Supporting Information for

Diastereoselective Synthesis of Cyclopropyl Sulfoxides via Hydrosulfenation

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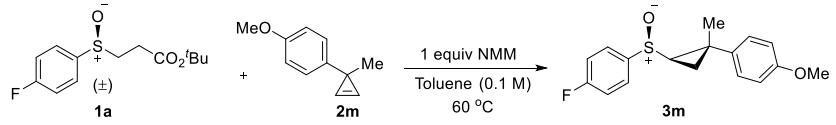
1. General Information

All chemicals and reagents were purchased and used without purification unless otherwise stated. All reactions were monitored by thin-layer chromatography (TLC) on gel F_{254} plates. The silica gel (300-400 meshes) was used for column chromatography, and the distillation range of petroleum ether was 60-90 °C. High-resolution mass spectral analysis (HRMS) data were measured by means of the ESI technique. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded in $CDCl_3$ solution on Bruker Aescend TM 400 MHz, Bruker Aescend TM 500 MHz and JNM-ECZ600R/SI instruments and spectral data were reported in ppm. The residual solvent peak or tetramethylsilane (TMS) was used as an internal reference: proton (TMS δ 0.0) and carbon ($CDCl_3$ δ 77.0). Regioselective ratios were determined by isolation yield ratio or ^{1}H NMR analysis. Optical rotations were measured by Perkin-Elmer-343 polarimeter.

2. Optimization of reaction conditions.

Table S1. Effect of bases[1,2]**.**



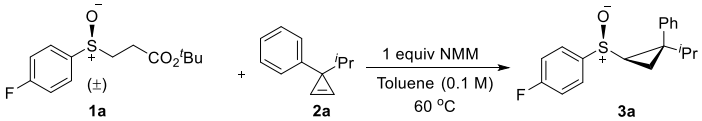
Entry[a]	Base	Solvent	T(°C)	Yield(3m)[b]	dr(3m)[c]
1	K_3PO_4	Toluene	60	47	6:1
2	K_2CO_3	Toluene	60	25	6:1
3	Cs_2CO_3	Toluene	60	47	5:1
4	NaOMe	Toluene	60	N.R.	--
5	^{t}BuCOOK	Toluene	60	25	5:1
6	NEt_3	Toluene	60	72	5:1
7	DBU	Toluene	60	N.R.	--
8	DIPEA	Toluene	60	41	5:1
9	DABCO	Toluene	60	66	4:1
10	NMM	Toluene	60	84	5:1

[a] Reaction conditions: 0.05 mmol **1a**, 0.055 mmol **2m**, 0.05 mmol **Base** (1 equiv), in toluene (0.5 mL), and at 60 °C.

[b] Isolated yield.

[c] Determined by ^{1}H NMR analysis.

Table S2. Effect of substrate's steric.



Entry[a]	Base	Solvent	T(°C)	Yield(3a)[b]	dr(3a)[c]
1	NMM	Toluene	60	84	>20:1

[a] Reaction conditions: 0.05 mmol **1a**, 0.055 mmol **2a**, 0.05 mmol NMM (1 equiv), in toluene (0.5 mL) and at 60 °C.

[b] Isolated yield.

[c] Determined by ^{1}H NMR analysis.

3. General Procedure for the synthesis of cyclopropyl sulfoxides.

General procedure 1 for the synthesis of racemic precursor of sulfenic acid (GP1)

Racemic precursor of sulfenic acid was synthesized by following the literature-reported procedure. [3]

General procedure 2 for the synthesis of chiral precursor of sulfenic acid (GP2)

Chiral precursor of sulfenic acid was synthesized by following the literature-reported procedure.[4–6]

General procedure 2 for the synthesis of cyclopropene (GP3)

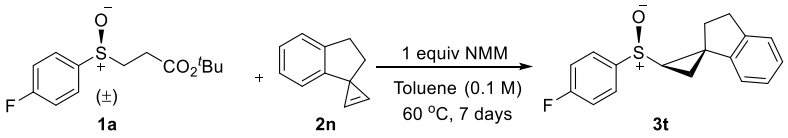
Cyclopropene was synthesized by following the literature-reported procedure.[7]

General procedure 3 for the synthesis of product 3a-3ac, 4a-4m (GP4)

To a 4 mL vial equipped with a stirring bar was charged with sulfoxide (0.1 mmol), cyclopropene (1.1 equiv), 4-Methylmorpholine (1 equiv) and toluene (1.0 mL). The vial was capped and stirred for 3 d to 7 d at 60 °C. Upon completion of the reaction, the mixture was cooled to ambient temperature and directly purified by preparative thin-layer chromatography to afford the corresponding product.

4. Synthetic applications.

4.1 Scale-up synthesis.



A 200 mL Schlenk tube equipped with a stirring bar was charged with sulfoxide **1a** (5 mmol), cyclopropene **2**(5.5 mmol), 4-Methylmorpholine (5 mmol) and toluene (50 mL). The tube was capped and stirred for 7 d at 60 ℃. Upon completion of the reaction, the mixture was cooled to ambient temperature. The organic phase was subsequently concentrated under reduced pressure and subjected to flash column chromatography purification to afford the desired product **3t** (72% yield, >20:1 dr).

4.2 Synthesis of 5b

A dried 4 mL vial equipped with a stirring bar was charged with **3t** (0.1 mmol, 1.0 equiv) and THF (1 mL) in N_2. After the mixture was cooled to 0 ℃, LDA (1.5 equiv) was added dropwise. Then the reaction mixture was stirred at 0 ℃ for 20 minutes and CH_3I (1.5 equiv) was added dropwise. Upon completion of the reaction, the mixture was quenched with water, concentrated under reduced pressure and purified by flash column chromatography to afford the product **5b, 5b′** (41% yield, 1.5:1 dr).

4.3 Synthesis of 5c

A dried 4 mL vial equipped with a stirring bar was charged with **3t** (0.1 mmol, 1 equiv) and magnesium monoperoxyphthalate (2 equiv) in MeOH (1 mL). The mixture was stirred at 25 ºC until TLC analysis indicated completion, and directly subjected to preparative thin-layer chromatography to afford the corresponding product **5e** (56% yield, >20:1 dr).

4.4 Synthesis of 5d and 5e

A dried 4 mL vial equipped with a stirring bar was charged with $Cu(OTf)_2$ (10 mol%) in MeCN (1 mL), **3t** or **4a** (0.1 mmol, 1 equiv) and PhI=NTs (0.15 mmol, 1.5 equiv). The mixture was stirred at 25 ºC until TLC analysis indicated completion, and directly subjected to preparative thin-layer chromatography to afford the corresponding product **5d** (56% yield, >20:1 dr) or **5e** (46% yield, >20:1 dr).

4.5 Synthesis of 5f, 5g, 5h, 5i

A dried 4 mL vial equipped with a stirring bar was charged with $Pd(PPh_3)_4$ (10 mol%) in dioxane (1 mL), Cs_2CO_3 (3 equiv), **3ad** (0.1 mmol, 1 equiv) and Ar-$B(OH)_2$ (1.5 equiv). The mixture was stirred at 80 ºC until TLC analysis indicated completion, and directly subjected to preparative thin-layer chromatography to afford the corresponding product **5f** (70% yield)**, 5g** (99% yield)**, 5h** (99% yield)**, 5i** (99% yield).

5. DFT Computational Studies.

To gain a deeper insight into the reactivity and selectivity, DFT computations were conducted. All the structures went through conformer search with the help of CREST/xTB program[8-10], and the low-energy conformers were then re-optimized using DFT at the **M062X/def2-TZVP**/SMD(Toluene)//**B3LYP-D3/def2-SVP** level with Gaussian 16[11-13]. Vibrational frequency calculations were conducted for all stationary points to confirm whether the optimized structures correspond to local minima or transition states. All optimized transition state structures have only one imaginary (negative) frequency, and all minima (reactants, products, and intermediates) have no imaginary frequencies. The M062X functional was used in single-point energy calculations with the def2-TZVP basis set in toluene solvent with the SMD continuum solvation model[14].Only the lowest-energy conformer from the DFT calculations is reported in this work. The calculated 3D optimized structures were visualized using CYLview program.[15]

Since the reaction system contains only a stoichiometric base and no catalyst, we propose that the reaction proceeds via a concerted reaction mechanism analogous to the Michael addition. In accordance with this mechanism, we calculated the energy of other species (**Table S3**).

	EE	ZPEC	TCH	TCG	H	G
1o	-1208.6816	0.3444	0.3662	0.2922	-1208.3154	-1208.3895
2n	-425.0847	0.1724	0.1819	0.1389	-424.9028	-424.9458
^{t}Bu-acrylate	-424.3993	0.1789	0.1901	0.1439	-424.2092	-424.2554
Int-1	-784.2535	0.1620	0.1729	0.1259	-784.0806	-784.1276
TS-1	-1208.6362	0.3389	0.3602	0.2884	-1208.2760	-1208.3479
TS-2-R_S	-1209.3271	0.3332	0.3528	0.2847	-1208.9744	-1209.0425
TS-2-S_S	-1209.3192	0.3332	0.3527	0.2848	-1208.9665	-1209.0344
TS-3-R_S	-1209.3238	0.3336	0.3530	0.2857	-1208.9708	-1209.0381
TS-3-S_S	-1209.3185	0.3336	0.3530	0.2854	-1208.9655	-1209.0332
TS-4-S_S	-1209.3253	0.3328	0.3523	0.2848	-1208.9730	-1209.0405
TS-4-R_S	-1209.3212	0.3333	0.3528	0.2847	-1208.9684	-1209.0365
TS-5-S_S	-1209.3217	0.3334	0.3529	0.2852	-1208.9688	-1209.0365
TS-5-R_S	-1209.3212	0.3339	0.3533	0.2862	-1208.9679	-1209.0349
4a	-1209.4047	0.3401	0.3596	0.2929	-1209.0451	-1209.1118
4a-S_S	-1209.4020	0.3399	0.3595	0.2914	-1209.0426	-1209.1107
4a′-R_S	-1209.4030	0.3400	0.3594	0.2930	-1209.0436	-1209.1100
4a′-S_S	-1209.4013	0.3397	0.3593	0.2911	-1209.0420	-1209.1102
4a″-S_S	-1209.4031	0.3398	0.3593	0.2921	-1209.0439	-1209.1110
4a″-R_S	-1209.4029	0.3397	0.3594	0.2909	-1209.0435	-1209.1120
4a‴-S_S	-1209.4018	0.3402	0.3596	0.2929	-1209.0422	-1209.1089
4a‴-R_S	-1209.4017	0.3398	0.3594	0.2913	-1209.0423	-1209.1103

Table S3. Energies of computed structures. All energies are shown in Hartree/Particle, EE is the all-electronic energy calculated at M062X/def2-TZVP/SMD(Toluene) level; ZPEC, TCH and TCG are zero-point energy correction, thermal correction to enthalpy and thermal correction to Gibbs free energy calculated under B3LYP-D3/def2-SVP level in gas phase, respectively. H=EE+TCH and G=EE+TCG.

To comprehensively reconstruct the reaction pathway, we calculated the energy barriers of a retro-Michael addition-type mechanism. Some important structures are shown in **Figure S1**. Starting from the reactant, the process proceeds through a five-membered cyclic transition state (**TS-1**), ultimately generating the olefin product (^{t}Bu-acrylate) along with sulfenic acid (**Int-1**) poised to react with cyclopropene.

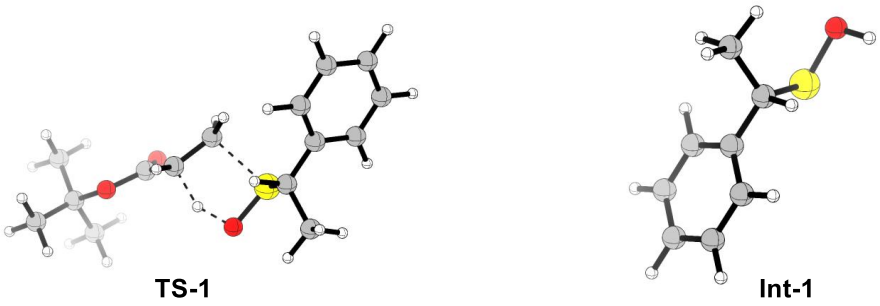
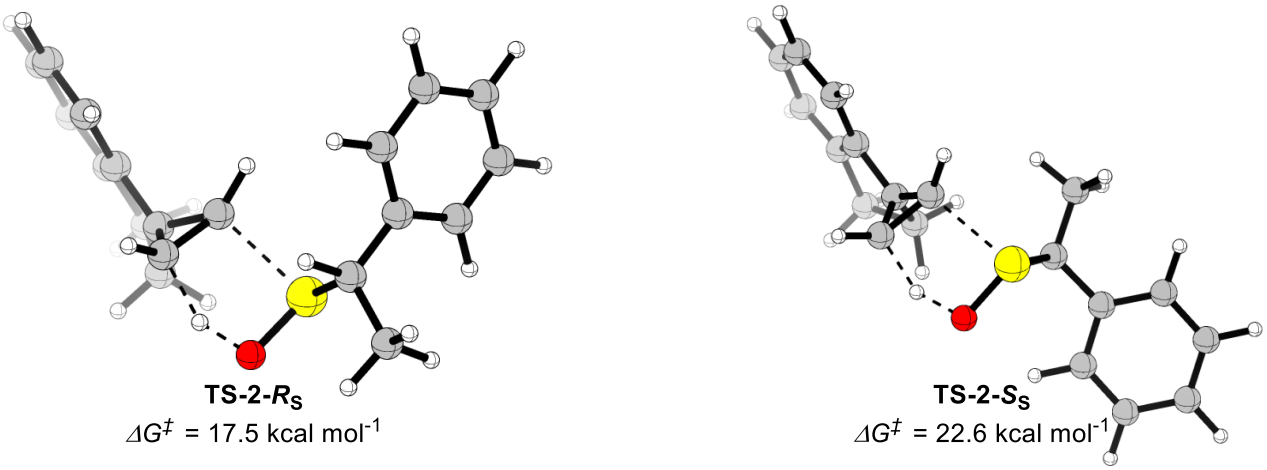


Figure S1. Optimized structure of **TS-1** and **Int-1**.

To gain deeper insights into the origins of diastereoselectivity and sulfur-centered chirality, computational studies were performed on the reaction between sulfenic acid and cyclopropene (**Figure S2**). These DFT investigations focused on the formation of product **4a**, which contains four stereogenic centers (**Figure S4**, **1*-4***). The configurationally fixed **1*** center is inherited from the sulfoxide substrate **1o**, while **2*-3*** emerge through cyclopropene desymmetrization during cycloaddition with sulfenic acid intermediate **Int-1**. The sulfur stereocenter (**4***) is dictated by the spatial geometry of this key bond-forming event. Collectively, these stereochemical determinants generate eight possible diastereomeric transition states, corresponding to permutations of three variable stereochemical parameters beyond the fixed **1*** center.

The dominant stereodifferentiation arises from the sulfur substituent's spatial orientation during cycloaddition. While the reaction proceeds through a coplanar five-membered transition state involving the S-O-H moiety and alkene π-system, the benzyl substituent adopts either *endo* (facing the benzannulated system) or *exo* (the lone pair inward) configurations. Severe steric repulsion in *endo*-type TSs elevates their energy by 5.0 kcal/mol relative to *exo*-counterparts (**TS-2-*R*s** vs. **TS-2-*S*s**), establishing this as the primary stereochemical gatekeeper.
Beyond sulfur orientation, facial selectivity imposed by cyclopropene's benzannulation introduces secondary energy differentiation. Attack at the methylene face minimizes steric repulsion, whereas approach from the benzene face induces destabilizing allylic strain. A 2.7 kcal/mol energy gap was found between **TS-2-*R*s** and **TS-3-*R*s**, rationalizing the observed preference for less hindered-face addition.
The residual stereochemical modulation stems from the side selectivity of enantiotopic cyclopropene carbons. While pseudo-enantiomeric pathways involving opposite cyclopropene carbons exhibit closely spaced energy profiles ($\Delta\Delta G^{\ddagger}$ = 1.2 kcal/mol, **TS-2-*R*s** vs. **TS-4-*R*s**), the fixed **1*** center breaks this symmetry through differential van der Waals interactions at the cyclopropane-sulfoxide interface, thus determined the side selectivity.



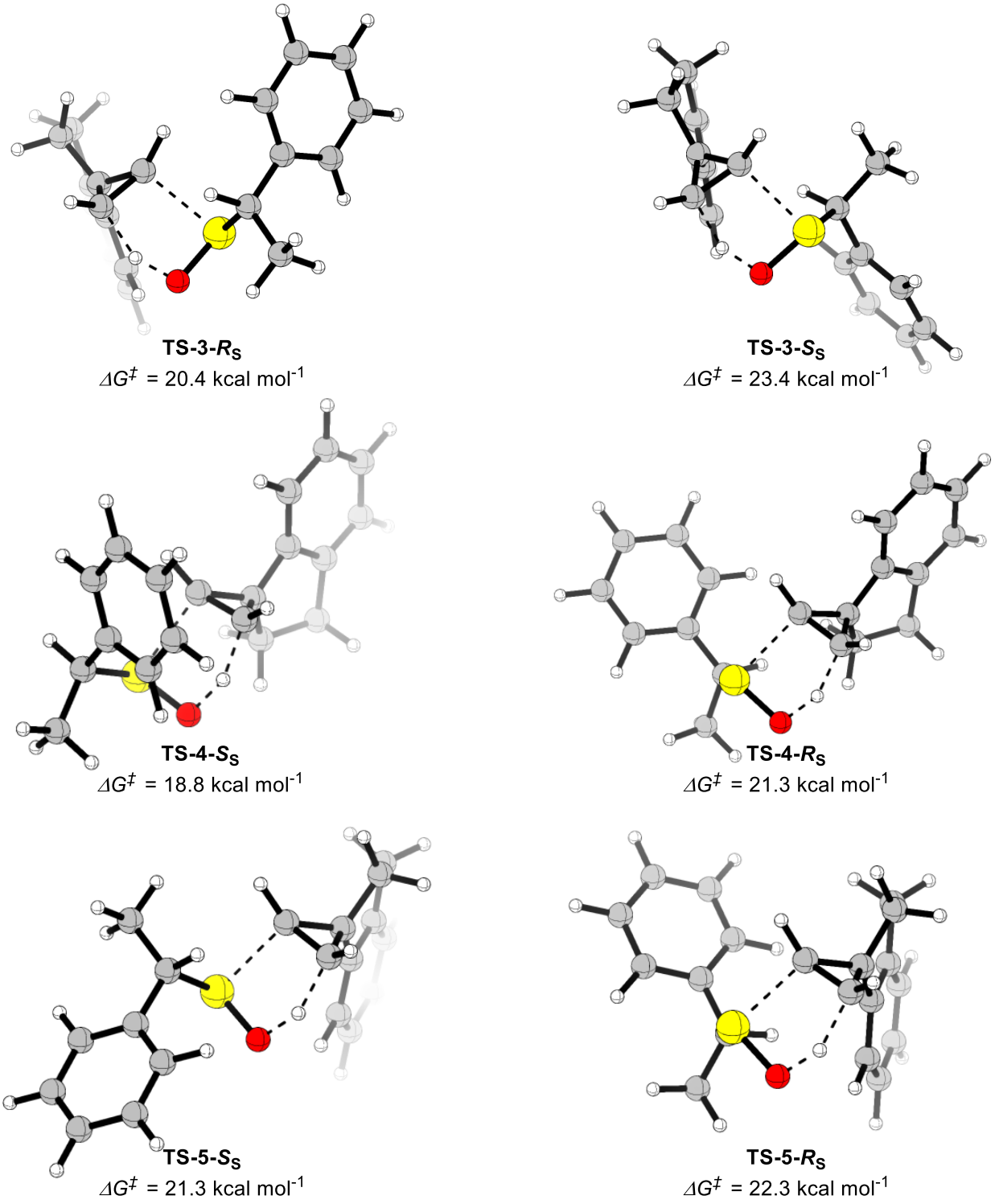


Figure S2. Five-membered cyclic transition states of the reaction.

Following this step, we computationally evaluated the products corresponding to these eight transition states and provided their three-dimensional structural representations (**Figure S3**). Single-crystal X-ray diffraction unambiguously confirmed the structure of major diastereomer **4a**, which aligns with the lowest-energy transition state (methylene-face *exo* attack) predicted by DFT calculations. While computational models identified **4a″-*Ss***—the pseudo-enantiomer differing solely in enantiotopic carbon selectivity—as the most probable minor product, its experimental isolation proved infeasible due to the exceptionally high diastereomeric ratio (dr >20:1). To circumvent this limitation, we analyzed the stereochemical outcome of substrate **4i**. X-ray characterization of **4i**'s two

predominant diastereomers revealed the pseudo-enantiomeric relationship expected for **4a** (between **4a** and **4a″-*S*s**), except for the benzene-face preference inherent to **4i**'s open-chain design (as rationalized in the facial selectivity analysis). This structural congruence validates our computational results, as both systems share identical stereochemical determinants despite divergent substitution patterns. The conserved configuration relationships across substrates demonstrate the generalizability of the stereocontrol model, particularly the dominance of sulfur orientation and facial selectivity.

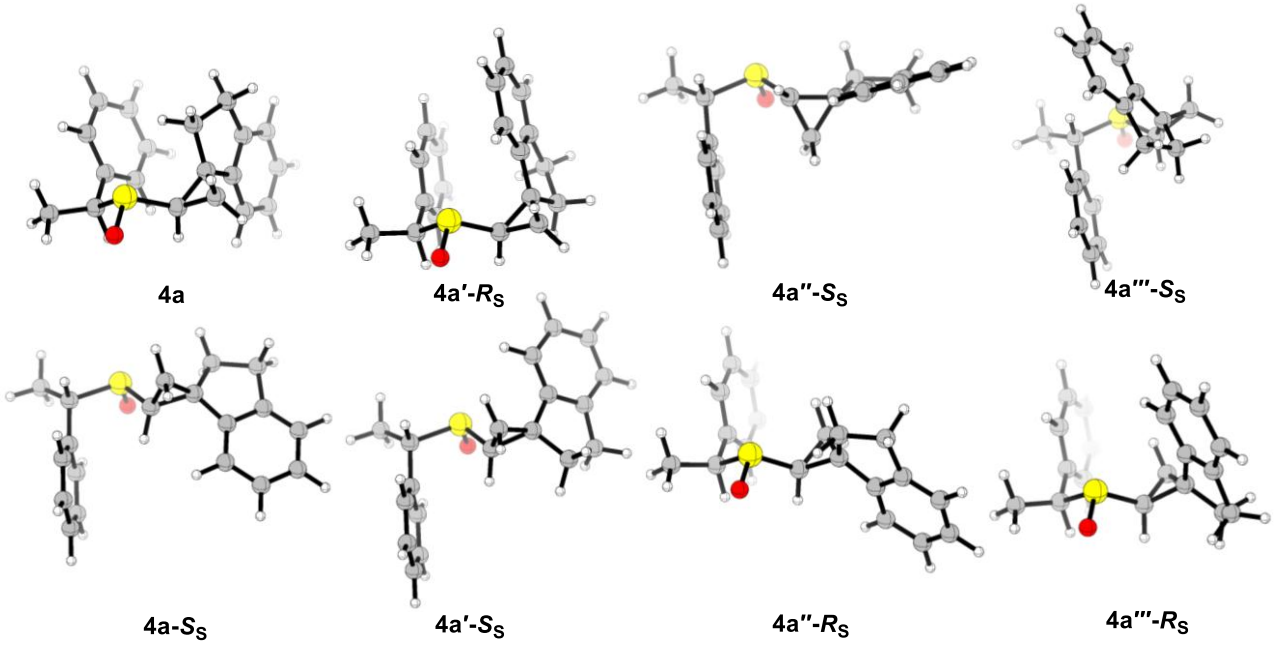
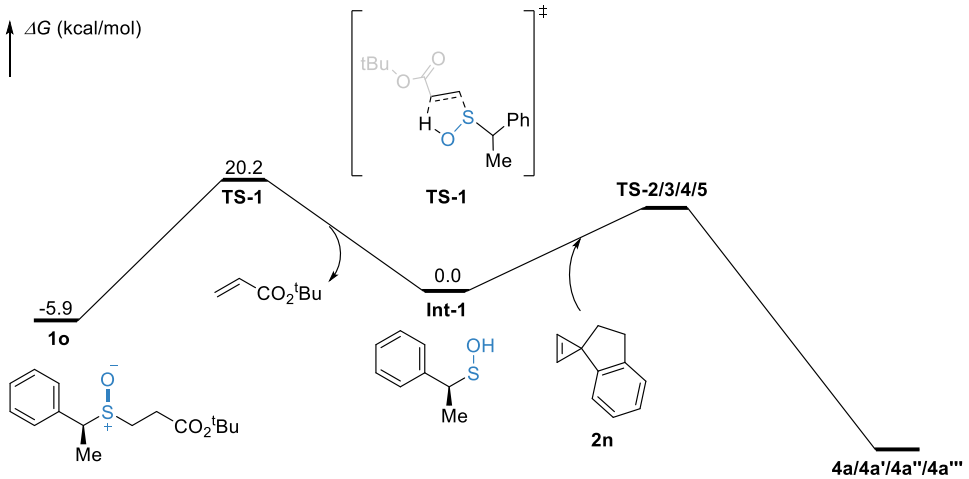
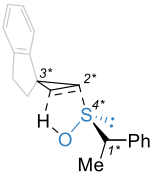
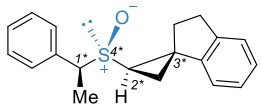


Figure S3. Product structures.

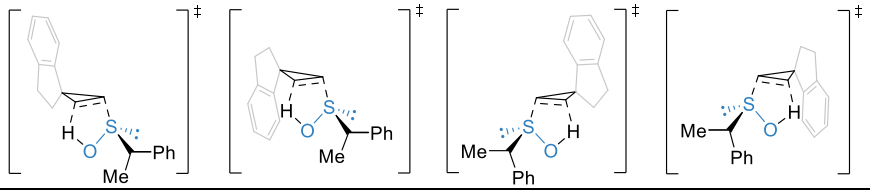
Based on the computational results, we propose the following reaction mechanism (**Figure S4**). Initially, the precursor **1o** undergoes decomposition via transition state **TS-1** to yield the olefin product (^{t}Bu-acrylate) and sulfenic acid **Int-1**. Subsequently, the sulfenic acid reacts with cyclopropane substrate **2n** through a concerted five-membered cyclic transition state to form the product. Notably, the **TS-3-*R*s** exhibits the lowest activation energy barrier ($\Delta G^{\ddagger}$ = 17.5 kcal/mol), ultimately generating the thermodynamically most stable product **4a** (ΔG = -26.0 kcal/mol).



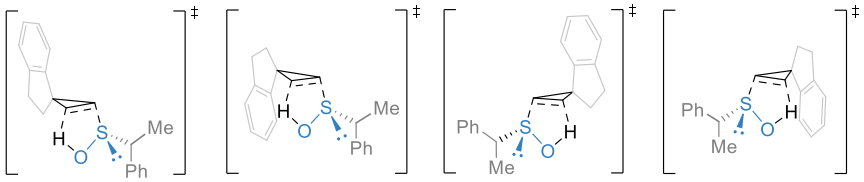




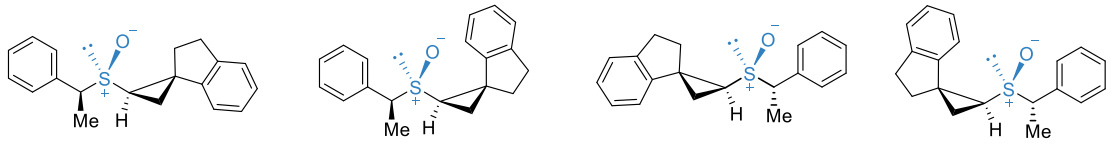
configuration = ***(1*,2*,3*,4*)***



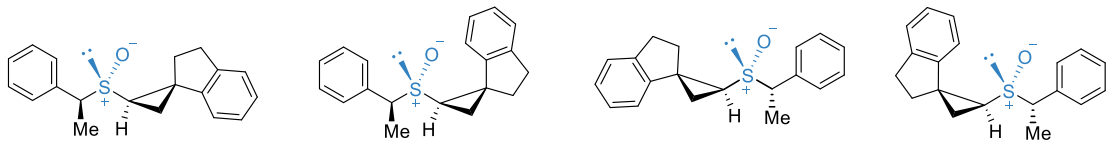
	TS-2-R_S	**TS-3-R_S**	**TS-4-S_S**	**TS-5-S_S**
$\Delta G^{\ddagger}$ (kcal/mol)	17.5	20.4	18.8	21.3
$\Delta\Delta G^{\ddagger}$ (kcal/mol)	0	2.7	1.2	3.7
configuration	**(*S*,*R*,*S*,R_S)**	**(*S*,*R*,*R*,R_S)**	**(*S*,*S*,*R*,S_S)**	**(*S*,*S*,*S*,S_S)**



	TS-2-S_S	**TS-3-S_S**	**TS-4-R_S**	**TS-5-R_S**
$\Delta G^{\ddagger}$ (kcal/mol)	22.6	23.4	21.3	22.3
$\Delta\Delta G^{\ddagger}$ (kcal/mol)	5.0	5.8	3.7	4.7
configuration	**(*S*,*R*,*S*,S_S)**	**(*S*,*R*,*R*,S_S)**	**(*S*,*S*,*R*,R_S)**	**(*S*,*S*,*S*,R_S)**



	4a	**4a′-R_S**	**4a″-S_S**	**4a‴-S_S**
ΔG (kcal/mol)	-26.0	-24.8	-25.5	-24.1
configuration	**(*S*,*R*,*S*,R_S)**	**(*S*,*R*,*R*,R_S)**	**(*S*,*S*,*R*,S_S)**	**(*S*,*S*,*S*,S_S)**



	4a-S_S	**4a′-S_S**	**4a″-R_S**	**4a‴-R_S**
ΔG (kcal/mol)	-25.3	-25.0	-26.1	-25.0
configuration	**(*S*,*R*,*S*,S_S)**	**(*S*,*R*,*R*,S_S)**	**(*S*,*S*,*R*,R_S)**	**(*S*,*S*,*S*,R_S)**

Figure S4. Proposed reaction process. All energies are shown in kcal mol^{-1}.

Cartesian Coordinates:

1o

S	1.40890	-1.66160	-0.52540
O	0.87280	-2.97570	0.01100
C	2.77940	-1.13700	0.66680
H	2.27170	-1.12270	1.64400
C	3.82030	-2.25410	0.65240
H	3.32970	-3.21920	0.84870
H	4.34140	-2.31840	-0.31560
H	4.57510	-2.07070	1.43280
C	3.26510	0.23660	0.29270
C	3.91030	0.46310	-0.93640
C	3.03930	1.33190	1.14260
C	4.32320	1.74690	-1.30000
H	4.08070	-0.37250	-1.61960
C	3.45550	2.61610	0.78210
H	2.53050	1.17450	2.09750

C	4.09940	2.82790	-0.44090
H	4.82140	1.90430	-2.26010
H	3.27440	3.45470	1.45930
H	4.42430	3.83200	-0.72470
C	0.17210	-0.37980	-0.01730
H	0.49290	0.58710	-0.43240
H	0.18140	-0.31320	1.08060
C	-1.20270	-0.80890	-0.50280
H	-1.37010	-1.86480	-0.22470
H	-1.29990	-0.75970	-1.59860
C	-2.31230	0.01100	0.13040
O	-2.16770	0.71330	1.10480
O	-3.46130	-0.17960	-0.52820
C	-4.72760	0.43290	-0.10200
C	-5.09380	-0.05490	1.30230
C	-4.61630	1.95840	-0.17310
C	-5.72180	-0.09060	-1.13790
H	-5.10590	-1.15550	1.33130
H	-4.37750	0.31200	2.04800
H	-6.09910	0.30750	1.56730
H	-4.29340	2.26950	-1.17880
H	-5.60080	2.40910	0.02680
H	-3.89690	2.33670	0.56380
H	-6.72940	0.30010	-0.93010
H	-5.42400	0.22310	-2.14970
H	-5.75810	-1.19010	-1.11440

2n

C	-0.02550	-0.32150	-0.03340
C	-0.66180	0.92710	0.03570
C	-2.05480	1.00650	0.06140
C	-2.80800	-0.17440	0.01690
C	-2.17050	-1.42080	-0.04630
C	-0.77290	-1.50020	-0.06990
H	-2.55490	1.97810	0.11460
H	-3.90000	-0.12360	0.03050
H	-2.76900	-2.33510	-0.08170
H	-0.26800	-2.46940	-0.11900
C	0.35880	2.04510	0.11170
H	0.40960	2.43170	1.14610
H	0.09990	2.90180	-0.53090
C	1.68680	1.36240	-0.29430
H	2.56140	1.74740	0.25160
H	1.87700	1.52300	-1.37000
C	1.46600	-0.14660	-0.04830
C	2.42440	-1.21370	-0.49840
C	2.39000	-1.00520	0.78490
H	2.82090	-1.76070	-1.35220
H	2.72840	-1.24600	1.79090

^{t}Bu-acrylate

C	1.05440	0.11290	0.00010
O	1.07100	1.32430	0.00000
O	-0.05080	-0.65070	0.00030
C	-1.40130	-0.07810	-0.00000
C	-1.61660	0.74940	1.27080
C	-1.61650	0.74990	-1.27050
C	-2.29560	-1.31770	-0.00050
H	-1.39780	0.14050	2.16170
H	-0.96970	1.63550	1.27920
H	-2.66710	1.07470	1.32500
H	-1.39730	0.14170	-2.16180
H	-2.66730	1.07440	-1.32440
H	-0.97020	1.63640	-1.27830
H	-3.35590	-1.02310	-0.00080
H	-2.10030	-1.93200	-0.89240
H	-2.10090	-1.93250	0.89120
C	2.27290	-0.74930	0.00020
H	2.11070	-1.83020	0.00060
C	3.49440	-0.20630	-0.00030
H	3.60670	0.88220	-0.00070
H	4.39710	-0.82240	-0.00030

Int-1

S	-1.83210	0.08240	-0.95220
O	-3.43960	0.19640	-0.42740
H	-3.68440	1.13370	-0.46720
C	-0.92960	0.26130	0.65700
H	-1.11750	1.28750	1.01320
C	-1.44360	-0.73350	1.69700
H	-1.25120	-1.77200	1.38920
H	-0.94810	-0.55800	2.66600
H	-2.52940	-0.61420	1.82560
C	0.53900	0.13030	0.30900
C	1.39710	1.23700	0.40470
C	1.06770	-1.09220	-0.14160
C	2.75090	1.12500	0.07730
H	0.99810	2.19740	0.74340
C	2.41990	-1.20510	-0.47360
H	0.41110	-1.95960	-0.24100
C	3.26680	-0.09780	-0.36260
H	3.40470	1.99670	0.16460
H	2.81400	-2.16320	-0.82220
H	4.32520	-0.18700	-0.62040

TS-1

S	-1.05780	0.98360	-0.75000
O	0.15620	1.84320	-0.21620
C	-2.28700	1.08990	0.65450
H	-1.72230	0.73930	1.53230
C	-2.68900	2.54940	0.86110
H	-1.79180	3.16900	1.00720
H	-3.24750	2.94370	-0.00150
H	-3.33050	2.63560	1.75270
C	-3.41580	0.13610	0.34790
C	-4.24140	0.33300	-0.77320
C	-3.64600	-0.98420	1.16250
C	-5.27040	-0.56450	-1.06710
H	-4.07380	1.19370	-1.42570
C	-4.67870	-1.88030	0.87280
H	-3.01340	-1.15110	2.03910
C	-5.49340	-1.67320	-0.24400
H	-5.90090	-0.39760	-1.94410
H	-4.84620	-2.74340	1.52190
H	-6.29970	-2.37420	-0.47350
C	-0.07070	-0.91100	-0.09510
H	0.06910	-1.36920	-1.07880
H	-0.88220	-1.34190	0.49800
C	1.09300	-0.39570	0.54950
H	1.15660	-0.41890	1.64190
H	0.83090	0.96900	0.29140
C	2.37540	-0.51460	-0.18490
O	2.46630	-0.74990	-1.37330
O	3.41900	-0.28080	0.63560
C	4.79760	-0.23930	0.15070
C	5.19930	-1.60470	-0.41680
C	4.95660	0.88130	-0.88200
C	5.59470	0.07550	1.41730
H	4.62300	-1.83780	-1.32050
H	6.27210	-1.60220	-0.66590
H	5.02070	-2.39290	0.33140
H	4.60370	1.83590	-0.46160
H	6.01930	0.99230	-1.14880
H	4.38180	0.66260	-1.79040
H	6.66970	0.13600	1.18870
H	5.27020	1.03610	1.84540
H	5.43840	-0.70870	2.17360

TS-2-*R*$_S$

S	-1.32280	-1.51770	0.46320
O	-0.73430	-2.81430	-0.27850
H	0.08840	-2.39110	-0.91460
C	2.92400	0.15290	-0.32150
C	3.69250	0.09130	0.85270
C	4.82240	0.89610	0.99450
C	5.17940	1.76410	-0.04740
C	4.40860	1.82790	-1.21530
C	3.27240	1.02140	-1.35770
H	5.42580	0.85150	1.90590
H	6.06760	2.39400	0.05090
H	4.69970	2.50680	-2.02140
H	2.66830	1.06210	-2.26870
C	3.08070	-0.88870	1.83220
H	2.54290	-0.33380	2.62280
H	3.83230	-1.51440	2.33940
C	2.09640	-1.70630	0.96430
H	1.20820	-2.04500	1.51360
H	2.59900	-2.60830	0.57740
C	1.76510	-0.79290	-0.23430
C	0.94430	-1.22960	-1.42690
C	0.40360	-0.27500	-0.60310
H	1.13600	-1.26180	-2.50350
H	-0.04180	0.72060	-0.64740
C	-2.63440	-0.94210	-0.72710
H	-2.09500	-0.80180	-1.67670
C	-3.69640	-2.02590	-0.90410
H	-3.21980	-2.96970	-1.20780
H	-4.25540	-2.20540	0.02670
H	-4.41380	-1.72290	-1.68390
C	-3.12870	0.39200	-0.21910
C	-2.84950	1.57210	-0.92750
C	-3.84270	0.48630	0.98820
C	-3.28100	2.81290	-0.45070
H	-2.29270	1.51500	-1.86700
C	-4.27050	1.72630	1.46870
H	-4.06040	-0.41860	1.56110
C	-3.99280	2.89340	0.74990
H	-3.05940	3.71970	-1.01910
H	-4.82300	1.78130	2.41020
H	-4.32910	3.86300	1.12530

TS-2-*S*$_S$

S	1.31060	-1.57770	-0.08210
O	1.10280	-1.28410	-1.64530
H	-0.02200	-1.27090	-1.76080
C	-3.27490	-0.13070	0.00420
C	-3.66070	1.19710	-0.24290
C	-4.96140	1.61570	0.03550

C	-5.87630	0.69570	0.56650
C	-5.49370	-0.63130	0.80230
C	-4.18990	-1.05390	0.51570
H	-5.26650	2.64830	-0.15750
H	-6.89660	1.01450	0.79540
H	-6.21790	-1.34000	1.21260
H	-3.89170	-2.09170	0.68950
C	-2.51360	1.96990	-0.85790
H	-2.42310	2.99580	-0.46740
H	-2.66880	2.05520	-1.94880
C	-1.28070	1.09180	-0.54420
H	-0.84960	1.41800	0.41710
H	-0.49700	1.14970	-1.31200
C	-1.84230	-0.33540	-0.38970
C	-1.42960	-1.50680	-1.26300
C	-1.10360	-1.55930	0.06950
H	-2.00080	-2.18390	-1.90600
H	-1.24440	-2.22860	0.92020
C	1.79490	0.07640	0.63770
H	1.20080	0.79240	0.05920
C	1.36030	0.09500	2.10100
H	1.79600	-0.74000	2.67330
H	1.68670	1.03090	2.58050
H	0.26580	0.02560	2.17960
C	3.26340	0.32850	0.36540
C	3.66470	0.64460	-0.94580
C	4.24480	0.23890	1.36360
C	5.00810	0.86760	-1.24710
H	2.91080	0.68750	-1.73530
C	5.59230	0.46470	1.06180
H	3.96750	-0.00600	2.39060
C	5.97890	0.78070	-0.24240
H	5.30040	1.11060	-2.27200
H	6.34250	0.39350	1.85380
H	7.03150	0.95810	-0.47680

TS-3-*R*$_S$

S	0.65800	1.29670	0.21890
O	-0.07470	2.43410	-0.65420
H	-0.60700	1.84290	-1.43590
C	-2.64910	-0.00810	-0.12590
C	-3.43400	-1.11000	0.25920
C	-4.34110	-1.00560	1.31360
C	-4.46980	0.21580	1.98660
C	-3.69830	1.31690	1.59700
C	-2.78680	1.21410	0.53840
H	-4.95090	-1.86560	1.60600
H	-5.18200	0.31260	2.81050
H	-3.81290	2.27160	2.11750
H	-2.20120	2.08280	0.23670
C	-3.13090	-2.31730	-0.60220
H	-4.03550	-2.87890	-0.88510
H	-2.47830	-3.01920	-0.05090
C	-2.38570	-1.70990	-1.80830
H	-3.10430	-1.45160	-2.60640
H	-1.63580	-2.38400	-2.25130
C	-1.76000	-0.40410	-1.27780
C	-0.26200	-0.29460	-1.30440
C	-0.95320	0.52300	-2.16080
H	0.54750	-1.02740	-1.30500
H	-0.91000	0.66550	-3.24490
C	2.33780	1.22500	-0.58240
H	2.12860	1.02680	-1.64500
C	3.06250	0.04590	0.02400
C	3.39870	0.02980	1.38910
C	3.38870	-1.07220	-0.76060
C	4.04610	-1.07300	1.95100
H	3.14510	0.88580	2.01960
C	4.04150	-2.17410	-0.20110
H	3.13470	-1.07430	-1.82440
C	4.37120	-2.17780	1.15740
H	4.29720	-1.06980	3.01470
H	4.29300	-3.03250	-0.82920
H	4.87950	-3.03950	1.59720
C	3.04150	2.57460	-0.44810
H	3.26260	2.81460	0.60280
H	3.99250	2.55720	-1.00490
H	2.40440	3.37180	-0.85870

TS-3-*S*$_S$

S	0.67180	-2.18860	-0.13670
O	0.50320	-1.71340	-1.65990
H	-0.59990	-1.71000	-1.80140
C	-2.03410	0.49180	-0.38820
C	-2.85150	1.26380	0.45770
C	-2.65570	2.63970	0.57580
C	-1.64750	3.25370	-0.17930
C	-0.85310	2.49090	-1.04410
C	-1.03930	1.10670	-1.15320
H	-3.29430	3.23570	1.23420
H	-1.49330	4.33350	-0.10720
H	-0.08050	2.97770	-1.64480
H	-0.40510	0.51830	-1.81720
C	-3.90410	0.39700	1.11560

H	-4.88350	0.89540	1.18830
H	-3.59690	0.14060	2.14660
C	-3.91710	-0.86130	0.22260
H	-4.62970	-0.72470	-0.61050
H	-4.20810	-1.78050	0.75440
C	-2.49150	-0.94420	-0.36130
C	-1.69110	-2.18510	-0.01700
C	-2.05520	-2.01120	-1.33000
H	-1.83240	-2.92550	0.77260
H	-2.60740	-2.64980	-2.02690
C	1.05940	-0.68010	0.87770
H	0.21810	0.01030	0.75040
C	2.34130	-0.01140	0.43050
C	2.35570	1.37030	0.19240
C	3.53980	-0.73160	0.29620
C	3.53970	2.01960	-0.17200
H	1.42940	1.94040	0.28910
C	4.72180	-0.08560	-0.06920
H	3.54350	-1.81180	0.46390
C	4.72610	1.29410	-0.30480
H	3.53160	3.09720	-0.35580
H	5.64460	-0.66200	-0.17480
H	5.65130	1.79910	-0.59410
C	1.10360	-1.17010	2.33110
H	1.31070	-0.31530	2.99280
H	0.14250	-1.61440	2.63660
H	1.90210	-1.91310	2.48680

TS-4-*S*$_S$

S	-1.39000	-1.89680	-0.63130
O	-1.30940	-1.97310	0.96680
H	-0.63930	-1.07910	1.23840
C	2.67810	0.27010	-0.06570
C	3.79160	-0.54900	0.18350
C	5.08260	-0.03470	0.06360
C	5.25360	1.30630	-0.30750
C	4.14160	2.12500	-0.54490
C	2.84520	1.61120	-0.41990
H	5.95300	-0.66840	0.25700
H	6.26140	1.71750	-0.40980
H	4.28820	3.17020	-0.82990
H	1.97380	2.24870	-0.59610
C	3.34550	-1.93130	0.61110
H	3.46190	-2.03410	1.70540
H	3.94250	-2.73590	0.15280
C	1.85400	-1.97940	0.20660
H	1.23110	-2.57100	0.89050
H	1.75820	-2.42460	-0.79870
C	1.41120	-0.50190	0.13390
C	0.12990	-0.01440	-0.45330
C	0.22810	0.07550	0.90970
H	-0.14050	0.60400	-1.30950
H	0.11320	0.91730	1.59780
C	-3.01180	-1.00610	-0.92050
H	-3.03590	-0.93870	-2.02180
C	-4.15200	-1.90020	-0.42740
H	-5.11980	-1.39520	-0.57680
H	-4.16380	-2.85720	-0.97080
H	-4.03780	-2.12340	0.64330
C	-3.00070	0.38320	-0.33380
C	-2.83960	1.50330	-1.16530
C	-3.11340	0.58580	1.05220
C	-2.78470	2.79260	-0.63090
H	-2.75340	1.36210	-2.24700
C	-3.05500	1.87480	1.58790
H	-3.22600	-0.27160	1.71620
C	-2.88890	2.98220	0.75070
H	-2.66190	3.65170	-1.29550
H	-3.13710	2.01410	2.66890
H	-2.84470	3.98950	1.17250

TS-4-*R*$_S$

S	1.74670	-1.56140	-1.00920
O	0.96580	-2.93730	-0.74740
H	-0.11570	-2.66080	-0.95360
C	-2.67590	0.13850	-0.28900
C	-3.36880	-0.00050	0.92560
C	-4.55000	0.70640	1.14740
C	-5.03390	1.55910	0.14510
C	-4.34810	1.68910	-1.06940
C	-3.16640	0.97250	-1.29620
H	-5.09350	0.59900	2.09050
H	-5.95460	2.12470	0.31100
H	-4.73820	2.35440	-1.84430
H	-2.63520	1.06480	-2.24770
C	-2.66700	-1.00700	1.81250
H	-3.18100	-1.98300	1.74240
H	-2.66270	-0.72220	2.87640
C	-1.25130	-1.08830	1.19970
H	-0.76070	-2.06150	1.33650
H	-0.62590	-0.31570	1.67880
C	-1.45620	-0.73530	-0.28680
C	-0.41220	-0.57910	-1.35720
C	-1.19050	-1.70990	-1.41970

H	-0.13740	0.26410	-1.99270
H	-1.83290	-2.11510	-2.20780
C	2.18950	-0.91210	0.68140
H	1.24570	-0.86000	1.23190
C	3.13030	-1.89110	1.37590
H	3.39350	-1.51750	2.37890
H	2.63510	-2.86760	1.48050
H	4.05970	-2.04850	0.80810
C	2.70250	0.48970	0.43710
C	4.05210	0.74990	0.15070
C	1.79550	1.56540	0.43160
C	4.48630	2.05160	-0.11830
H	4.77560	-0.06750	0.13870
C	2.22800	2.86540	0.16480
H	0.73840	1.37600	0.63380
C	3.57730	3.11300	-0.11060
H	5.54170	2.23590	-0.33490
H	1.50880	3.68830	0.17200
H	3.91830	4.13030	-0.31890

TS-5-*S*$_S$

S	-0.63370	0.14880	0.55720
O	-0.66510	0.65420	-0.96660
H	0.03690	-0.04190	-1.48120
C	2.83840	0.24200	-0.30640
C	4.11120	0.00530	0.24320
C	4.90970	1.06450	0.67510
C	4.43290	2.37530	0.54990
C	3.17150	2.61360	-0.00840
C	2.36820	1.55150	-0.44250
H	5.90020	0.87380	1.09860
H	5.05150	3.21480	0.87850
H	2.81040	3.64000	-0.11600
H	1.39350	1.75220	-0.88770
C	4.41830	-1.47650	0.27880
H	4.27760	-1.86650	1.30380
H	5.45700	-1.70510	-0.00840
C	3.37200	-2.07520	-0.68350
H	3.05380	-3.09460	-0.41430
H	3.78290	-2.12180	-1.70760
C	2.20000	-1.07320	-0.67680
C	0.96200	-1.27350	-1.52410
C	0.86700	-1.56520	-0.18830
H	0.76680	-1.86180	-2.42590
H	0.56250	-2.38550	0.46570
C	-2.07980	-1.03330	0.63000
H	-1.85020	-1.79890	-0.12720
C	-2.06850	-1.65920	2.02460
H	-2.93390	-2.32940	2.14050
H	-1.15320	-2.24790	2.19030
H	-2.12360	-0.89890	2.81920
C	-3.34480	-0.31320	0.23010
C	-4.18000	0.31290	1.16950
C	-3.68110	-0.22540	-1.13090
C	-5.32520	1.00000	0.75890
H	-3.94020	0.27000	2.23380
C	-4.82370	0.46310	-1.54280
H	-3.03060	-0.69350	-1.87300
C	-5.65150	1.07760	-0.59840
H	-5.96580	1.47790	1.50460
H	-5.06800	0.52070	-2.60660
H	-6.54740	1.61550	-0.91860

TS-5-*R*$_S$

S	1.10680	-2.07150	-0.50510
O	-0.11830	-3.06910	-0.18880
H	-0.92550	-2.68170	-0.83640
C	-2.03680	0.00270	-0.03530
C	-2.33150	1.37520	0.04870
C	-2.68060	1.95250	1.26990
C	-2.75990	1.14240	2.41080
C	-2.50670	-0.23200	2.31920
C	-2.14880	-0.81100	1.09470
H	-2.90500	3.02120	1.33450
H	-3.04050	1.58130	3.37190
H	-2.59490	-0.86080	3.20910
H	-1.94420	-1.88060	1.02640
C	-2.21900	2.02350	-1.31550
H	-1.25080	2.55030	-1.40780
H	-3.00920	2.76760	-1.50200
C	-2.26660	0.81430	-2.27450
H	-1.72810	0.97810	-3.22060
H	-3.31480	0.57420	-2.52760
C	-1.67510	-0.34900	-1.45300
C	-1.46710	-1.74170	-1.98430
C	-0.36470	-0.92300	-1.94950
H	-1.93680	-2.30310	-2.79820
H	0.37420	-0.50940	-2.63730
C	1.20820	-0.91240	0.95020
H	0.18480	-0.56420	1.11810
C	1.70130	-1.66300	2.18450
H	1.02520	-2.50180	2.40890
H	2.71540	-2.06850	2.04710
H	1.71500	-0.98300	3.05170

C	2.05700	0.24590	0.48240
C	1.45500	1.48900	0.22240
C	3.43580	0.10200	0.25390
C	2.21480	2.56420	-0.24350
H	0.38230	1.60820	0.39310
C	4.19520	1.17660	-0.21830
H	3.92100	-0.85890	0.44280
C	3.58740	2.41080	-0.46700
H	1.73240	3.52680	-0.43200
H	5.26680	1.04870	-0.39170
H	4.18210	3.25170	-0.83290

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S	-2.35680	-1.20740	0.36060
O	-3.29650	-2.29560	-0.10960
H	-0.44520	-3.02420	1.69150
C	1.81370	-0.95800	-0.04940
C	2.61060	-0.14120	0.76850
C	3.83840	0.33230	0.30660
C	4.26690	-0.01620	-0.98130
C	3.47510	-0.83920	-1.79230
C	2.24300	-1.31690	-1.32820
H	4.45770	0.97440	0.93930
H	5.22370	0.35630	-1.35620
H	3.81810	-1.10630	-2.79510
H	1.62580	-1.95310	-1.96900
C	1.94500	0.08340	2.10720
H	2.02770	1.12530	2.45420
H	2.42420	-0.55170	2.87410
C	0.47750	-0.33940	1.86080
H	-0.11110	0.54720	1.58890
H	0.00050	-0.79570	2.73980
C	0.53970	-1.29780	0.65810
C	0.03490	-2.72250	0.75450
C	-0.68150	-1.73210	-0.11930
H	0.59650	-3.51510	0.25160
H	-0.59420	-1.85650	-1.20450
C	-2.51810	0.19170	-0.92570
H	-2.20840	-0.29780	-1.86230
C	-4.00250	0.53230	-1.00280
H	-4.17920	1.25840	-1.81170
H	-4.57850	-0.38190	-1.20690
H	-4.37930	0.96870	-0.06460
C	-1.57060	1.30410	-0.57250
C	-0.32230	1.39670	-1.21040
C	-1.85910	2.21330	0.46130
C	0.61760	2.35290	-0.82180
H	-0.06970	0.69000	-2.00400
C	-0.92510	3.17910	0.84510
H	-2.81570	2.15590	0.98480
C	0.31870	3.24950	0.20870
H	1.59140	2.38380	-1.31590
H	-1.16700	3.87470	1.65280
H	1.05300	3.99790	0.51690

4a-*S*$_S$

S	1.04940	-1.85970	-0.13070
O	1.05510	-1.70550	-1.63920
H	-0.54000	-1.73010	2.35570
C	-2.45100	0.29700	0.22390
C	-3.68050	-0.25920	-0.16400
C	-4.74880	0.56990	-0.50720
C	-4.57920	1.95980	-0.45910
C	-3.35270	2.51170	-0.06780
C	-2.27950	1.68150	0.27770
H	-5.70700	0.14110	-0.81390
H	-5.40760	2.61820	-0.73270
H	-3.23000	3.59740	-0.03850
H	-1.32120	2.11690	0.57510
C	-3.62470	-1.77040	-0.10610
H	-4.10660	-2.25140	-0.97160
H	-4.15510	-2.12930	0.79470
C	-2.11120	-2.07820	-0.02020
H	-1.69960	-2.24270	-1.02910
H	-1.88130	-2.97010	0.58050
C	-1.48210	-0.79590	0.55040
C	-0.70090	-0.77210	1.84920
C	0.00210	-0.54160	0.53670
H	-0.82020	0.08780	2.51500
H	0.34990	0.46060	0.26920
C	2.72880	-1.21510	0.48370
H	2.68500	-1.38670	1.57170
C	3.77240	-2.12510	-0.16520
H	3.69920	-2.07670	-1.26160
H	4.78390	-1.80990	0.13320
H	3.62920	-3.17460	0.13840
C	2.89750	0.24930	0.19220
C	2.98010	1.17760	1.24320
C	2.92370	0.72270	-1.13310
C	3.09830	2.54560	0.98360
H	2.94830	0.82260	2.27750
C	3.03290	2.09150	-1.39020
H	2.80860	0.01610	-1.95530
C	3.12570	3.00680	-0.33630

H	3.16840	3.25260	1.81440
H	3.04170	2.44620	-2.42410
H	3.21660	4.07630	-0.54290

4a′-*R*$_S$

S	-2.08070	0.93240	-0.51850
O	-3.44700	1.58030	-0.44730
H	-0.75970	3.41150	0.17550
C	1.21140	1.34680	-0.06000
C	2.26770	0.54110	0.39570
C	3.26240	0.11680	-0.48470
C	3.19460	0.49940	-1.83000
C	2.14050	1.30230	-2.28430
C	1.14380	1.73340	-1.40050
H	4.08290	-0.51250	-0.12920
H	3.97020	0.17500	-2.52870
H	2.09830	1.60160	-3.33460
H	0.32520	2.35820	-1.76290
C	2.10180	0.21780	1.86250
H	3.04750	0.26510	2.42500
H	1.71170	-0.80880	1.96360
C	1.06170	1.25410	2.34230
H	1.57600	2.15020	2.72890
H	0.40780	0.87650	3.14250
C	0.28310	1.65040	1.07870
C	-1.22020	1.39340	1.01520
C	-0.68610	2.79780	1.07970
H	-1.70940	0.98580	1.90750
H	-0.83720	3.35140	2.01120
C	-2.38080	-0.88030	-0.08950
H	-2.89280	-0.82020	0.88440
C	-1.09070	-1.64570	0.02860
C	-0.18170	-1.69930	-1.04250
C	-0.78070	-2.34290	1.20740
C	1.00190	-2.43090	-0.93700
H	-0.39240	-1.14550	-1.96020
C	0.39690	-3.08930	1.30880
H	-1.47650	-2.30810	2.05040
C	1.29270	-3.13450	0.23620
H	1.70590	-2.44000	-1.77160
H	0.61690	-3.63350	2.23090
H	2.21840	-3.70970	0.31680
C	-3.35540	-1.41440	-1.13950
H	-4.23090	-0.75150	-1.20730
H	-2.88150	-1.47860	-2.13190
H	-3.69010	-2.42490	-0.85800

4a′-*S*$_S$

S	0.22560	1.25600	0.16930
O	0.34900	1.17400	1.67630
H	-0.59700	0.10950	-2.48530
C	-2.56310	-0.25150	-0.44190
C	-3.35760	-0.95850	0.47730
C	-4.58300	-0.44000	0.89310
C	-5.01240	0.79190	0.38150
C	-4.22050	1.49440	-0.53440
C	-2.98830	0.97590	-0.95230
H	-5.20370	-0.98850	1.60710
H	-5.97380	1.20580	0.69660
H	-4.56660	2.45310	-0.92920
H	-2.37320	1.53170	-1.66350
C	-2.66900	-2.24080	0.89190
H	-3.35960	-3.09110	1.00310
H	-2.17090	-2.09210	1.86700
C	-1.62020	-2.44770	-0.22330
H	-2.07090	-3.01030	-1.05900
H	-0.72570	-2.99570	0.10800
C	-1.30530	-1.02650	-0.70260
C	0.07370	-0.44750	-0.42040
C	-0.35960	-0.73810	-1.83320
H	0.80840	-1.10050	0.06120
H	0.12580	-1.57650	-2.34200
C	1.97590	1.60300	-0.49310
H	1.82590	1.68590	-1.58200
C	2.91650	0.47470	-0.17990
C	3.45940	-0.30610	-1.21370
C	3.23420	0.14900	1.15210
C	4.30960	-1.37850	-0.93170
H	3.21080	-0.06950	-2.25240
C	4.07710	-0.92940	1.43230
H	2.77930	0.71700	1.96400
C	4.62200	-1.69320	0.39460
H	4.72890	-1.96970	-1.75000
H	4.30870	-1.17620	2.47180
H	5.28650	-2.53170	0.61860
C	2.36970	2.95530	0.10160
H	1.67600	3.74850	-0.22080
H	2.34870	2.91500	1.20070
H	3.38650	3.22790	-0.22030

4a′′-*S*$_S$

S	-1.03010	-1.72640	-0.68370
O	-1.34060	-2.20120	0.72590
H	-0.40630	-0.11630	1.63880

C	2.59610	0.27470	-0.13110
C	3.69480	-0.33710	0.49630
C	4.98450	0.15090	0.28660
C	5.17060	1.25640	-0.55450
C	4.07350	1.86960	-1.17210
C	2.77730	1.38230	-0.96090
H	5.84230	-0.32410	0.77120
H	6.17800	1.64210	-0.73110
H	4.22980	2.73140	-1.82620
H	1.92390	1.86590	-1.44510
C	3.23140	-1.47690	1.37800
H	3.22490	-1.14900	2.43360
H	3.88570	-2.36100	1.32270
C	1.79490	-1.75770	0.88270
H	1.10840	-2.13290	1.65150
H	1.82690	-2.51550	0.08100
C	1.33550	-0.42210	0.27590
C	0.05760	-0.26560	-0.50810
C	0.17090	0.36650	0.84440
H	0.06310	0.35380	-1.41180
H	0.23810	1.45680	0.89290
C	-2.59040	-0.81590	-1.28580
H	-2.31700	-0.48200	-2.30070
C	-3.68150	-1.88470	-1.34940
H	-3.41790	-2.67900	-2.06600
H	-3.82550	-2.35310	-0.36460
H	-4.63420	-1.43190	-1.66370
C	-2.89470	0.36430	-0.40970
C	-2.72090	1.67120	-0.89380
C	-3.30250	0.18700	0.92470
C	-2.94800	2.77710	-0.07150
H	-2.40170	1.82320	-1.92930
C	-3.52340	1.29350	1.74830
H	-3.40260	-0.82150	1.32570
C	-3.34890	2.59070	1.25540
H	-2.81240	3.78690	-0.46770
H	-3.83040	1.14040	2.78620
H	-3.52610	3.45370	1.90230

4a″-*R*$_S$

S	0.94900	1.64290	0.00280
O	0.36420	2.82080	-0.74700
H	0.41530	-0.83010	1.54740
C	-2.65100	-0.37960	-0.10760
C	-3.71560	0.02310	0.71510
C	-5.02960	-0.29120	0.36750
C	-5.27320	-1.01330	-0.80800
C	-4.20940	-1.41990	-1.62330
C	-2.88990	-1.10590	-1.27560
H	-5.86150	0.02430	1.00360
H	-6.29960	-1.25860	-1.09280
H	-4.41040	-1.98070	-2.53970
H	-2.06320	-1.42260	-1.91780
C	-3.20010	0.75100	1.93740
H	-3.24630	0.08240	2.81610
H	-3.79280	1.64510	2.18650
C	-1.73590	1.08990	1.57210
H	-1.05570	1.07050	2.43570
H	-1.68020	2.09680	1.12750
C	-1.35330	0.06540	0.49010
C	-0.11190	0.21350	-0.35430
C	-0.20200	-0.90550	0.64650
H	-0.18730	0.00410	-1.42770
H	-0.31580	-1.92020	0.25450
C	2.44140	1.07060	-1.01150
H	2.00840	0.84230	-1.99810
C	3.37380	2.27340	-1.13340
H	4.19550	2.04140	-1.82860
H	2.81250	3.13840	-1.51700
H	3.81720	2.54920	-0.16370
C	3.01870	-0.16760	-0.38190
C	2.94340	-1.40640	-1.03850
C	3.59570	-0.12310	0.89960
C	3.43460	-2.56810	-0.43760
H	2.49070	-1.45910	-2.03250
C	4.08300	-1.28390	1.50460
H	3.65000	0.82780	1.43510
C	4.00490	-2.51110	0.83790
H	3.37020	-3.52220	-0.96710
H	4.52490	-1.23030	2.50300
H	4.38750	-3.41920	1.31060

4a‴-*S*$_S$

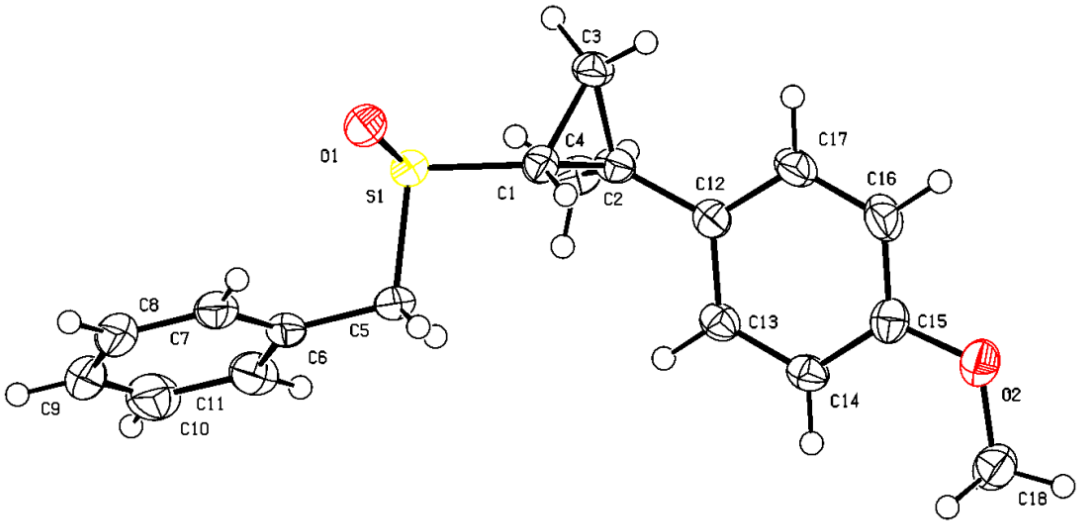
S	-0.61580	-2.11940	0.23380
O	-1.94920	-2.71960	0.63930
H	1.44560	-2.16100	2.31830
C	2.02790	-0.07940	0.42950
C	2.31870	1.24550	0.06280
C	3.16900	1.50710	-1.01320
C	3.73360	0.43690	-1.71840
C	3.45200	-0.88320	-1.34430
C	2.59850	-1.14910	-0.26710
H	3.39570	2.53780	-1.30020
H	4.40240	0.63220	-2.56060

H	3.90280	-1.71260	-1.89510
H	2.37340	-2.18080	0.01210
C	1.59180	2.23140	0.94970
H	0.78110	2.72470	0.38970
H	2.25590	3.03000	1.31730
C	1.02460	1.35830	2.09430
H	0.01560	1.66690	2.40400
H	1.67850	1.42410	2.97960
C	1.05730	-0.08840	1.57130
C	0.86560	-1.25110	2.50680
C	-0.22710	-0.90360	1.53300
H	0.69310	-1.03480	3.56570
H	-1.15070	-0.44040	1.89490
C	-0.96910	-0.95240	-1.21570
H	0.03730	-0.65880	-1.55280
C	-1.65910	-1.81970	-2.27030
H	-1.88710	-1.21330	-3.16030
H	-1.01720	-2.66120	-2.57770
H	-2.59820	-2.23360	-1.87460
C	-1.75350	0.26350	-0.80660
C	-1.23690	1.54550	-1.04860
C	-3.00800	0.14410	-0.17920
C	-1.95160	2.68740	-0.67490
H	-0.26210	1.64480	-1.53390
C	-3.71530	1.28640	0.20320
H	-3.39780	-0.85140	0.04130
C	-3.19330	2.56110	-0.04480
H	-1.53650	3.67860	-0.87680
H	-4.68360	1.18010	0.69950
H	-3.75360	3.45220	0.24980

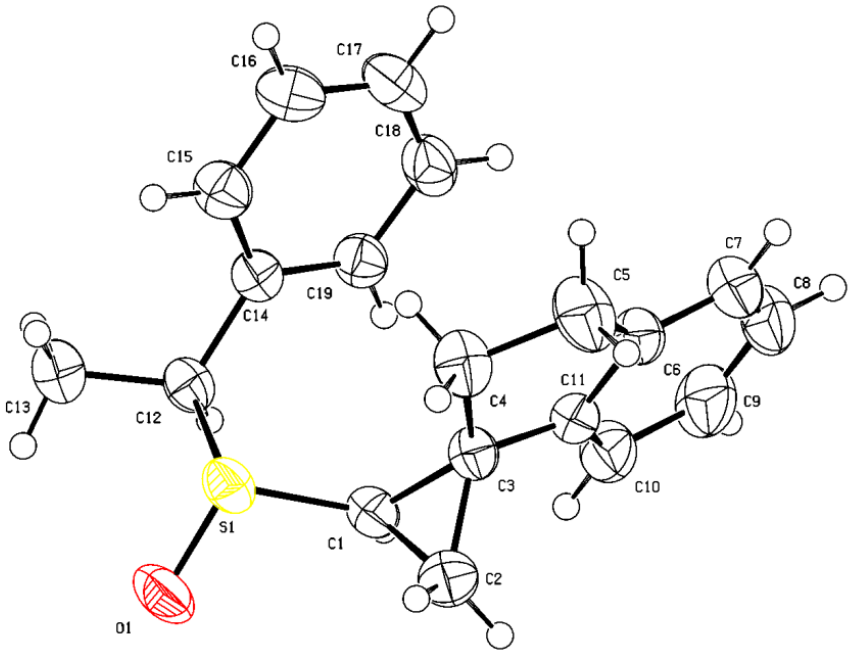
4a‴-*R*$_S$

S	0.30990	-1.29680	-0.60580
O	-0.29280	-2.67780	-0.73810
H	0.48380	1.38950	0.85200
C	-2.16810	0.59820	0.13930
C	-3.48650	0.15250	0.33560
C	-4.47300	0.43890	-0.60680
C	-4.13230	1.17700	-1.74850
C	-2.81860	1.62060	-1.94160
C	-1.82550	1.33280	-0.99670
H	-5.50030	0.09520	-0.45710
H	-4.89860	1.41200	-2.49180
H	-2.56600	2.19850	-2.83430
H	-0.80110	1.67880	-1.15250
C	-3.58780	-0.63430	1.62480
H	-3.54930	-1.71520	1.39840
H	-4.52050	-0.44750	2.17930
C	-2.32020	-0.20150	2.39560
H	-1.94390	-0.96730	3.09030
H	-2.53220	0.71020	2.98050
C	-1.31900	0.14570	1.28960
C	0.06380	0.66110	1.55170
C	-0.10840	-0.75640	1.07410
H	0.38980	0.79840	2.58700
H	0.03240	-1.58790	1.77500
C	2.16320	-1.56650	-0.30290
H	2.19940	-2.15980	0.62420
C	2.67320	-2.41020	-1.46890
H	2.64410	-1.85390	-2.41920
H	3.71570	-2.71380	-1.28530
H	2.04920	-3.31020	-1.57440
C	2.82490	-0.23000	-0.10800
C	2.81460	0.73400	-1.13220
C	3.41580	0.10700	1.12010
C	3.37520	1.99770	-0.93070
H	2.34880	0.49730	-2.09190
C	3.98310	1.36760	1.32200
H	3.42360	-0.62810	1.92960
C	3.96160	2.31960	0.29780
H	3.35290	2.73540	-1.73700
H	4.44090	1.60910	2.28480
H	4.40090	3.30780	0.45550

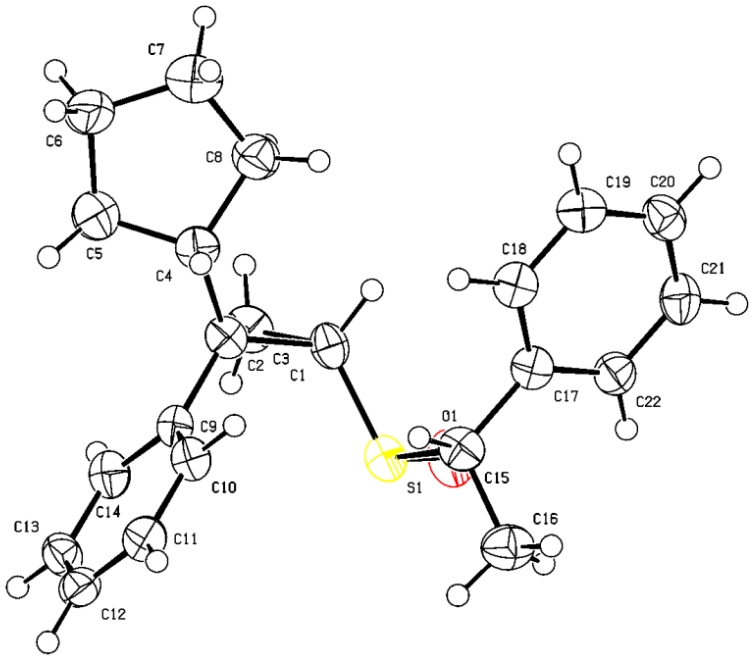
6. X-ray crystal structures.



