Electronic Supplementary Material (ESI) for ChemComm.

Photo/Ni dual-catalyzed radical defluorinative sulfonylation to synthesize *gem*-difluoro allylsulfones

Yiran Xu,[a] Shengchun Wang,[a] Zhao Liu,[a] Mian Guo*,[a] and Aiwen Lei*,[a]

[a] College of Chemistry and Molecular Sciences, The Institute for Advanced Studies (IAS), Wuhan University, Wuhan 430072, P.R. China.

E-mail: : aiwenlei@whu.edu.cn; whguomian@whu.edu.cn

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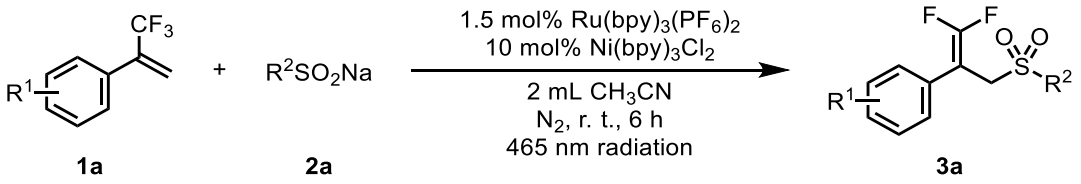
I. General Information

All manipulations were carried out by standard schlenk techniques. Unless otherwise stated, analytical grade solvents and commercially available reagents were used to conduct the reactions. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum ether (bp. 60-90 ºC). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum ether to the ethyl acetate. All the new compounds were characterized by ^{1}H NMR, ^{13}C NMR and ^{19}F NMR. The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. The chemical shifts (δ) were given in part per million related to internal tetramethyl silane (TMS, 0 ppm for ^{1}H NMR), $CDCl_3$ (77.16 ppm for ^{13}C NMR). All ^{1}H NMR spectra were reported in delta (δ) units, parts per million (ppm) downfield from the internal standard. Coupling constants are reported in Hertz (Hz). The multiplicities of signals are designated by the following abbreviations: s (singlet), d (doublet), t (triplet), q (quarter), m (multiplet), dd (doublet of doublets), dt (doublet of triplets), td (triplet of doublets), tt (triplets of triplets). High resolution mass spectroscopy (HRMS) was recorded on Thermo Fisher Scientific LTQ Orbitrap Elite. All kinds of photocatalysts were purchased from China Bidepharm company.

II. Experimental Procedures

1. Procedure A: General Procedures for Defluorinative sulfonation of α-trifluoromethyl alkenes



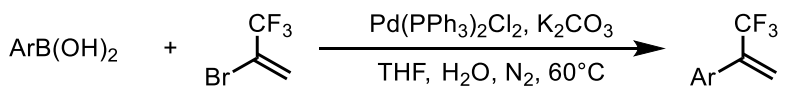
1a **2a** **3a**

To a 10 mL Schlenk tube was added a magnetic stirrer, $Ru(bpy)_3(PF_6)_2$ (1.5 mol%, 2.3 μmol), $Ni(bpy)_3Cl_2$ (10 mol%, 0.015 mmol), sulfinate salt **2a** (1.33 equiv., 0.2 mmol) and the tube was added and sealed with a septum. The tube was purged with N_2 and added alkene **1a** (1 equiv., 0.15 mmol), solvent under N_2 atmosphere. Then put the tube in the radiation of 465 nm LEDs and stirred for 6 hours. After reaction, solvent was removed under vacuum and solved with ethyl acetate, washed with 1 M HCl, saturated $NaHCO_3$. Organic layer was collected and dried with anhydrous Na_2SO_4. Solvent was removed under vacuum and the residue was purified by flash column chromatography over silica gel (ethyl acetate/petroleum ether as eluent) to give desired product.

2. Procedure B: Synthesis of 1-methoxy-4-(3,3,3-trifluoroprop-1-en-2-yl)benzene (1a)

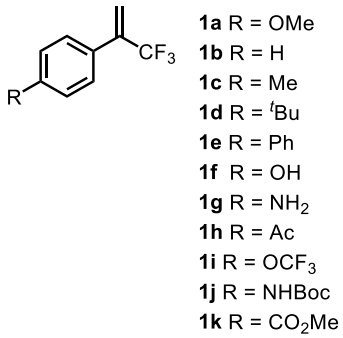
1a was prepared on large scale started with 2,2,2-trifluoro-1-(4-methoxyphenyl)ethan-1-one by Wittig reaction according to a reported procedure.[1]

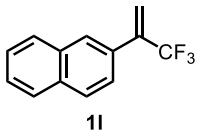
3. Procedure C: Synthesis of trifluoromethyl alkenes (1b-1o)



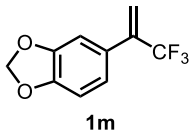
To a 25 mL Schlenk tube was added aryl borate (3 mmol, 1 equiv.), potassium carbonate (12 mmol, 4 equiv.), bis(triphenylphosphine)palladium(II) chloride (0.09 mmol, 3 mol%). Then removed air under vacuum and charged with N_2, the tube was added THF (9 mL), 2-bromo-3,3,3-trifluoropropene (4.5 mmol, 1.5 equiv.), degassed deionized H_2O (6 mL) subsequently and sealed tightly. The solution was heated to 60 ºC for 12 hours. The mixture was cooled to room temperature, extracted with ethyl acetate and remove solvent under vacuum. The residue was purified by column chromatography over silica gel with ethyl acetate and petroleum ether as eluent to give desired product. All the structures were previously reported. The spectra of **1a-1e**, **1h**, **1i**, **1k**, **1l**[2a], **1f**,**1m**[2b], **1g**[2c], **1j**[2d], **1n**[2e],**1o**[2f] were identical as previously reported.

List of alkenes

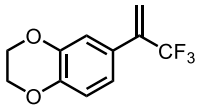




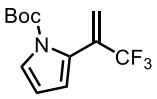
1l



1m

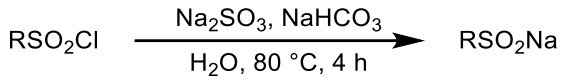


1n



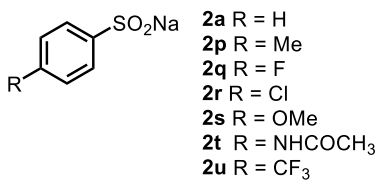
1o

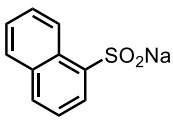
4. Procedure D: Synthesis of sulfinate salts



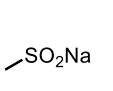
According to a reported procedure, sodium sulfite (10 mmol, 2 equiv.), sodium bicarbonate (10 mmol, 2 equiv.) and the corresponding sulfonyl chloride (5 mmol, 1 equiv.) were dissolved in distilled water (10 mL). The reaction mixture was stirred for 4 h at 80 °C. After cooling down to room temperature, water was removed in vacuo. 20 mL of methanol was then added to this white residue and the resulting heterogeneous solution was filtered. The filtrate was concentrated under reduced pressure and the desired sodium aryl sulfinates were obtained as white crystalline powders. All the structures are previously reported. **2a**, **2p-2r**, **2w**, **2x** were commercially available and the spectra of **2s**, **2y**[3a], **2t-2v**[3b] were identical as previously reported.

List of Sodium Sulfinate salts:

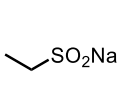




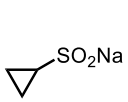
2v



2w

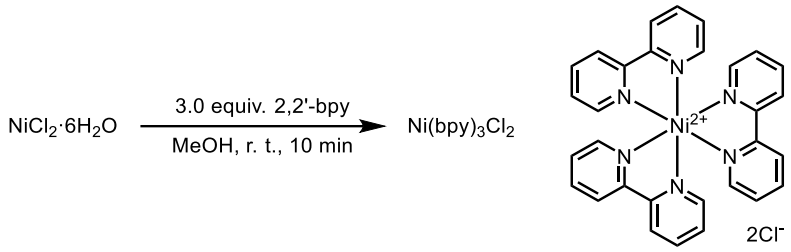


2x



2y

5. Procedure E: Synthesis of Ni co-catalyst $[Ni(bpy)_3]Cl_2$

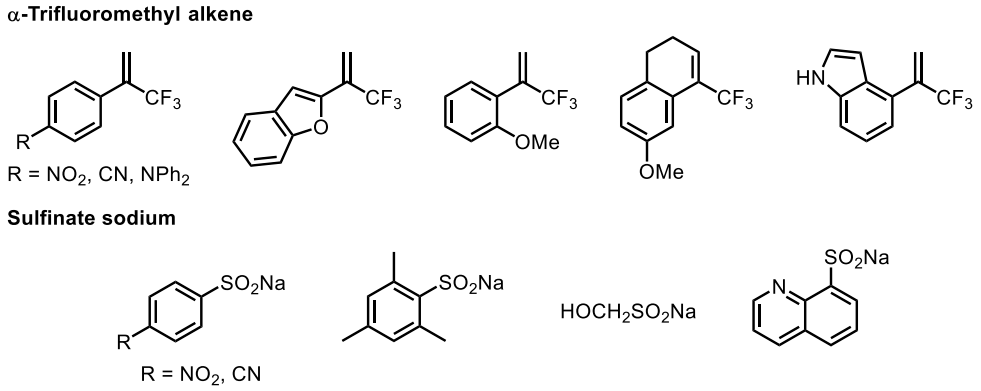


$Ni(bpy)_3Cl_2$ was synthesized according to a reported procedure with $NiCl_2•6H_2O$ instead of $NiBr_2•3H_2O$.[2] To a 250 mL Erlenmeyer flask equipped with a magnetic stirrer was added 2,2'-bpy (45 mmol) and 15 mL MeOH. Then a solution of 15 mL MeOH containing $NiCl_2•6H_2O$ (15 mmol) was added to the flask in one portion under vigorous stirring. The solution turned red and pink precipitate was formed. After stirring for 20 min, 30 mL acetone was added to the mixture and the precipitate was filtered and washed with 5 ml acetone twice to obtain pink solid. The solid was used directly without further purification (7.2 g, 80 % yield).

6. Procedure F: The Gram-Scale Experiment

1a (6 mmol, 1.0 equiv.), **2a** (8 mmol, 1.33 equiv.), $Ru(bpy)_3(PF_6)_2$ (0.09 mmol, 1.5 mol%), $Ni(bpy)_3Cl_2$ (0.6 mmol, 10 mol%), 80 mL CH_3CN were separated equally into four 25 mL Schlenk tubes equipped with magnetic stirrer and sealed with septum. The tubes were purged with nitrogen and stirred in the radiation of 465 nm LEDs for 12 hours. After the reactions were completed, solvent was removed under vacuum and solved with ethyl acetate, washed with 1 M HCl, saturated $NaHCO_3$. The residue was purified by column chromatography over silica gel with ethyl acetate and petroleum ether as eluent to give desired product **3a** (1.87 g, 96 % yield).

Failed Examples



III. Density Functional Theory (DFT) Studies

1. Computational Methods

All density functional theory (DFT) calculations were carried out using the Gaussian 16 software package.[3] All geometries were optimized using the M06-2X functional[4] with a basis set of 6-31G(d) for all atoms. Frequencies were calculated for all the stationary points to confirm if each optimized structure is a local minimum on the respective potential energy surface or a transition state structure with only one imaginary frequency. Solvation energy correction was calculated in acetonitrile

solvent with the SMD continuum solvation model[5] based on the gas phase optimized geometries. The M06-2X functional with a basis set of 6-311+G(d,p) for all atoms was used for single point energy calculations. SuperFineGrid is used for geometry optimization and single point energy calculation

DFT Calculations were first performed to investigate the number of the solvent coordinated with the Na atom in **2a**, **NaF** and **NaOH**. More than one acetonitrile can coordinate with the Na atom by the N atom. Calculation results suggest that one acetonitrile coordinated structures of all three species have the lowest free energies. Thus, the reaction energies are calculated based on the one acetonitrile solvent coordinated structures **2a-s**, **NaF-s** and **NaOH-2s**.

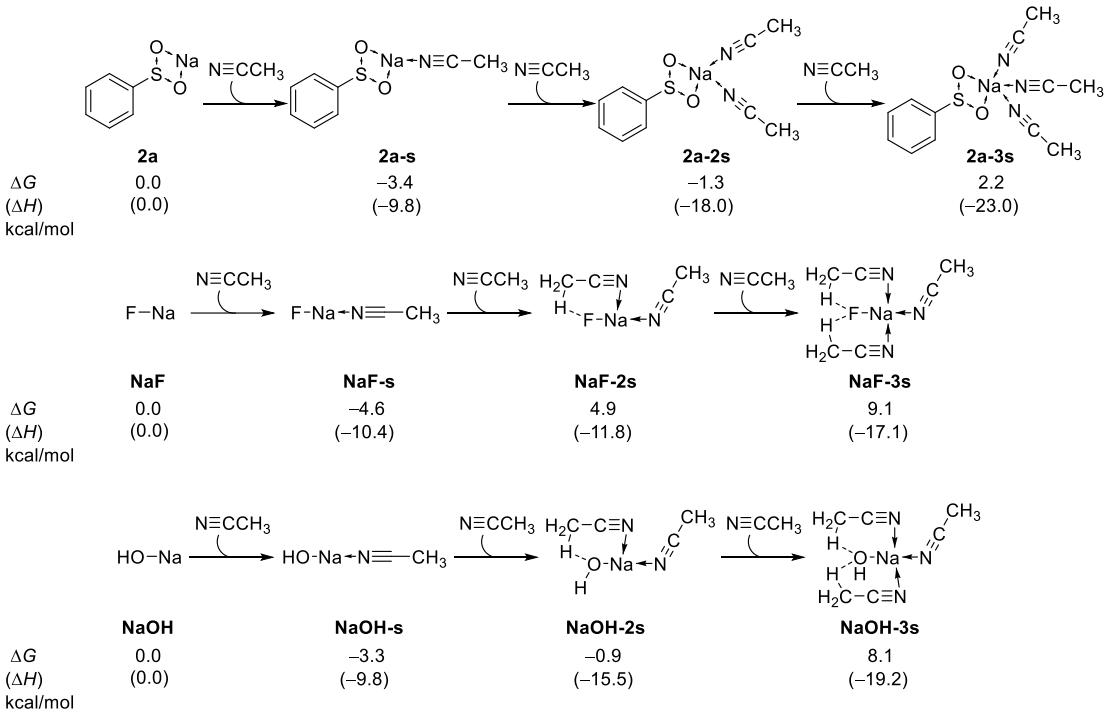


Figure S1. Calculated energy profiles of solvation energy of sodium salts with MeCN as solvent. All results were calculated at the M06-2X/6-31G(d) level of theory.

2. Cartesian Coordinates and Energies of Optimized Structures

1a

M06-2X SCF energy: -760.91089363 a.u.

M06-2X enthalpy: -760.722892 a.u.

M06-2X free energy: -760.775534 a.u.

M06-2X SCF energy in solution: -761.15982040 a.u.

M06-2X enthalpy in solution: -760.971819 a.u.

M06-2X free energy in solution: -761.024461 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.978706	1.484612	0.289857
C	-0.605211	1.619615	0.218863
C	0.218898	0.530407	-0.106683

C	-0.390584	-0.705678	-0.331937
C	-1.773517	-0.857607	-0.260360
C	-2.575716	0.241601	0.046747
H	-2.617791	2.321795	0.548683
H	-0.155463	2.581716	0.444614
H	0.212791	-1.571590	-0.579354
H	-2.206898	-1.832714	-0.446977
C	1.685077	0.712657	-0.202854
C	2.546459	-0.483176	0.117493
C	2.284299	1.852220	-0.550899
H	3.363645	1.940363	-0.567789
H	1.705441	2.723164	-0.838387
F	2.477241	-1.413045	-0.856275
F	3.838901	-0.163776	0.253197
F	2.158478	-1.082330	1.251007
O	-3.927210	0.205641	0.143477
C	-4.563897	-1.033631	-0.077613
H	-4.233417	-1.785858	0.648596
H	-5.630950	-0.852388	0.048092
H	-4.373871	-1.403374	-1.092342

2a

M06-2X SCF energy: -942.36049216 a.u.
M06-2X enthalpy: -942.249281 a.u.
M06-2X free energy: -942.295187 a.u.
M06-2X SCF energy in solution: -942.53746561 a.u.
M06-2X enthalpy in solution: -942.426254 a.u.
M06-2X free energy in solution: -942.472160 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.494217	-1.208527	0.236563
C	-1.157836	-1.212326	-0.156224
C	-0.500998	0.000011	-0.349207
C	-1.157843	1.212328	-0.156186
C	-2.494230	1.208511	0.236607
C	-3.161744	-0.000012	0.429602
H	-3.015132	-2.147915	0.395616
H	-0.610547	-2.139727	-0.296064
H	-0.610575	2.139747	-0.295997
H	-3.015144	2.147895	0.395686
H	-4.203861	-0.000025	0.734348
S	1.222944	0.000020	-0.909268
O	1.774444	1.241519	-0.178349

O	1.774456	-1.241509	-0.178385
Na	2.663469	-0.000026	1.365604

2a-s

M06-2X SCF energy: -1075.07661259 a.u.
M06-2X enthalpy: -1074.912718 a.u.
M06-2X free energy: -1074.975795 a.u.
M06-2X SCF energy in solution: -1075.29846202 a.u.
M06-2X enthalpy in solution: -1075.134567 a.u.
M06-2X free energy in solution: -1075.197644 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.303986	1.337665	-1.209705
C	2.405386	0.273214	-1.211155
C	1.962449	-0.248722	0.001085
C	2.403222	0.278904	1.211641
C	3.301842	1.343335	1.206802
C	3.754071	1.869710	-0.002284
H	3.651215	1.755931	-2.149942
H	2.024641	-0.147081	-2.137298
H	2.020795	-0.137063	2.139043
H	3.647401	1.765992	2.145692
H	4.455700	2.698526	-0.003605
S	0.833769	-1.671684	0.003418
O	-0.023801	-1.369326	1.244862
O	-0.020773	-1.375848	-1.241702
Na	-1.654918	-0.574664	-0.002498
N	-3.833487	0.348832	-0.002337
C	-4.894481	0.798178	-0.001387
C	-6.238996	1.367673	-0.000089
H	-6.973030	0.575029	-0.157371
H	-6.430946	1.852476	0.959047
H	-6.325860	2.104272	-0.801146

2a-2s

M06-2X SCF energy: -1207.79499541 a.u.
M06-2X enthalpy: -1207.578453 a.u.
M06-2X free energy: -1207.652671 a.u.
M06-2X SCF energy in solution: -1208.05676161 a.u.
M06-2X enthalpy in solution: -1207.840219 a.u.
M06-2X free energy in solution: -1207.914437 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	4.178587	0.019167	-0.466260
C	3.064169	-0.755784	-0.776160
C	1.993194	-0.811111	0.113034
C	2.028478	-0.112553	1.314025
C	3.141467	0.671582	1.618447
C	4.214073	0.738652	0.729686
H	5.017911	0.066231	-1.153720
H	3.019175	-1.310067	-1.711257
H	1.181219	-0.198884	1.988803
H	3.176401	1.224682	2.552517
H	5.082905	1.343097	0.972423
S	0.504379	-1.752767	-0.365568
O	-0.342971	-1.661086	0.905671
O	-0.112058	-0.794557	-1.403022
Na	-1.708795	-0.123349	0.066575
N	-0.837355	2.129441	0.307090
N	-4.089251	0.053889	0.106538
C	0.085569	2.113965	-0.390368
C	-5.237648	0.132121	0.156489
C	-6.693298	0.231340	0.220566
H	-7.067967	-0.390979	1.035451
H	-6.983404	1.268900	0.396532
H	-7.126737	-0.109681	-0.721509
C	1.231036	2.065547	-1.291850
H	1.228016	2.938762	-1.947350
H	2.156328	2.033634	-0.709538
H	1.135537	1.139707	-1.867845

2a-3s

M06-2X SCF energy: -1340.50475729 a.u.
M06-2X enthalpy: -1340.235615 a.u.
M06-2X free energy: -1340.323963 a.u.
M06-2X SCF energy in solution: -1340.80986704 a.u.
M06-2X enthalpy in solution: -1340.540725 a.u.
M06-2X free energy in solution: -1340.629073 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	4.414209	-0.312513	-0.258830
C	3.324941	0.430161	-0.706594
C	2.091077	-0.191831	-0.881357
C	1.934773	-1.549188	-0.627166
C	3.024357	-2.289374	-0.168310

C	4.261441	-1.672543	0.016499
H	5.380056	0.164588	-0.121907
H	3.428772	1.493387	-0.912873
H	0.959652	-1.998796	-0.793671
H	2.911186	-3.349388	0.039179
H	5.110202	-2.252739	0.365886
S	0.658029	0.820434	-1.379447
O	-0.417583	-0.236460	-1.600657
O	0.347351	1.540323	-0.049149
Na	-1.550582	0.134701	0.301422
N	-2.899958	2.193770	0.625595
N	-0.432602	-1.000335	2.170148
N	-3.440681	-1.328940	0.061666
C	0.594590	-0.477712	2.266122
C	-4.290817	-2.065442	-0.186946
C	-2.200769	3.048579	0.283314
C	-5.367451	-2.999965	-0.505253
H	-5.245398	-3.366218	-1.526374
H	-5.338683	-3.844842	0.185391
H	-6.331721	-2.495989	-0.416920
C	-1.288565	4.102685	-0.149112
H	-1.593488	4.479007	-1.127641
H	-1.291740	4.921400	0.572914
H	-0.297578	3.642256	-0.213986
C	1.877665	0.207616	2.374877
H	2.060731	0.496598	3.411846
H	2.676884	-0.449721	2.020781
H	1.820895	1.086596	1.726017

3a

M06-2X SCF energy: -1441.11748253 a.u.
M06-2X enthalpy: -1440.821685 a.u.
M06-2X free energy: -1440.891307 a.u.
M06-2X SCF energy in solution: -1441.49081586 a.u.
M06-2X enthalpy in solution: -1441.195018 a.u.
M06-2X free energy in solution: -1441.264640 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.925038	3.286671	0.753020
C	0.370897	2.783553	0.686133
C	0.677865	1.857693	-0.306768
C	-0.261478	1.439422	-1.243381
C	-1.553474	1.949836	-1.165419

C	-1.884105	2.864092	-0.166180
H	-1.185145	4.011249	1.517716
H	1.142126	3.109782	1.377641
H	0.025760	0.722737	-2.005589
H	-2.304316	1.628484	-1.880295
H	-2.896152	3.251802	-0.105217
S	2.304055	1.130407	-0.322849
O	2.497689	0.469126	-1.609768
O	3.250592	2.124024	0.178183
C	2.223868	-0.159879	0.959570
H	3.273991	-0.423268	1.109345
H	1.864344	0.340621	1.862718
C	1.393258	-1.338652	0.559306
C	-0.085246	-1.238278	0.525329
C	-0.771776	-0.506899	1.507208
C	-0.829647	-1.787497	-0.519124
C	-2.139932	-0.322256	1.437774
H	-0.228151	-0.063494	2.336497
C	-2.210630	-1.617612	-0.598759
H	-0.323702	-2.338564	-1.304872
C	-2.870830	-0.871845	0.377903
H	-2.671280	0.254915	2.186775
H	-2.749284	-2.054597	-1.431128
C	2.033438	-2.434147	0.157375
F	3.344054	-2.561052	0.113797
F	1.457435	-3.553224	-0.230178
O	-4.203061	-0.615954	0.383285
C	-4.971741	-1.149712	-0.671740
H	-5.999545	-0.839215	-0.486023
H	-4.642145	-0.758187	-1.642251
H	-4.919133	-2.244814	-0.689378

4a

M06-2X SCF energy: -1616.76615977 a.u.
M06-2X enthalpy: -1616.448244 a.u.
M06-2X free energy: -1616.520303 a.u.
M06-2X SCF energy in solution: -1617.20499782 a.u.
M06-2X enthalpy in solution: -1616.887082 a.u.
M06-2X free energy in solution: -1616.959141 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.772584	1.650296	-0.342545
C	1.475751	1.614714	-0.846628

C	0.443109	2.100874	-0.053687
C	0.666826	2.639734	1.210879
C	1.966657	2.660984	1.704670
C	3.014352	2.162831	0.930116
H	3.593119	1.264708	-0.939247
H	1.254304	1.207784	-1.827170
H	-0.159988	3.047852	1.785096
H	2.163988	3.073582	2.688474
H	4.026653	2.177375	1.321174
S	-1.225643	2.036277	-0.664928
O	-1.890614	3.283658	-0.310156
O	-1.168421	1.587023	-2.065248
C	-2.067431	0.739904	0.269626
H	-1.822467	0.890769	1.323712
H	-3.127537	0.967108	0.118092
C	-1.775349	-0.692677	-0.218532
C	-0.303443	-1.069491	-0.072763
C	0.392550	-0.879883	1.131057
C	0.381685	-1.591960	-1.161316
C	1.739172	-1.174908	1.223045
H	-0.116056	-0.489703	2.007143
C	1.743484	-1.891432	-1.084824
H	-0.155154	-1.764973	-2.087241
C	2.428605	-1.671014	0.108568
H	2.291932	-1.015135	2.142497
H	2.247653	-2.290746	-1.956764
C	-2.638899	-1.636750	0.631049
F	-3.936906	-1.344274	0.508353
F	-2.459834	-2.903604	0.272424
O	3.754837	-1.892063	0.288426
C	4.480865	-2.412300	-0.803447
H	5.508360	-2.525217	-0.458801
H	4.090182	-3.388830	-1.112821
H	4.456495	-1.727679	-1.660534
F	-2.328775	-1.523060	1.935627
O	-2.258680	-0.881389	-1.517992
H	-1.931645	-0.140237	-2.064255

H_2O

M06-2X SCF energy: -76.37222092 a.u.

M06-2X enthalpy: -76.346943 a.u.

M06-2X free energy: -76.368376 a.u.

M06-2X SCF energy in solution: -76.42964184 a.u.

M06-2X enthalpy in solution: -76.404364 a.u.

M06-2X free energy in solution: -76.425797 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	0.000000	0.000000	0.118307
H	0.000000	0.763087	-0.473229
H	0.000000	-0.763087	-0.473229

MeCN

M06-2X SCF energy: -132.69017945 a.u.
M06-2X enthalpy: -132.639442 a.u.
M06-2X free energy: -132.666933 a.u.
M06-2X SCF energy in solution: -132.74336349 a.u.
M06-2X enthalpy in solution: -132.692626 a.u.
M06-2X free energy in solution: -132.720117 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.000000	0.000000	1.436247
C	0.000000	0.000000	0.281798
C	0.000000	0.000000	-1.180594
H	0.000000	1.026239	-1.553651
H	0.888749	-0.513120	-1.553651
H	-0.888749	-0.513120	-1.553651

NaF-s

M06-2X SCF energy: -394.79525992 a.u.
M06-2X enthalpy: -394.738175 a.u.
M06-2X free energy: -394.780974 a.u.
M06-2X SCF energy in solution: -394.94328349 a.u.
M06-2X enthalpy in solution: -394.886199 a.u.
M06-2X free energy in solution: -394.928998 a.u.

Cartesian coordinates

ATOM	X	Y	Z
F	3.483318	0.000217	-0.000394
Na	1.587351	-0.000092	0.000370
N	-0.785802	-0.000410	0.000212
C	-1.937972	-0.000107	0.000029
C	-3.398034	0.000257	-0.000219
H	-3.764591	-0.301214	-0.983341
H	-3.764989	-0.700239	0.752395
H	-3.764496	1.002475	0.230092

NaF-2s

M06-2X SCF energy: -527.52475766 a.u.
M06-2X enthalpy: -527.415667 a.u.
M06-2X free energy: -527.468553 a.u.
M06-2X SCF energy in solution: -527.69014996 a.u.
M06-2X enthalpy in solution: -527.581059 a.u.
M06-2X free energy in solution: -527.633945 a.u.

Cartesian coordinates

ATOM	X	Y	Z
F	2.294727	1.416724	0.000160
Na	0.341151	1.362825	-0.000072
N	0.115281	-1.268194	0.000030
N	-2.026708	1.316647	-0.000100
C	1.272303	-1.337109	-0.000016
C	-2.545260	0.284469	-0.000020
C	2.727558	-1.287623	-0.000081
H	2.932648	-0.190182	-0.000008
H	3.120123	-1.776723	0.893240
H	3.120041	-1.776620	-0.893494
C	-3.166231	-1.035086	0.000083
H	-3.784227	-1.156067	0.891652
H	-3.784128	-1.156250	-0.891531
H	-2.359886	-1.772827	0.000199

NaF-3s

M06-2X SCF energy: -660.24686397 a.u.
M06-2X enthalpy: -660.084918 a.u.
M06-2X free energy: -660.150293 a.u.
M06-2X SCF energy in solution: -660.44397448 a.u.
M06-2X enthalpy in solution: -660.282029 a.u.
M06-2X free energy in solution: -660.347404 a.u.

Cartesian coordinates

ATOM	X	Y	Z
F	1.868388	0.000071	1.394340
Na	-0.137168	-0.000100	1.270744
N	-0.336790	1.711744	-0.673729
N	-0.336258	-1.711556	-0.674143
N	-2.523720	-0.000433	1.414959
C	0.809832	1.872188	-0.658618
C	-2.815300	-0.000266	0.296131
C	0.810369	-1.871942	-0.658864
C	2.259175	1.996419	-0.551995

H	2.521617	1.296070	0.262084
H	2.731173	1.710211	-1.494196
H	2.532470	3.023483	-0.303590
C	-3.139291	-0.000059	-1.125598
H	-4.221230	-0.000691	-1.268375
H	-2.694062	0.889842	-1.575434
H	-2.692967	-0.889181	-1.575899
C	2.259701	-1.996124	-0.552024
H	2.521983	-1.295815	0.262138
H	2.532995	-3.023194	-0.303640
H	2.731837	-1.709839	-1.494132

NaOH

M06-2X SCF energy: -238.03393817 a.u.
M06-2X enthalpy: -238.018129 a.u.
M06-2X free energy: -238.045394 a.u.
M06-2X SCF energy in solution: -238.11799176 a.u.
M06-2X enthalpy in solution: -238.102183 a.u.
M06-2X free energy in solution: -238.129448 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Na	0.000000	0.000000	-0.905710
O	0.000000	0.000000	1.000540
H	0.000000	0.000000	1.958489

NaOH-s

M06-2X SCF energy: -370.74966411 a.u.
M06-2X enthalpy: -370.681580 a.u.
M06-2X free energy: -370.725895 a.u.
M06-2X SCF energy in solution: -370.87855154 a.u.
M06-2X enthalpy in solution: -370.810467 a.u.
M06-2X free energy in solution: -370.854782 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Na	1.558747	-0.000616	0.000573
O	3.485611	0.000996	-0.000433
H	4.443928	0.001140	-0.001025
N	-0.816001	-0.001480	0.000055
C	-1.968075	-0.000368	-0.000055
C	-3.428230	0.001019	-0.000194
H	-3.795188	-0.003134	1.027949
H	-3.794154	0.894060	-0.510418

H	-3.795856	-0.886804	-0.518238

NaOH-2s

M06-2X SCF energy: -503.47482099 a.u.
M06-2X enthalpy: -503.355071 a.u.
M06-2X free energy: -503.414024 a.u.
M06-2X SCF energy in solution: -503.63185973 a.u.
M06-2X enthalpy in solution: -503.512110 a.u.
M06-2X free energy in solution: -503.571063 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Na	0.287532	0.788038	0.000588
O	2.092862	1.720174	-0.000328
H	2.403046	2.631119	-0.000482
N	-2.074132	0.457560	0.000462
C	-3.157273	0.064867	0.000015
C	-4.528048	-0.438575	-0.000588
H	-5.052278	-0.078496	-0.887813
H	-4.515504	-1.530182	-0.007175
H	-5.049094	-0.089245	0.892792
N	1.058853	-1.579601	0.000596
C	2.171143	-1.252171	0.000083
C	3.514279	-0.692190	-0.000575
H	3.305266	0.416634	-0.000619
H	4.054976	-1.008361	0.893451
H	4.054185	-1.008572	-0.895005

NaOH-3s

M06-2X SCF energy: -636.19785153 a.u.
M06-2X enthalpy: -636.025455 a.u.
M06-2X free energy: -636.091555 a.u.
M06-2X SCF energy in solution: -636.38312343 a.u.
M06-2X enthalpy in solution: -636.210727 a.u.
M06-2X free energy in solution: -636.276827 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Na	0.122962	0.000024	-1.257526
O	-1.963183	-0.000017	-1.413525
H	-2.489254	-0.000010	-2.222252
N	2.518807	-0.000021	-1.450843
C	2.820092	-0.000012	-0.334535
C	3.159834	0.000003	1.083643

H	2.718630	-0.889337	1.538418
H	4.243343	0.000147	1.214183
H	2.718393	0.889215	1.538441
N	0.365144	-1.708946	0.678962
C	-0.779304	-1.886915	0.691793
C	-2.227700	-2.030237	0.618995
H	-2.516278	-1.323639	-0.194534
H	-2.490715	-3.060255	0.370155
H	-2.681387	-1.755896	1.573721
N	0.365125	1.709018	0.678920
C	-0.779332	1.886932	0.691780
C	-2.227737	2.030182	0.619015
H	-2.516297	1.323576	-0.194515
H	-2.681388	1.755806	1.573749
H	-2.490810	3.060189	0.370193

NaF

M06-2X SCF energy: -262.07850362 a.u.
M06-2X enthalpy: -262.073672 a.u.
M06-2X free energy: -262.098241 a.u.
M06-2X SCF energy in solution: -262.18176134 a.u.
M06-2X enthalpy in solution: -262.176930 a.u.
M06-2X free energy in solution: -262.201498 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Na	0.000000	0.000000	-1.031899
O	0.000000	0.000000	0.844281

O_2

M06-2X SCF energy: -150.25576847 a.u.
M06-2X enthalpy: -150.248395 a.u.
M06-2X free energy: -150.271652 a.u.
M06-2X SCF energy in solution: -150.31235706 a.u.
M06-2X enthalpy in solution: -150.304983 a.u.
M06-2X free energy in solution: -150.328241 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	0.000000	0.000000	0.598588
O	0.000000	0.000000	-0.598588

IV. References

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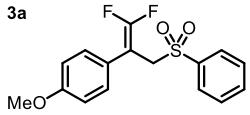
V. Characterization of Products



1-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)-4-methoxybenzene (3a)

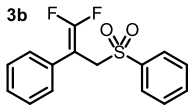
The reaction was carried out as Procedure A using **1a** and **2a**. The product was obtained as pale yellow oil in 90 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.76 (m, 2H), 7.62 – 7.54 (m, 1H), 7.50 – 7.42 (m, 2H), 7.21 – 7.14 (m, 2H), 6.85 – 6.77 (m, 2H), 4.14 (t, *J* = 2.1 Hz, 2H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.29, 156.02 (t, *J* = 294.7 Hz), 138.69, 133.96, 129.58 (t, *J* = 3.3 Hz), 129.18, 128.45, 123.06 (t, *J* = 3.4 Hz), 114.16, 84.26 (dd, *J* = 20.7, 19.1 Hz), 56.32 (d, *J* = 3.1 Hz), 55.37.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.48 (d, *J* = 24.3 Hz, 1F), -85.19 (d, *J* = 23.8 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{16}H_{14}F_2O_3S + NH_4]^+$ 342.0970, measured 342.0969.



