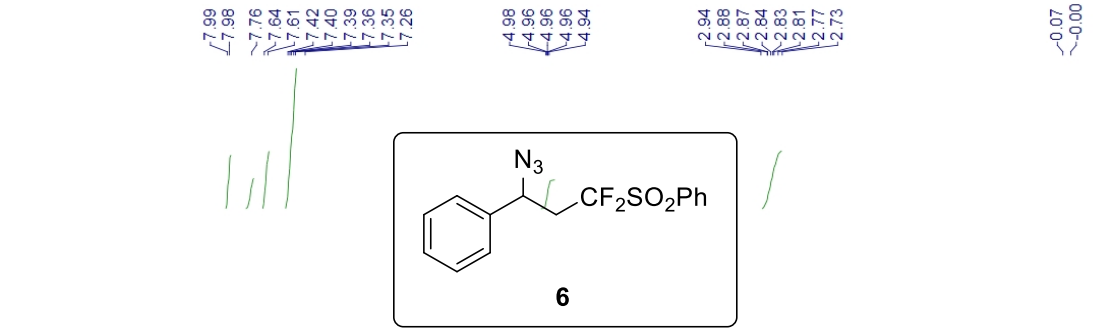
7.61
7.61
7.59
7.58
7.55
7.55
7.52
7.50
7.48
7.26
6.46
6.43
6.42
6.40
6.39
6.36
0.09
0.00
CF2SO2Ph
CF3
3q
2.00
1.09
2.01
4.04
1.06
1.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
138.40
138.31
138.29
138.22
135.59
132.78
132.57
132.40
130.94
129.98
129.49
129.19
128.89
128.59
128.28
128.21
126.37
126.31
126.26
126.20
125.27
123.80
122.55
120.97
119.83
118.15
117.47
117.25
117.02
77.48
77.16
76.84
CF2SO2Ph
CF3
3q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