ORTEP drawing of **3n** at 50% probability (**CCDC 2450631**).
These X-ray data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

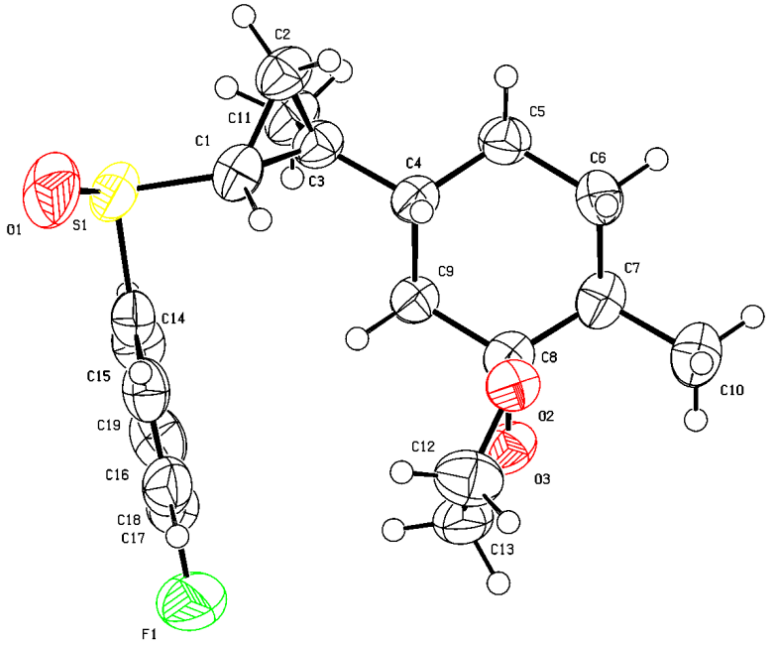


ORTEP drawing of **4a** at 50% probability (**CCDC 2431747**).
These X-ray data can be obtained free of charge from The Cambridge Crystallographic Data Centre.



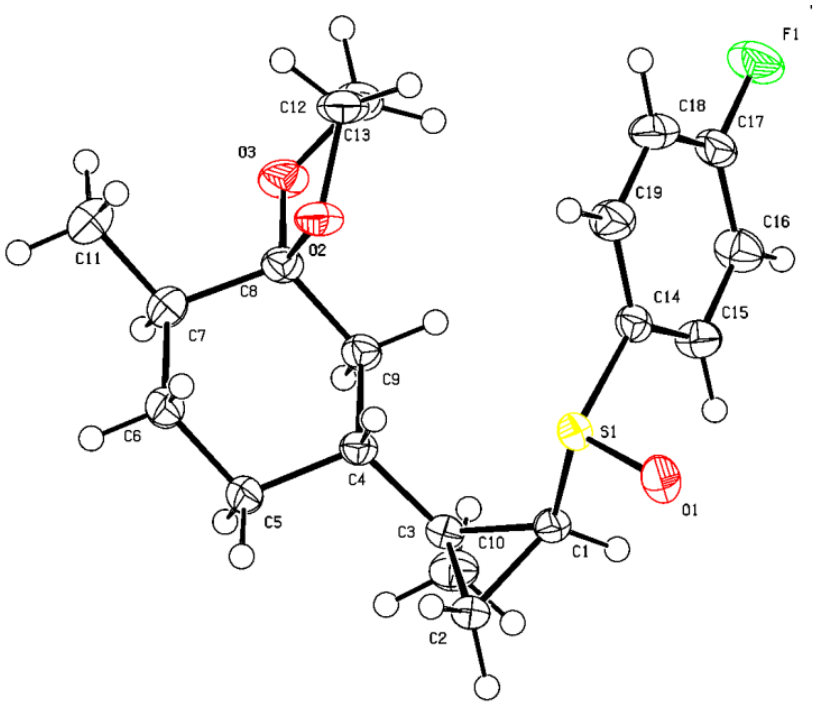
ORTEP drawing of **4i′** at 50% probability (**CCDC 2451688**).

These X-ray data can be obtained free of charge from The Cambridge Crystallographic Data Centre.



ORTEP drawing of **4k** at 50% probability (**CCDC 2450395**).

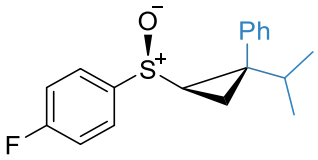
These X-ray data can be obtained free of charge from The Cambridge Crystallographic Data Centre.



ORTEP drawing of **4k″** at 50% probability (**CCDC 2450394**).

These X-ray data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

7. Spectroscopic data of products.



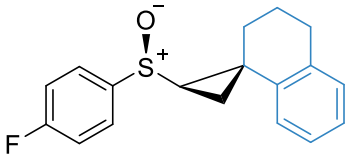
3a, 84% yield, >20:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 – 7.65 (m, 2H), 7.35 – 7.23 (m, 3H), 7.27 – 7.14 (m, 4H), 2.45 (dd, *J* = 8.6, 5.1 Hz, 1H), 1.90 (t, *J* = 5.1 Hz, 1H), 1.35 – 1.26 (m, 2H), 0.86 (d, *J* = 6.8 Hz, 3H), 0.78 (d, *J* = 6.8 Hz, 3H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.07.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.40 (d, *J* = 251.7 Hz), 140.05 (d, *J* = 3.3 Hz), 135.22, 130.15, 126.88, 126.42, 126.35 (d, *J* = 8.8 Hz), 115.53 (d, *J* = 22.5 Hz), 45.82, 38.70, 36.63, 19.06, 17.74, 13.92.

HRMS (ESI) calcd for $C_{18}H_{20}FOS^+$ $[M+H]^+$ 303.1212, Found 303.1215.



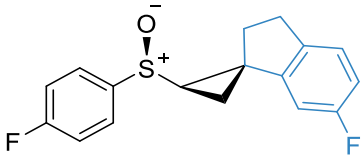
3b, 74% yield, >20:1 dr, colorless solid.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.66 – 7.56 (m, 2H), 7.17 – 7.06 (m, 2H), 7.05 – 6.95 (m, 3H), 6.54 – 6.49 (m, 1H), 2.81 (td, J = 6.4, 2.1 Hz, 2H), 2.47 (dd, J = 8.8, 5.8 Hz, 1H), 2.10 (ddd, J = 13.7, 8.2, 3.3 Hz, 1H), 2.05 – 1.98 (m, 1H), 1.95 – 1.87 (m, 1H), 1.86 – 1.79 (m, 1H), 1.77 (t, J = 6.0 Hz, 1H), 1.50 (dd, J = 8.8, 6.1 Hz, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.37.

^{13}C NMR (126 MHz, Chloroform-d) δ 164.36 (d, J = 251.6 Hz), 141.11 (d, J = 3.1 Hz), 138.17, 137.62, 129.27, 126.68 (d, J = 8.8 Hz), 126.43, 126.10, 121.78, 116.73 (d, J = 22.5 Hz), 51.33, 30.23, 29.64, 27.50, 22.31, 19.66.

HRMS (ESI) calcd for $C_{18}H_{17}FNaOS^+$ $[M+Na]^+$ 323.0876, Found 323.0878.



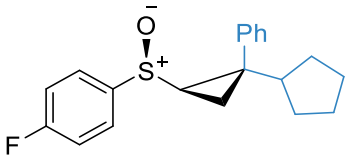
3c, 72% yield, >20:1 dr, colorless solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.62 – 7.56 (m, 2H), 7.17 – 7.10 (m, 2H), 7.10 – 7.05 (m, 1H), 6.77 (td, *J* = 8.6, 2.4 Hz, 1H),6.24 (dd, *J* = 8.9, 2.4 Hz, 1H), 3.04 – 2.86 (m, 2H), 2.53 (ddd, *J* = 13.6, 9.0, 6.1 Hz, 1H), 2.36 (dd, *J* = 8.8, 5.9 Hz, 1H), 2.29 (ddd, *J* = 13.6, 9.0, 5.8 Hz, 1H), 1.91 (t, *J* = 5.9 Hz, 1H), 1.32 (dd, *J* = 8.9, 6.0 Hz, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.23, -116.22.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.47 (d, *J* = 241.3 Hz), 162.50 (d, *J* = 233.1 Hz), 147.00 (d, *J* = 7.9 Hz), 140.53 (d, *J* = 3.2 Hz), 138.99 (d, *J* = 2.3 Hz), 126.51 (d, *J* = 9.0 Hz), 125.59 (d, *J* = 8.8 Hz), 116.79 (d, *J* = 22.5 Hz), 113.93 (d, *J* = 22.4 Hz), 106.04 (d, *J* = 23.0 Hz), 47.73, 34.26 (d, *J* = 2.5 Hz), 30.65, 30.27, 16.69.

HRMS (ESI) calcd for $C_{17}H_{14}F_2NaOS^+$ $[M+Na]^+$ 327.0626, Found 327.0630.



3d, 74% yield, 16:1 dr, colorless oil.

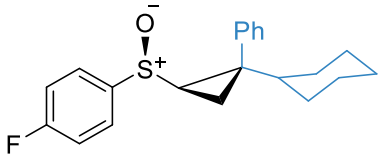
^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.61 – 7.56 (m, 2H), 7.25 (dd, *J* = 8.1, 6.3 Hz, 2H), 7.22 – 7.17 (m, 1H), 7.15 (ddd, *J* = 8.5, 5.2, 3.7 Hz, 4H), 2.44 (dd, *J* = 8.6, 5.1 Hz, 1H), 1.94 – 1.88 (m, 1H), 1.88 – 1.83 (m, 1H), 1.49 (dtd, *J* =

13.2, 6.8, 3.1 Hz, 1H), 1.46 – 1.36 (m, 4H), 1.32 (dd, *J* = 8.6, 5.9 Hz, 1H), 1.22 – 1.15(m, 1H), 1.14 – 1.04 (m, 1H), 0.91 (ddt, *J* = 12.1, 10.1, 8.4 Hz, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.19.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.40 (d, *J* = 251.8 Hz), 141.01 (d, *J* = 3.1 Hz), 138.66, 130.39, 128.17, 127.40, 127.32, 116.53 (d, *J* = 22.4 Hz), 48.19, 46.06, 36.60, 29.89, 28.07, 24.44, 24.40, 12.82.

HRMS (ESI) calcd for $C_{20}H_{22}FOS^+$ $[M+H]^+$ 329.1370, Found 329.1369.



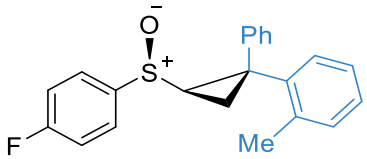
3e, 76% yield, 12:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.68 – 7.60 (m, 2H), 7.26 – 7.20 (m, 3H), 7.16 (t, *J* = 8.5 Hz, 2H), 7.10 (dd, *J* = 7.7, 1.8 Hz, 2H), 2.39 (dd, *J* = 8.6, 5.1 Hz, 1H), 1.81 (t, *J* = 5.4 Hz, 1H), 1.62 – 1.56 (m, 3H), 1.49 (dd, *J* = 24.3, 11.8 Hz, 2H), 1.22 (dd, *J* = 8.6, 5.6 Hz, 1H), 1.11 – 0.90 (m, 3H), 0.88 – 0.78 (m, 2H), 0.66 (qd, *J* = 12.1, 3.3 Hz, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.15.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.38 (d, *J* = 251.5 Hz), 140.09 (d, *J* = 3.2 Hz), 135.95, 130.12, 126.84, 126.37, 126.34 (d, *J* = 7.7 Hz), 115.53 (d, *J* = 22.3 Hz), 46.83, 45.28, 38.59, 29.56, 28.42, 25.45, 25.31, 24.94, 13.75.

HRMS (ESI) calcd for $C_{21}H_{23}FNaOS^+$ $[M+Na]^+$ 365.1346, Found 365.1347.



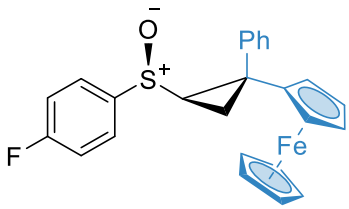
3f, 70% yield, >20:1 dr, colorless solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.55 (m, 2H), 7.46 – 7.37 (m, 1H), 7.22 – 7.17 (m, 2H), 7.14 (tq, *J* = 8.4, 2.2 Hz, 5H), 7.10 – 7.04 (m, 1H), 6.90 – 6.83 (m, 2H), 2.89 (dd, *J* = 8.8, 5.6 Hz, 1H), 2.39 (t, *J* = 5.7 Hz, 1H), 2.12 (s, 3H), 1.60 – 1.52 (m, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.30.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.46 (d, *J* = 251.8 Hz), 142.79, 141.02 (d, *J* = 3.2 Hz), 138.43, 135.83, 131.17, 131.07, 128.49, 128.12, 126.91 (d, *J* = 9.0 Hz), 126.32, 126.18, 125.71, 116.69 (d, *J* = 22.5 Hz), 49.38, 35.45, 20.34, 16.56.

HRMS (ESI) calcd for $C_{22}H_{20}FOS^+$ $[M+H]^+$ 351.1213, Found 351.1213.



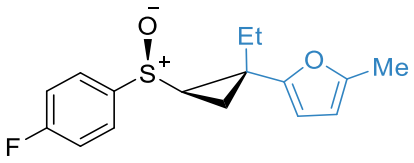
3g, 60% yield, >20:1 dr, orange solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (dd, *J* = 8.8, 5.1 Hz, 2H), 7.42 – 7.28 (m, 5H), 7.20 (t, *J* = 8.6 Hz, 2H), 4.04 (s, 5H), 4.04 (2H), 3.84 – 3.79 (m, 1H), 3.73 – 3.68 (m, 1H), 2.83 (dd, *J* = 8.6, 5.7 Hz, 1H), 2.44 (t, *J* = 5.8 Hz, 1H), 1.83 (dd, *J* = 8.7, 5.7 Hz, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -107.77.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.47 (d, *J* = 251.9 Hz), 140.62 (d, *J* = 3.1 Hz), 137.76, 130.07, 128.31, 127.68, 127.16 (d, *J* = 8.8 Hz), 116.62 (d, *J* = 22.5 Hz), 94.67, 68.70, 67.71, 67.46, 67.20, 66.13, 51.33, 32.96, 18.47.

HRMS (ESI) calcd for $C_{25}H_{21}FFeNaOS^+$ $[M+Na]^+$ 467.0539, Found 467.0550.



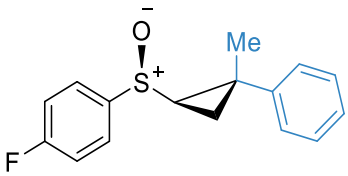
3h, 77% yield, 5:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 – 7.68 (m, 2H), 7.23 (t, *J* = 8.6 Hz, 2H), 5.89 (d, *J* = 3.1 Hz, 1H), 5.82 (dd, *J* = 3.1, 1.2 Hz, 1H), 2.47 (dd, *J* = 8.8, 5.9 Hz, 1H), 2.19 (s, 3H), 2.13 (dq, *J* = 14.4, 7.2 Hz, 1H), 1.89 (dq, *J* = 14.6, 7.4 Hz, 1H), 1.67 (t, *J* = 5.8 Hz, 1H), 1.62 (ddd, *J* = 8.8, 5.7, 1.4 Hz, 1H), 1.06 (t, *J* = 7.3 Hz, 3H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.92.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.27 (d, *J* = 251.3 Hz), 153.12, 151.07, 141.06 (d, *J* = 3.1 Hz), 126.54 (d, *J* = 8.9 Hz), 116.58 (d, *J* = 22.5 Hz), 106.37, 106.10, 48.29, 29.18, 24.79, 15.01, 13.52, 11.90.

HRMS (ESI) calcd for $C_{16}H_{17}FNaO_2S^+$ $[M+Na]^+$ 315.0825, Found 315.0831.



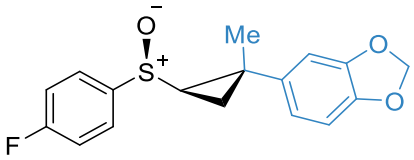
3i, 72% yield, 4:1 dr, colorless oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.78 – 7.73 (m, 2H), 7.27 – 7.20 (m, 4H), 7.19 – 7.15 (m, 1H), 7.03 – 6.99 (m, 2H), 2.46 (dd, *J* = 8.8, 5.6 Hz, 1H), 1.71 (t, *J* = 5.8 Hz, 1H), 1.69 (s, 3H), 1.61 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -108.20.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.42 (d, *J* = 251.5 Hz), 144.04, 141.27 (d, *J* = 3.3 Hz), 128.79, 127.02, 126.99, 126.43 (d, *J* = 8.9 Hz), 116.88 (d, *J* = 22.6 Hz), 48.97, 29.47, 22.57, 18.46.

HRMS (ESI) calcd for $C_{16}H_{15}FNaOS^+$ $[M+Na]^+$ 297.0720, Found 297.0720.



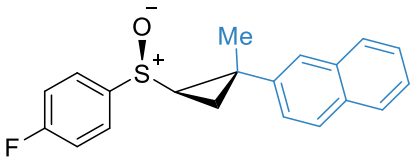
3j, 93% yield, 5:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.64 (m, 2H), 7.24 – 7.16 (m, 2H), 6.58 (dd, *J* = 7.7, 0.7 Hz, 1H), 6.43 – 6.40 (m, 2H), 5.82 (s, 2H), 2.35 (dd, *J* = 8.8, 5.6 Hz, 1H), 1.60 (t, *J* = 5.7 Hz, 1H), 1.58 (s, 3H), 1.49 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.24.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.36 (d, *J* = 251.5 Hz), 147.72, 146.42, 141.21 (d, *J* = 3.2 Hz), 138.08, 126.31 (d, *J* = 9.0 Hz), 120.12, 116.81 (d, *J* = 22.5 Hz), 108.27, 107.72, 101.10, 48.98, 29.45, 22.91, 18.50.

HRMS (ESI) calcd for $C_{17}H_{15}FNaO_3S^+$ $[M+Na]^+$ 319.0799, Found 319.0797.



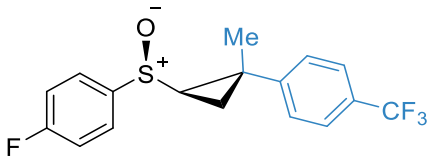
3k, 94% yield, 4:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.81 – 7.77 (m, 2H), 7.77 – 7.74 (m, 1H), 7.73 – 7.68 (m, 2H), 7.47 (d, *J* = 1.8 Hz, 1H), 7.46 – 7.40 (m, 2H), 7.27 (t, *J* = 8.6 Hz, 2H), 7.10 (dd, *J* = 8.5, 1.9 Hz, 1H), 2.55 (dd, *J* = 8.7, 5.5 Hz, 1H), 1.80 (t, *J* = 5.8 Hz, 1H), 1.78 (s, 3H), 1.74 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -108.14.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.47 (d, *J* = 251.7 Hz), 141.38, 141.36, 133.30, 132.32, 128.68, 127.70 (d, *J* = 8.0 Hz), 126.52, 126.46, 126.11, 125.52, 125.09, 116.88 (d, *J* = 22.5 Hz), 49.06, 29.57, 22.36, 18.38.

HRMS (ESI) calcd for $C_{20}H_{17}FNaOS^+$ $[M+H]^+$ 347.0876, Found 347.0881.



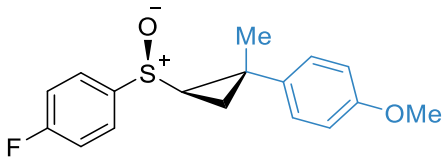
3l, 75% yield, 5:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 (dd, *J* = 8.8, 5.0 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 2.45 (dd, *J* = 8.9, 5.6 Hz, 1H), 1.80 (t, *J* = 5.8 Hz, 1H), 1.72 (s, 3H), 1.62 (dd, *J* = 8.9, 5.8 Hz, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -62.59, -107.84.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.45 (d, J = 251.9 Hz), 147.91, 140.96 (d, J = 3.2 Hz), 129.10 (q, J = 32.5 Hz), 127.24, 126.33 (d, J = 8.8 Hz), 125.73 (q, J = 3.8 Hz), 123.95 (q, J = 272.1 Hz), 116.90 (d, J = 22.5 Hz)., 48.91, 28.92, 21.76, 17.88.

HRMS (ESI) calcd for $C_{17}H_{15}F_4OS^+$ $[M+H]^+$ 343.0774, Found 343.0772.



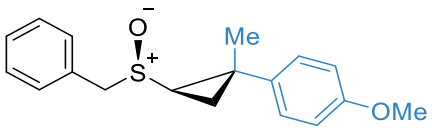
3m, 84% yield, 5:1 dr, white solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.75 (dd, *J* = 8.5, 5.1 Hz, 2H), 7.29 – 7.23 (m, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.75 (d, *J* = 8.5 Hz, 2H), 3.73 (s, 3H), 2.42 (dd, *J* = 8.7, 5.5 Hz, 1H), 1.68 (m, 1H), 1.65 (s, 3H), 1.58 (dd, *J* = 8.7, 5.8 Hz, 1H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -108.28.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.40 (d, *J* = 251.5 Hz), 158.49, 141.35 (d, *J* = 2.2 Hz), 136.22, 128.11, 126.40 (d, *J* = 8.7 Hz), 116.85 (d, *J* = 21.9 Hz), 114.09, 55.36, 49.04, 28.96, 22.93, 18.67.

HRMS (ESI) calcd for $C_{17}H_{18}FO_2S^+$ $[M+Na]^+$ 305.1006, Found 305.1006.

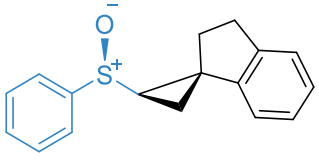


3n, 78% yield, 5:1 dr, white solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.33 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.28 – 7.26 (m, 2H), 6.94 – 6.89 (m, 2H), 6.83 – 6.78 (m, 2H), 4.26 (d, *J* = 12.8 Hz, 1H), 4.09 (d, *J* = 12.7 Hz, 1H), 3.79 (s, 3H), 2.33 (dd, *J* = 8.9, 5.8 Hz, 1H), 1.60 (dd, *J* = 8.9, 5.9 Hz, 1H), 1.50 (t, *J* = 5.8 Hz, 1H), 1.27 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 158.35, 135.87, 130.30, 129.80, 129.04, 128.39, 127.49, 113.90, 60.81, 55.40, 44.53, 27.92, 21.41, 19.23.

HRMS (ESI) calcd for $C_{18}H_{20}NaO_2S^+$ $[M+Na]^+$ 323.1076, Found 323.1086.

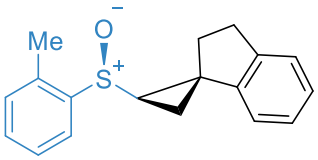


3o, 73% yield, >20:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.66 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.56 – 7.43 (m, 3H), 7.25 – 7.21 (m, 1H), 7.14 (dtd, *J* = 22.2, 7.3, 1.2 Hz, 2H), 6.64 (dd, *J* = 7.4, 1.3 Hz, 1H), 3.17 – 3.00 (m, 2H), 2.60 (ddd, *J* = 13.4, 8.9, 6.1 Hz, 1H), 2.54 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.34 (ddd, *J* = 13.4, 9.0, 6.0 Hz, 1H), 1.97 (t, *J* = 5.8 Hz, 1H), 1.45 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 145.20, 144.76, 143.77, 131.06, 129.41, 127.00, 126.80, 124.63, 124.22, 118.80, 47.73, 34.34, 30.99, 30.31, 17.34.

HRMS (ESI) calcd for $C_{17}H_{16}NaOS^+$ $[M+Na]^+$ 291.0814, Found 291.0820.

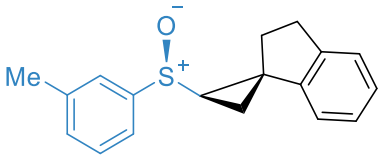


3p, 73% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.88 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.39 (dtd, *J* = 19.9, 7.4, 1.5 Hz, 2H), 7.24 – 7.18 (m, 2H), 7.16 (td, *J* = 7.4, 1.2 Hz, 1H), 7.11 (td, *J* = 7.4, 1.2 Hz, 1H), 6.64 – 6.60 (m, 1H), 3.16 – 3.01 (m, 2H), 2.62 (ddd, *J* = 13.5, 9.1, 6.1 Hz, 1H), 2.44 (dd, *J* = 9.0, 5.8 Hz, 1H), 2.41 (s, 3H), 2.31 (ddd, *J* = 13.6, 9.1, 5.9 Hz, 1H), 1.97 (t, *J* = 5.7 Hz, 1H), 1.28 (dd, *J* = 9.0, 5.7 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.32, 144.06, 143.40, 134.75, 130.91, 130.89, 127.37, 126.97, 126.83, 124.72, 124.30, 118.87, 46.24, 34.34, 31.10, 29.69, 18.49, 14.82.

HRMS (ESI) calcd for $C_{18}H_{19}OS^+$ $[M+H]^+$ 283.1151, Found 283.1151.

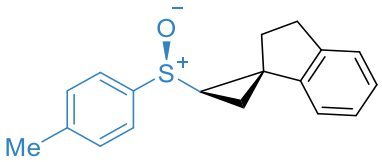


3q, 81% yield, >20:1 dr, colorless oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.49 (dq, *J* = 1.7, 0.9 Hz, 1H), 7.40 (dt, *J* = 7.7, 1.7 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.26 (dp, *J* = 7.5, 0.9 Hz, 1H), 7.22 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.15 (td, *J* = 7.4, 1.3 Hz, 1H), 7.11 (ddd, *J* = 8.5, 7.0, 1.1 Hz, 1H), 6.63 (dd, *J* = 7.3, 1.3 Hz, 1H), 3.15 – 3.07 (m, 1H), 3.03 (ddd, *J* = 15.8, 9.0, 6.0 Hz, 1H), 2.59 (ddd, *J* = 13.4, 9.0, 5.9 Hz, 1H), 2.51 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.39 (s, 3H), 2.37 – 2.29 (m, 1H), 1.95 (t, *J* = 5.8 Hz, 1H), 1.44 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.02, 144.92, 143.87, 139.70, 132.00, 129.28, 127.05, 126.86, 124.70, 124.62, 121.35, 118.90, 47.87, 34.34, 31.07, 30.31, 21.57, 17.33.

HRMS (ESI) calcd for $C_{18}H_{18}NaOS^+$ $[M+Na]^+$ 305.0971, Found 305.0971.

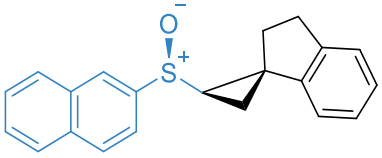


3r, 72% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.62 (d, *J* = 7.4 Hz, 1H), 3.13 – 2.96 (m, 2H), 2.56 (td, *J* = 11.4, 8.8, 5.9 Hz, 1H), 2.52 (dd, *J* = 8.8, 5.9 Hz, 1H), 2.38 (s, 3H), 2.31 (dt, *J* = 14.4, 7.0 Hz, 1H), 1.95 (t, *J* = 5.8 Hz, 1H), 1.44 (dd, *J* = 8.9, 5.9 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.89, 143.84, 142.00, 141.66, 130.19, 127.04, 126.87, 124.68, 124.35, 118.87, 47.79, 34.29, 31.06, 30.34, 21.51, 17.61.

HRMS (ESI) calcd for $C_{18}H_{19}OS^+$ $[M+H]^+$ 283.1151, Found 283.1151.

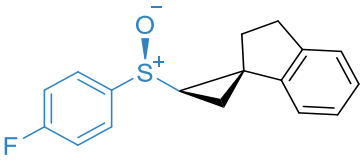


3s, 78% yield, >20:1 dr, colorless solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.20 (d, *J* = 1.7 Hz, 1H), 7.93 (d, *J* = 8.6 Hz, 1H), 7.92 – 7.85 (m, 2H), 7.64 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.14 (td, *J* = 7.4, 1.2 Hz, 1H), 7.09 (td, *J* = 7.4, 1.2 Hz, 1H), 6.63 – 6.58 (m, 1H), 3.10 (qdd, *J* = 15.9, 8.9, 6.1 Hz, 2H), 2.67 (ddd, *J* = 13.6, 8.8, 6.1 Hz, 1H), 2.59 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.38 (ddd, *J* = 13.5, 8.9, 6.1 Hz, 1H), 2.02 (t, *J* = 5.8 Hz, 1H), 1.46 (dd, *J* = 8.8, 5.8 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.75, 143.76, 142.25, 134.47, 132.94, 129.72, 128.59, 128.06, 127.79, 127.29, 127.02, 126.83, 124.68, 124.64, 120.16, 118.79, 47.77, 34.42, 31.02, 30.34, 17.33.

HRMS (ESI) calcd for $C_{21}H_{18}NaOS^+$ $[M+Na]^+$ 341.0971, Found 341.0974.



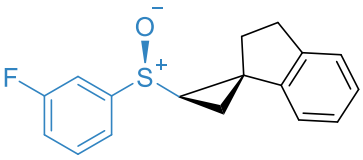
3t, 76% yield, >20:1 dr, colorless solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.61 (m, 2H), 7.25 – 7.09 (m, 5H), 6.67 – 6.62 (m, 1H), 3.12 (ddd, *J* = 15.4, 9.0, 6.0 Hz, 1H), 3.03 (ddd, *J* = 15.9, 9.0, 5.9 Hz, 1H), 2.57 (ddd, *J* = 13.4, 9.0, 6.0 Hz, 1H), 2.50 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.34 (ddd, *J* = 13.5, 9.0, 5.9 Hz, 1H), 1.97 (t, *J* = 5.8 Hz, 1H), 1.46 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.49.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.35 (d, *J* = 251.6 Hz), 144.58, 143.72, 140.72 (d, *J* = 3.1 Hz), 127.08, 126.85, 126.54 (d, *J* = 8.8 Hz), 124.67, 118.76, 116.73 (d, *J* = 22.5 Hz), 47.76, 34.34, 30.98, 30.24, 17.26.

HRMS (ESI) calcd for $C_{17}H_{15}FNaOS^+$ $[M+Na]^+$ 309.0720, Found 309.0723.



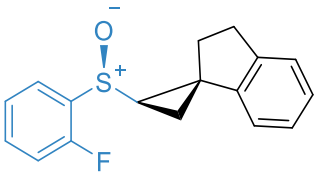
3u, 72% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.46 (td, *J* = 8.0, 5.2 Hz, 1H), 7.42 (ddd, *J* = 8.1, 2.6, 1.5 Hz, 1H), 7.38 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.24 – 7.21 (m, 1H), 7.18 – 7.14 (m, 2H), 7.14 – 7.10 (m, 1H), 6.65 – 6.61 (m, 1H), 3.16 – 3.02 (m, 2H), 2.58 (ddd, *J* = 13.4, 9.0, 6.1 Hz, 1H), 2.51 (dd, *J* = 8.8, 5.7 Hz, 1H), 2.34 (ddd, *J* = 13.5, 9.0, 5.9 Hz, 1H), 1.95 (t, *J* = 5.8 Hz, 1H), 1.44 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -109.30.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.21 (d, *J* = 251.6 Hz), 147.79 (d, *J* = 5.7 Hz), 144.58, 143.82, 131.17 (d, *J* = 7.4 Hz), 127.21, 126.94, 124.78, 119.83 (d, *J* = 3.5 Hz), 118.87, 118.29 (d, *J* = 21.5 Hz), 111.57 (d, *J* = 23.3 Hz), 47.87, 34.55, 31.05, 30.36, 17.21.

HRMS (ESI) calcd for $C_{17}H_{15}FNaOS^+$ $[M+Na]^+$ 309.0720, Found 309.0724.



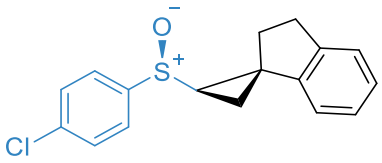
3v, 67% yield, >20:1 dr, colorless oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.85 (ddd, *J* = 8.2, 6.9, 1.8 Hz, 1H), 7.47 (tdd, *J* = 7.4, 5.2, 1.8 Hz, 1H), 7.36 (td, *J* = 7.6, 1.1 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.18 – 7.14 (m, 1H), 7.13 – 7.07 (m, 2H), 6.64 (d, *J* = 7.5 Hz, 1H), 3.14 – 3.03 (m, 2H), 2.70 – 2.65 (m, 1H), 2.65 – 2.61 (m, 1H), 2.31 (ddd, *J* = 13.5, 8.6, 6.6 Hz, 1H), 1.89 (t, *J* = 5.9 Hz, 1H), 1.38 (dd, *J* = 8.7, 5.8 Hz, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -114.26.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 157.96 (d, *J* = 247.4 Hz), 144.91, 144.13, 132.86 (d, *J* = 7.4 Hz), 132.34 (d, *J* = 17.2 Hz), 127.06, 126.78, 126.05(d, *J* = 1.51 Hz), 125.47(d, *J* = 1.5 Hz), 124.72, 118.89, 116.02 (d, *J* = 20.3 Hz), 46.90, 34.80, 31.11, 29.83, 16.23.

HRMS (ESI) calcd for $C_{17}H_{15}FNaOS^+$ $[M+Na]^+$ 309.0720, Found 309.0719.

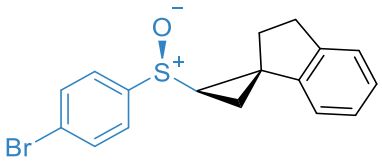


3w, 73% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.58 (dd, *J* = 8.5, 1.3 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.16 (td, *J* = 7.4, 1.3 Hz, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.62 (d, *J* = 7.5 Hz, 1H), 3.11 (ddd, *J* = 15.4, 9.0, 6.0 Hz, 1H), 3.03 (ddd, *J* = 15.8, 9.0, 5.9 Hz, 1H), 2.56 (ddd, *J* = 14.5, 9.0, 6.0 Hz, 1H), 2.49 (ddd, *J* = 8.8, 5.7, 1.1 Hz, 1H), 2.33 (ddd, *J* = 13.2, 9.0, 5.9 Hz, 1H), 1.95 (t, *J* = 5.9 Hz, 1H), 1.44 (dd, *J* = 8.8, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.55, 143.79, 143.74, 137.36, 129.79, 127.22, 126.96, 125.69, 124.77, 118.85, 47.85, 34.53, 31.05, 30.38, 17.40.

HRMS (ESI) calcd for $C_{17}H_{16}ClOS^+$ $[M+H]^+$ 303.0605, Found 303.0605.

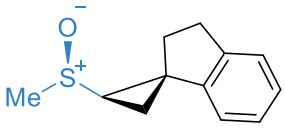


3x, 65% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 7.8 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.26 – 7.20 (m, 1H), 7.13 (dt, *J* = 28.0, 7.2 Hz, 2H), 6.62 (t, *J* = 6.4 Hz, 1H), 3.11 (ddd, *J* = 15.3, 9.2, 5.9 Hz, 1H), 3.03 (td, *J* = 10.0, 9.6, 4.5 Hz, 1H), 2.55 (ddd, *J* = 14.4, 8.9, 6.0 Hz, 1H), 2.48 (dd, *J* = 8.8, 5.6 Hz, 1H), 2.33 (ddt, *J* = 14.1, 8.9, 5.7 Hz, 1H), 1.94 (t, *J* = 5.8 Hz, 1H), 1.44 (dd, *J* = 8.8, 5.8 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.53, 144.36, 143.79, 132.71, 127.22, 126.96, 125.85, 125.61, 124.78, 118.85, 47.81, 34.56, 31.05, 30.38, 17.41.

HRMS (ESI) calcd for $C_{17}H_{16}BrOS^+$ $[M+H]^+$ 347.0111, Found 347.0098.

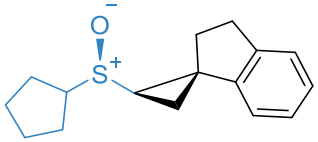


3y, 63% yield, >20:1 dr, colorless oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.24 – 7.22 (m, 1H), 7.20 – 7.14 (m, 2H), 6.74 – 6.70 (m, 1H), 3.09 (ddd, *J* = 15.5, 8.9, 6.2 Hz, 1H), 3.00 (ddd, *J* = 15.7, 9.0, 6.0 Hz, 1H), 2.68 (s, 3H), 2.48 (dd, *J* = 8.7, 5.7 Hz, 1H), 2.29 (ddd, *J* = 13.2, 8.9, 6.2 Hz, 1H), 2.20 (ddd, *J* = 13.2, 8.9, 5.9 Hz, 1H), 1.77 (t, *J* = 5.9 Hz, 1H), 1.55 (dd, *J* = 8.7, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.61, 143.64, 127.22, 127.03, 124.75, 118.86, 45.18, 40.31, 33.62, 31.06, 29.95, 19.33.

HRMS (ESI) calcd for $C_{12}H_{14}NaOS^+$ $[M+Na]^+$ 229.0658, Found 229.0658.

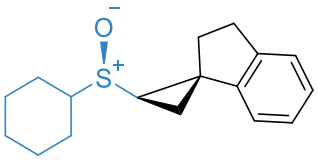


3z, 77% yield, 16:1 dr, colorless oil.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 – 7.15 (m, 1H), 7.12 – 7.08 (m, 2H), 6.67 – 6.63 (m, 1H), 3.12 – 2.90 (m, 3H), 2.37 – 2.28 (m, 2H), 2.20 – 2.04 (m, 2H), 1.92 – 1.82 (m, 2H), 1.71 (t, *J* = 5.8 Hz, 1H), 1.69 – 1.61 (m, 3H), 1.61 – 1.51 (m, 2H), 1.42 – 1.37 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.93, 143.70, 126.95, 126.84, 124.62, 118.69, 61.60, 42.45, 33.55, 30.87, 30.26, 27.48, 26.01, 25.60, 25.23, 17.96.

HRMS (ESI) calcd for $C_{16}H_{20}NaOS^+$ $[M+Na]^+$ 283.1127, Found 283.1132.

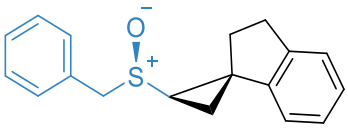


3aa, 73% yield, 16:1 dr, colorless oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.24 – 7.20 (m, 1H), 7.19 – 7.14 (m, 2H), 6.74 – 6.69 (m, 1H), 3.06 (ddd, *J* = 15.4, 9.0, 6.0 Hz, 1H), 2.99 (ddd, *J* = 15.8, 9.1, 6.0 Hz, 1H), 2.67 (tt, *J* = 11.7, 3.7 Hz, 1H), 2.43 (dd, *J* = 9.0, 5.8 Hz, 1H), 2.34 (ddd, *J* = 13.3, 9.0, 6.0 Hz, 1H), 2.20 (ddd, *J* = 13.4, 9.0, 6.0 Hz, 1H), 2.14 (dtd, *J* = 11.1, 3.7, 1.8 Hz, 1H), 1.89 – 1.85 (m, 1H), 1.81 – 1.77 (m, 1H), 1.75 (t, *J* = 5.8 Hz, 1H), 1.66 (dt, *J* = 12.7, 3.7 Hz, 1H), 1.57 – 1.46 (m, 2H), 1.41 (qd, *J* = 12.1, 3.5 Hz, 1H), 1.38 – 1.17 (m, 4H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.80, 143.80, 127.11, 126.95, 124.75, 118.86, 61.19, 41.47, 34.04, 30.86, 30.53, 26.09, 25.64, 25.33, 25.32, 25.29, 18.72.

HRMS (ESI) calcd for $C_{17}H_{23}OS^+$ $[M+Na]^+$ 275.1464, Found 275.1463

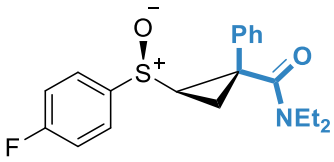


3ab, 80% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.24 – 7.22 (m, 1H), 7.18 – 7.10 (m, 7H), 6.66 – 6.61 (m, 1H), 4.15 (d, *J* = 12.7 Hz, 1H), 4.05 (d, *J* = 12.7 Hz, 1H), 2.90 (ddd, *J* = 15.7, 9.2, 6.2 Hz, 1H), 2.55 (ddd, *J* = 16.2, 9.3, 5.5 Hz, 1H), 2.40 (dd, *J* = 8.9, 5.9 Hz, 1H), 2.01 (ddd, *J* = 13.2, 9.2, 5.5 Hz, 1H), 1.81 (ddd, *J* = 13.3, 9.4, 6.1 Hz, 1H), 1.69 (t, *J* = 5.9 Hz, 1H), 1.50 (dd, *J* = 8.9, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.29, 143.80, 130.33, 129.23, 128.83, 128.29, 127.10, 126.89, 124.62, 118.81, 60.49, 43.11, 34.21, 30.77, 30.19, 19.75.

HRMS (ESI) calcd for $C_{18}H_{18}NaOS^+$ $[M+Na]^+$ 305.0971, Found 305.0970.



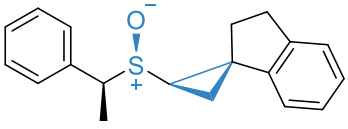
3ac, 41% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.99 (dd, *J* = 8.6, 5.2 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.18 (dd, *J* = 22.1, 8.0 Hz, 4H), 3.39 (dq, *J* = 26.7, 7.1 Hz, 4H), 2.40 (t, *J* = 7.7 Hz, 1H), 2.17 (t, *J* = 6.5 Hz, 1H), 2.07 (t, *J* = 7.7 Hz, 1H), 1.17 (t, *J* = 7.1 Hz, 3H), 0.88 (t, *J* = 7.1 Hz, 3H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -109.78.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.68, 164.22 (d, *J* = 250.8 Hz), 141.01, 137.48, 129.18, 127.74, 127.33 (d, *J* = 8.7 Hz), 125.77, 116.29 (d, *J* = 22.8 Hz), 50.53, 42.02, 39.78, 38.46, 14.84, 13.22, 12.53.

HRMS (ESI) calcd for $C_{20}H_{23}FNO_2S^+$ $[M+H]^+$ 360.1428, Found 360.1434.



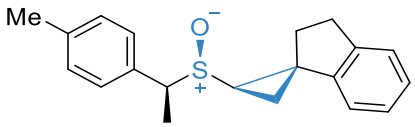
4a, 48% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.18 (d, *J* = 6.9 Hz, 1H), 7.13 (dt, *J* = 9.7, 5.3 Hz, 6H), 7.10 – 7.06 (m, 1H), 6.59 – 6.56 (m, 1H), 3.94 (q, *J* = 7.2 Hz, 1H), 2.80 (ddd, *J* = 15.8, 9.3, 6.2 Hz, 1H), 2.39 (ddd, *J* = 25.2, 9.4, 5.6 Hz, 2H), 1.91 (ddd, *J* = 14.1, 9.3, 5.3 Hz, 1H), 1.76 (d, *J* = 7.2 Hz, 3H), 1.69 – 1.61 (m, 2H), 1.42 (dd, *J* = 9.0, 5.8 Hz, 1H).

^{13}C NMR (151 M**Hz,** Chloroform-*d*) δ 144.42, 143.91, 135.57, 128.83, 128.50, 128.33, 126.89, 126.68, 124.52, 118.69, 64.99, 43.05, 34.47, 30.58, 30.07, 19.09, 15.29.

HRMS (ESI) calcd for $C_{19}H_{20}NaOS^+$ $[M+Na]^+$ 319.1127, Found 319.1130.

Optical Rotation: $[a]_D^{20}$ = -171.2 (c = 0.52, acetone).



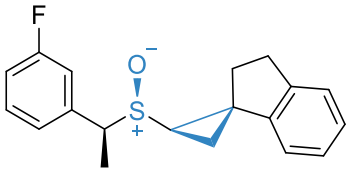
4b, 48% yield, 6:1 dr, colorless solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.13 – 7.00 (m, 3H), 6.99 – 6.92 (m, 2H), 6.83 (d, *J* = 7.8 Hz, 2H), 6.55 – 6.47 (m, 1H), 3.85 (q, *J* = 7.2 Hz, 1H), 2.75 (ddd, *J* = 15.8, 9.4, 6.1 Hz, 1H), 2.34 – 2.26 (m, 2H), 2.17 (s, 3H), 1.86 (ddd, *J* = 13.4, 9.4, 5.4 Hz, 1H), 1.69 (d, *J* = 7.2 Hz, 3H), 1.66 – 1.56 (m, 2H), 1.41 – 1.33 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.50, 144.01, 138.23, 132.37, 129.47, 128.35, 126.86, 126.67, 124.37, 118.75, 64.89, 43.31, 34.56, 30.54, 29.95, 21.14, 19.17, 15.39.

HRMS (ESI) calcd for $C_{20}H_{22}NaOS^+$ $[M+Na]^+$ 333.1284, Found 333.1297.

Optical Rotation: $[a]_D^{20}$ = +124.24 (c = 0.56, acetone).



4c, 41% yield, >20:1 dr, colorless solid.

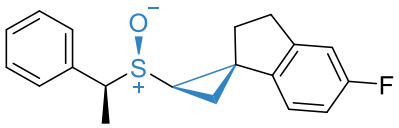
^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.10 – 7.05 (m, 3H), 7.04 – 6.99 (m, 1H), 6.87 (dt, *J* = 7.7, 1.3 Hz, 1H), 6.85 – 6.81 (m, 2H), 6.55 – 6.49 (m, 1H), 3.87 (q, *J* = 7.2 Hz, 1H), 2.82 (ddd, *J* = 15.8, 9.3, 6.2 Hz, 1H), 2.47 (ddd, *J* = 16.6, 9.5, 5.4 Hz, 1H), 2.28 (dd, *J* = 9.0, 5.9 Hz, 1H), 1.93 (ddd, *J* = 13.3, 9.3, 5.3 Hz, 1H), 1.74 (ddd, *J* = 13.4, 9.5, 6.2 Hz, 1H), 1.68 (d, *J* = 7.1 Hz, 3H), 1.62 (t, *J* = 5.9 Hz, 1H), 1.41 – 1.36 (m, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -111.93.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.74 (d, *J* = 247.7 Hz), 143.09, 142.63, 137.12 (d, *J* = 7.0 Hz), 129.25 (d, *J* = 8.2 Hz), 125.92, 125.69, 123.48, 123.20 (d, *J* = 2.9 Hz), 117.53, 114.16 (d, *J* = 21.1 Hz), 114.14 (d, *J* = 21.9 Hz), 63.22, 41.68, 33.25, 29.50, 29.01, 17.80, 13.86.

HRMS (ESI) calcd for $C_{19}H_{19}FNaOS^+$ $[M+Na]^+$ 337.1033, Found 337.1047.

Optical Rotation: $[a]_D^{20}$ = -127.7 (c = 0.53, acetone).



4d, 48% yield, 3:1 dr, colorless solid.

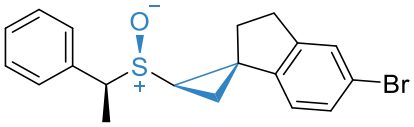
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.16 – 7.11 (m, 1H), 7.07 (d, *J* = 3.5 Hz, 4H), 6.77 – 6.67 (m, 2H), 6.43 (dd, *J* = 8.4, 4.9 Hz, 1H), 3.88 (q, *J* = 7.2 Hz, 1H), 2.76 – 2.63 (m, 1H), 2.31 – 2.19 (m, 2H), 1.86 (ddd, *J* = 13.4, 9.4, 5.4 Hz, 1H), 1.71 (d, *J* = 7.2 Hz, 3H), 1.61 – 1.52 (m, 2H), 1.34 (dd, *J* = 9.1, 5.9 Hz, 1H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -116.59.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 162.41 (d, *J* = 243.4 Hz), 146.00 (d, *J* = 8.0 Hz), 139.90, 135.44, 128.83, 128.50, 128.37, 119.61 (d, *J* = 8.8 Hz), 113.63 (d, *J* = 23.0 Hz), 111.55 (d, *J* = 22.4 Hz), 65.26, 43.25, 33.95, 30.47, 30.41, 19.10, 15.50.

HRMS (ESI) calcd for $C_{19}H_{19}FNaOS^+$ $[M+Na]^+$ 337.1033, Found 337.1039.

Optical Rotation: $[a]_D^{20}$ = -109.3 (c = 0.66, acetone).



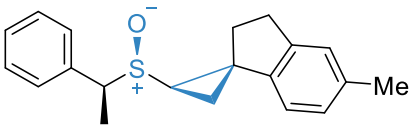
4e, 47% yield, 3:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.23 – 7.21 (m, 1H), 7.19 (dd, *J* = 7.3, 2.9 Hz, 2H), 7.13 (d, *J* = 4.3 Hz, 4H), 6.42 (d, *J* = 8.1 Hz, 1H), 3.94 (q, *J* = 7.2 Hz, 1H), 2.76 (ddd, *J* = 15.9, 9.4, 6.2 Hz, 1H), 2.32 (qd, *J* = 8.2, 5.3 Hz, 2H), 1.90 (ddd, *J* = 14.3, 9.4, 5.4 Hz, 1H), 1.76 (d, *J* = 7.2 Hz, 3H), 1.65 (t, *J* = 6.0 Hz, 1H), 1.63 – 1.58 (m, 1H), 1.40 (dd, *J* = 9.1, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 146.20, 143.65, 135.44, 129.73, 128.89, 128.49, 128.44, 127.65, 120.49, 120.18, 65.24, 43.25, 34.14, 30.35, 30.06, 19.10, 15.49.

HRMS (ESI) calcd for $C_{19}H_{19}BrNaOS^+$ $[M+Na]^+$ 397.0232, Found 397.0242.

Optical Rotation: $[a]_D^{20}$ = -96.47 (c = 0.44, acetone).



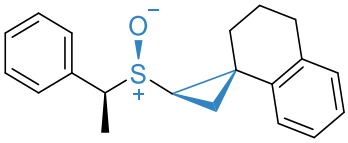
4f, 47% yield, 3:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.19 (td, *J* = 6.1, 2.4 Hz, 1H), 7.16 – 7.11 (m, 4H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 7.7 Hz, 1H), 6.36 (s, 1H), 3.93 (q, *J* = 7.1 Hz, 1H), 2.75 (ddd, *J* = 15.6, 9.3, 6.2 Hz, 1H), 2.35 (ddd, *J* = 15.2, 9.2, 5.6 Hz, 2H), 2.28 (s, 3H), 1.91 (ddd, *J* = 14.3, 9.3, 5.4 Hz, 1H), 1.75 (d, *J* = 7.2 Hz, 3H), 1.67 – 1.63 (m, 2H), 1.40 (dd, *J* = 9.1, 5.8 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.55, 140.94, 136.33, 135.71, 128.83, 128.51, 128.31, 127.77, 124.24, 119.27, 64.75, 42.90, 34.28, 30.36, 30.18, 21.44, 18.90, 15.13.

HRMS (ESI) calcd for $C_{20}H_{22}NaOS^+$ $[M+Na]^+$ 333.1284, Found 333.1289.

Optical Rotation: $[a]_D^{20}$ = +140.9 (c = 0.36, acetone).



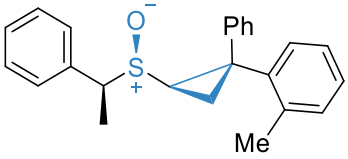
4g, 50% yield, 5:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.23 – 7.17 (m, 1H), 7.16 – 7.05 (m, 6H), 6.98 (d, *J* = 7.4 Hz, 1H), 6.56 (d, *J* = 7.6 Hz, 1H), 3.93 (q, *J* = 7.3 Hz, 1H), 2.70 – 2.64 (m, 1H), 2.55 (t, *J* = 7.6 Hz, 1H), 2.46 (dt, *J* = 15.5, 6.9 Hz, 1H), 1.77 (d, *J* = 7.2, 3H), 1.66 – 1.58 (m, 1H), 1.54 (q, *J* = 5.6, 5.2 Hz, 2H), 1.50 – 1.41 (m, 2H), 1.09 (dd, *J* = 13.4, 10.4 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 138.09, 137.80, 135.61, 129.14, 128.82, 128.71, 128.34, 126.39, 125.85, 121.66, 65.31, 46.15, 30.48, 30.11, 27.37, 22.38, 21.59, 14.94.

HRMS (ESI) calcd for $C_{20}H_{22}NaOS^+$ $[M+Na]^+$ 333.1284, Found 333.1281.

Optical Rotation: $[a]_D^{20}$ = -129.2 (c = 0.60, acetone).



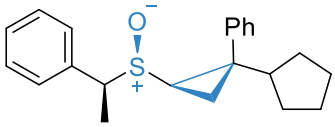
4h, 52% yield, 4:1 dr, colorless solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.19 (m, 6H), 7.15 – 7.02 (m, 6H), 6.74 (dd, *J* = 7.1, 1.8 Hz, 2H), 3.83 (q, *J* = 7.1 Hz, 1H), 2.82 – 2.70 (m, 1H), 2.23 (t, *J* = 5.8 Hz, 1H), 1.98 (s, 3H), 1.63 (d, *J* = 7.1 Hz, 3H), 1.49 – 1.39 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 143.22, 138.44, 136.98, 136.02, 131.25, 130.84, 129.29, 128.61, 128.48, 128.43, 127.94, 126.18, 126.03, 125.95, 64.04, 34.26, 29.81, 20.19, 15.81, 15.65.

HRMS (ESI) calcd for $C_{24}H_{24}NaOS^+$ $[M+Na]^+$ 383.1440, Found 383.1440.

Optical Rotation: $[a]_D^{20}$ = +124.2 (c = 0.56, acetone).



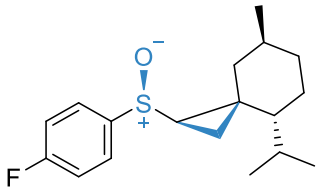
4i, 53% yield, 4:1 dr, colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.27 (m, 3H), 7.25 – 7.18 (m, 2H), 7.16 – 7.08 (m, 3H), 6.87 – 6.78 (m, 2H), 3.85 (q, *J* = 7.1 Hz, 1H), 2.26 (dd, *J* = 8.9, 5.3 Hz, 1H), 1.76 (tt, *J* = 10.6, 6.6 Hz, 1H), 1.68 (t, *J* = 5.5 Hz, 1H), 1.63 (d, *J* = 7.1 Hz, 3H), 1.51 – 1.24 (m, 5H), 1.22 – 1.16 (m, 2H), 1.02 – 0.92 (m, 1H), 0.84 (tdd, *J* = 11.6, 9.9, 7.2 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 138.91, 137.01, 130.45, 129.07, 128.70, 128.48, 128.00, 126.99, 63.95, 48.10, 40.55, 36.31, 29.79, 29.42, 28.01, 24.52, 15.06, 11.39.

HRMS (ESI) calcd for $C_{22}H_{26}NaOS^+$ $[M+Na]^+$ 361.1597, Found 361.1597.

Optical Rotation: $[a]_D^{20}$ = -45.2 (c = 0.57, acetone).



4j, 39% yield, 1:1 dr, colorless oil.

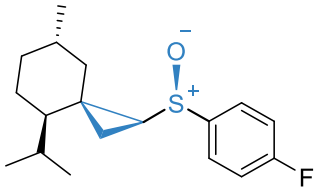
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 – 7.70 (m, 2H), 7.26 – 7.19 (m, 2H), 2.16 (dd, *J* = 8.7, 5.2 Hz, 1H), 1.95 (dd, *J* = 13.7, 4.4 Hz, 1H), 1.74 (tt, *J* = 12.0, 8.2 Hz, 4H), 1.54 (d, *J* = 6.7 Hz, 1H), 1.46 (dd, *J* = 13.7, 6.4 Hz, 1H), 1.31 (t, *J* = 5.5 Hz, 1H), 1.26 (d, *J* = 3.3 Hz, 1H), 1.10 (dd, *J* = 8.8, 5.9 Hz, 1H), 1.04 (d, *J* = 6.8 Hz, 3H), 0.80 (td, *J* = 7.2, 3.3 Hz, 1H), 0.69 (d, *J* = 6.7 Hz, 3H), 0.64 (d, *J* = 6.7 Hz, 3H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -108.33.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.40 (d, *J* = 251.3 Hz), 141.52, 126.70 (d, *J* = 8.6 Hz), 116.65 (d, *J* = 22.0 Hz), 48.08, 46.27, 36.76, 30.28, 29.79, 29.50, 25.48, 24.11, 22.78, 20.80, 20.44, 15.81.

HRMS (ESI) calcd for $C_{18}H_{25}FNaOS^+$ $[M+Na]^+$ 331.1502, Found 331.1500.

Optical Rotation: $[a]_D^{20}$ = 48.6(c = 0.47, acetone).



4j′, 39% yield, colorless oil.

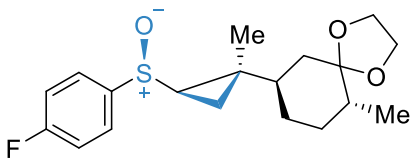
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.69 – 7.63 (m, 2H), 7.23 (t, *J* = 8.4 Hz, 2H), 2.45 (t, *J* = 6.9 Hz, 1H), 1.83 (dp, *J* = 13.1, 3.3 Hz, 1H), 1.70 (ddd, *J* = 13.1, 6.8, 3.1 Hz, 3H), 1.40 (q, *J* = 11.7, 9.9 Hz, 1H), 1.26 – 1.22 (m, 3H), 1.15 (qd, *J* = 12.5, 3.4 Hz, 1H), 1.10 – 1.01 (m, 1H), 0.99 (dd, *J* = 12.1, 3.4 Hz, 1H), 0.94 (d, *J* = 6.4 Hz, 3H), 0.67 (dd, *J* = 6.8, 3.3 Hz, 6H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -109.15.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.16 (d, *J* = 250.7 Hz), 141.61 (d, *J* = 3.3 Hz), 126.20 (d, *J* = 8.7 Hz), 116.64 (d, *J* = 22.4 Hz), 45.72, 45.69, 43.77, 35.27, 32.05, 31.90, 26.78, 25.15, 24.39, 22.26, 18.93, 14.88.

HRMS (ESI) calcd for $C_{18}H_{25}FNaOS^+$ $[M+Na]^+$ 331.1502, Found 331.1506.

Optical Rotation: $[a]_D^{20}$ = 18.3 (c = 0.48, acetone).



4k, 39% (88%) yield, 4:3:1:1 dr, white solid.

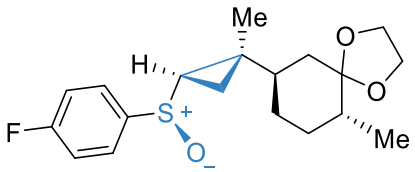
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (ddq, *J* = 10.8, 5.7, 2.9 Hz, 2H), 7.22 – 7.12 (m, 2H), 3.82 – 3.60 (m, 4H), 1.92 (dd, *J* = 8.6, 5.2 Hz, 1H), 1.73 – 1.65 (m, 1H), 1.57 (ddd, *J* = 11.7, 6.6, 3.4 Hz, 1H), 1.54 – 1.41 (m, 2H), 1.26 (t, *J* = 5.5 Hz, 1H), 1.18 (s, 3H), 1.06 (tdd, *J* = 12.9, 11.1, 7.3 Hz, 4H), 0.91 (d, *J* = 8.6 Hz, 1H), 0.73 (d, *J* = 6.5 Hz, 3H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.54.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.30 (d, *J* = 251.1 Hz), 141.76, 126.30 (d, *J* = 8.4 Hz), 116.56 (d, *J* = 23.0 Hz), 110.42, 65.34, 64.83, 48.65, 44.38, 39.58, 38.42, 31.59, 28.37, 27.86, 18.97, 15.49, 13.77.

HRMS (ESI) calcd for $C_{19}H_{25}FNaO_3S^+$ $[M+Na]^+$ 375.1401, Found 375.1406.

Optical Rotation: $[a]_D^{20}$ = -26.7 (c = 0.56, acetone).



4k″, 11% yield, white solid.

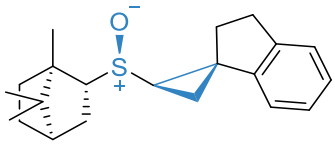
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.62 (m, 2H), 7.20 – 7.10 (m, 2H), 3.95 – 3.78 (m, 4H), 2.03 (dd, *J* = 8.6, 5.2 Hz, 1H), 1.73 – 1.56 (m, 4H), 1.52 (dd, *J* = 3.2, 2.2 Hz, 1H), 1.40 – 1.25 (m, 4H), 0.96 (dd, *J* = 8.7, 5.7 Hz, 1H), 0.90 (s, 3H), 0.80 (d, *J* = 6.4 Hz, 3H).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.54.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.32 (d, *J* = 251.7 Hz), 142.23, 126.98 (d, *J* = 8.7 Hz), 116.62 (d, *J* = 21.9 Hz), 110.75, 65.66, 65.10, 49.23, 39.85, 39.66, 39.15, 31.74, 29.54, 29.08, 19.10, 18.05, 13.93.

HRMS (ESI) calcd for $C_{19}H_{25}FNaO_3S^+$ $[M+Na]^+$ 375.1401, Found 375.1400.

Optical Rotation: $[a]_D^{20}$ = 35.7 (c = 0.29, acetone).



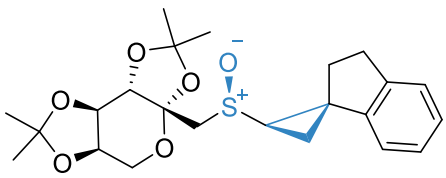
4l, 48% yield, >20:1 dr, colorless solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 – 7.15 (m, 1H), 7.13 – 7.07 (m, 2H), 6.67 – 6.61 (m, 1H), 3.06 – 2.90 (m, 2H), 2.82 (t, *J* = 8.1 Hz, 1H), 2.35 (dd, *J* = 9.2, 5.9 Hz, 1H), 2.34 (s, 1H), 2.19 (ddd, *J* = 13.6, 8.9, 6.1 Hz, 1H), 1.68 (m, 2H), 1.62 – 1.55 (m, 1H), 1.47 – 1.42 (m, 2H), 1.34 (dd, *J* = 9.1, 5.8 Hz, 1H), 1.29 (ddd, *J* = 12.9, 9.3, 3.4 Hz, 1H), 1.21 – 1.17 (m, 1H), 1.15 (s, 3H), 1.10 (ddd, *J* = 12.0, 9.3, 4.6 Hz, 1H), 0.89 (s, 3H), 0.81 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 143.90, 142.66, 125.89, 125.77, 123.58, 117.66, 71.54, 48.49, 46.54, 43.78, 42.60, 37.96, 33.60, 30.21, 30.14, 29.68, 25.98, 19.06, 18.54, 16.13, 12.72.

HRMS (ESI) calcd for $C_{21}H_{28}NaOS^+$ $[M+Na]^+$ 351.1753, Found 351.1746.

Optical Rotation: $[a]_D^{20}$ = -37.7 (c = 0.45, acetone).



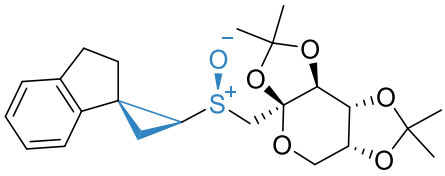
4m, 52% yield, 1.5:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.21 – 7.17 (m, 1H), 7.16 – 7.10 (m, 2H), 6.69 – 6.65 (m, 1H), 4.58 (dd, *J* = 7.9, 2.7 Hz, 1H), 4.41 (d, *J* = 2.7 Hz, 1H), 4.16 (d, *J* = 7.9 Hz, 1H), 3.83 (dd, *J* = 13.0, 1.9 Hz, 1H), 3.57 (d, *J* = 13.0 Hz, 1H), 3.42 (d, *J* = 13.5 Hz, 1H), 3.19 (d, *J* = 13.5 Hz, 1H), 3.02 (qdd, *J* = 15.8, 9.1, 6.4 Hz, 2H), 2.72 – 2.67 (m, 1H), 2.40 (ddd, *J* = 14.6, 8.9, 6.3 Hz, 1H), 2.21 – 2.13 (m, 1H), 1.77 (t, *J* = 5.9 Hz, 1H), 1.53 (s, 3H), 1.49 – 1.46 (m, 1H), 1.45 (s, 3H), 1.38 (s, 3H), 1.30 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.95, 143.84, 126.99, 126.86, 124.62, 118.80, 109.62, 109.22, 101.17, 72.93, 70.50, 70.13, 64.22, 61.75, 45.03, 33.84, 31.06, 29.67, 26.54, 26.02, 25.25, 24.13, 18.32.