((3,3-Difluoro-2-phenylallyl)sulfonyl)benzene (3b)

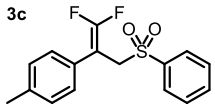
The reaction was carried out as Procedure A using **1b** and **2a**. The product was obtained as pale yellow oil in 80 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.73 (m, 2H), 7.63 – 7.52 (m, 1H), 7.49 – 7.39 (m, 2H), 7.29 – 7.20 (m, 5H), 4.18 (t, *J* = 2.0 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.18 (t, *J* = 295.7 Hz), 138.52, 133.98, 130.92 (t, *J* = 3.4 Hz), 129.16, 128.64, 128.38, 128.27 (t, *J* = 3.2 Hz), 128.08, 84.71 (dd, *J* = 20.5, 19.1 Hz), 56.10 (d, *J* = 3.0 Hz).

^{19}F NMR (377 MHz, Chloroform-*d*) δ -83.31 (d, *J* = 21.2 Hz, 1F), -84.22 (d, *J* = 21.0 Hz, 1F).

HR-MS (APCI+) *m*/*z*: calculated for $[C_{15}H_{12}F_2O_2S + H]^+$ 295.0599, measured 295.0599.



1-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)-4-methylbenzene (3c)

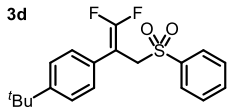
The reaction was carried out as Procedure A using **1c** and **2a**. The product was obtained as pale yellow oil in 76 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.76 (m, 2H), 7.62 – 7.53 (m, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 6.9 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 4.16 (t, *J* = 2.0 Hz, 2H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.99 (t, *J* = 295.1 Hz), 138.53, 137.91, 133.86, 129.31, 129.09, 128.35, 128.10 (t, *J* = 3.3 Hz), 127.87 (t, *J* = 3.3 Hz), 84.52 (dd, *J* = 20.6, 18.9 Hz), 56.10 (d, *J* = 3.2 Hz), 21.14.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -83.98 (d, *J* = 23.0 Hz), -84.73 (d, *J* = 22.6 Hz).

HR-MS (ESI) m/z: calculated for $[C_{16}H_{14}F_2O_2S + NH_4]^+$ 326.1021, measured 326.1024.



1-(*Tert*-butyl)-4-(1,1-difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)benzene (3d)

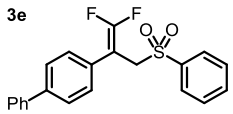
The reaction was carried out as Procedure A using **1d** and **2a**. The product was obtained as colorless oil in 65 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 – 7.72 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.28 – 7.22 (m, 2H), 7.14 (dd, *J* = 8.5, 1.5 Hz, 2H), 4.18 (t, *J* = 2.0 Hz, 2H), 1.28 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.62 – 152.67 (m), 150.90, 138.64, 133.80, 129.03, 128.39, 127.85 (t, *J* = 3.3 Hz), 127.74 (t, *J* = 3.4 Hz), 125.52, 84.53 (dd, *J* = 20.3, 18.9 Hz), 56.04 (d, *J* = 3.1 Hz), 34.54, 31.21.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -83.62 (d, *J* = 22.1 Hz), -84.59 (d, *J* = 22.3 Hz).

HR-MS (ESI) *m/z*: calculated for $[C_{19}H_{20}F_2O_2S + NH_4]^+$ 368.1490, measured 368.1491.



4-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)-1,1'-biphenyl (3e)

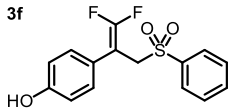
The reaction was carried out as Procedure A using **1e** and **2a**. The product was obtained as white solid in 91 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.79 (m, 2H), 7.59 – 7.54 (m, 3H), 7.52 – 7.36 (m, 8H), 7.32 (dt, *J* = 8.8, 1.9 Hz, 2H), 4.23 (d, *J* = 2.1 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.55 – 151.36 (m), 140.77, 140.26, 138.58, 133.90, 129.79 (t, *J* = 3.5 Hz), 129.16, 128.92, 128.64 (t, *J* = 3.3 Hz), 128.42, 127.68, 127.27, 127.04, 84.53 (t, *J* = 19.7 Hz), 56.00 (d, *J* = 3.0 Hz).

^{19}F NMR (377 MHz, Chloroform-*d*) δ -82.82 (d, *J* = 20.6 Hz), -83.74 (d, *J* = 20.9 Hz).

HR-MS (ESI) *m/z*: calculated for $[C_{21}H_{16}F_2O_2S + Na]^+$ 393.0731, measured 393.0737.



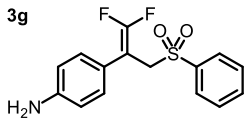
4-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)phenol (3f)

The reaction was carried out as Procedure A using **1f** and **2a**. The product was obtained as yellow oil in 55 % yield by flash column chromatography with ethyl acetate : petroleum ether = 2 : 1 as eluent.

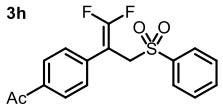
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.75 (m, 2H), 7.64 – 7.55 (m, 1H), 7.51 – 7.42 (m, 2H), 7.12 – 7.05 (m, 2H), 6.75 – 6.68 (m, 2H), 5.92 (s, 1H), 4.16 (t, *J* = 2.0 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.99 (t, *J* = 294.9 Hz), 155.85, 138.26, 134.23, 129.69 (t, *J* = 3.2 Hz), 129.34, 128.40, 122.68 (t, *J* = 3.3 Hz), 115.78, 84.13 (dd, *J* = 20.9, 19.1 Hz), 56.43 (d, *J* = 3.2 Hz).

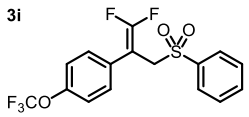
^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.58 (d, *J* = 23.9 Hz, 1F), -85.02 (d, *J* = 23.8 Hz, 1F).
HR-MS (ESI) *m*/*z*: calculated for $[C_{15}H_{12}F_2O_3S + Na]^+$ 333.0367, measured 333.0371.



4-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)aniline (3g)
The reaction was carried out as Procedure A using **1g** and **2a**. The product was obtained as yellow oil in 58 % yield by flash column chromatography with ethyl acetate : petroleum ether = 2 : 1 as eluent.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 7.0 Hz, 1H), 7.62 – 7.52 (m, 1H), 7.46 (m, 2H), 7.02 (d, *J* = 7.1 Hz, 1H), 6.56 (d, *J* = 8.6 Hz, 1H), 4.12 (t, *J* = 2.1 Hz, 2H), 3.62 (s, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.87 (t, *J* = 294.4 Hz), 146.35, 138.67, 133.87, 129.30 (t, *J* = 3.3 Hz), 129.13, 128.45, 120.40 (t, *J* = 3.3 Hz), 115.01, 84.43 (dd, *J* = 20.7, 18.9 Hz), 56.34 (d, *J* = 3.2 Hz).
^{19}F NMR (377 MHz, Chloroform-*d*) δ -85.19 (dt, *J* = 25.8, 2.3 Hz, 1F), -85.80 (d, *J* = 25.9 Hz, 1F).
HR-MS (ESI) *m*/*z*: calculated for $[C_{15}H_{13}F_2NO_2S + H]^+$ 310.0708, measured 310.0705.



1-(4-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)phenyl)ethan-1-one (3h)
The reaction was carried out as Procedure A using **1h** and **2a**. The product was obtained as yellow oil in 69 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 2 as eluent.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.84 (m, 2H), 7.81 – 7.77 (m, 2H), 7.61 – 7.54 (m, 1H), 7.49 – 7.42 (m, 2H), 7.36 (dd, *J* = 8.4, 1.6 Hz, 2H), 4.19 (t, *J* = 2.0 Hz, 2H), 2.56 (s, 1H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.36, 163.00 – 149.93 (m), 138.34, 136.35, 135.85 (t, *J* = 3.8 Hz), 134.18, 129.31, 128.60, 128.47 (t, *J* = 3.5 Hz), 128.37, 84.44 (t, *J* = 19.6 Hz), 55.64 (d, *J* = 2.9 Hz), 26.69.
^{19}F NMR (377 MHz, Chloroform-*d*) δ -81.02 (dt, *J* = 16.3, 2.2 Hz, 1F), -81.94 (d, *J* = 16.3 Hz, 1F).
HR-MS (ESI) *m*/*z*: calculated for $[C_{17}H_{14}F_2O_3S + Na]^+$ 359.0524, measured 359.0529.

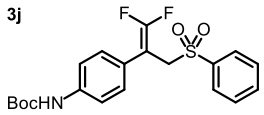


1-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)-4-(trifluoromethoxy)benzene (3i)
The reaction was carried out as Procedure A using **1i** and **2a**. The product was obtained as colorless oil in 90 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.74 (m, 2H), 7.62 – 7.53 (m, 1H), 7.47 – 7.39 (m, 2H), 7.30 – 7.24 (m, 2H), 7.13 – 7.07 (m, 2H), 4.17 (t, *J* = 2.1 Hz, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.37 (t, *J* = 296.3 Hz), 148.65, 138.46, 134.12, 129.90 (t, *J* = 3.3 Hz), 129.70 (t, *J* = 3.6 Hz), 129.26, 128.36, 121.10, 120.45 (q, *J* = 257.7 Hz), 83.91 (t, *J* = 20.2 Hz),

55.96 (d, *J* = 2.9 Hz).

^{19}F NMR (377 MHz, Chloroform-*d*) δ -57.83 (s, 3F), -82.39 (d, *J* = 19.1 Hz, 1F), -83.38 (d, *J* = 19.1 Hz, 1F).

HR-MS (APCI+) *m/z*: calculated for $[C_{16}H_{11}F_5O_3S + H]^+$ 379.0422, measured 379.0421.



***Tert*-butyl (4-(1,1-difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)phenyl)carbamate (3j)**

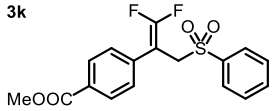
The reaction was carried out as Procedure A using **1j** and **2a**. The product was obtained as wihte solid in 78 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 2 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (dd, *J* = 7.8, 1.5 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.7 Hz, 2H), 7.16 (d, *J* = 8.3 Hz, 2H), 6.51 (s, 1H), 4.14 (d, *J* = 2.1 Hz, 2H), 1.52 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.99 (t, *J* = 295.2 Hz), 152.69, 138.40, 138.36, 133.98, 129.13, 128.80 (t, *J* = 3.3 Hz), 128.30, 124.97 (t, *J* = 3.3 Hz), 118.35, 85.08 – 83.34 (m), 80.62, 56.05 (d, *J* = 3.0 Hz), 28.28.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -83.81 (d, *J* = 22.5 Hz, 1F), -84.52 (d, *J* = 22.4 Hz, 1F).

HR-MS (ESI) *m/z*: calculated for $[C_{20}H_{21}F_2NO_4S - C_5H_{11}NO]^+$ 308.0551, measured 308.0442.



Methyl 4-(1,1-difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)benzoate (3k)

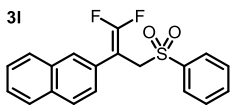
The reaction was carried out as Procedure A using **1k** and **2a**. The product was obtained as colorless oil in 75 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 2 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.5 Hz, 2H), 7.81 – 7.74 (m, 2H), 7.59 – 7.53 (m, 1H), 7.46 – 7.41 (m, 2H), 7.34 – 7.29 (m, 2H), 4.18 (t, *J* = 2.0 Hz, 2H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.44, 161.52 – 152.00 (m), 138.33, 135.68 (t, *J* = 3.8 Hz), 134.16, 129.81, 129.27, 128.36, 128.24 (t, *J* = 3.4 Hz), 84.47 (t, *J* = 19.7 Hz), 55.68 (d, *J* = 2.9 Hz), 52.30.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -81.09 (d, *J* = 16.4 Hz, 1F), -82.07 (d, *J* = 16.4 Hz, 1F).

HR-MS (ESI) *m/z*: calculated for $[C_{17}H_{14}F_2O_4S + Na]^+$ 375.0473, measured 375.0477.



2-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)naphthalene (3l)

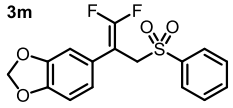
The reaction was carried out as Procedure A using **1l** and **2a**. The product was obtained as colorless oil in 90 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.71 (m, 5H), 7.67 (s, 1H), 7.51 – 7.42 (m, 3H), 7.40 – 7.31 (m, 3H), 4.28 (t, *J* = 2.0 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.38 (t, *J* = 296.1 Hz), 138.57, 133.87, 133.04, 132.63, 129.05, 128.38, 128.36, 128.05, 127.92 (t, *J* = 3.3 Hz), 127.60, 126.68, 126.54, 125.60 – 125.36 (m), 85.97 – 83.49 (m), 56.20 (d, *J* = 2.9 Hz).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -82.80 (dt, *J* = 20.5, 2.3 Hz, 1F), -83.83 (dt, *J* = 20.5, 1.6 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{19}H_{14}F_2O_2S + Na]^+$ 367.0575, measured 367.0579.



5-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)benzo[d][1,3]dioxole (3m)

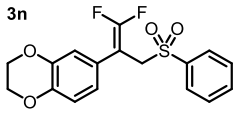
The reaction was carried out as Procedure A using **1m** and **2a**. The product was obtained as colorless oil in 92 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.76 (m, 2H), 7.63 – 7.54 (m, 1H), 7.51 – 7.43 (m, 2H), 6.70 (q, *J* = 1.1 Hz, 3H), 5.92 (s, 2H), 4.10 (t, *J* = 2.1 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.05 (t, *J* = 295.0 Hz), 147.80, 147.39, 138.57, 133.97, 129.16, 128.38, 124.48 (t, *J* = 3.4 Hz), 122.23 (t, *J* = 3.2 Hz), 101.38, 84.44 (t, *J* = 19.7 Hz), 56.34 (d, *J* = 2.9 Hz).

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.15 (d, *J* = 23.1 Hz, 1F), -84.48 (d, *J* = 23.0 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{16}H_{12}F_2O_4S + NH_4]^+$ 356.0763, measured 356.0768.



6-(1,1-Difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)-2,3-dihydrobenzo[b][1,4]dioxine

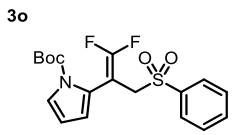
The reaction was carried out as Procedure A using 1n and 2a. The product was obtained as colorless oil in 88 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (dt, *J* = 7.1, 1.3 Hz, 2H), 7.60 – 7.53 (m, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 6.78 – 6.67 (m, 3H), 4.23 – 4.16 (m, 4H), 4.10 (t, *J* = 2.1 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.94 (t, *J* = 295.0 Hz), 143.37, 143.33, 138.51, 133.85, 129.06, 128.35, 123.80 (t, *J* = 3.4 Hz), 121.38 (t, *J* = 3.3 Hz), 117.38, 117.27 (t, *J* = 3.3 Hz), 84.15 (t, *J* = 20.0 Hz), 64.36, 64.25, 56.04 (d, *J* = 3.0 Hz).

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.22 (d, *J* = 23.1 Hz, 1F), -84.69 (d, *J* = 23.1 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{17}H_{14}F_2O_4S + Na]^+$ 375.0473, measured 375.0478.



***Tert*-butyl 2-(1,1-difluoro-3-(phenylsulfonyl)prop-1-en-2-yl)-1H-pyrrole-1-carboxylate (3o)**

The reaction was carried out as Procedure A using **1o** and **2a**. The product was obtained as colorless oil in 90 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as

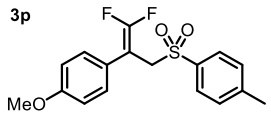
eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.77 (m, 2H), 7.61 (d, *J* = 717.2 Hz, 1H), 7.54 – 7.45 (m, 2H), 7.15 (dd, *J* = 3.4, 1.8 Hz, 1H), 6.17 (dd, *J* = 3.4, 1.7 Hz, 1H), 6.09 (t, *J* = 3.4 Hz, 1H), 4.14 (s, 1H), 1.54 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.53 (dd, *J* = 296.4, 292.2 Hz), 148.62, 138.98, 133.80, 129.20, 128.22, 123.00, 122.30 (dd, *J* = 6.6, 2.6 Hz), 117.46 (t, *J* = 2.0 Hz), 110.88, 84.46, 78.72 (dd, *J* = 25.2, 22.4 Hz), 56.00 (t, *J* = 1.8 Hz), 28.00.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -81.53 (d, *J* = 17.5 Hz, 1F), -84.10 (d, *J* = 17.3 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{18}H_{19}F_2NO_4S + Na]^+$ 406.0895, measured 406.0895.



1-((3,3-Difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)-4-methylbenzene (3p)

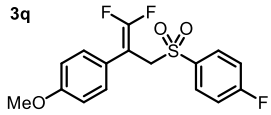
The reaction was carried out as Procedure A using **1a** and **2p**. The product was obtained as pale yellow oil in 75 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.19 – 7.14 (m, 2H), 6.83 – 6.77 (m, 2H), 4.11 (t, *J* = 2.1 Hz, 2H), 3.77 (s, 3H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.19, 155.93 (t, *J* = 294.6 Hz), 144.95, 135.63, 129.74, 129.55 (t, *J* = 3.2 Hz), 128.41, 123.10, 114.03, 84.31 (dd, *J* = 20.6, 19.2 Hz), 56.27 (d, *J* = 3.1 Hz), 55.30, 21.64.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.64 (d, *J* = 24.6 Hz), -85.40 (d, *J* = 24.4 Hz).

HR-MS (ESI) *m*/*z*: calculated for $[C_{17}H_{16}F_2O_3S + Na]^+$ 361.0680, measured 361.0680.



1-((3,3-Difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)-4-fluorobenzene (3q)

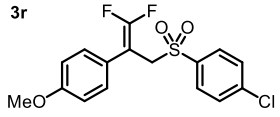
The reaction was carried out as Procedure A using **1a** and **2q**. The product was obtained as colorless oil in 78 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 – 7.74 (m, 2H), 7.17 – 7.07 (m, 4H), 6.83 – 6.77 (m, 2H), 4.14 (t, *J* = 2.1 Hz, 2H), 3.77 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.21, 164.66, 159.32, 155.98 (t, *J* = 295.8 Hz), 134.63 (d, *J* = 3.2 Hz), 131.34 (d, *J* = 9.6 Hz), 129.49 (t, *J* = 3.2 Hz), 122.78 (t, *J* = 3.3 Hz), 116.43 (d, *J* = 22.7 Hz), 114.16, 84.23 (dd, *J* = 20.6, 19.1 Hz), 56.33 (d, *J* = 3.2 Hz), 55.35.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.43 (d, *J* = 23.9 Hz, 1F), -85.11 (d, *J* = 23.8 Hz, 1F), -103.13 (1F).

HR-MS (APCI+) *m*/*z*: calculated for $[C_{16}H_{13}F_3O_3S + H]^+$ 343.0160, measured 343.0162.



1-Chloro-4-((3,3-difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)benzene (3r)

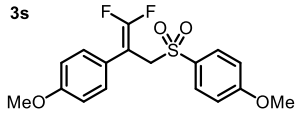
The reaction was carried out as Procedure A using **1a** and **2r**. The product was obtained as colorless oil in 69 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.6 Hz, 2H), 7.44 – 7.32 (m, 2H), 7.11 (dd, *J* = 8.9, 1.3 Hz, 2H), 6.84 – 6.72 (m, 2H), 4.14 (d, *J* = 2.0 Hz, 2H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.33, 155.98 (t, *J* = 295.0 Hz), 140.63, 137.08, 129.90, 129.49 (t, *J* = 3.1 Hz), 129.39, 114.13, 84.14 (dd, *J* = 20.8, 19.2 Hz), 56.26 (d, *J* = 3.2 Hz), 55.35.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.28 (d, *J* = 23.6 Hz, 1F), -84.98 (d, *J* = 23.5 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{16}H_{13}ClF_2O_3S + Na]^+$ 381.0134, measured 381.0136.



1-((3,3-Difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)-4-methoxybenzene (3s)

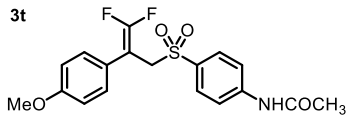
The reaction was carried out as Procedure A using **1a** and **2s**. The product was obtained as colorless oil in 79 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.9 Hz, 1H), 7.16 (dd, *J* = 8.9, 1.3 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 1H), 6.80 (d, *J* = 8.9 Hz, 1H), 4.10 (s, 1H), 3.83 (s, 3H), 3.77 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.91, 159.15, 155.93 (t, *J* = 294.6 Hz), 130.61, 129.98, 129.54 (t, *J* = 3.3 Hz), 123.11 (t, *J* = 3.3 Hz), 114.32, 114.07, 84.73 – 84.15 (m), 56.38 (d, *J* = 3.0 Hz), 55.73, 55.32.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.75 (d, *J* = 24.5 Hz, 1F), -85.50 (d, *J* = 24.5 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{17}H_{16}F_2O_4S + Na]^+$ 377.0627, measured 377.0627.



***N*-(4-((3,3-difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)phenyl)acetamide (3t)**

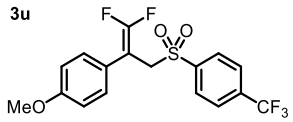
The reaction was carried out as Procedure A using **1a** and **2t**. The product was obtained as pale yellow oil in 80 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 1 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.68 (m, 2H), 7.61 (d, *J* = 8.6 Hz, 2H), 7.49 (s, 1H), 7.22 – 7.15 (m, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.12 (d, *J* = 2.0 Hz, 2H), 3.79 (s, 3H), 2.21 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.38, 159.30, 155.97 (t, *J* = 294.8 Hz), 143.66, 132.49, 129.59, 129.53 (t, *J* = 3.2 Hz), 122.95, 119.23, 114.18, 84.58 – 83.86 (m), 56.41 (d, *J* = 3.0 Hz), 55.34, 24.67.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -84.49 (d, *J* = 24.1 Hz), -85.11 (d, *J* = 24.0 Hz).

HR-MS (ESI) *m*/*z*: calculated for $[C_{18}H_{17}F_2NO_4S + H]^+$ 382.0919, measured 382.0923.



1-((3,3-Difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)-4-(trifluoromethyl)benzene (3u)

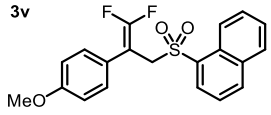
The reaction was carried out as Procedure A using **1a** and **2u**. The product was obtained as colorless oil in 54 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.64 (d, *J* = 8.1 Hz, 2H), 7.08 – 7.01 (m, 2H), 6.73 (d, *J* = 8.8 Hz, 2H), 4.20 (d, *J* = 2.1 Hz, 2H), 3.74 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.35, 156.09 (t, *J* = 295.2 Hz), 142.19, 135.39 (q, *J* = 33.1 Hz), 129.43, 129.13, 126.14 (q, *J* = 3.7 Hz), 123.12 (d, *J* = 273.2 Hz), 122.40 (t, *J* = 3.3 Hz), 114.11, 83.97 (dd, *J* = 21.2, 19.3 Hz), 56.14 (d, *J* = 3.2 Hz), 55.21.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -63.35, -84.15 (d, *J* = 22.9 Hz, 1F), -84.87 (d, *J* = 23.3 Hz, 1F).

HR-MS (APCI+) *m*/*z*: calculated for $[C_{17}H_{13}F_5O_3S + H]^+$ 394.0578, measured 394.0581.



1-((3,3-Difluoro-2-(4-methoxyphenyl)allyl)sulfonyl)naphthalene (3v)

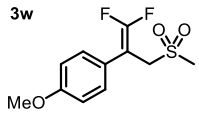
The reaction was carried out as Procedure A using 1a and 2v. The product was obtained as colorless oil in 68 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 8.3 Hz, 1H), 8.18 – 8.12 (m, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 1.4 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.64 – 7.55 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 2H), 6.60 (d, *J* = 8.8 Hz, 2H), 4.33 (t, *J* = 2.0 Hz, 2H), 3.73 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.87, 155.99 (t, *J* = 294.8 Hz), 135.42, 134.06, 133.79, 131.25, 129.22, 129.18, 128.96, 128.75, 126.94, 124.26, 123.78, 122.62 (t, *J* = 3.3 Hz), 113.66, 84.12 (dd, *J* = 21.2, 19.5 Hz), 55.54 (d, *J* = 3.1 Hz), 55.23.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -84.41 (d, *J* = 23.9 Hz), -85.25 (d, *J* = 23.9 Hz).

HR-MS (ESI) *m*/*z*: calculated for $[C_{20}H_{16}F_2O_3S + NH_4]^+$ 392.1127, measured 392.1124.



1-(1,1-Difluoro-3-(methylsulfonyl)prop-1-en-2-yl)-4-methoxybenzene (3w)

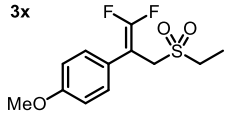
The reaction was carried out as Procedure A using **1b** and **2w**. The product was obtained as colorless oil in 94 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.29 (m, 2H), 6.96 – 6.89 (m, 2H), 4.03 (s, 2H), 3.81 (s, 3H), 2.67 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.62, 156.05 (t, *J* = 294.6 Hz), 129.69 (t, *J* = 3.2 Hz), 122.99, 114.54, 84.36 (dd, *J* = 21.2, 19.7 Hz), 55.37, 55.03 (d, *J* = 2.9 Hz), 41.16 (d, *J* = 1.6 Hz).

^{19}F NMR (377 MHz, Chloroform-*d*) δ -84.04 (d, *J* = 25.1 Hz, 1F), -84.92 (d, *J* = 24.6 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{11}H_{12}F_2O_3S + Na]^+$ 285.0367, measured 285.0370.



1-(3-(Ethylsulfonyl)-1,1-difluoroprop-1-en-2-yl)-4-methoxybenzene (3x)

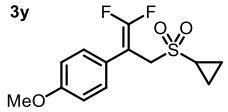
The reaction was carried out as Procedure A using **1b** and **2x**. The product was obtained as pale yellow oil in 78 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.28 (m, 2H), 6.96 – 6.88 (m, 2H), 3.99 (d, *J* = 1.7 Hz, 1H), 3.80 (s, 3H), 2.76 (q, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.56, 156.07 (t, *J* = 294.5 Hz), 129.70 (t, *J* = 3.1 Hz), 123.16, 114.45, 84.09 (dd, *J* = 21.3, 19.8 Hz), 55.36, 52.49 (d, *J* = 2.8 Hz), 47.55, 6.28.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -84.21 (d, *J* = 25.0 Hz, 1F), -85.04 (d, *J* = 25.0 Hz, 1F).

HR-MS (ESI) *m*/*z*: calculated for $[C_{12}H_{14}F_2O_3S + Na]^+$ 299.0524, measured 299.0527.



1-(3-(Cyclopropylsulfonyl)-1,1-difluoroprop-1-en-2-yl)-4-methoxybenzene (3y)

The reaction was carried out as Procedure A using **1b** and **2y**. The product was obtained as colorless oil in 59 % yield by flash column chromatography with ethyl acetate : petroleum ether = 1 : 4 as eluent.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.30 (m, 2H), 6.95 – 6.87 (m, 2H), 4.06 (t, *J* = 2.0 Hz, 2H), 3.79 (s, 2H), 2.12 (tt, *J* = 8.0, 4.8 Hz, 1H), 1.18 – 1.09 (m, 2H), 0.89 – 0.80 (m, 2H).

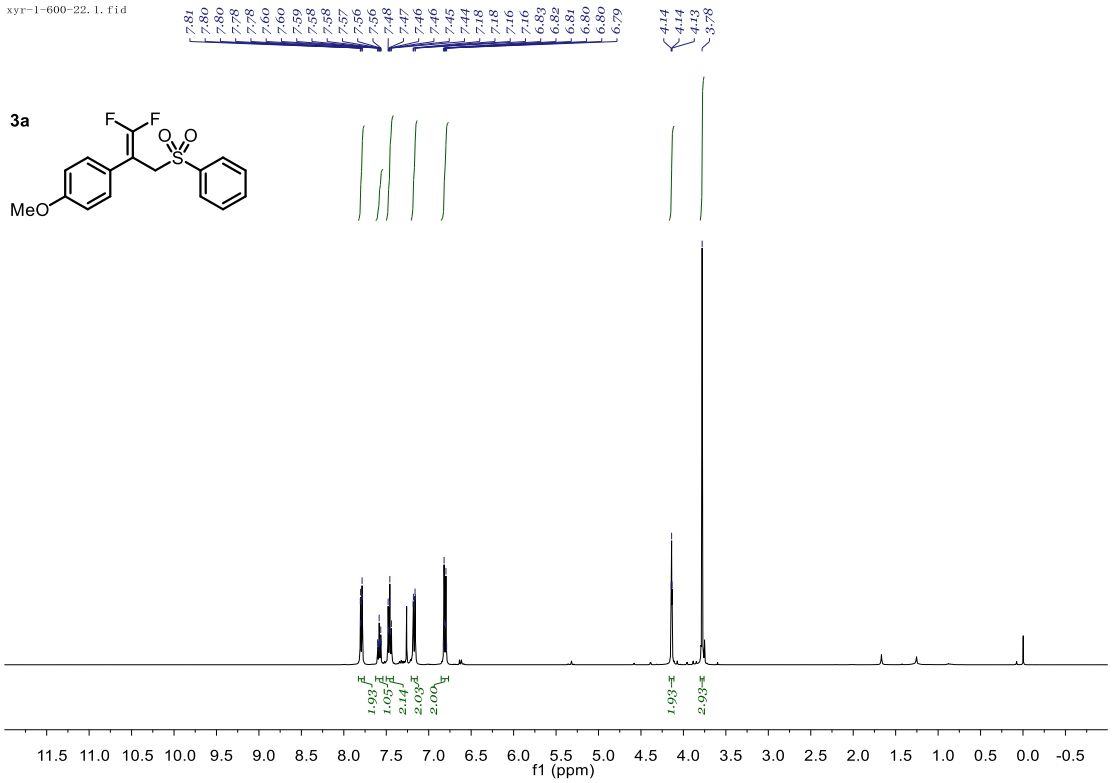
^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.38, 155.98 (t, *J* = 294.3 Hz), 129.61 (t, *J* = 3.3 Hz), 123.39, 114.26, 86.34 – 83.18 (m), 57.96 – 52.63 (m), 29.95 (d, *J* = 1.6 Hz), 5.10.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -84.24 (dt, *J* = 25.4, 2.3 Hz, 1F), -85.42 (d, *J* = 25.3 Hz, 1F).

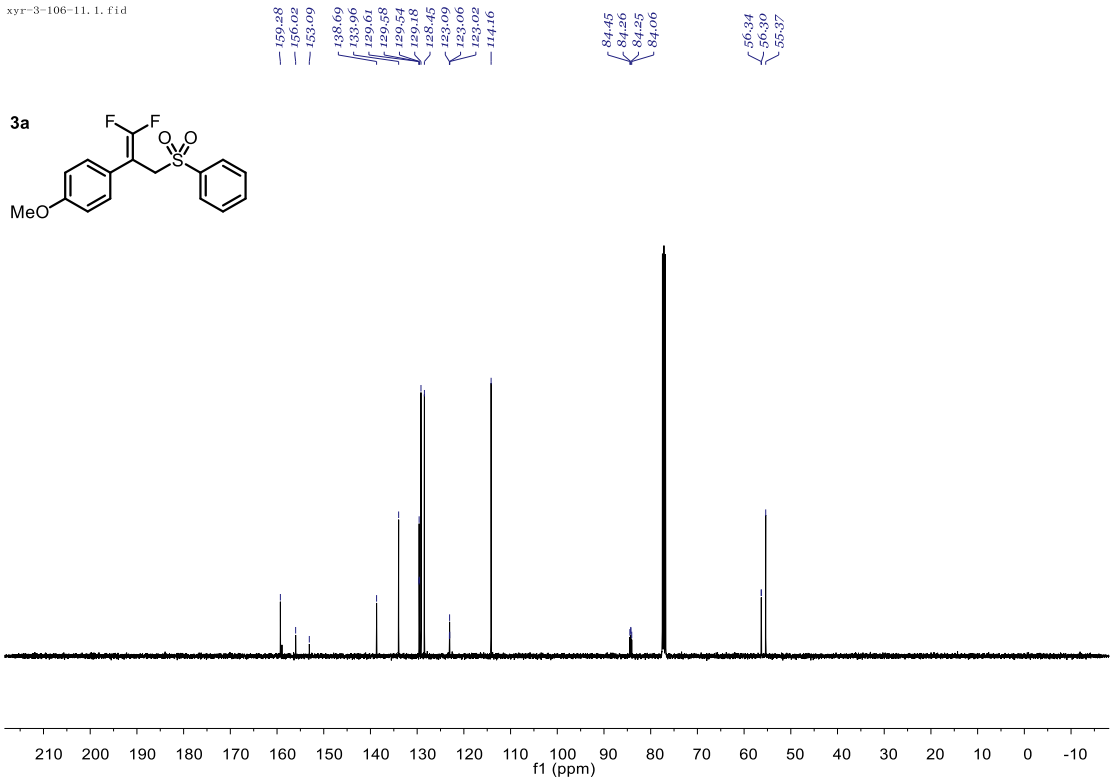
HR-MS (ESI) *m*/*z*: calculated for $[C_{13}H_{14}F_2O_3S + Na]^+$ 311.0524, measured 311.0545.