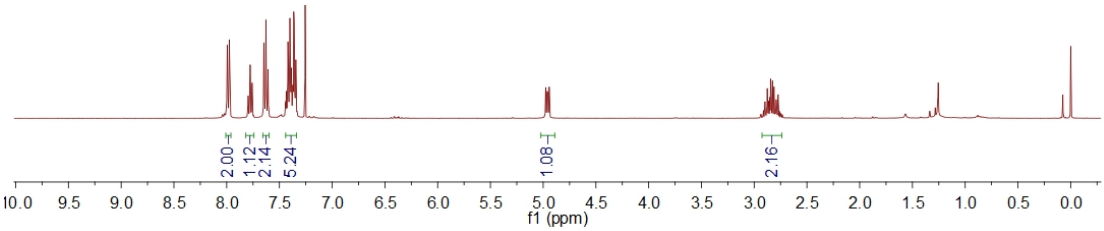

-59.03
-102.20
CF2SO2Ph
CF3
3q

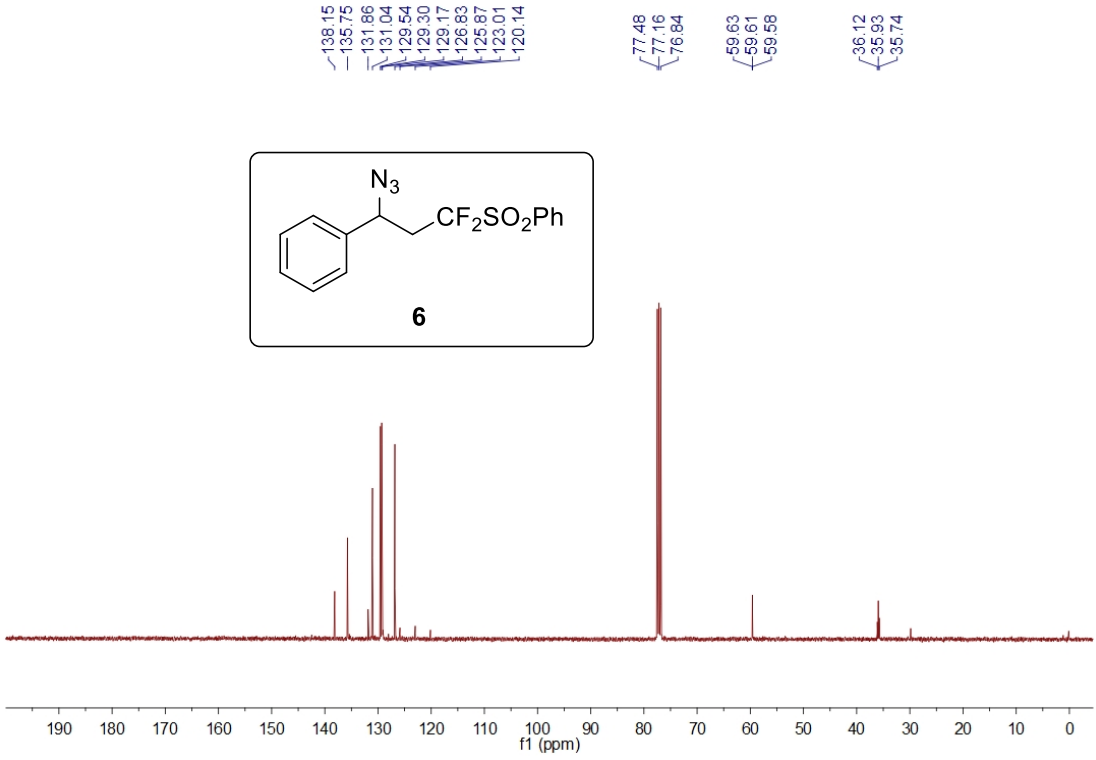

8.04
8.02
7.67
7.55
7.12
6.56
6.53
6.52
6.51
6.49
6.47
-0.00
CF2SO2Ph
NC
3r
1.98
1.05
6.01
1.01
1.00