HRMS (ESI) calcd for $C_{23}H_{30}NaO_6S^+$ $[M+Na]^+$ 457.1655, Found 457.1655.

Optical Rotation: $[a]_D^{20}$ = -46.8 (c = 0.47, acetone).



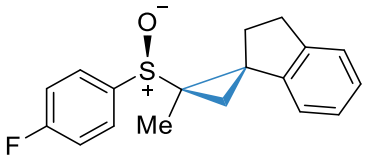
4m′, 35% yield, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.20 – 7.16 (m, 1H), 7.14 (dd, *J* = 5.6, 3.1 Hz, 2H), 6.68 (dd, *J* = 5.4, 3.3 Hz, 1H), 4.56 (dd, *J* = 7.8, 2.6 Hz, 1H), 4.20 (d, *J* = 2.6 Hz, 1H), 4.18 (dd, *J* = 7.8, 1.7 Hz, 1H), 3.77 – 3.68 (m, 2H), 3.54 (d, *J* = 13.2 Hz, 1H), 3.24 (d, *J* = 13.2 Hz, 1H), 3.08 – 2.94 (m, 2H), 2.72 (dd, *J* = 8.9, 5.9 Hz, 1H), 2.50 (ddd, *J* = 13.4, 9.2, 5.7 Hz, 1H), 2.17 (ddd, *J* = 13.3, 9.2, 6.2 Hz, 1H), 1.72 (t, *J* = 6.0 Hz, 1H), 1.56 (dd, *J* = 8.9, 6.0 Hz, 1H), 1.46 (s, 3H), 1.32 (s, 3H), 1.14 (s, 3H), 1.10 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.35, 144.13, 126.88, 126.71, 124.60, 118.68, 109.48, 109.00, 101.43, 73.18, 70.43, 70.28, 65.80, 61.57, 46.77, 34.75, 31.08, 29.75, 25.96, 25.60, 24.63, 24.23, 20.02.

HRMS (ESI) calcd for $C_{23}H_{30}NaO_6S^+$ $[M+Na]^+$ 457.1655, Found 457.1655.

Optical Rotation: $[a]_D^{20}$ = 42.5 (c = 0.43, acetone).



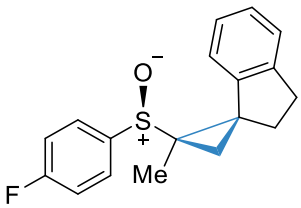
5b, 41% yield, 1.5:1 dr, colorless solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.64 – 7.56 (m, 2H), 7.27 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.21 – 7.12 (m, 4H), 6.85 (dd, *J* = 7.5, 1.3 Hz, 1H), 3.02 (dd, *J* = 9.8, 4.7 Hz, 2H), 2.82 – 2.71 (m, 1H), 2.50 (dt, *J* = 13.7, 9.8 Hz, 1H), 2.02 (d, *J* = 6.4 Hz, 1H), 1.51 (d, *J* = 6.4 Hz, 1H), 1.12 (s, 3H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -108.94.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.16 (d, *J* = 251.4 Hz), 145.10, 141.71, 137.83(d, *J* = 3.0 Hz), 127.25 (d, *J* = 8.8 Hz), 127.11, 126.05, 124.82, 122.54, 116.36 (d, *J* = 22.2 Hz), 47.86, 39.08, 32.02, 31.11, 24.28, 10.46.

HRMS (ESI) calcd for $C_{18}H_{17}FNaOS^+$ $[M+Na]^+$ 323.0876, Found 323.0869.



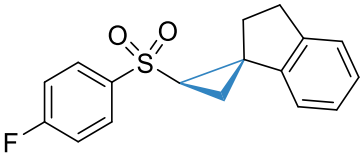
5b′, 27 % yield, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.67 – 7.61 (m, 2H), 7.28 – 7.22 (m, 3H), 7.21 – 7.17 (m, 3H), 3.12 (dt, *J* = 16.8, 8.8 Hz, 1H), 2.93 (ddd, *J* = 15.8, 8.5, 2.9 Hz, 1H), 2.30 – 2.20 (m, 2H), 1.79 (d, *J* = 6.4 Hz, 1H), 1.24 (s, 3H), 1.15 (d, *J* = 6.4 Hz, 1H).

^{19}F NMR (565 MHz, Chloroform-*d*) δ -109.89.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.23 (d, *J* = 250.1 Hz), 145.31, 141.57, 138.38 (d, *J* = 3.0 Hz), 127.26, 127.03 (d, *J* = 8.6 Hz), 125.96, 124.77, 123.42, 116.27 (d, *J* = 22.5 Hz), 47.53, 39.57, 32.17, 30.88, 23.57, 11.41.

HRMS (ESI) calcd for $C_{18}H_{17}FNaOS^+$ $[M+Na]^+$ 323.0876, Found 323.0876.



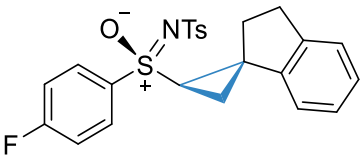
5c, 56% yield, colorless solid.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.98 – 7.89 (m, 2H), 7.25 – 7.20 (m, 3H), 7.17 (td, *J* = 7.4, 1.3 Hz, 1H), 7.13 (td, *J* = 7.4, 1.3 Hz, 1H), 6.65 – 6.60 (m, 1H), 3.07 (ddd, *J* = 15.2, 8.9, 5.8 Hz, 1H), 2.96 (ddd, *J* = 15.7, 8.9, 5.9 Hz, 1H), 2.84 (ddd, *J* = 13.6, 8.9, 5.9 Hz, 1H), 2.71 (dd, *J* = 8.6, 6.0 Hz, 1H), 2.43 (ddd, *J* = 13.8, 8.9, 5.9 Hz, 1H), 1.99 (t, *J* = 5.7 Hz, 1H), 1.57 (dd, *J* = 8.7, 5.6 Hz, 1H).

^{19}F NMR (471 MHz, Chloroform-*d*) δ -104.09.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.57 (d, *J* = 255.9 Hz), 143.18, 142.77, 136.55 (d, *J* = 3.2 Hz), 129.16 (d, *J* = 9.4 Hz), 126.36, 125.73, 123.75, 117.55, 115.55 (d, *J* = 22.5 Hz), 44.97, 35.44, 29.89, 28.36, 19.81.

HRMS (ESI) calcd for $C_{17}H_{16}FNaO_2S^+$ $[M+H]^+$ 303.0850, Found 303.0844.



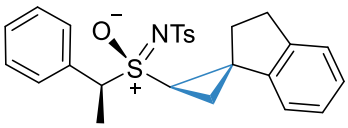
5d, 56% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.04 – 7.99 (m, 2H), 7.75 (d, *J* = 8.1 Hz, 2H), 7.27 (t, *J* = 8.5 Hz, 2H), 7.24 – 7.15 (m, 4H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.56 (d, *J* = 7.6 Hz, 1H), 2.96 (t, *J* = 7.4 Hz, 2H), 2.83 (dd, *J* = 8.5, 6.0 Hz, 1H), 2.65 (dt, *J* = 14.1, 7.0 Hz, 1H), 2.38 (s, 3H), 2.23 (dt, *J* = 13.7, 7.6 Hz, 1H), 1.81 (t, *J* = 6.0 Hz, 1H), 1.47 (dd, *J* = 8.5, 6.0 Hz, 1H).

^{19}F NMR NMR (565 MHz, Chloroform-*d*) δ -102.70.

^{13}C NMR (151 MHz, Chloroform-*d*) δ 166.15 (d, *J* = 257.5 Hz), 144.55, 143.06, 142.87, 140.86, 135.83 (d, *J* = 2.3 Hz), 130.84 (d, *J* = 9.7 Hz), 129.26, 127.84, 126.88, 126.67, 124.94, 118.73, 117.14 (d, *J* = 23.0 Hz), 47.48, 38.22, 31.06, 28.93, 21.64, 19.49.

HRMS (ESI) calcd for $C_{24}H_{22}NFNaO_3S_2^+$ $[M+Na]^+$ 478.0917, Found 478.0924.



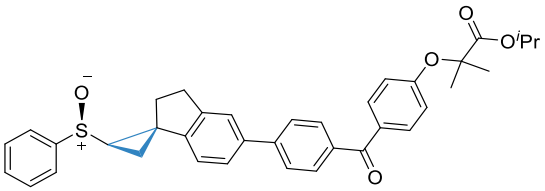
5e, 46% yield, >20:1 dr, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.72 – 7.68 (m, 2H), 7.52 – 7.47 (m, 2H), 7.42 – 7.32 (m, 3H), 7.18 – 7.15 (m, 2H), 7.10 (d, *J* = 8.1 Hz, 3H), 6.46 (d, *J* = 7.6 Hz, 1H), 5.03 (q, *J* = 7.2 Hz, 1H), 2.86 – 2.80 (m, 2H), 2.49 (dd, *J* = 8.5, 6.2 Hz, 1H), 2.43 (ddd, *J* = 14.3, 8.1, 6.5 Hz, 1H), 2.34 (s, 3H), 2.05 – 2.01 (m, 1H), 1.99 (d, *J* = 7.2 Hz, 3H), 1.39 (t, *J* = 6.1 Hz, 1H), 1.28 (dd, *J* = 8.5, 6.1 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 144.67, 142.98, 142.42, 140.97, 132.43, 130.03, 129.68, 129.11, 128.78, 127.70, 126.75, 126.40, 124.86, 118.56, 68.70, 38.80, 36.00, 30.87, 28.69, 21.61, 20.28, 14.75.

HRMS (ESI) calcd for $C_{26}H_{27}NNaO_3S_2^+$ $[M+Na]^+$ 488.1325, Found 488.1327.

Optical Rotation: $[a]_D^{20}$ = -29.7 (c = 0.50, acetone).

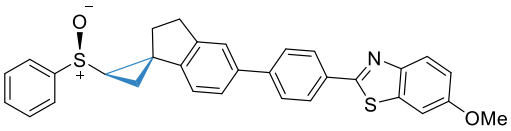


5f, 70% yield, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.82 – 7.75 (m, 4H), 7.69 – 7.65 (m, 2H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.50 (qt, *J* = 6.4, 3.6 Hz, 4H), 7.39 (dd, *J* = 7.9, 1.7 Hz, 1H), 6.88 – 6.84 (m, 2H), 6.73 (d, *J* = 7.9 Hz, 1H), 5.08 (hept, *J* = 6.2 Hz, 1H), 3.18 (ddd, *J* = 15.4, 9.0, 6.1 Hz, 1H), 3.11 (ddd, *J* = 15.8, 9.0, 5.9 Hz, 1H), 2.66 (ddd, *J* = 13.4, 9.0, 6.0 Hz, 1H), 2.57 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.39 (ddd, *J* = 13.5, 9.0, 5.9 Hz, 1H), 2.04 – 1.99 (m, 1H), 1.65 (s, 6H), 1.48 (dd, *J* = 8.9, 5.9 Hz, 1H), 1.19 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.18, 173.27, 159.62, 145.21, 145.15, 144.78, 139.32, 136.80, 132.07, 131.21, 130.82, 130.52, 129.53, 126.89, 126.25, 124.30, 123.60, 119.38, 117.29, 79.46, 69.40, 47.91, 34.23, 31.07, 30.47, 29.78, 25.46, 21.61, 17.30.

HRMS (ESI) calcd for $C_{37}H_{37}O_5S^+$ $[M+H]^+$ 593.2356, Found 593.2355.

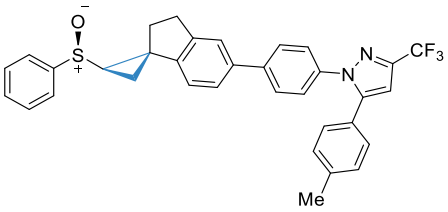


5g, 99% yield, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.08 – 8.04 (m, 2H), 7.96 – 7.88 (m, 1H), 7.69 – 7.66 (m, 2H), 7.64 – 7.61 (m, 2H), 7.53 – 7.44 (m, 4H), 7.41 – 7.37 (m, 1H), 7.34 (d, *J* = 2.5 Hz, 1H), 7.08 (dd, *J* = 8.9, 2.6 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 3.18 (ddd, *J* = 15.4, 9.0, 6.0 Hz, 1H), 3.10 (ddd, *J* = 15.8, 9.0, 5.9 Hz, 1H), 2.64 (ddd, *J* = 13.5, 8.9, 6.0 Hz, 1H), 2.58 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.39 (ddd, *J* = 13.4, 9.0, 5.9 Hz, 1H), 2.01 (t, *J* = 5.9 Hz, 1H), 1.49 (dd, *J* = 8.8, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 165.23, 157.88, 148.83, 145.14, 144.86, 144.74, 143.22, 139.37, 136.50, 132.65, 131.24, 129.55, 127.74, 127.60, 126.05, 124.30, 123.76, 123.40, 119.36, 115.79, 104.25, 55.91, 47.89, 34.27, 31.09, 30.52, 17.45.

HRMS (ESI) calcd for $C_{31}H_{26}NO_2S_2^+$ $[M+H]^+$ 508.1399, Found 508.1390.

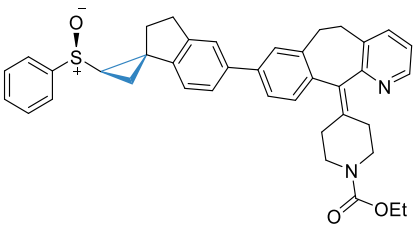


5h, 99% yield, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.69 – 7.65 (m, 2H), 7.54 – 7.45 (m, 5H), 7.44 (d, *J* = 1.6 Hz, 1H), 7.39 – 7.30 (m, 3H), 7.13 (d, *J* = 1.1 Hz, 4H), 6.73 – 6.67 (m, 2H), 3.16 (ddd, *J* = 15.4, 9.0, 6.0 Hz, 1H), 3.09 (ddd, *J* = 15.8, 9.0, 5.9 Hz, 1H), 2.64 (ddd, *J* = 13.4, 9.0, 6.0 Hz, 1H), 2.56 (dd, *J* = 8.8, 5.8 Hz, 1H), 2.38 (ddd, *J* = 13.4, 9.0, 6.0 Hz, 1H), 2.35 (s, 3H), 2.01 (t, *J* = 5.9 Hz, 1H), 1.47 (dd, *J* = 8.8, 5.9 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.19, 144.83, 144.79, 144.74, 143.30 (q, *J* = 38.2 Hz), 141.13, 139.23, 139.04, 138.45, 131.23, 129.54, 128.79, 127.67, 126.36, 126.06, 125.74, 124.29, 123.44, 121.41 (q, *J* = 268.9 Hz), 119.33, 105.53, 47.90, 34.22, 31.07, 30.50, 21.40, 17.37.

HRMS (ESI) calcd for $C_{34}H_{28}F_3N_2OS^+$ $[M+H]^+$ 569.1869, Found 569.1865.



5i, 99% yield, colorless solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 4.8, 1.7 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.50 – 7.45 (m, 3H), 7.43 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.40 (d, *J* = 1.6 Hz, 1H), 7.32 (dq, *J* = 4.1, 1.9 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.07 (dd, *J* = 7.7, 4.8 Hz, 1H), 6.66 (d, *J* = 7.9 Hz, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 3.89 – 3.75 (m, 2H), 3.45 (tt, *J* = 10.1, 4.5 Hz, 1H), 3.37 (ddd, *J* = 15.4, 8.6, 4.6 Hz, 1H), 3.18 – 3.02 (m, 4H), 2.91 – 2.82 (m, 2H), 2.62 (ddd, *J* = 13.4, 9.0, 6.1 Hz, 1H), 2.54 (ddd, *J* = 8.9, 5.8, 1.1 Hz, 1H), 2.51 – 2.45 (m, 1H), 2.41 (t, *J* = 5.8 Hz, 2H), 2.40 – 2.34 (m, 1H), 2.34 – 2.27 (m, 1H), 1.98 (t, *J* = 5.9 Hz, 1H), 1.45 (dd, *J* = 8.8, 5.9 Hz, 1H), 1.23 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 157.73, 155.62, 146.70, 145.25, 144.51, 144.11, 140.29, 140.06, 138.11, 138.08, 137.48, 137.03, 135.03, 133.77, 131.16, 129.94, 129.49, 127.92, 125.92, 124.81, 124.29, 123.32, 122.27, 119.16, 61.39, 47.82, 45.00, 44.92, 34.23, 32.19, 31.79, 31.06, 30.89, 30.66, 30.49, 17.26, 14.78.

HRMS (ESI) calcd for $C_{39}H_{39}N_2O_3S^+$ $[M+H]^+$ 615.2676, Found 615.2671.

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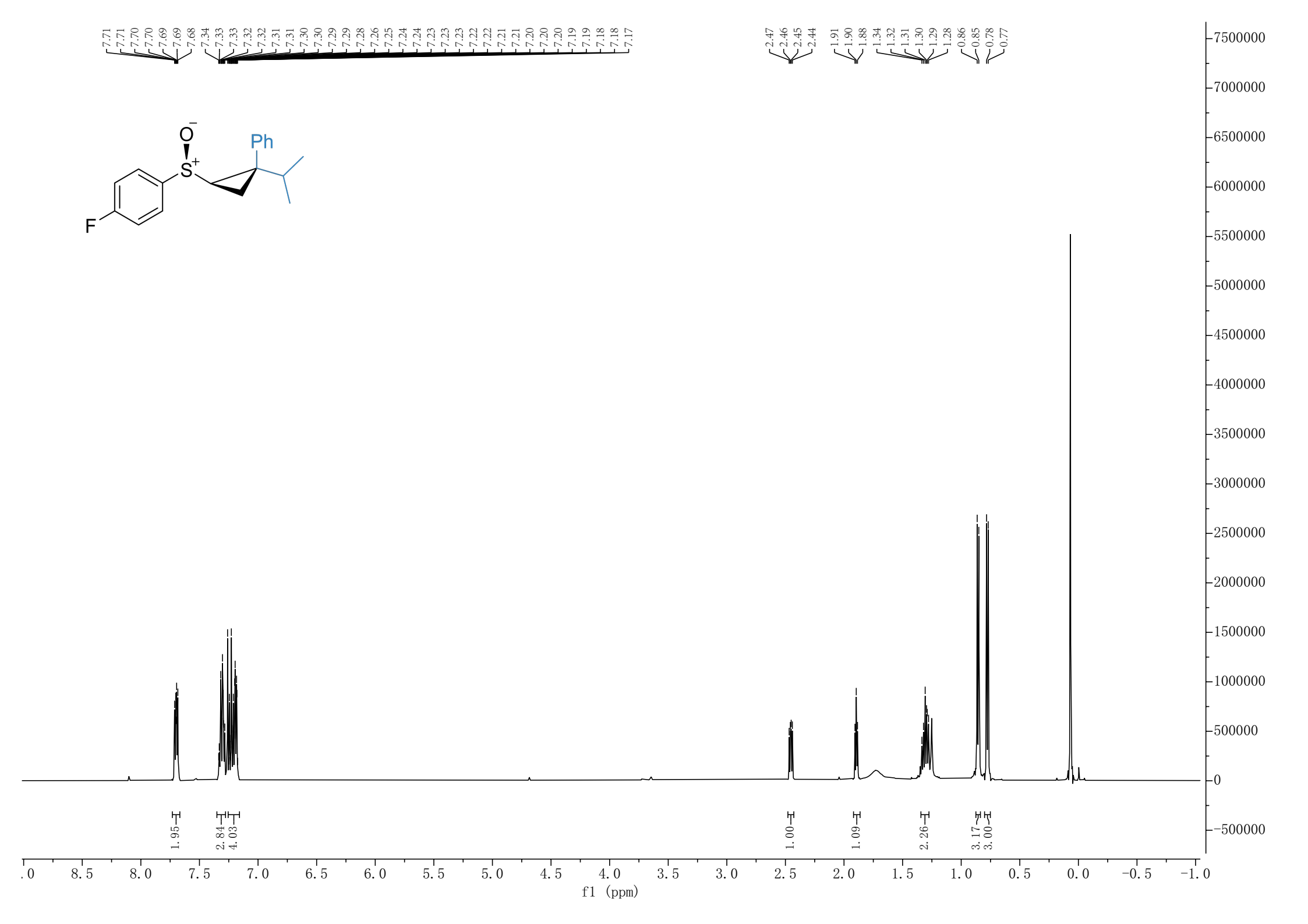
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2.47 2.46 2.45 2.44 1.91 1.90 1.88 1.34 1.32 1.31 1.30 1.29 1.28 0.86 0.85 0.78 0.77
O
S+
Ph
F
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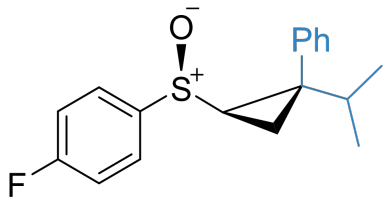
f1 (ppm)



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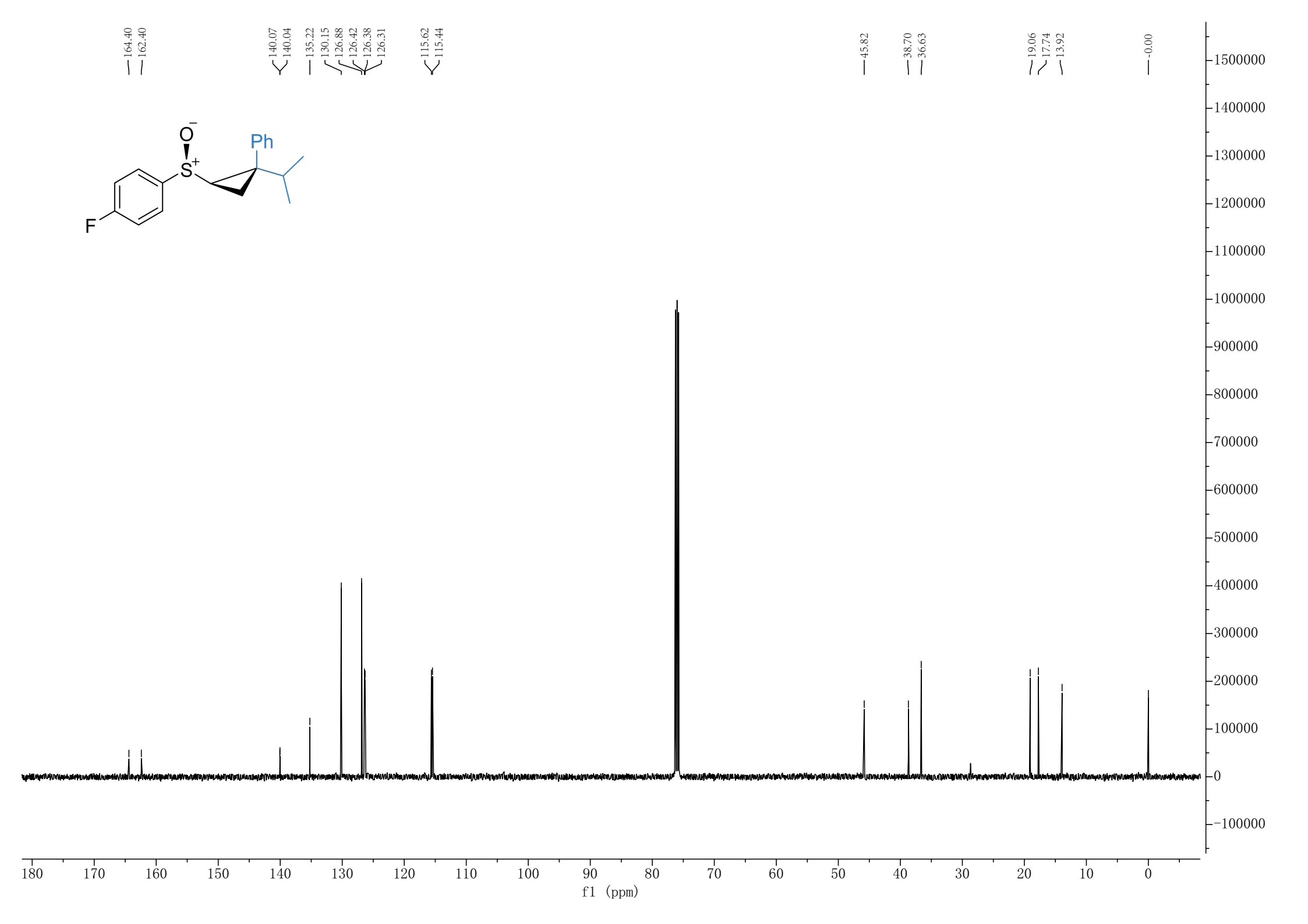
164.40
162.40
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140.04
135.22
130.15
126.88
126.42
126.38
126.31
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115.44
45.82
38.70
36.63
19.06
17.74
13.92
-0.00
O
S+
Ph
F
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
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400000
300000
200000
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-100000
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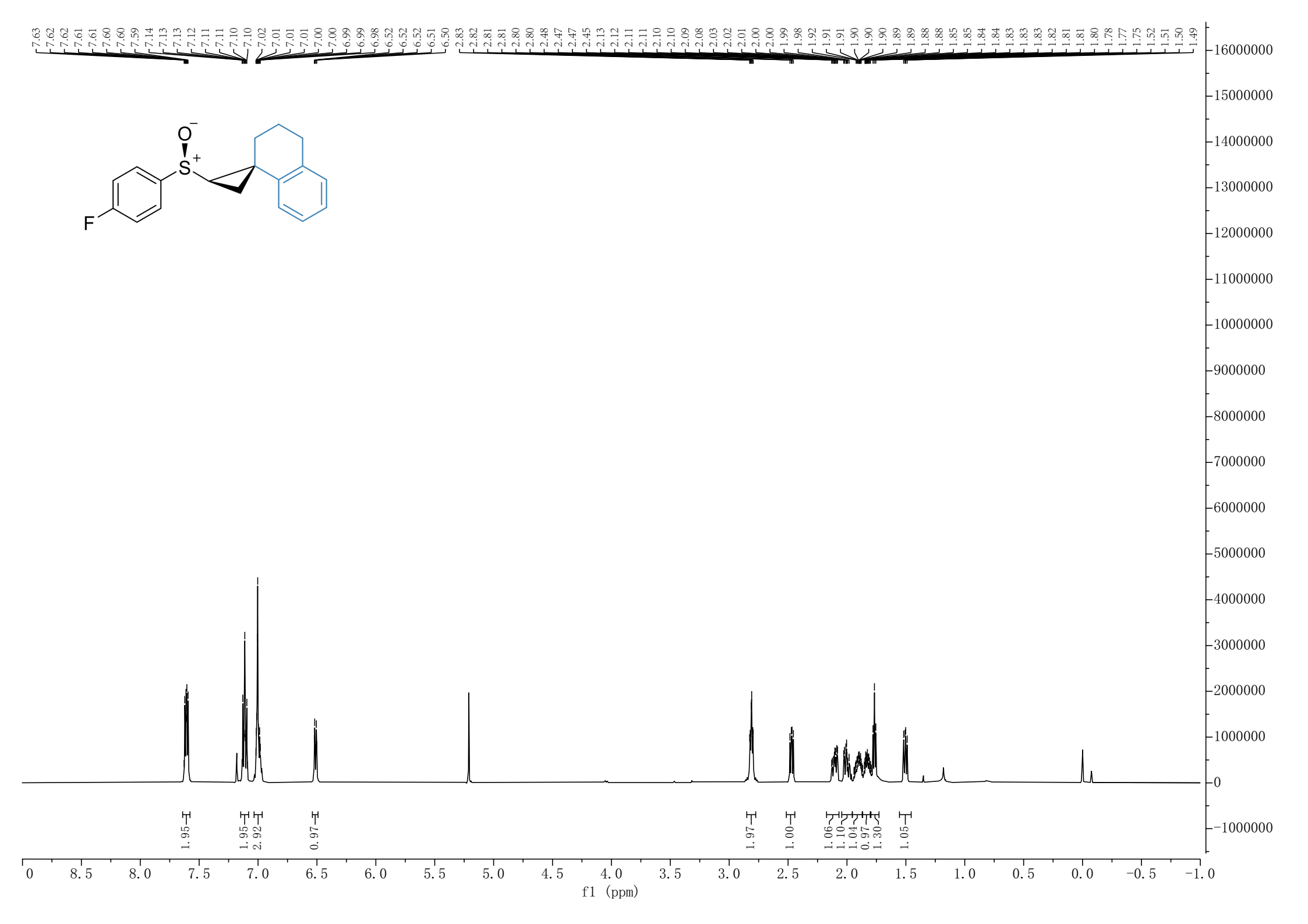
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2.83 2.82 2.81 2.81 2.80 2.80 2.48 2.47 2.47 2.45 2.13 2.12 2.11 2.11 2.10 2.10 2.09 2.08 2.03 2.02 2.01 2.00 2.00 1.99 1.98 1.92 1.91 1.91 1.90 1.90 1.90 1.89 1.89 1.88 1.88 1.85 1.85 1.84 1.84 1.83 1.83 1.83 1.82 1.81 1.81 1.80 1.78 1.77 1.75 1.52 1.51 1.50 1.49
O
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0
-1000000
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1.95
2.92
0.97
1.97
1.00
1.06
1.10
1.04
0.97
1.30
1.05
0
8.5
8.0
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
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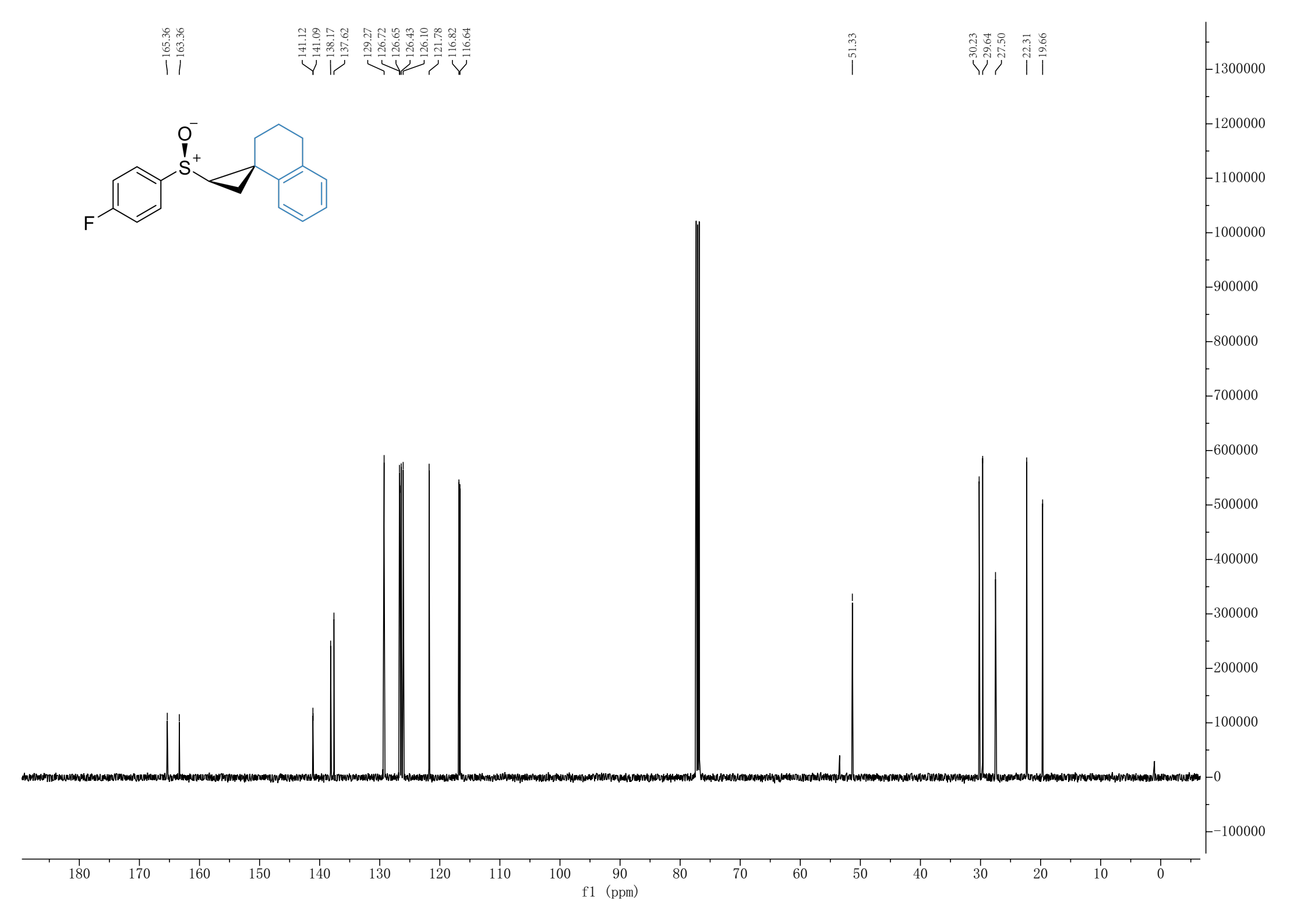
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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116.64
51.33
30.23
29.64
27.50
22.31
19.66
O
S
F
1300000
1200000
1100000
1000000
900000
800000
700000
600000
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400000
300000
200000
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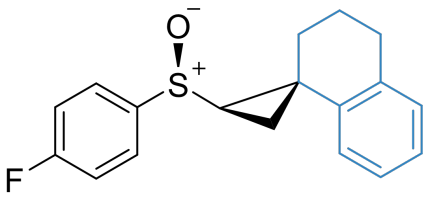
f1 (ppm)



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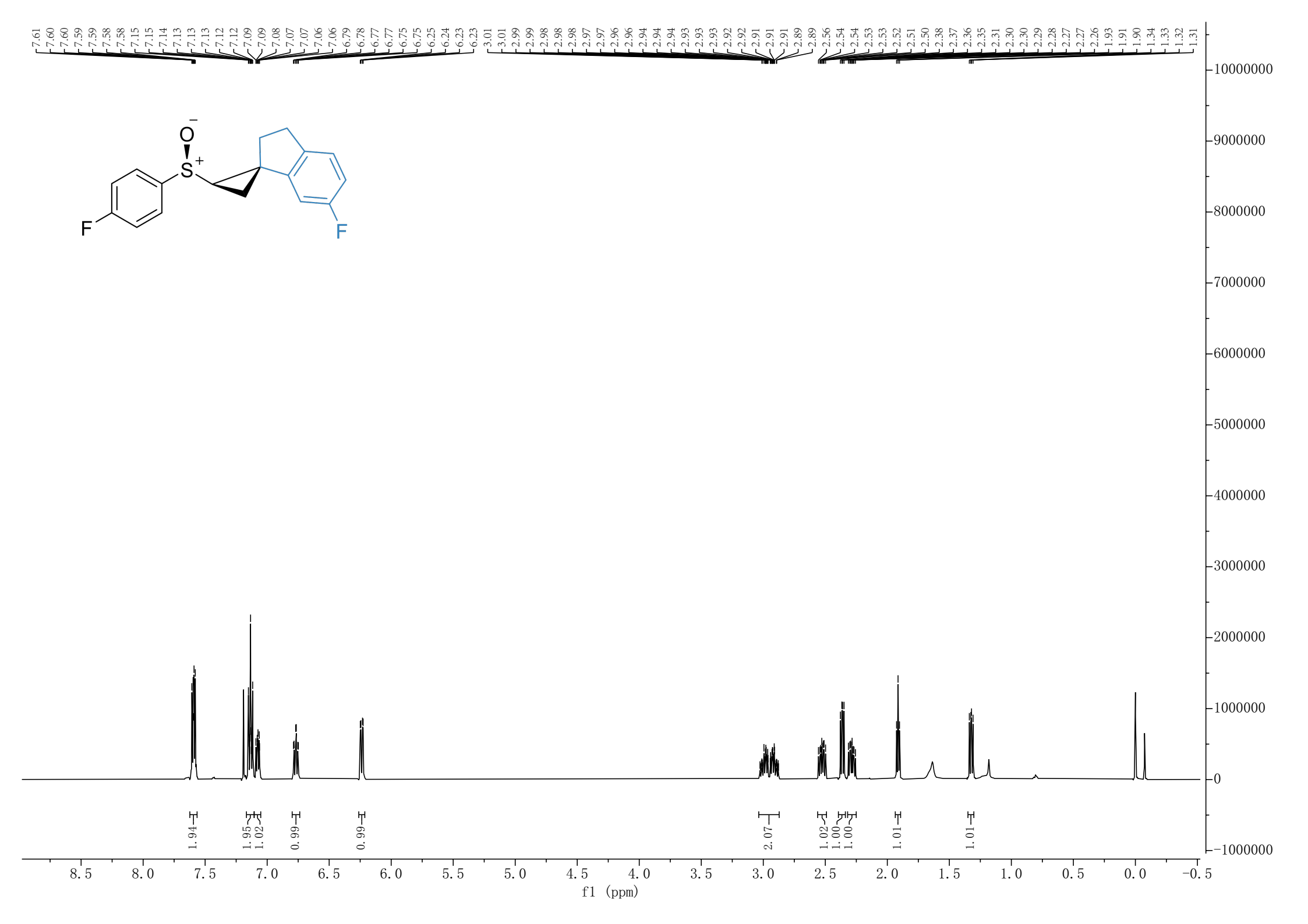
f1 (ppm)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3.01 3.01 2.99 2.99 2.98 2.98 2.98 2.97 2.97 2.96 2.96 2.94 2.94 2.94 2.93 2.93 2.93 2.92 2.92 2.91 2.91 2.91 2.89 2.89
2.56 2.54 2.54 2.53 2.53 2.52 2.51 2.50 2.38 2.37 2.36 2.35 2.31 2.30 2.30 2.29 2.28 2.27 2.27 2.26 1.93 1.91 1.90 1.34 1.33 1.32 1.31
O
S+
F
F
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6000000
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3000000
2000000
1000000
0
-1000000
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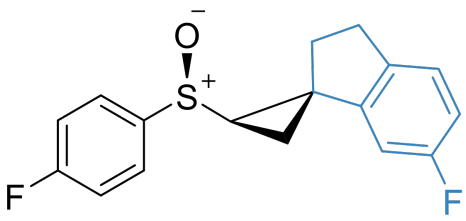
1.95
1.02
0.99
0.99
2.07
1.02
1.00
1.00
1.01
1.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


O
S
F
F

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-116.22
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10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
10
0
-10
-20
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-50
-60
-70
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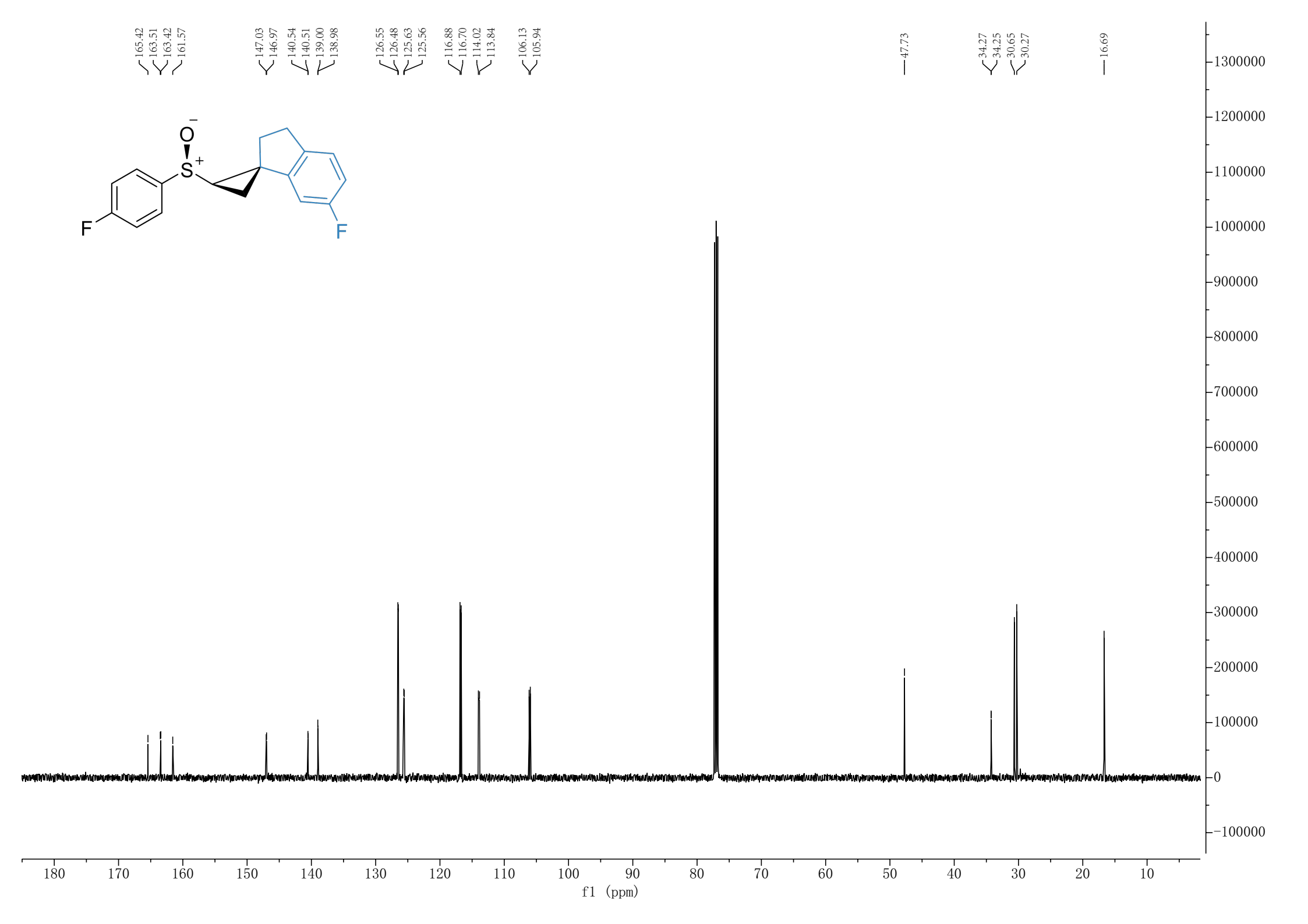
-170
-180
-190
-200
-210
f1 (ppm)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140.54
140.51
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125.63
125.56
116.88
116.70
114.02
113.84
106.13
105.94
47.73
34.27
34.25
30.65
30.27
16.69
O
S+
F
F
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
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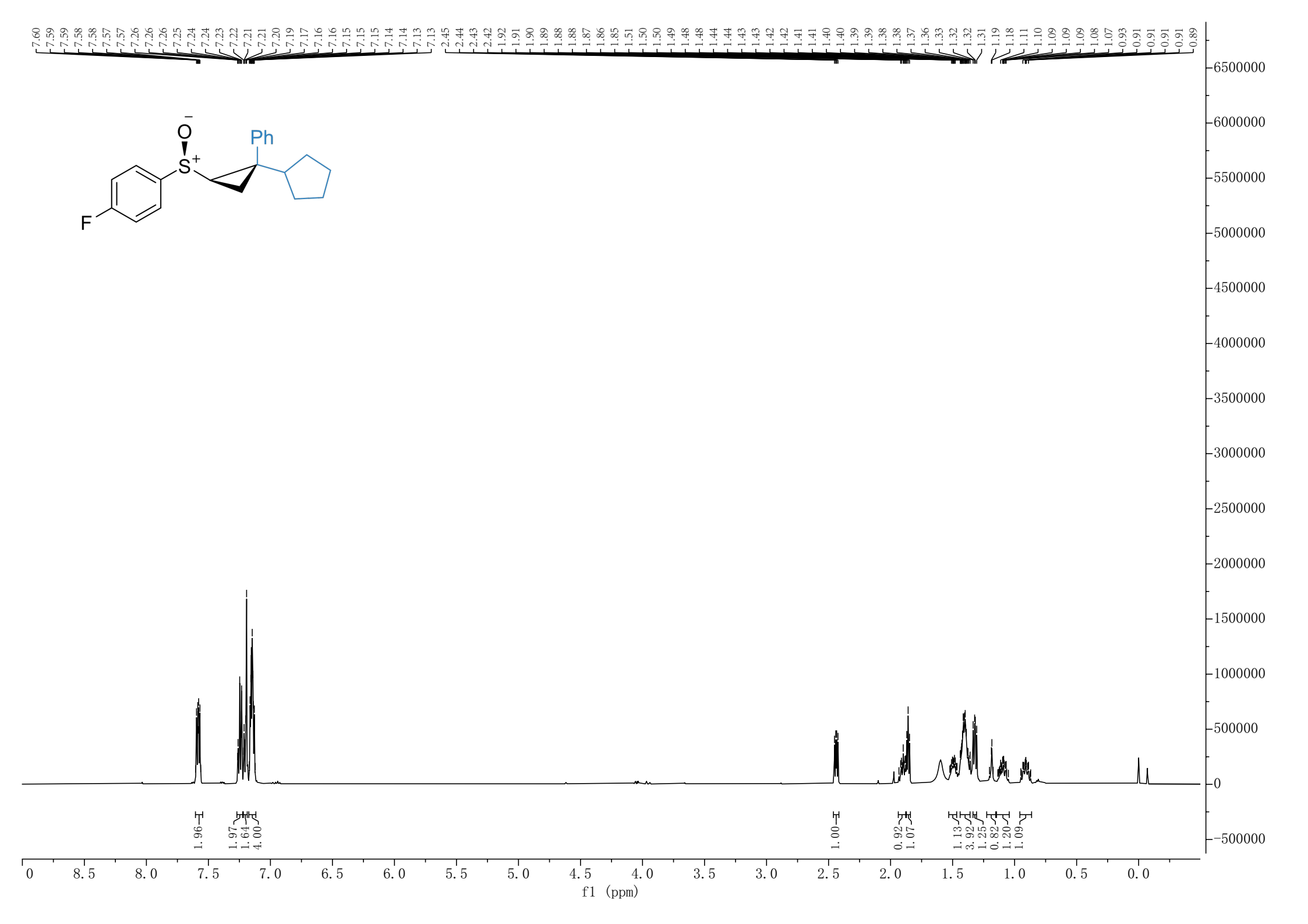
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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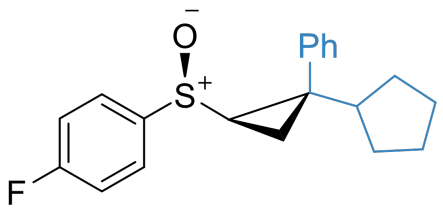
2.45 2.44 2.43 2.42 1.92 1.91 1.90 1.89 1.88 1.88 1.87 1.86 1.85 1.51 1.50 1.50 1.49 1.48 1.48 1.44 1.44 1.43 1.43 1.42 1.42 1.41 1.41 1.40 1.40 1.39 1.39 1.38 1.38 1.37 1.36 1.33 1.32 1.32 1.31 1.19 1.18 1.11 1.10 1.09 1.09 1.09 1.08 1.07 0.93 0.91 0.91 0.91 0.91 0.89
O
S+
Ph
F
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
-500000
1.96
1.97
1.64
4.00
1.00
0.92
1.07
1.13
3.92
1.25
0.82
1.20
1.09
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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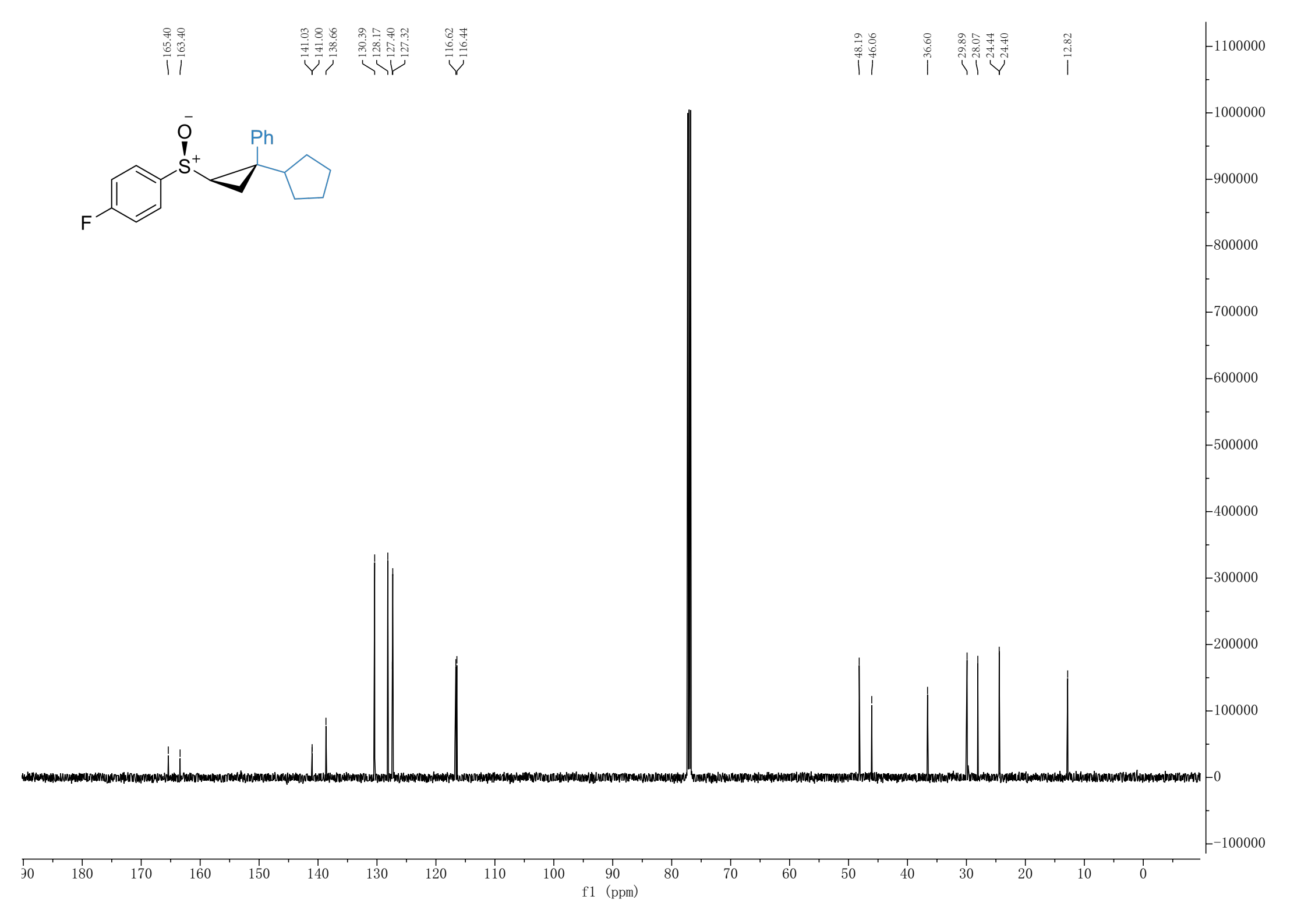
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

f1 (ppm)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138.66
130.39
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127.40
127.32
116.62
116.44
48.19
46.06
36.60
29.89
28.07
24.44
24.40
12.82
O
S+
Ph
F
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
190
180
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150
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130
120
110
100
90
80
70
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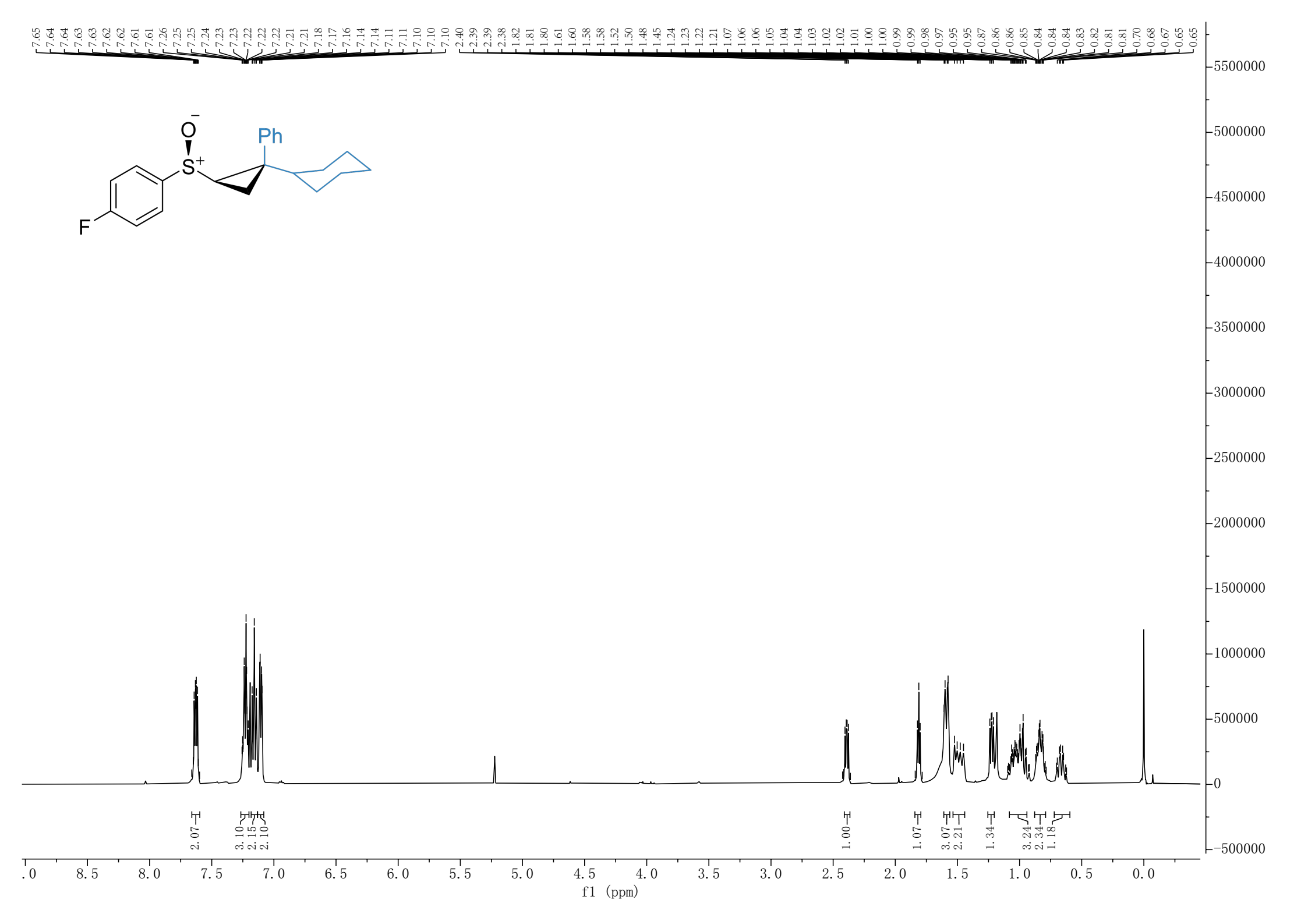
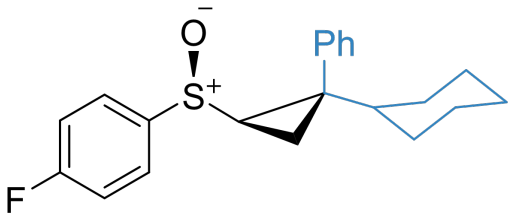
50
40
30
20
10
0
f1 (ppm)


O
S+
Ph
F
f1 (ppm)



-108.15

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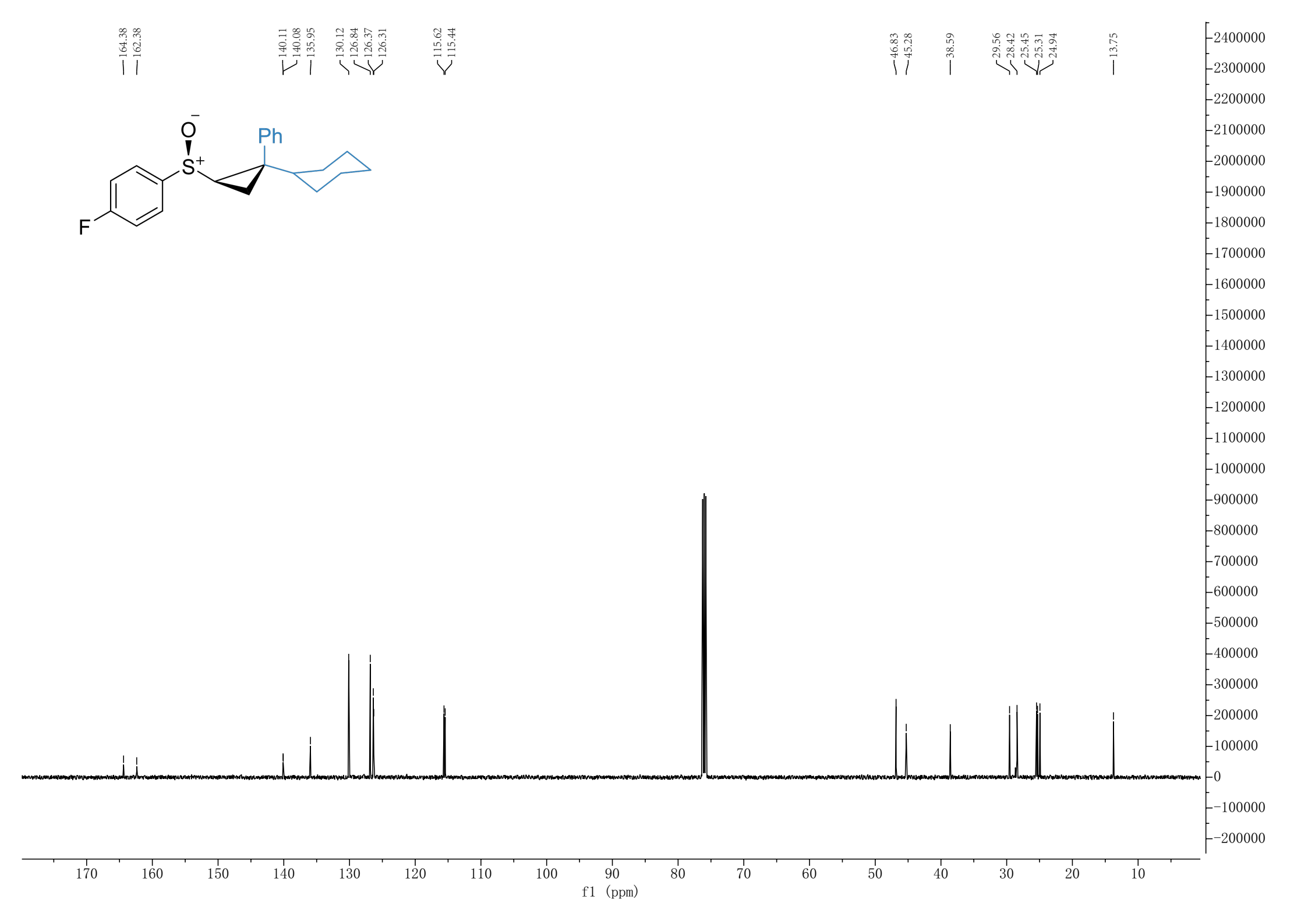
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

f1 (ppm)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126.37
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115.62
115.44
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45.28
38.59
29.56
28.42
25.45
25.31
24.94
13.75
O
S+
Ph
F
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2300000
2200000
2100000
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1900000
1800000
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1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
−200000
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140
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120
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100
90
80
70
60
50
40
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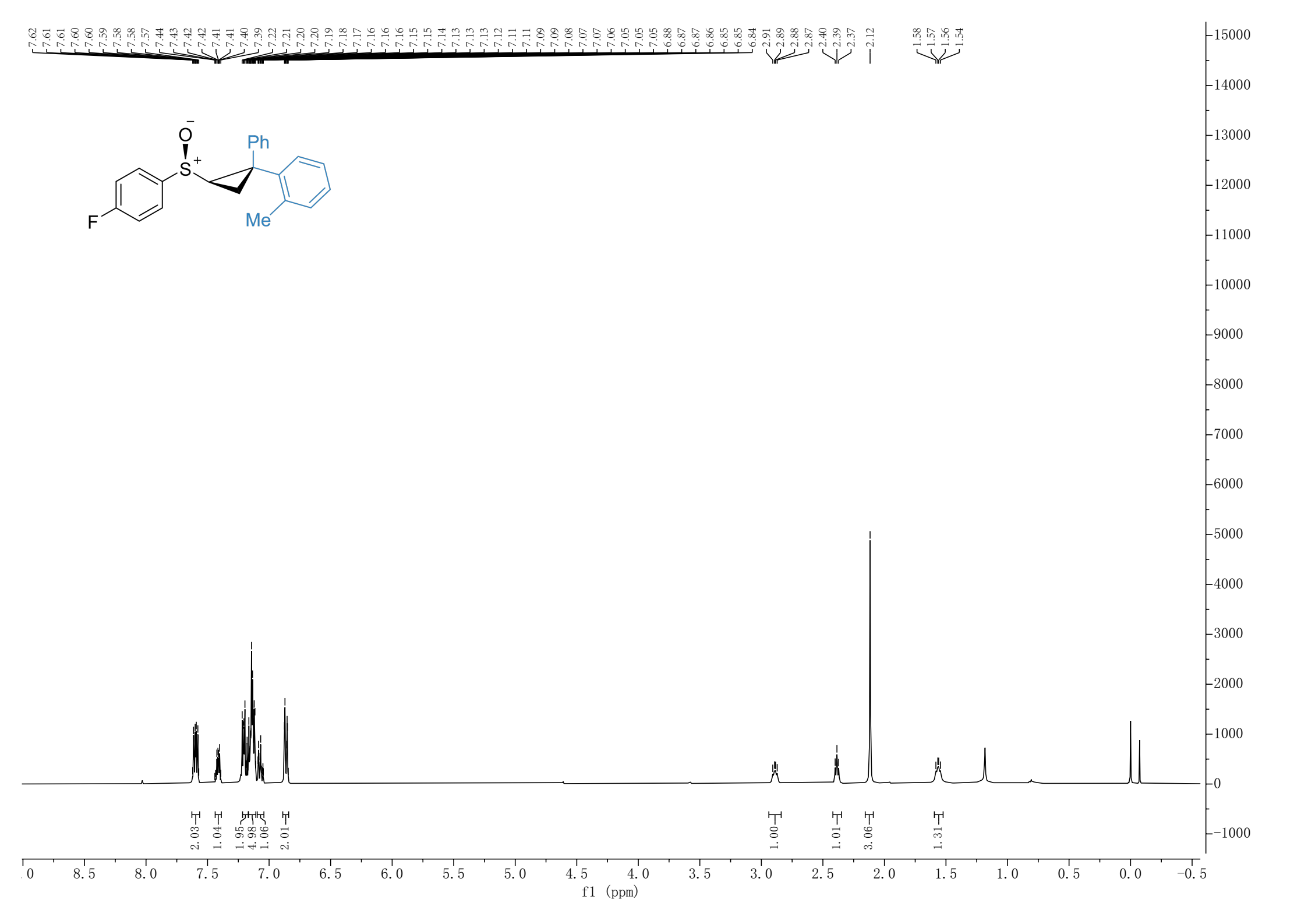
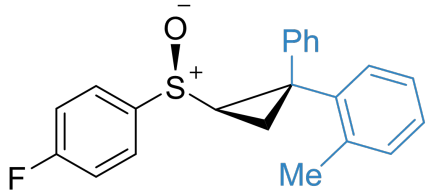
20
10
f1 (ppm)


7.62 7.61 7.61 7.60 7.60 7.59 7.58 7.58 7.57 7.44 7.43 7.42 7.42 7.41 7.41 7.40 7.39 7.22 7.21 7.20 7.20 7.19 7.18 7.17 7.16 7.16 7.16 7.15 7.15 7.14 7.13 7.13 7.13 7.12 7.11 7.11 7.09 7.09 7.08 7.07 7.07 7.06 7.05 7.05 7.05 6.88 6.87 6.87 6.86 6.85 6.84 2.91 2.89 2.88 2.87 2.40 2.39 2.37 2.12 1.58 1.57 1.56 1.54
O
S+
Ph
F
Me
15000 14000 13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
2.03 1.04 1.95 4.98 1.06 2.01 1.00 1.01 3.06 1.31
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
f1 (ppm)