VI. NMR Spectrum

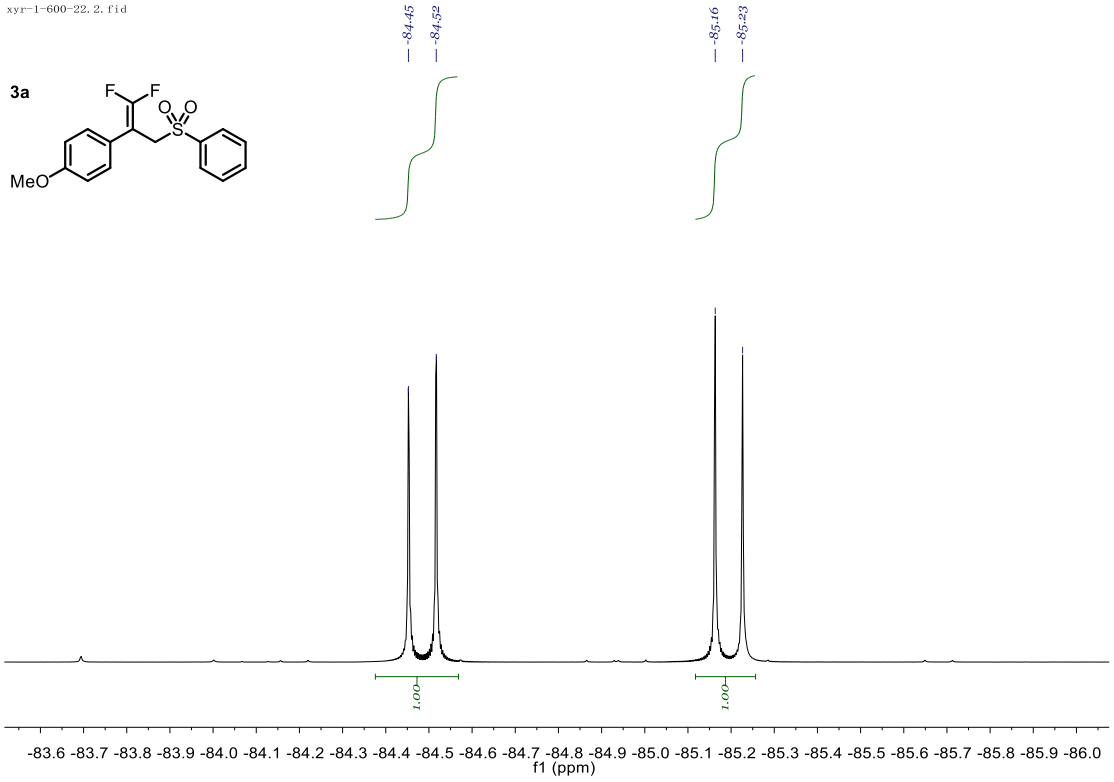
^{1}H NMR (400 MHz, Chloroform-*d*)



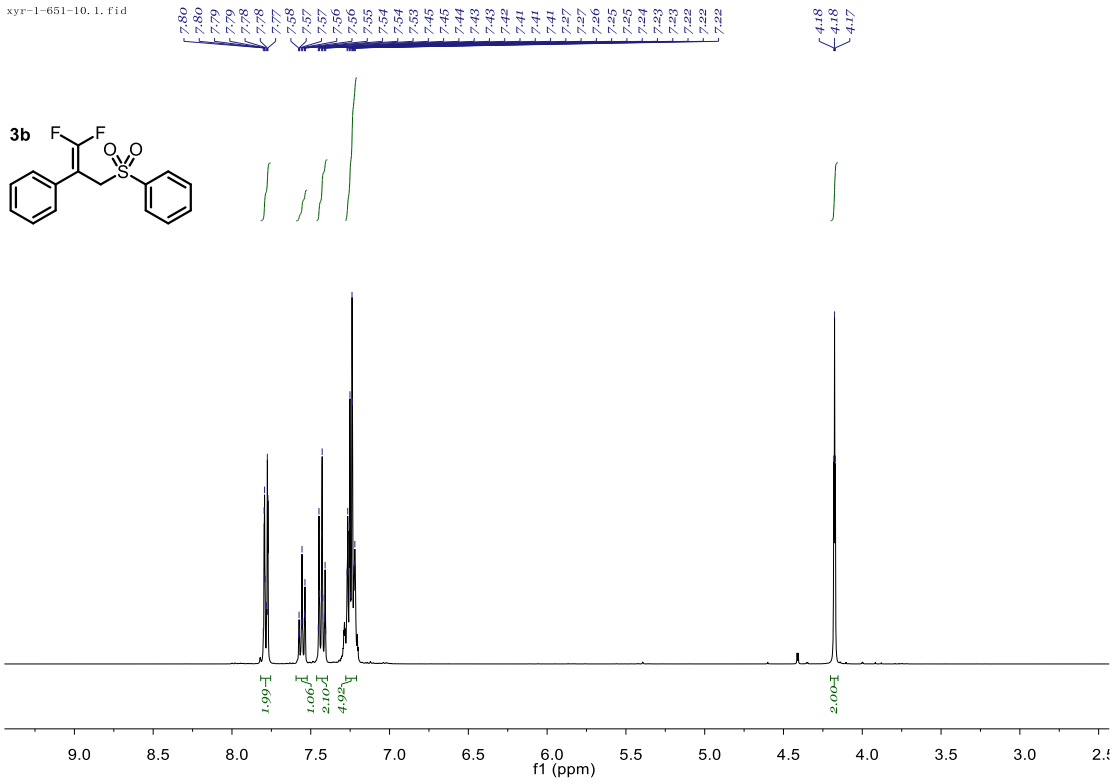
^{13}C NMR (101 MHz, Chloroform-*d*)



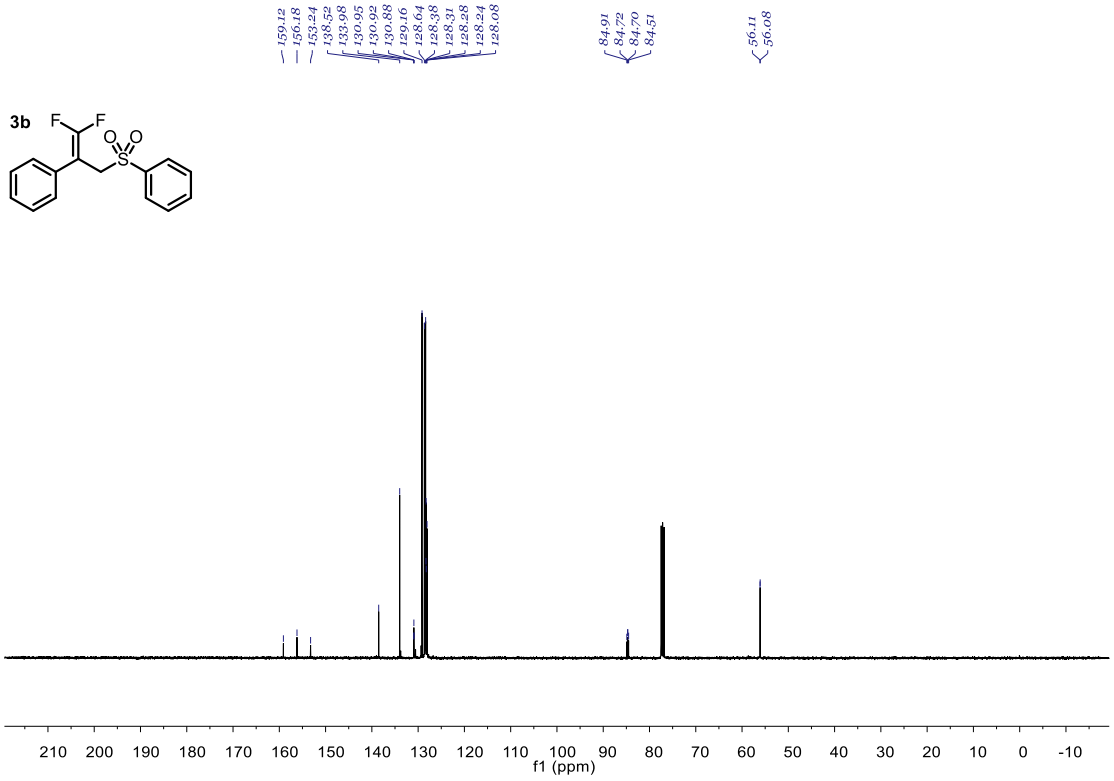
^{19}F NMR (377 MHz, Chloroform-*d*)



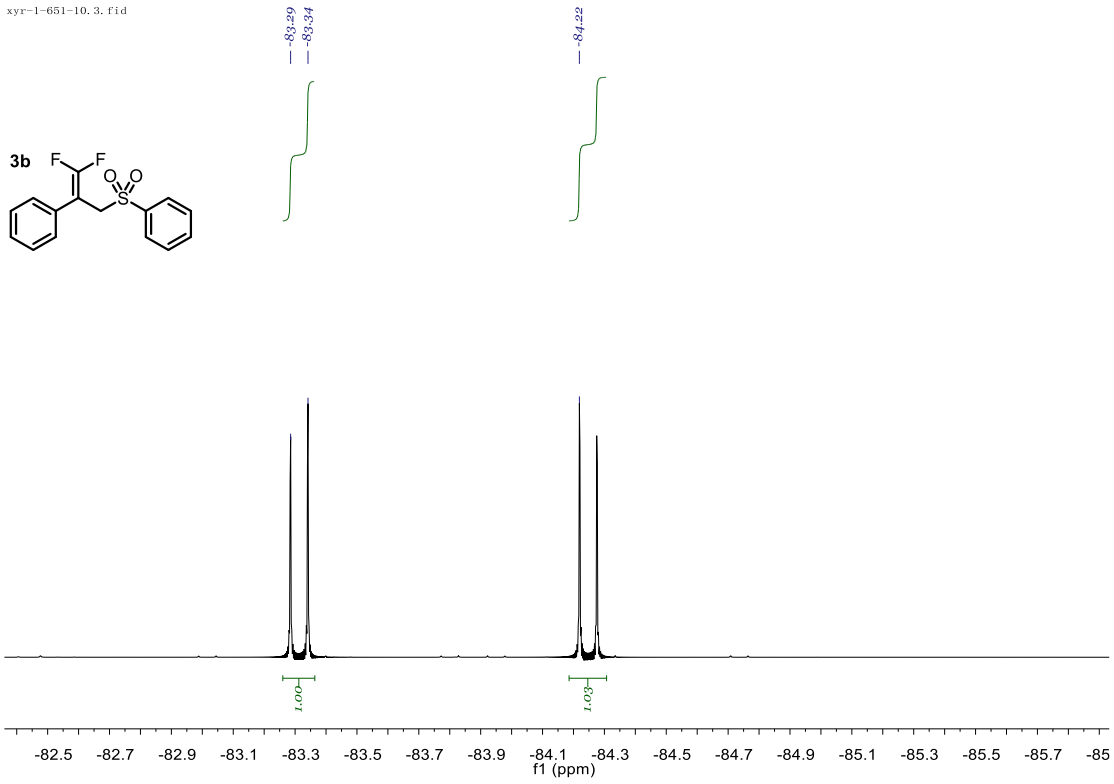
^{1}H NMR (400 MHz, Chloroform-*d*)



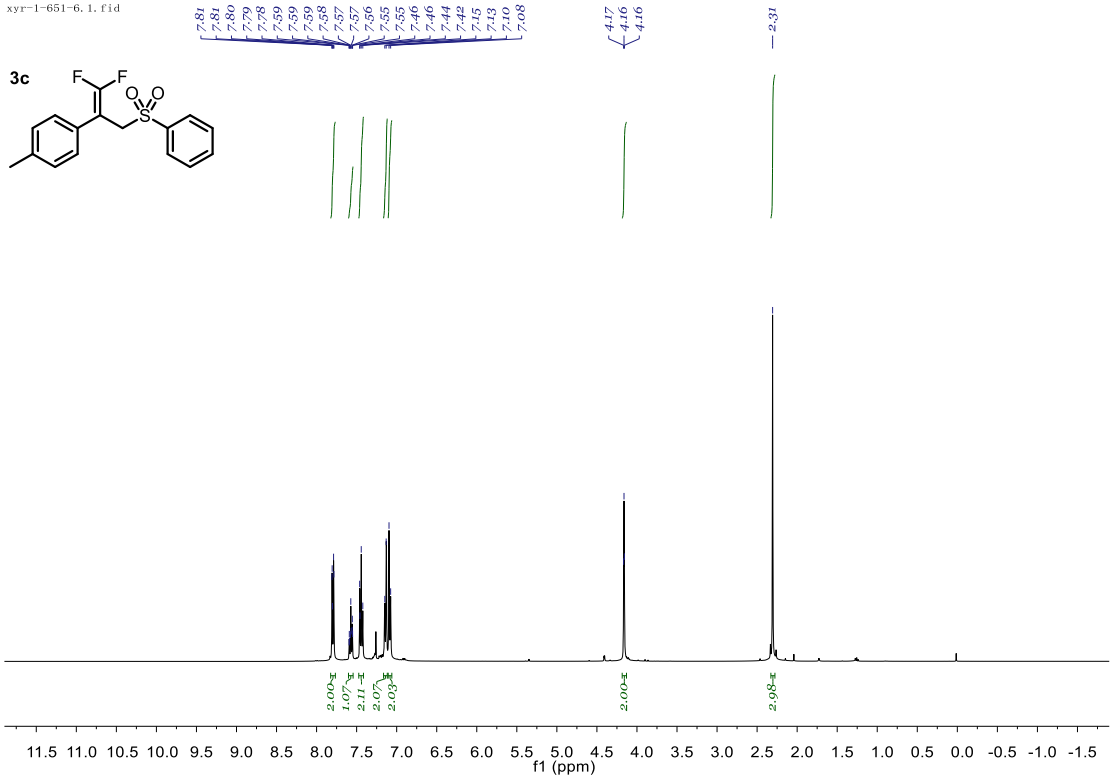
^{13}C NMR (101 MHz, Chloroform-*d*)



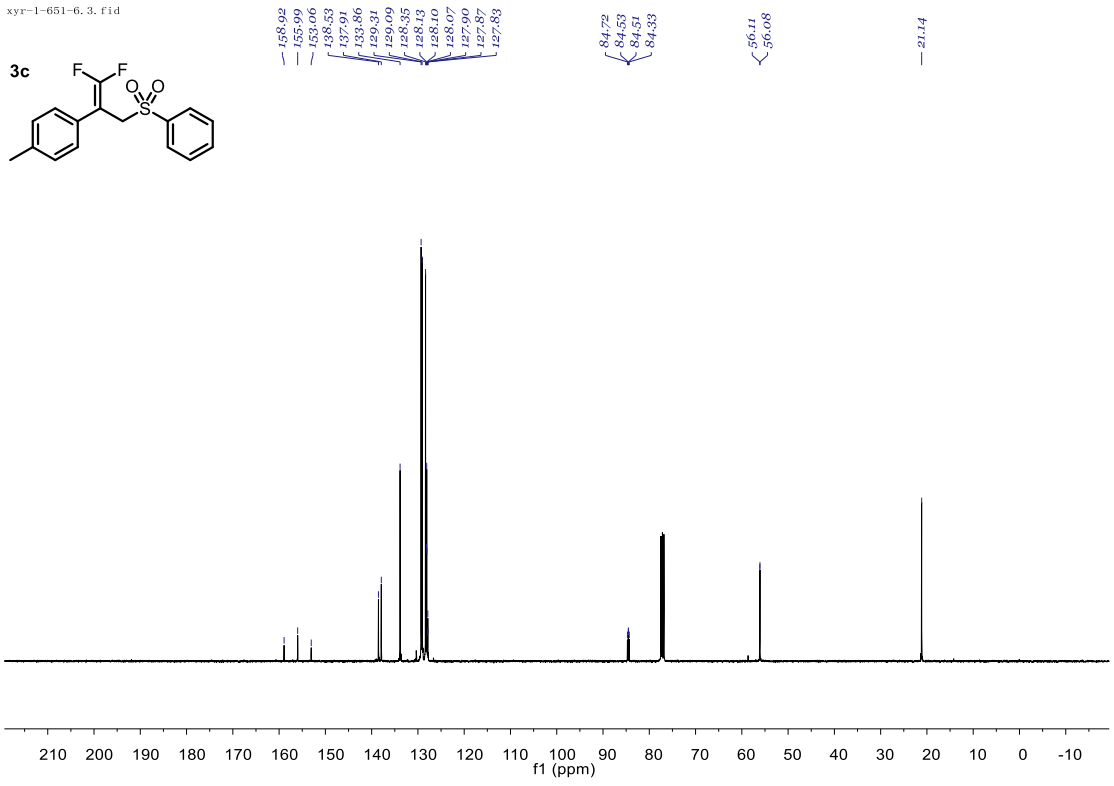
^{19}F NMR (377 MHz, Chloroform-*d*)



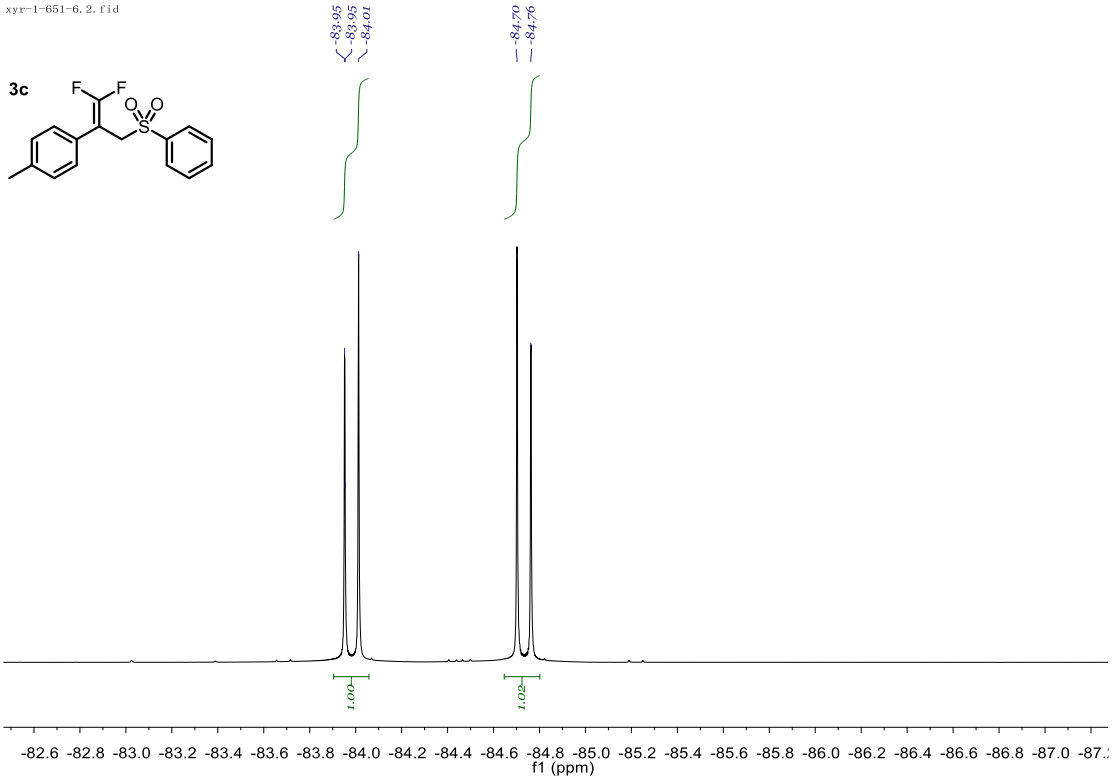
^{1}H NMR (400 MHz, Chloroform-*d*)



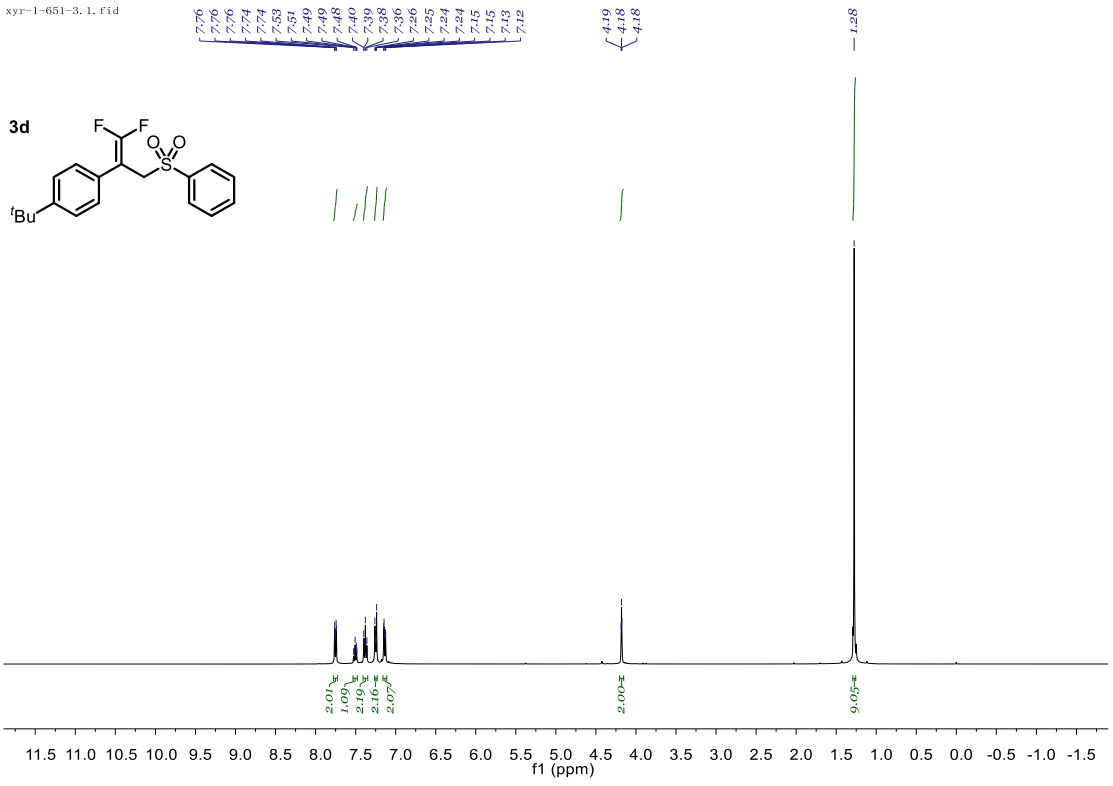
^{13}C NMR (101 MHz, Chloroform-*d*)



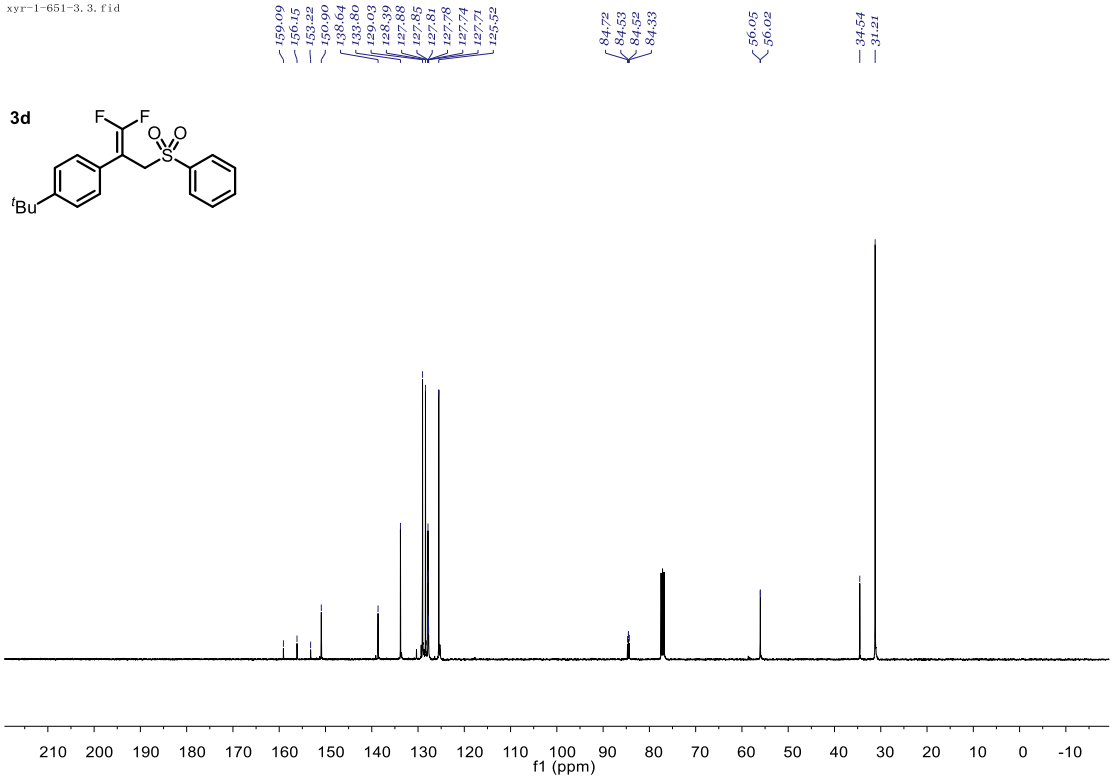
^{19}F NMR (377 MHz, Chloroform-*d*)



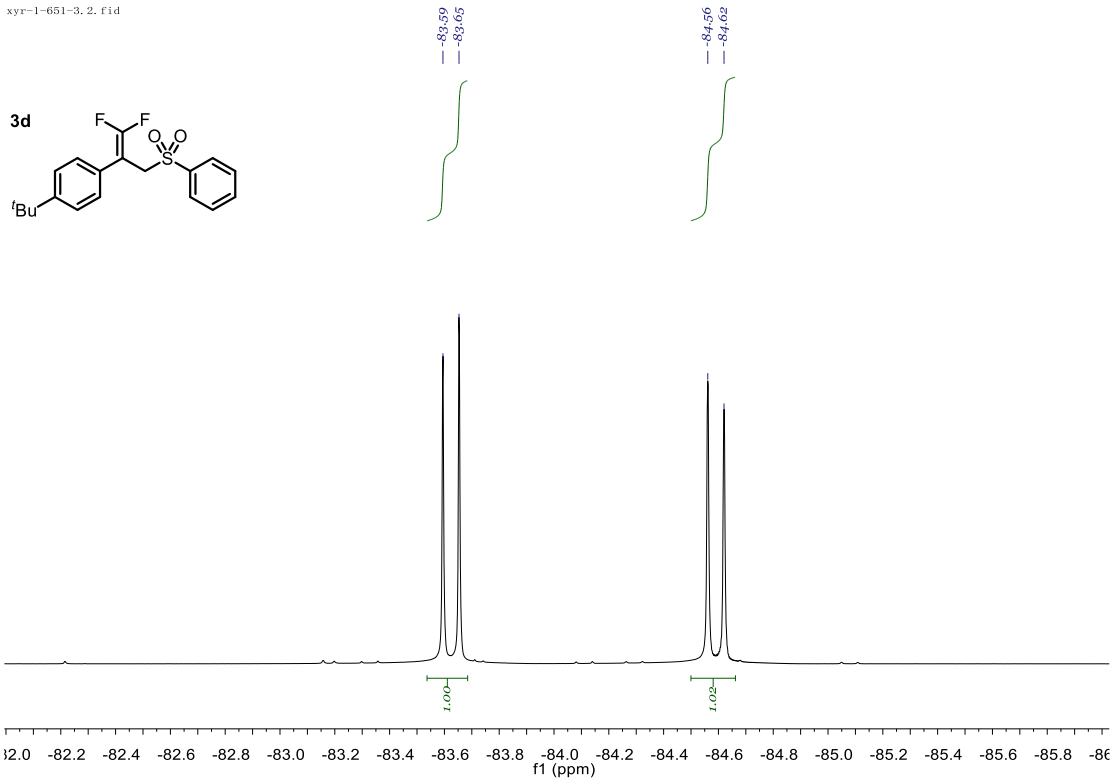
^{1}H NMR (400 MHz, Chloroform-*d*)



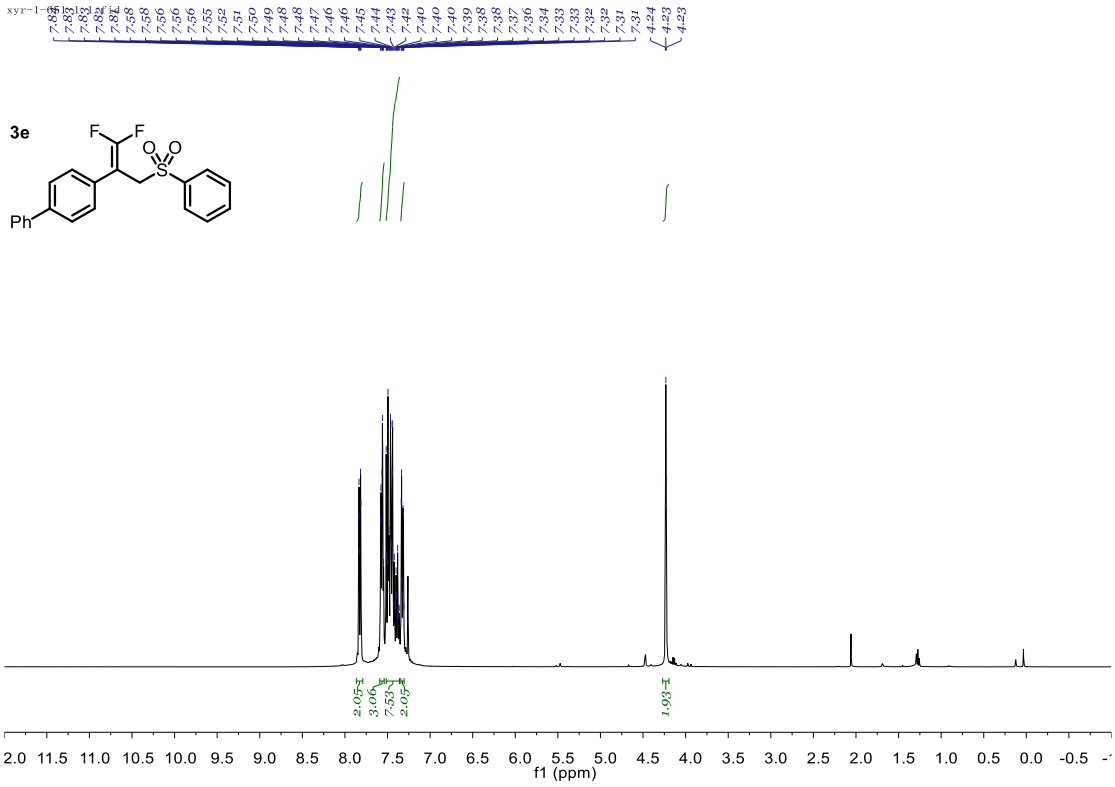
^{13}C NMR (101 MHz, Chloroform-*d*)