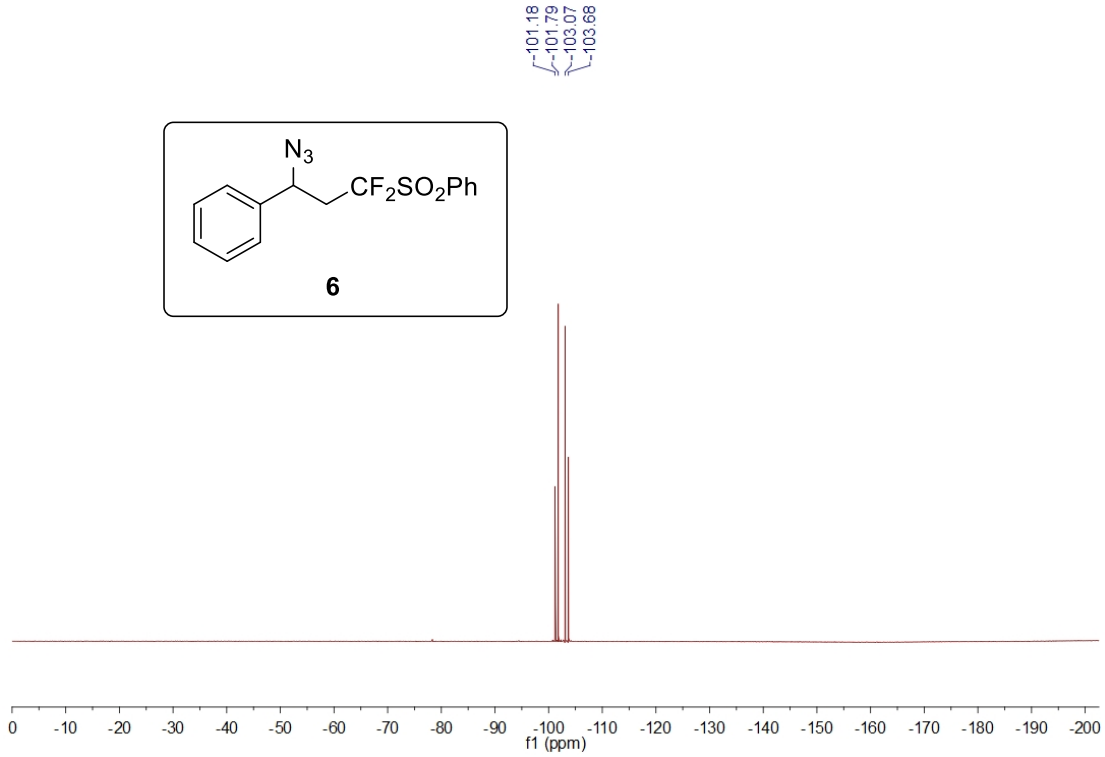

140.43
140.34
140.25
137.80
135.67
132.81
132.69
130.95
129.52
128.42
123.90
121.07
118.31
118.25
116.77
116.54
116.32
113.76
77.48
77.16
76.84
CF2SO2Ph
NC
3r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