-108.30

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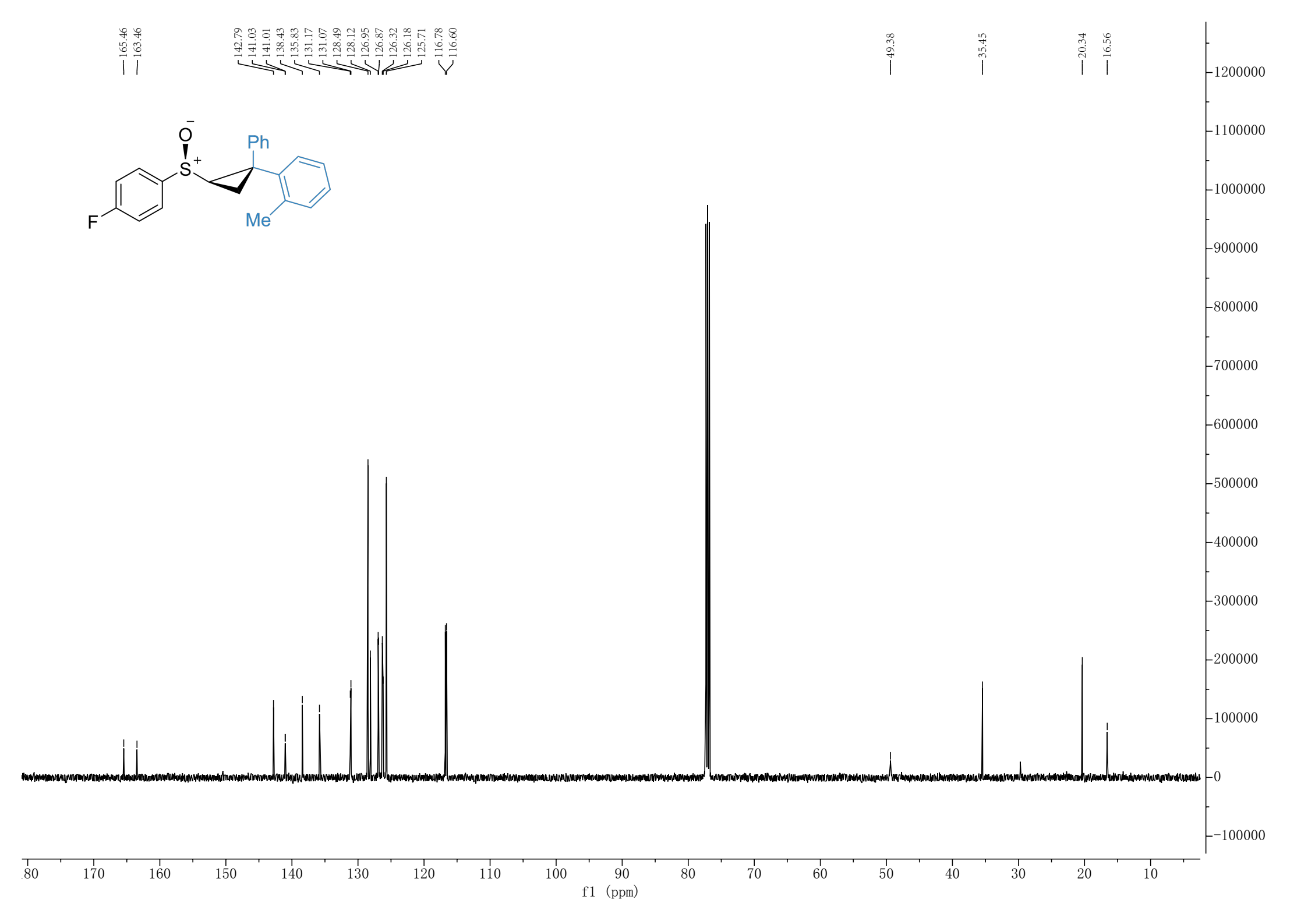
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)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128.12
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126.87
126.32
126.18
125.71
116.78
116.60
49.38
35.45
20.34
16.56
O
S+
Ph
Me
F
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
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100
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80
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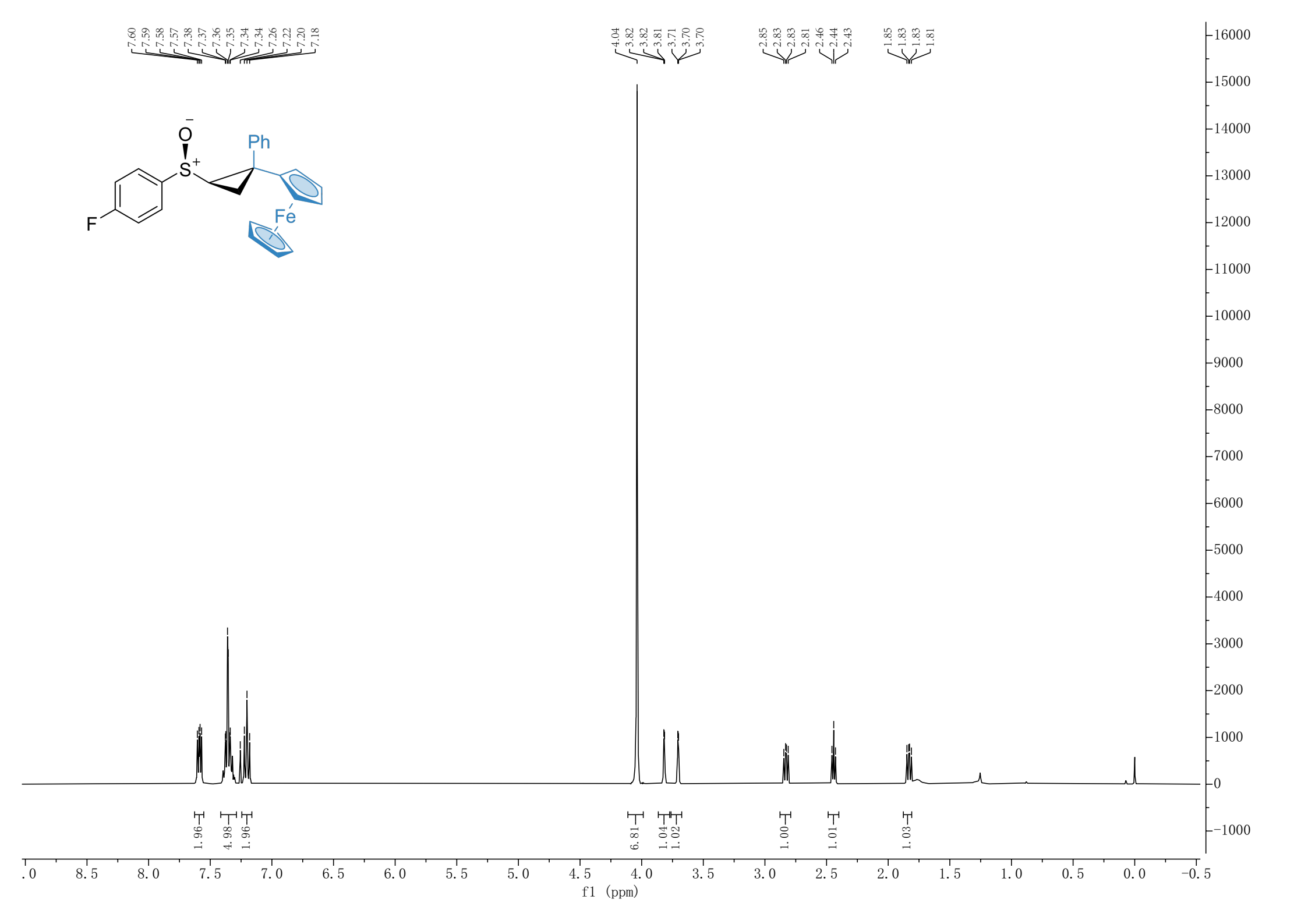
60
50
40
30
20
10
f1 (ppm)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7.22
7.20
7.18
4.04
3.82
3.82
3.81
3.71
3.70
3.70
2.85
2.83
2.83
2.81
2.46
2.44
2.43
1.85
1.83
1.83
1.81
O
S+
Ph
F
Fe
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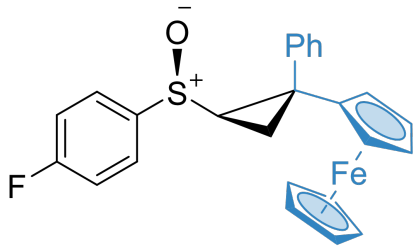
4.98
1.96
6.81
1.04
1.02
1.00
1.01
1.03
f1 (ppm)



-107.77

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16000
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11000
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9000
8000
7000
6000
5000
4000
3000
2000
1000
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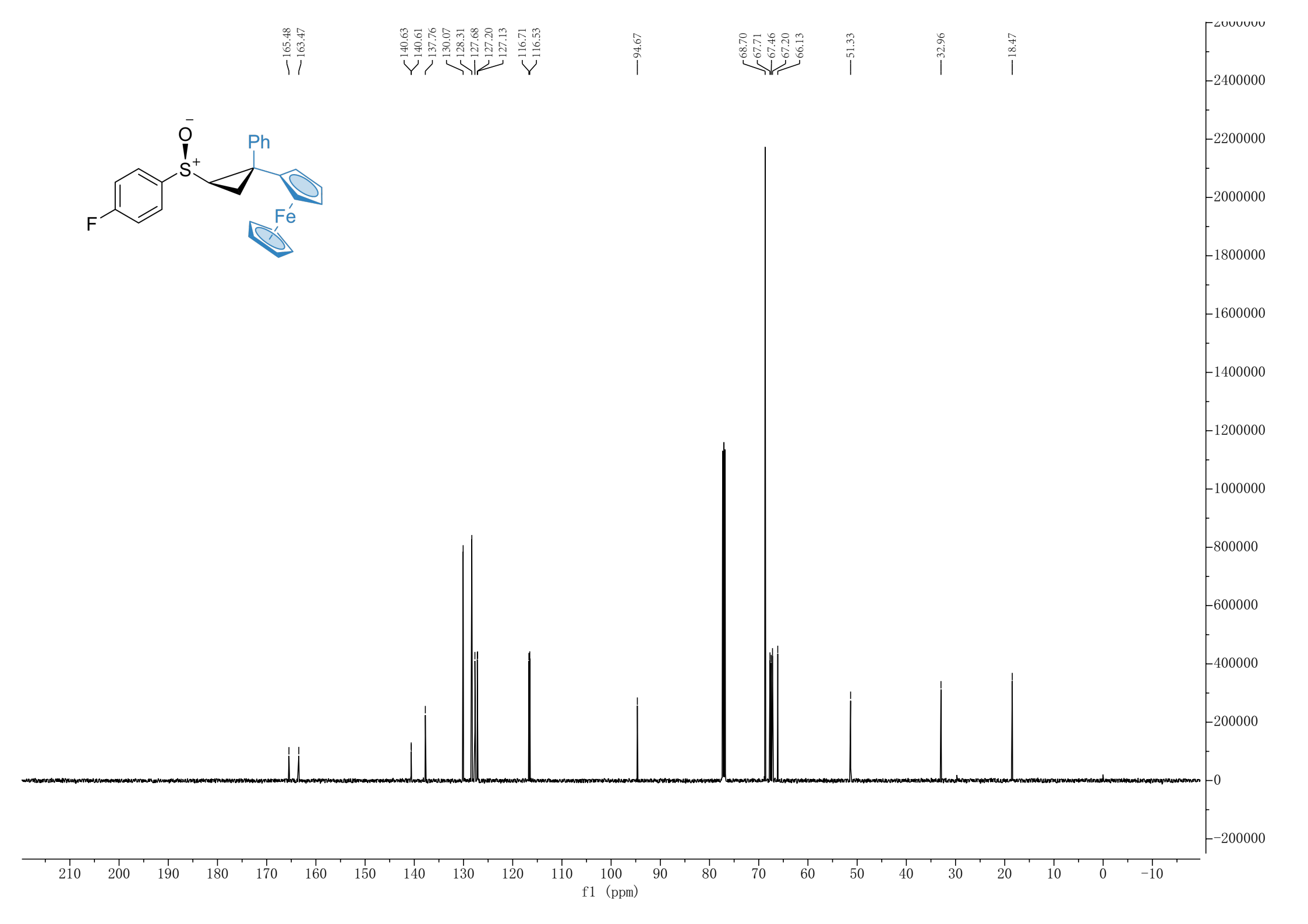
-1000

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)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127.13
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116.53
94.67
68.70
67.71
67.46
67.20
66.13
51.33
32.96
18.47
O
S+
Ph
F
Fe
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
-200000
210
200
190
180
170
160
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140
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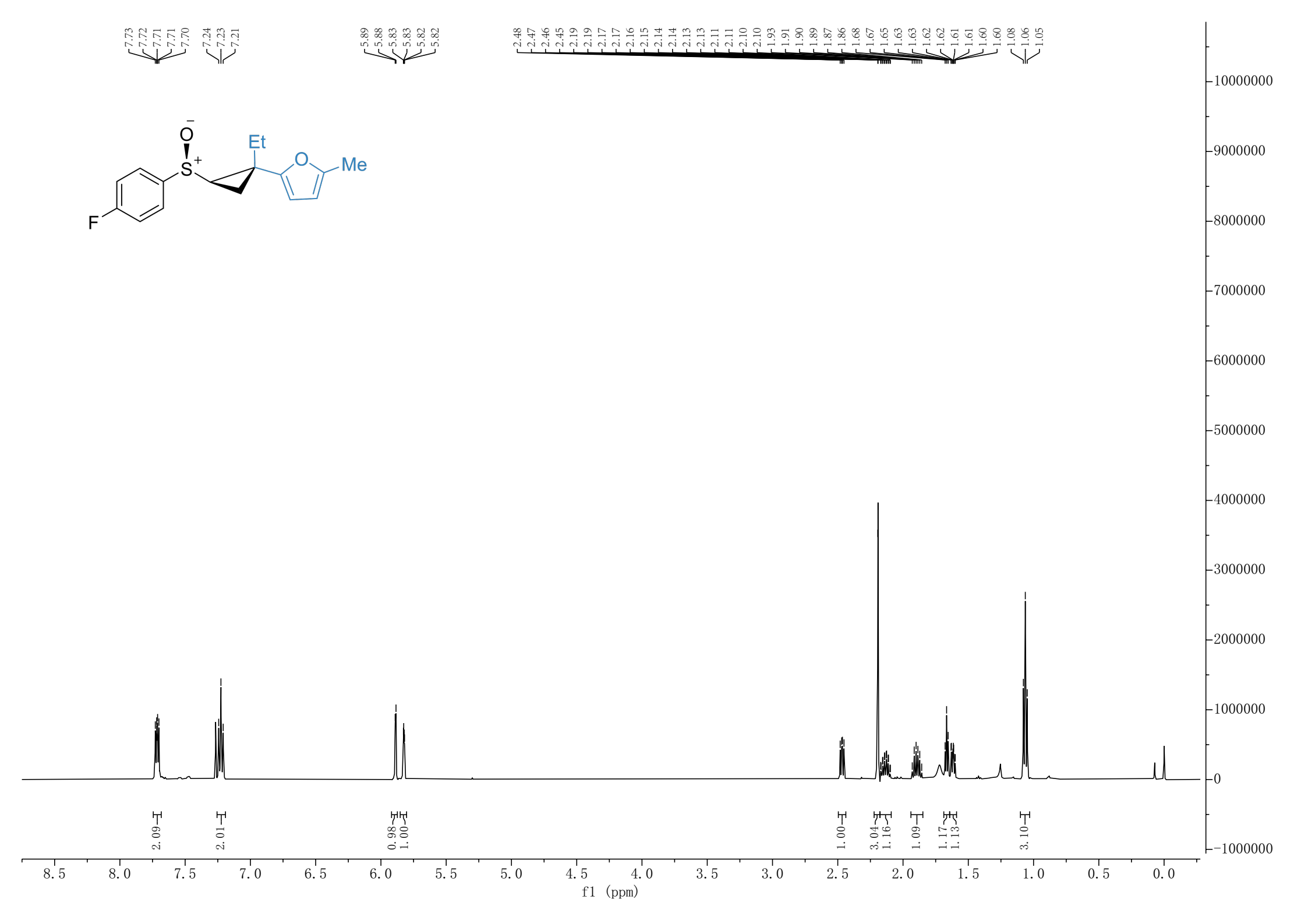
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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5.82
5.82
2.48
2.47
2.46
2.45
2.19
2.19
2.17
2.17
2.16
2.15
2.14
2.14
2.13
2.13
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2.11
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2.10
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1.65
1.63
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1.62
1.61
1.61
1.60
1.60
1.08
1.06
1.05
O
S+
Et
O
Me
F
10000000
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8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000
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2.01
0.98
1.00
1.00
3.04
1.16
1.09
1.17
1.13
3.10
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7.5
7.0
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6.0
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2.0
1.5
1.0
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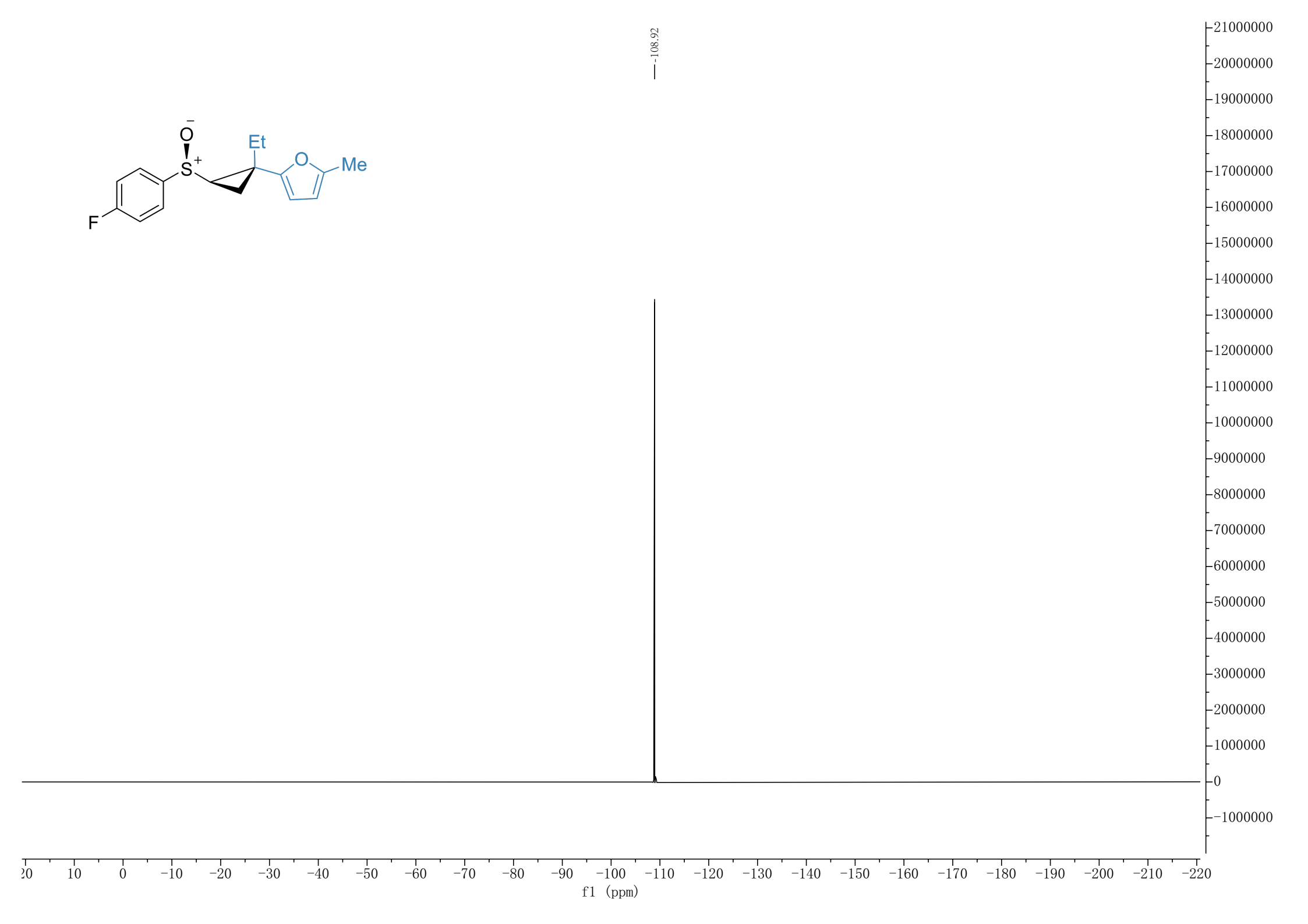
0.0
f1 (ppm)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7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
20
10
0
-10
-20
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-70
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-90
-100
-110
-120
-130
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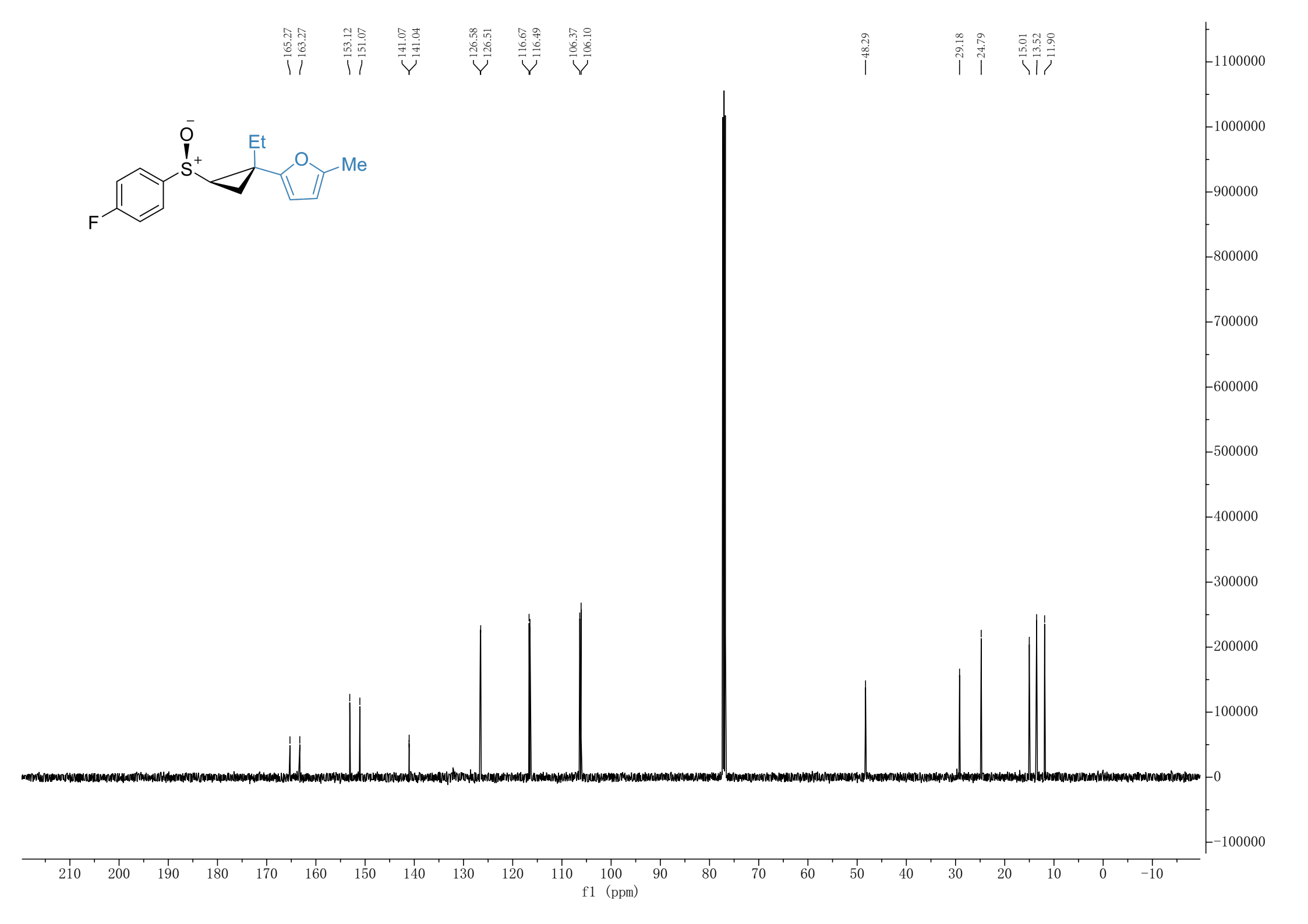
-150
-160
-170
-180
-190
-200
-210
-220
f1 (ppm)
O
S+
Et
O
Me
F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151.07
141.07
141.04
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126.51
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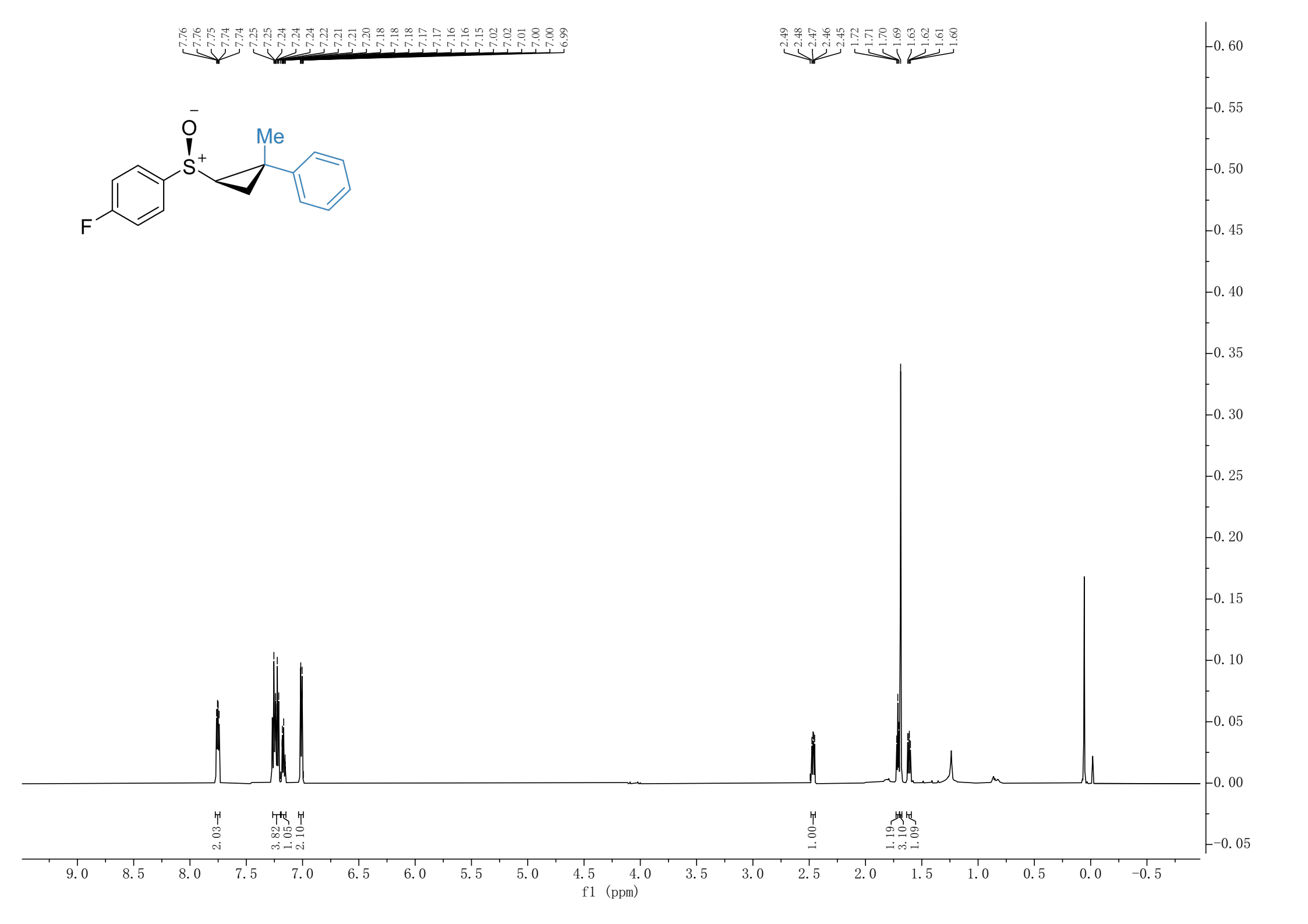
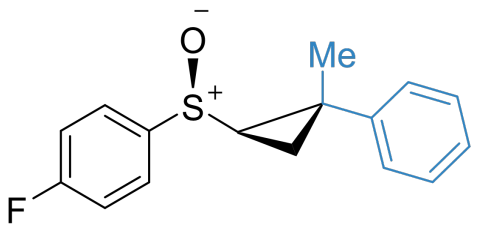
116.49
106.37
106.10
48.29
29.18
24.79
15.01
13.52
11.90
O
S+
Et
O
Me
F
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


7.76 7.76 7.75 7.74 7.74 7.25 7.25 7.24 7.24 7.24 7.22 7.21 7.21 7.20 7.18 7.18 7.18 7.17 7.17 7.16 7.16 7.15 7.02 7.02 7.01 7.00 7.00 6.99
2.49 2.48 2.47 2.46 2.45 1.72 1.71 1.70 1.69 1.63 1.62 1.61 1.60
O
S+
Me
F
2.03
3.82
1.05
2.10
1.00
1.19
3.10
1.09
f1 (ppm)

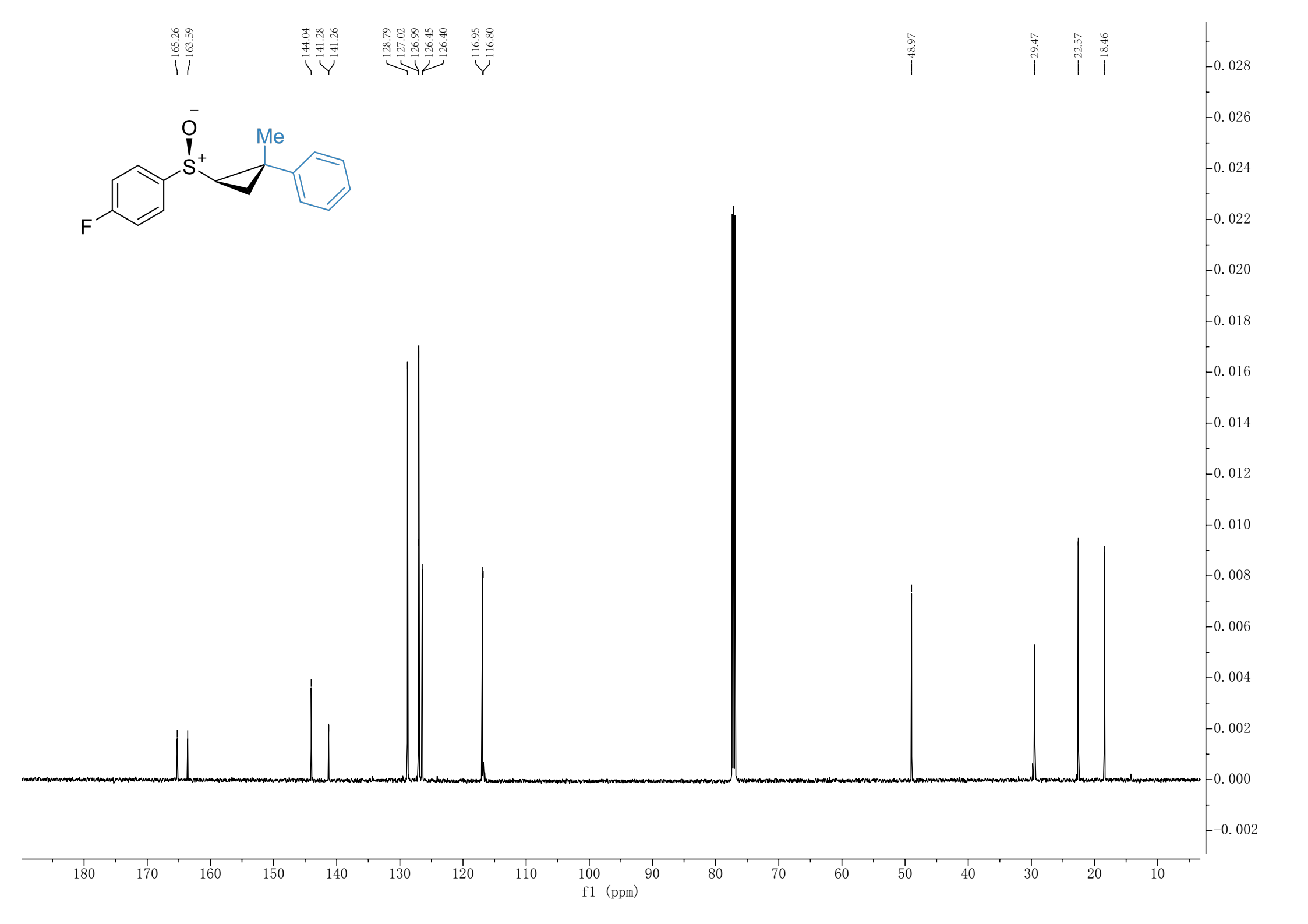


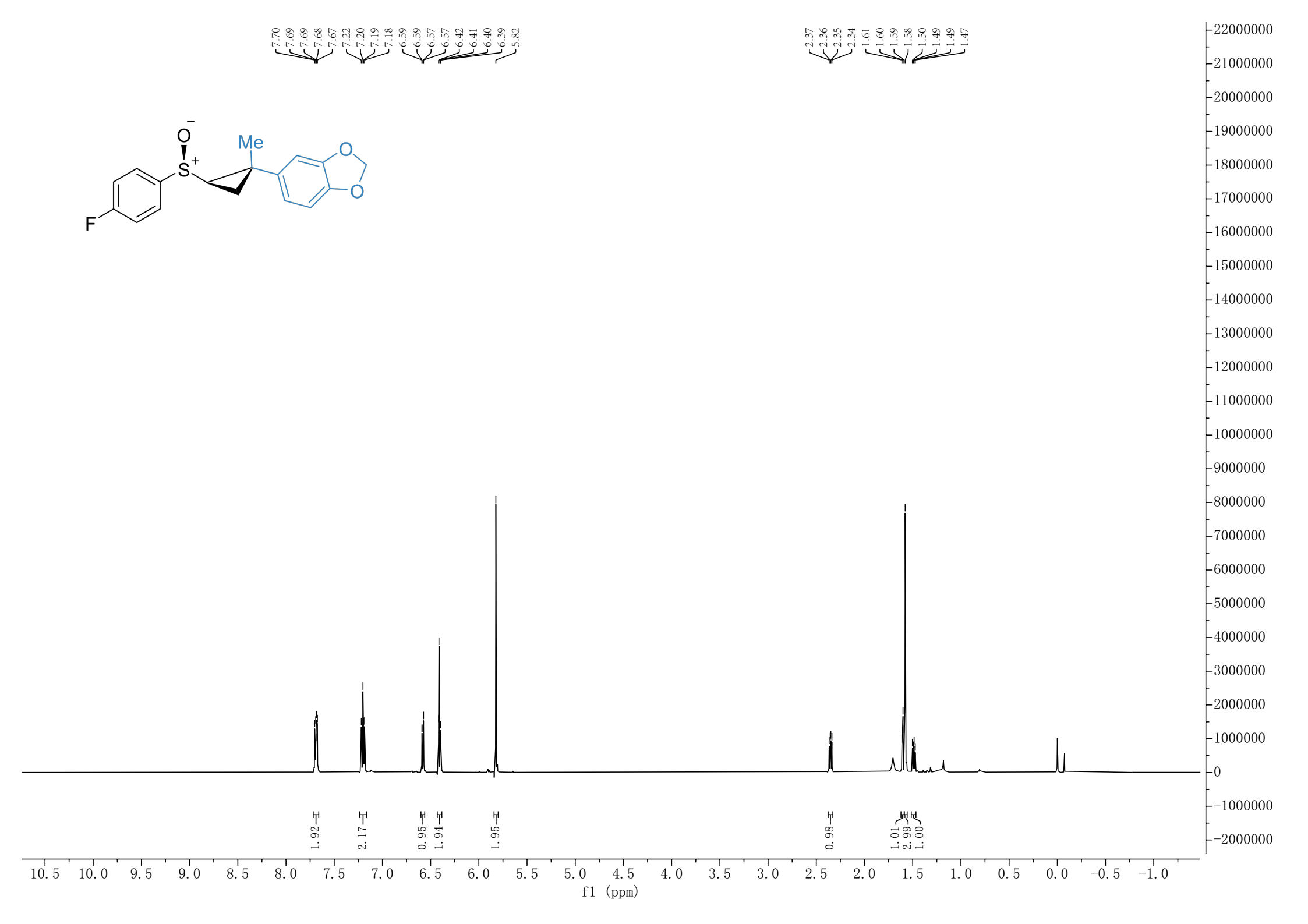
-108.20

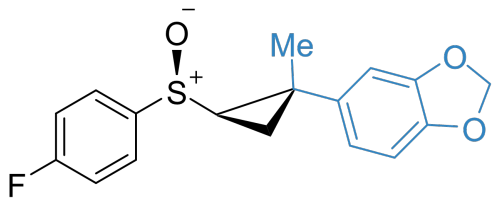
9 8 7 6 5 4 3 2 1 0 -1

40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

f1 (ppm)


165.26
163.59
144.04
141.28
141.26
128.79
127.02
126.99
126.45
126.40
116.95
116.80
48.97
29.47
22.57
18.46
O
S+
Me
F
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.70
7.69
7.69
7.68
7.67
7.22
7.20
7.19
7.18
6.59
6.59
6.57
6.57
6.42
6.41
6.40
6.39
5.82
2.37
2.36
2.35
2.34
1.61
1.60
1.59
1.58
1.50
1.49
1.49
1.47
O
S+
Me
O
O
F
1.92
2.17
0.95
1.94
1.95
0.98
1.01
2.99
1.00
f1 (ppm)

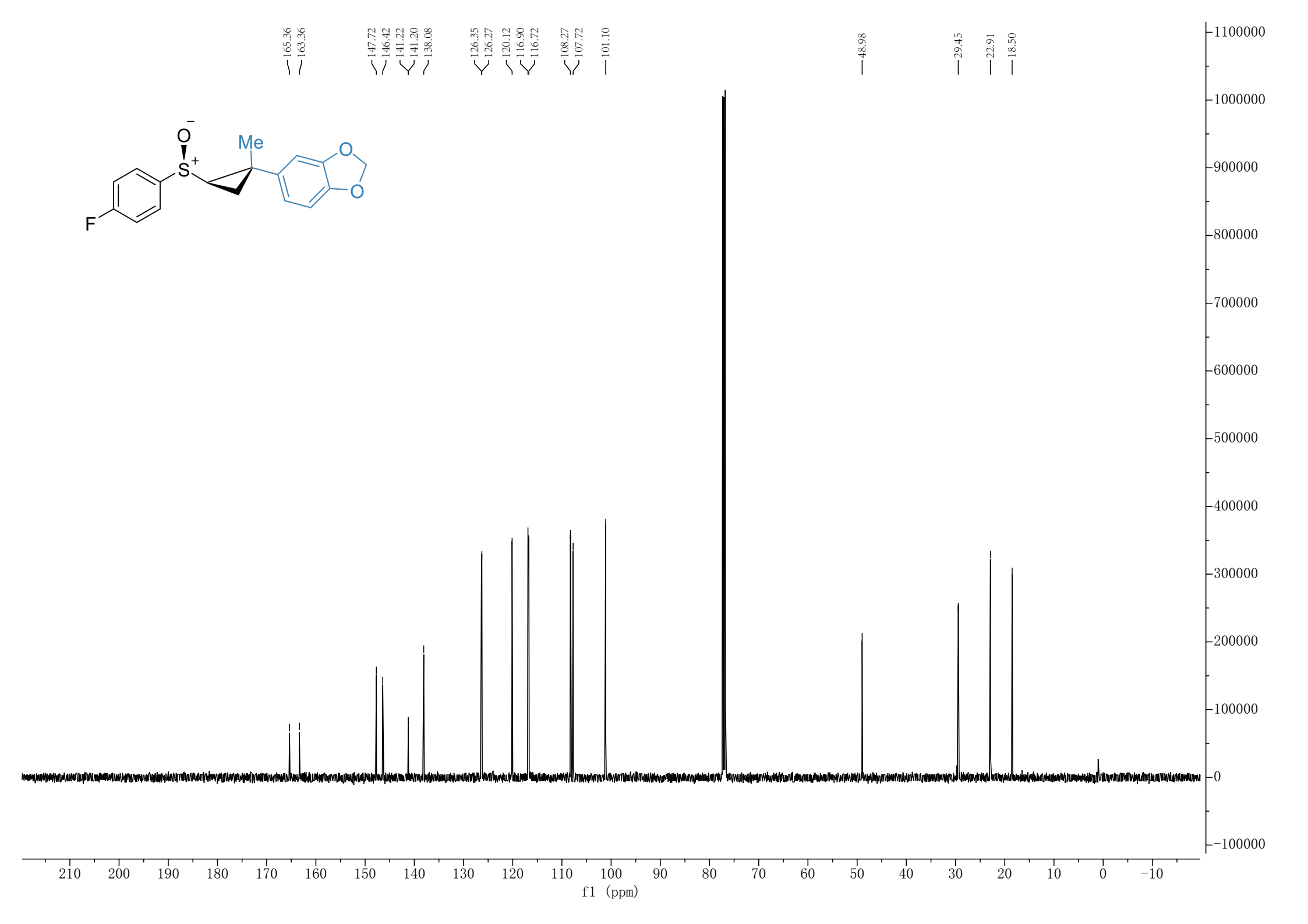


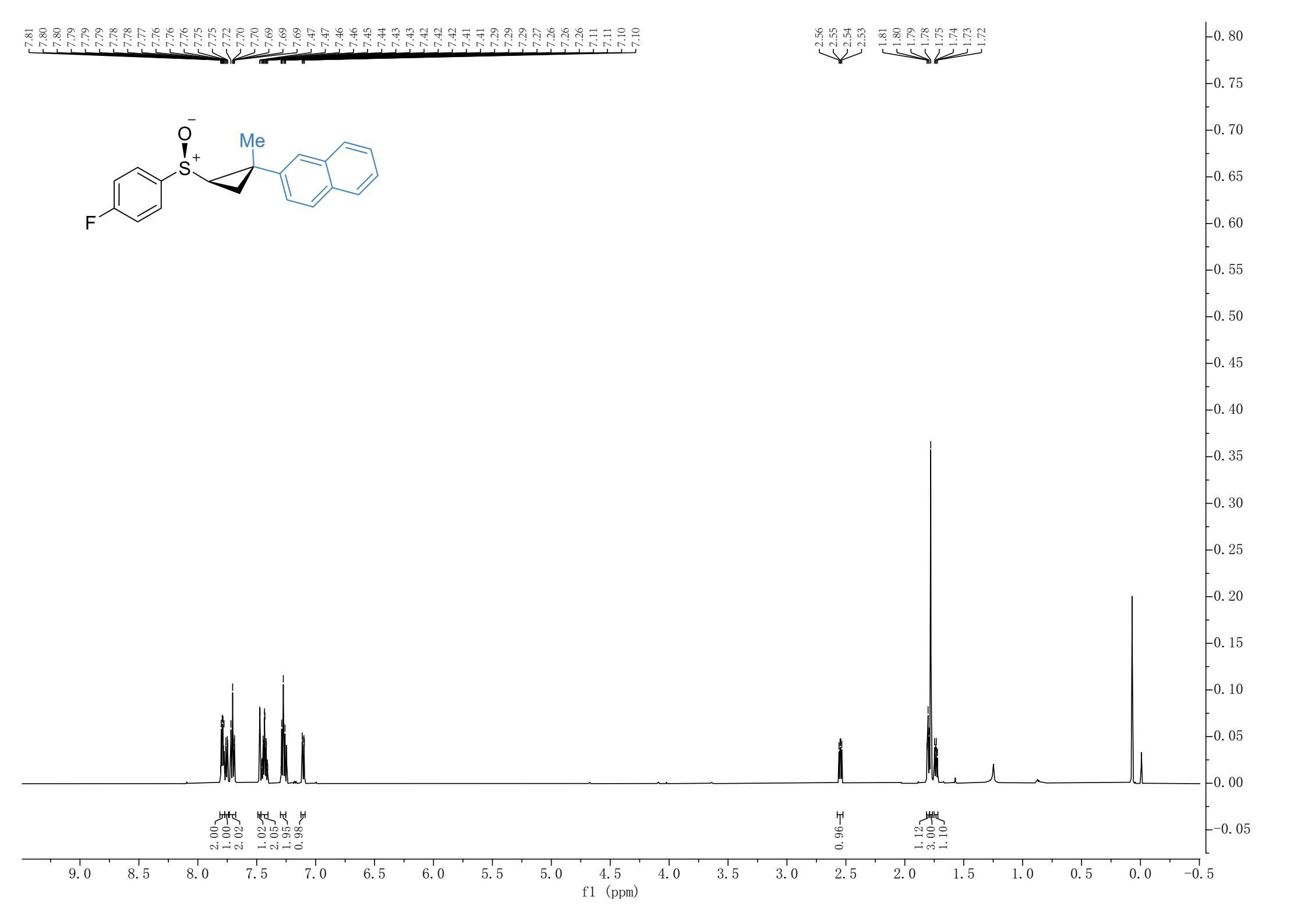
-108.24

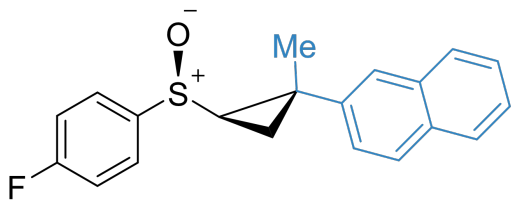
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)


165.36
163.36
147.72
146.42
141.22
141.20
138.08
126.35
126.27
120.12
116.90
116.72
108.27
107.72
101.10
48.98
29.45
22.91
18.50
O
S+
Me
O
O
F
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


7.81 7.80 7.80 7.79 7.79 7.79 7.78 7.78 7.77 7.76 7.76 7.76 7.75 7.75 7.72 7.70 7.70 7.69 7.69 7.69 7.47 7.47 7.46 7.46 7.45 7.44 7.43 7.43 7.42 7.42 7.42 7.41 7.41 7.29 7.29 7.27 7.26 7.26 7.26 7.11 7.11 7.10 7.10
2.56 2.55 2.54 2.53
1.81 1.80 1.79 1.78 1.75 1.74 1.73 1.72
O
S
Me
F
2.00 1.00 2.02 1.02 2.05 1.95 0.98 0.96 1.12 3.00 1.10
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
f1 (ppm)
0.80 0.75 0.70 0.65 0.60 0.55 0.50 0.45 0.40 0.35 0.30 0.25 0.20 0.15 0.10 0.05 0.00 -0.05

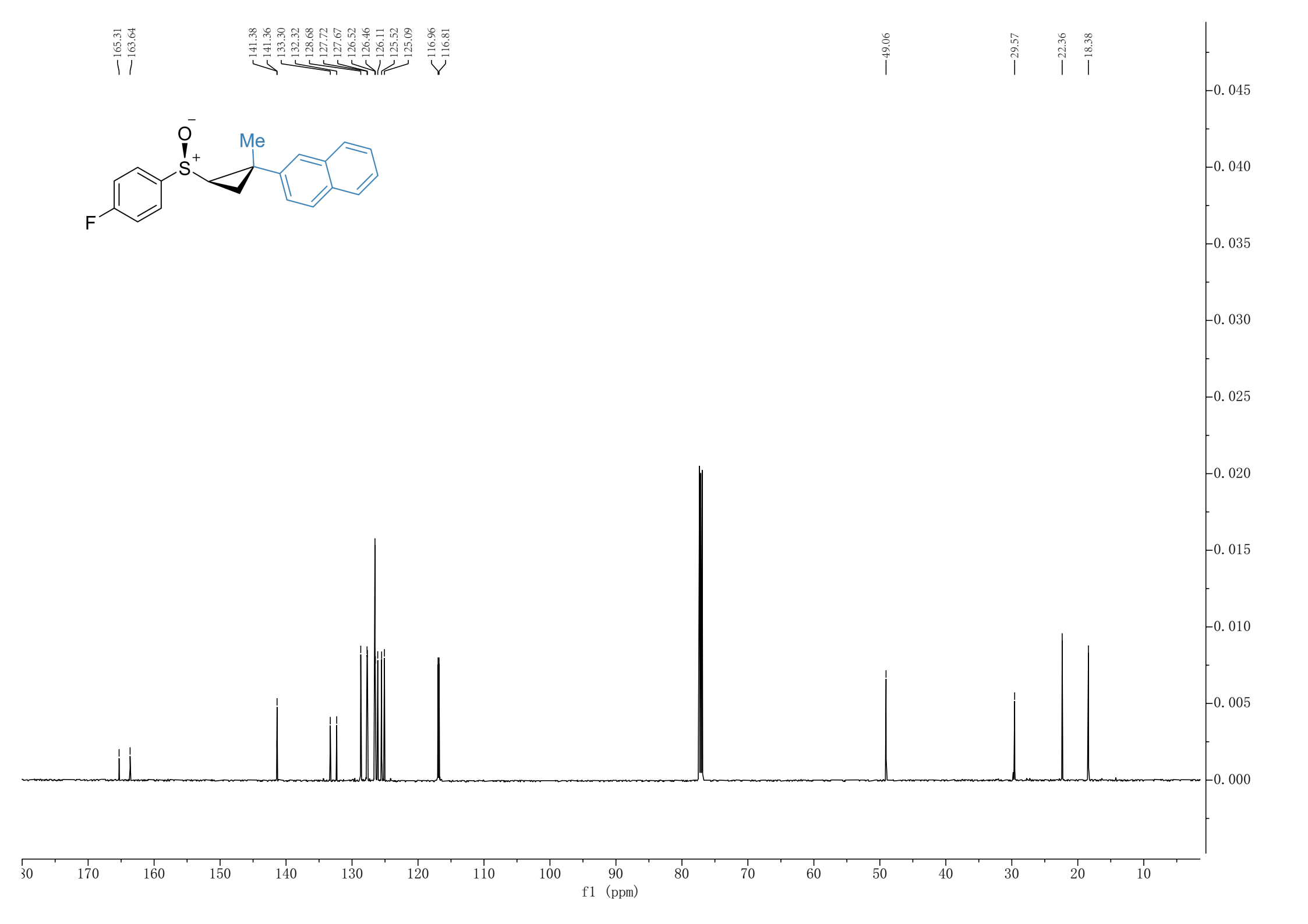


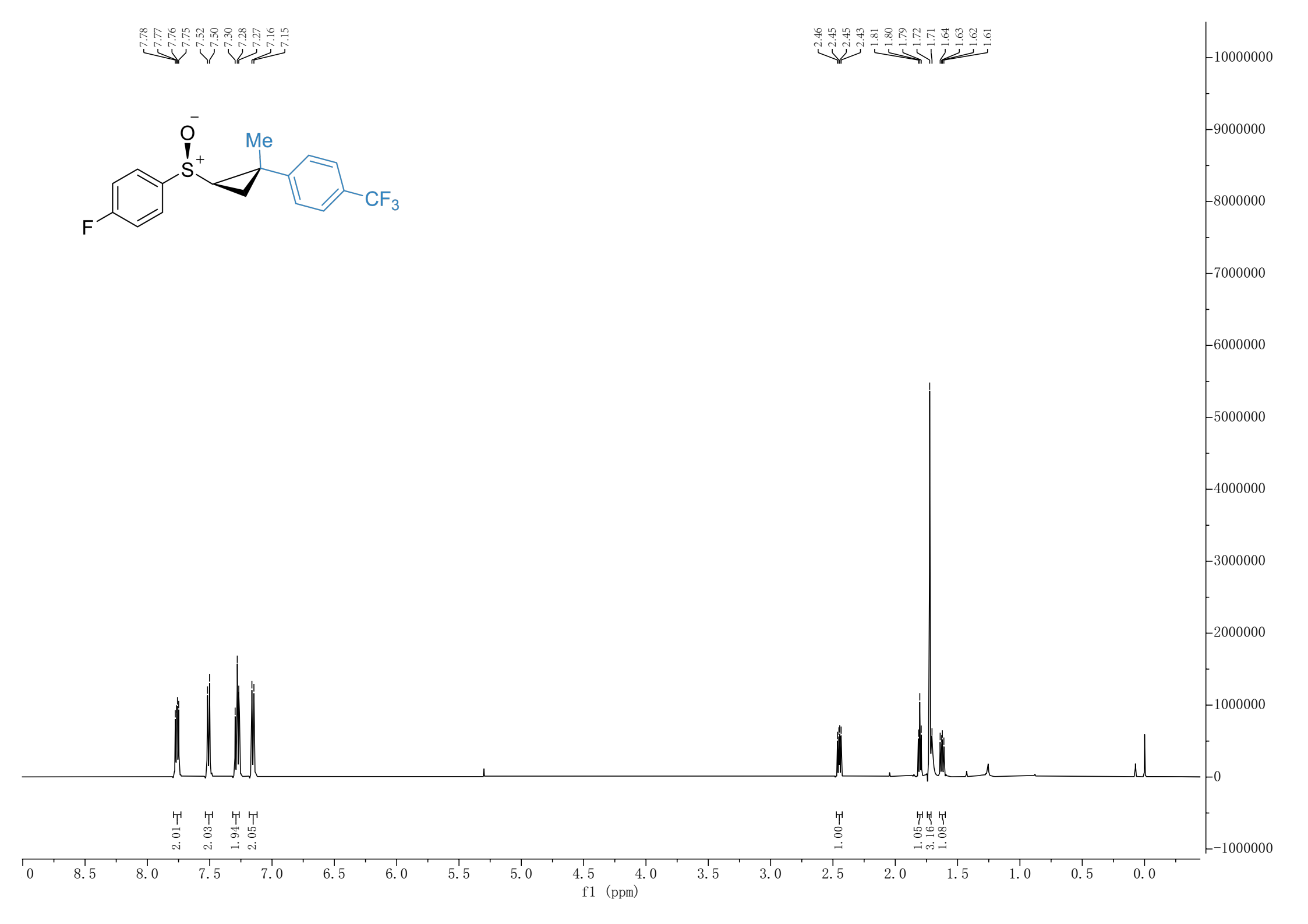
-108.14

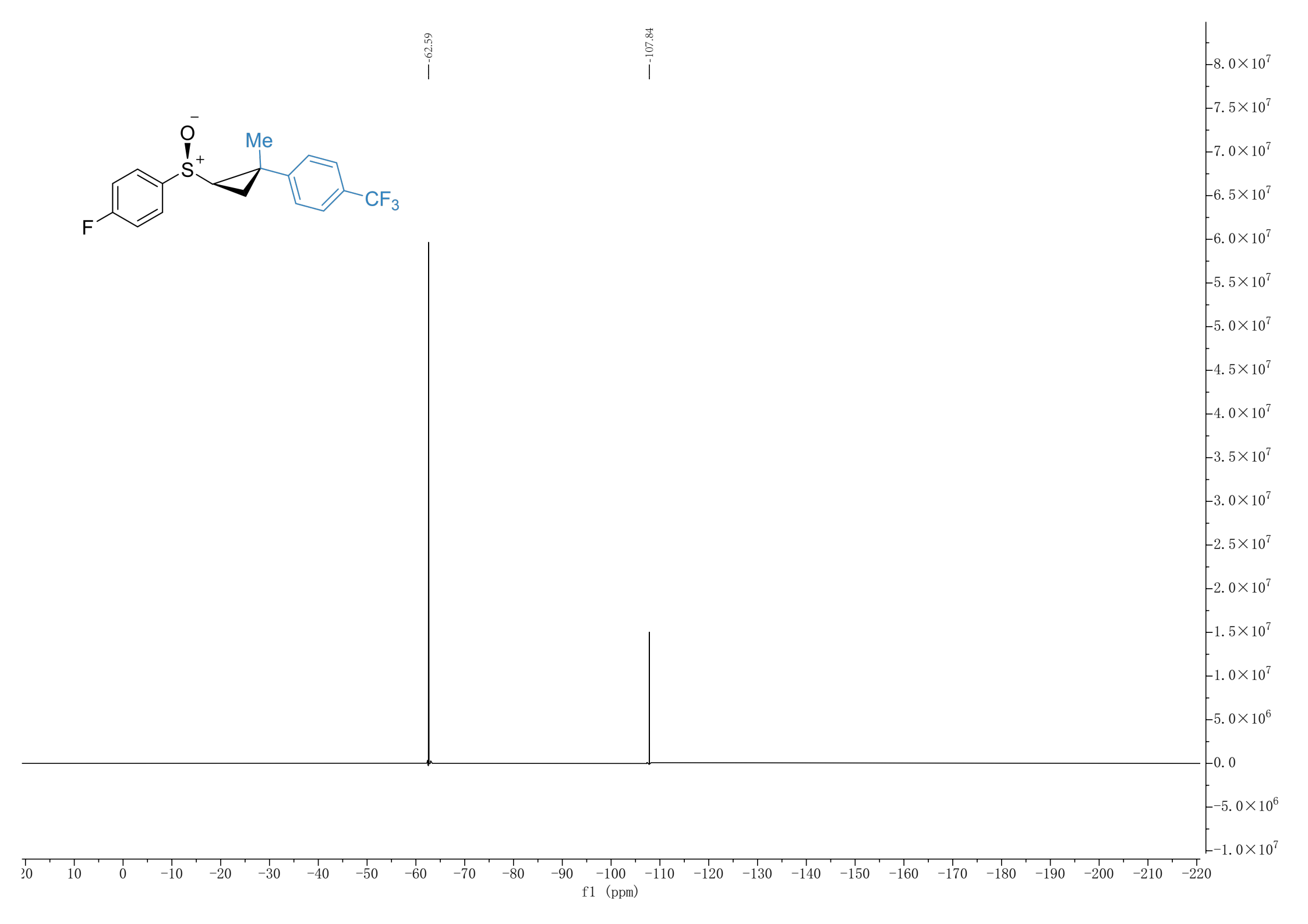
28 26 24 22 20 18 16 14 12 10 8 6 4 2 0 -2

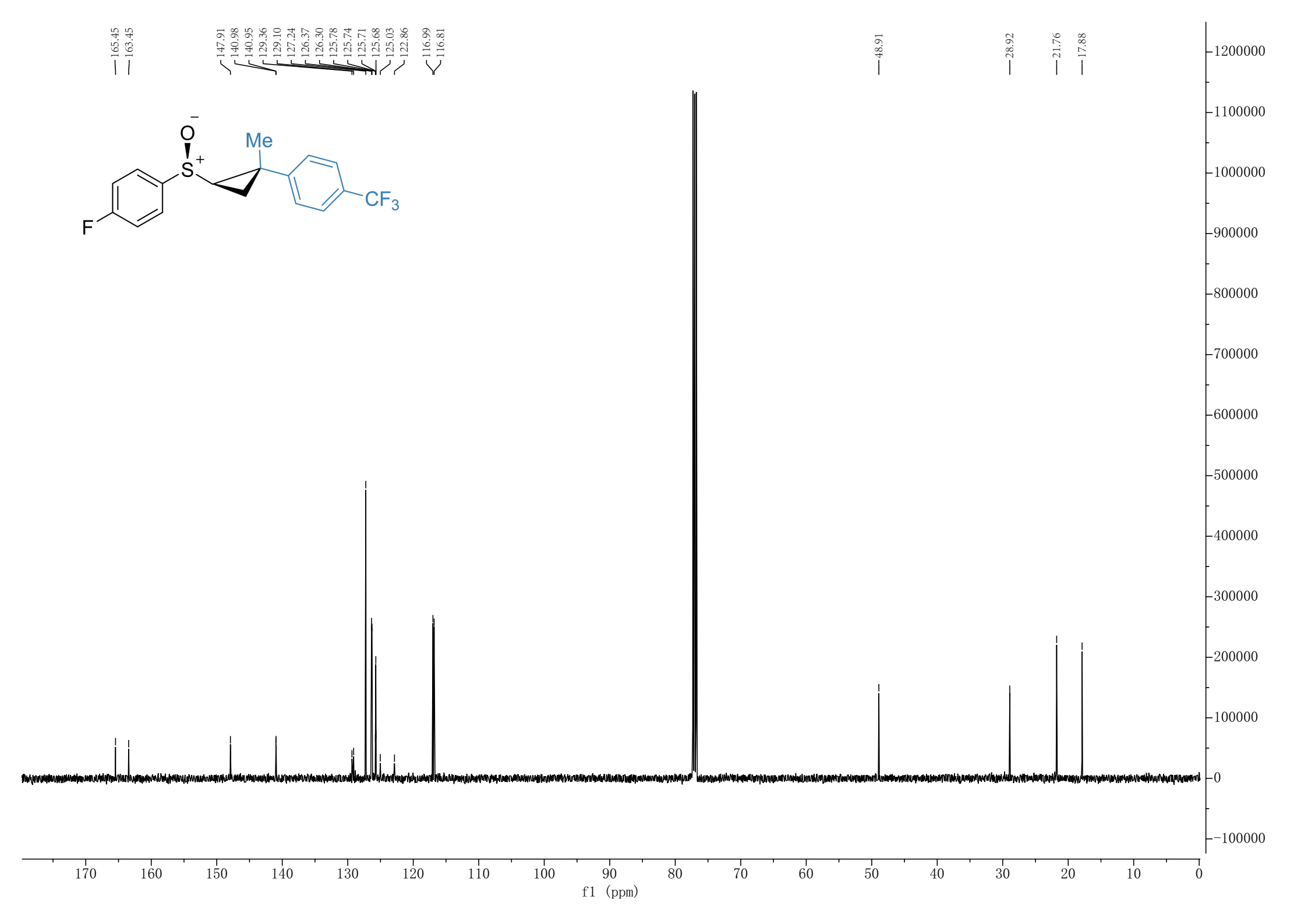
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

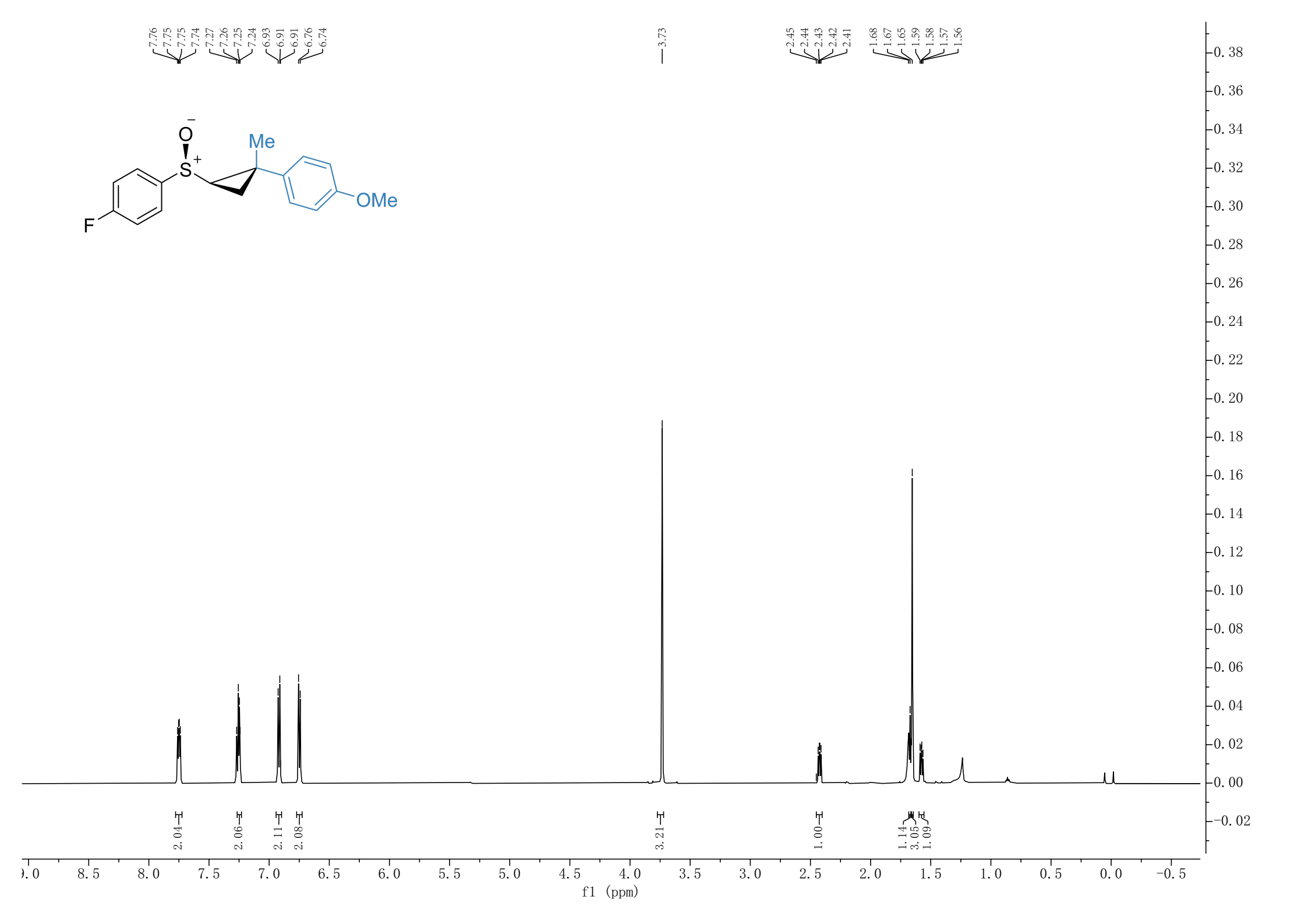
f1 (ppm)

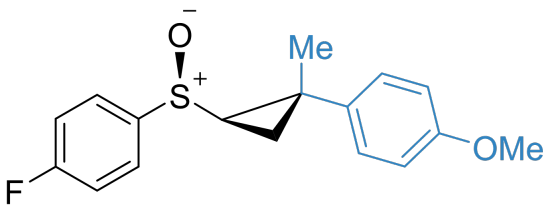

165.31
163.64
141.38
141.36
133.30
132.32
128.68
127.72
127.67
126.52
126.46
126.11
125.52
125.09
116.96
116.81
49.06
29.57
22.36
18.38
O
S
+
Me
F
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.78
7.77
7.76
7.75
7.52
7.50
7.30
7.28
7.27
7.16
7.15
2.46
2.45
2.45
2.43
1.81
1.80
1.79
1.72
1.71
1.64
1.63
1.62
1.61
O
S+
Me
CF3
F
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
2.01
2.03
1.94
2.05
1.00
1.05
3.16
1.08
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)


-62.59
-107.84
O
S+
Me
F
CF3
8.0×10^7
7.5×10^7
7.0×10^7
6.5×10^7
6.0×10^7
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
-1.0×10^7
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)


165.45
163.45
147.91
140.98
140.95
129.36
129.10
127.24
126.37
126.30
125.78
125.74
125.71
125.68
125.03
122.86
116.99
116.81
48.91
28.92
21.76
17.88
O
S+
Me
CF3
F
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.76
7.75
7.75
7.74
7.27
7.26
7.25
7.24
6.93
6.91
6.91
6.76
6.74
3.73
2.45
2.44
2.43
2.42
2.41
1.68
1.67
1.65
1.59
1.58
1.57
1.56
O
S
Me
OMe
F
2.04
2.06
2.11
2.08
3.21
1.00
1.14
3.05
1.09
f1 (ppm)