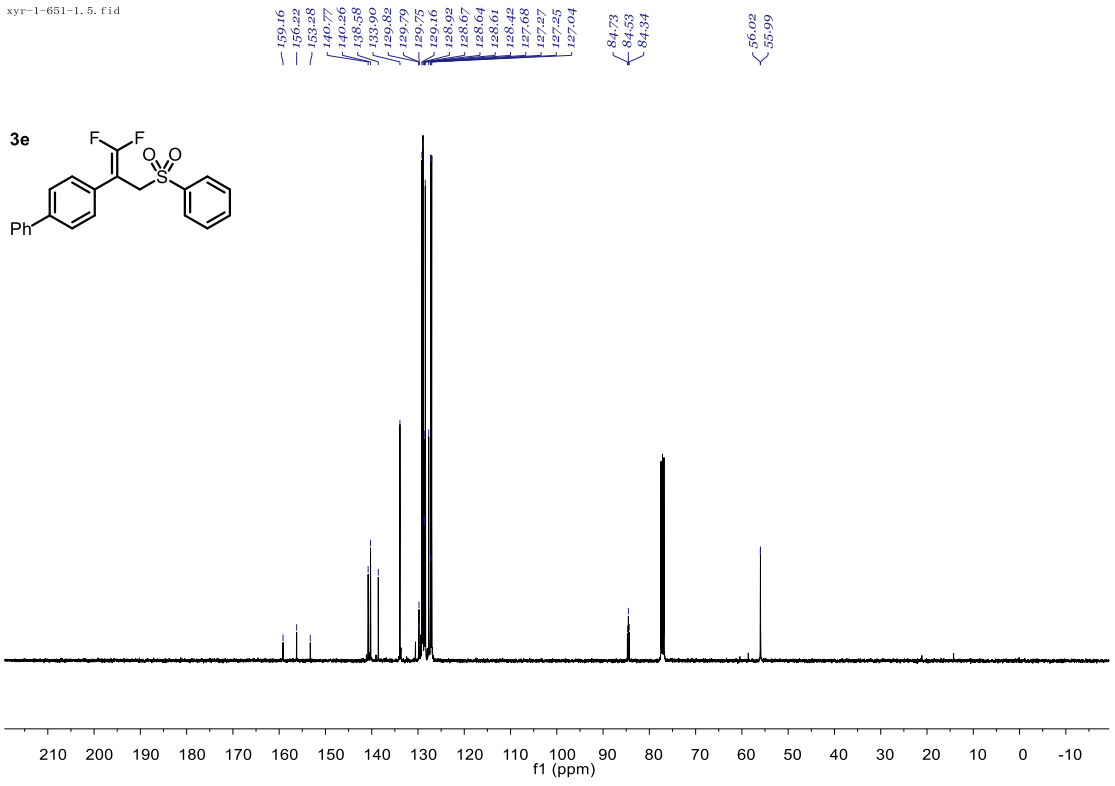
^{19}F NMR (377 MHz, Chloroform-*d*)



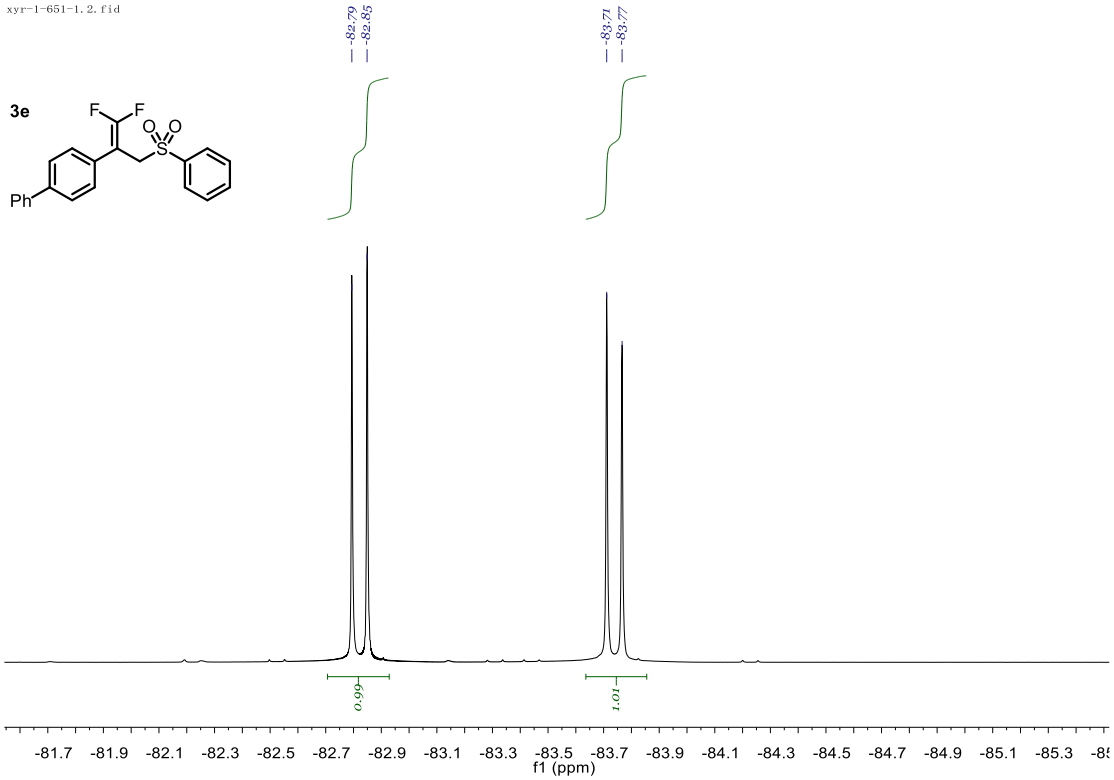
^{1}H NMR (400 MHz, Chloroform-*d*)



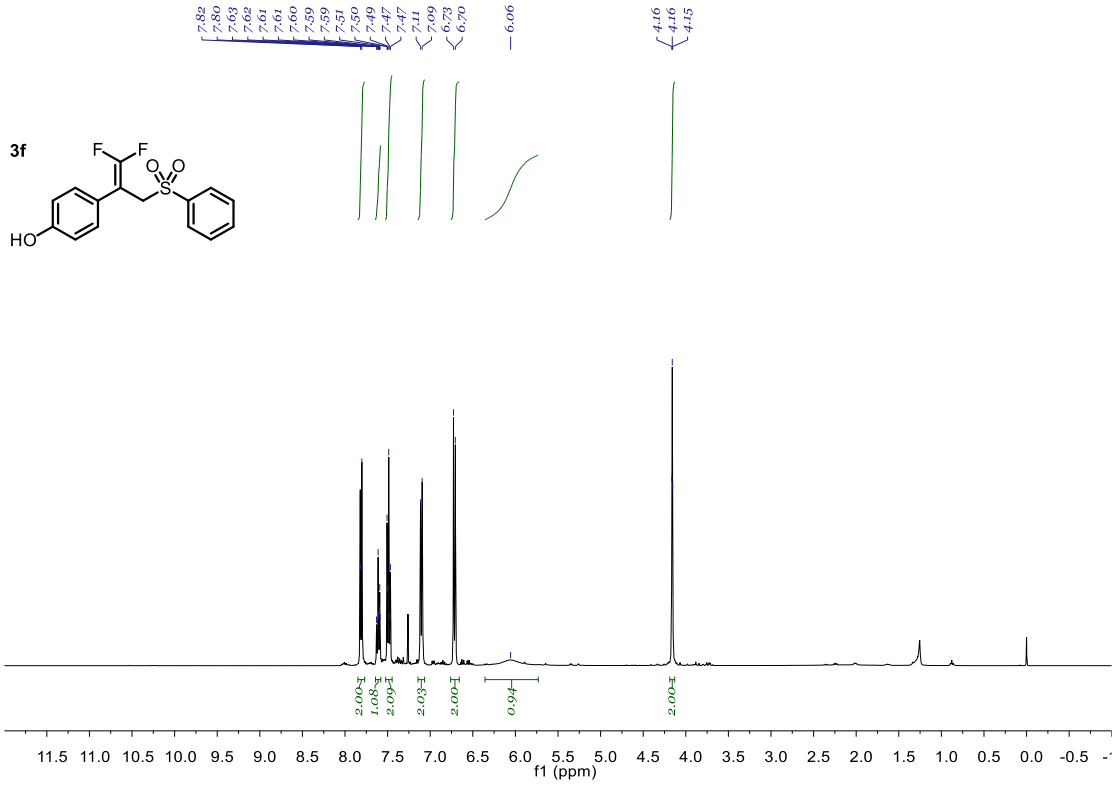
^{13}C NMR (101 MHz, Chloroform-*d*)



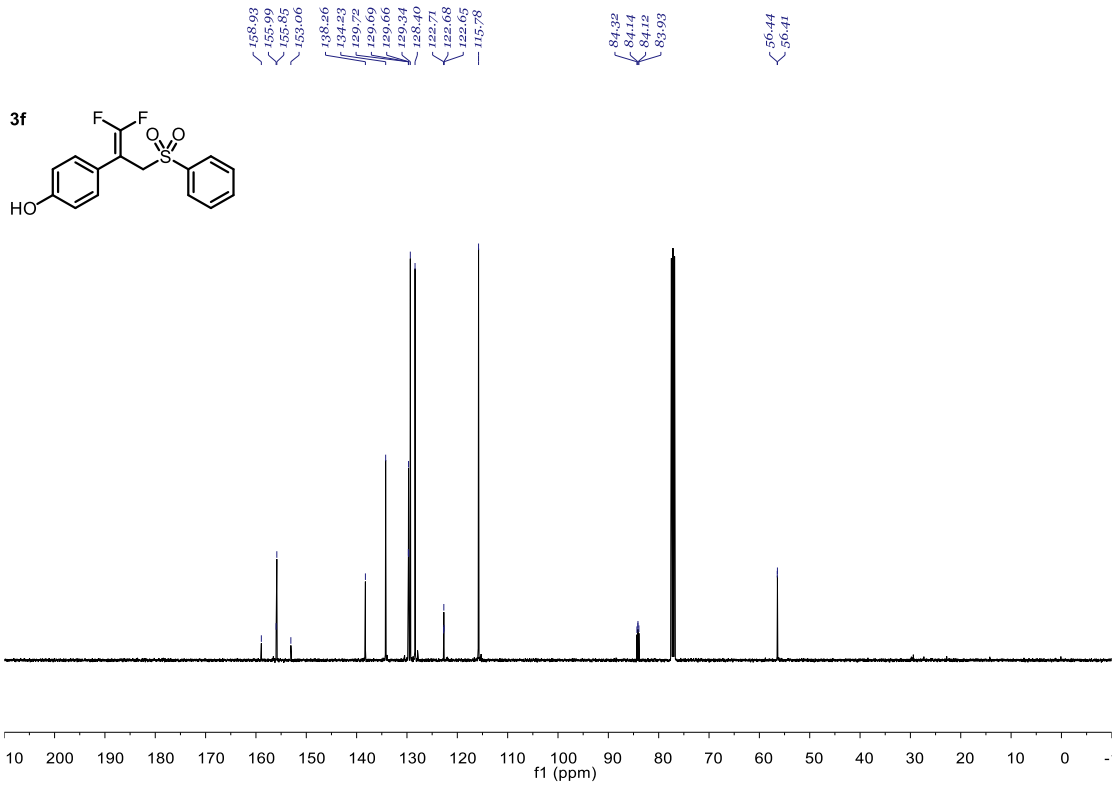
^{19}F NMR (377 MHz, Chloroform-*d*)



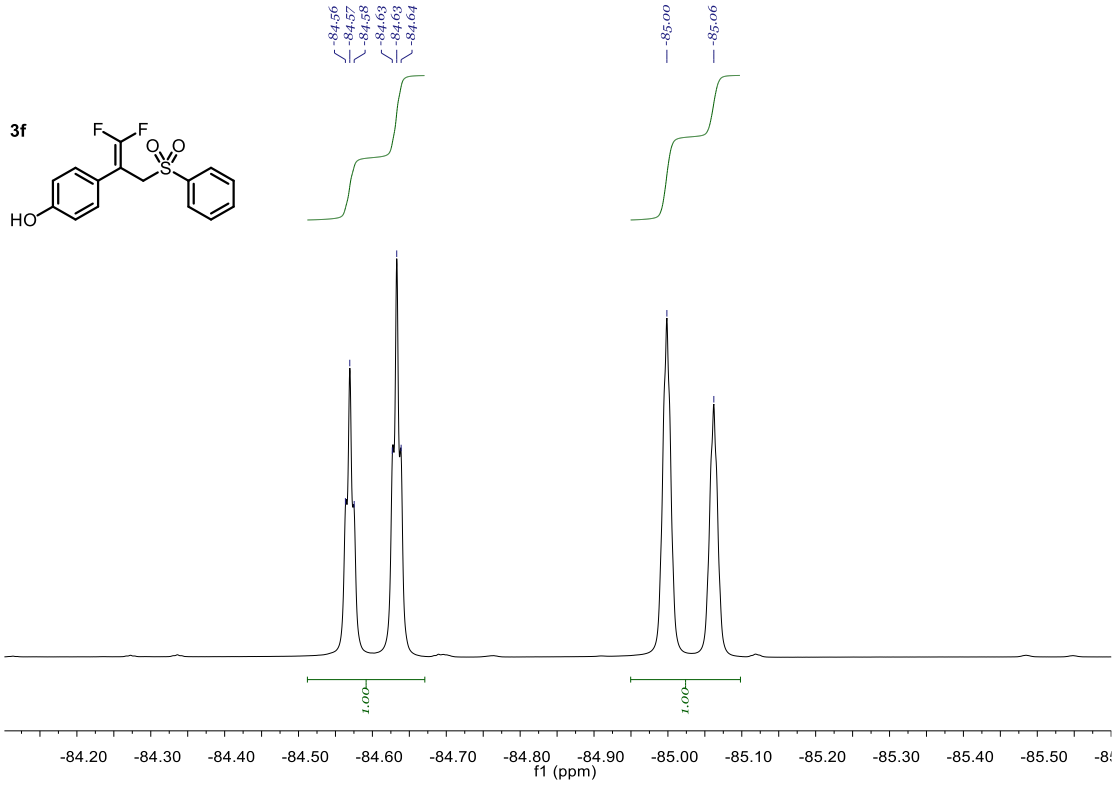
^{1}H NMR (400 MHz, Chloroform-*d*)



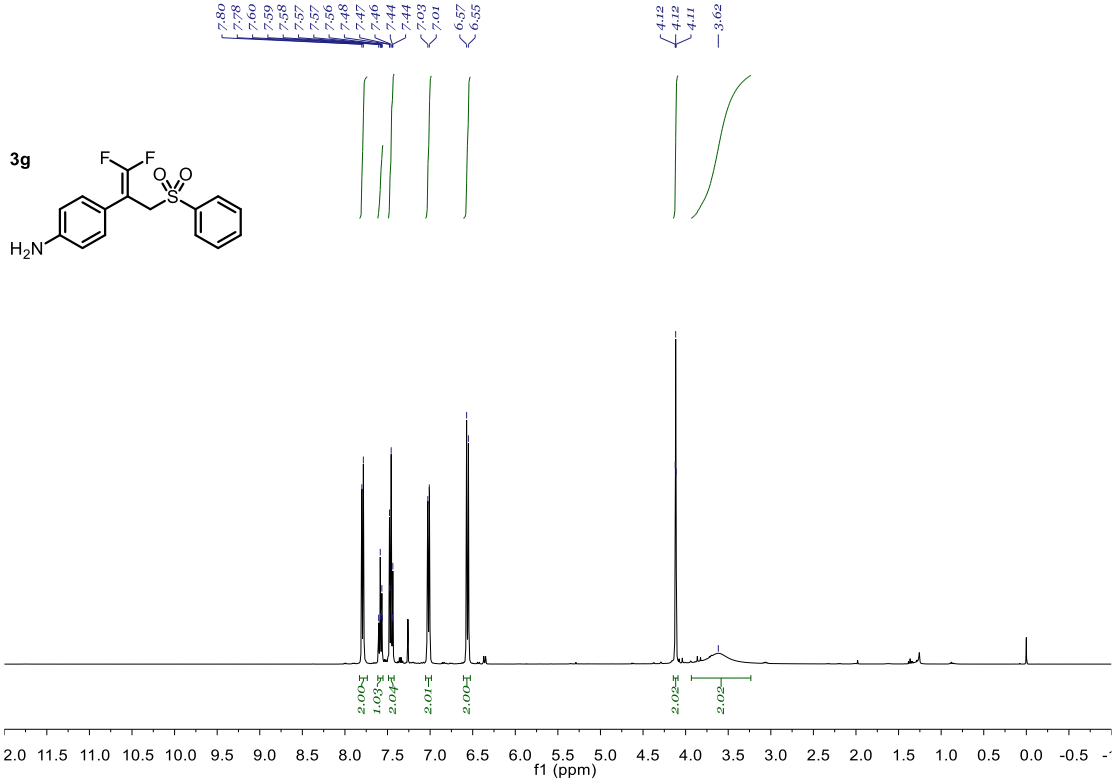
^{13}C NMR (101 MHz, Chloroform-*d*)



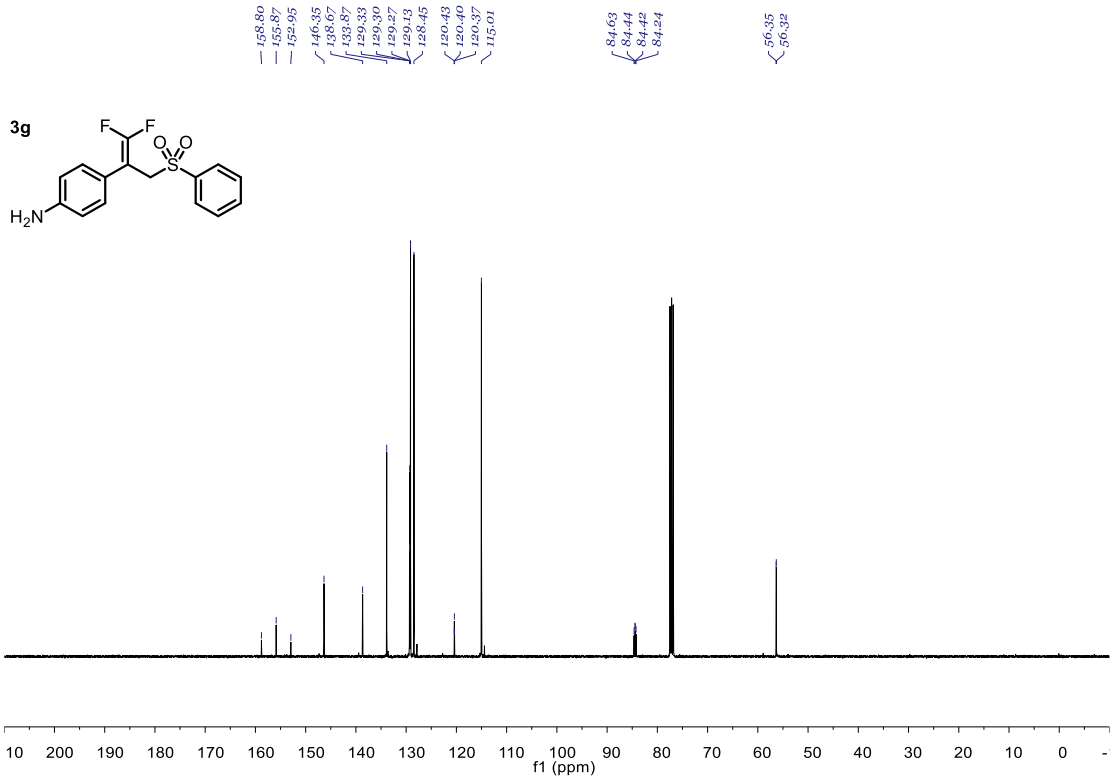
^{19}F NMR (377 MHz, Chloroform-*d*)



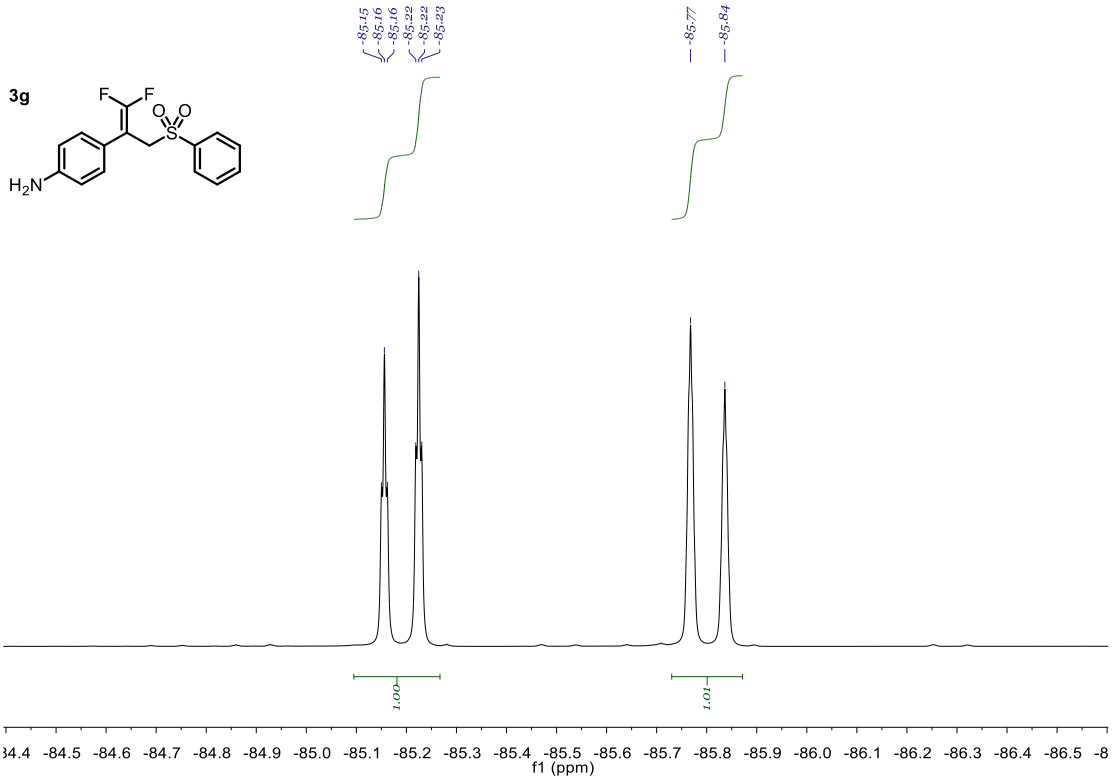
^{1}H NMR (400 MHz, Chloroform-*d*)



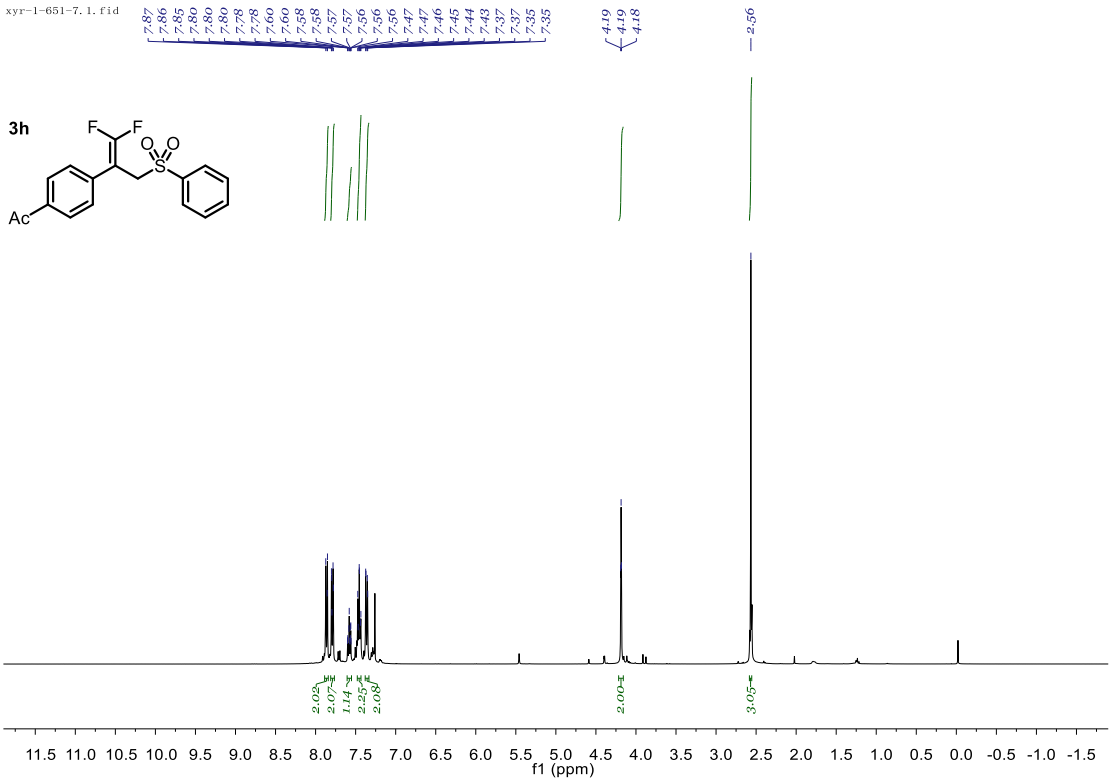
^{13}C NMR (101 MHz, Chloroform-*d*)



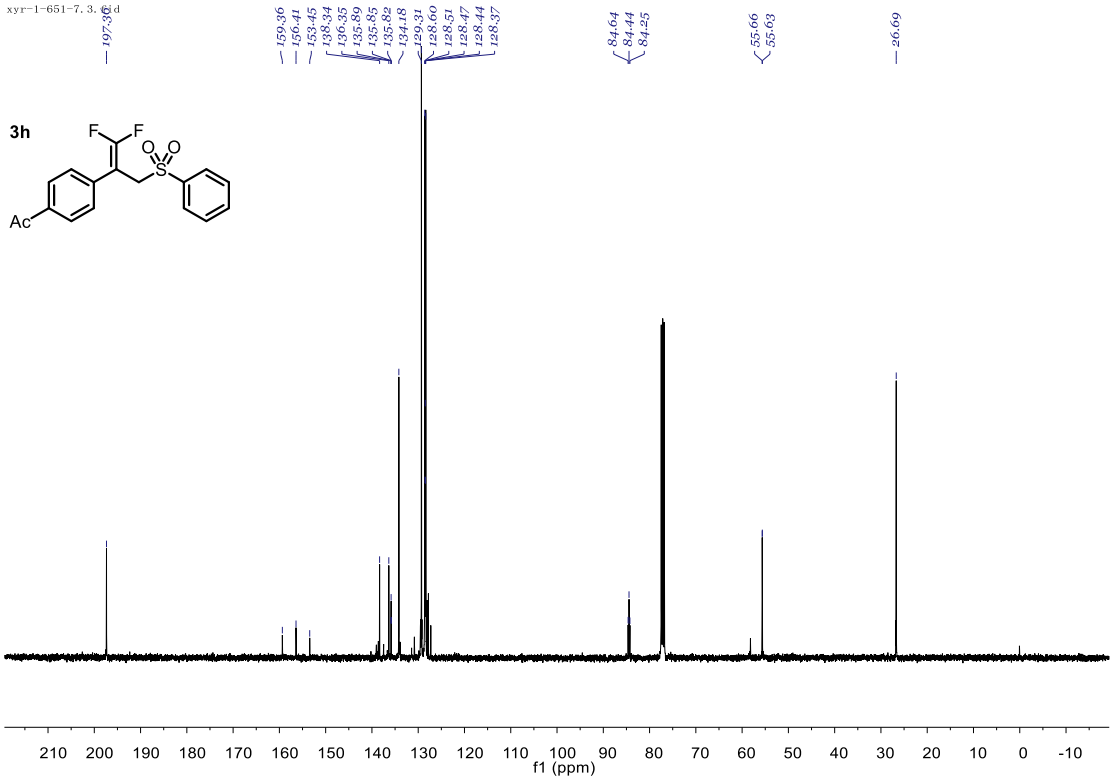
^{19}F NMR (377 MHz, Chloroform-*d*)



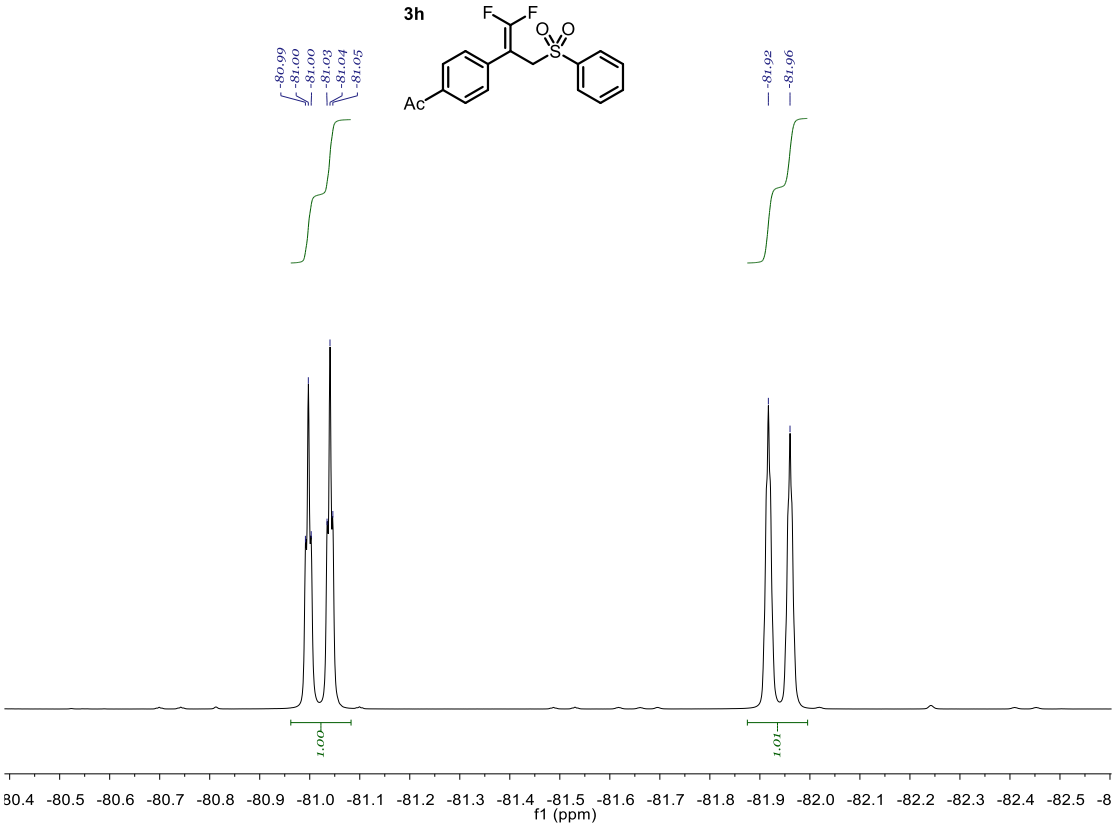
^{1}H NMR (400 MHz, Chloroform-*d*)



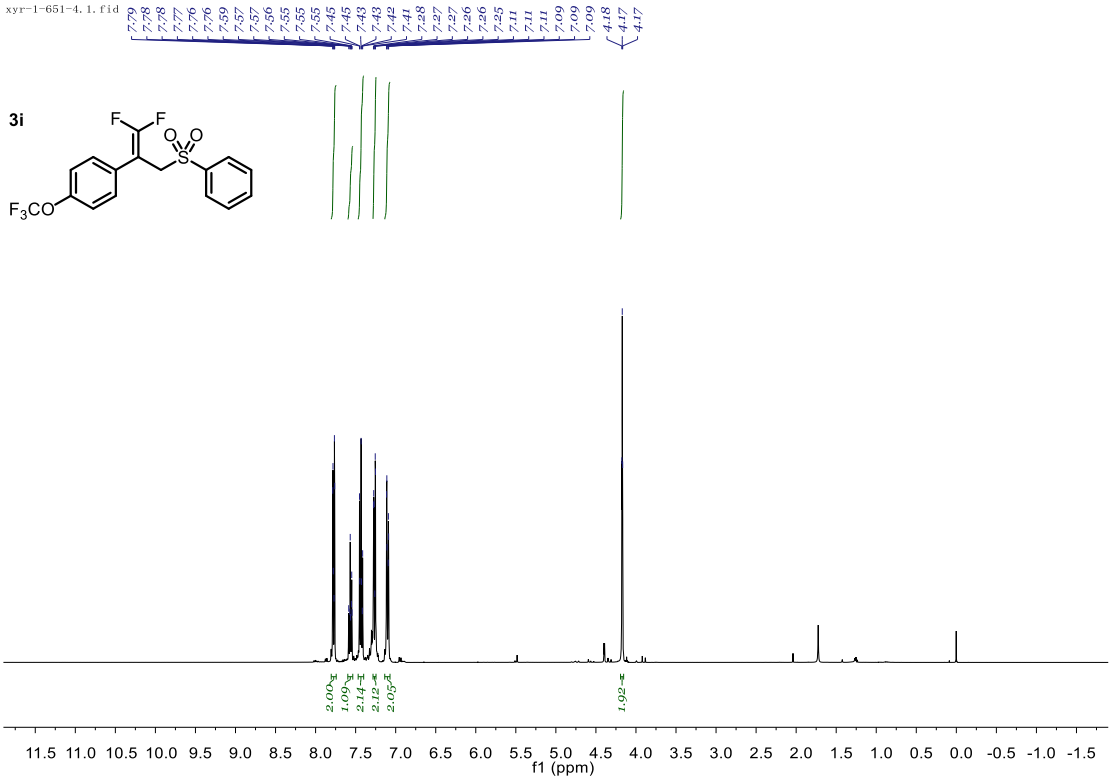
^{13}C NMR (101 MHz, Chloroform-*d*)