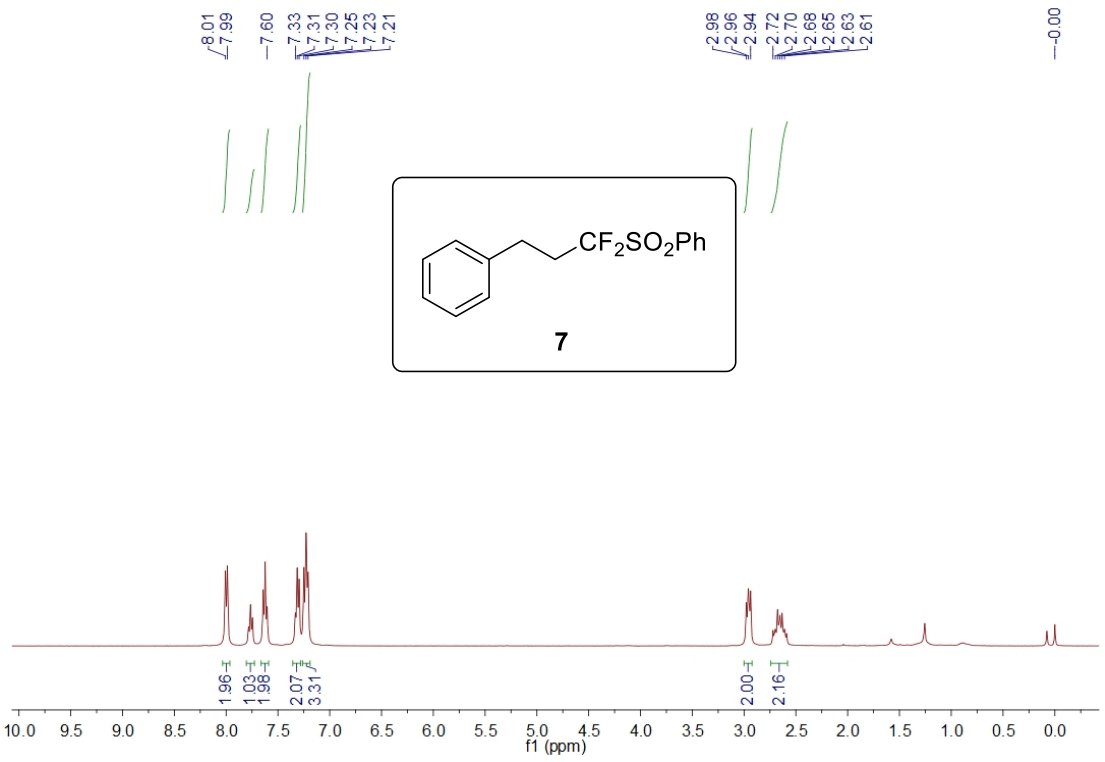

-101.73
CF2SO2Ph
NC
3r
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200

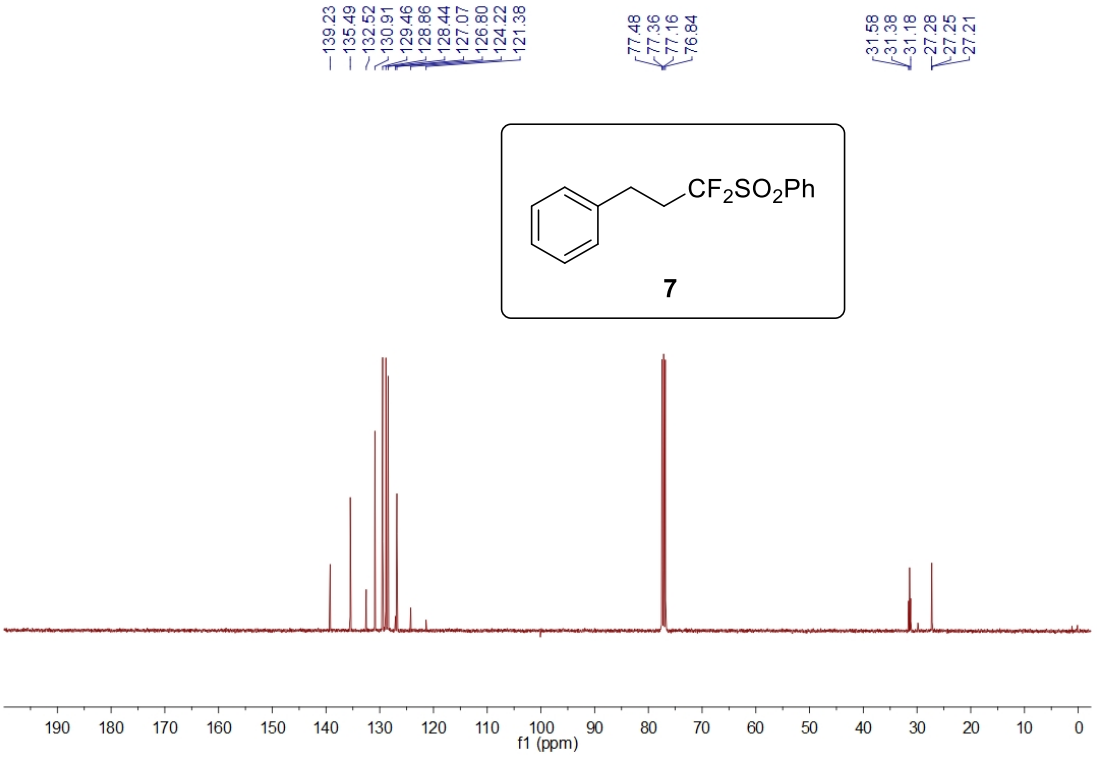

7.99
7.98
7.76
7.64
7.61
7.42
7.40
7.39
7.36
7.35
7.26
4.98
4.96
4.96
4.96
4.94
2.94
2.88
2.87
2.84
2.83
2.81
2.77
2.73
0.07
-0.00
N3
CF2SO2Ph
6