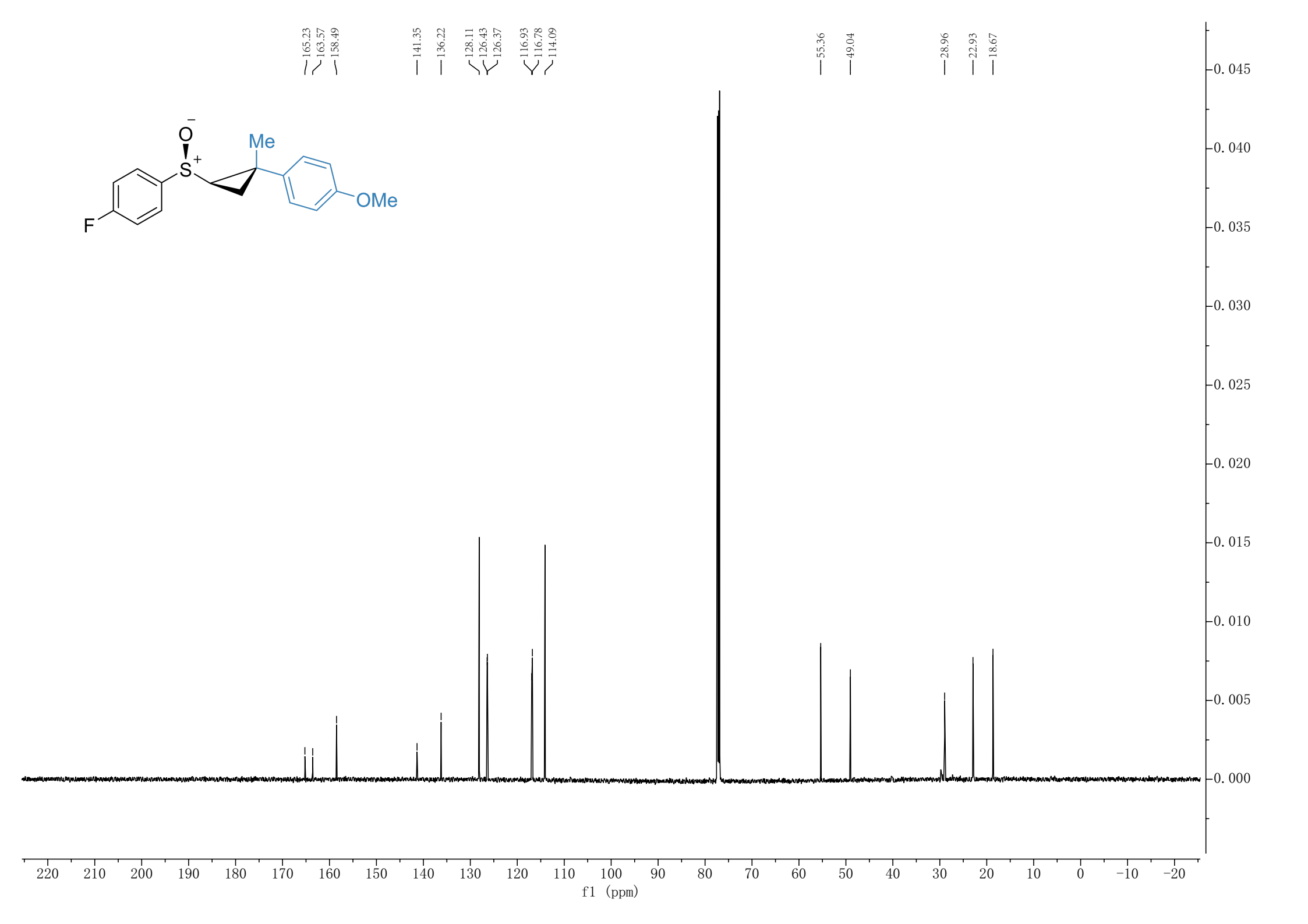


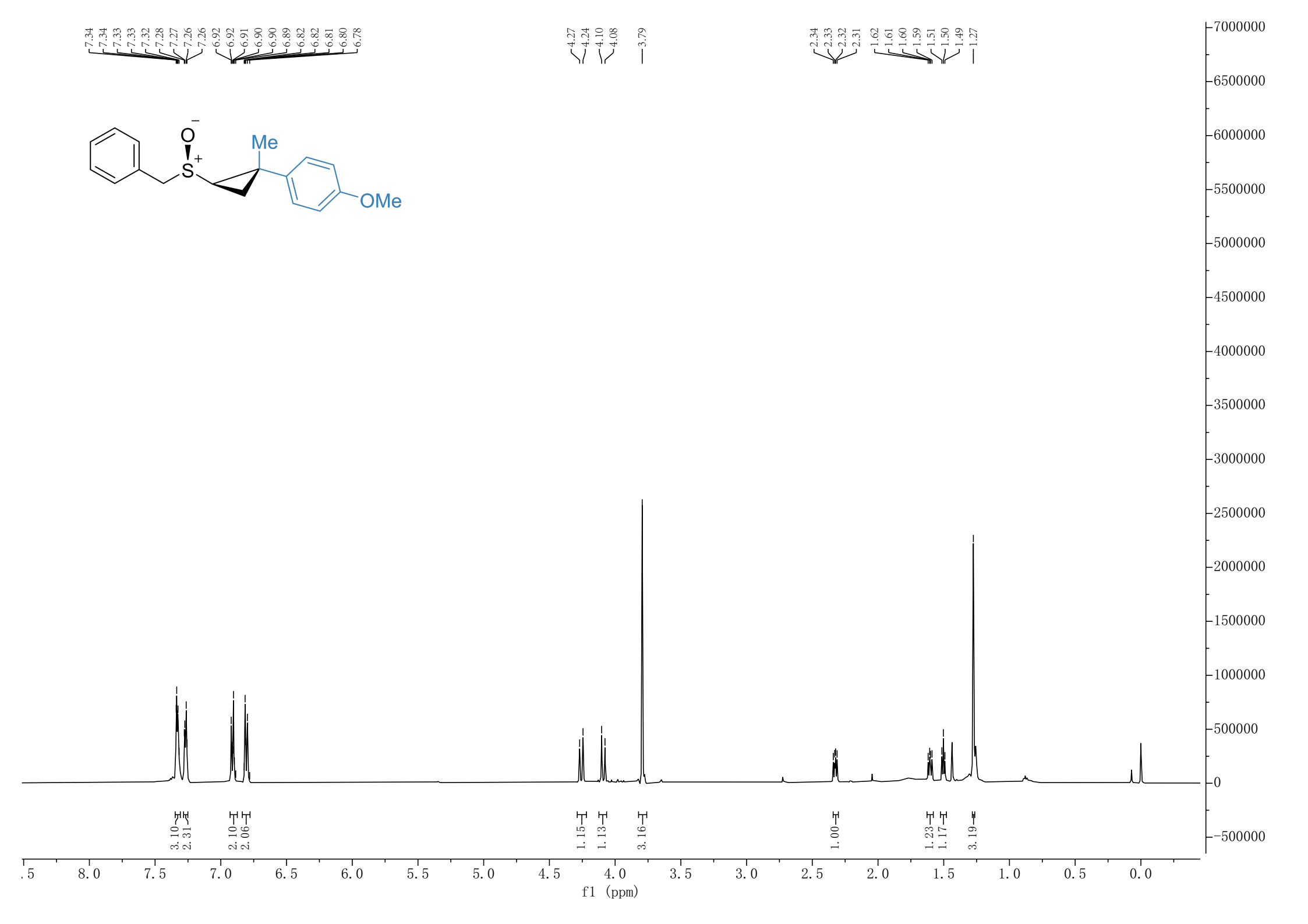
-108.28

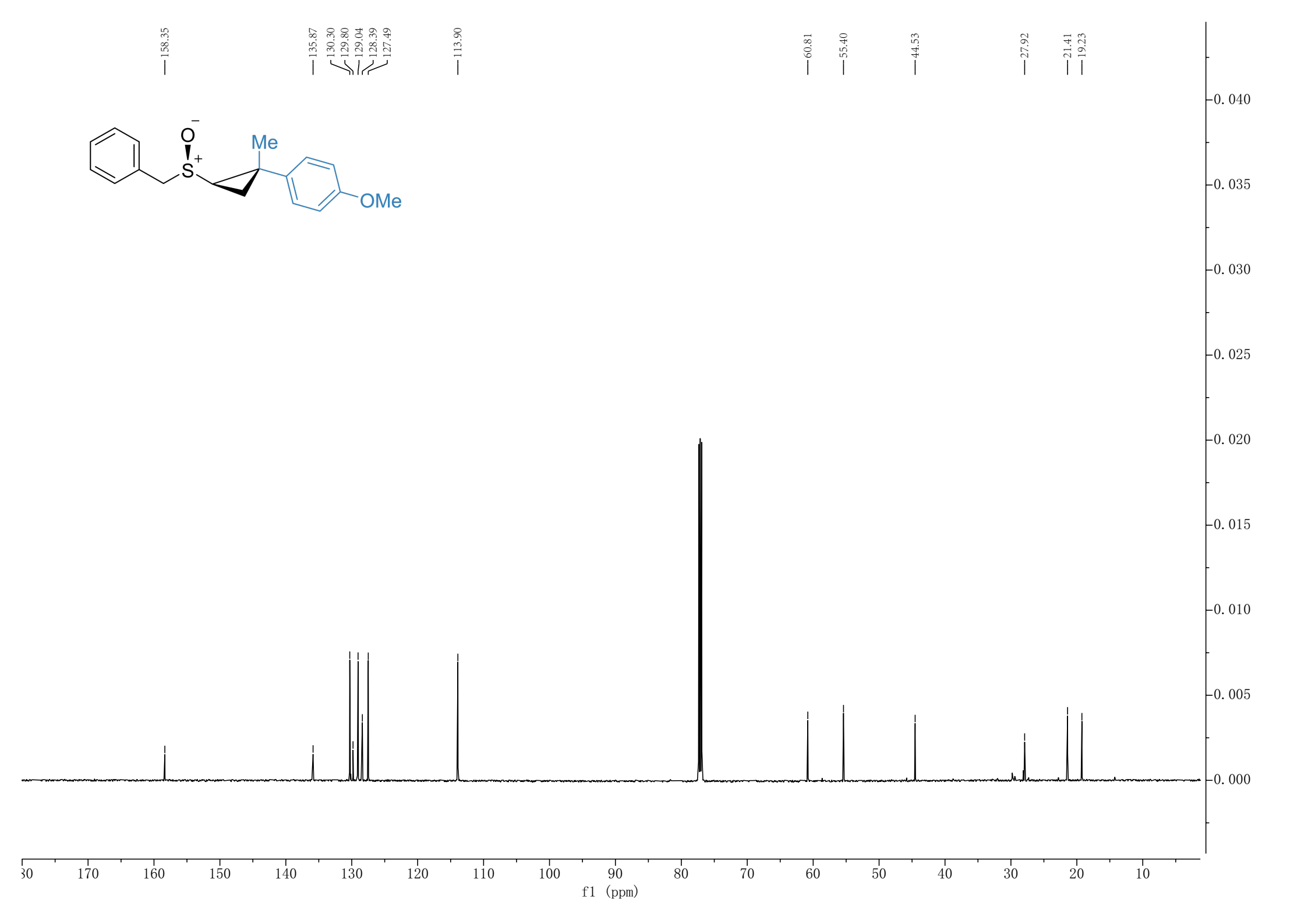
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1

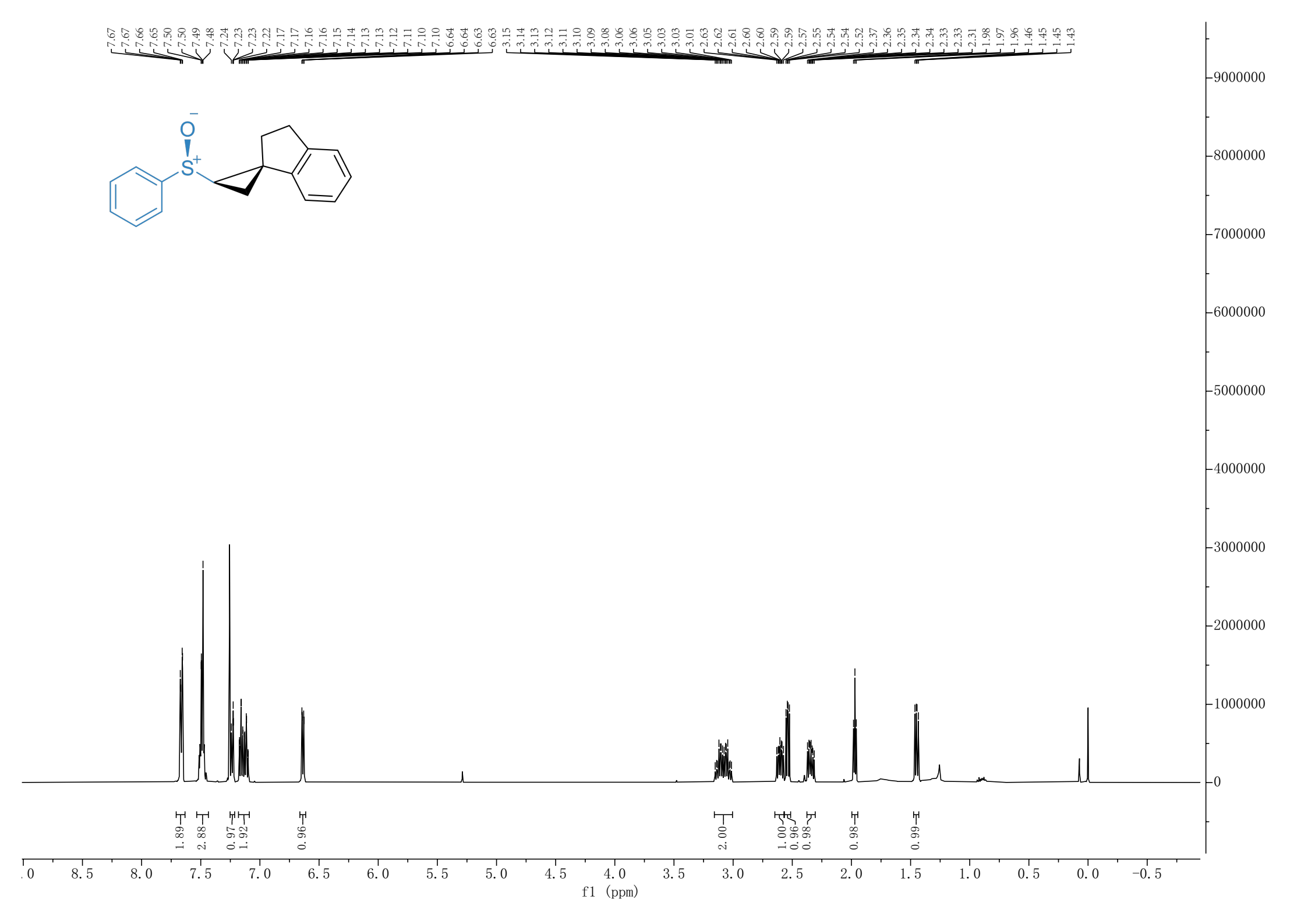
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

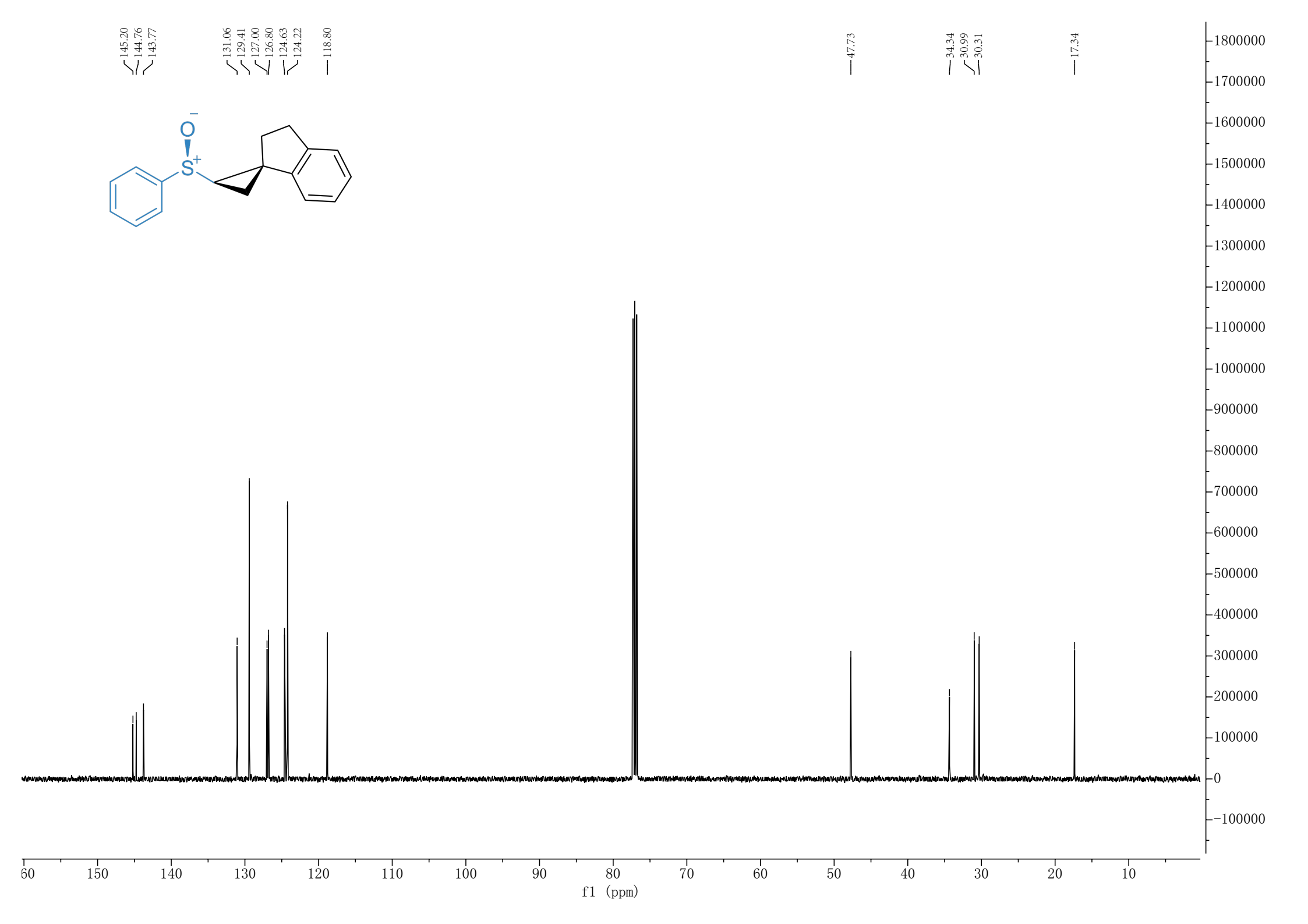
f1 (ppm)

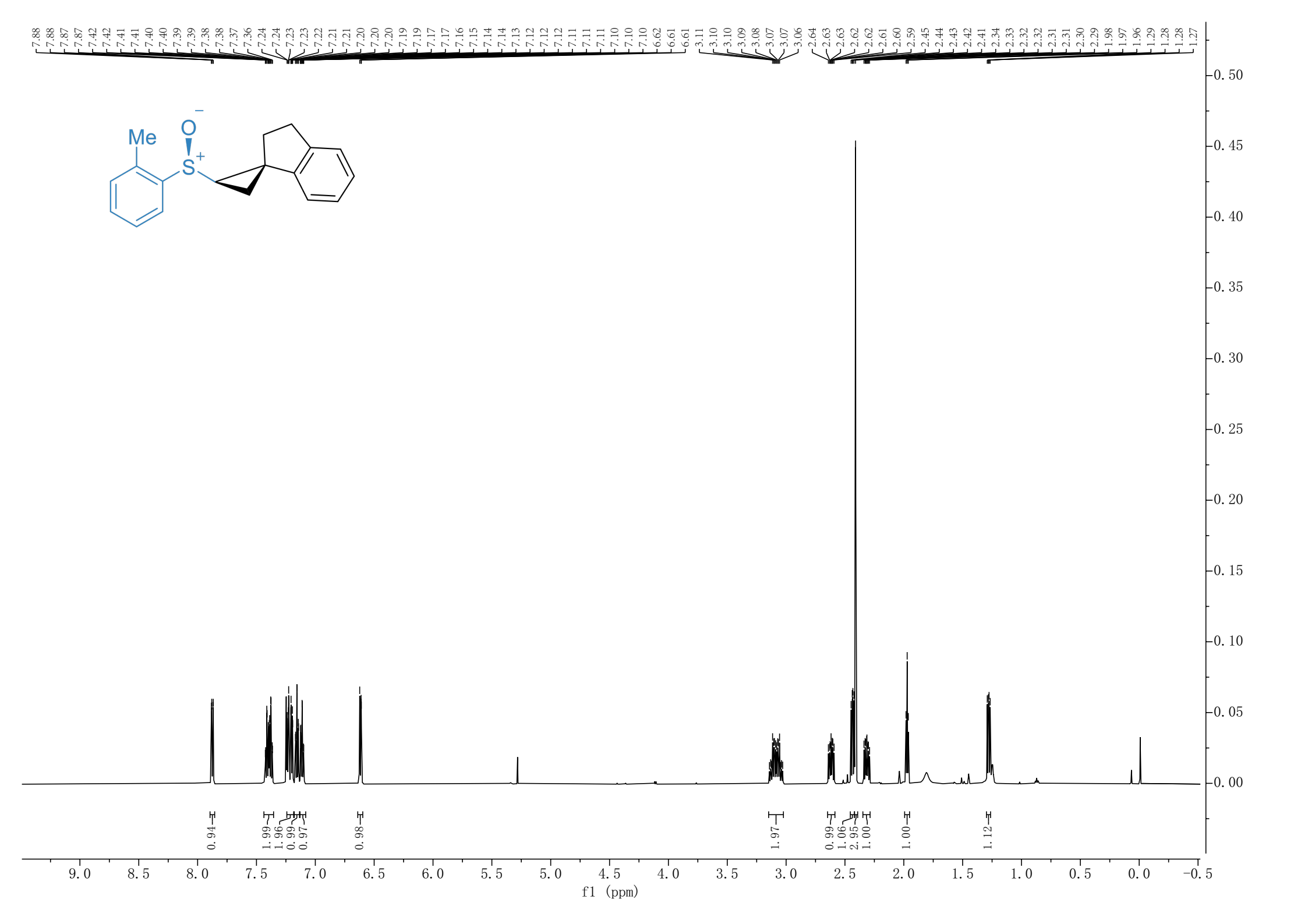

165.23
163.57
158.49
141.35
136.22
128.11
126.43
126.37
116.93
116.78
114.09
55.36
49.04
28.96
22.93
18.67
O
S+
Me
OMe
F
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

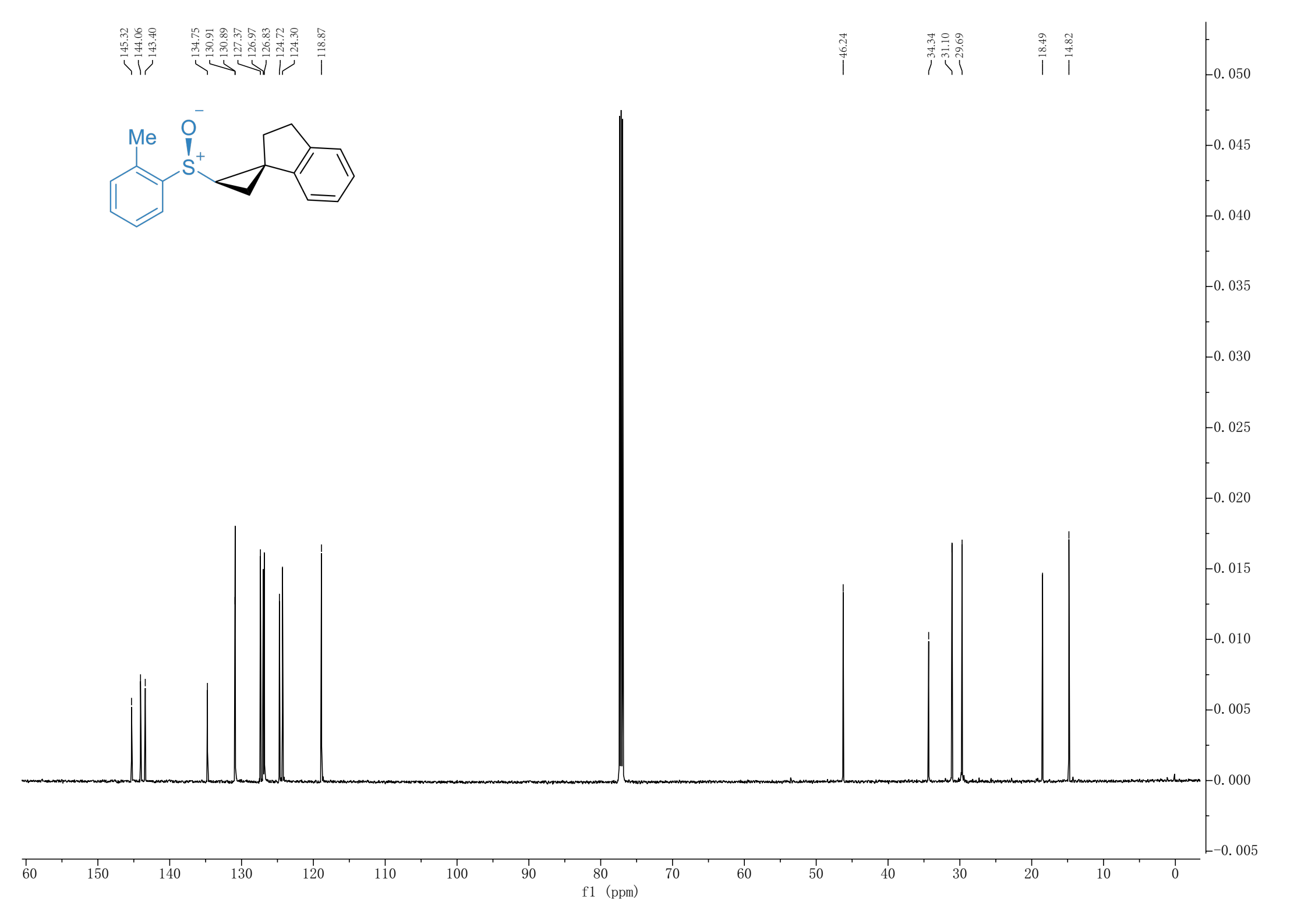

7.34
7.34
7.33
7.33
7.32
7.28
7.27
7.26
7.26
6.92
6.92
6.91
6.90
6.90
6.89
6.82
6.82
6.81
6.80
6.78
4.27
4.24
4.10
4.08
3.79
2.34
2.33
2.32
2.31
1.62
1.61
1.60
1.59
1.51
1.50
1.49
1.27
O
S+
Me
OMe
3.10
2.31
2.10
2.06
1.15
1.13
3.16
1.00
1.23
1.17
3.19
f1 (ppm)

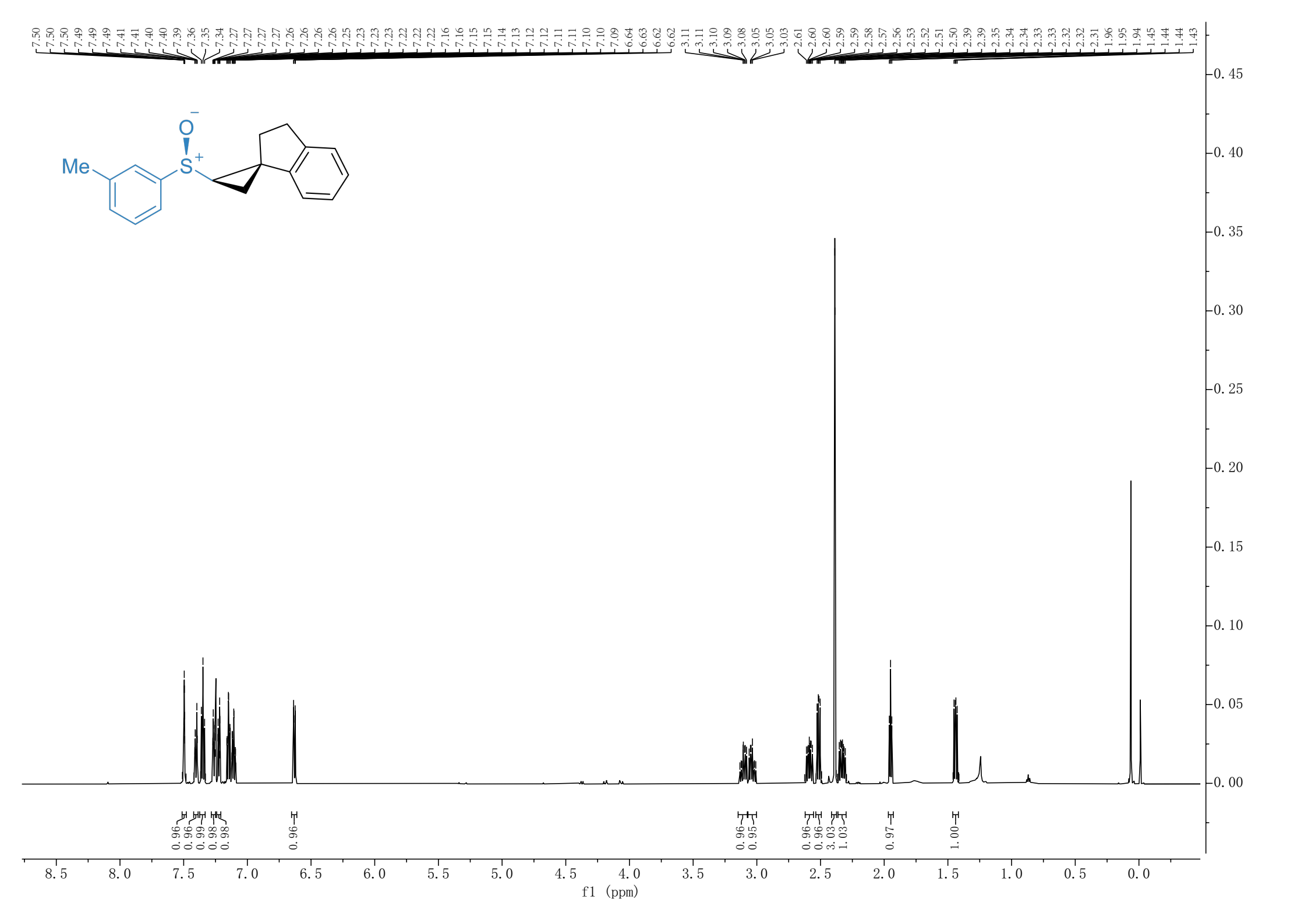

158.35
135.87
130.30
129.80
129.04
128.39
127.49
113.90
60.81
55.40
44.53
27.92
21.41
19.23
O
S+
Me
OMe
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

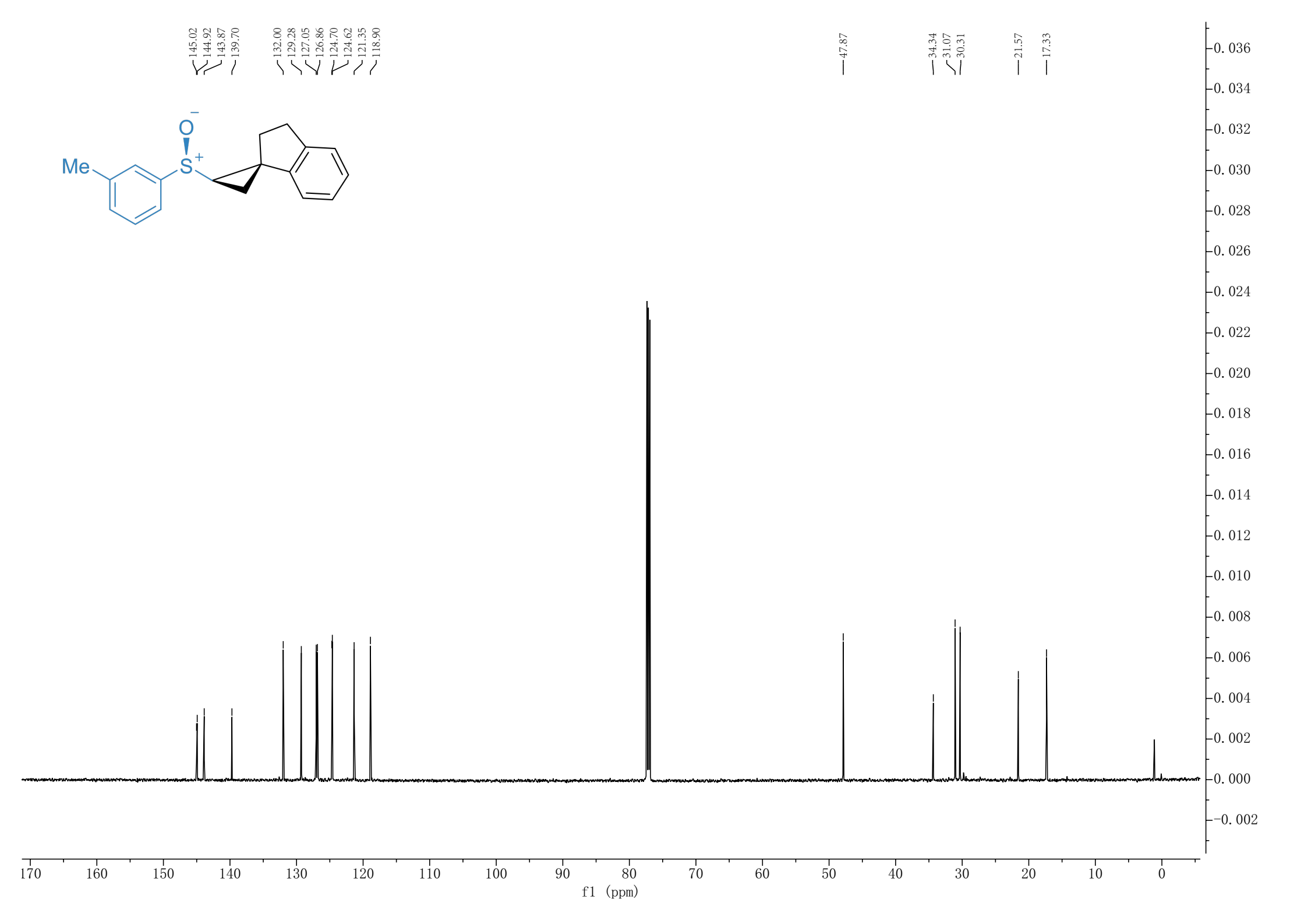

7.67 7.67 7.66 7.65 7.50 7.50 7.49 7.48 7.24 7.23 7.23 7.22 7.17 7.17 7.16 7.16 7.15 7.14 7.13 7.13 7.12 7.11 7.10 7.10 6.64 6.64 6.63 6.63
3.15 3.14 3.13 3.12 3.11 3.10 3.09 3.08 3.06 3.06 3.05 3.03 3.03 3.01 2.63 2.62 2.61 2.60 2.60 2.59 2.59 2.57 2.55 2.54 2.54 2.52 2.37 2.36 2.35 2.34 2.34 2.33 2.33 2.31 1.98 1.97 1.96 1.46 1.45 1.45 1.43
O
S+
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
1.89 2.88 0.97 1.92 0.96 2.00 1.00 0.96 0.98 0.98 0.99
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
f1 (ppm)

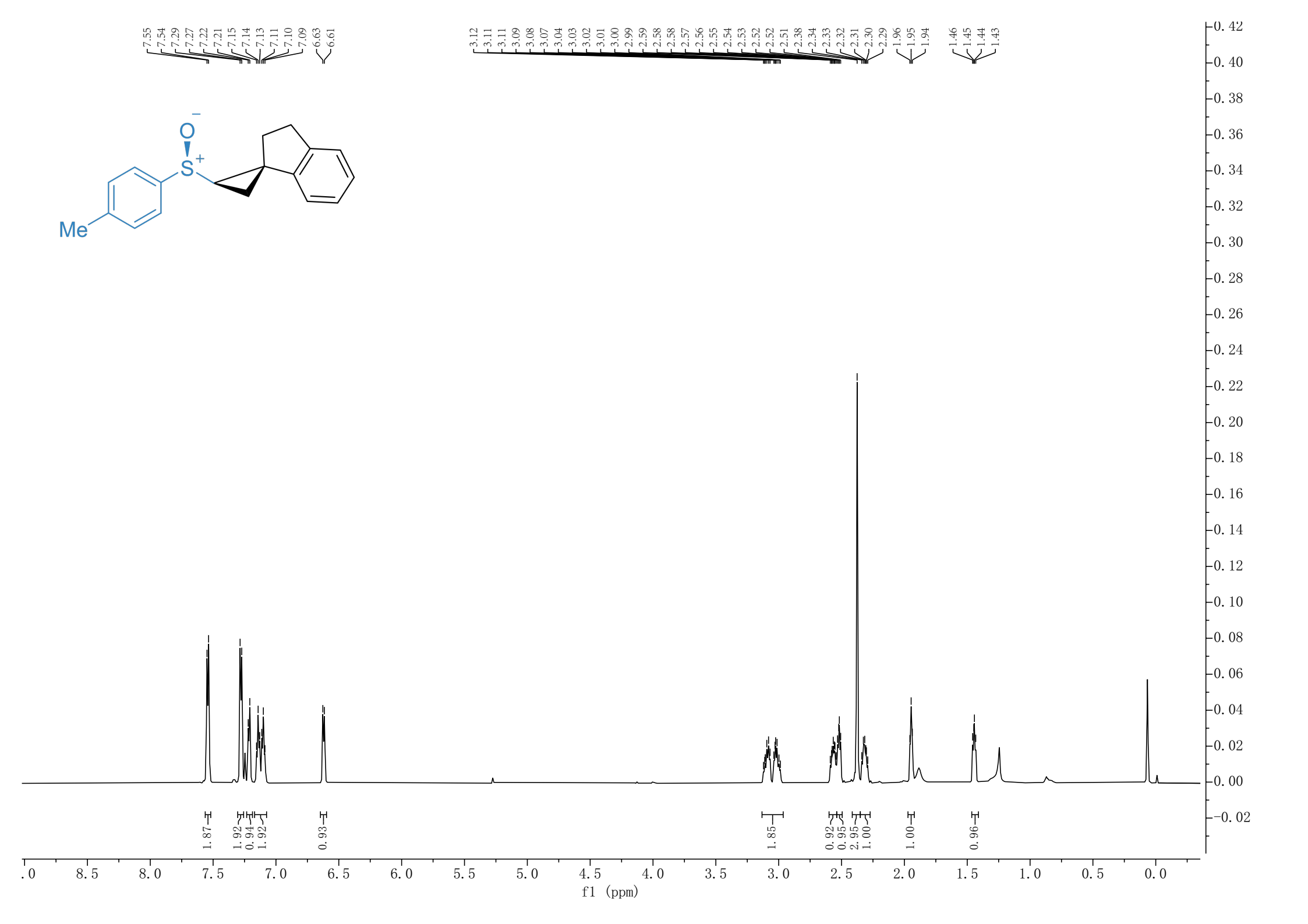

145.20
144.76
143.77
131.06
129.41
127.00
126.80
124.63
124.22
118.80
47.73
34.34
30.99
30.31
17.34
O
S+
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

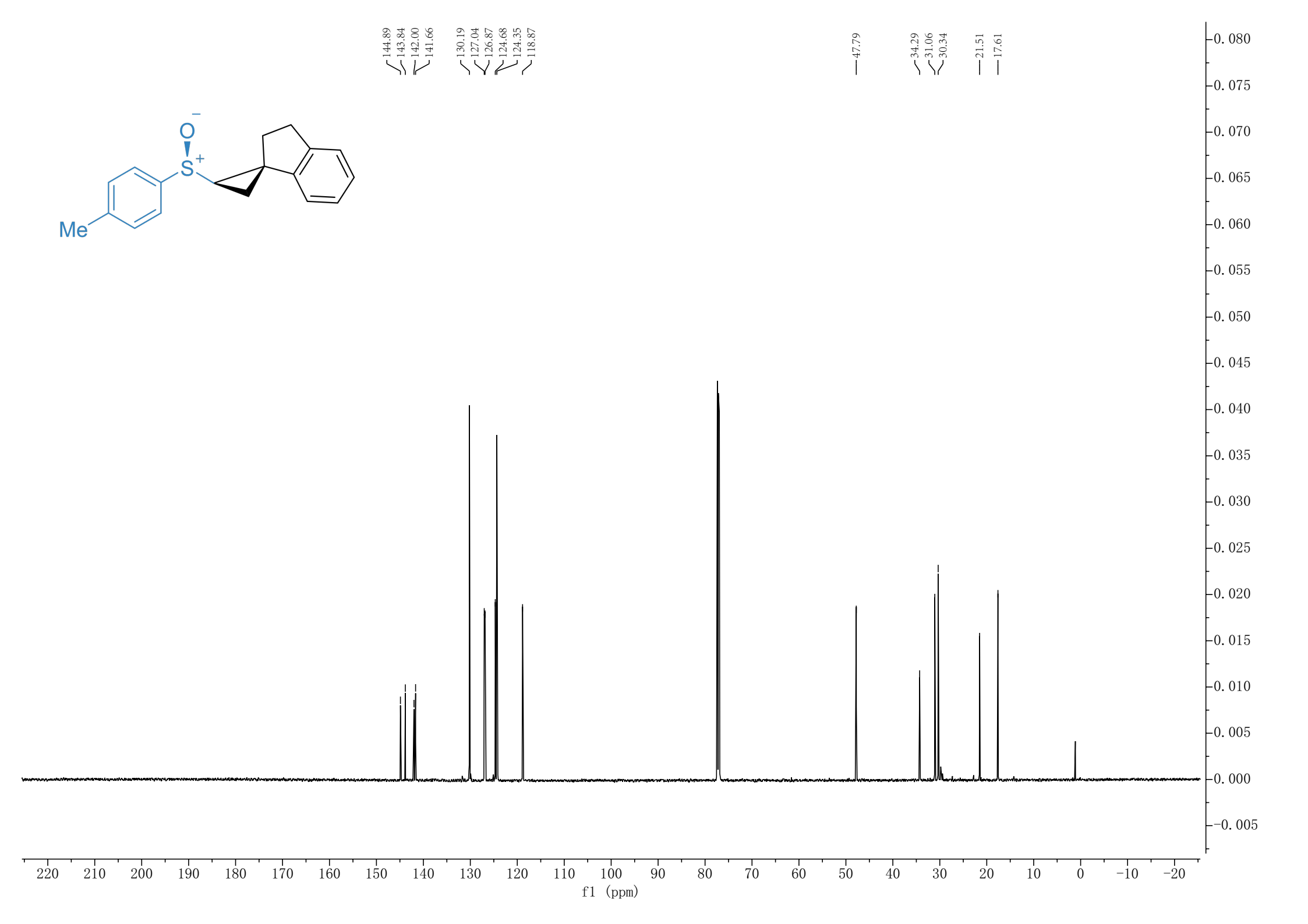

Me
O
S+
f1 (ppm)

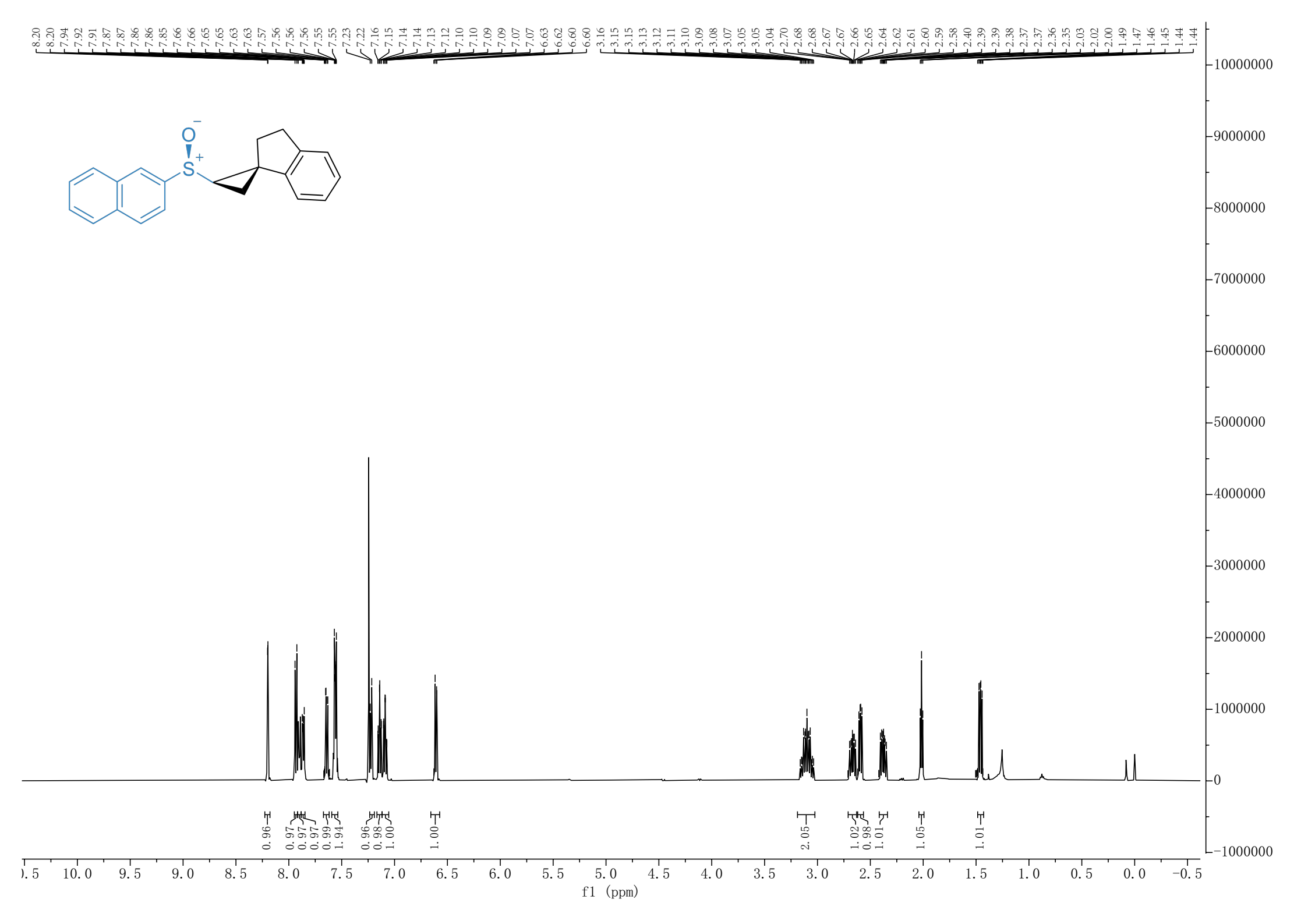

145.32
144.06
143.40
134.75
130.91
130.89
127.37
126.97
126.83
124.72
124.30
118.87
46.24
34.34
31.10
29.69
18.49
14.82
Me
O
S+
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

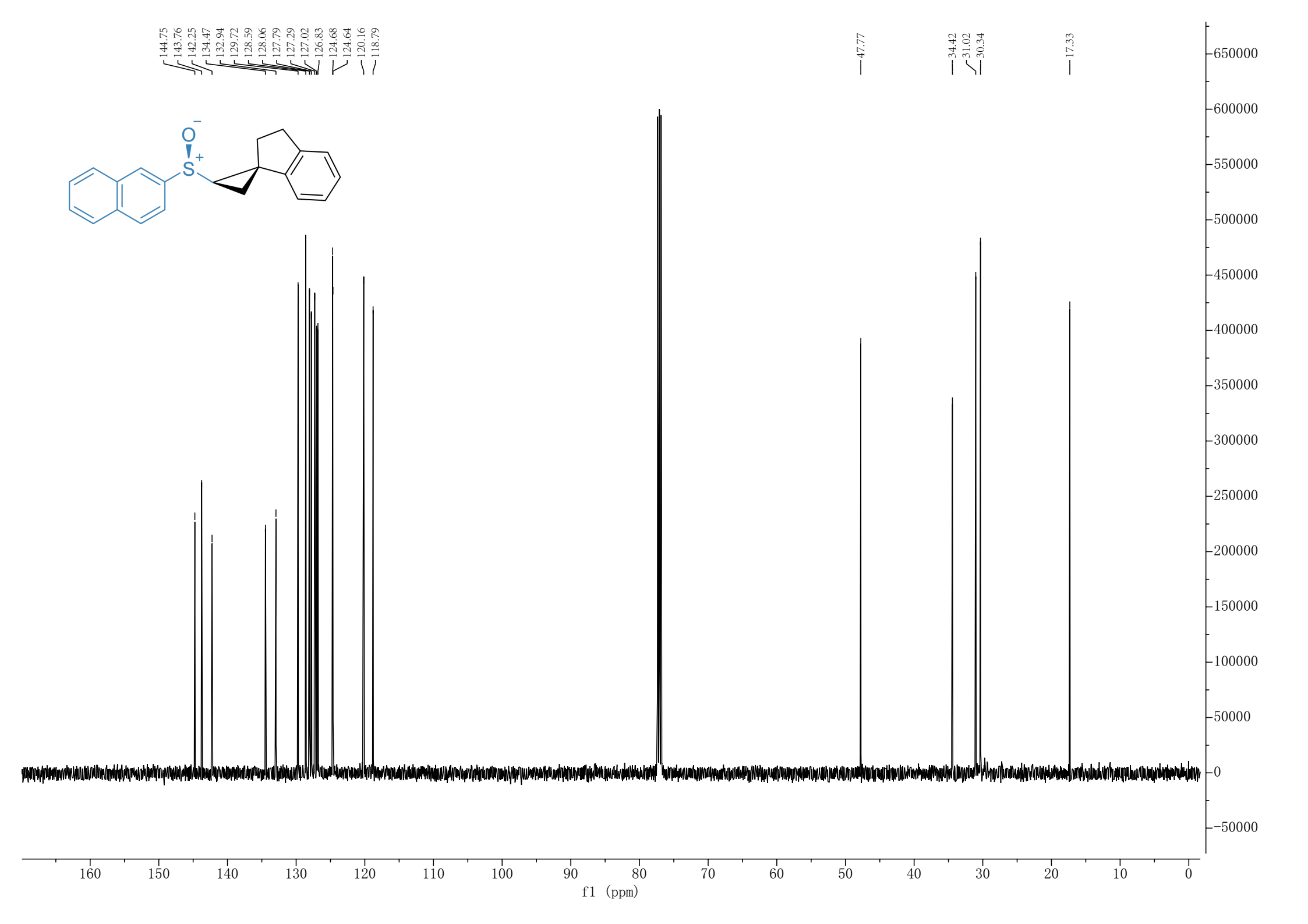

Me
O
S
f1 (ppm)

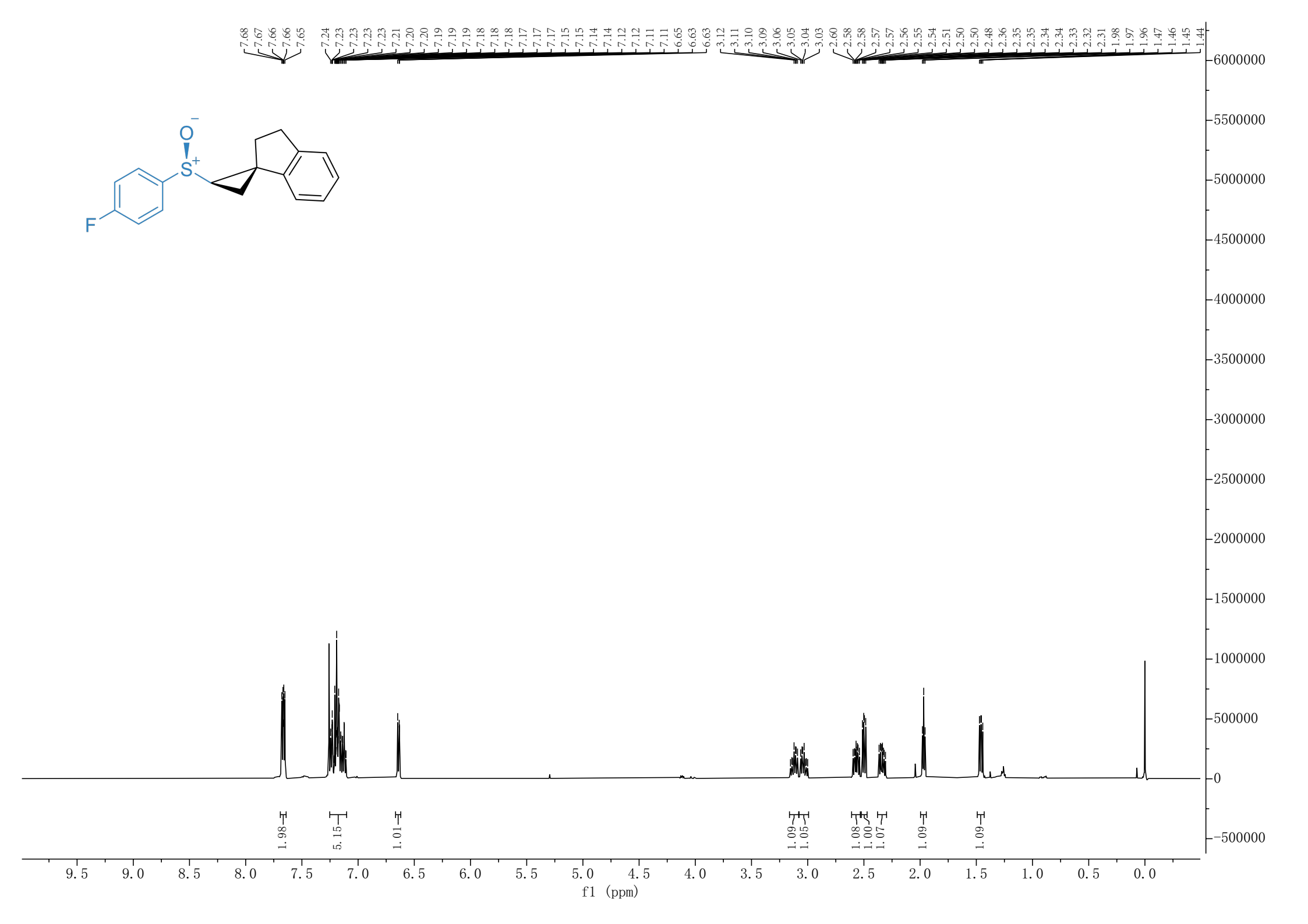

145.02
144.92
143.87
139.70
132.00
129.28
127.05
126.86
124.70
124.62
121.35
118.90
47.87
34.34
31.07
30.31
21.57
17.33
Me
O
S
f1 (ppm)

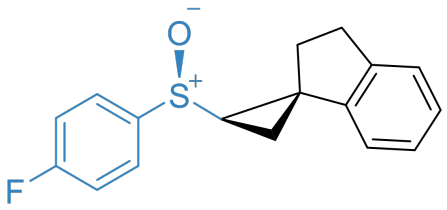

7.55
7.54
7.29
7.27
7.22
7.21
7.15
7.14
7.13
7.11
7.10
7.09
6.63
6.61
3.12
3.11
3.11
3.09
3.08
3.07
3.04
3.03
3.02
3.01
3.00
2.99
2.59
2.58
2.58
2.57
2.56
2.55
2.54
2.53
2.52
2.52
2.51
2.38
2.34
2.33
2.32
2.31
2.30
2.29
1.96
1.95
1.94
1.46
1.45
1.44
1.43
O
S+
Me
1.87
1.92
0.94
1.92
0.93
1.85
0.92
0.95
2.95
1.00
1.00
0.96
f1 (ppm)


144.89
143.84
142.00
141.66
130.19
127.04
126.87
124.68
124.35
118.87
47.79
34.29
31.06
30.34
21.51
17.61
O
S+
Me
f1 (ppm)


8.20 8.20 7.94 7.92 7.91 7.87 7.87 7.86 7.86 7.85 7.66 7.66 7.65 7.65 7.63 7.63 7.57 7.56 7.56 7.56 7.55 7.55 7.23 7.22 7.16 7.15 7.14 7.14 7.13 7.12 7.10 7.10 7.09 7.09 7.07 7.07 6.63 6.62 6.60 6.60 3.16 3.15 3.15 3.13 3.12 3.11 3.10 3.09 3.08 3.07 3.05 3.05 3.04 2.70 2.68 2.68 2.67 2.67 2.66 2.65 2.64 2.62 2.61 2.60 2.59 2.58 2.40 2.39 2.39 2.38 2.37 2.37 2.36 2.35 2.03 2.02 2.00 1.49 1.47 1.46 1.45 1.44 1.44
O
S+
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000
0.96
0.97
0.97
0.99
1.94
0.96
0.98
1.00
1.00
2.05
1.02
0.98
1.01
1.05
1.01
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
f1 (ppm)


144.75
143.76
142.25
134.47
132.94
129.72
128.59
128.06
127.79
127.29
127.02
126.83
124.68
124.64
120.16
118.79
47.77
34.42
31.02
30.34
17.33
O
S
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.68 7.67 7.66 7.66 7.65 7.24 7.23 7.23 7.23 7.23 7.21 7.20 7.20 7.19 7.19 7.19 7.18 7.18 7.18 7.17 7.17 7.17 7.15 7.15 7.14 7.14 7.12 7.12 7.11 7.11 6.65 6.63 6.63 3.12 3.11 3.10 3.09 3.06 3.05 3.04 3.03 2.60 2.58 2.58 2.57 2.57 2.56 2.55 2.54 2.51 2.50 2.50 2.48 2.36 2.35 2.34 2.34 2.33 2.32 2.31 1.98 1.97 1.96 1.47 1.46 1.45 1.44
O
S+
F
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
-500000
1.98
5.15
1.01
1.09
1.05
1.08
1.00
1.07
1.09
1.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


O
S+
F

-108.49
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22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
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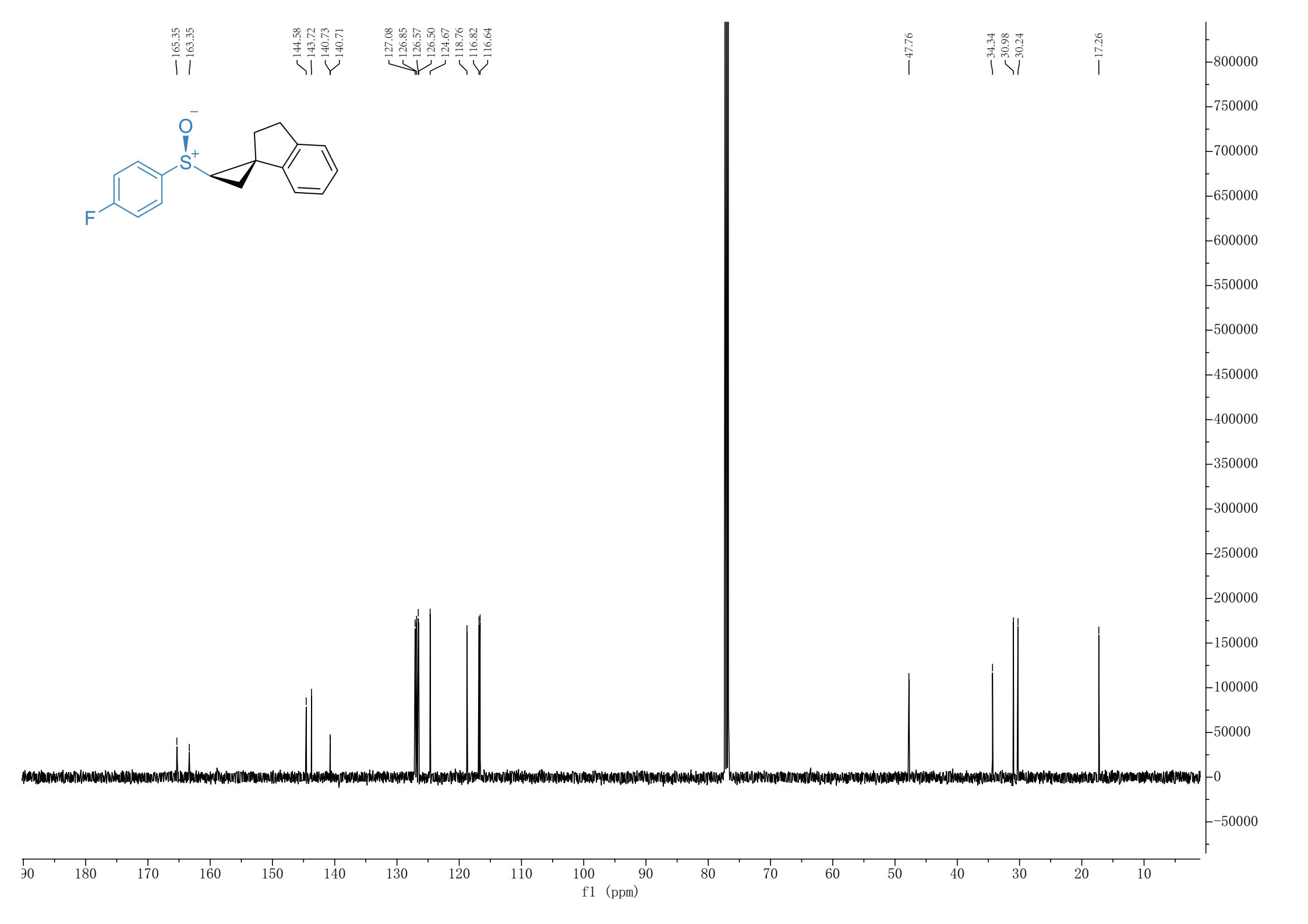
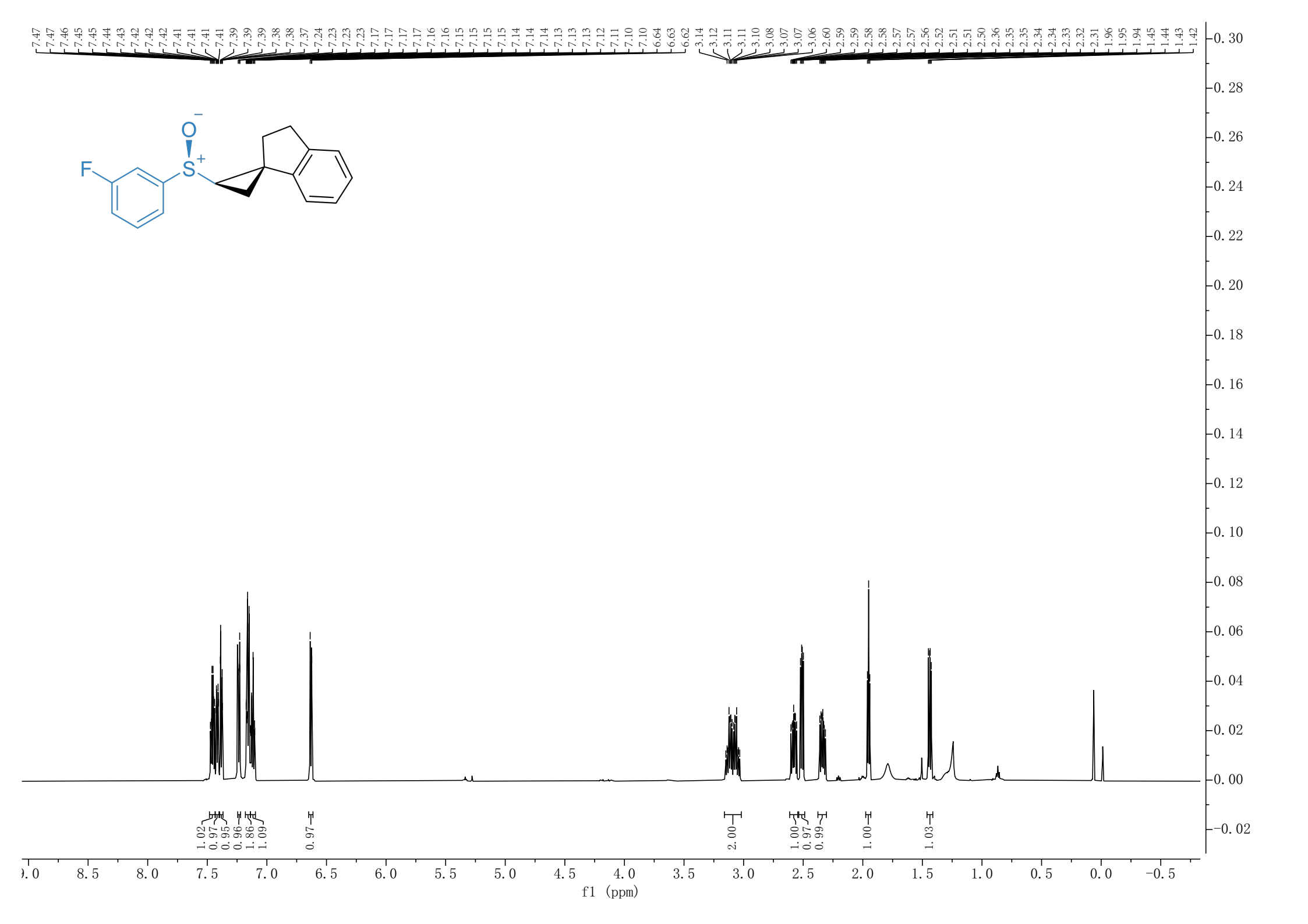
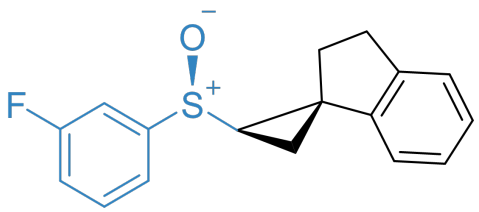
-180
-190
-200
-210
-220
f1 (ppm)


165.35
163.35
144.58
143.72
140.73
140.71
127.08
126.85
126.57
126.50
124.67
118.76
116.82
116.64
47.76
34.34
30.98
30.24
17.26
O
S+
F
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


F
S+
O−
f1 (ppm)

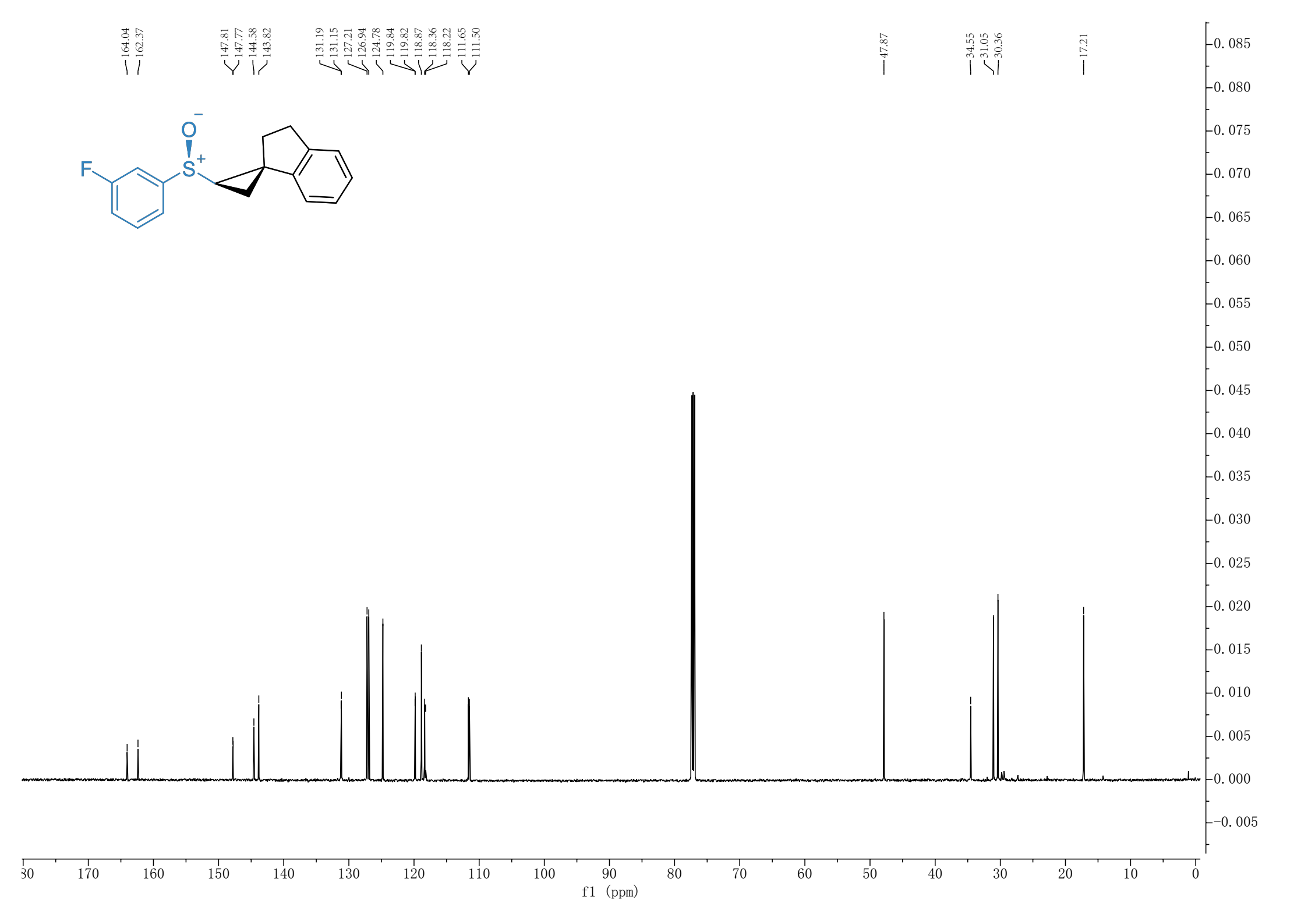


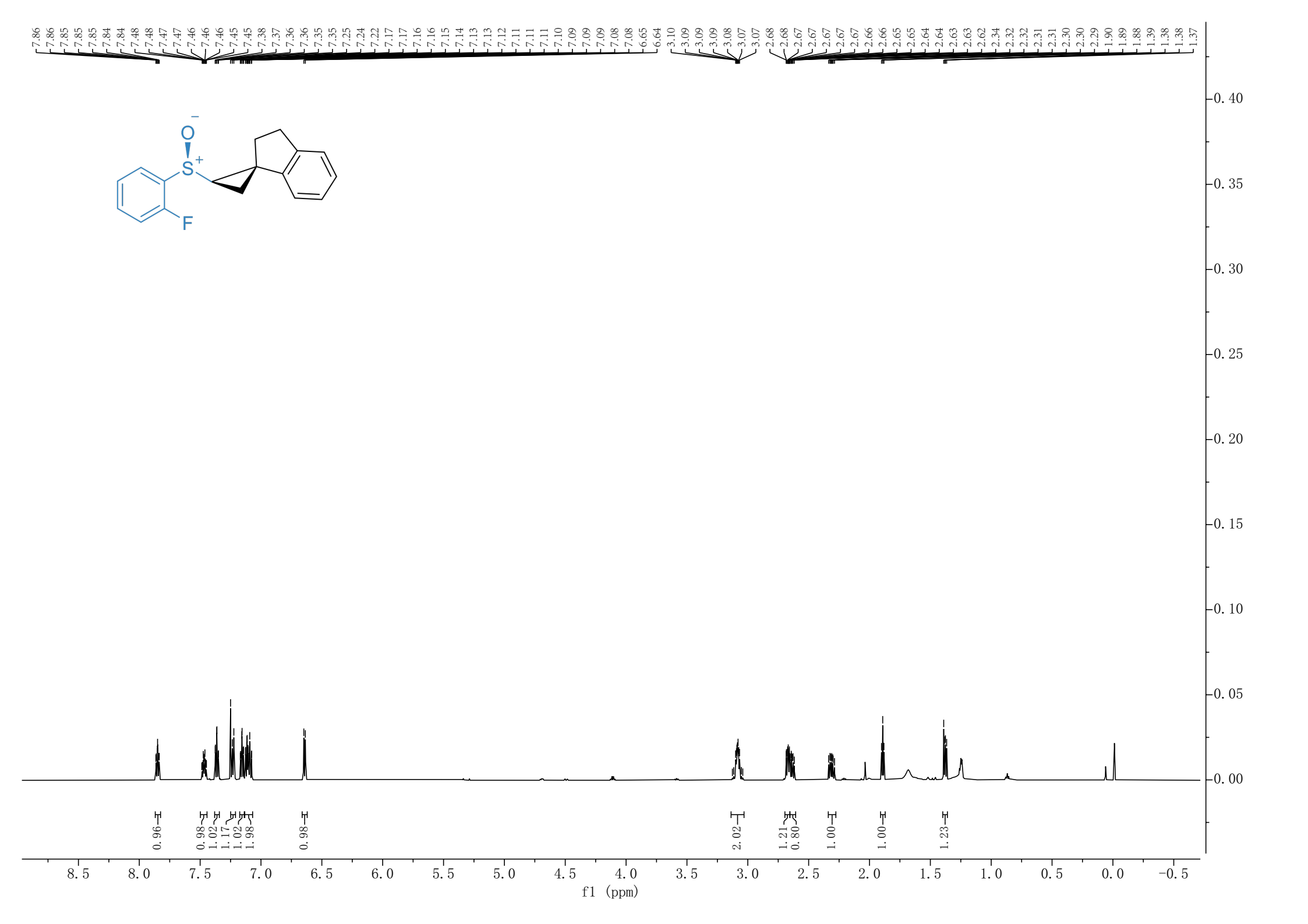
-109.30

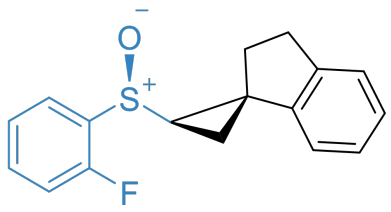
22 21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2