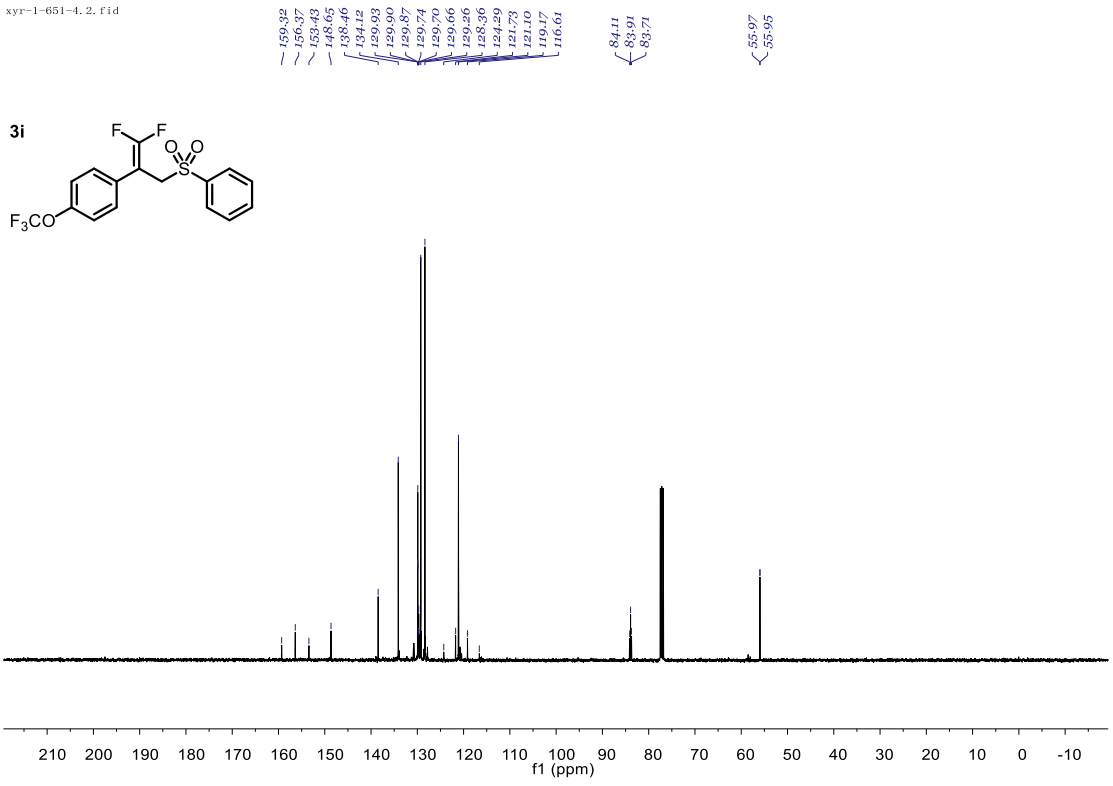
^{19}F NMR (377 MHz, Chloroform-*d*)



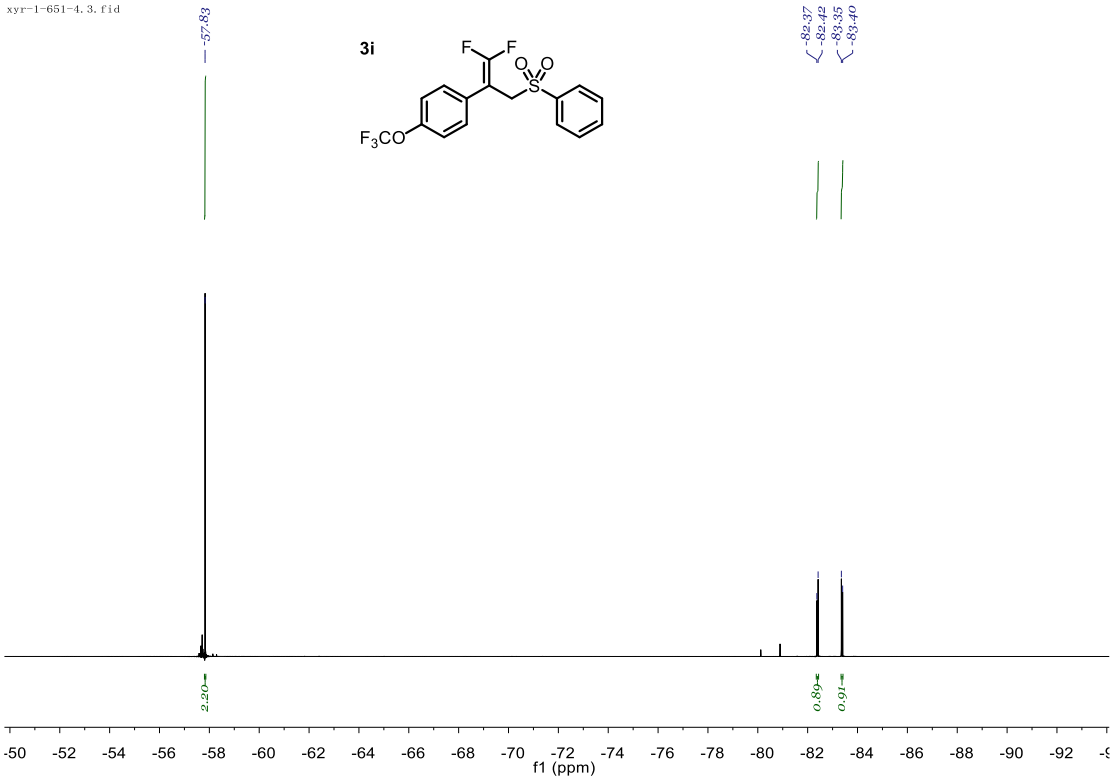
^{1}H NMR (400 MHz, Chloroform-*d*)



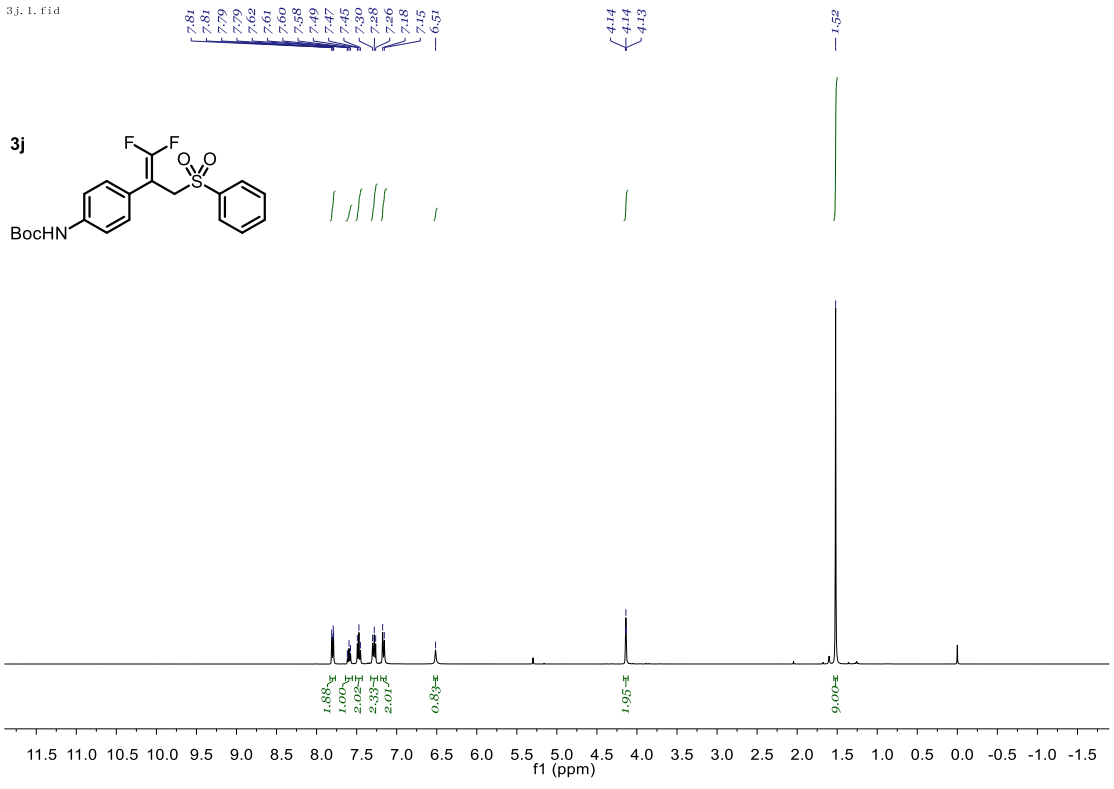
^{13}C NMR (101 MHz, Chloroform-*d*)



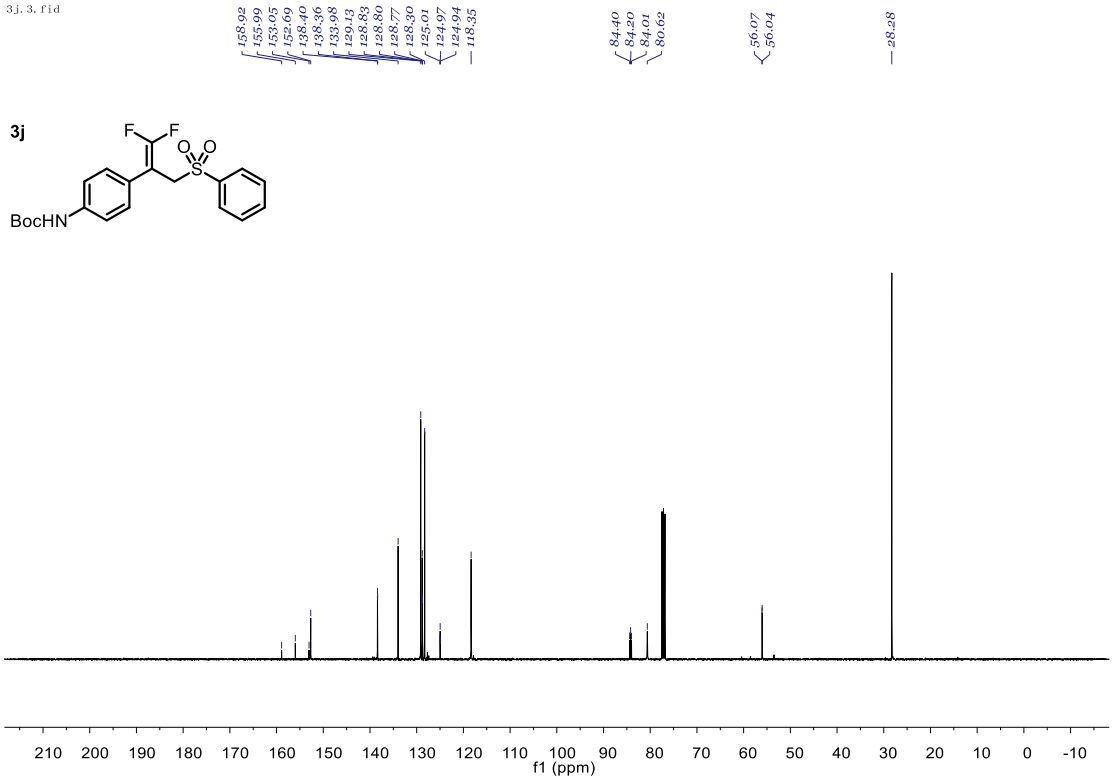
^{19}F NMR (377 MHz, Chloroform-*d*)



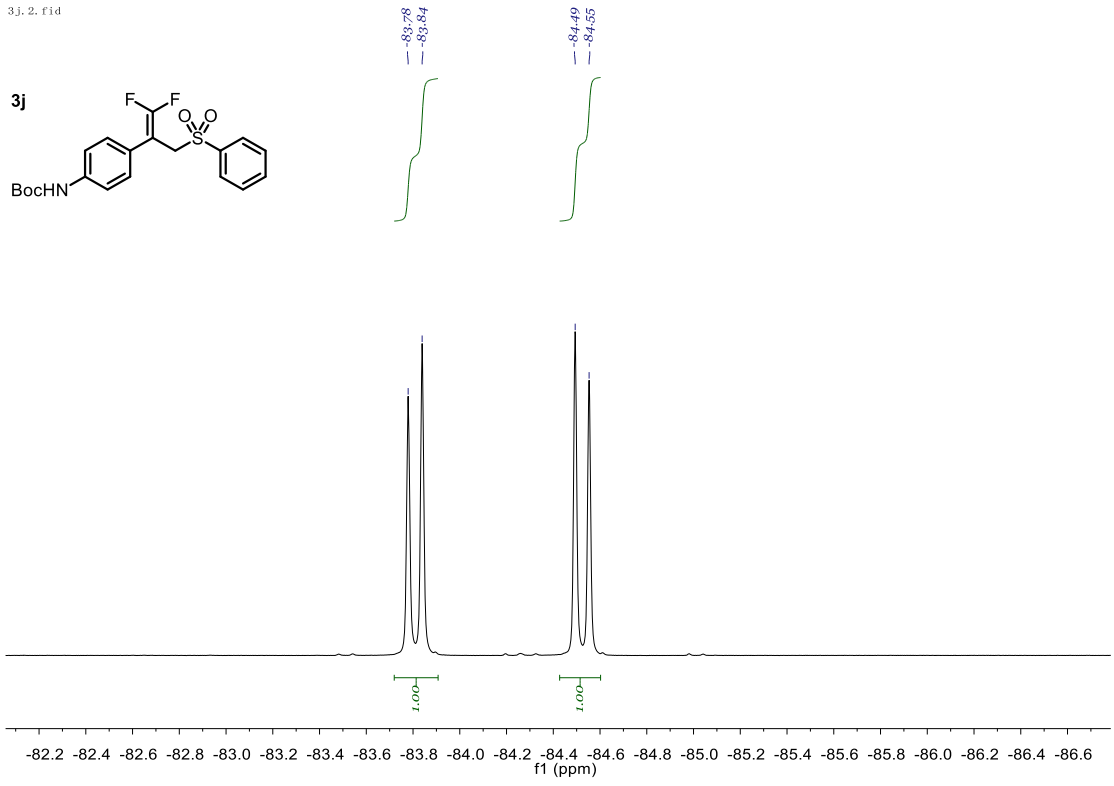
^{1}H NMR (400 MHz, Chloroform-*d*)



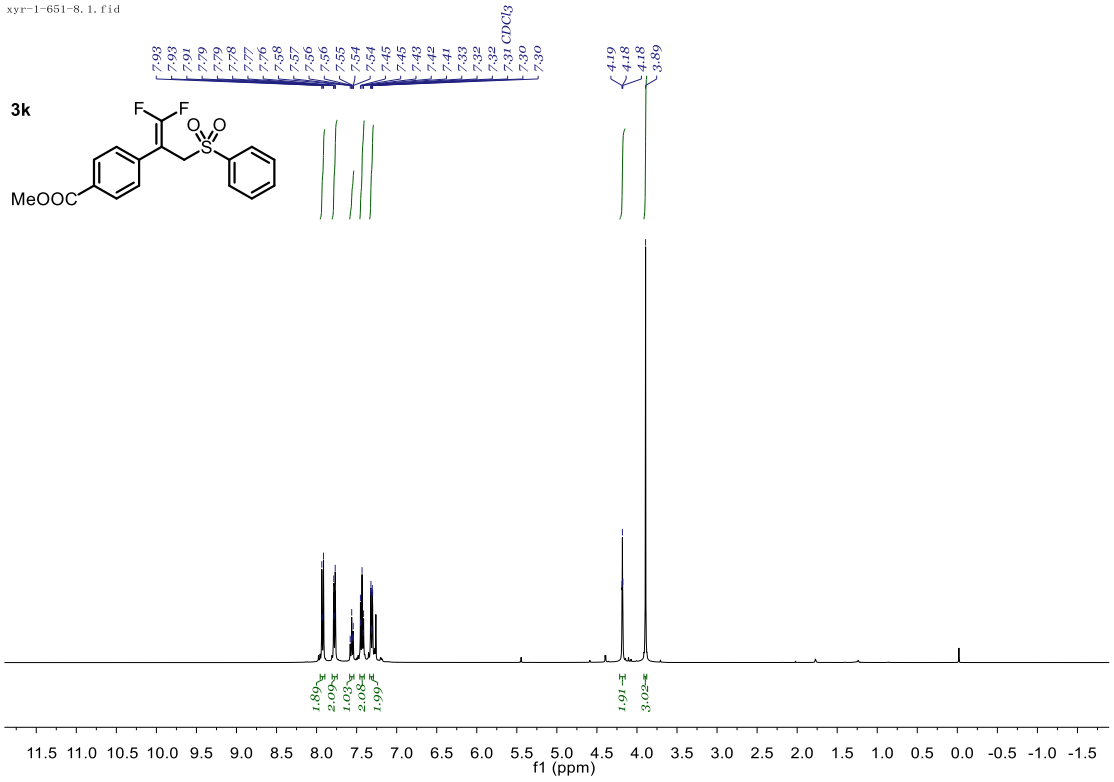
^{13}C NMR (101 MHz, Chloroform-*d*)



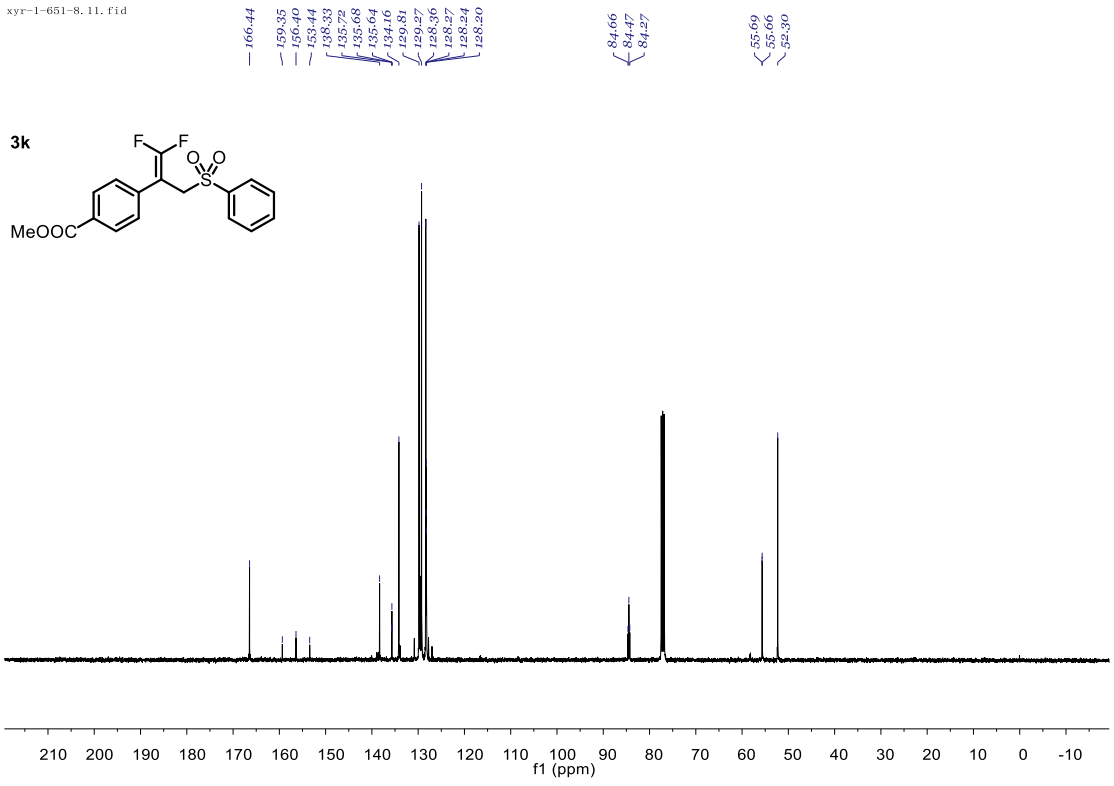
^{19}F NMR (377 MHz, Chloroform-*d*)



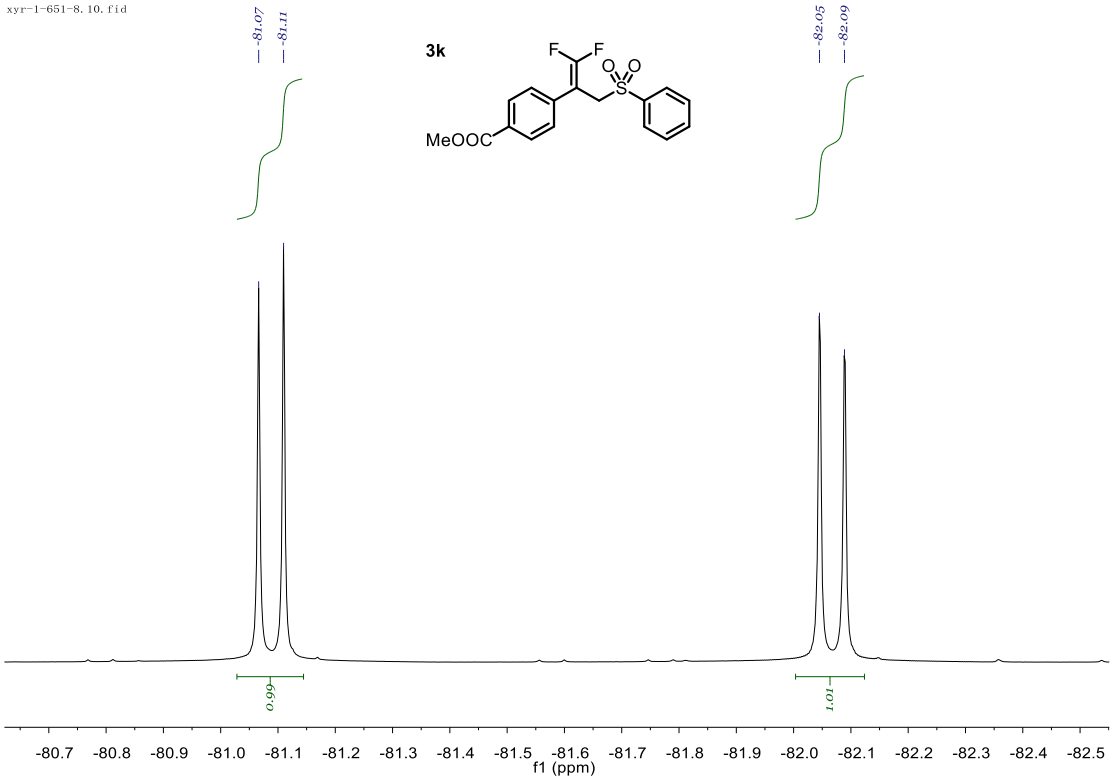
^{1}H NMR (400 MHz, Chloroform-*d*)



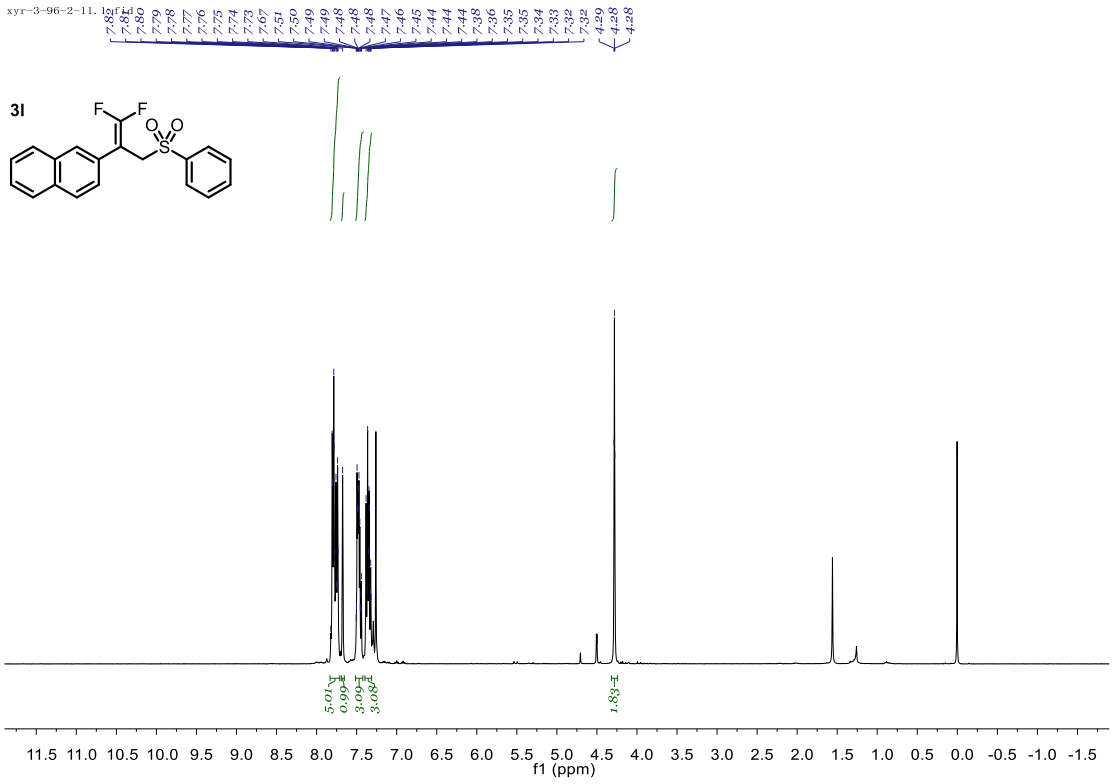
^{13}C NMR (101 MHz, Chloroform-*d*)



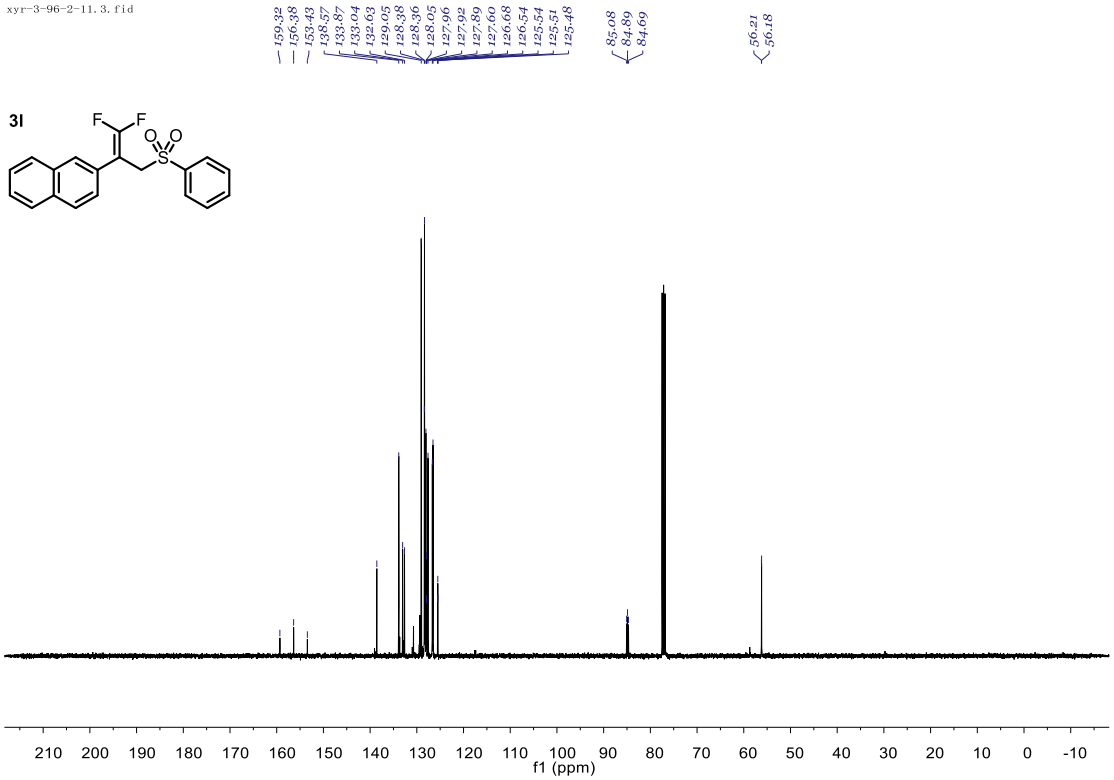
^{19}F NMR (377 MHz, Chloroform-*d*)



^{1}H NMR (400 MHz, Chloroform-*d*)



^{13}C NMR (101 MHz, Chloroform-*d*)



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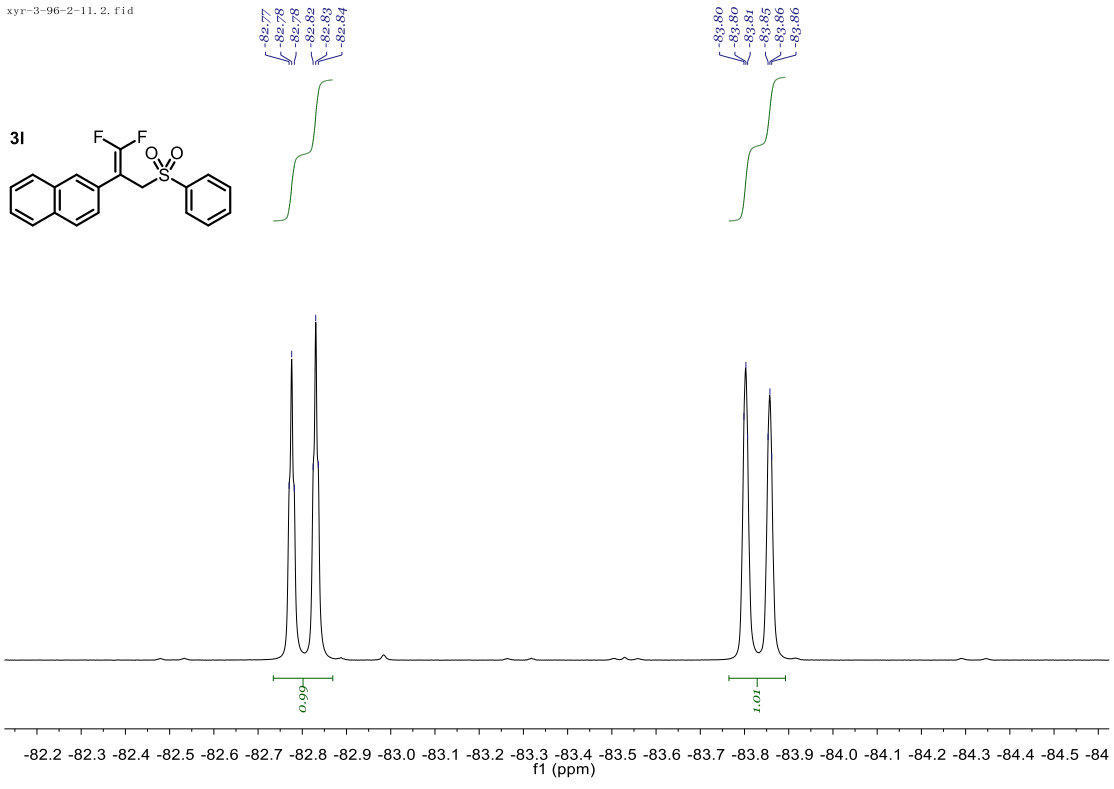
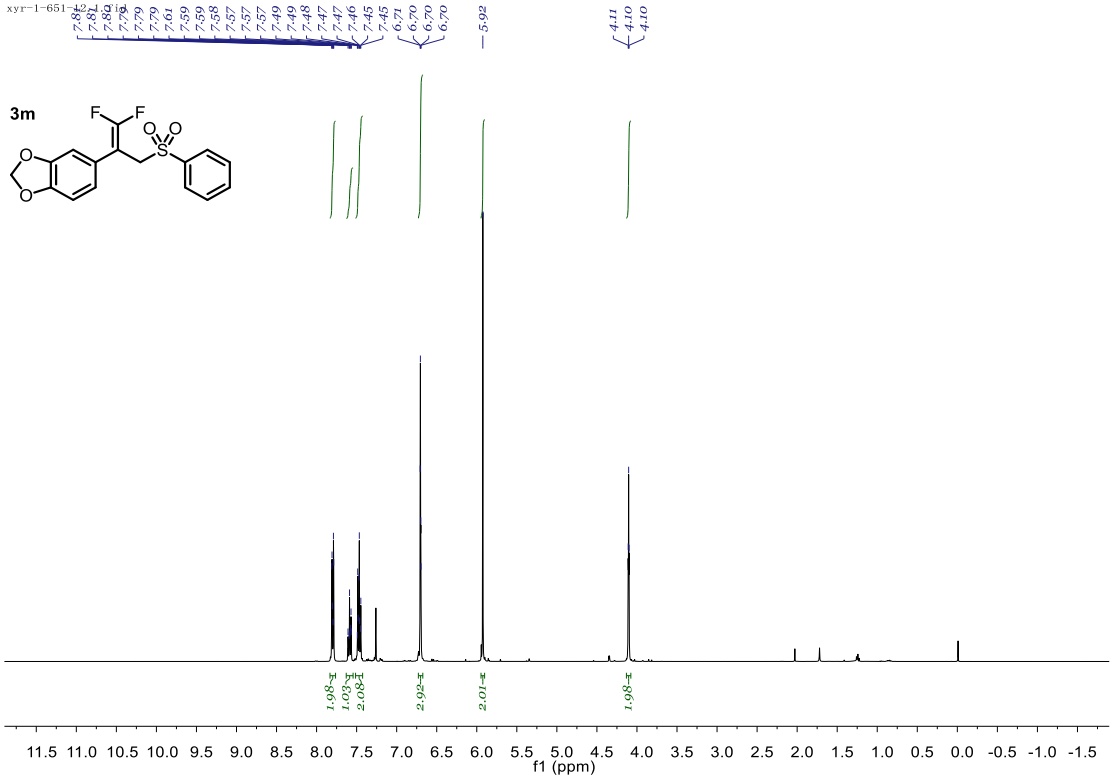


^{1}H NMR (400 MHz, Chloroform-*d*)