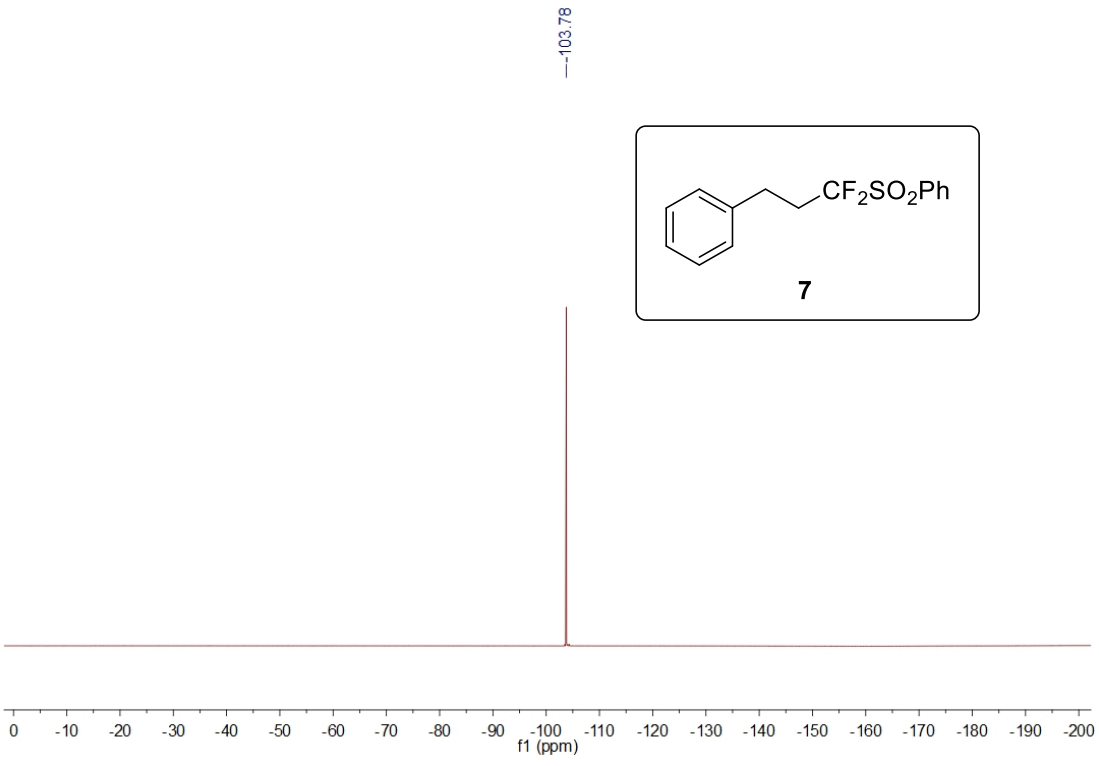

2.00
1.12
2.14
5.24
1.08
2.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

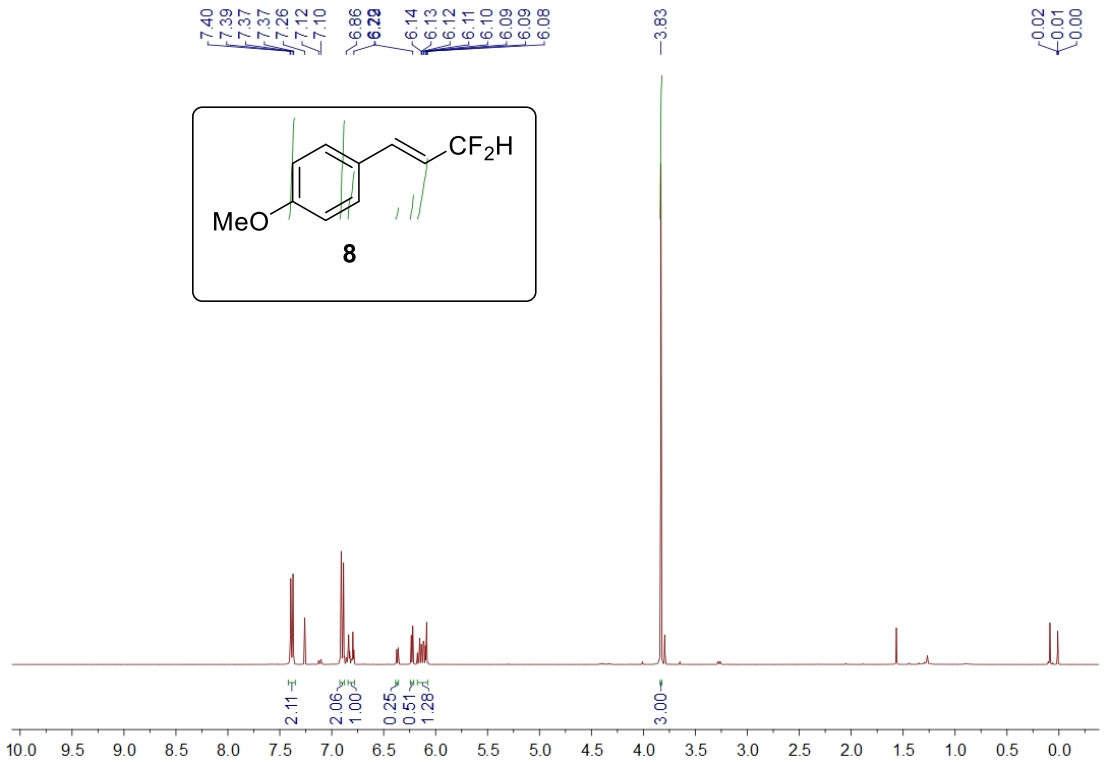

138.15
135.75
131.86
131.04
129.54
129.30
129.17
126.83
125.87