40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

f1 (ppm)


164.04
162.37
147.81
147.77
144.58
143.82
131.19
131.15
127.21
126.94
124.78
119.84
119.82
118.87
118.36
118.22
111.65
111.50
47.87
34.55
31.05
30.36
17.21
O
S+
F
0.085
0.080
0.075
0.070
0.065
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
−0.005
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.86 7.86 7.85 7.85 7.85 7.84 7.84 7.48 7.47 7.47 7.46 7.46 7.46 7.45 7.45 7.38 7.37 7.36 7.36 7.35 7.35 7.25 7.24 7.22 7.17 7.17 7.16 7.16 7.15 7.14 7.13 7.13 7.12 7.11 7.11 7.11 7.10 7.09 7.09 7.09 7.08 7.08 6.65 6.64
3.10 3.09 3.09 3.09 3.08 3.07 3.07
2.68 2.68 2.67 2.67 2.67 2.67 2.67 2.66 2.66 2.65 2.65 2.64 2.64 2.63 2.63 2.62 2.34 2.32 2.32 2.31 2.31 2.30 2.30 2.29 1.90 1.89 1.88 1.39 1.38 1.38 1.37
O
S+
F
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.96
0.98
1.02
1.17
1.02
1.98
0.98
2.02
1.21
0.80
1.00
1.00
1.23
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
f1 (ppm)

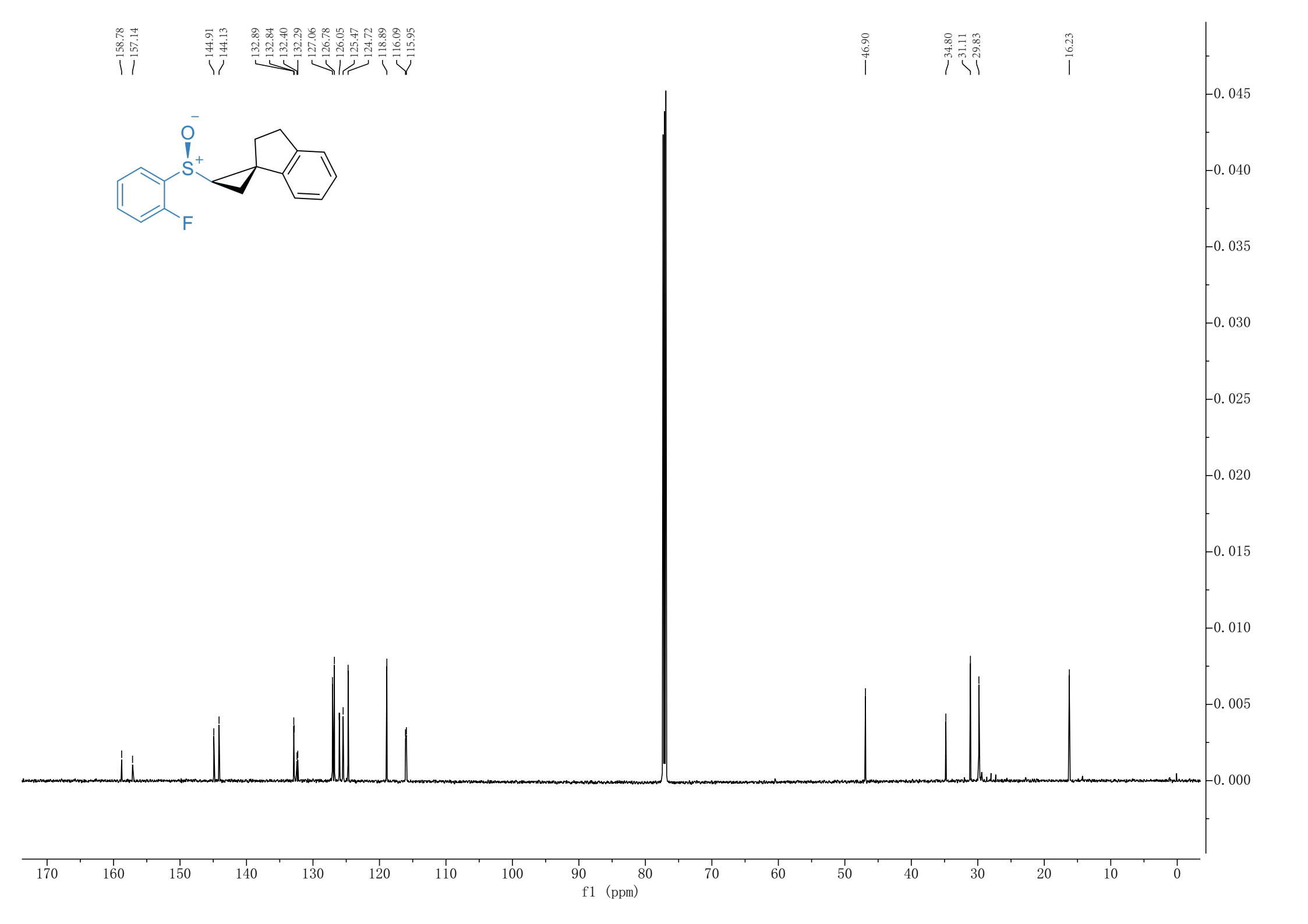


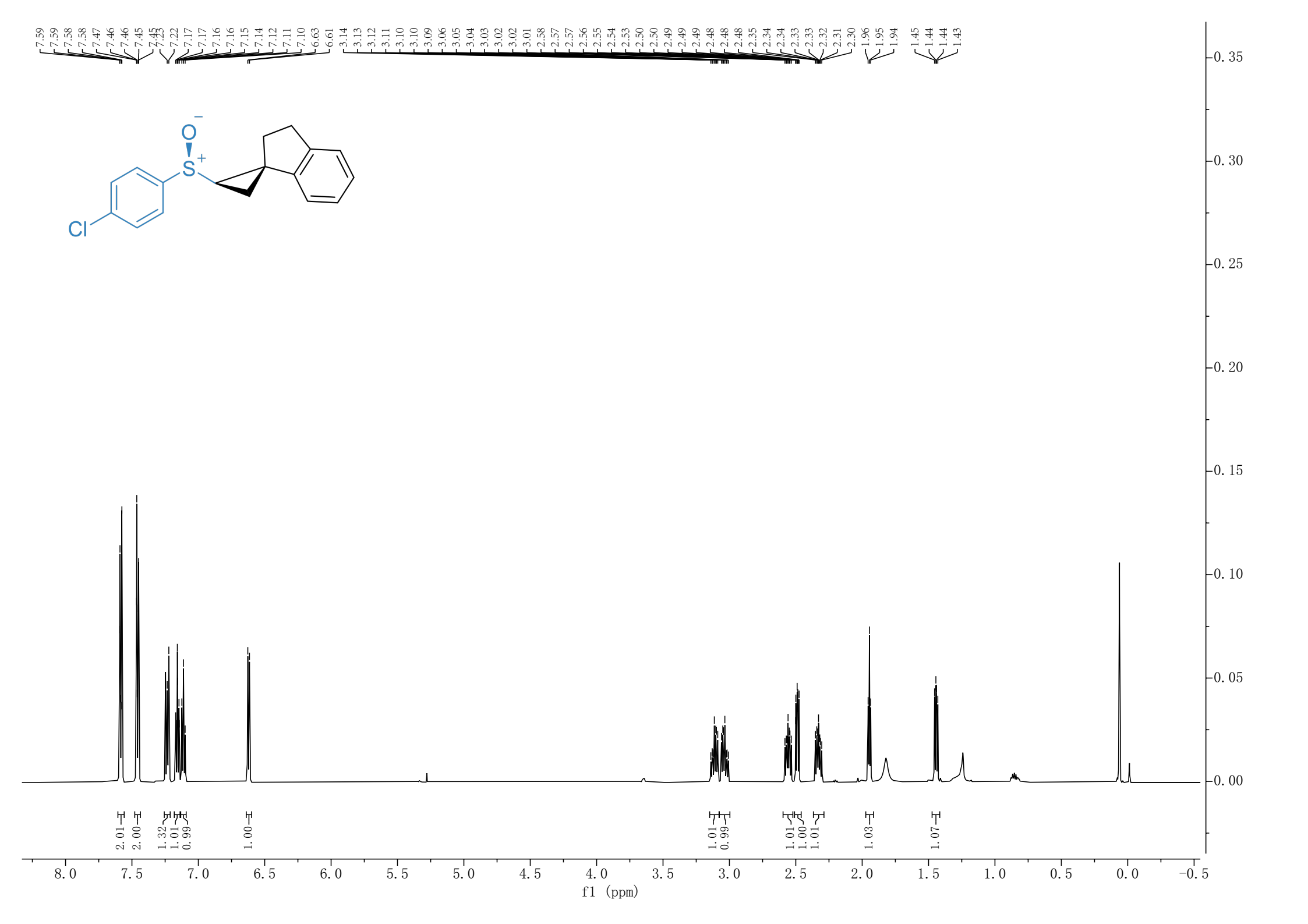
-114.26

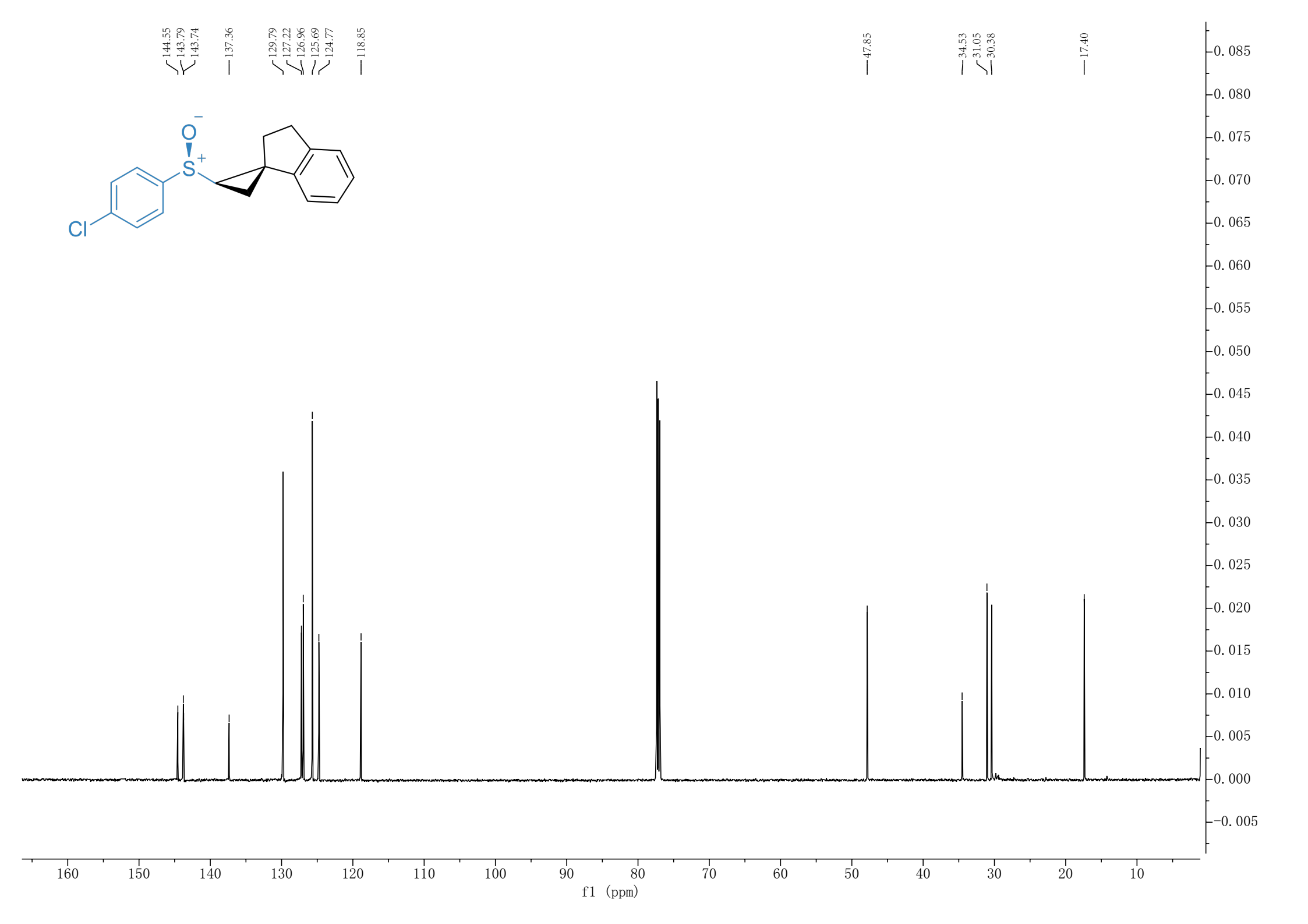
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
−100

10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210

f1 (ppm)


158.78
157.14
144.91
144.13
132.89
132.84
132.40
132.29
127.06
126.78
126.05
125.47
124.72
118.89
116.09
115.95
46.90
34.80
31.11
29.83
16.23
O
S+
F
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.59 7.59 7.58 7.58 7.47 7.46 7.46 7.45 7.45 7.23 7.22 7.17 7.17 7.16 7.16 7.15 7.14 7.12 7.11 7.10 6.63 6.61
3.14 3.13 3.12 3.11 3.10 3.10 3.09 3.06 3.05 3.04 3.03 3.02 3.02 3.01 2.58 2.57 2.57 2.56 2.55 2.54 2.53 2.50 2.50 2.49 2.49 2.49 2.48 2.48 2.35 2.34 2.34 2.33 2.33 2.32 2.31 2.30
1.96 1.95 1.94
1.45 1.44 1.44 1.43
O
S+
Cl
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
2.01 2.00 1.32 1.01 0.99 1.00 1.01 0.99 1.01 1.00 1.01 1.03 1.07
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
f1 (ppm)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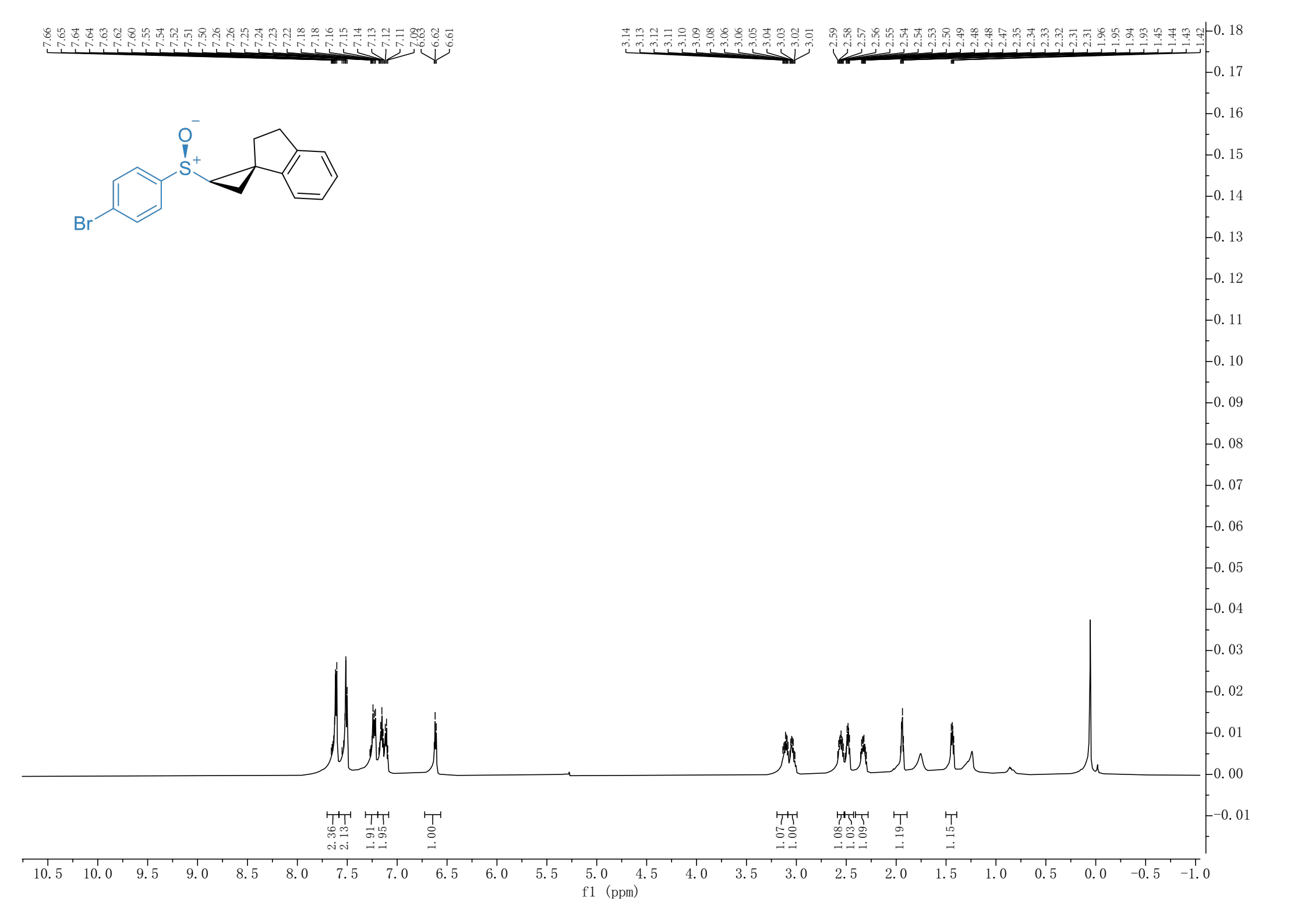
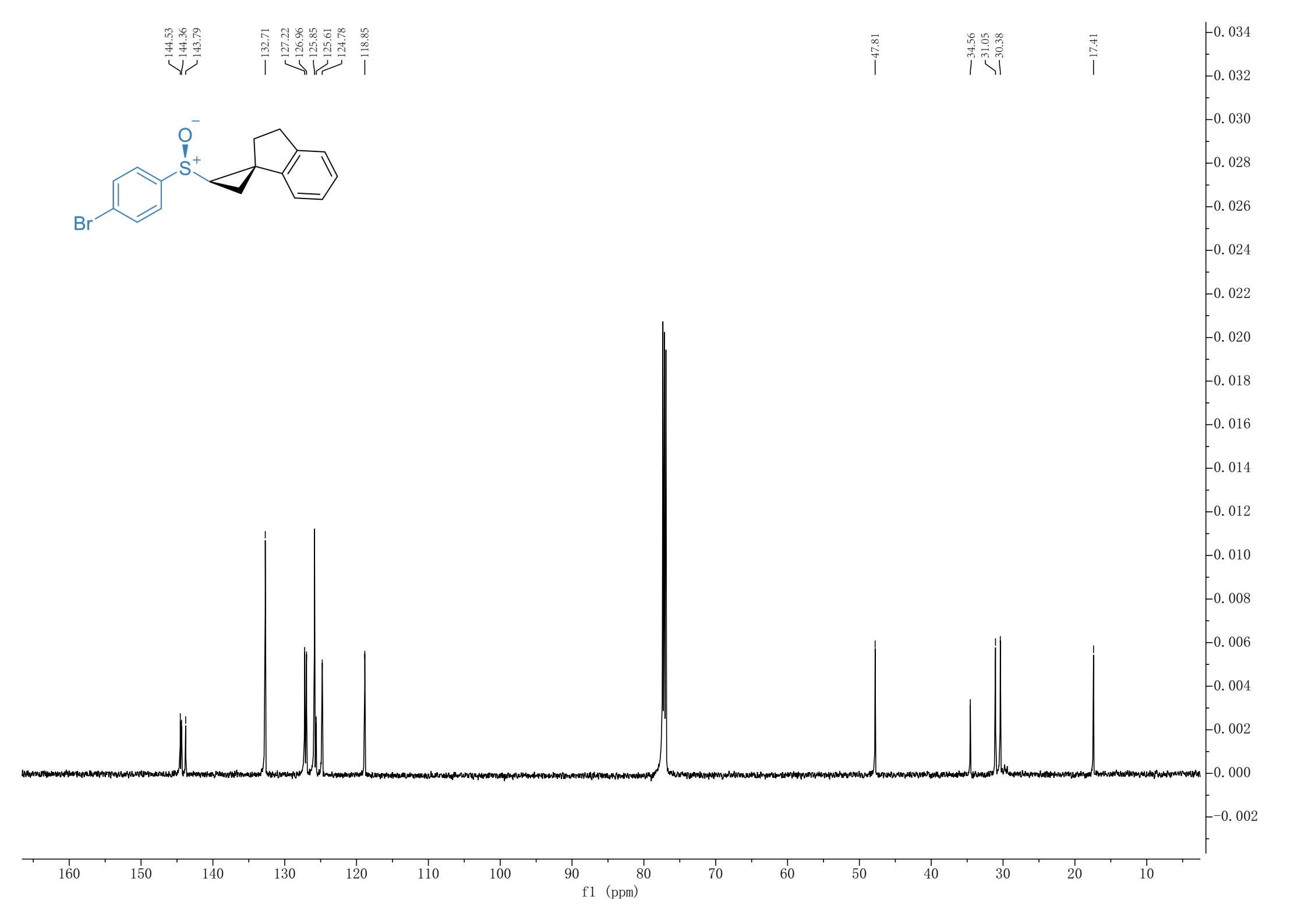
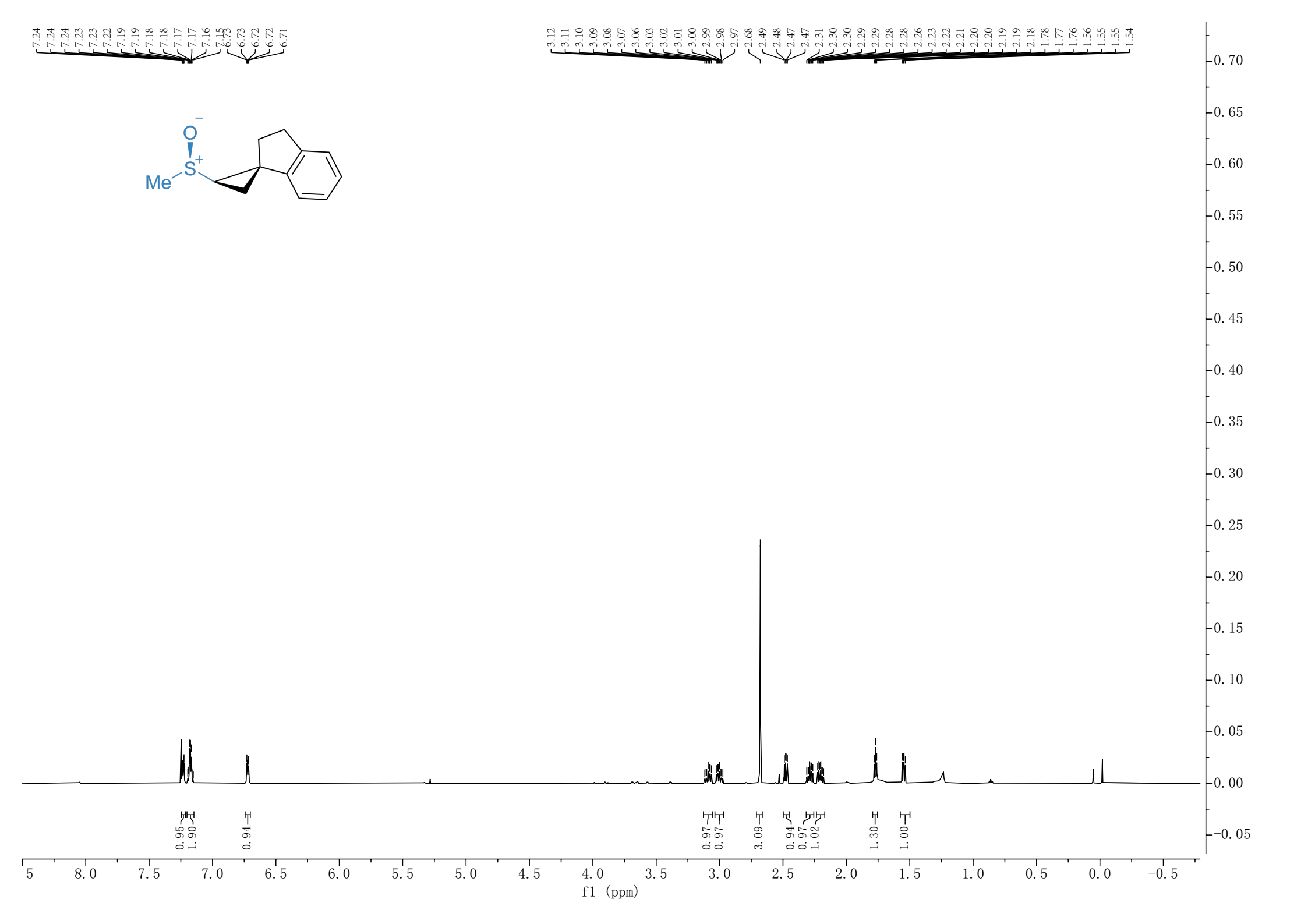
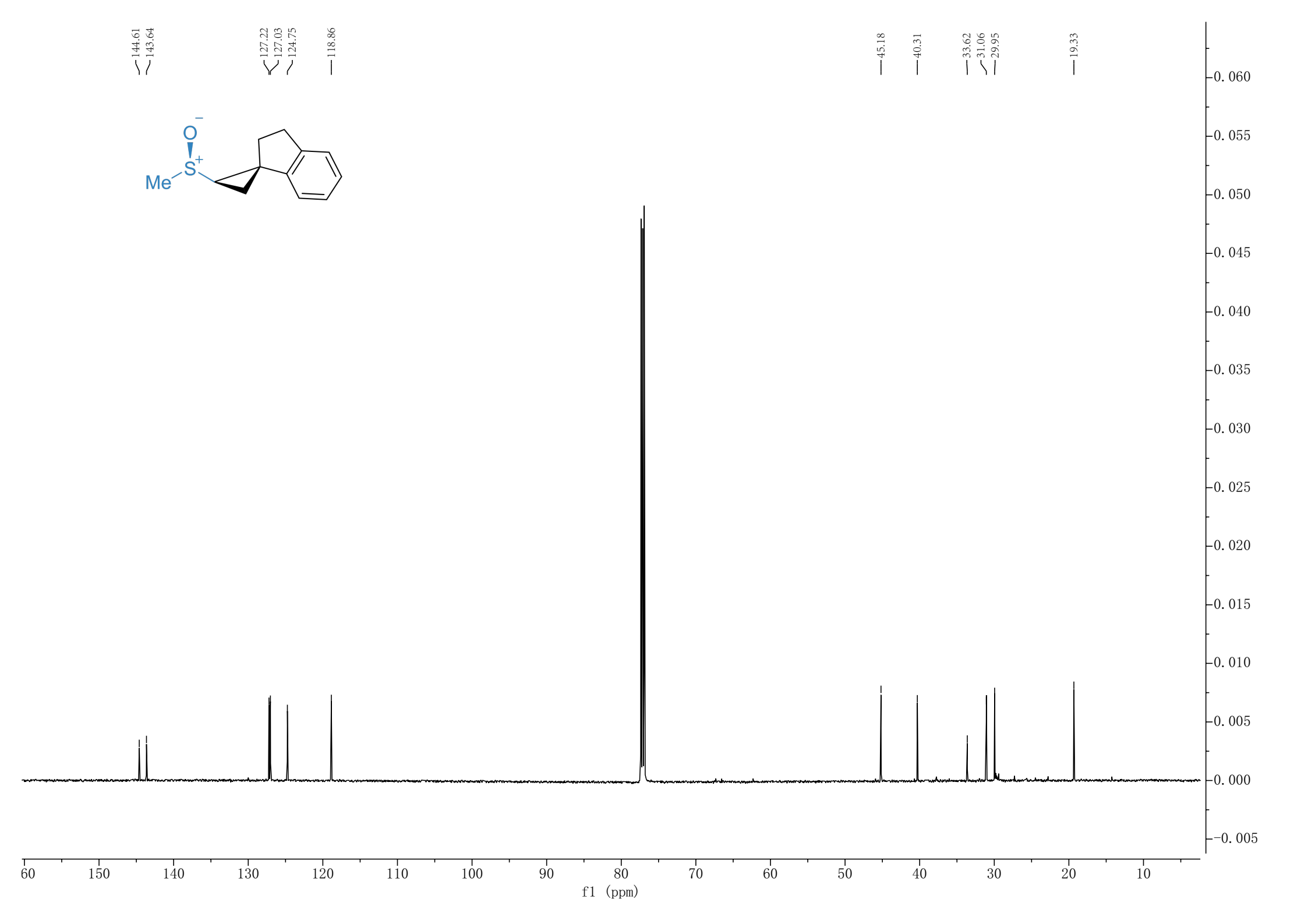
143.79
143.74
137.36
129.79
127.22
126.96
125.69
124.77
118.85
47.85
34.53
31.05
30.38
17.40
O
S+
Cl
0.085
0.080
0.075
0.070
0.065
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.66 7.65 7.64 7.64 7.63 7.62 7.60 7.55 7.54 7.52 7.51 7.50 7.26 7.25 7.24 7.23 7.22 7.18 7.18 7.16 7.15 7.14 7.13 7.12 7.11 7.09 7.03 6.62 6.61
3.14 3.13 3.12 3.11 3.10 3.09 3.08 3.06 3.06 3.05 3.04 3.03 3.02 3.01
2.59 2.58 2.57 2.56 2.55 2.54 2.54 2.53 2.50 2.49 2.48 2.48 2.47 2.35 2.34 2.33 2.32 2.31 2.31 1.96 1.95 1.94 1.93 1.45 1.44 1.43 1.42
O
S+
Br
2.36 2.13 1.91 1.95 1.00 1.07 1.00 1.08 1.03 1.09 1.19 1.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
0.18 0.17 0.16 0.15 0.14 0.13 0.12 0.11 0.10 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0.00 -0.01


144.53
144.36
143.79
132.71
127.22
126.96
125.85
125.61
124.78
118.85
47.81
34.56
31.05
30.38
17.41
O
S+
Br
0.034
0.032
0.030
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.24 7.24 7.24 7.23 7.23 7.22 7.19 7.19 7.18 7.18 7.17 7.17 7.16 7.15 6.73 6.73 6.72 6.72 6.71
3.12 3.11 3.10 3.09 3.08 3.07 3.06 3.03 3.02 3.01 3.00 2.99 2.98 2.97 2.68 2.49 2.48 2.47 2.47 2.31 2.30 2.30 2.29 2.29 2.28 2.28 2.26 2.23 2.22 2.21 2.20 2.20 2.19 2.19 2.18 1.78 1.77 1.76 1.56 1.55 1.55 1.54
O
S+
Me
0.95
1.90
0.94
0.97
0.97
3.09
0.94
0.97
1.02
1.30
1.00
f1 (ppm)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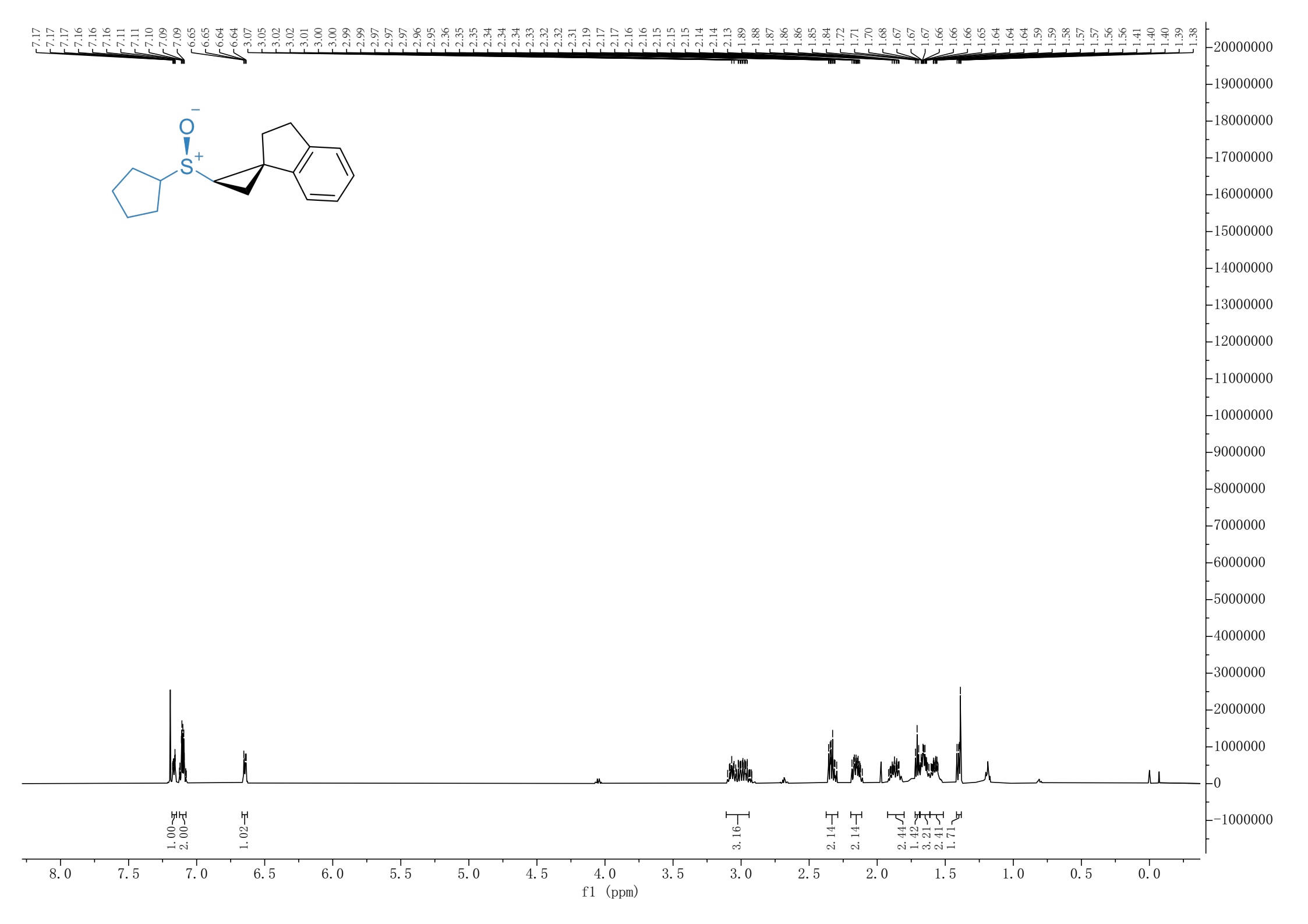
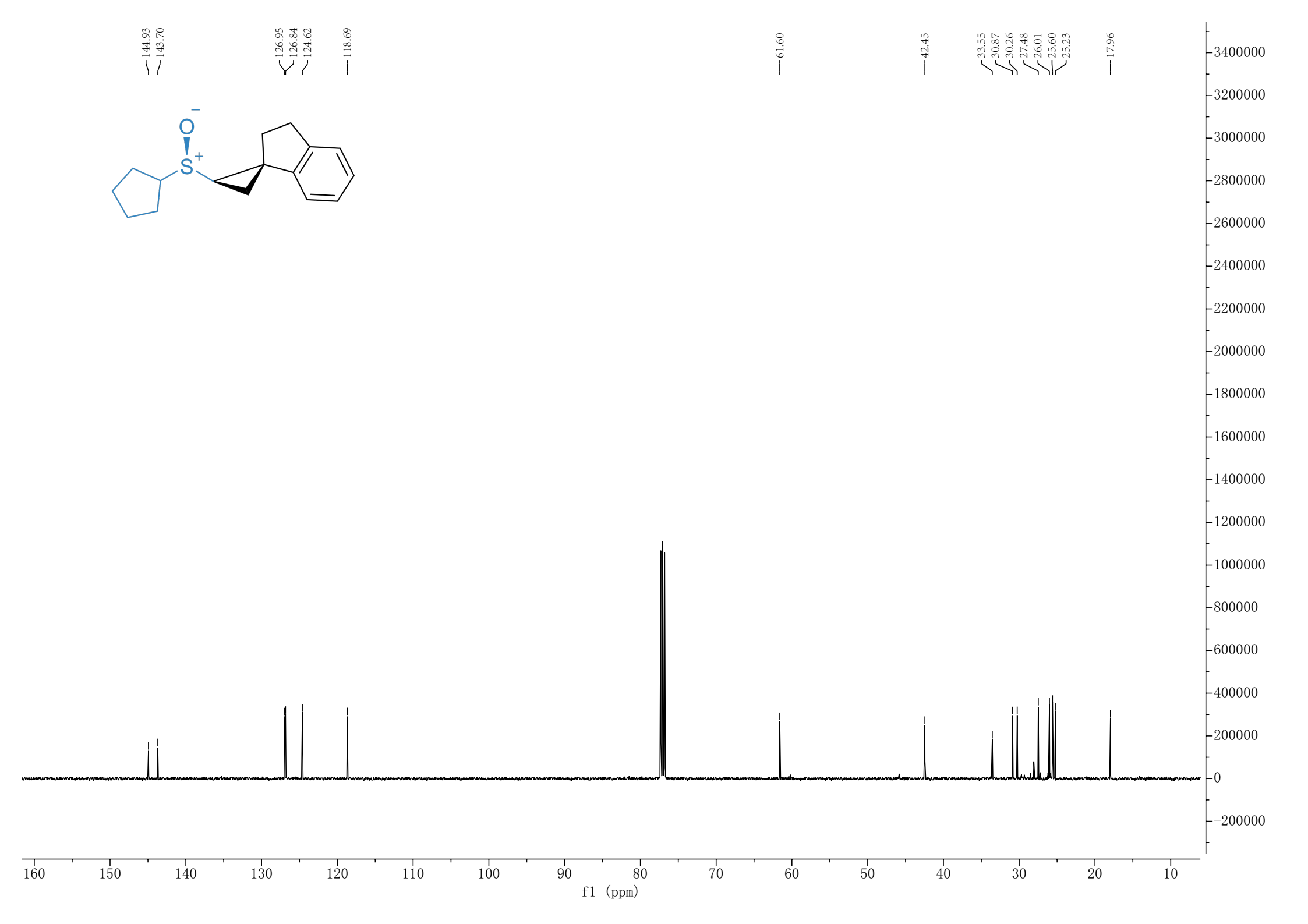
143.64
127.22
127.03
124.75
118.86
45.18
40.31
33.62
31.06
29.95
19.33
O
S+
Me
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.17 7.17 7.17 7.16 7.16 7.16 7.11 7.11 7.10 7.09 7.09 6.65 6.65 6.64 6.64 3.07 3.05 3.02 3.02 3.01 3.00 3.00 2.99 2.99 2.97 2.97 2.97 2.96 2.95 2.36 2.35 2.34 2.34 2.34 2.33 2.32 2.31 2.19 2.17 2.17 2.16 2.16 2.15 2.15 2.14 2.14 2.13 1.89 1.88 1.87 1.86 1.86 1.85 1.84 1.72 1.71 1.70 1.68 1.67 1.67 1.67 1.66 1.66 1.66 1.65 1.64 1.64 1.64 1.59 1.59 1.58 1.57 1.57 1.56 1.56 1.41 1.40 1.40 1.39 1.38
O
S+
20000000 19000000 18000000 17000000 16000000 15000000 14000000 13000000 12000000 11000000 10000000 9000000 8000000 7000000 6000000 5000000 4000000 3000000 2000000 1000000 0 −1000000
1.00 2.00 1.02 3.16 2.14 2.14 2.44 1.42 3.21 2.41 1.71
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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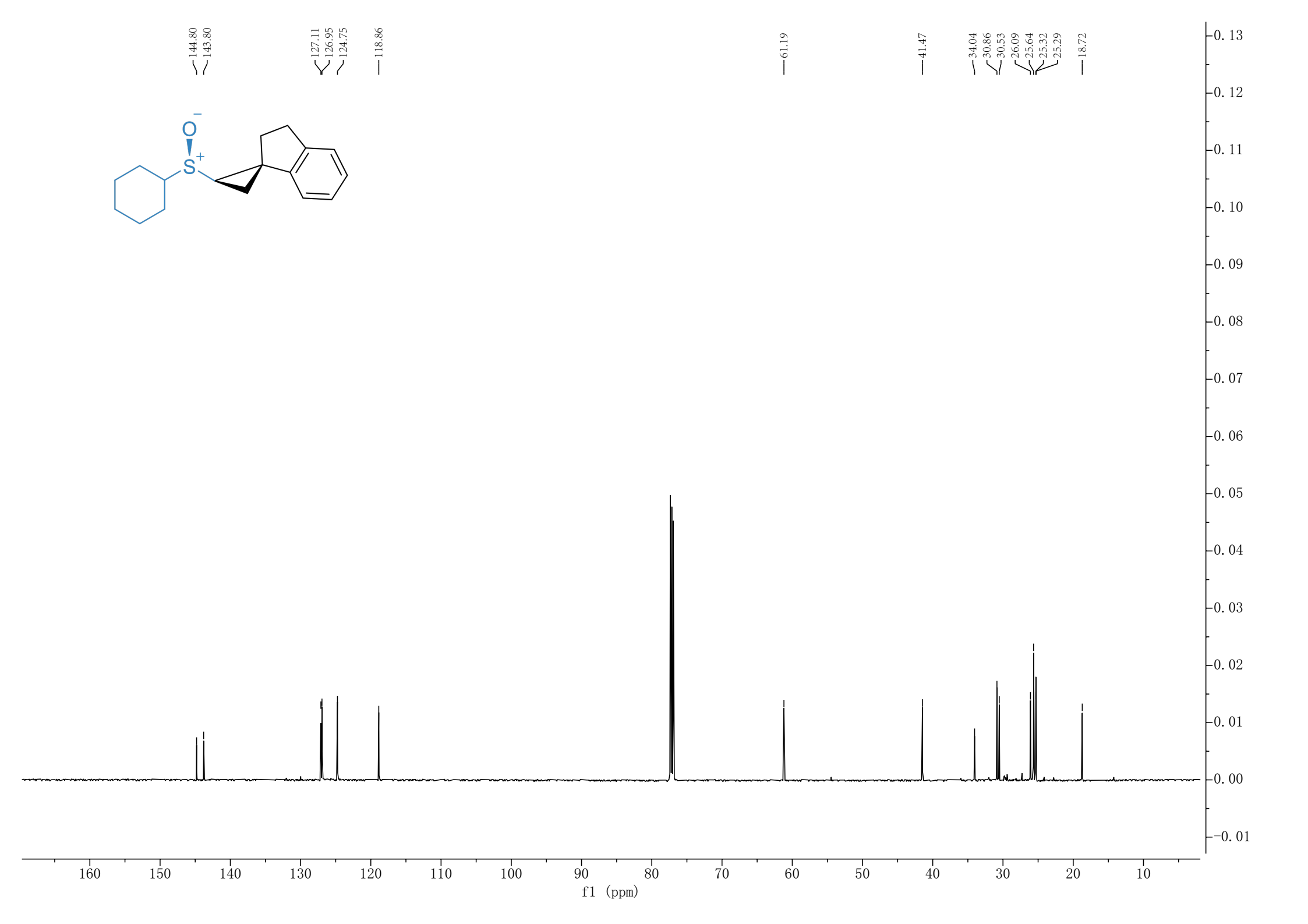
126.95
126.84
124.62
118.69
61.60
42.45
33.55
30.87
30.26
27.48
26.01
25.60
25.23
17.96
O
S+
3400000
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
−200000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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124.75
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61.19
41.47
34.04
30.86
30.53
26.09
25.64
25.32
25.29
18.72
O
S+
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01
160
150
140
130
120
110
100
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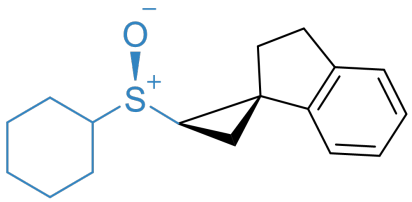
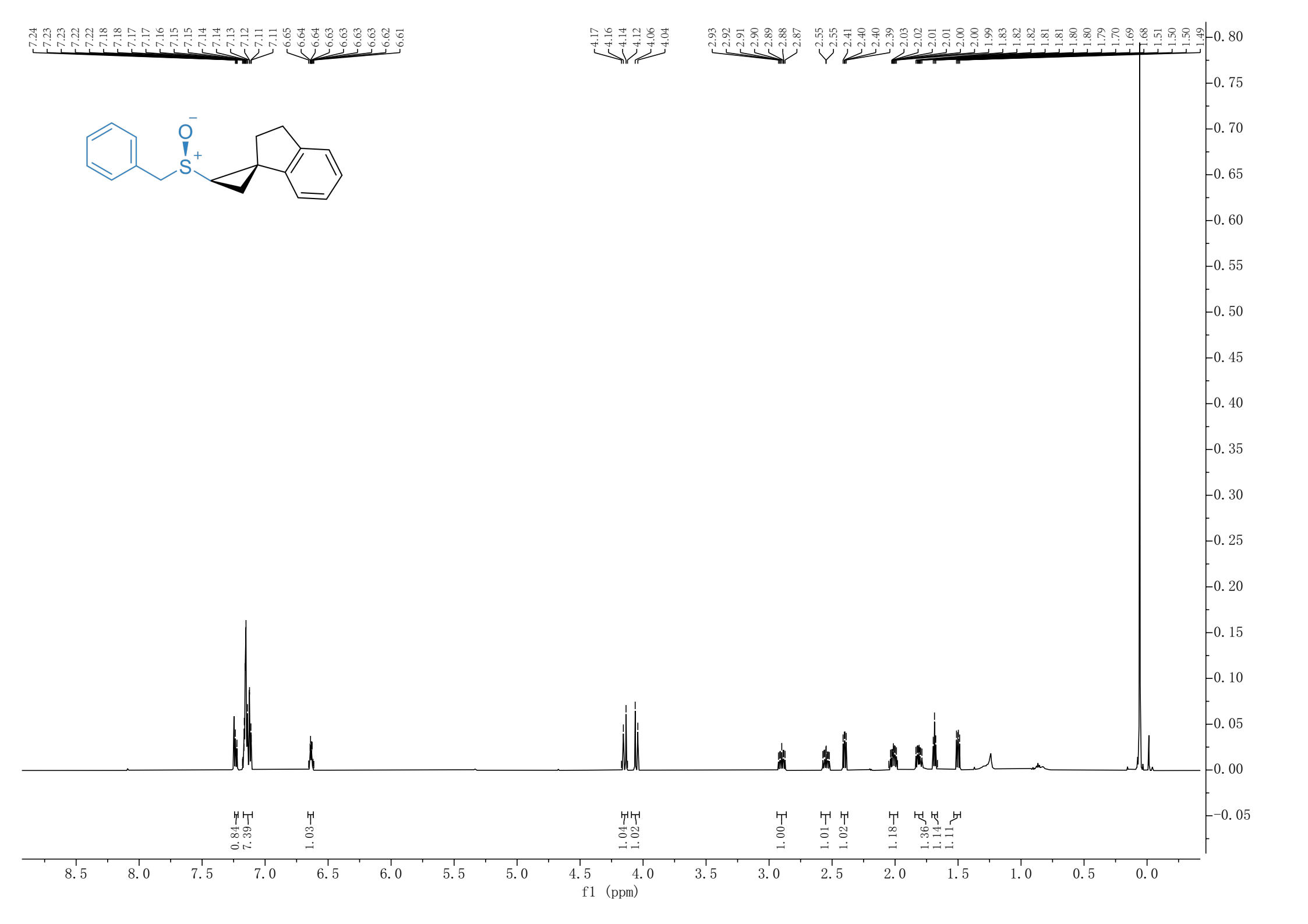
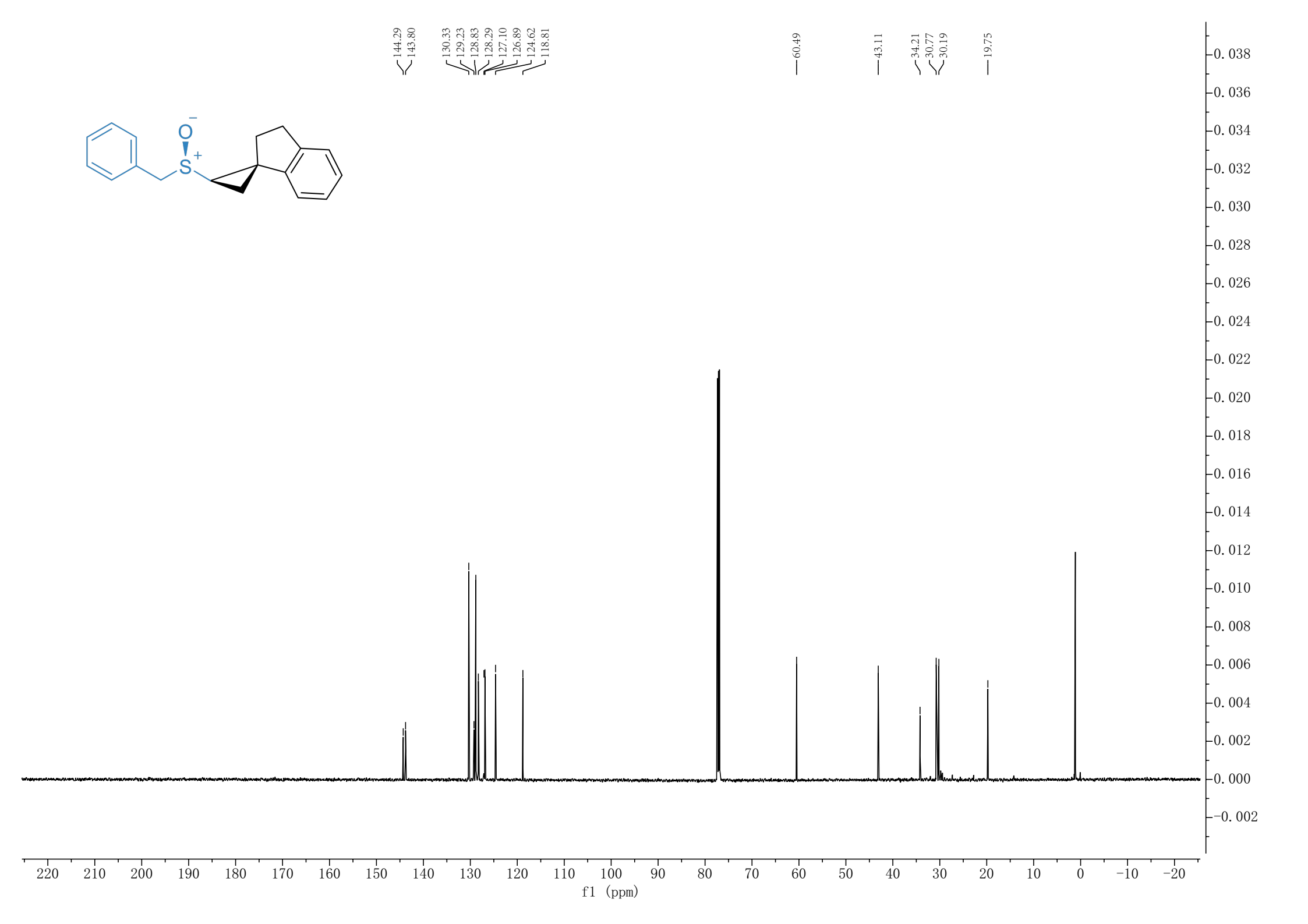
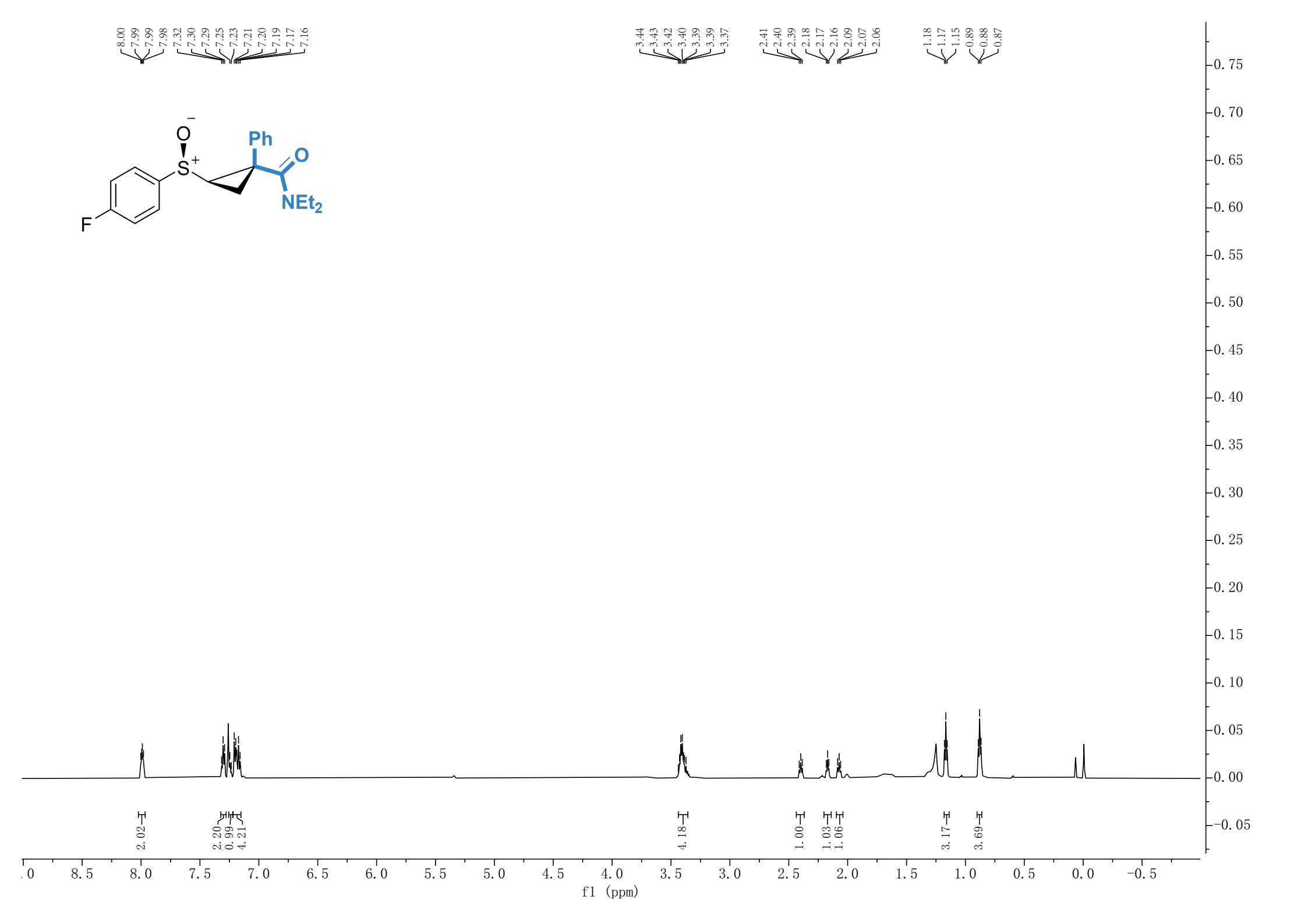
80
70
60
50
40
30
20
10
f1 (ppm)

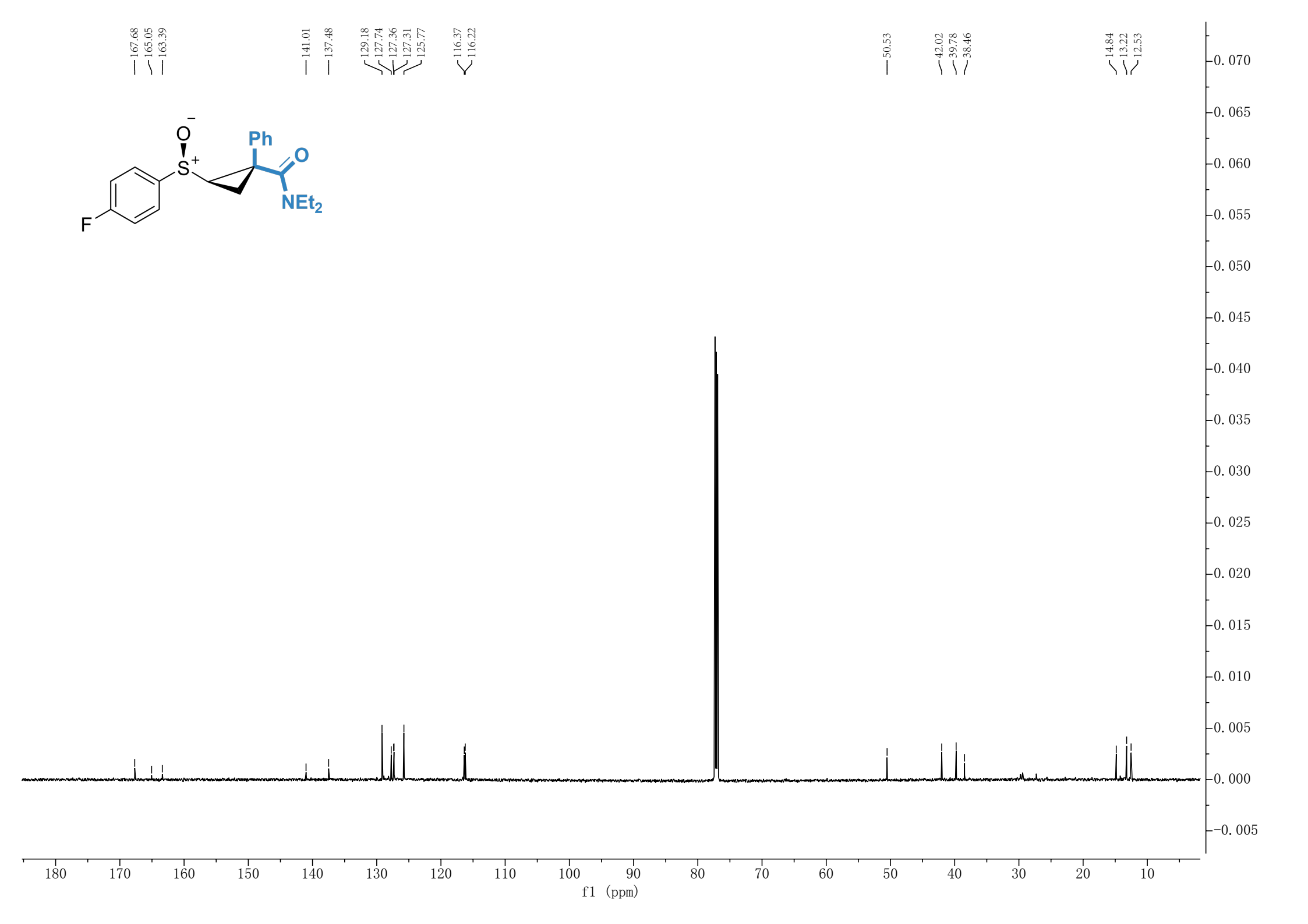


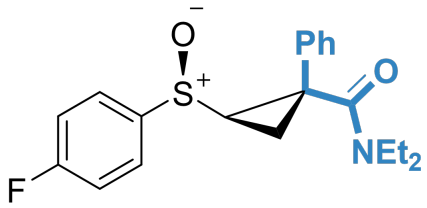
f1 (ppm)


7.24 7.23 7.23 7.22 7.22 7.18 7.18 7.17 7.17 7.16 7.15 7.15 7.14 7.14 7.13 7.12 7.11 7.11
6.65 6.64 6.64 6.63 6.63 6.63 6.63 6.62 6.61
4.17 4.16 4.14 4.12 4.06 4.04
2.93 2.92 2.91 2.90 2.89 2.88 2.87
2.55 2.55 2.41 2.40 2.40 2.39 2.03 2.02 2.01 2.01 2.00 2.00 1.99 1.83 1.82 1.81 1.81 1.80 1.80 1.79 1.70 1.69 1.68 1.51 1.50 1.50 1.49
O
S
0.84
7.39
1.03
1.04
1.02
1.00
1.01
1.02
1.18
1.36
1.14
1.11
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)
0.80 0.75 0.70 0.65 0.60 0.55 0.50 0.45 0.40 0.35 0.30 0.25 0.20 0.15 0.10 0.05 0.00 -0.05


144.29
143.80
130.33
129.23
128.83
128.29
127.10
126.89
124.62
118.81
60.49
43.11
34.21
30.77
30.19
19.75
O
S+
0.038
0.036
0.034
0.032
0.030
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.00
7.99
7.99
7.98
7.32
7.30
7.29
7.25
7.23
7.21
7.20
7.19
7.17
7.16
3.44
3.43
3.42
3.40
3.39
3.39
3.37
2.41
2.40
2.39
2.18
2.17
2.16
2.09
2.07
2.06
1.18
1.17
1.15
0.89
0.88
0.87
O
S+
Ph
O
NEt2
F
2.02
2.20
0.99
4.21
4.18
1.00
1.03
1.06
3.17
3.69
f1 (ppm)


167.68
165.05
163.39
141.01
137.48
129.18
127.74
127.36
127.31
125.77
116.37
116.22
50.53
42.02
39.78
38.46
14.84
13.22
12.53
O
S+
Ph
O
NEt2
F
0.070
0.065
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