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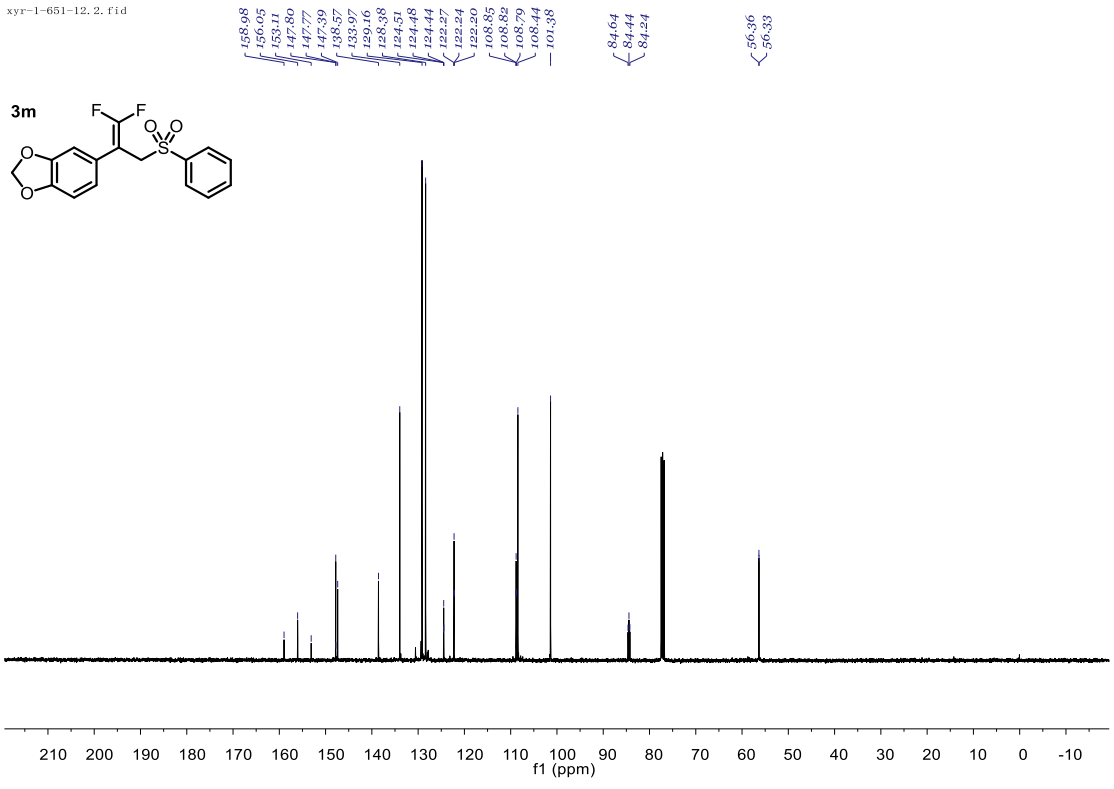

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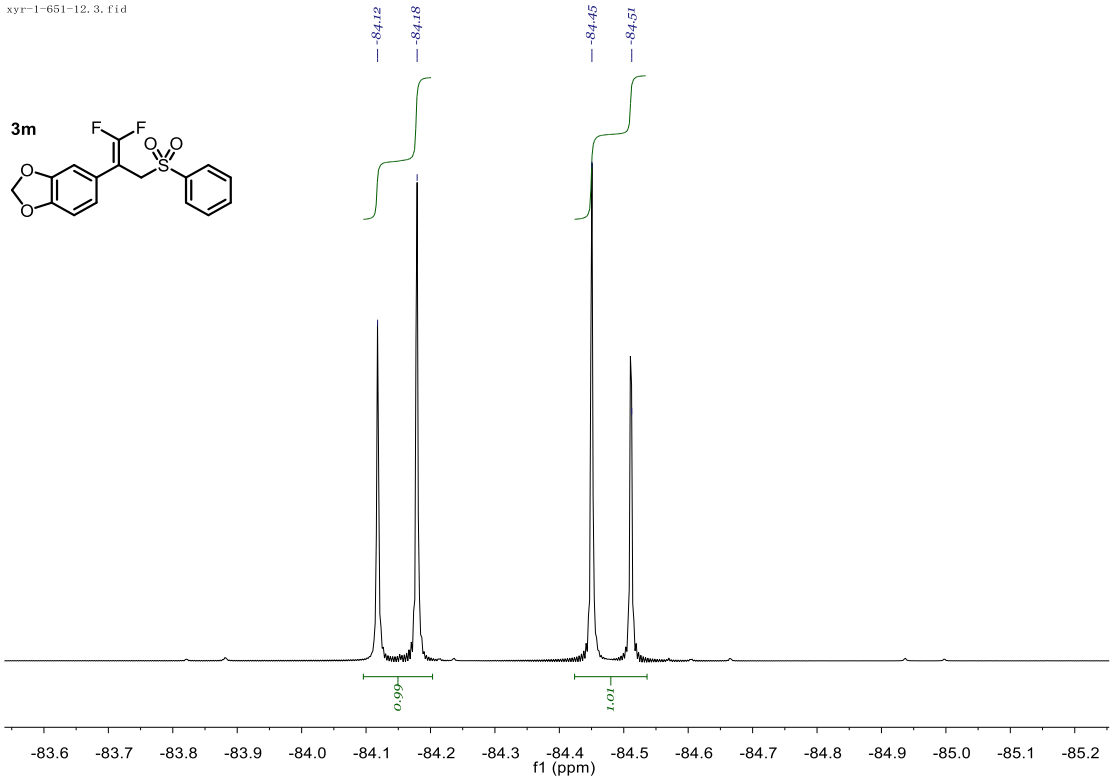

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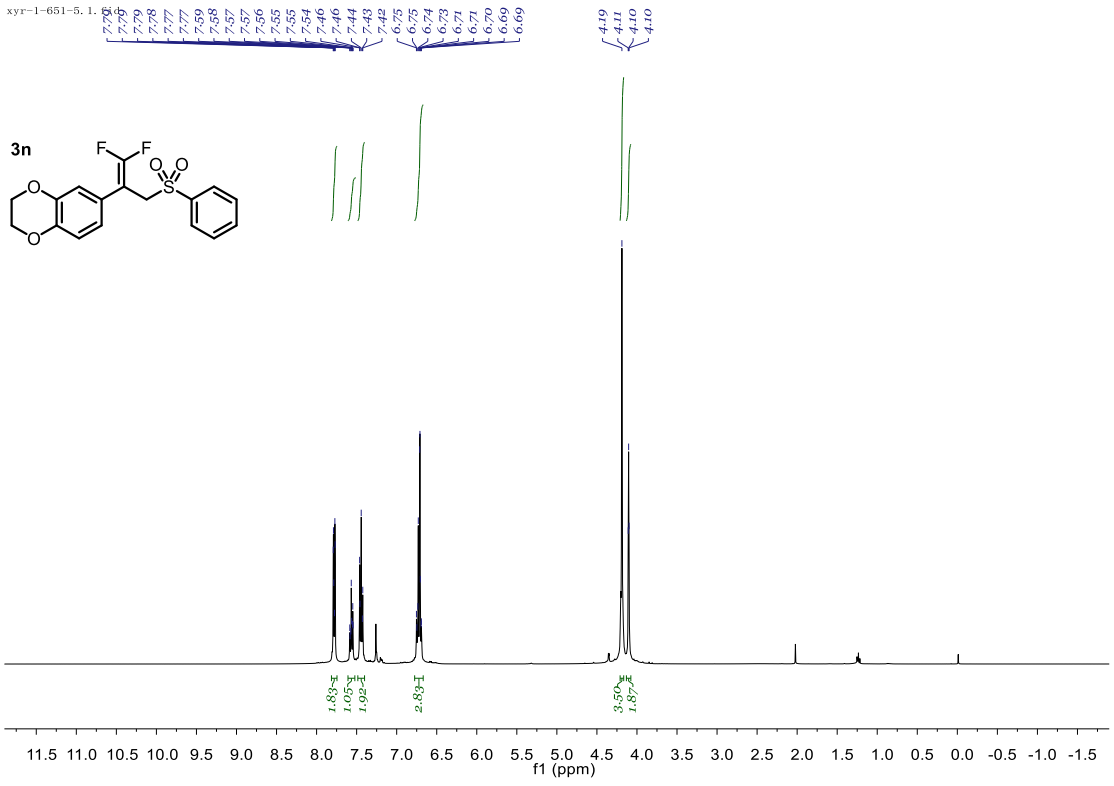

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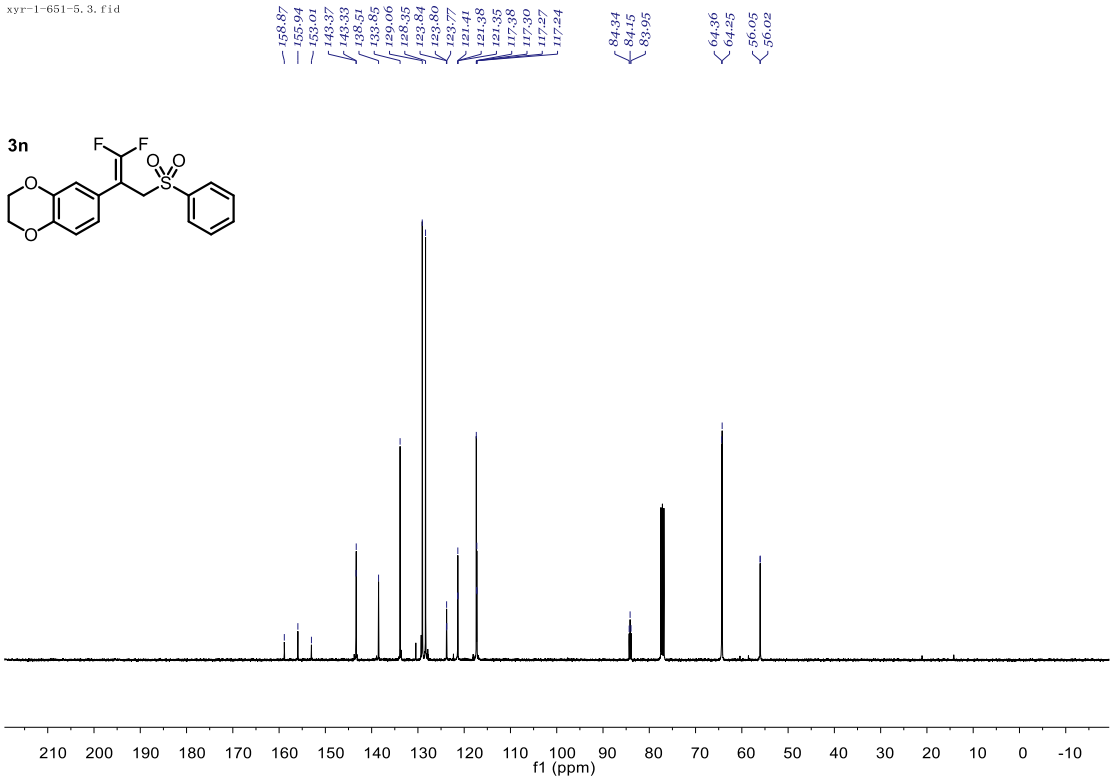

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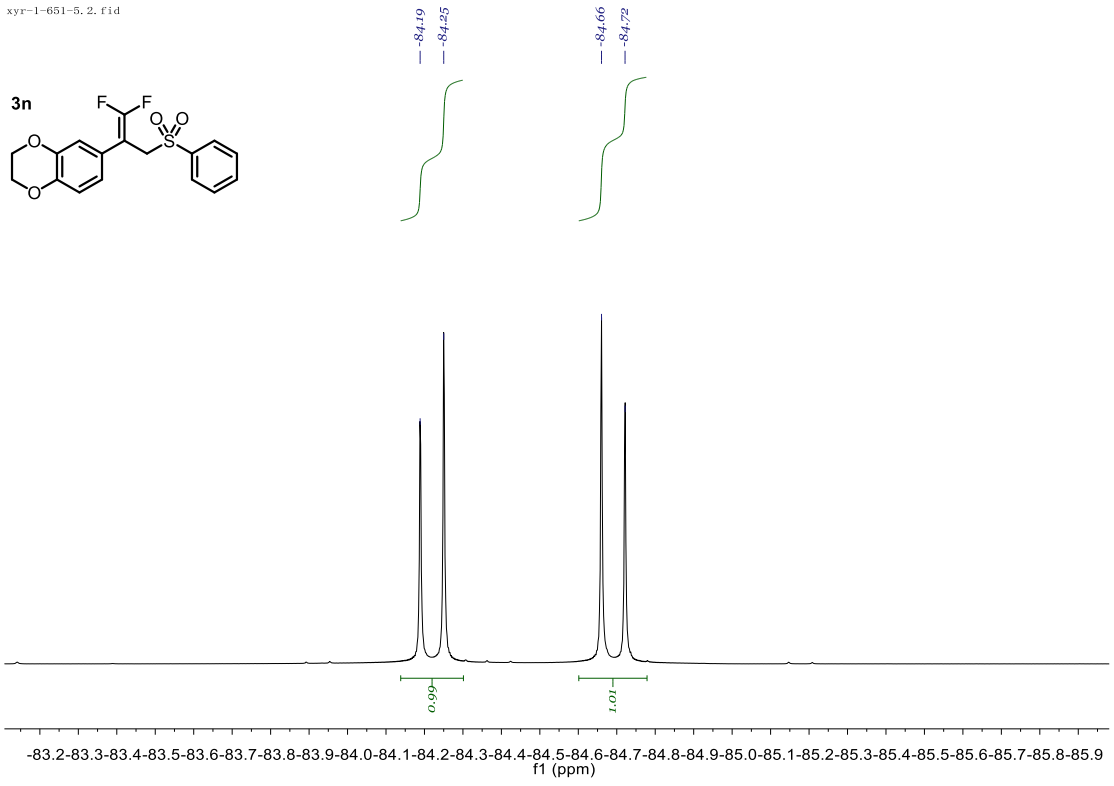

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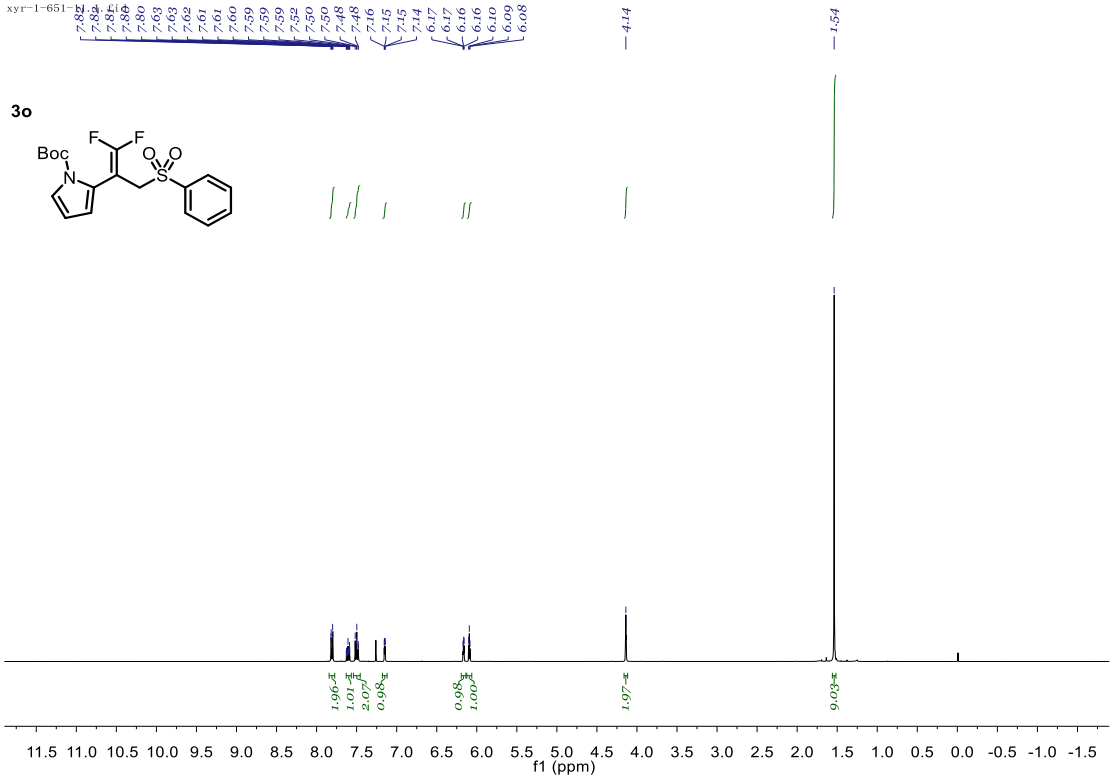

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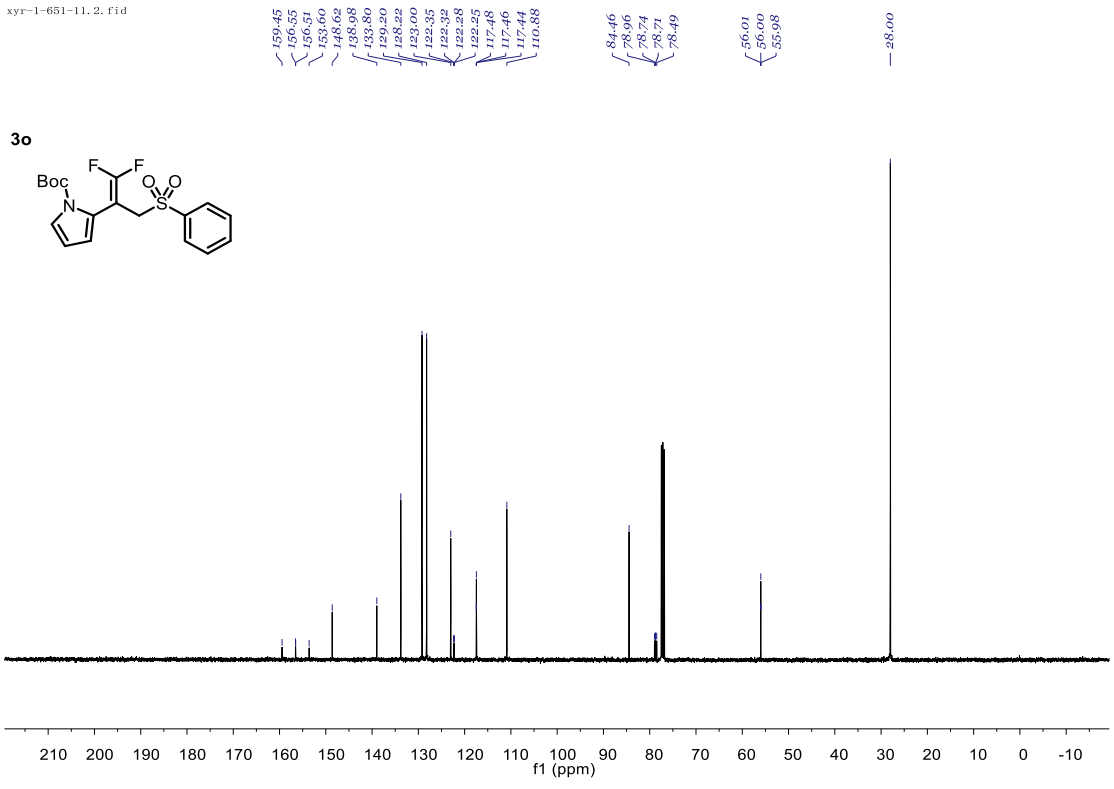

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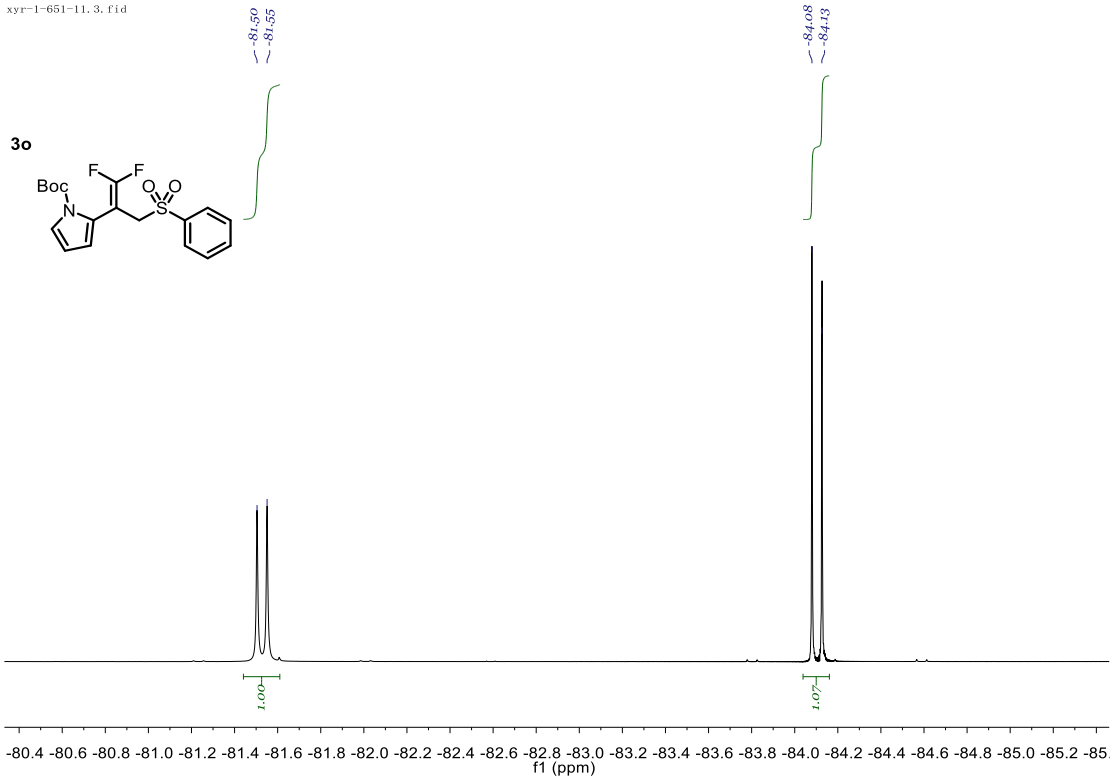

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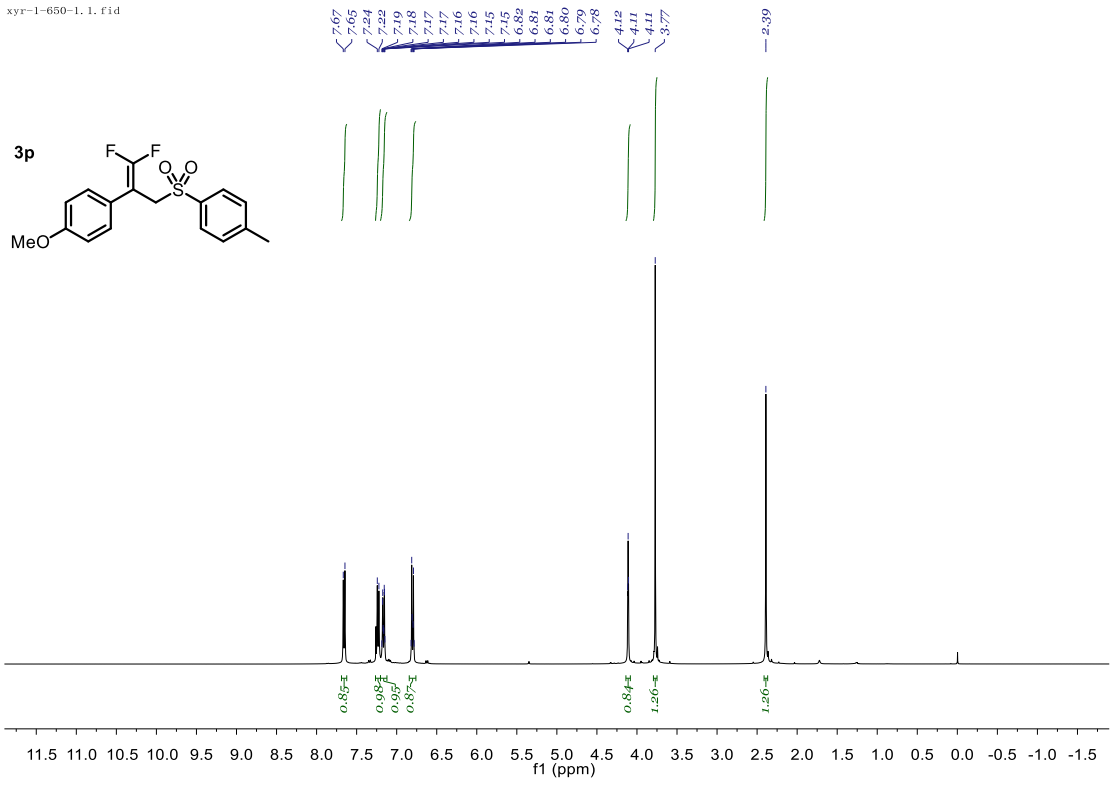

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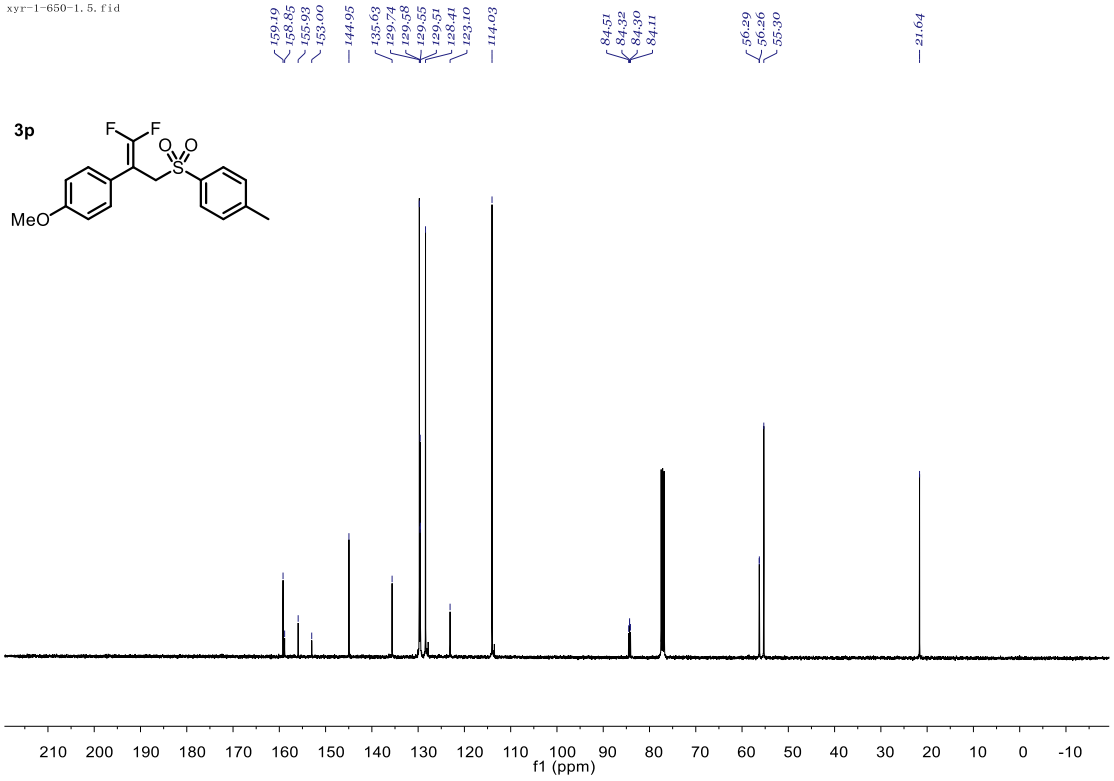

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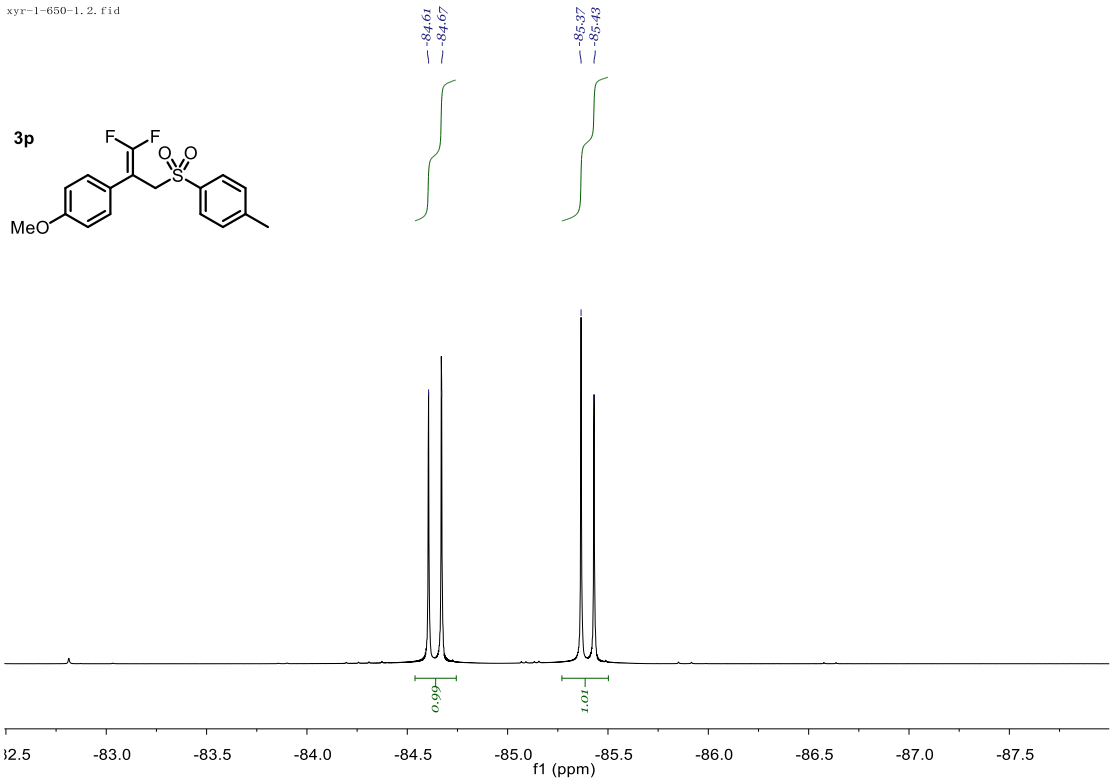

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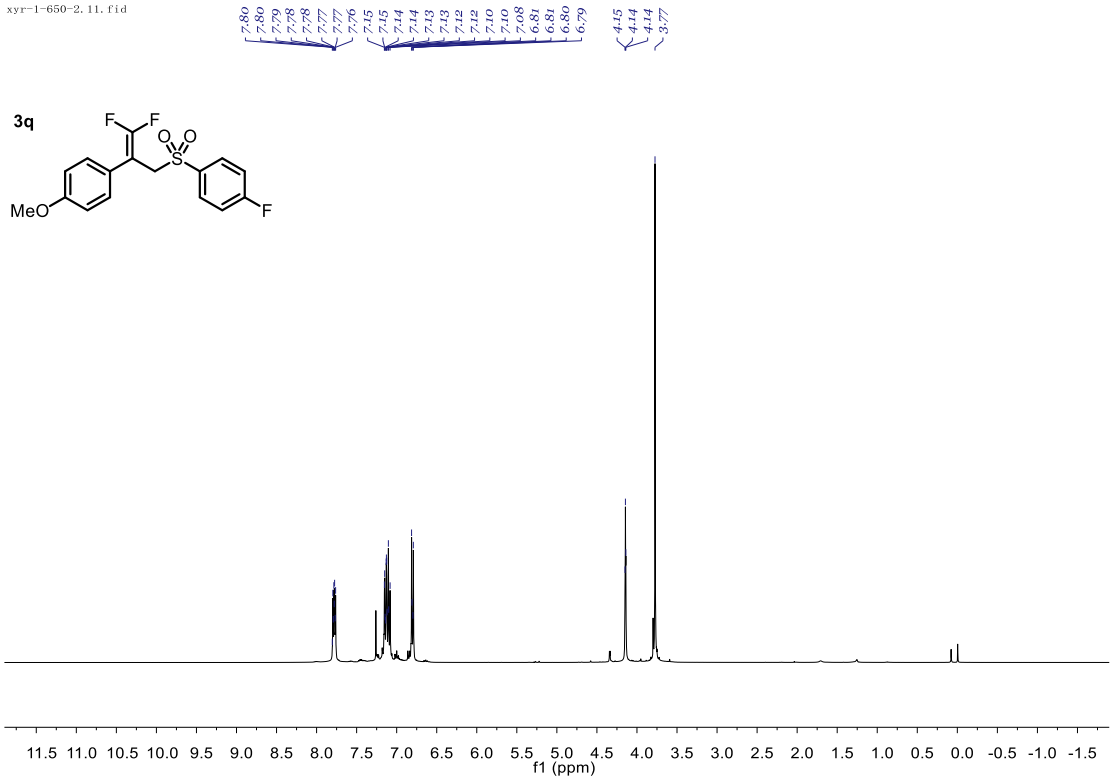

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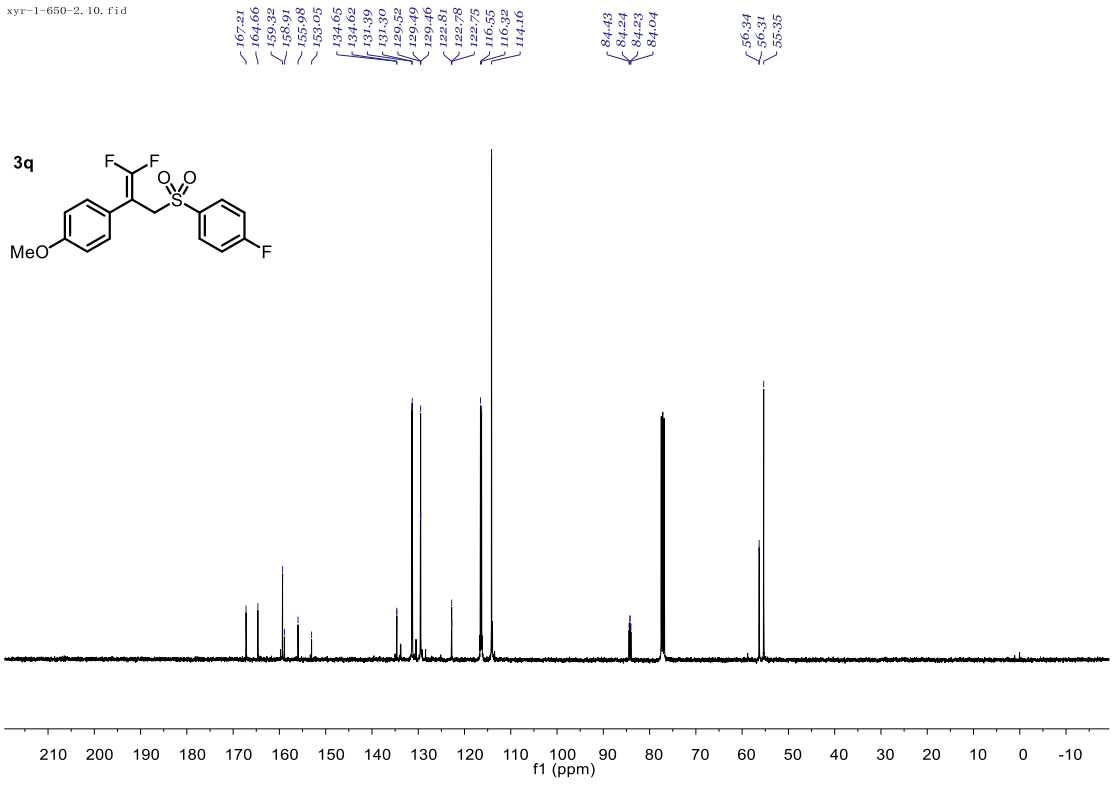