123.01
120.14
77.48
77.16
76.84
59.63
59.61
59.58
36.12
35.93
35.74
N3
CF2SO2Ph
6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

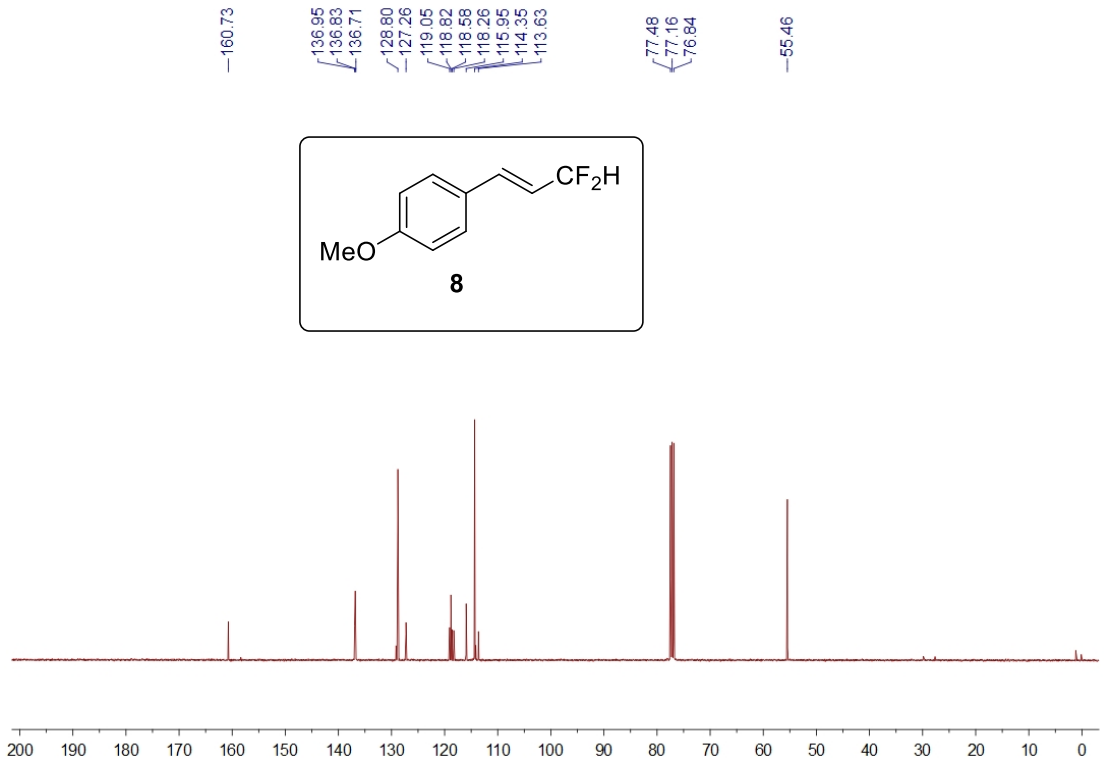

-101.18
-101.79
-103.07
-103.68
N3
CF2SO2Ph
6
f1 (ppm)