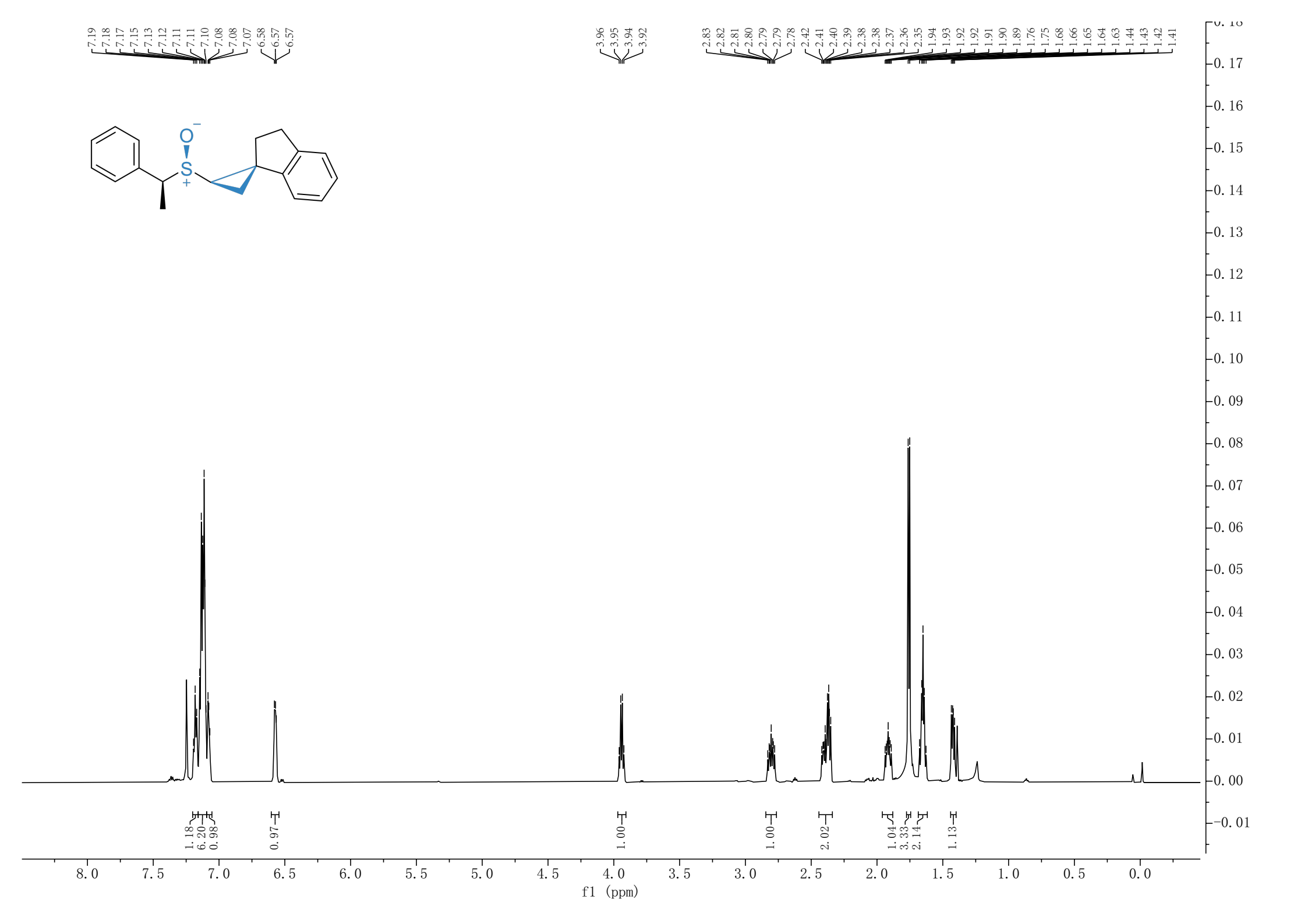


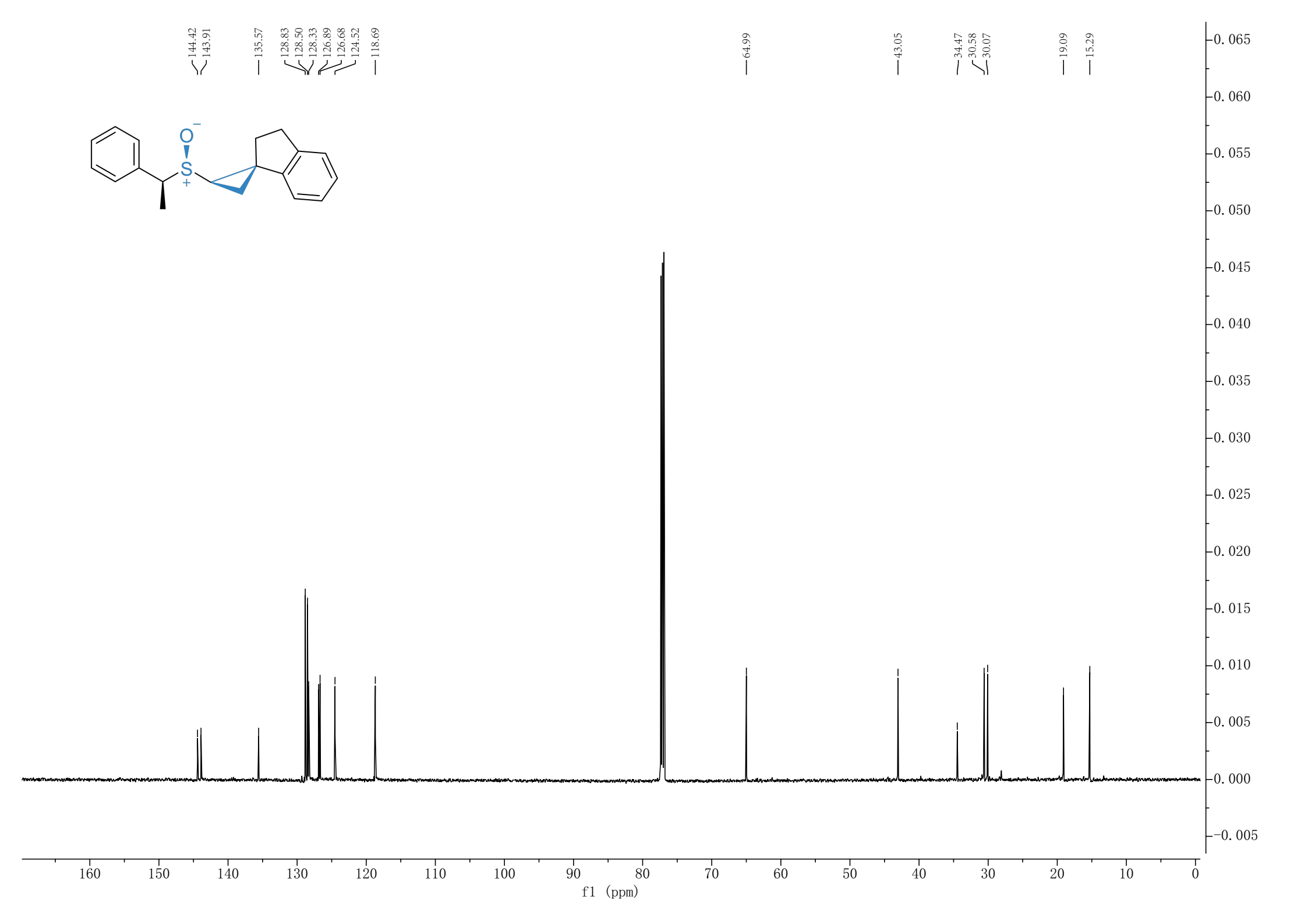
-109.78

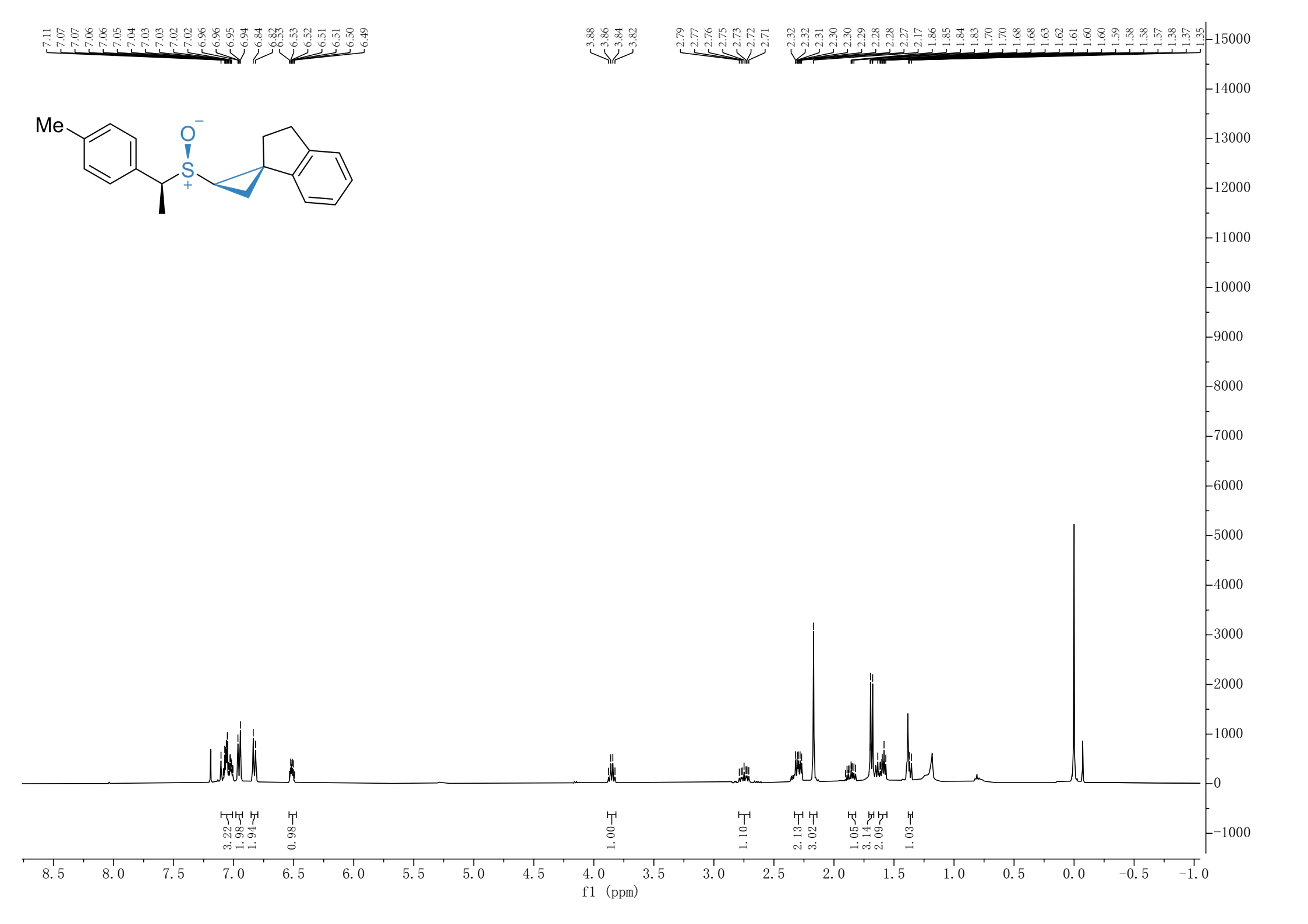
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1

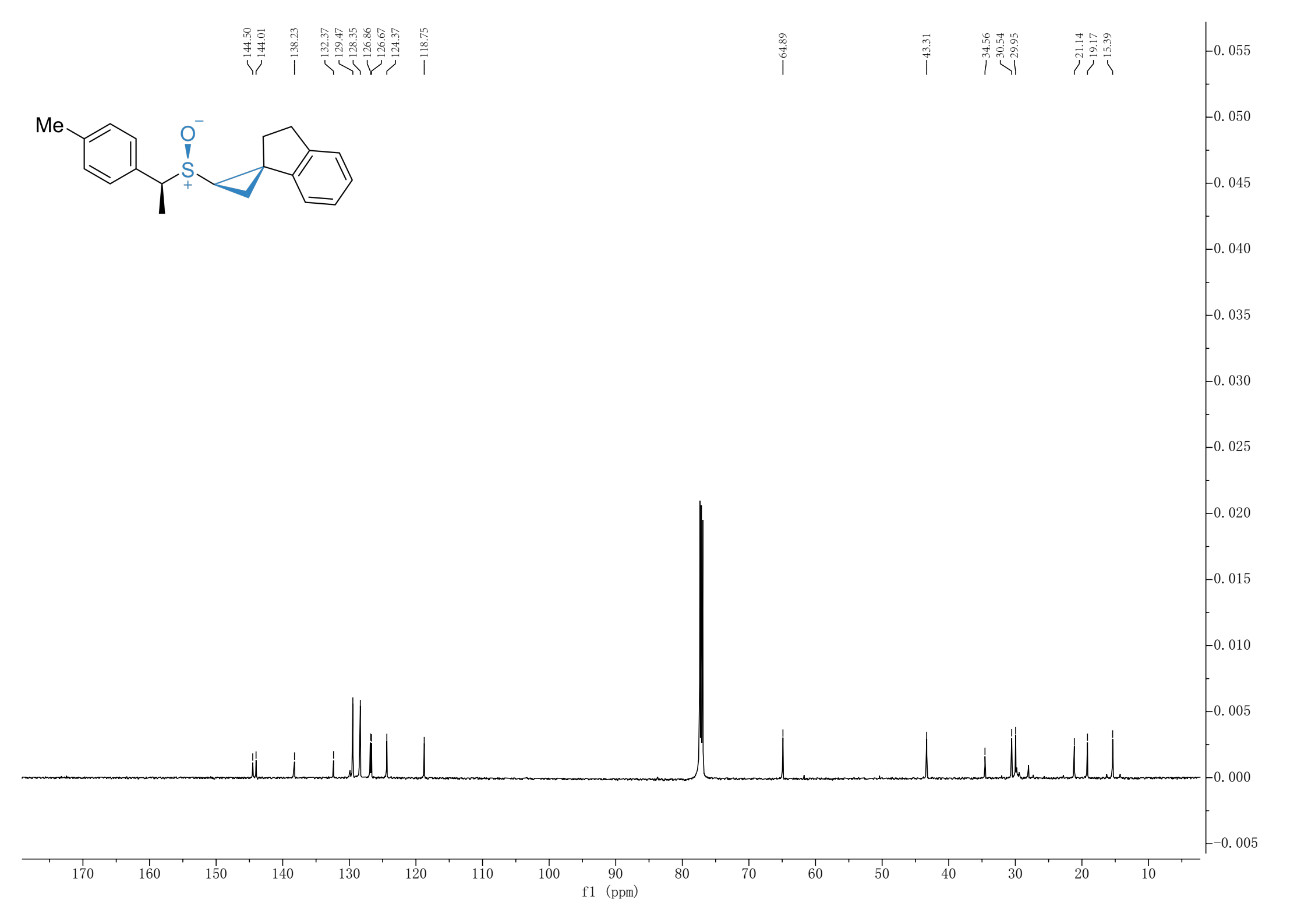
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

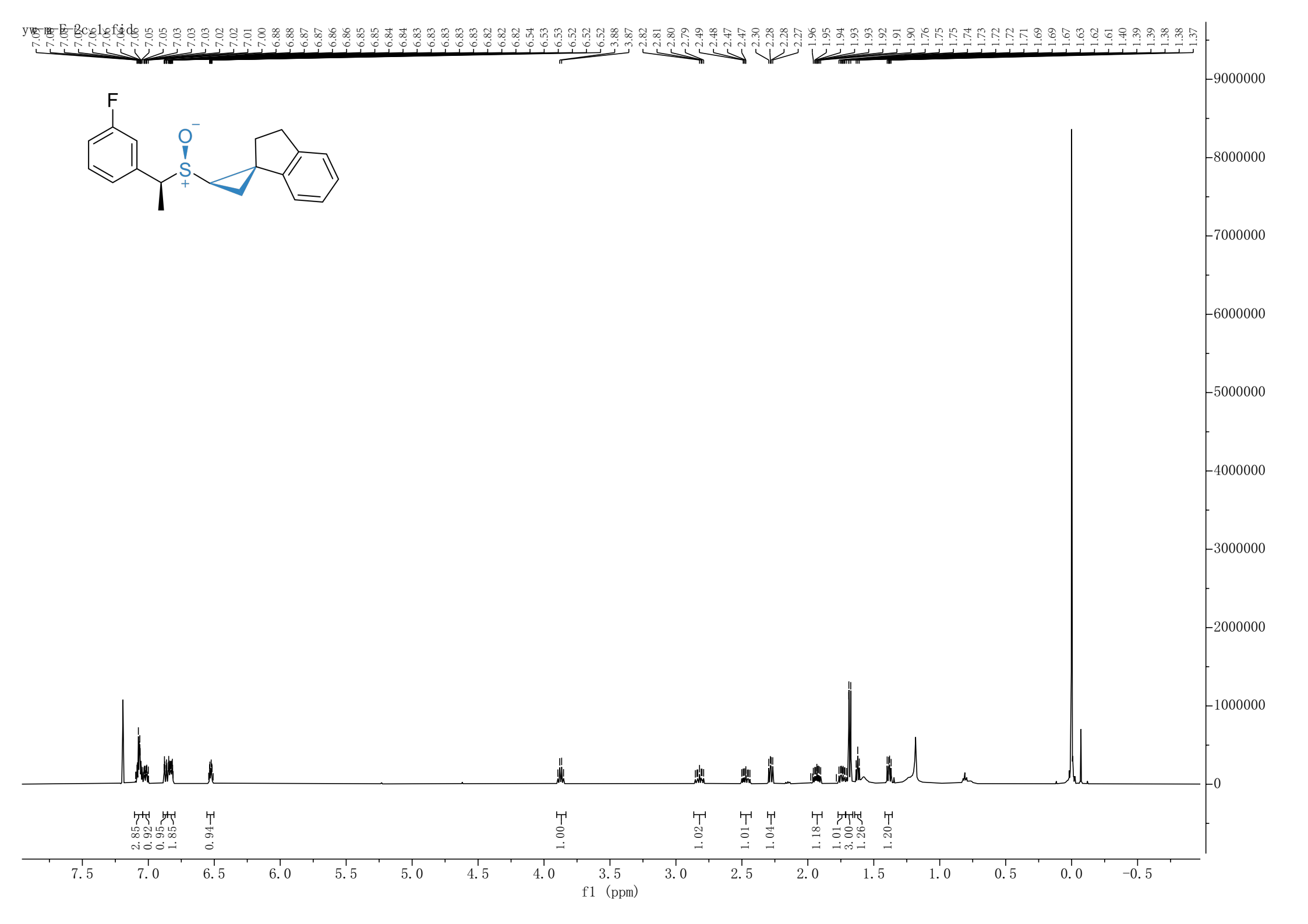
f1 (ppm)


7.19 7.18 7.17 7.15 7.13 7.12 7.11 7.11 7.10 7.08 7.08 7.07 6.58 6.57 6.57
3.96 3.95 3.94 3.92
2.83 2.82 2.81 2.80 2.79 2.79 2.78 2.42 2.41 2.40 2.39 2.38 2.38 2.37 2.36 2.35 1.94 1.93 1.92 1.92 1.91 1.90 1.89 1.76 1.75 1.68 1.66 1.65 1.64 1.63 1.44 1.43 1.42 1.41
O
S
+
1.18 6.20 0.98 0.97 1.00 1.00 2.02 1.04 3.33 2.14 1.13
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)
0.17 0.16 0.15 0.14 0.13 0.12 0.11 0.10 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0.00 -0.01

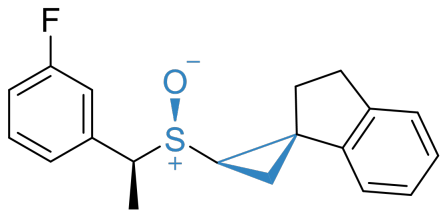

144.42
143.91
135.57
128.83
128.50
128.33
126.89
126.68
124.52
118.69
64.99
43.05
34.47
30.58
30.07
19.09
15.29
O
S
+
−
0.065
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
−0.005
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.11 7.07 7.07 7.06 7.06 7.05 7.04 7.03 7.03 7.02 7.02 6.96 6.95 6.94 6.84 6.82 6.53 6.52 6.51 6.51 6.50 6.49
3.88 3.86 3.84 3.82
2.79 2.77 2.76 2.75 2.73 2.72 2.71
2.32 2.32 2.31 2.30 2.30 2.29 2.28 2.28 2.27 2.17 1.86 1.85 1.84 1.83 1.70 1.70 1.68 1.68 1.63 1.62 1.61 1.60 1.60 1.59 1.58 1.58 1.57 1.38 1.37 1.35
Me
O
S
+
3.22
1.98
1.94
0.98
1.00
1.10
2.13
3.02
1.05
3.14
2.09
1.03
f1 (ppm)


144.50
144.01
138.23
132.37
129.47
128.35
126.86
126.67
124.37
118.75
64.89
43.31
34.56
30.54
29.95
21.14
19.17
15.39
Me
O
S
+
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


yw-m-E-2cc1cfid
F
O
S
+
f1 (ppm)

yw-m-F-2c.2.fid

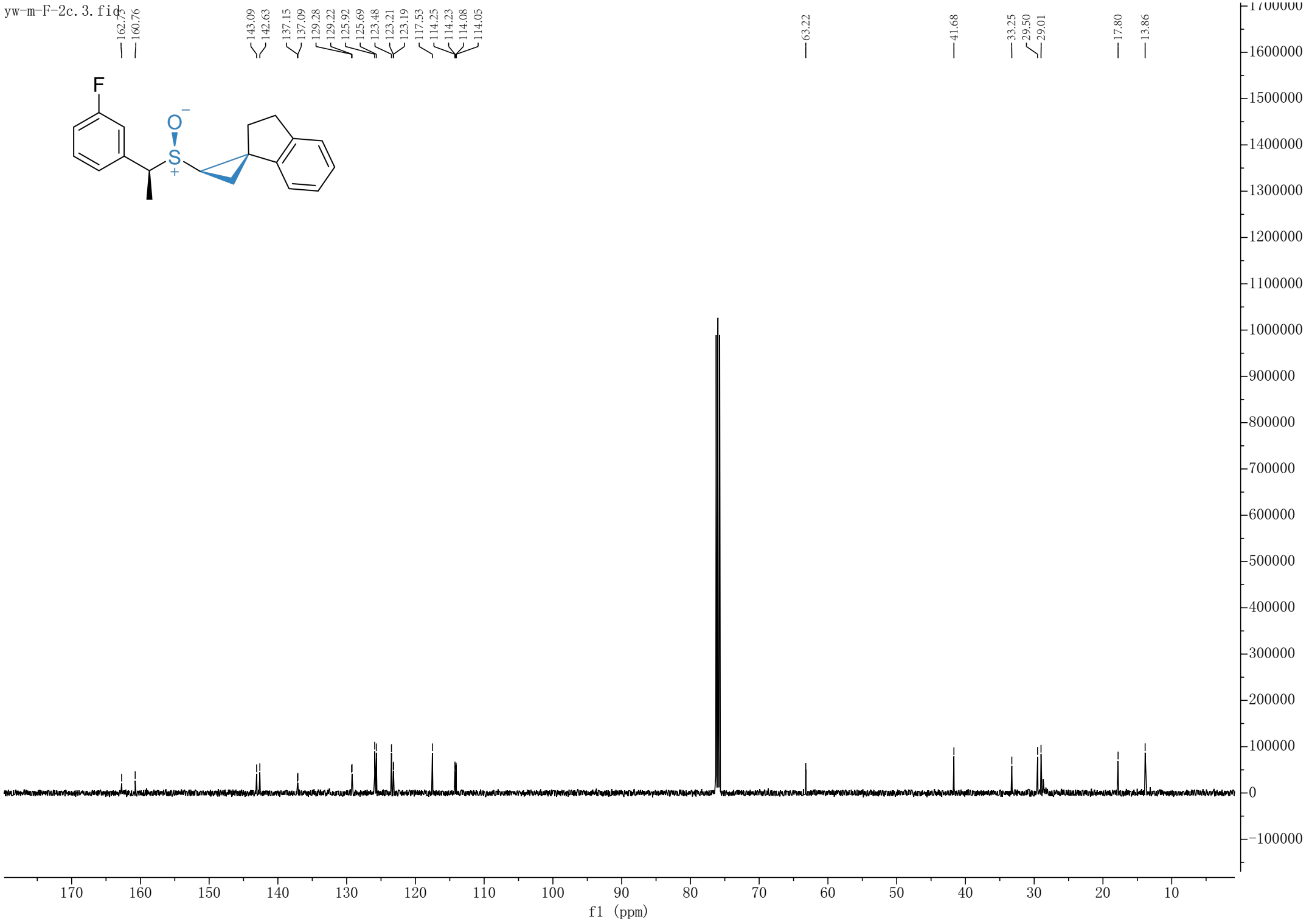


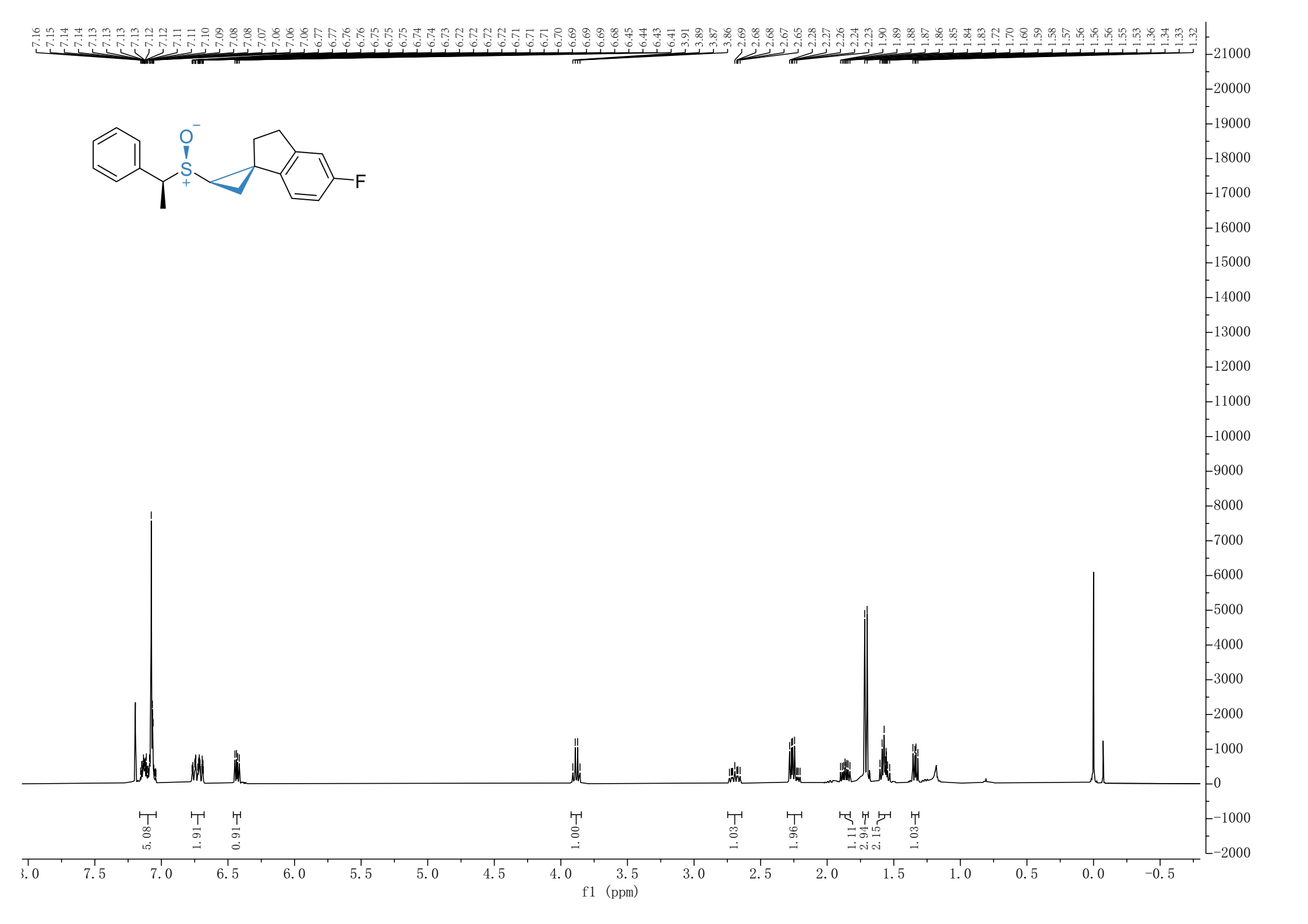
-111.93

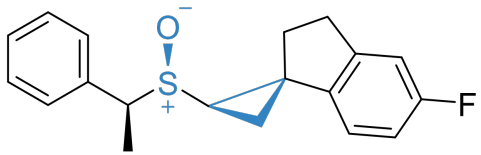
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

f1 (ppm)


yw-m-F-2c.3.fid
162.75
160.76
143.09
142.63
137.15
137.09
129.28
129.22
125.92
125.69
123.48
123.21
123.19
117.53
114.25
114.23
114.08
114.05
63.22
41.68
33.25
29.50
29.01
17.80
13.86
F
O
S
+
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
S
+
F
5.08
1.91
0.91
1.00
1.03
1.96
1.11
2.94
2.15
1.03
f1 (ppm)

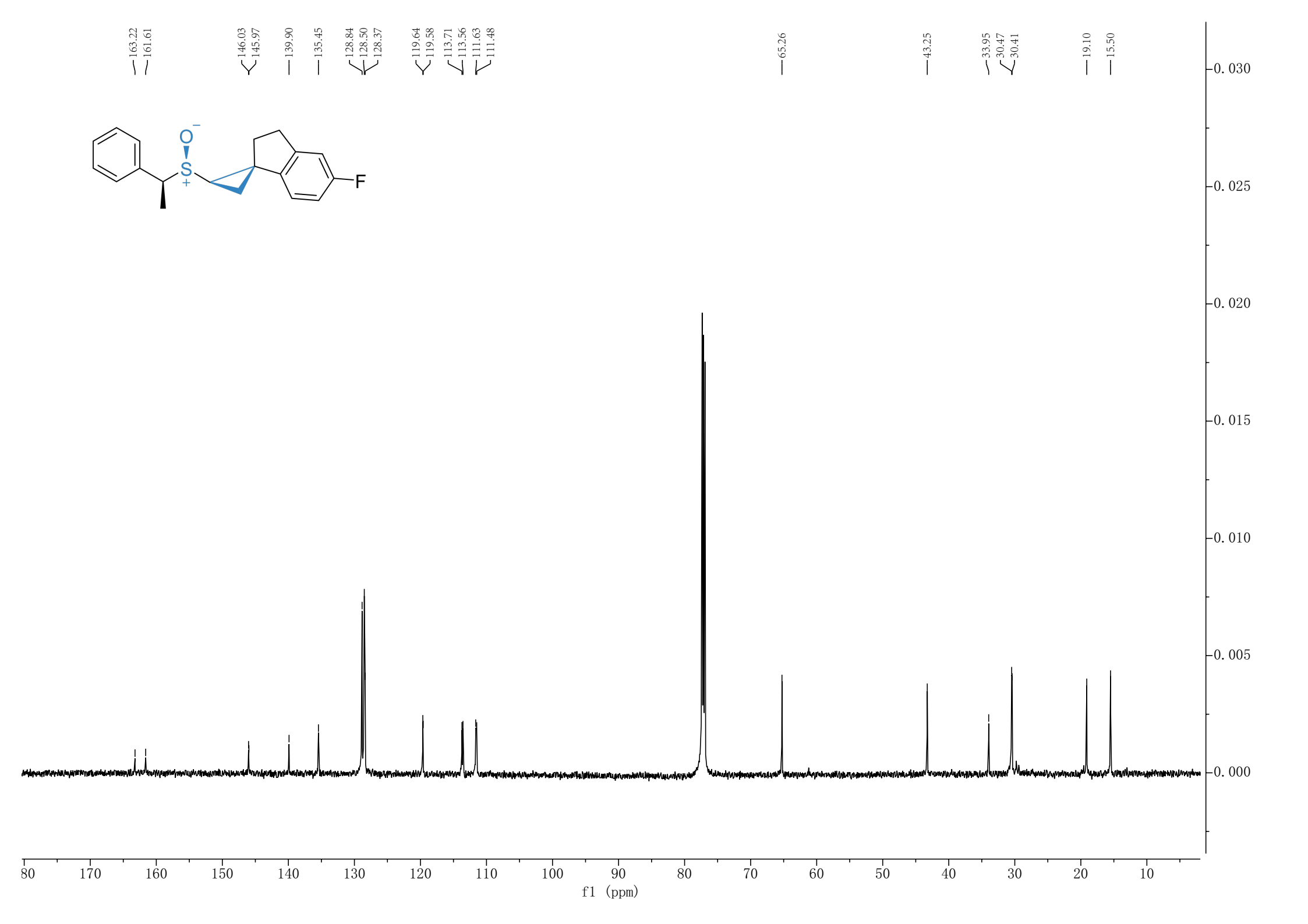


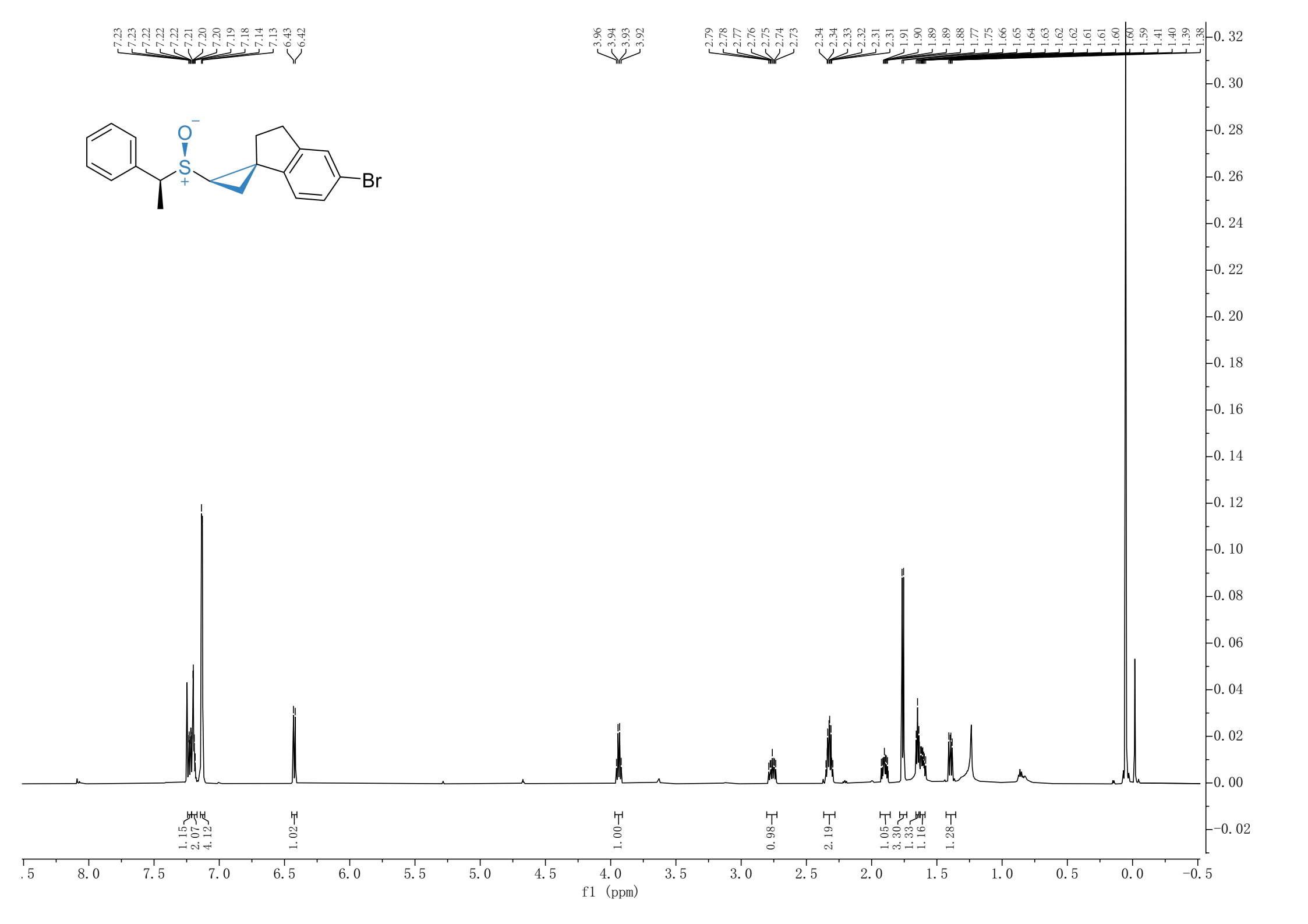
-116.59

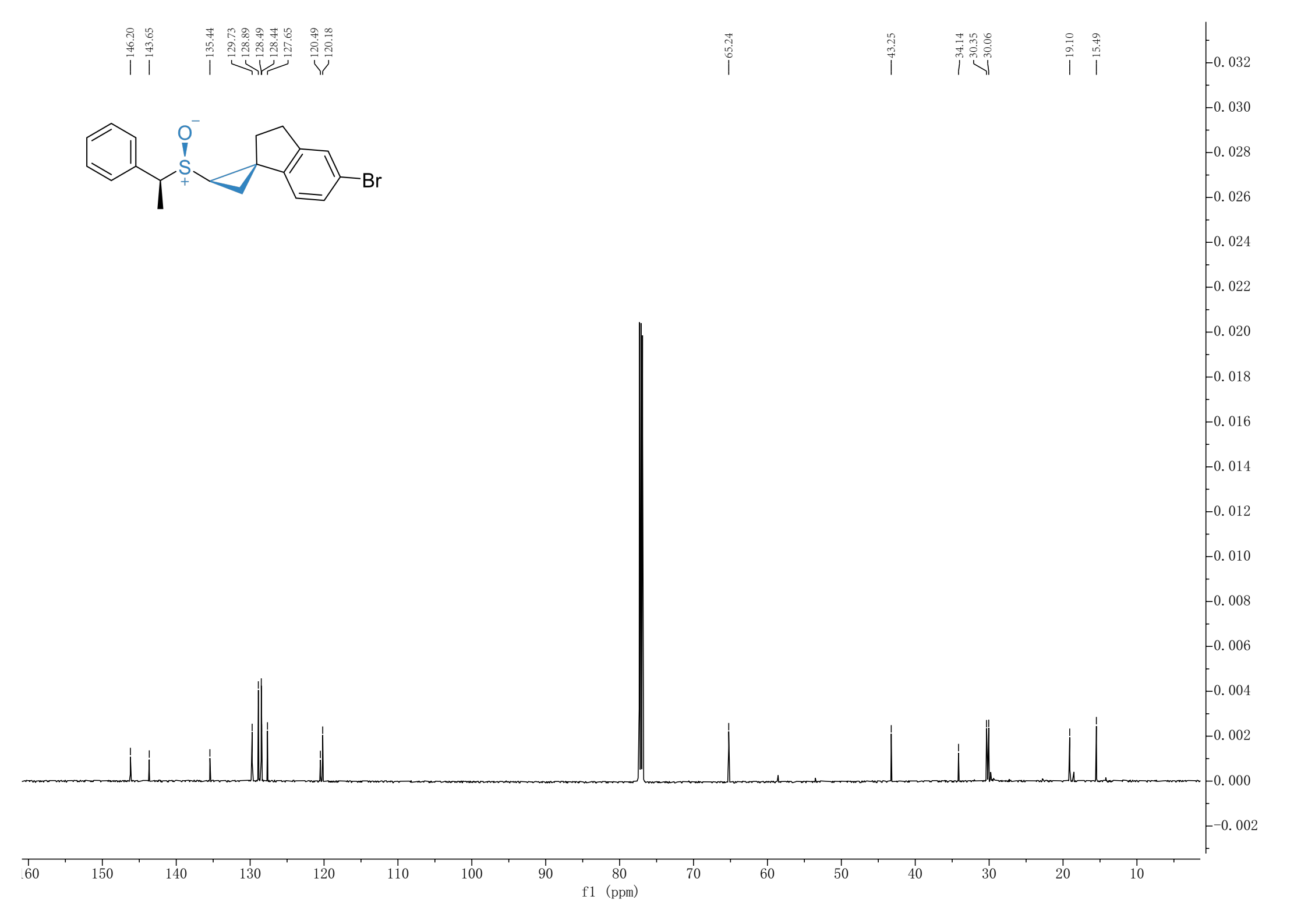
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)


163.22
161.61
146.03
145.97
139.90
135.45
128.84
128.50
128.37
119.64
119.58
113.71
113.56
111.63
111.48
65.26
43.25
33.95
30.47
30.41
19.10
15.50
O
S
+
F
0.030
0.025
0.020
0.015
0.010
0.005
0.000
f1 (ppm)


7.23 7.23 7.22 7.22 7.22 7.21 7.20 7.20 7.19 7.18 7.14 7.13 6.43 6.42
3.96 3.94 3.93 3.92
2.79 2.78 2.77 2.76 2.75 2.74 2.73
2.34 2.34 2.33 2.32 2.31 2.31 1.91 1.90 1.89 1.89 1.88 1.77 1.75 1.66 1.65 1.64 1.63 1.62 1.62 1.61 1.61 1.60 1.60 1.59 1.41 1.40 1.39 1.38
O
S
+
Br
1.15 2.07 4.12 1.02 1.00 0.98 2.19 1.05 3.30 1.33 1.16 1.28
f1 (ppm)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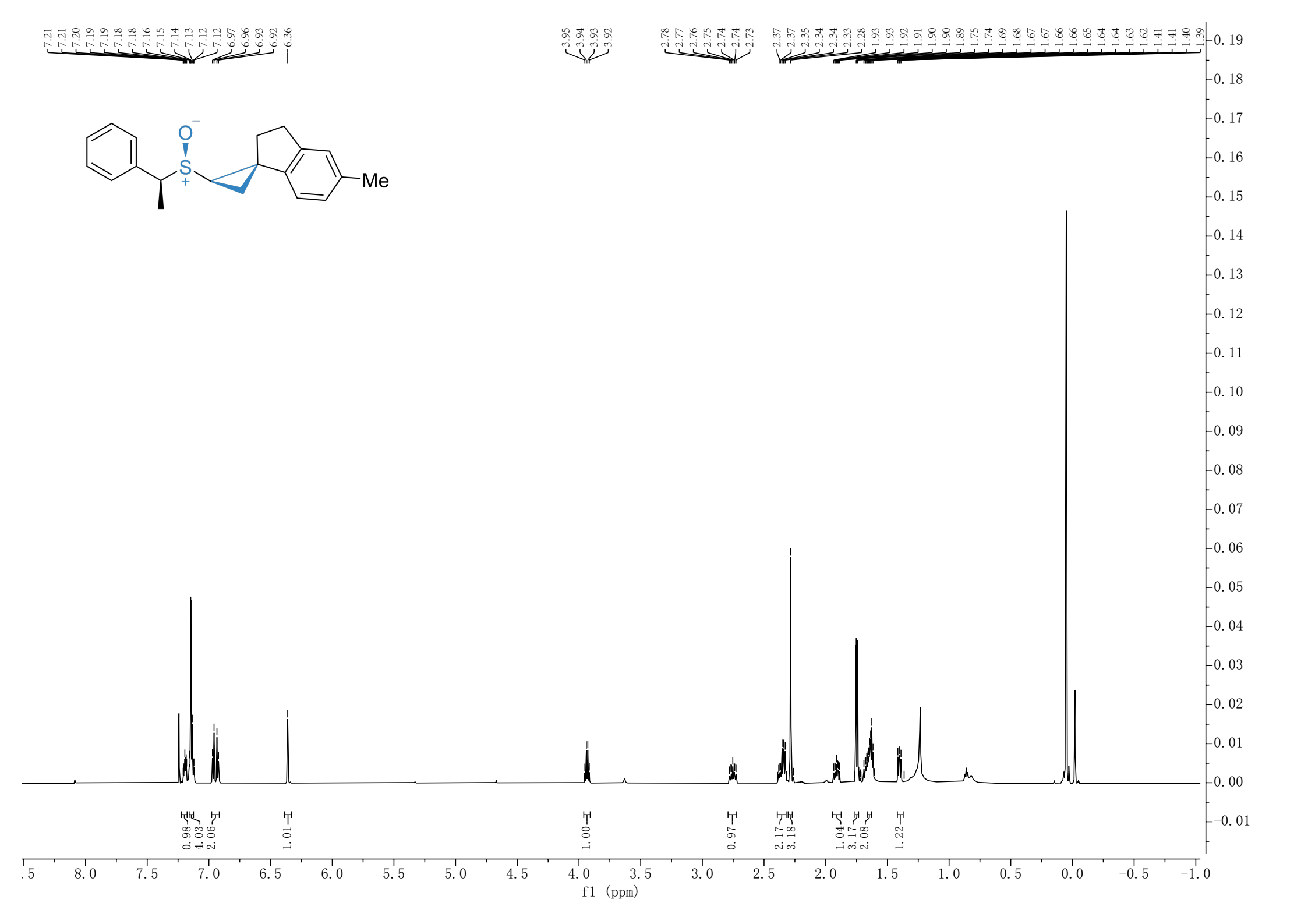
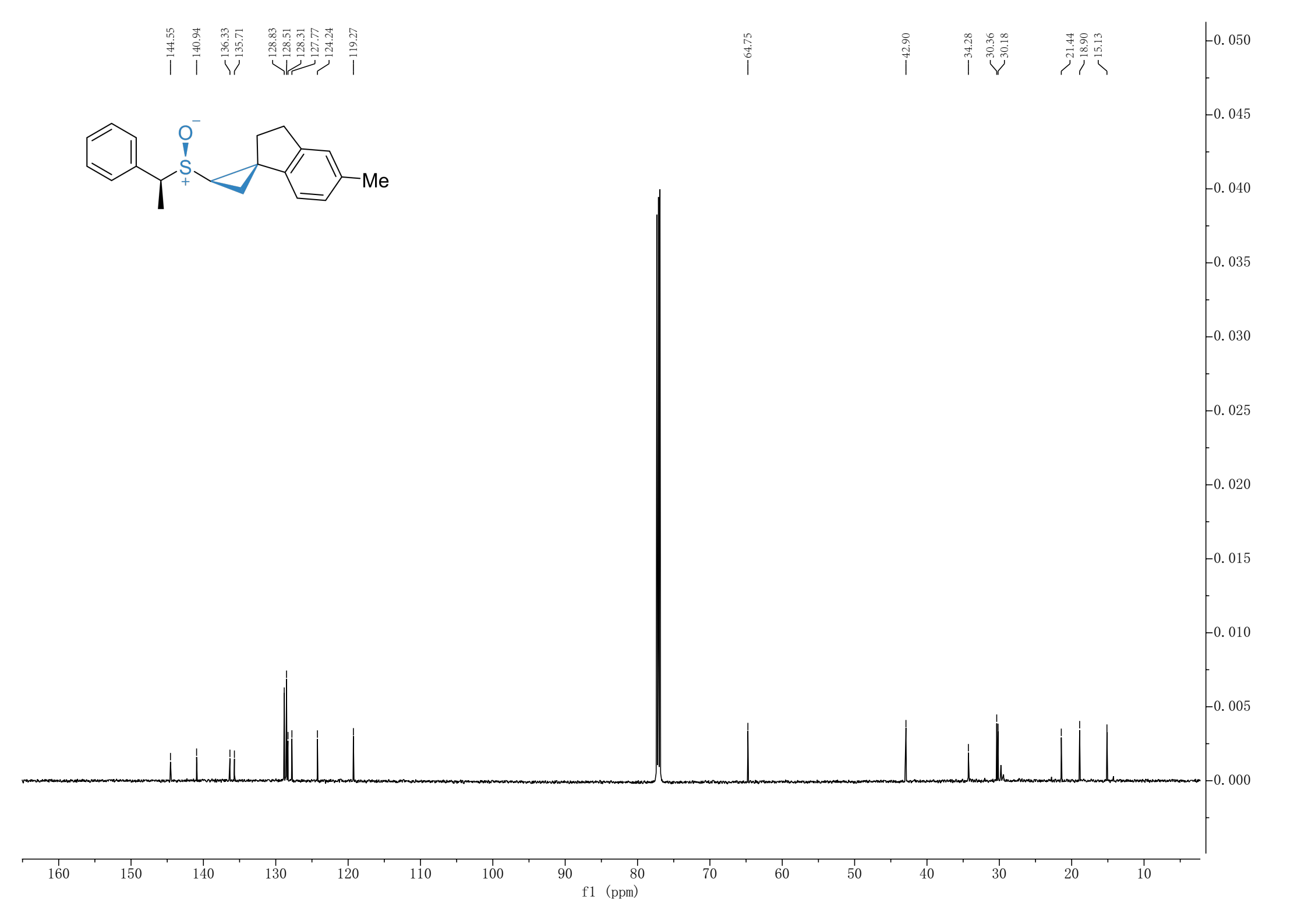
143.65
135.44
129.73
128.89
128.49
128.44
127.65
120.49
120.18
65.24
43.25
34.14
30.35
30.06
19.10
15.49
O
S
+
Br
0.032
0.030
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.21 7.21 7.20 7.19 7.19 7.18 7.18 7.16 7.15 7.14 7.13 7.12 7.12 6.97 6.96 6.93 6.92 6.36
3.95 3.94 3.93 3.92
2.78 2.77 2.76 2.75 2.74 2.74 2.73
2.37 2.37 2.35 2.34 2.34 2.33 2.28 1.93 1.93 1.92 1.91 1.90 1.90 1.89 1.75 1.74 1.69 1.68 1.67 1.67 1.66 1.66 1.65 1.64 1.64 1.63 1.62 1.41 1.41 1.40 1.39
O
S
+
Me
0.98 4.03 2.06 1.01 1.00 0.97 2.17 3.18 1.04 3.17 2.08 1.22
f1 (ppm)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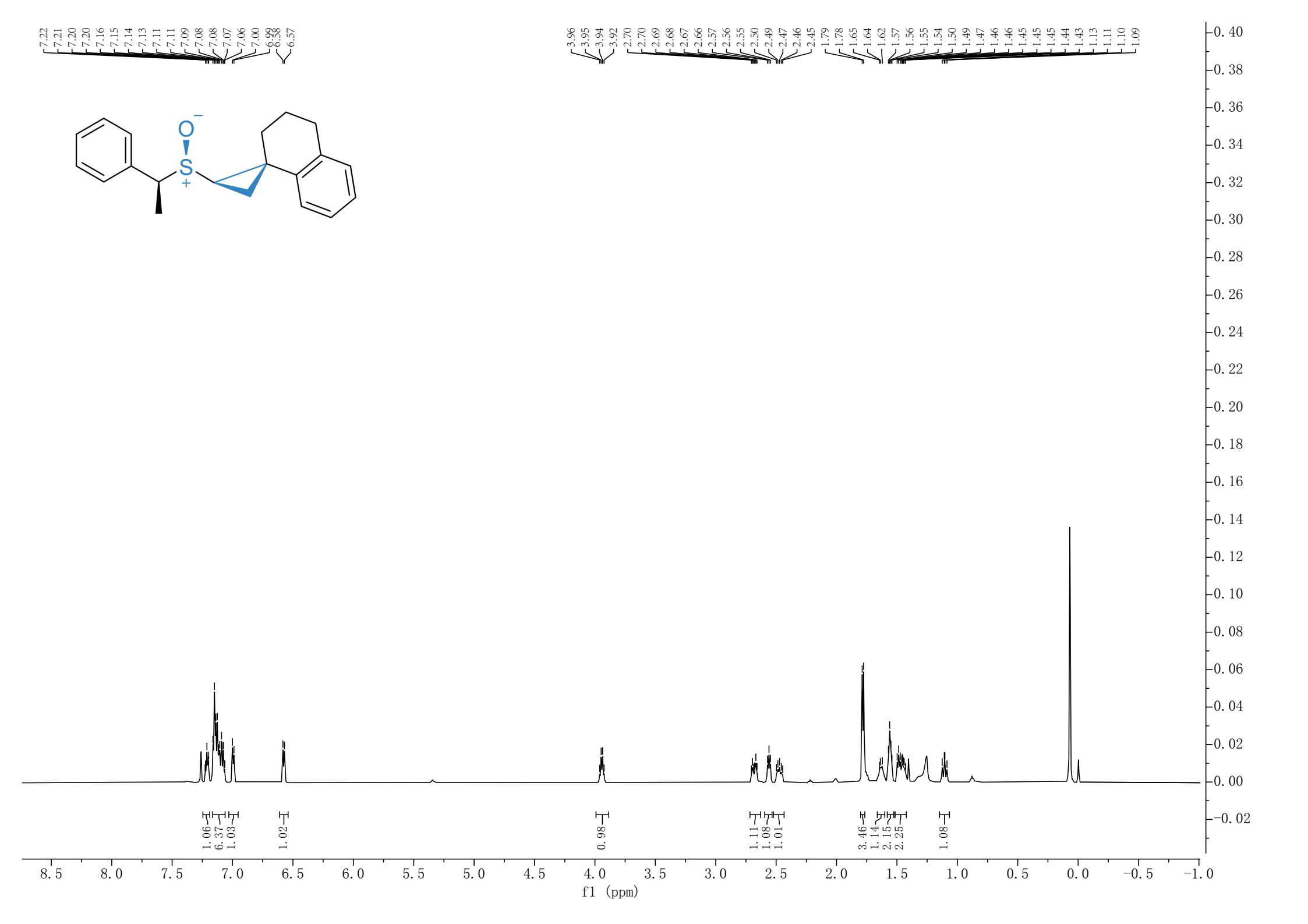
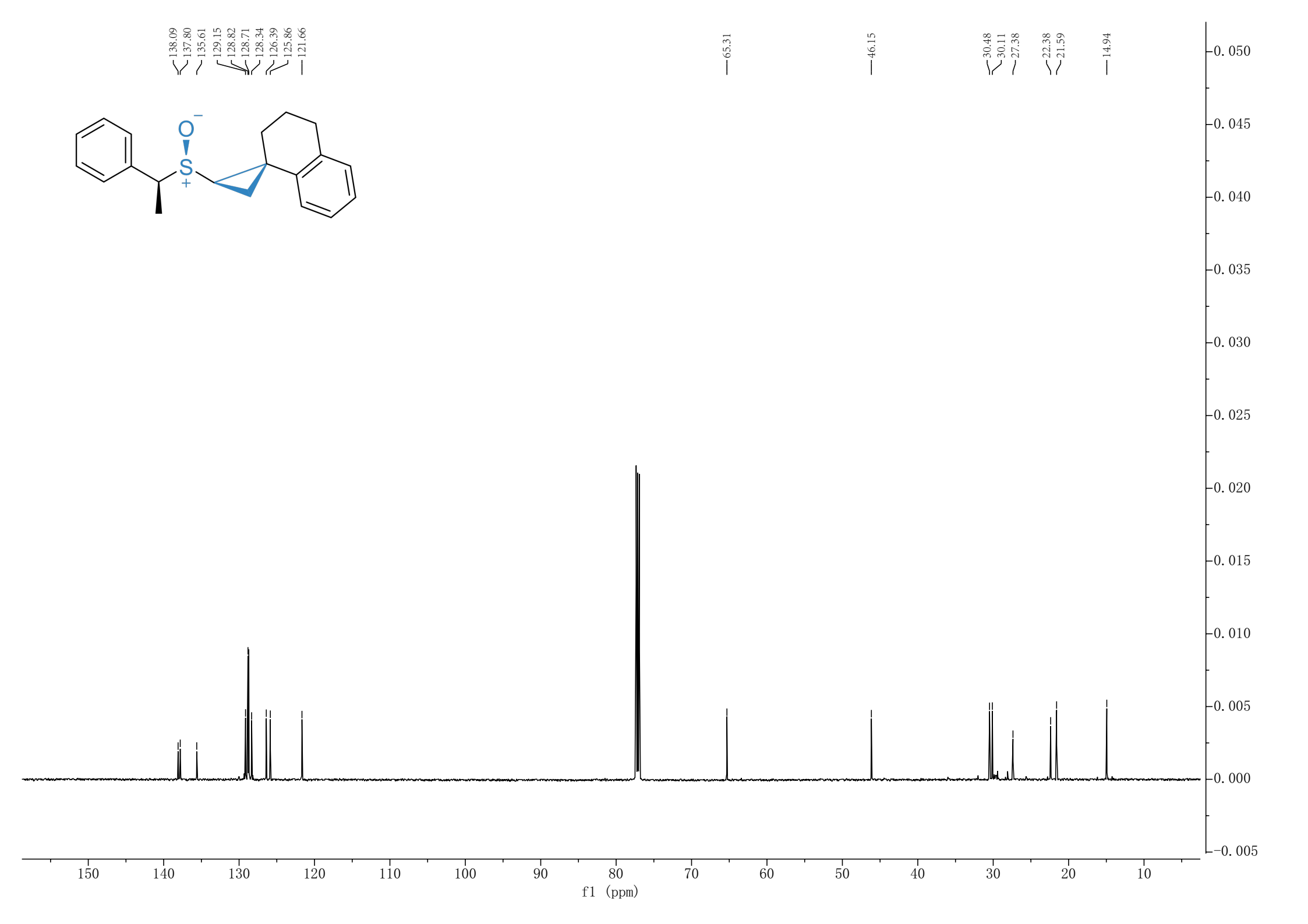
140.94
136.33
135.71
128.83
128.51
128.31
127.77
124.24
119.27
64.75
42.90
34.28
30.36
30.18
21.44
18.90
15.13
O
S
+
Me
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.22 7.21 7.20 7.20 7.16 7.15 7.14 7.13 7.11 7.11 7.09 7.08 7.08 7.07 7.06 7.00 6.59 6.58 6.57
3.96 3.95 3.94 3.92 2.70 2.70 2.68 2.67 2.66 2.57 2.56 2.55 2.50 2.49 2.47 2.46 2.45 1.79 1.78 1.65 1.64 1.62 1.57 1.56 1.55 1.54 1.50 1.49 1.47 1.46 1.46 1.45 1.45 1.45 1.44 1.43 1.13 1.11 1.10 1.09
O
S
+
1.06 6.37 1.03 1.02 0.98 1.11 1.08 1.01 3.46 1.14 2.15 2.25 1.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
0.40 0.38 0.36 0.34 0.32 0.30 0.28 0.26 0.24 0.22 0.20 0.18 0.16 0.14 0.12 0.10 0.08 0.06 0.04 0.02 0.00 -0.02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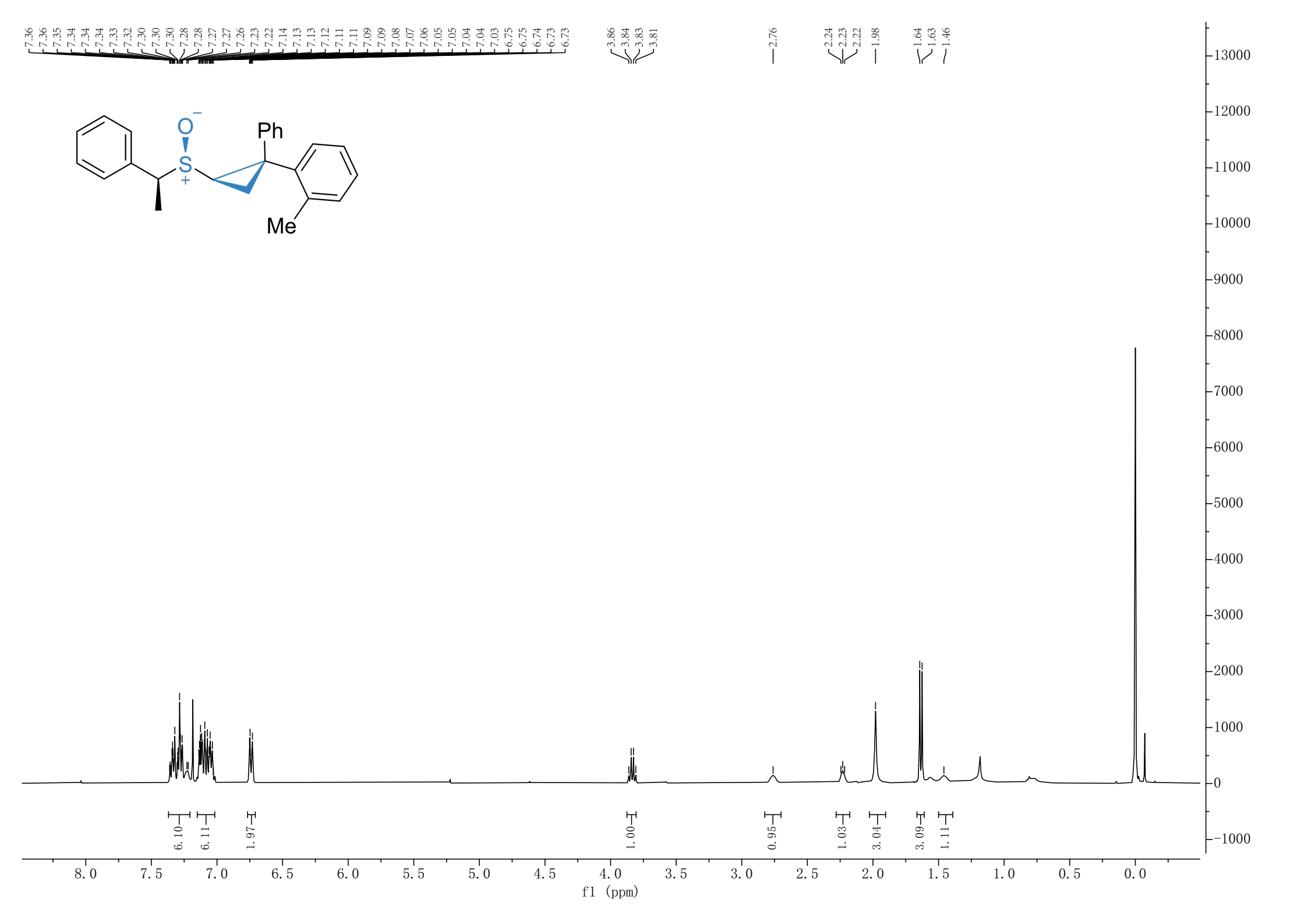
137.80
135.61
129.15
128.82
128.71
128.34
126.39
125.86
121.66
65.31
46.15
30.48
30.11
27.38
22.38
21.59
14.94
O
S
+
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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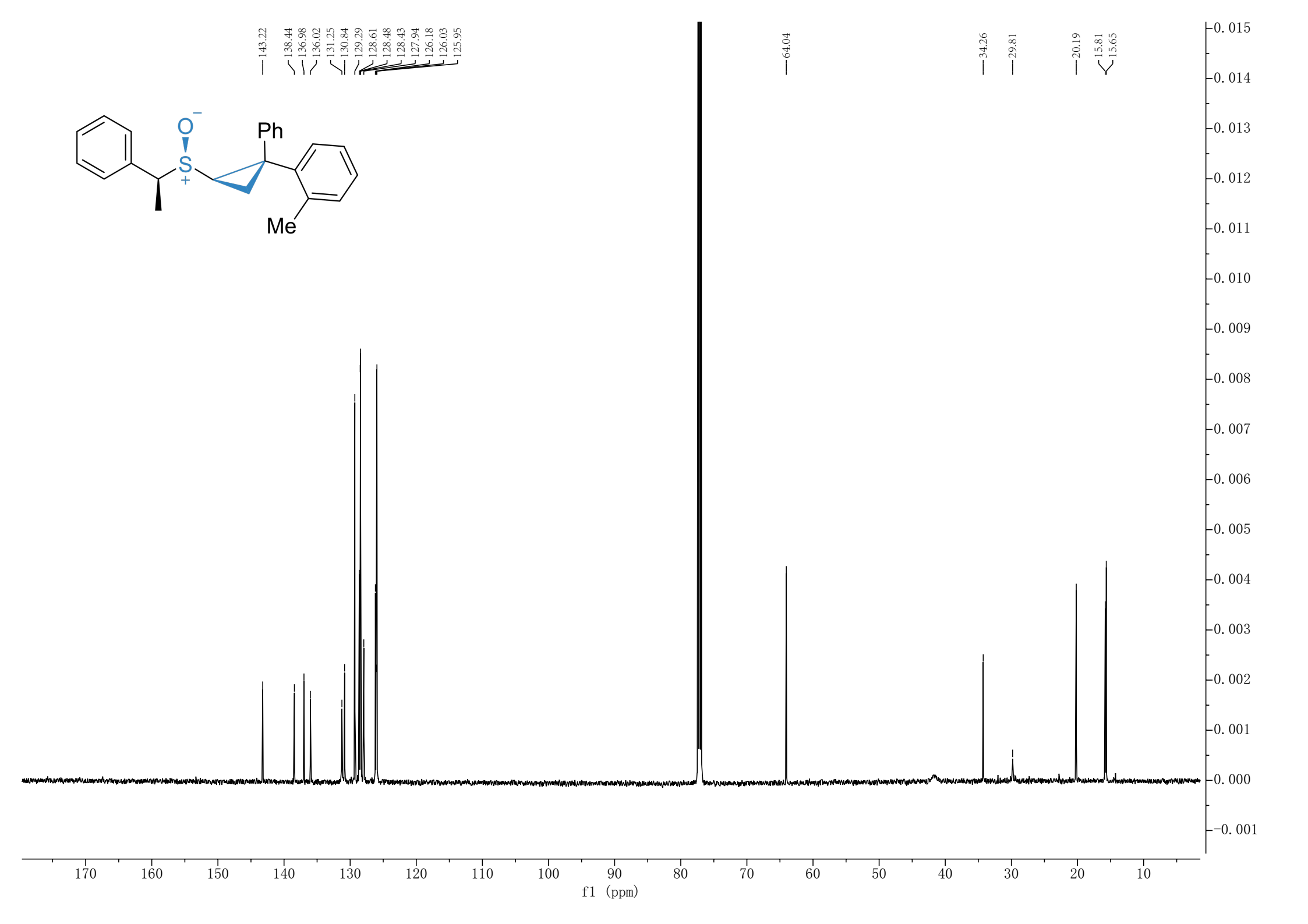
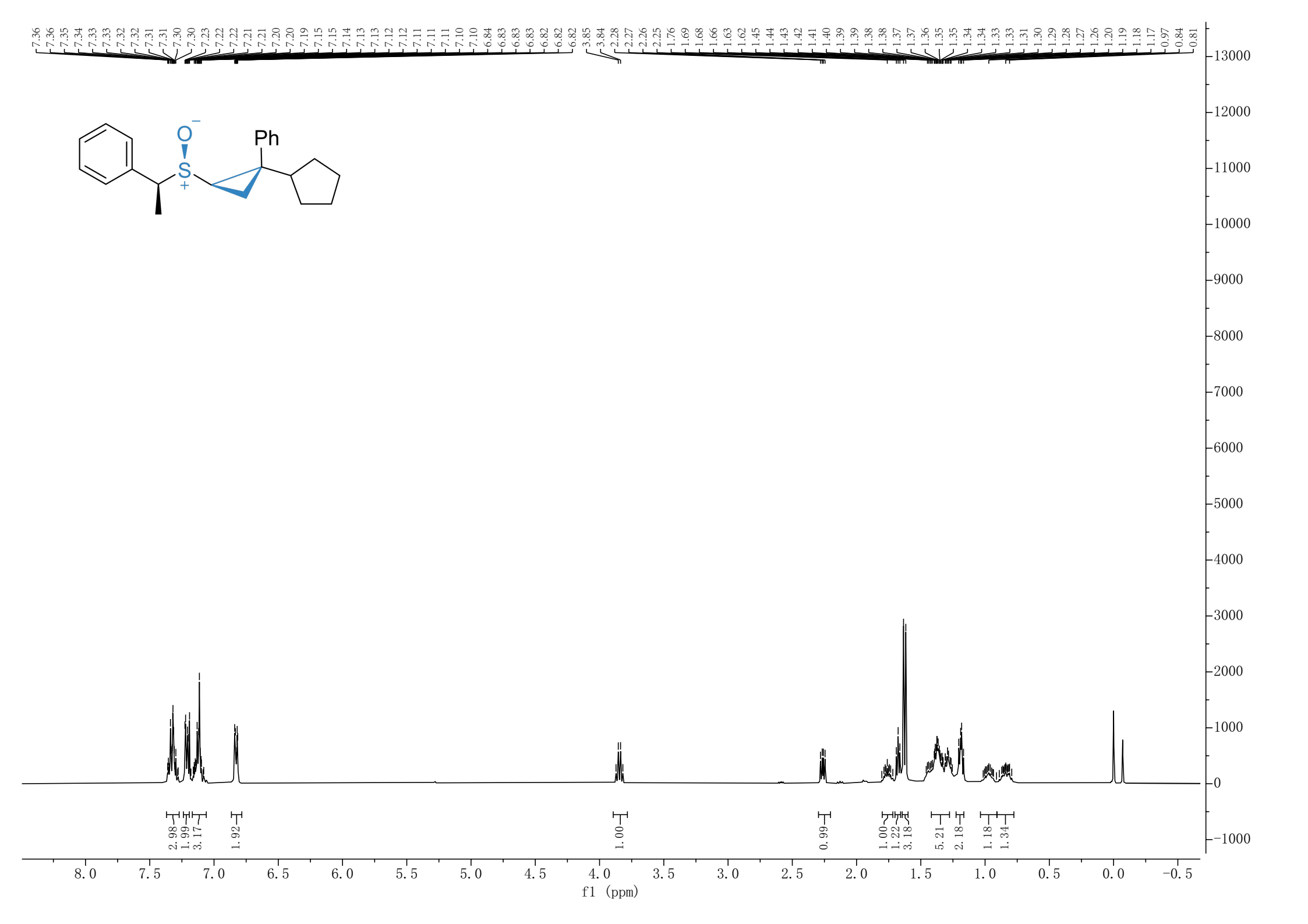
3.86 3.84 3.83 3.81
2.76
2.24 2.23 2.22
1.98
1.64 1.63 1.46
O
S
+
Ph
Me
13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
6.10 6.11 1.97 1.00 0.95 1.03 3.04 3.09 1.11
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.22
138.44
136.98
136.02
131.25
130.84
129.29
128.61
128.48
128.43
127.94
126.18
126.03
125.95
64.04
34.26
29.81
20.19
15.81
15.65
O
S
Ph
Me
f1 (ppm)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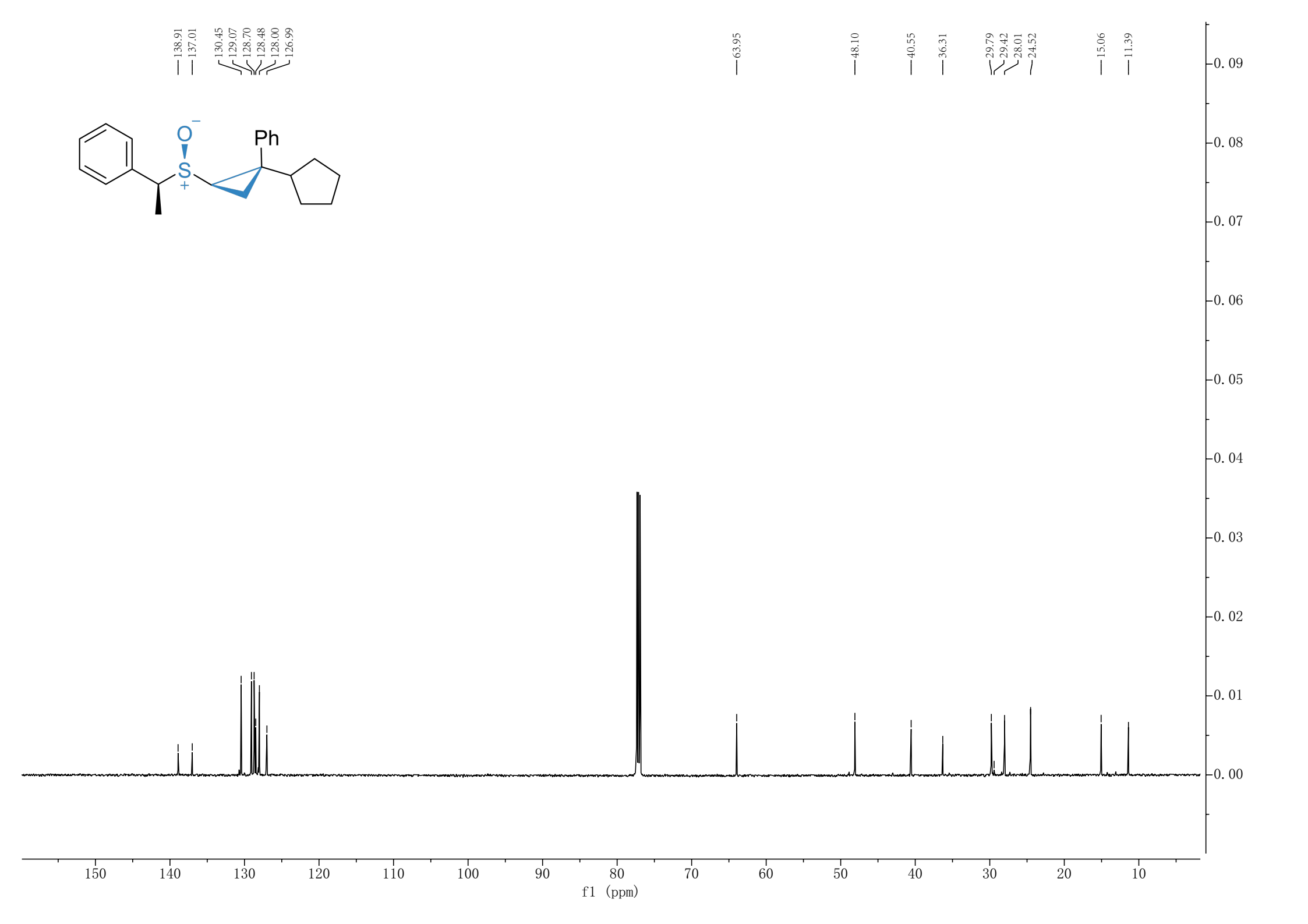
3.85 3.84 2.28 2.27 2.26 2.25 1.76 1.69 1.68 1.66 1.63 1.62 1.45 1.44 1.43 1.42 1.41 1.40 1.39 1.39 1.38 1.38 1.37 1.37 1.36 1.35 1.35 1.34 1.34 1.33 1.33 1.31 1.30 1.29 1.28 1.27 1.26 1.20 1.19 1.18 1.17 0.97 0.84 0.81
O
S
+
Ph
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
2.98
1.99
3.17
1.92
1.00
0.99
1.00
1.22
3.18
5.21
2.18
1.18
1.34
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
f1 (ppm)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130.45
129.07
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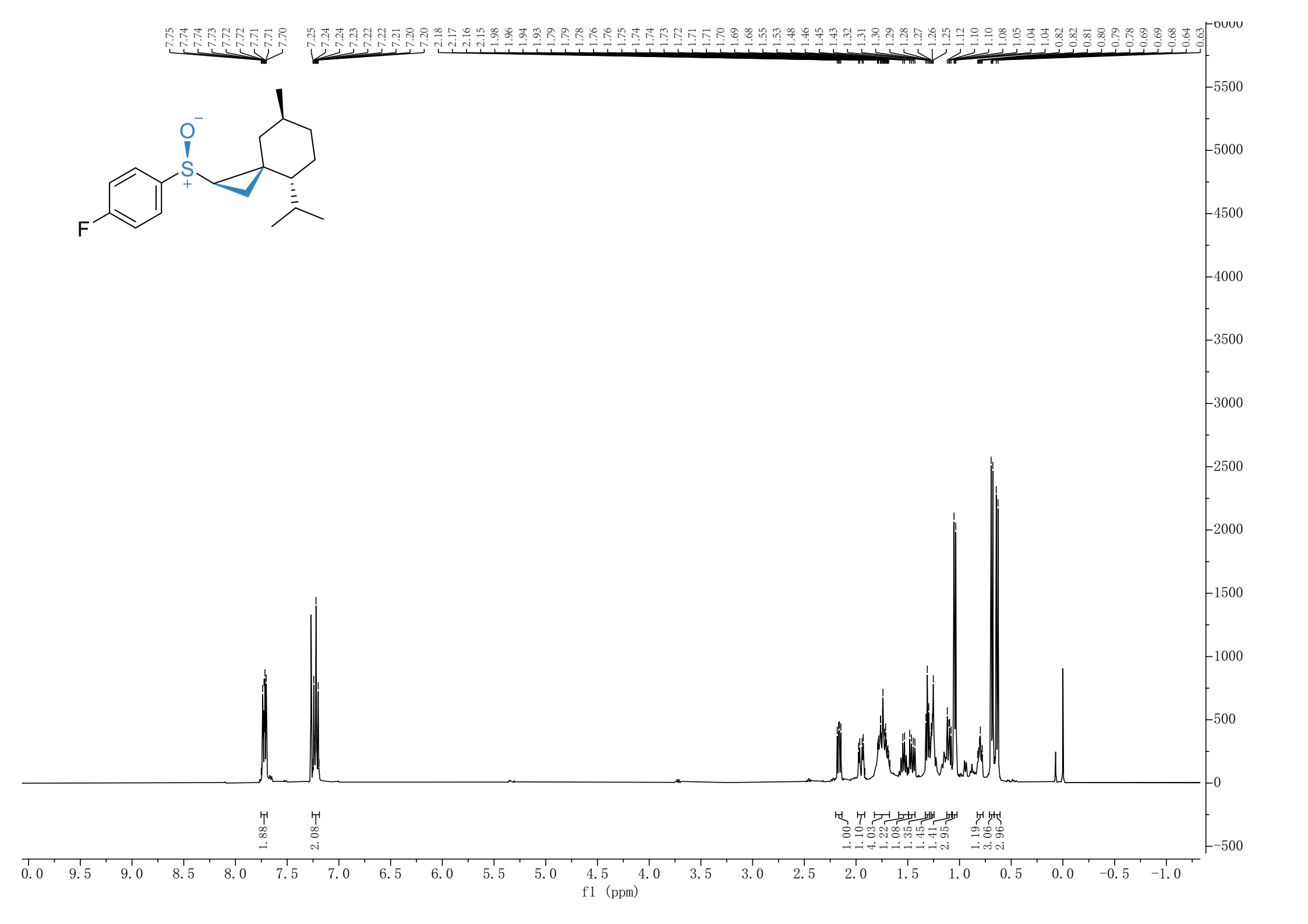
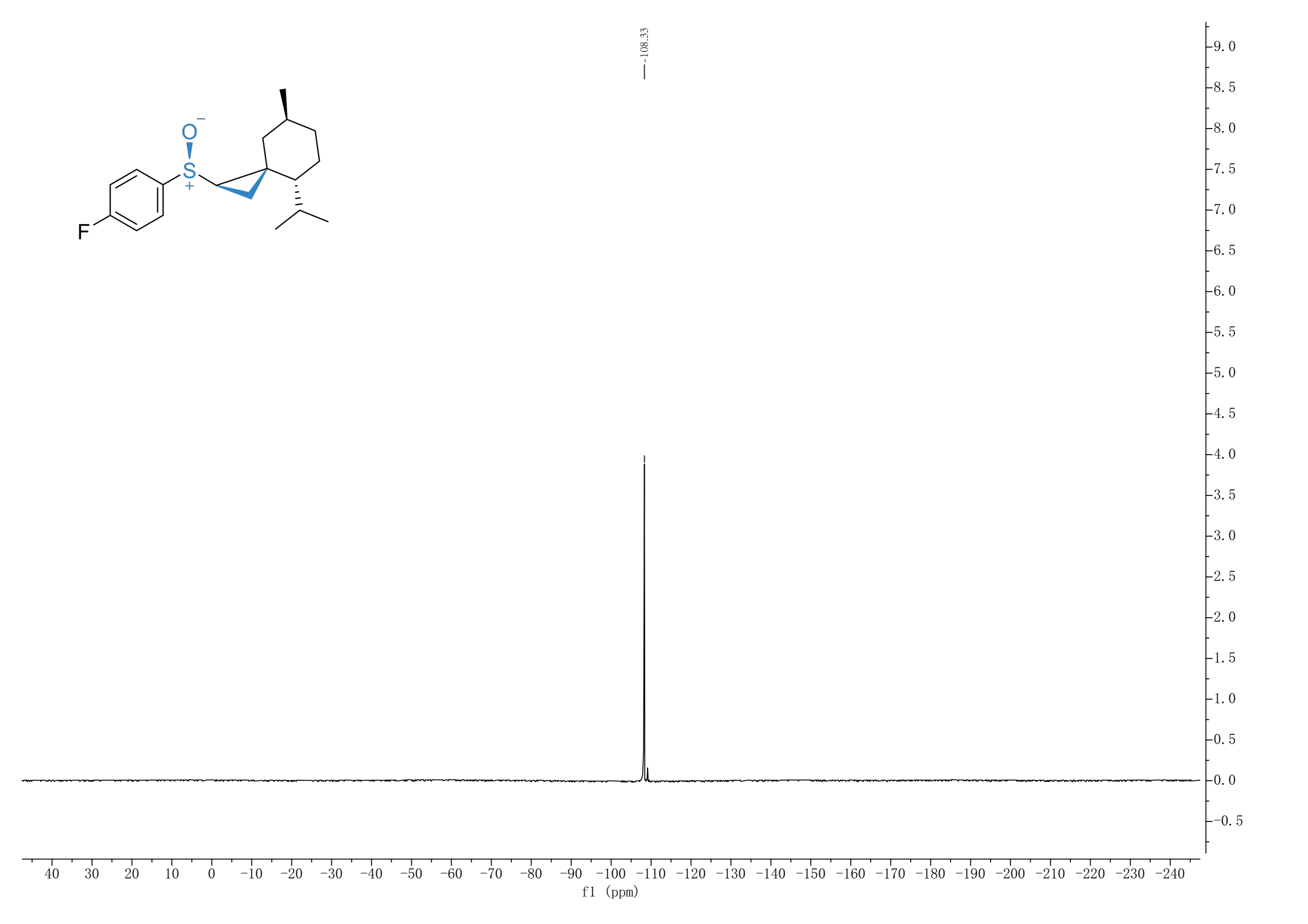
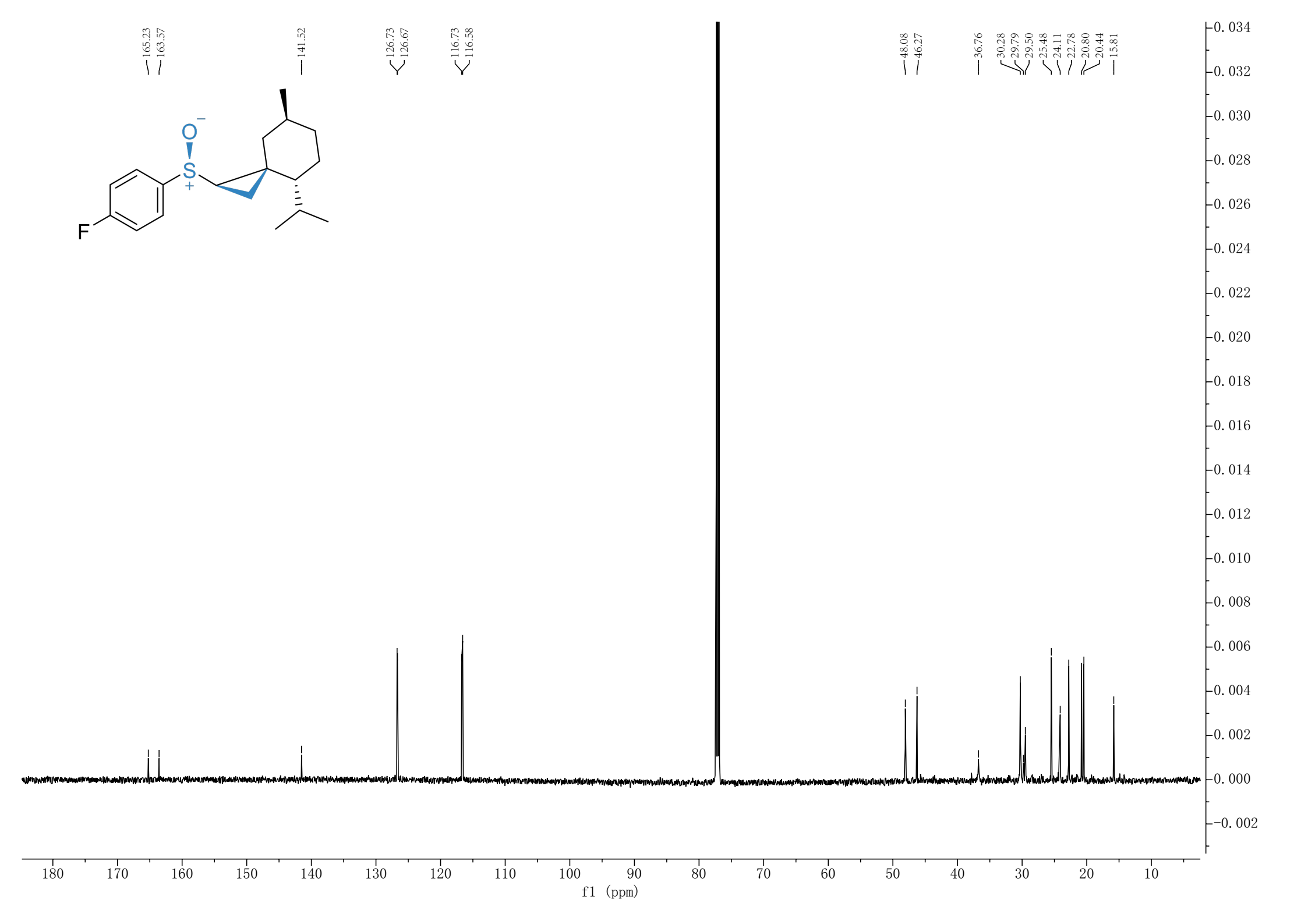
128.48
128.00
126.99
63.95
48.10
40.55
36.31
29.79
29.42
28.01
24.52
15.06
11.39
O
S
Ph
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.75 7.74 7.74 7.73 7.72 7.72 7.71 7.71 7.70
7.25 7.24 7.24 7.23 7.22 7.22 7.21 7.20 7.20
2.18 2.17 2.16 2.15 1.98 1.96 1.94 1.93 1.79 1.79 1.78 1.76 1.76 1.75 1.74 1.74 1.73 1.72 1.71 1.71 1.70 1.69 1.68 1.55 1.53 1.48 1.46 1.45 1.43 1.32 1.31 1.30 1.29 1.28 1.27 1.26 1.25 1.12 1.10 1.10 1.08 1.05 1.04 1.04 0.82 0.82 0.81 0.80 0.79 0.78 0.69 0.69 0.68 0.64 0.63
O
S
+
F
1.88
2.08
1.00
1.10
4.03
1.22
1.08
1.35
1.45
1.41
2.95
1.19
3.06
2.96
f1 (ppm)