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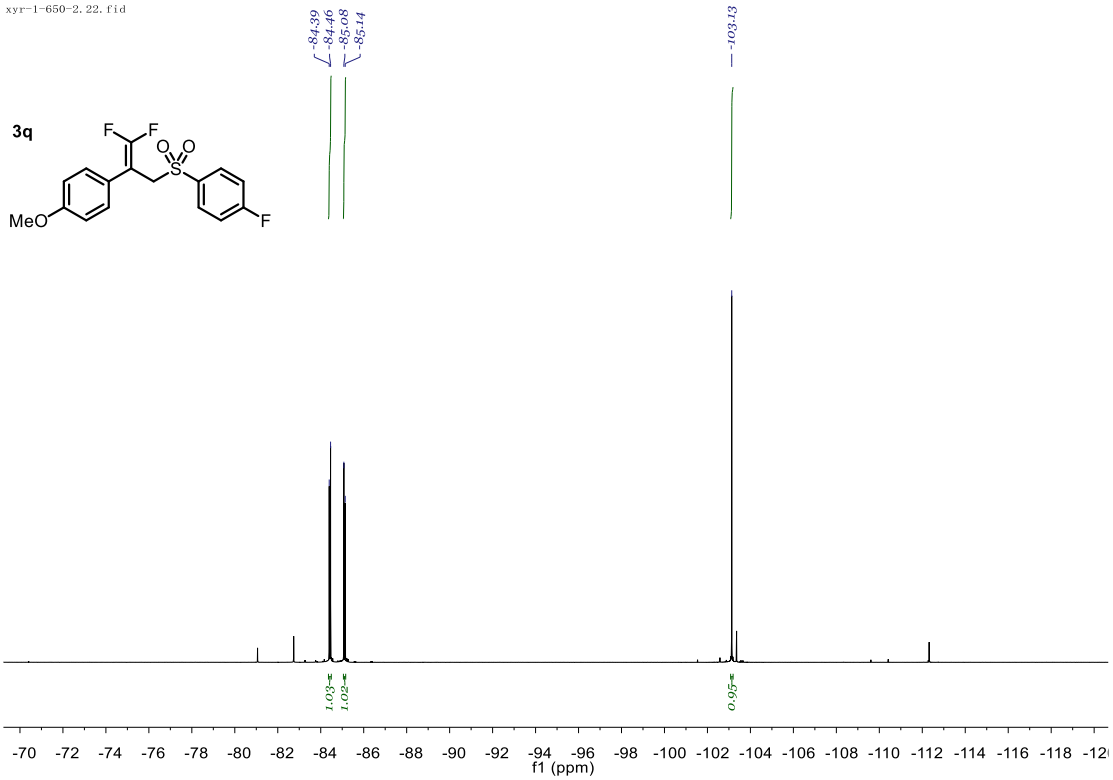

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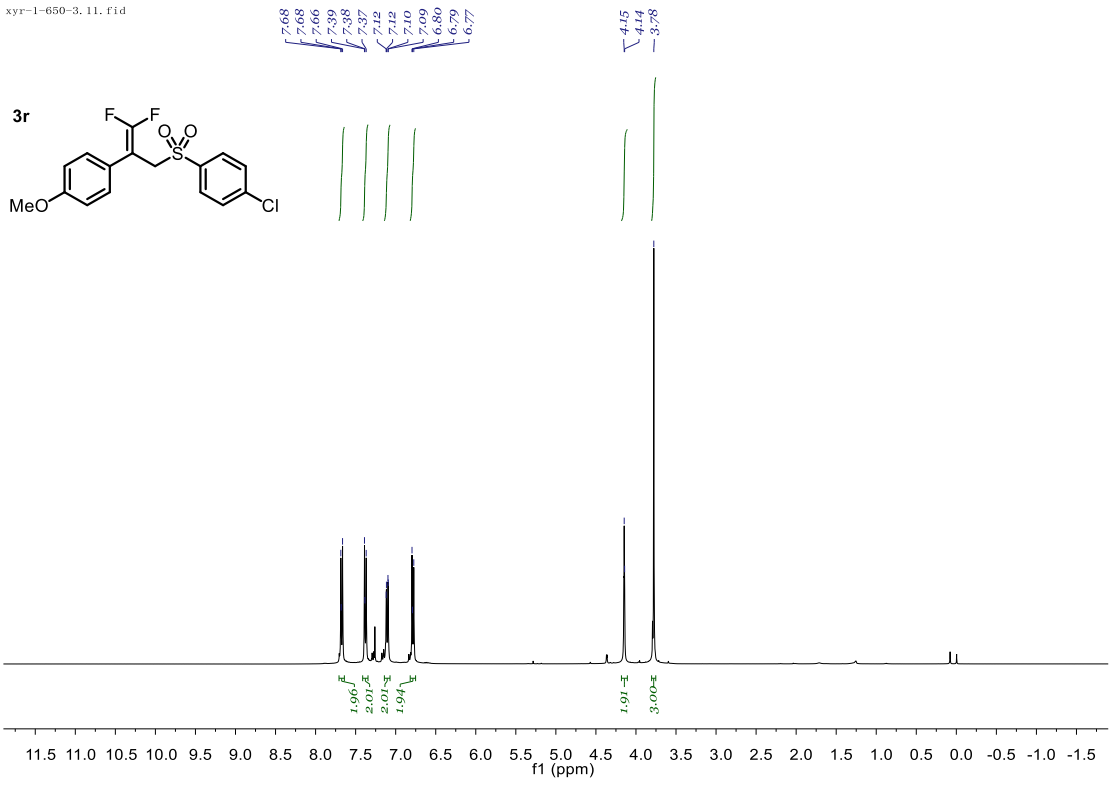

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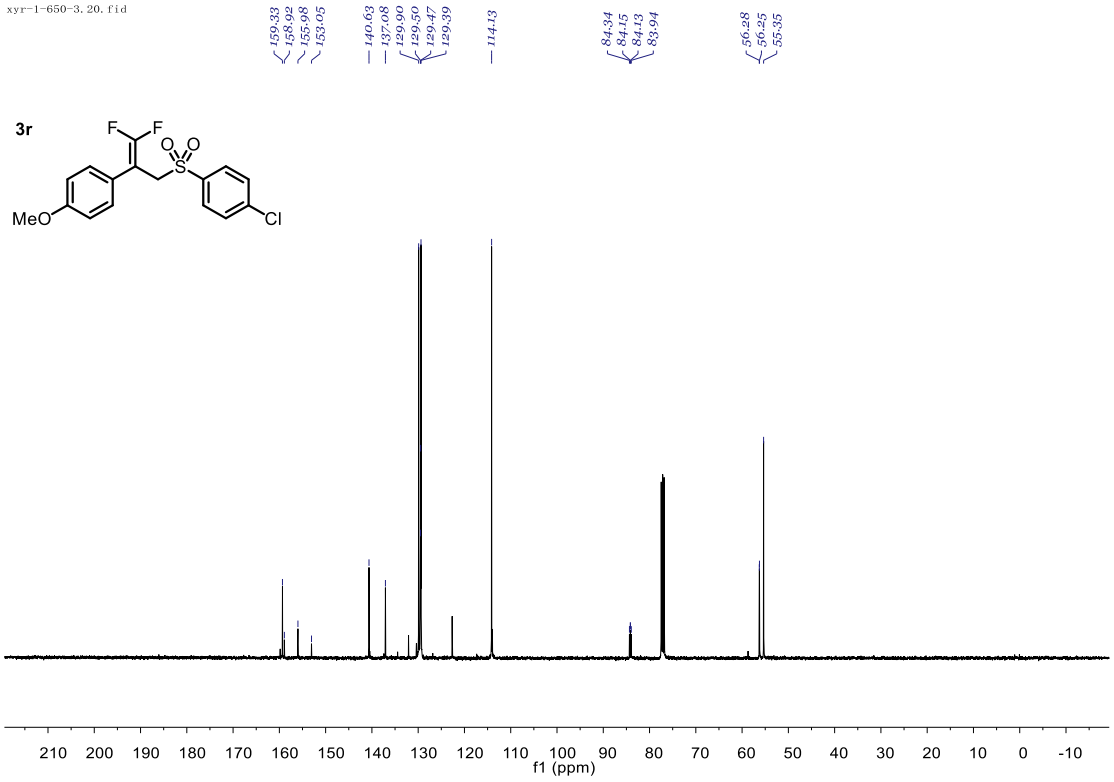

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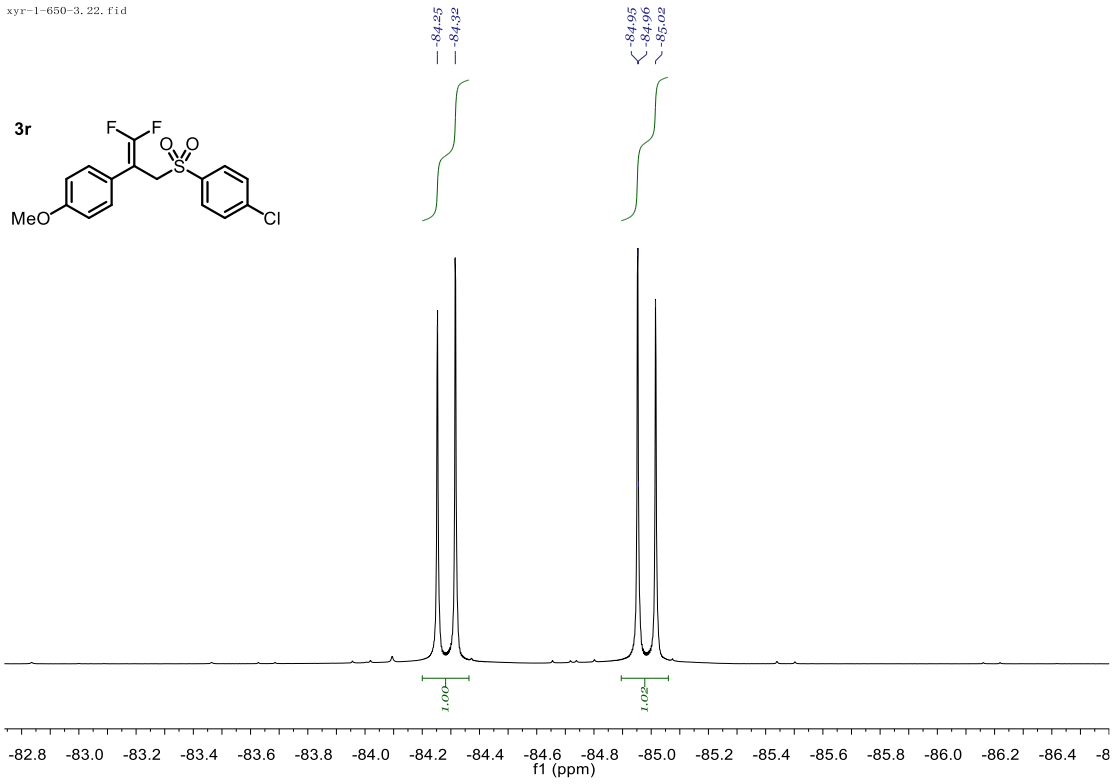

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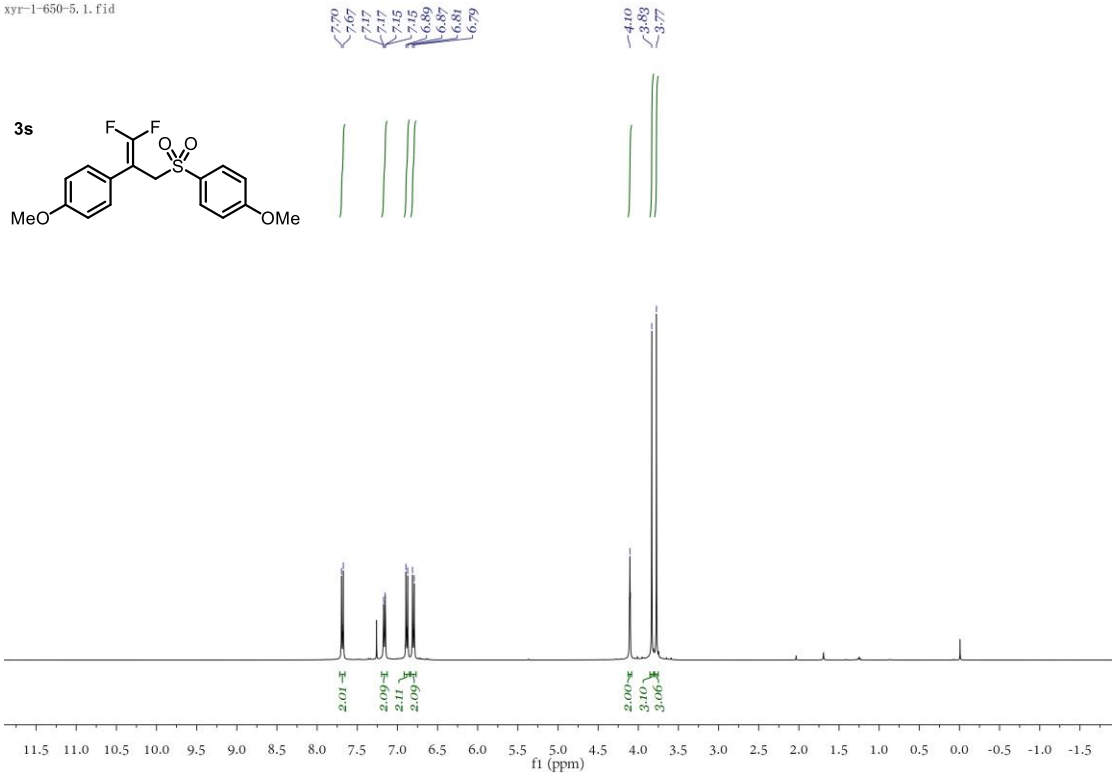

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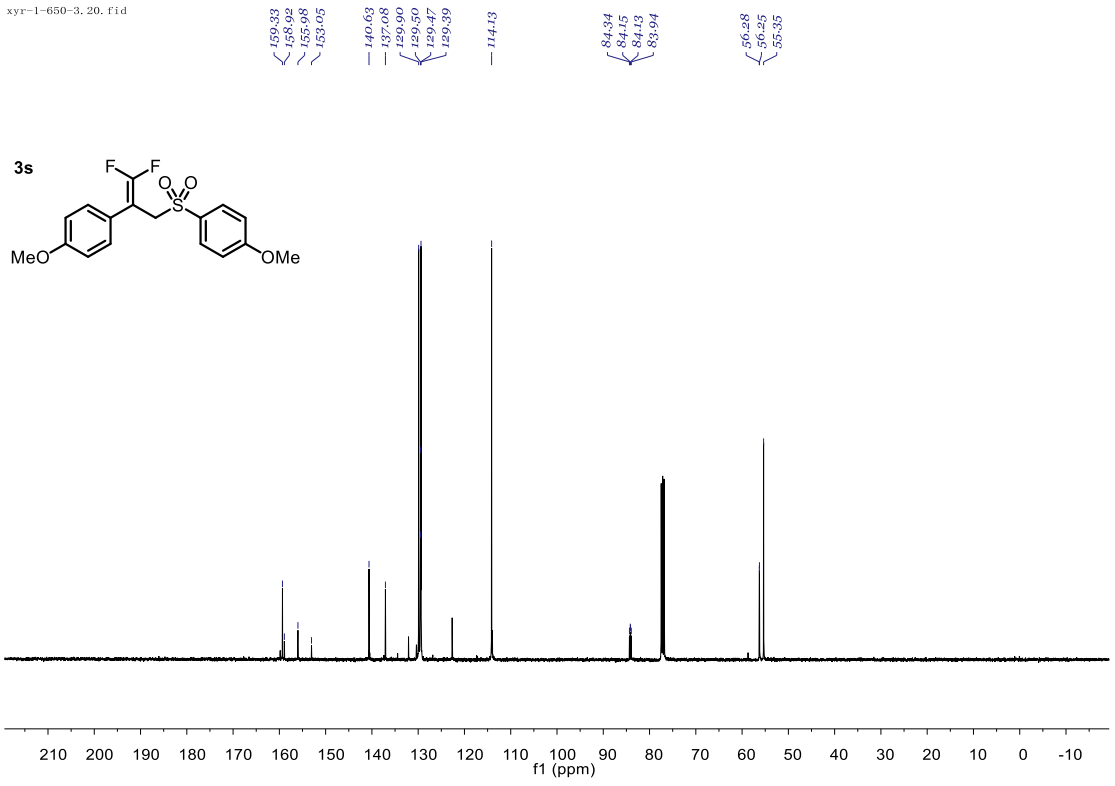

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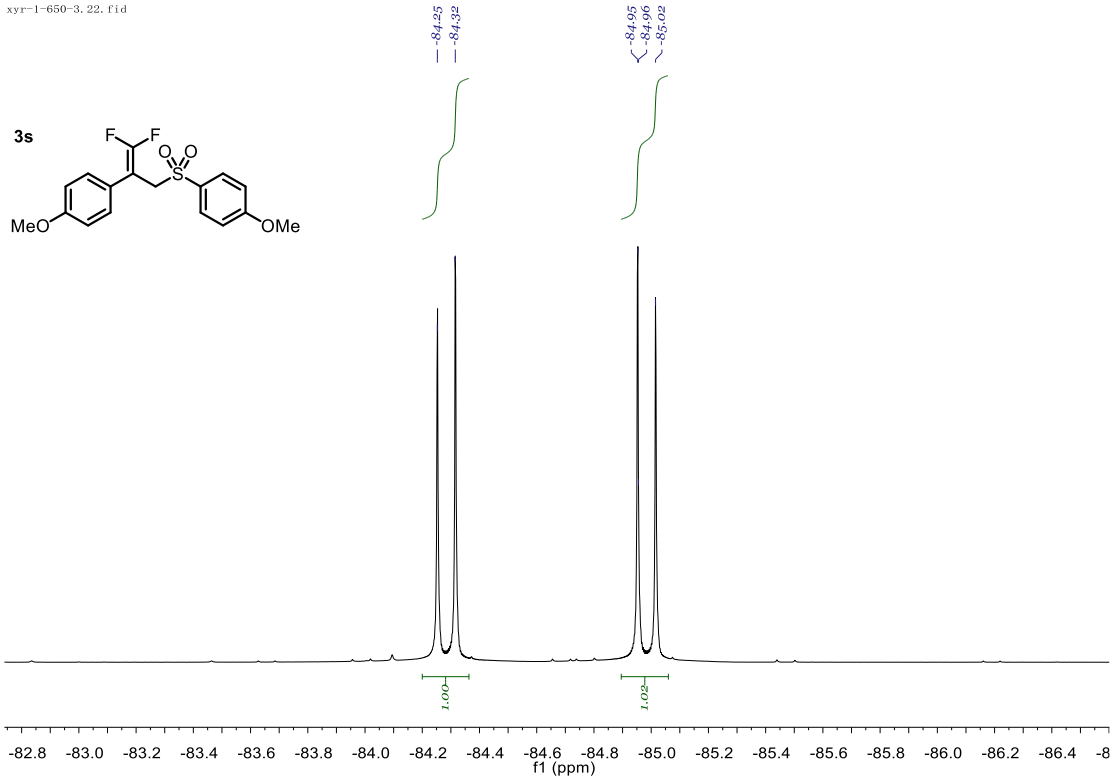

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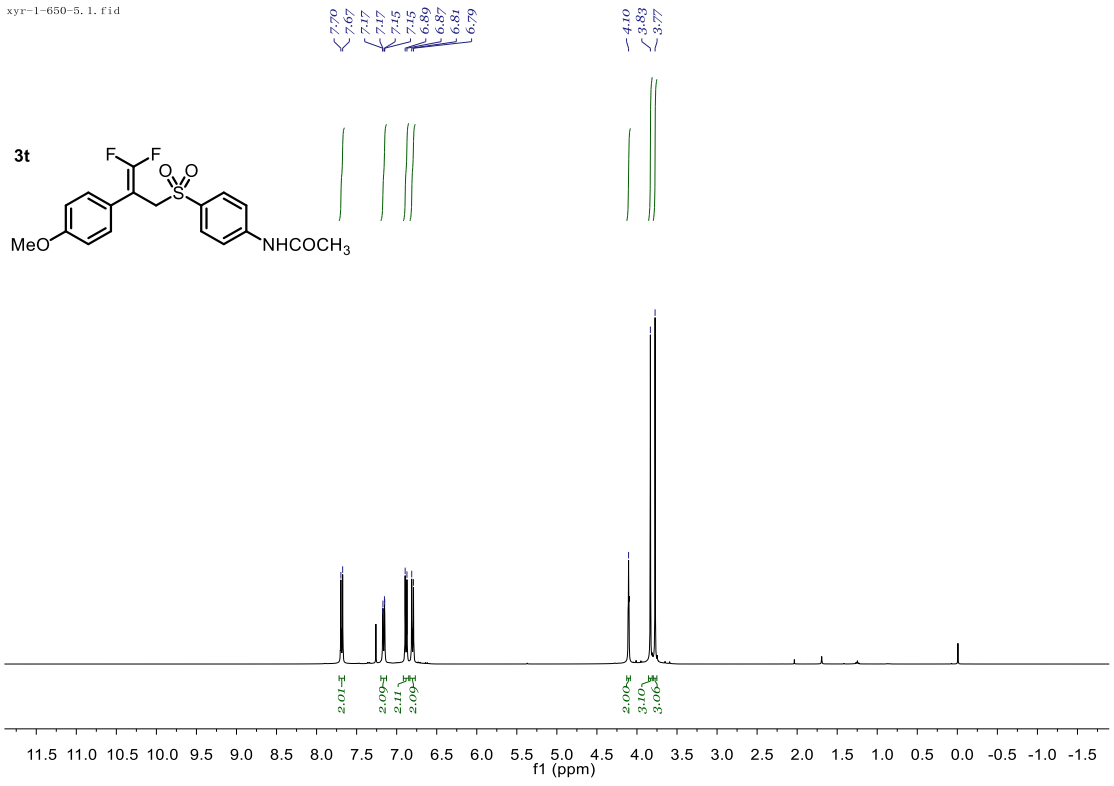

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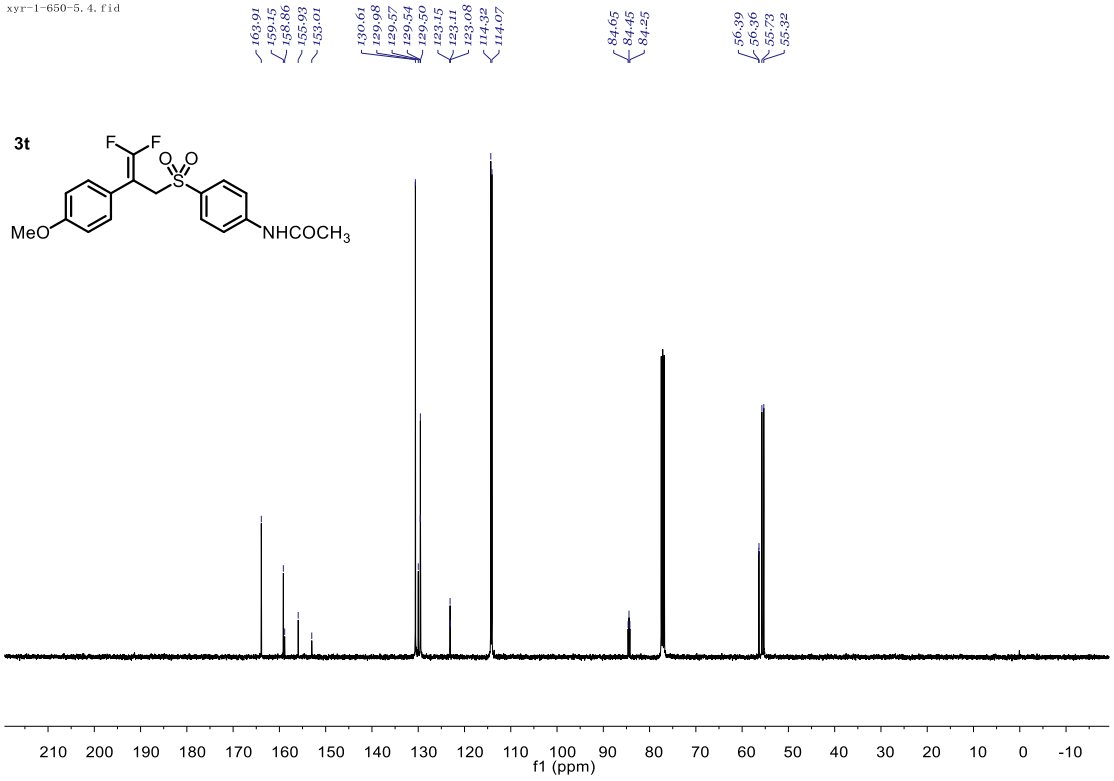

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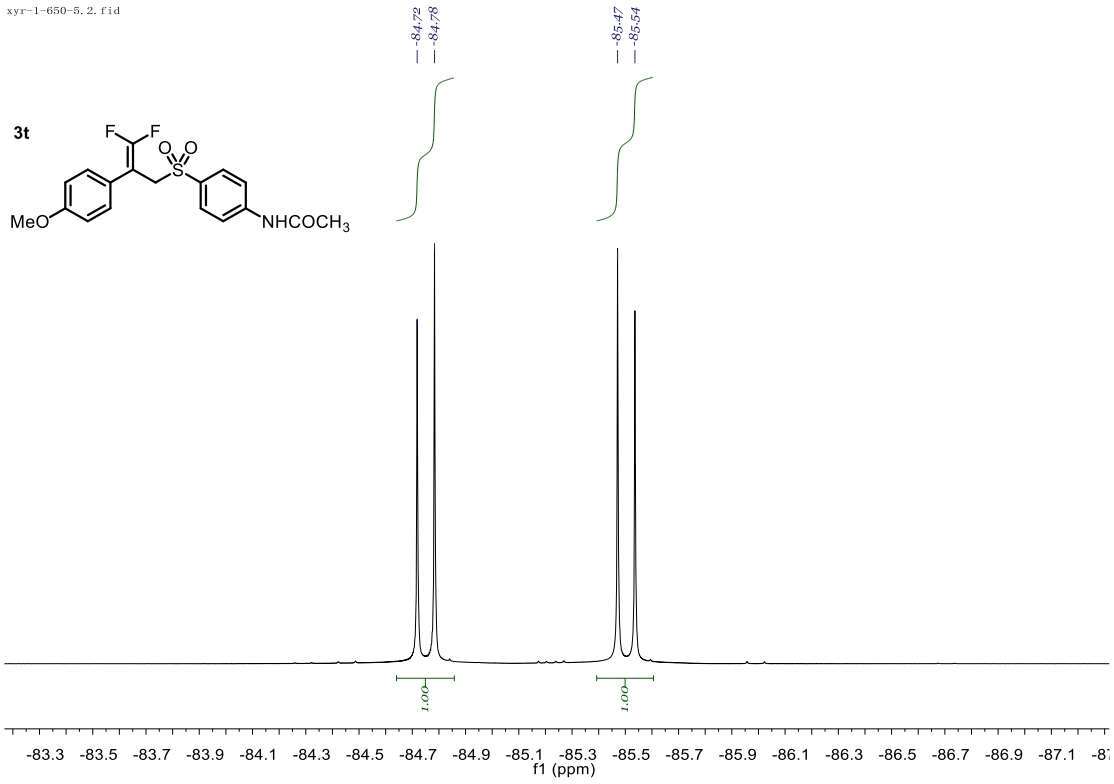

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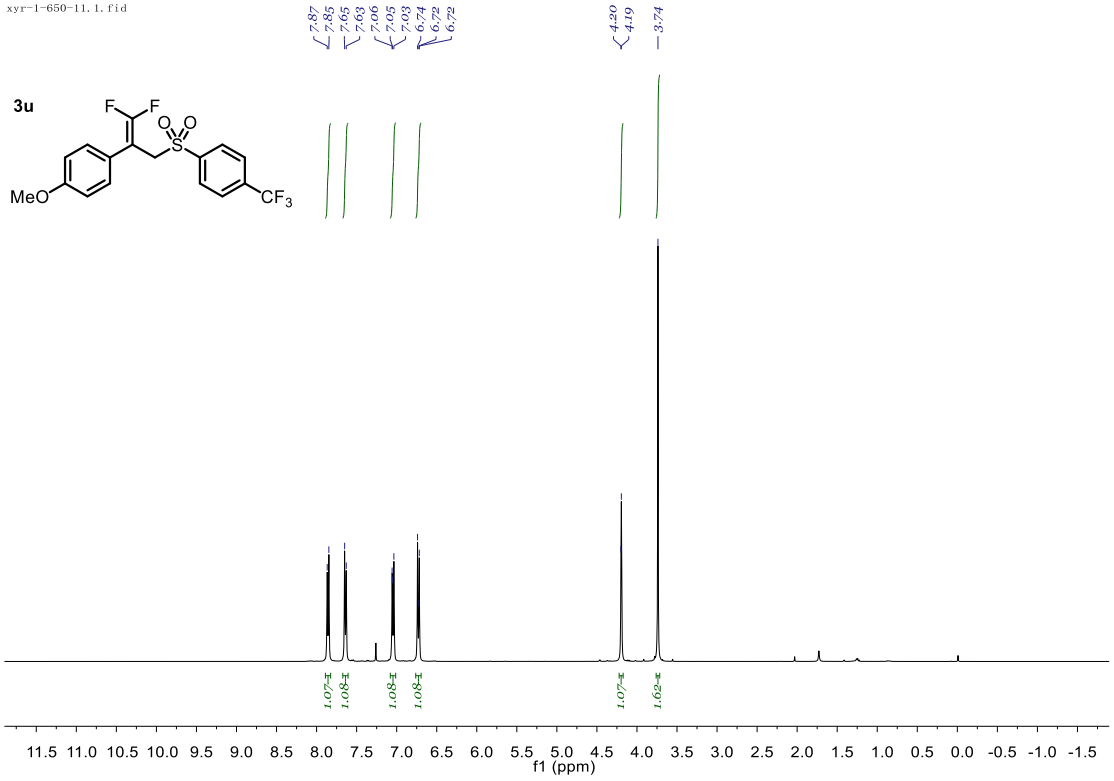

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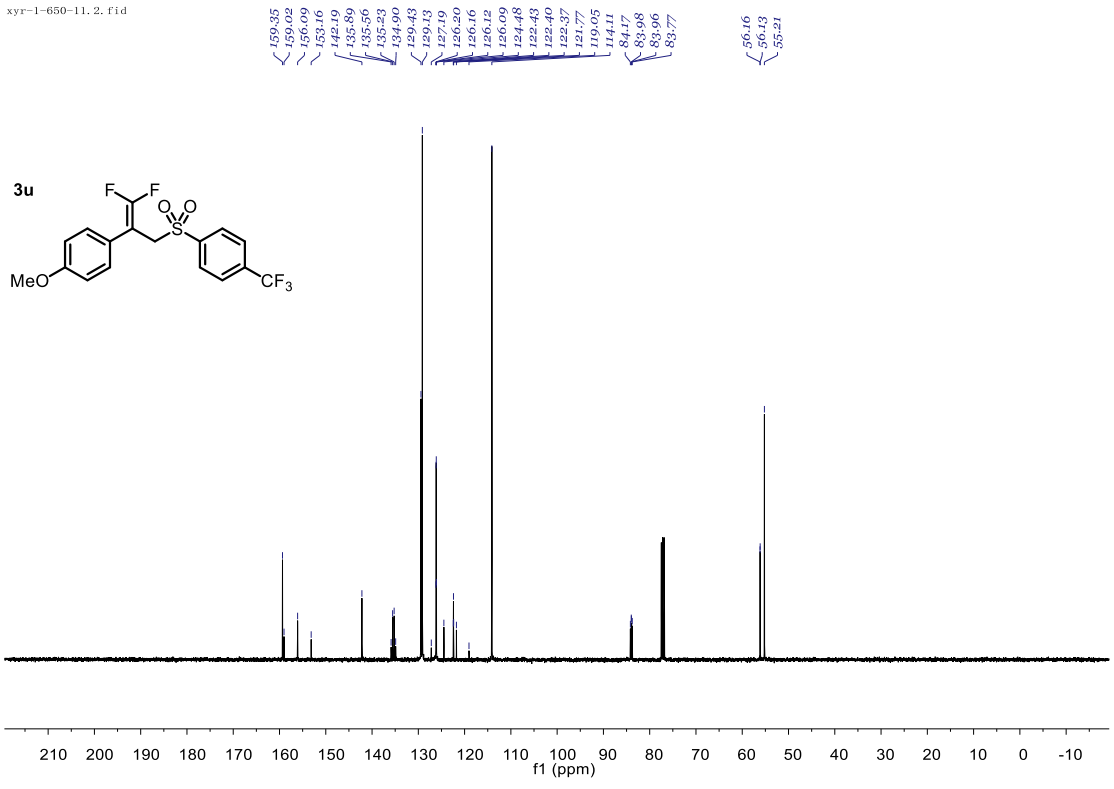