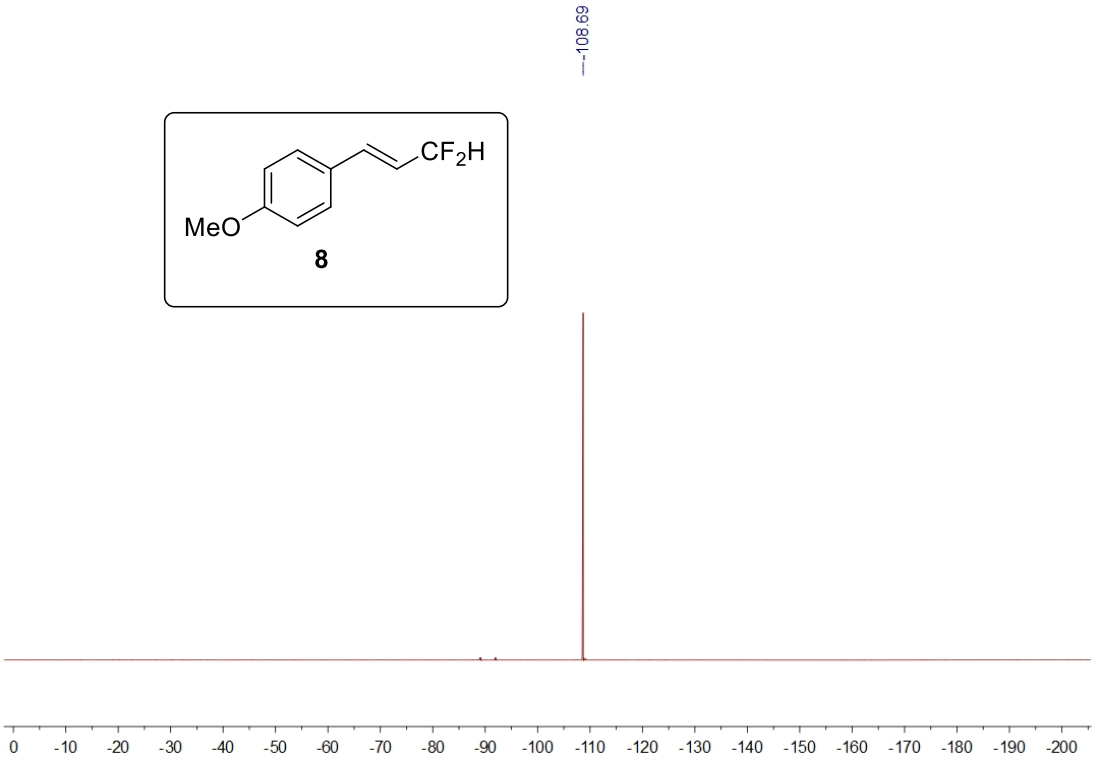

8.01
7.99
7.60
7.33
7.31
7.30
7.25
7.23
7.21
2.98
2.96
2.94
2.72
2.70
2.68
2.65
2.63
2.61
0.00
CF2SO2Ph
7
1.96
1.03
1.98
2.07
3.31
2.00
2.16
f1 (ppm)


139.23
135.49
132.52
130.91
129.46
128.86
128.44
127.07
126.80
124.22
121.38
77.48
77.36
77.16
76.84
31.58
31.38
31.18
27.28
27.25
27.21
CF2SO2Ph
7
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


103.78
CF2SO2Ph
7
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.40
7.39
7.37
7.37
7.26
7.12
7.10
6.86
6.29
6.14
6.13
6.12
6.11
6.10
6.09
6.09
6.08
3.83
0.02
0.01
0.00
CF2H
MeO
8
2.11
2.06
1.00
0.25
0.51
1.28
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


160.73
136.95
136.83
136.71
128.80
127.26
119.05
118.82
118.58
118.26
115.95
114.35
113.63
77.48
77.16
76.84
55.46
CF2H
MeO
8
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


-108.69
CF2H
MeO
8
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200