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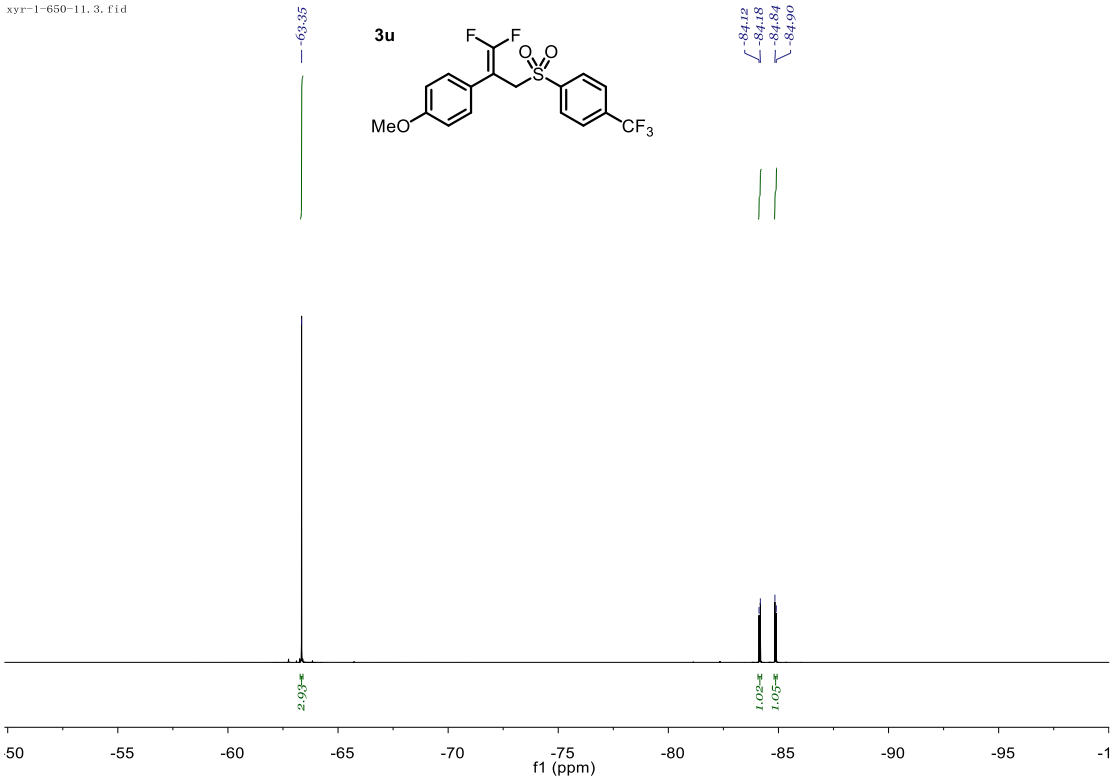

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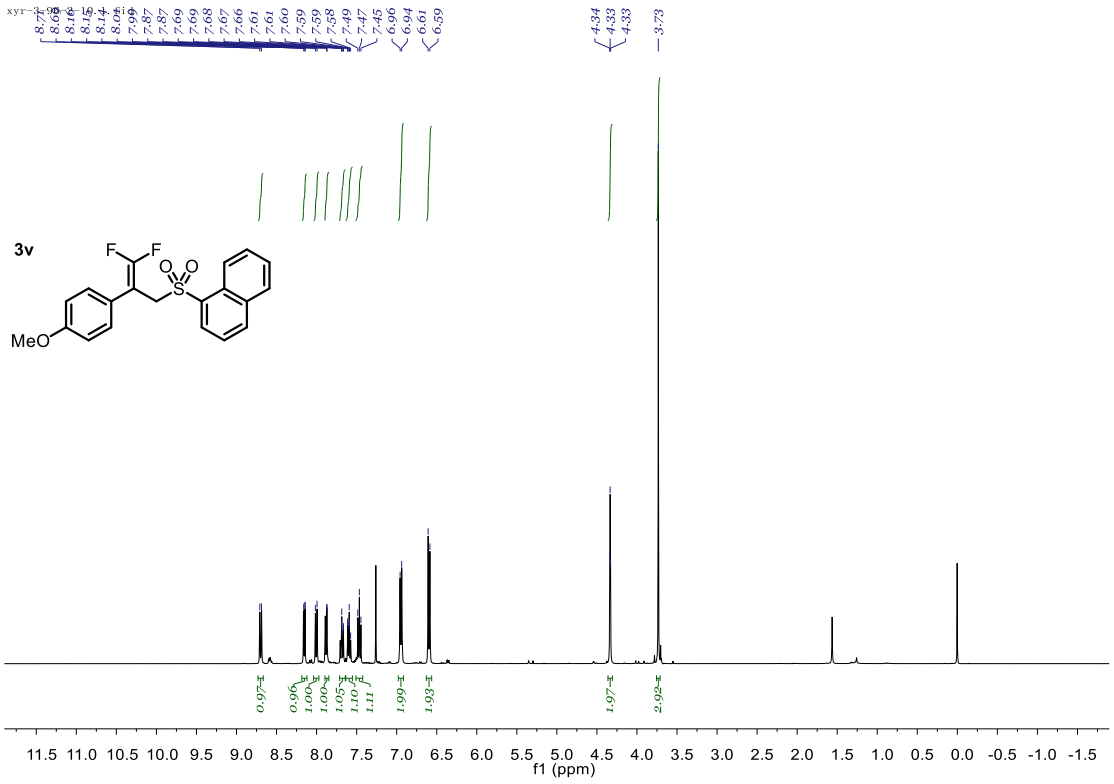

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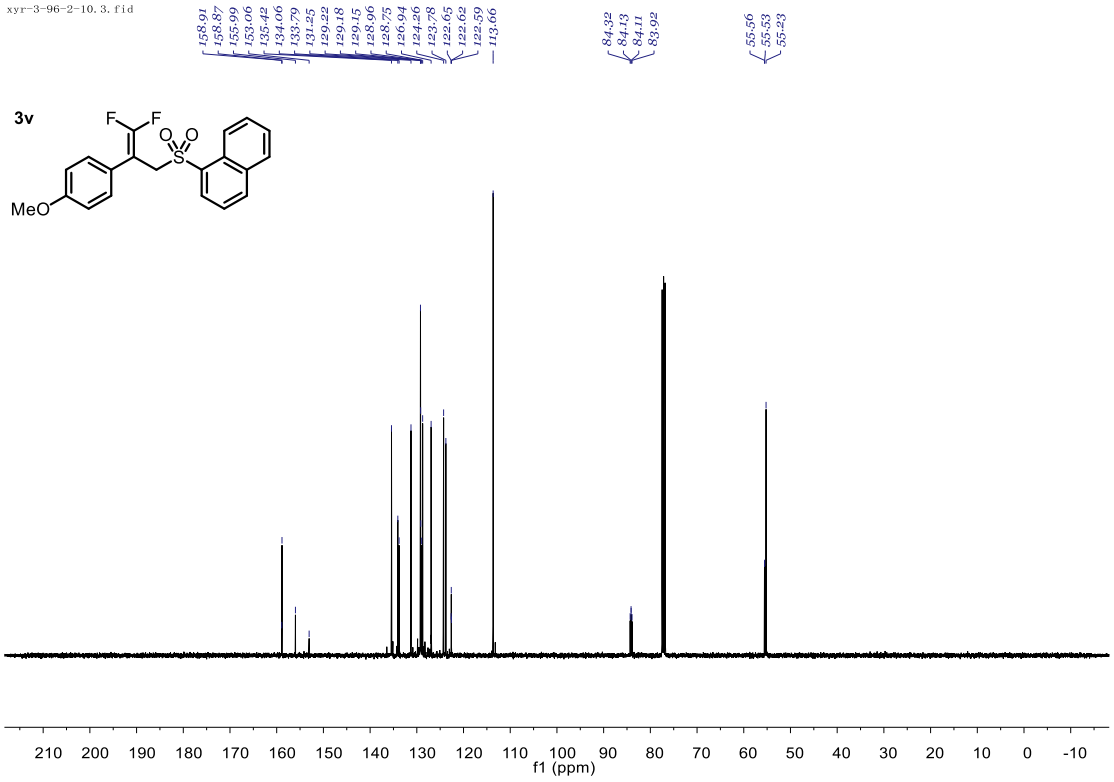

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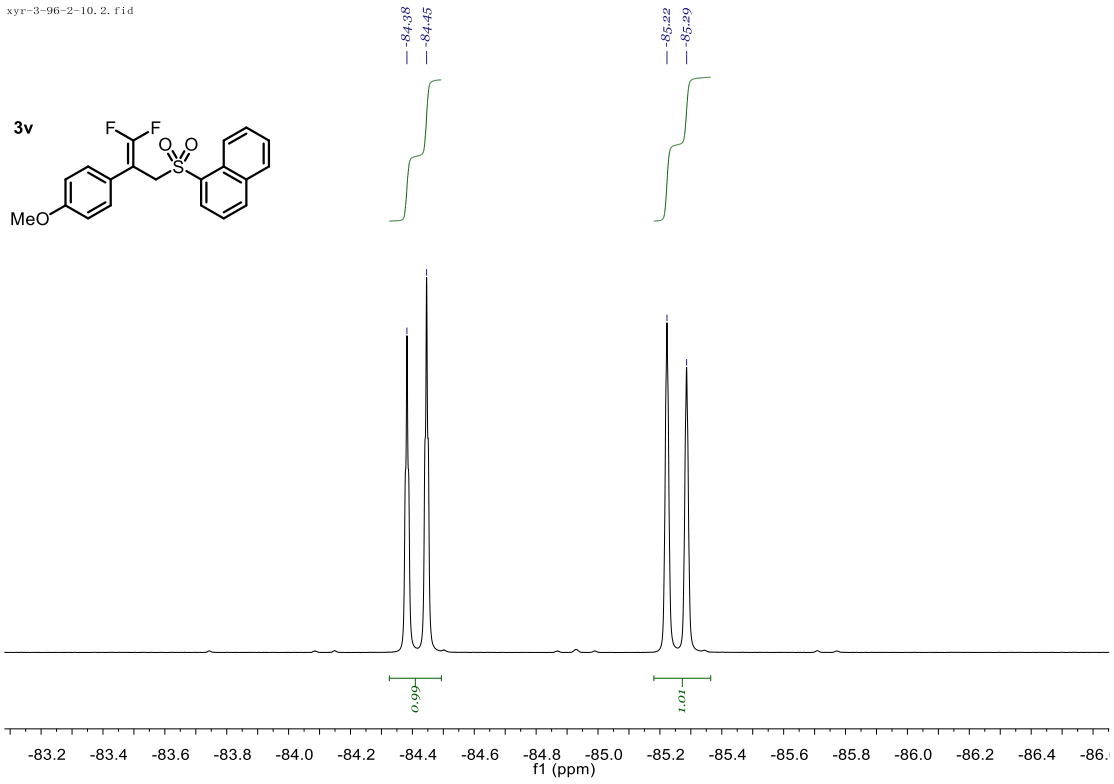

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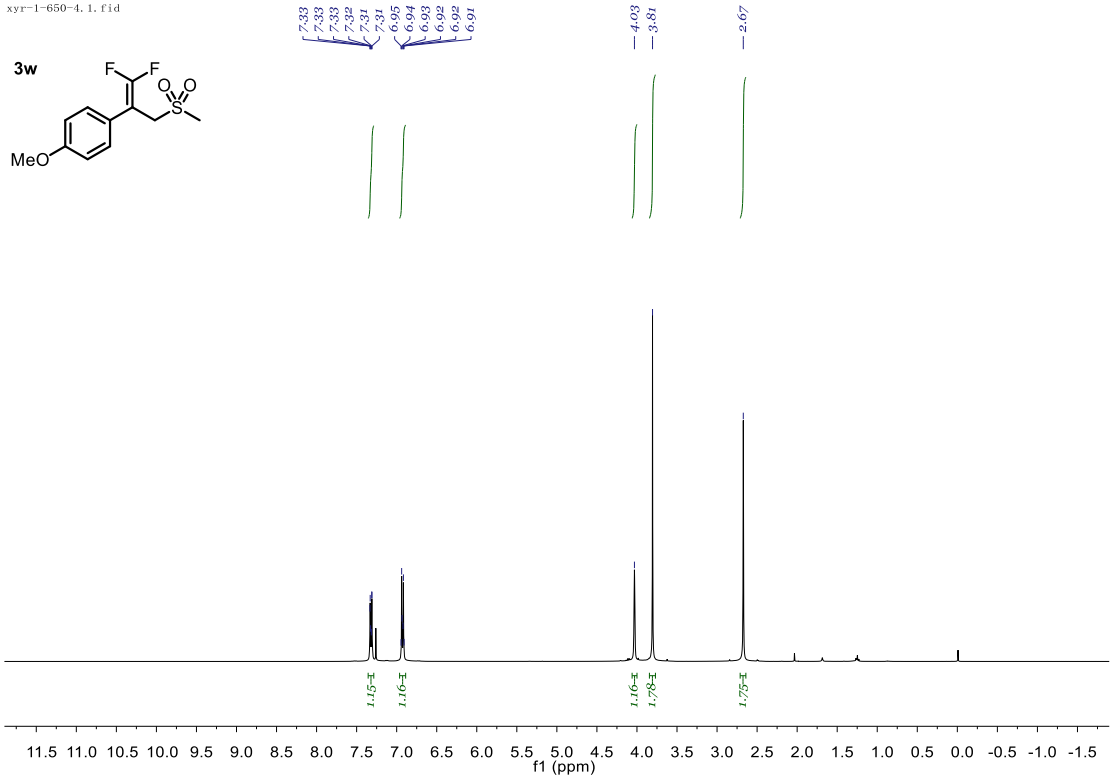

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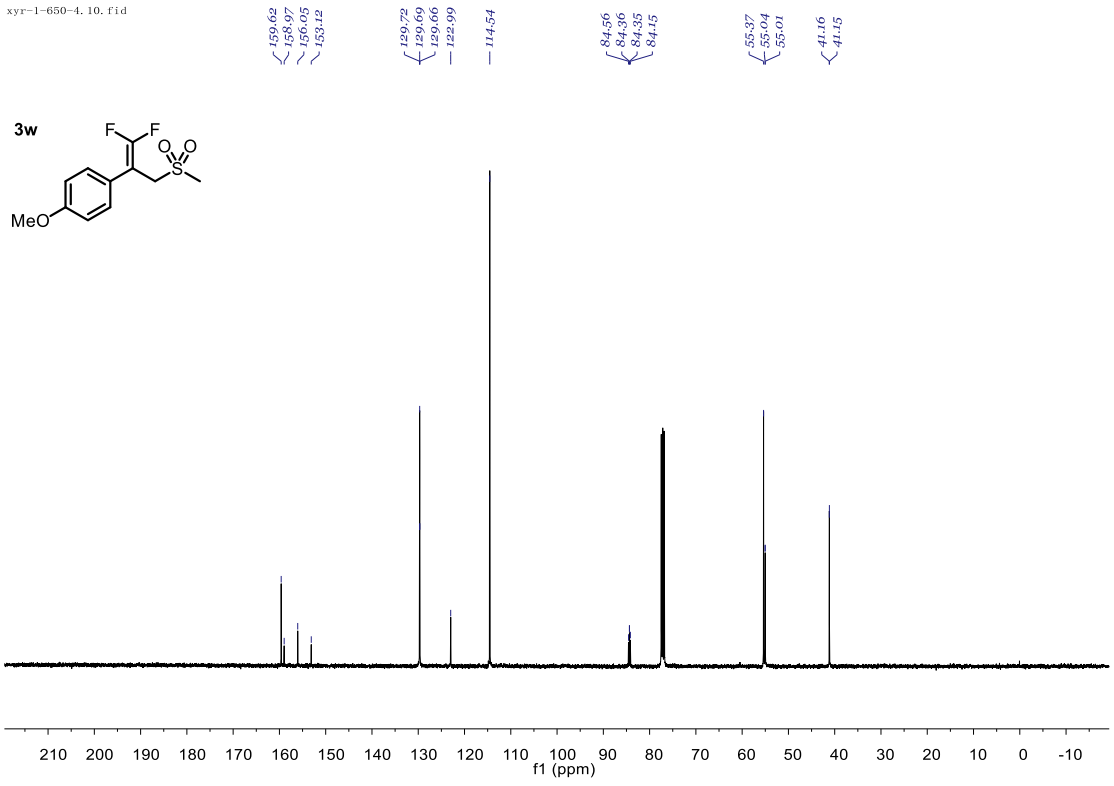

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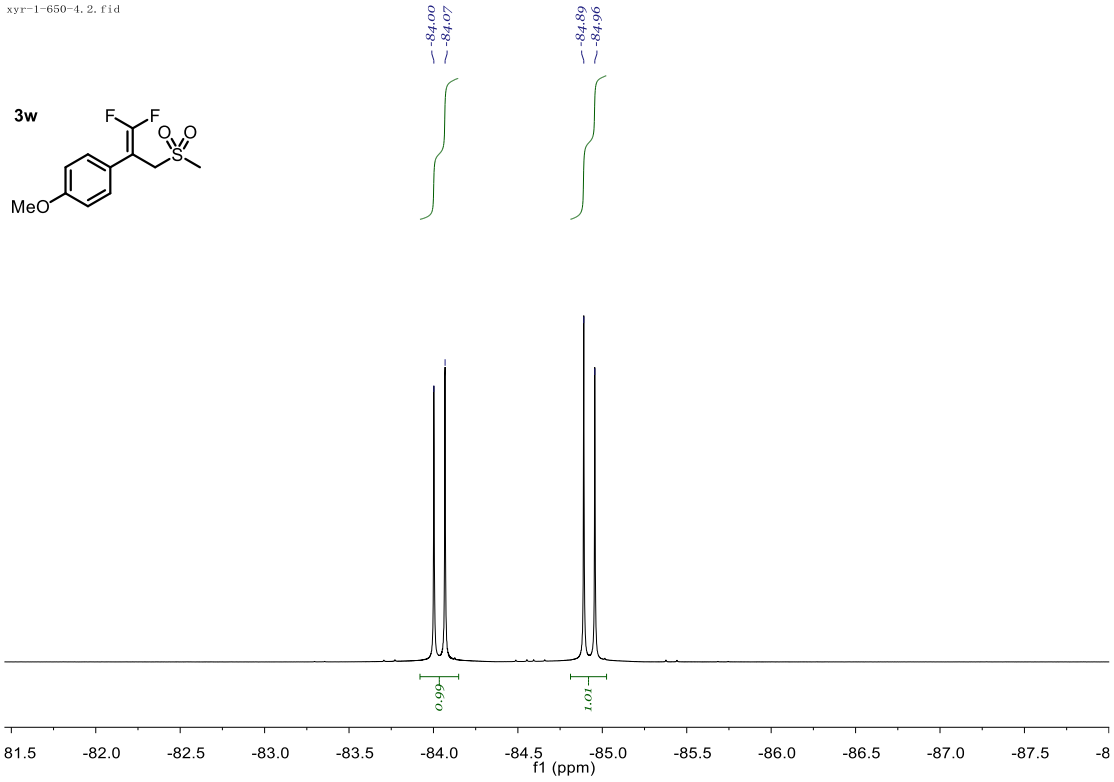

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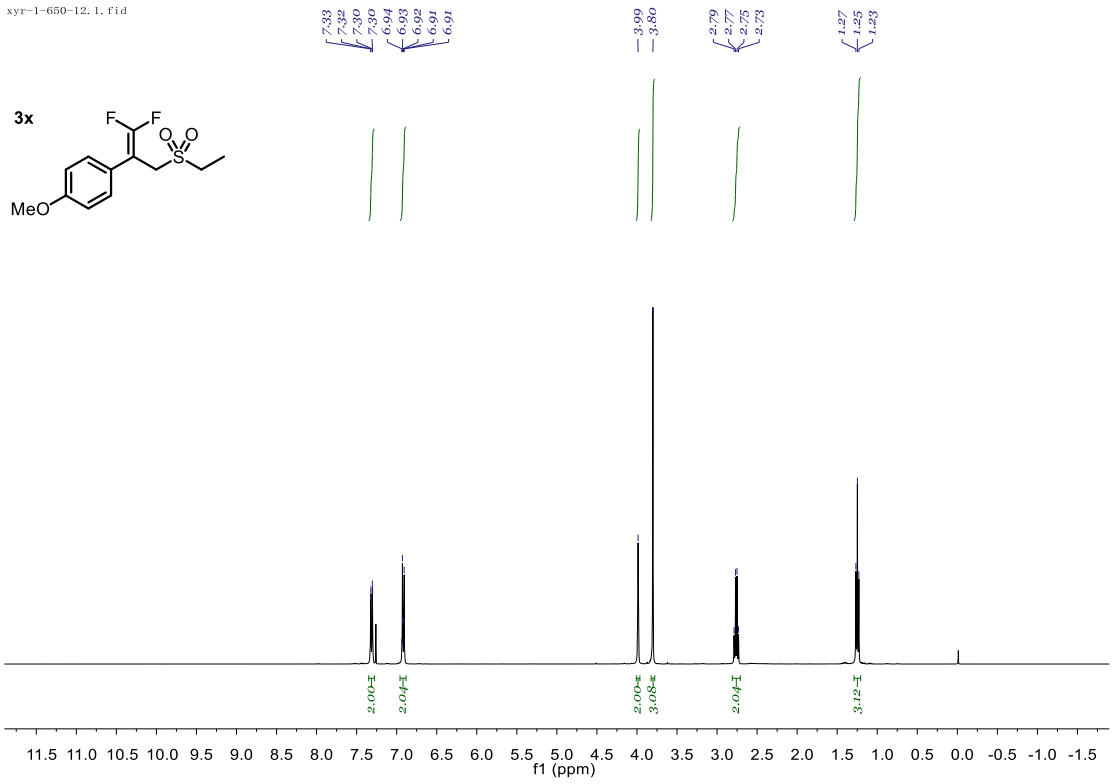

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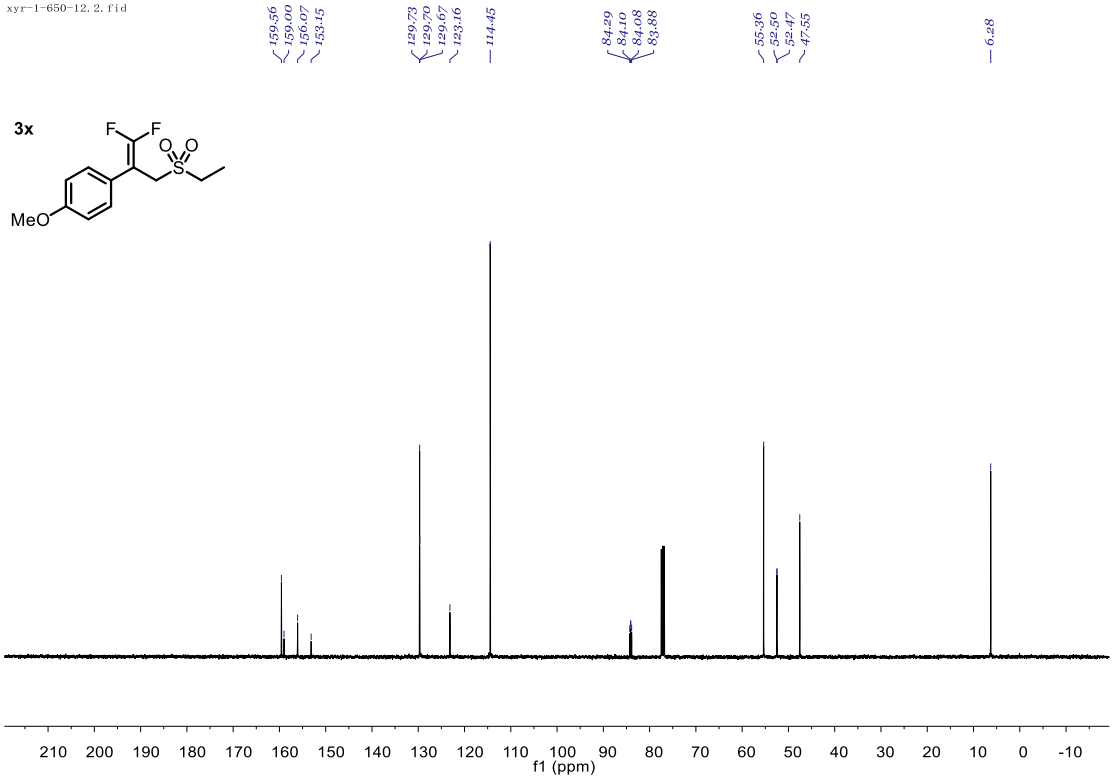

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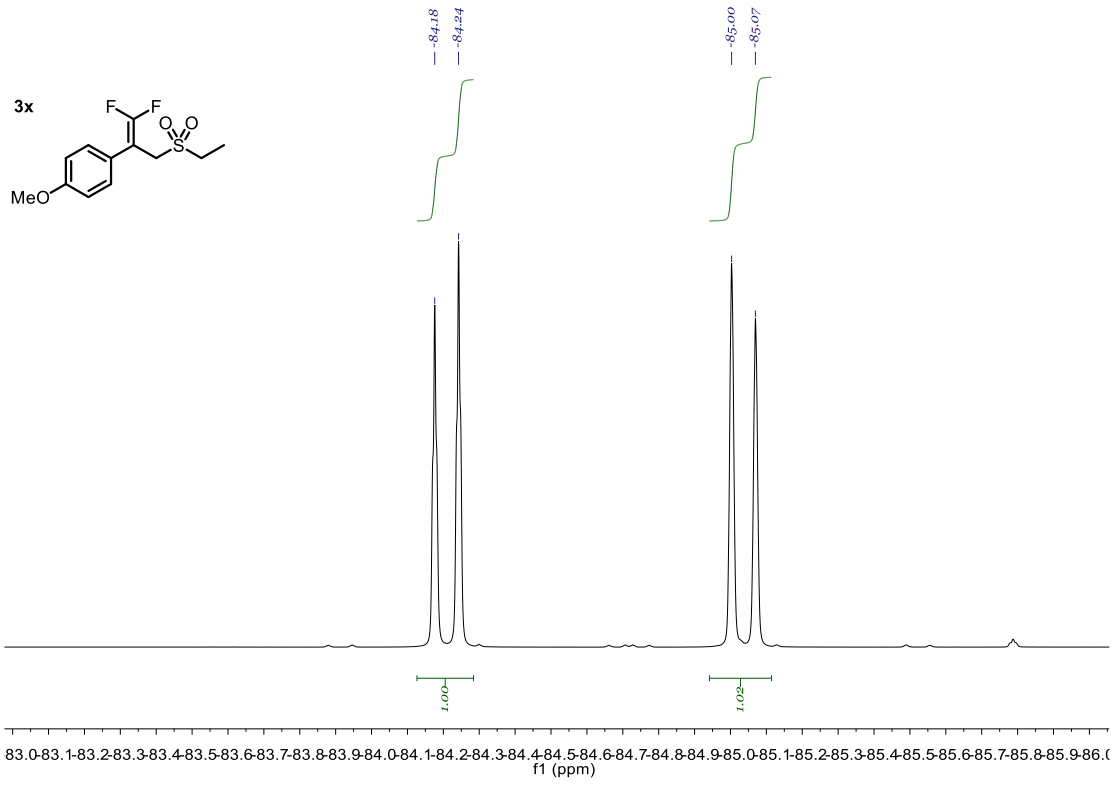

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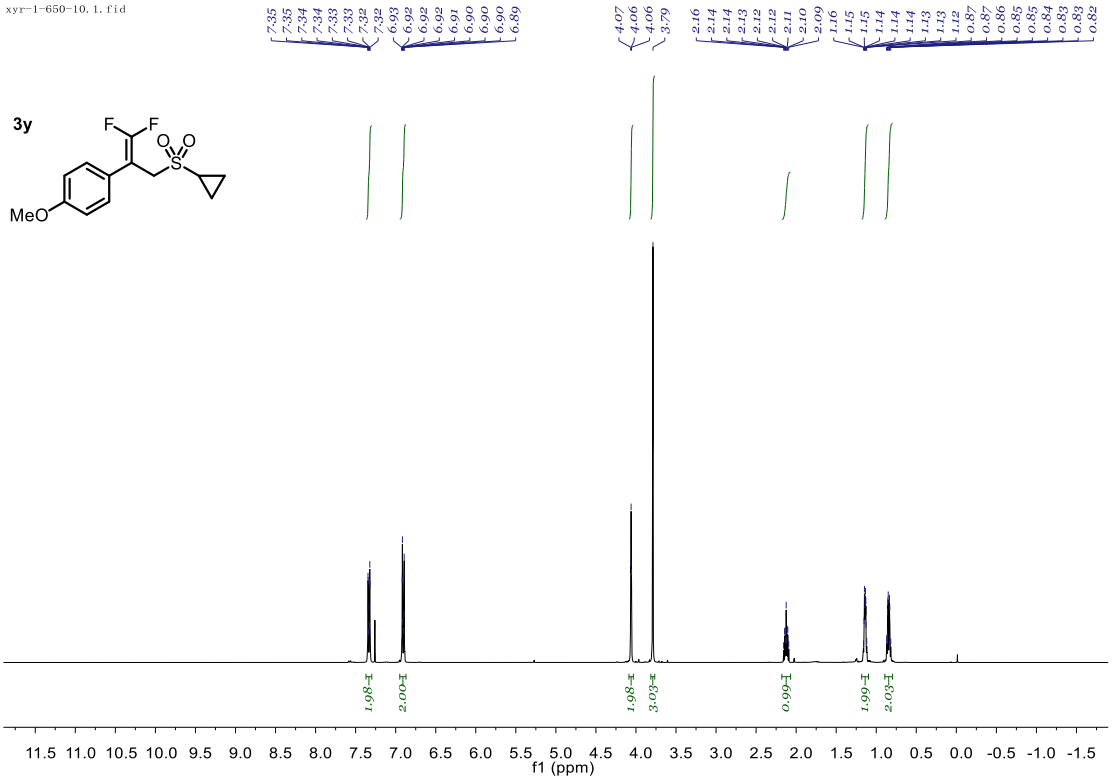
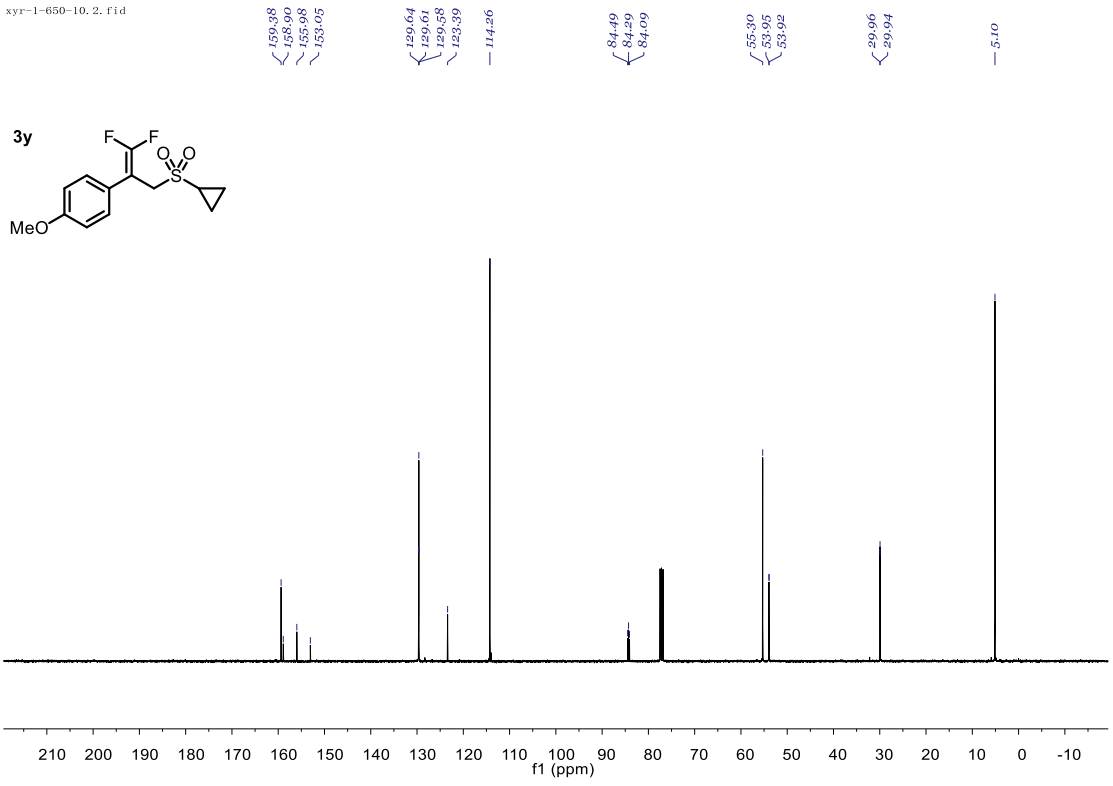


^{13}C NMR (101 MHz, Chloroform-*d*)



^{19}F NMR (377 MHz, Chloroform-*d*)