-108.33
O
S
F
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
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)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163.57
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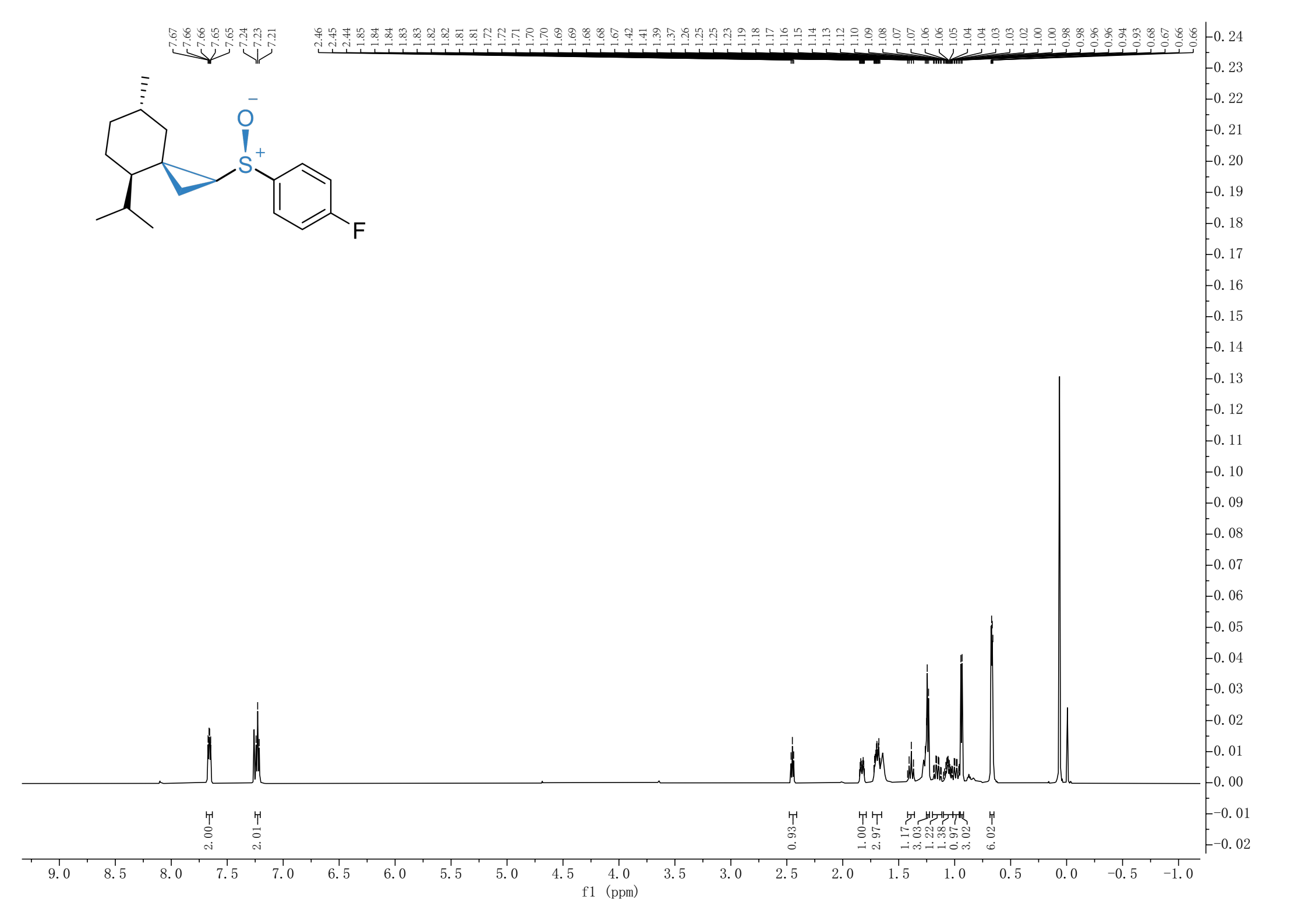
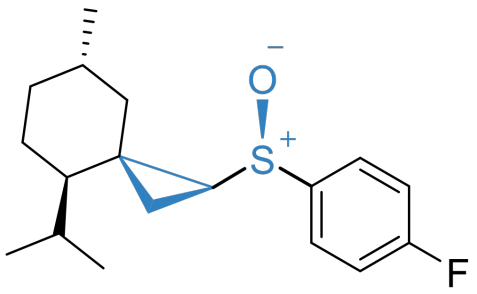
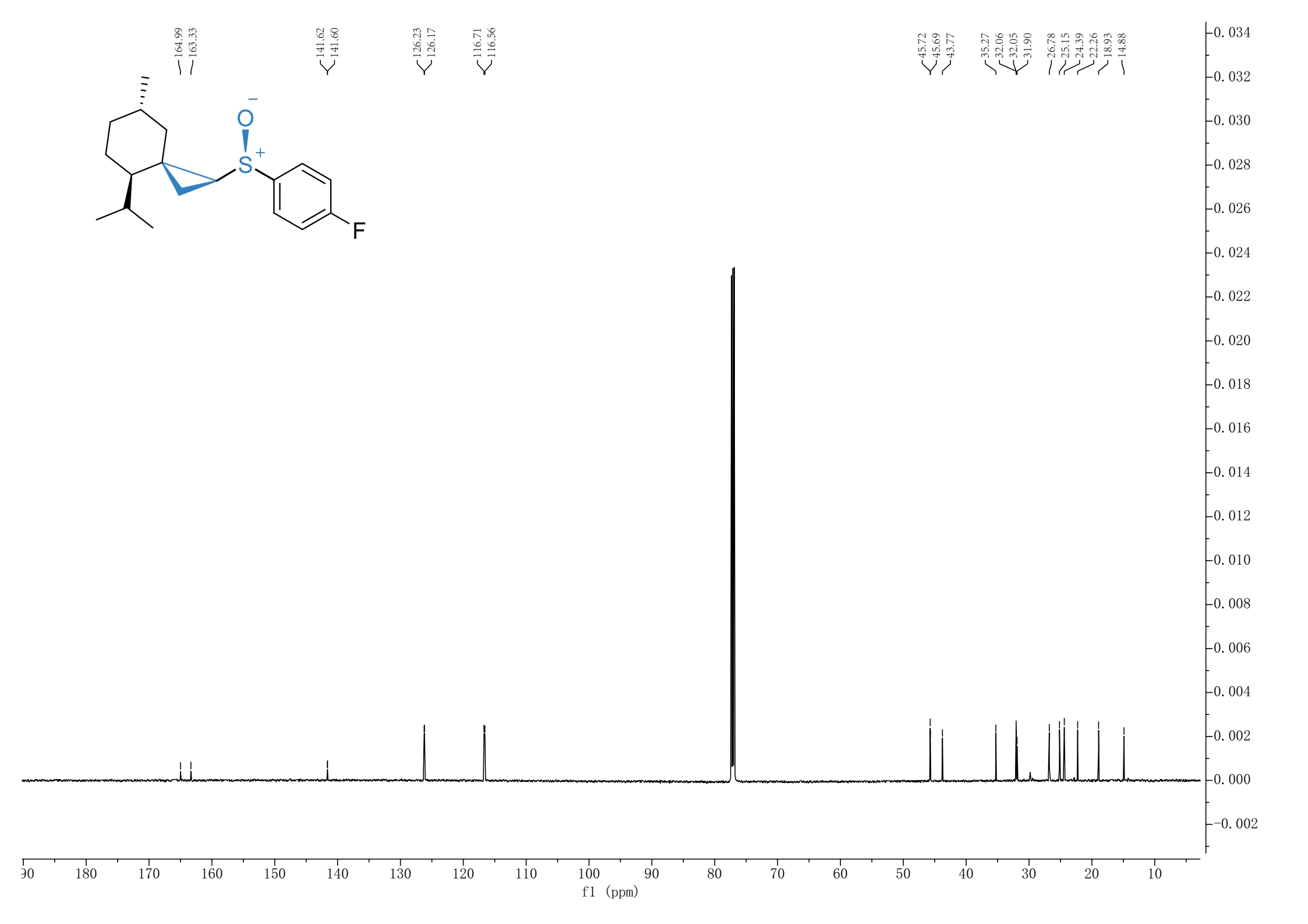
126.67
116.73
116.58
48.08
46.27
36.76
30.28
29.79
29.50
25.48
24.11
22.78
20.80
20.44
15.81
O
S
+
F
0.034
0.032
0.030
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.67 7.66 7.66 7.65 7.65 7.24 7.23 7.21
2.46 2.45 2.44 1.85 1.84 1.84 1.83 1.83 1.82 1.82 1.81 1.81 1.72 1.72 1.71 1.70 1.70 1.69 1.69 1.68 1.68 1.67 1.42 1.41 1.39 1.37 1.26 1.25 1.25 1.23 1.19 1.18 1.17 1.16 1.15 1.14 1.13 1.12 1.10 1.09 1.08 1.07 1.07 1.06 1.06 1.05 1.04 1.04 1.03 1.03 1.02 1.00 1.00 0.98 0.98 0.96 0.96 0.94 0.93 0.68 0.67 0.66 0.66
O
S
F
2.00
2.01
0.93
1.00
2.97
1.17
3.03
1.22
1.38
0.97
3.02
6.02
f1 (ppm)


O
S
F

-109.15
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


164.99
163.33
141.62
141.60
126.23
126.17
116.71
116.56
45.72
45.69
43.77
35.27
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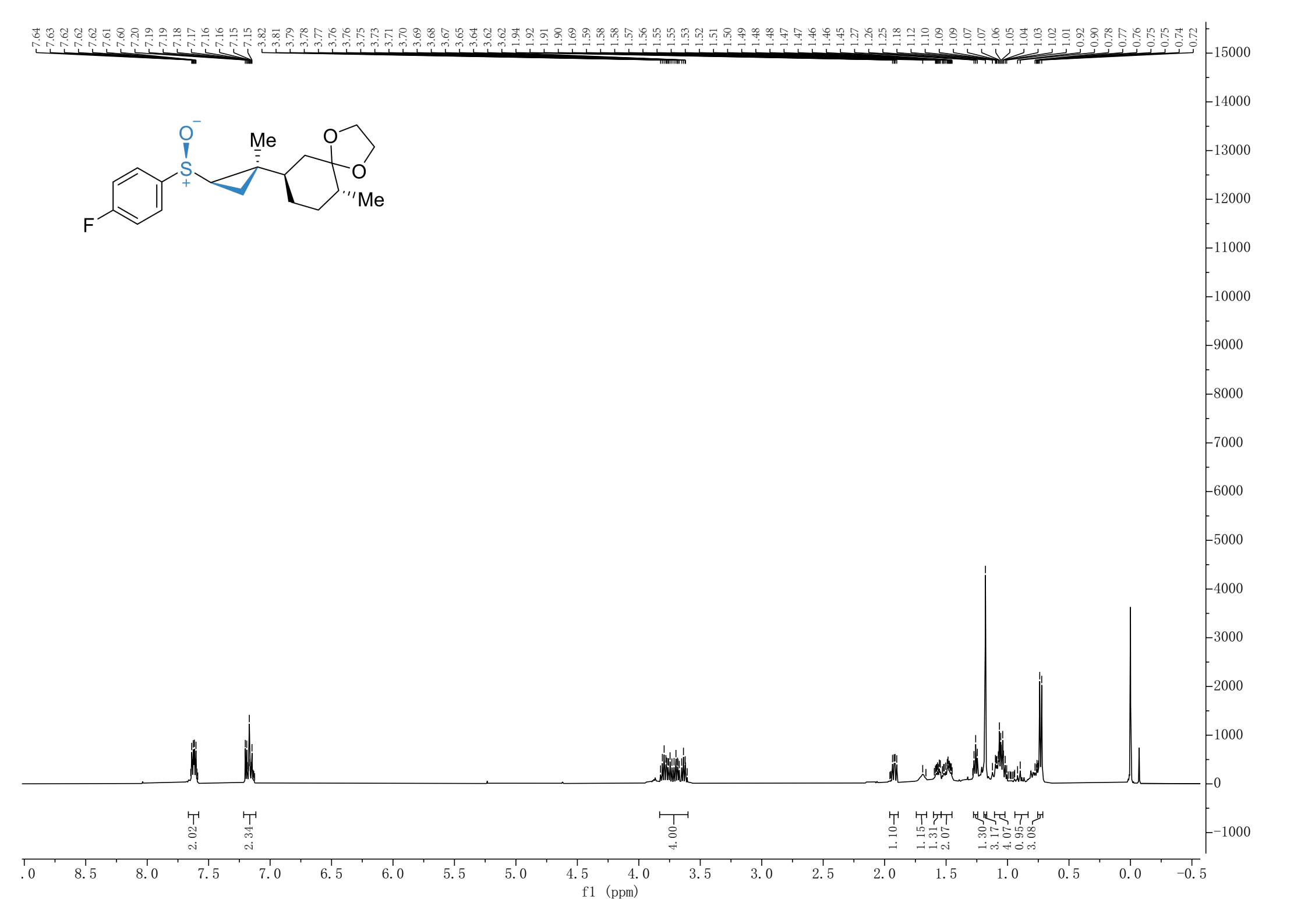
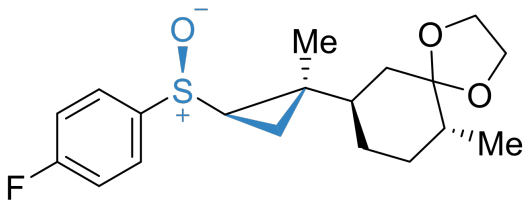
22.26
18.93
14.88
O
S
F
f1 (ppm)


7.64 7.63 7.62 7.62 7.62 7.61 7.60 7.20 7.19 7.19 7.18 7.17 7.16 7.16 7.15 7.15
3.82 3.81 3.79 3.78 3.77 3.76 3.76 3.75 3.73 3.71 3.70 3.69 3.68 3.67 3.65 3.64 3.62 3.62 1.94 1.92 1.91 1.90 1.69 1.59 1.58 1.58 1.57 1.56 1.55 1.55 1.53 1.52 1.51 1.50 1.49 1.48 1.48 1.47 1.47 1.46 1.46 1.45 1.27 1.26 1.25 1.18 1.12 1.10 1.09 1.09 1.07 1.07 1.06 1.05 1.04 1.03 1.02 1.01 0.92 0.90 0.78 0.77 0.76 0.75 0.75 0.74 0.72
O
S
+
Me
O
O
Me
F
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
2.02
2.34
4.00
1.10
1.15
1.31
2.07
1.30
3.17
4.07
0.95
3.08
.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
f1 (ppm)

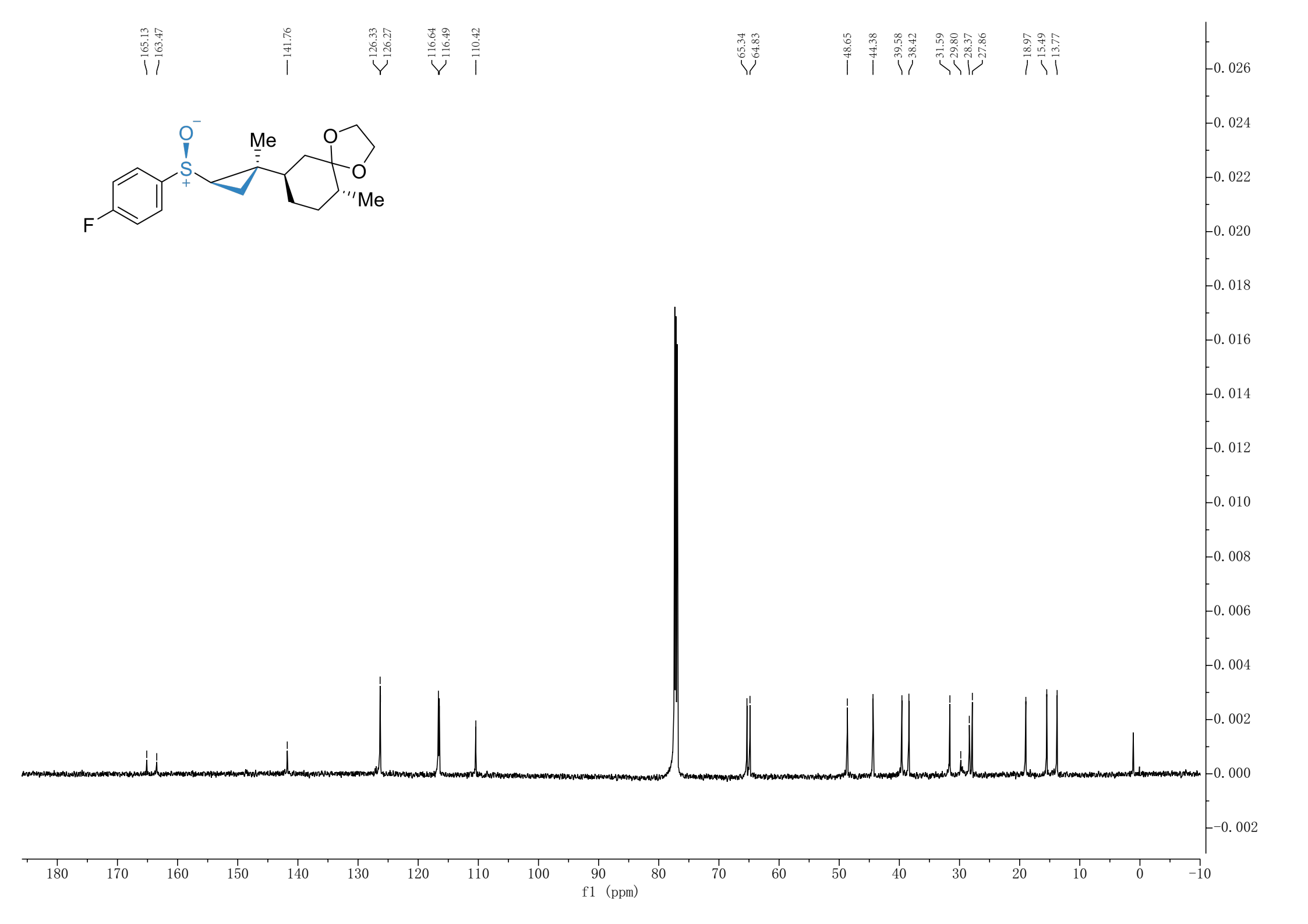


-108.54

3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)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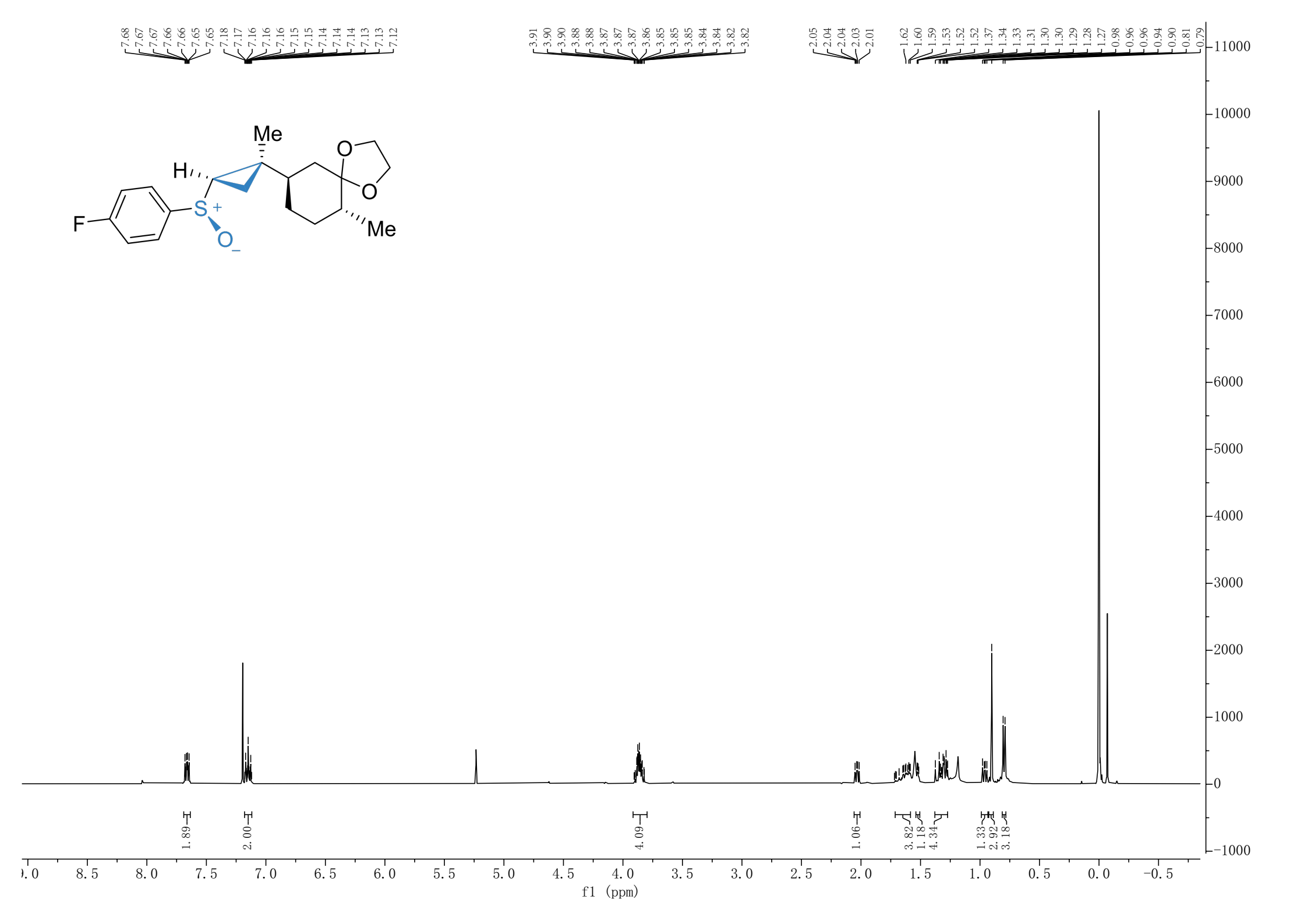
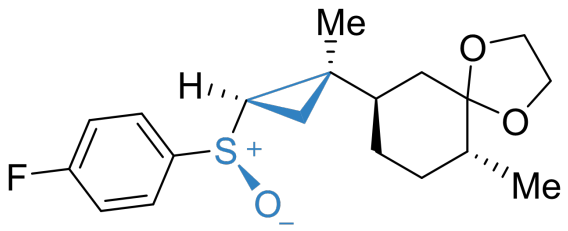
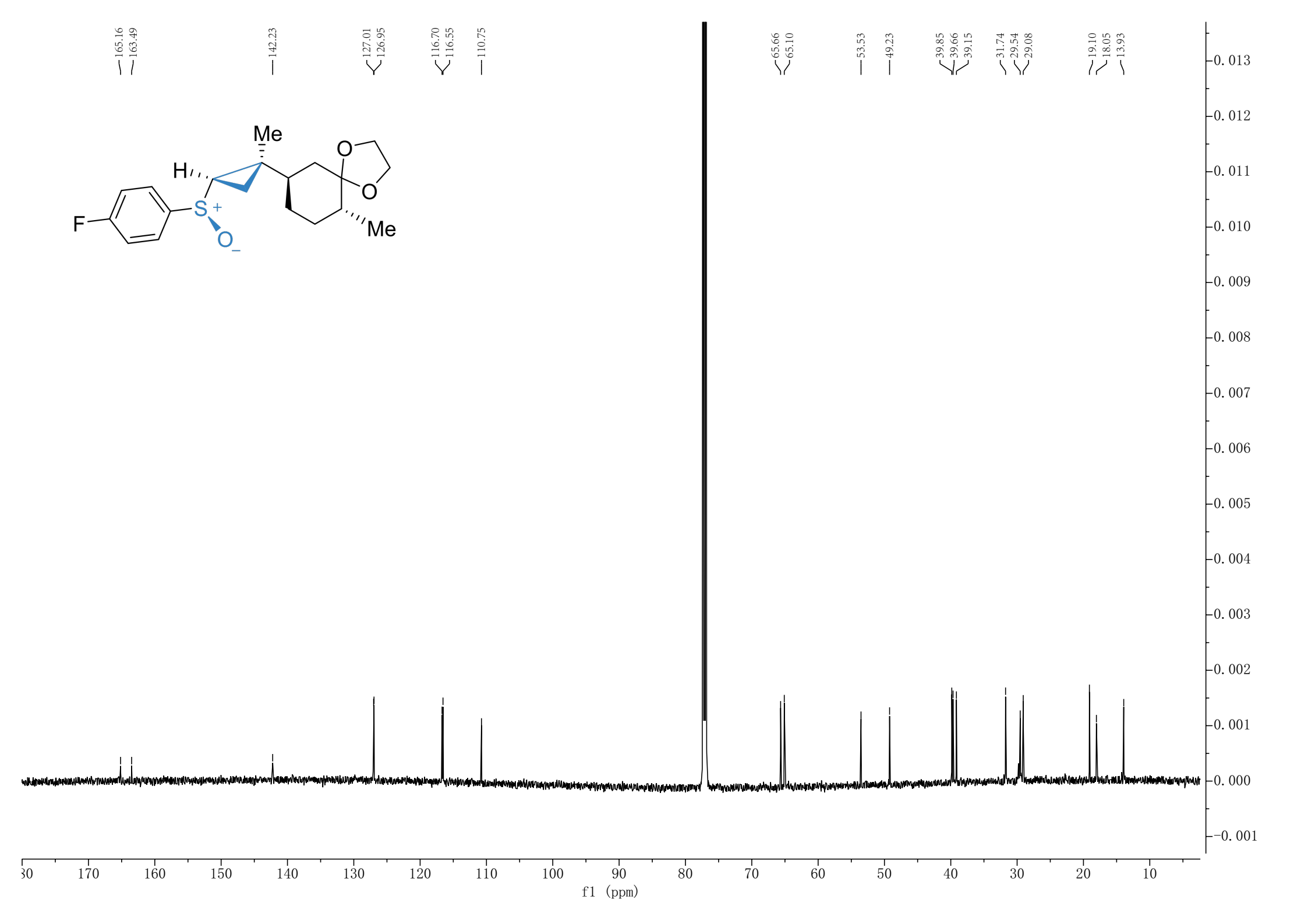
141.76
126.33
126.27
116.64
116.49
110.42
65.34
64.83
48.65
44.38
39.58
38.42
31.59
29.80
28.37
27.86
18.97
15.49
13.77
O
S
+
Me
O
O
Me
F
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Me
H
O
O
S +
O_
F
Me
f1 (ppm)


Me
H
O
O
S
+
F
O
Me

-108.54
4000
3500
3000
2500
2000
1500
1000
500
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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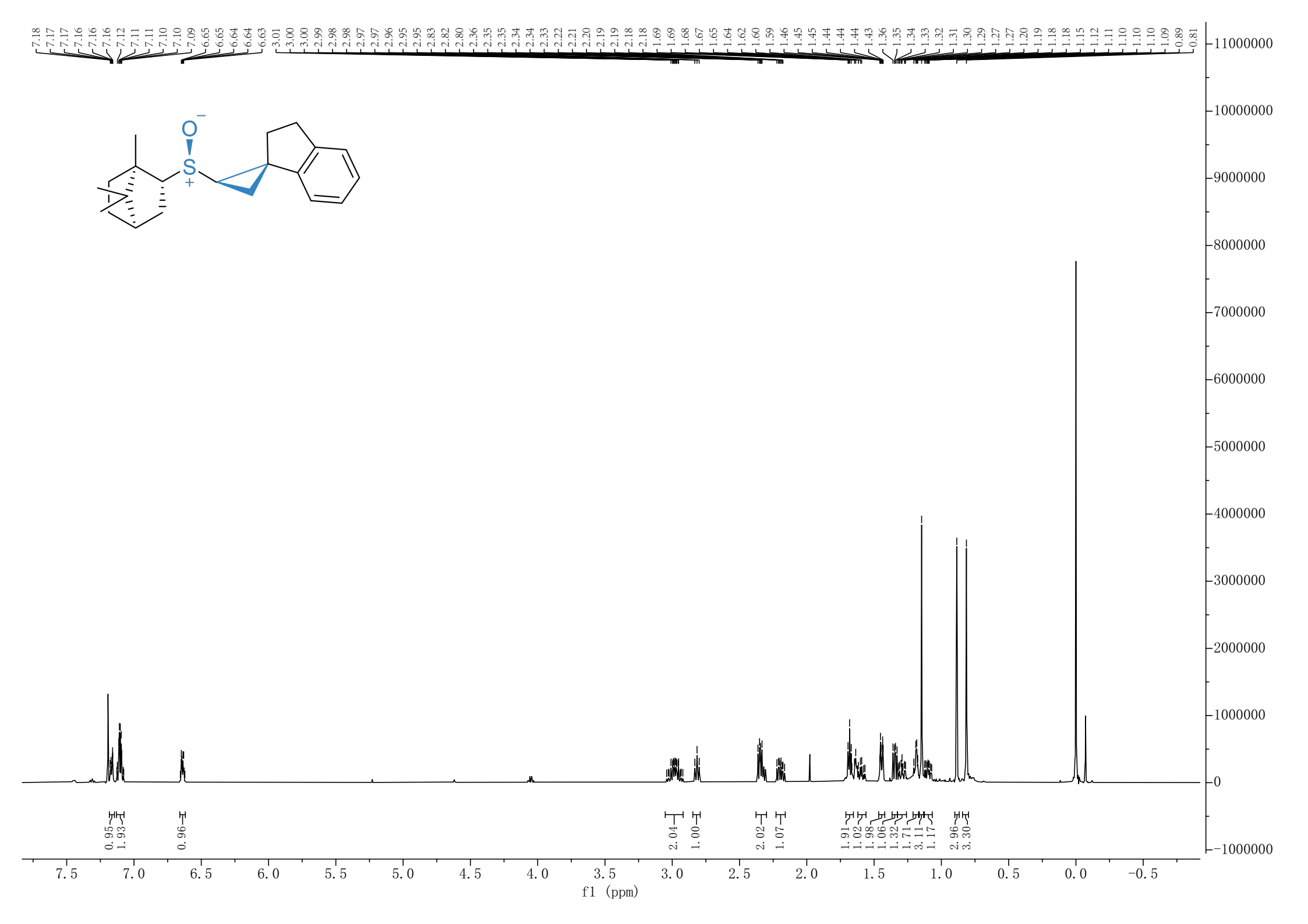
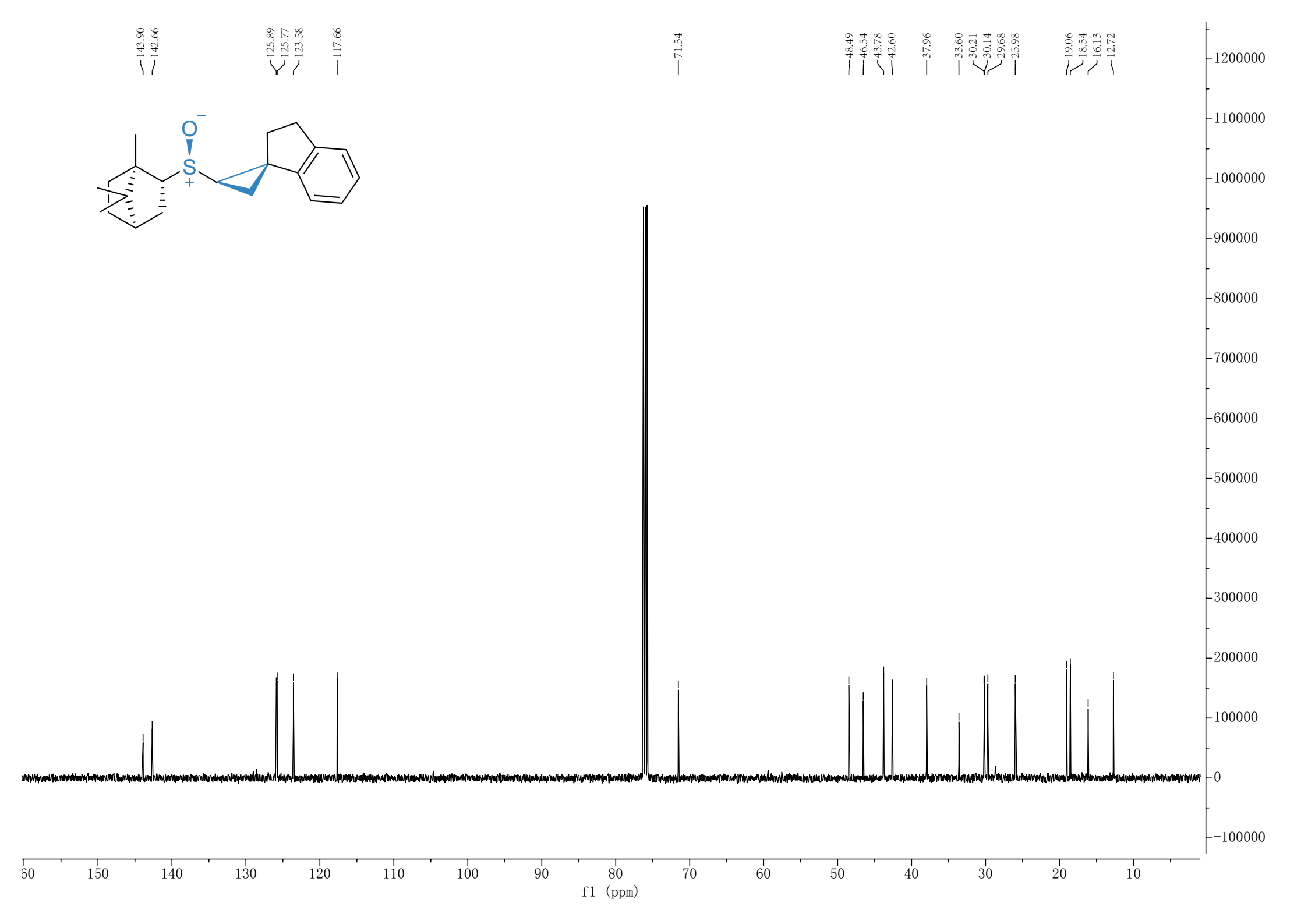
142.23
127.01
126.95
116.70
116.55
110.75
65.66
65.10
53.53
49.23
39.85
39.66
39.15
31.74
29.54
29.08
19.10
18.05
13.93
Me
H
O
O
S +
O_
F
Me
0.013
0.012
0.011
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
-0.001
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.18 7.17 7.17 7.16 7.16 7.16 7.12 7.11 7.11 7.10 7.10 7.09 6.65 6.65 6.64 6.64 6.63
3.01 3.00 3.00 2.99 2.98 2.98 2.97 2.97 2.96 2.95 2.95 2.83 2.82 2.80 2.36 2.35 2.35 2.34 2.34 2.33 2.22 2.21 2.20 2.19 2.19 2.18 2.18 1.69 1.69 1.68 1.67 1.65 1.64 1.62 1.60 1.59 1.46 1.45 1.45 1.44 1.44 1.44 1.43 1.36 1.35 1.34 1.33 1.32 1.31 1.30 1.29 1.27 1.27 1.20 1.19 1.18 1.18 1.15 1.12 1.11 1.10 1.10 1.10 1.09 0.89 0.81
O
S
+
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
0.95 1.93 0.96 2.04 1.00 2.02 1.07 1.91 1.02 1.98 1.06 1.32 1.71 3.11 1.17 2.96 3.30
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
f1 (ppm)


143.90
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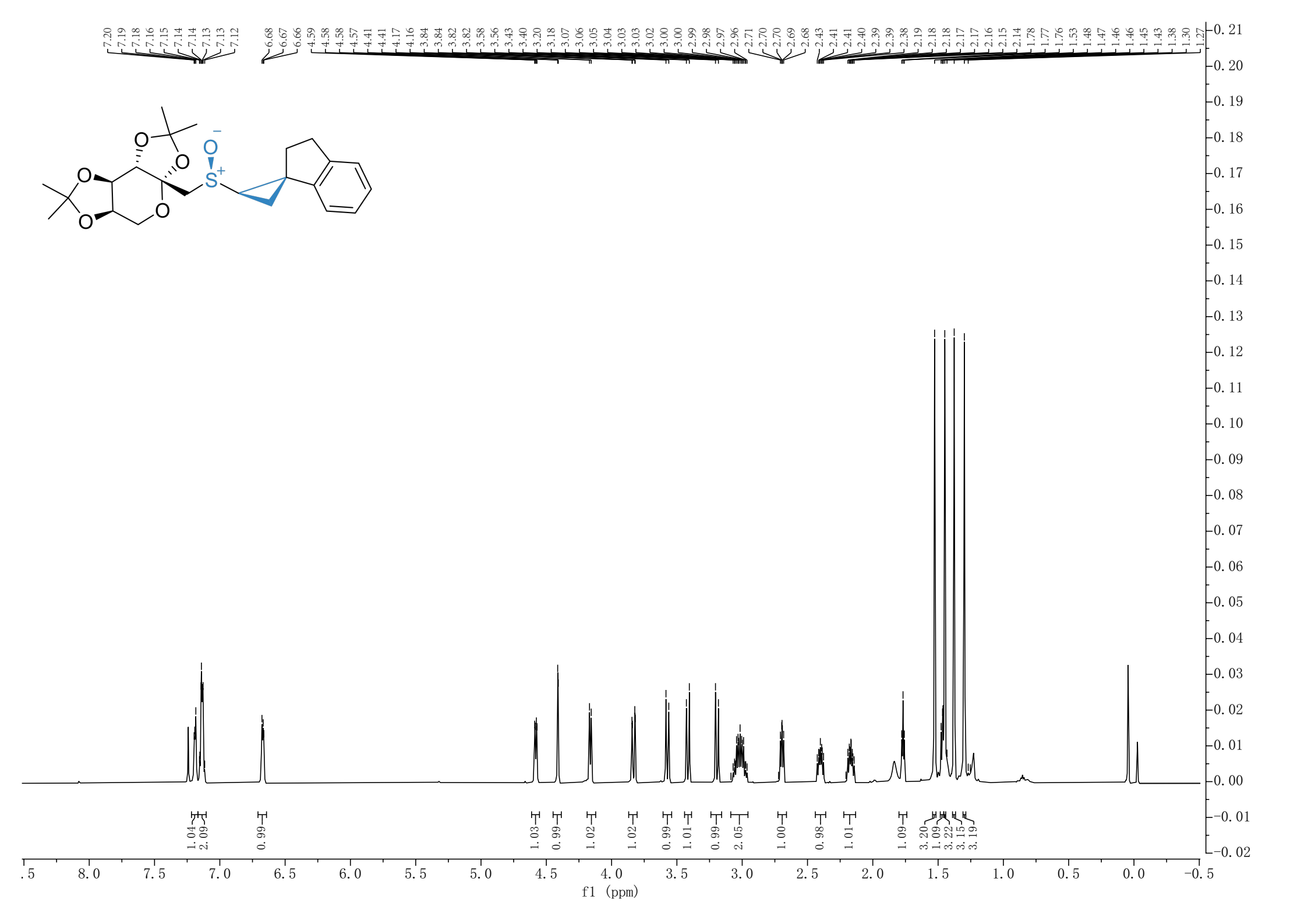
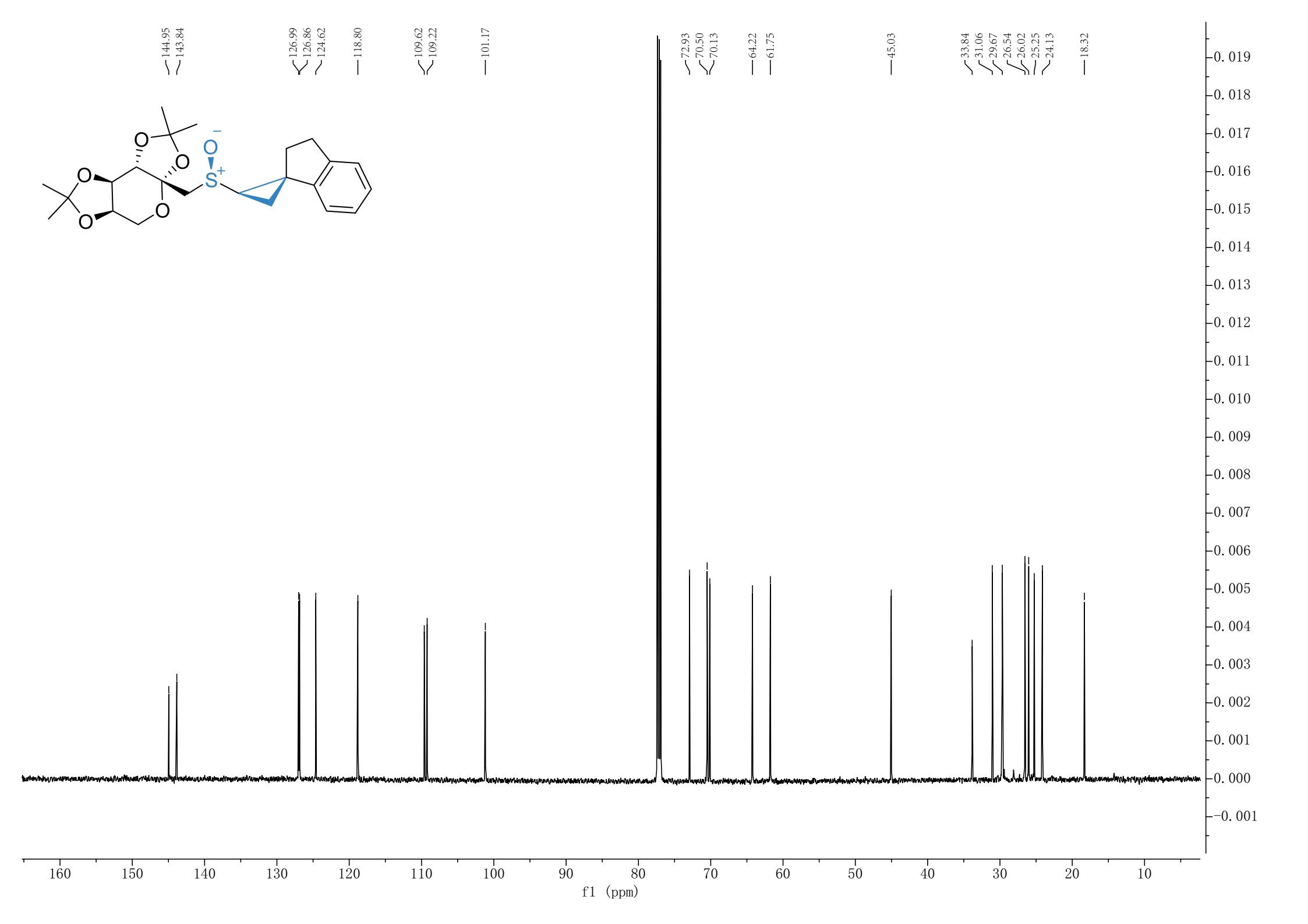
125.89
125.77
123.58
117.66
71.54
48.49
46.54
43.78
42.60
37.96
33.60
30.21
30.14
29.68
25.98
19.06
18.54
16.13
12.72
O
S
+
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.20 7.19 7.18 7.16 7.15 7.14 7.14 7.13 7.13 7.12
6.68 6.67 6.66
4.59 4.58 4.58 4.57 4.41 4.41 4.17 4.16 3.84 3.84 3.82 3.82 3.58 3.56 3.43 3.40 3.20 3.18 3.07 3.06 3.05 3.04 3.03 3.03 3.02 3.00 3.00 2.99 2.98 2.97 2.96 2.71 2.70 2.70 2.69 2.68
2.43 2.41 2.41 2.40 2.39 2.39 2.38 2.19 2.18 2.18 2.17 2.17 2.16 2.15 2.14 1.78 1.77 1.76 1.53 1.48 1.47 1.46 1.46 1.45 1.43 1.38 1.30 1.27
O
O
O
O
O
S+
O−
1.04
2.09
0.99
1.03
0.99
1.02
1.02
0.99
1.01
0.99
2.05
1.00
0.98
1.01
1.09
3.20
1.09
3.22
3.15
3.19
f1 (ppm)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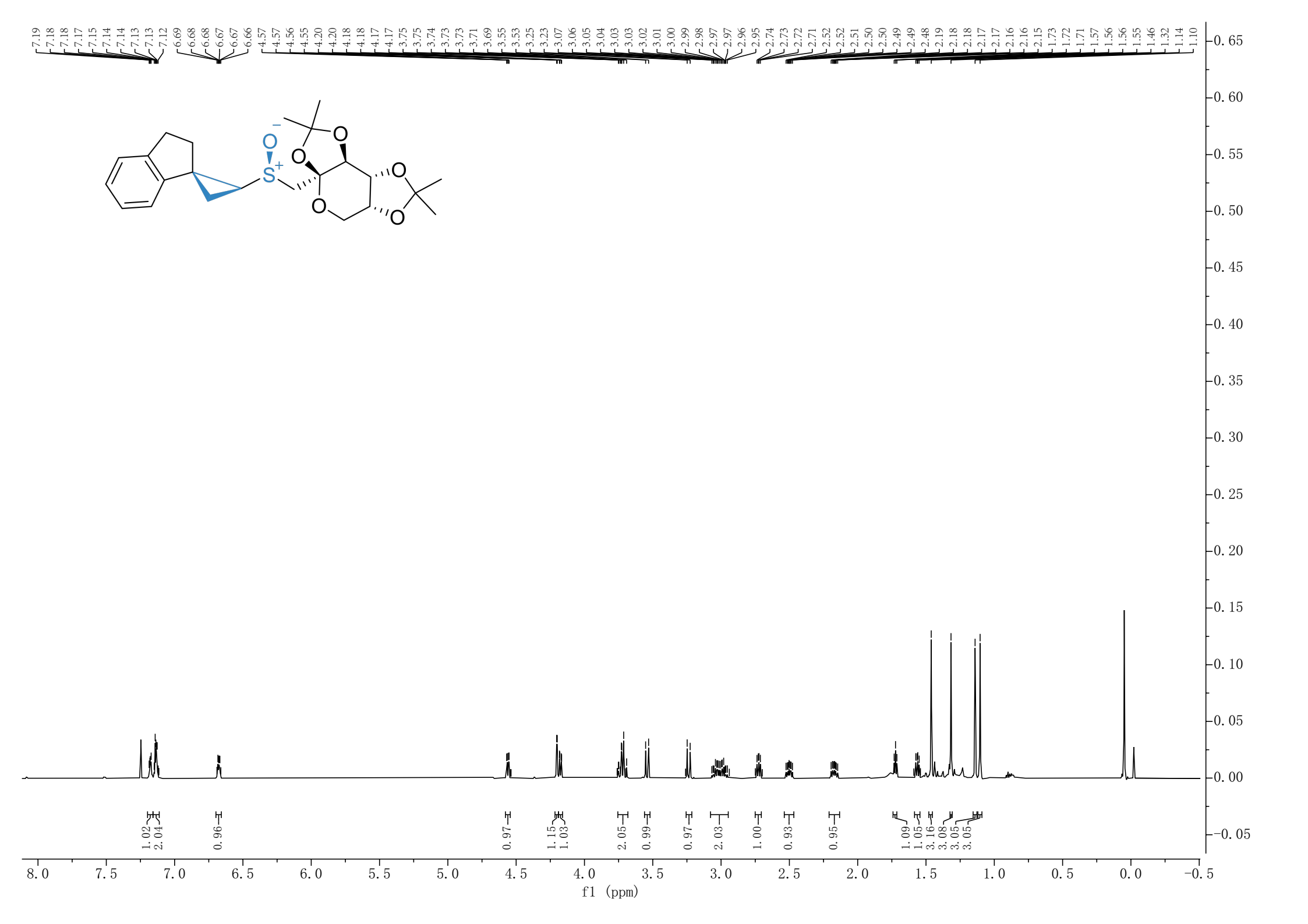
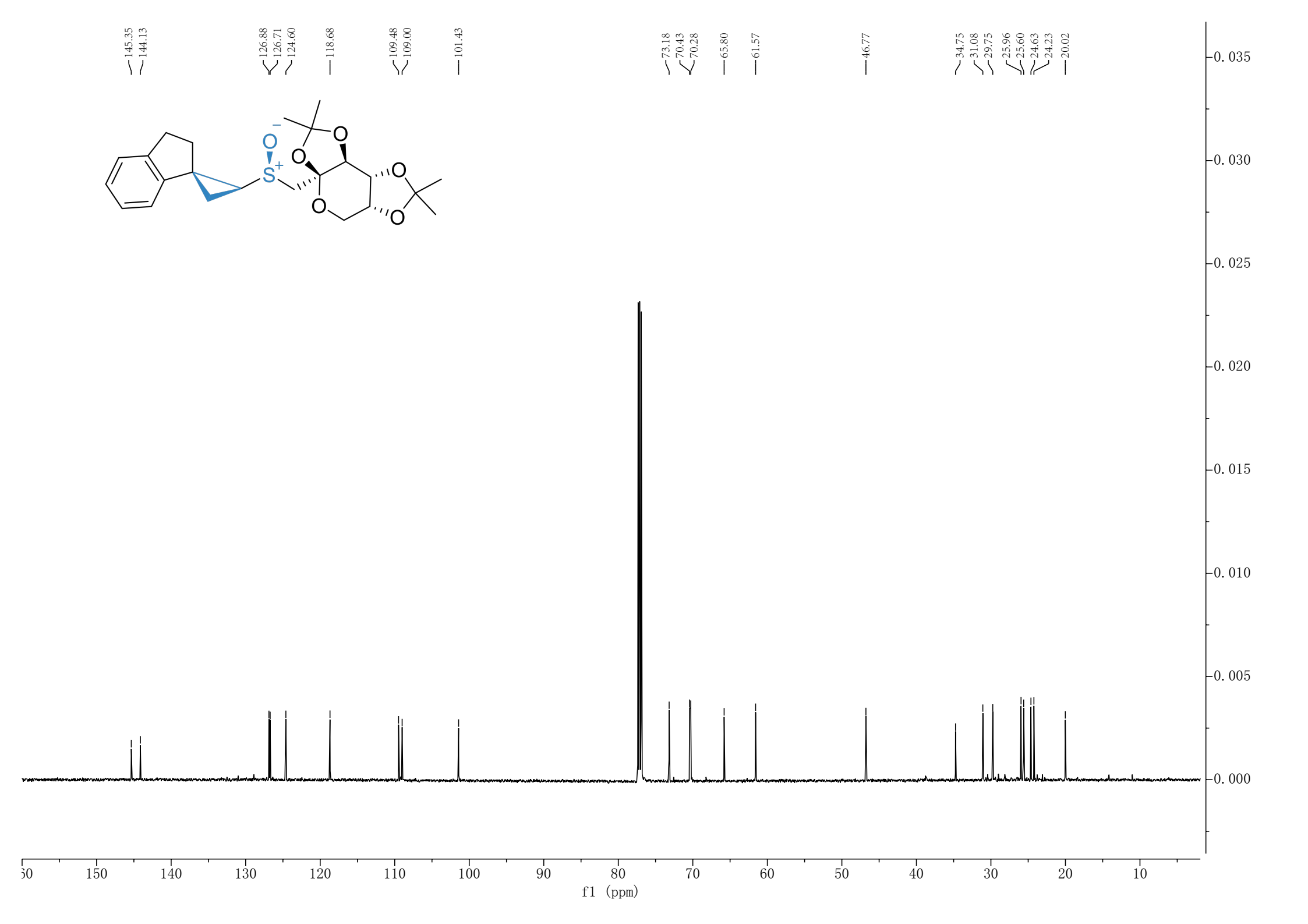
143.84
126.99
126.86
124.62
118.80
109.62
109.22
101.17
72.93
70.50
70.13
64.22
61.75
45.03
33.84
31.06
29.67
26.54
26.02
25.25
24.13
18.32
O
O
O
O
O
S+
O−
0.019
0.018
0.017
0.016
0.015
0.014
0.013
0.012
0.011
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
−0.001
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.19 7.18 7.18 7.17 7.15 7.14 7.14 7.13 7.13 7.12 6.69 6.68 6.68 6.67 6.67 6.66 4.57 4.57 4.56 4.55 4.20 4.20 4.18 4.18 4.17 4.17 3.75 3.75 3.74 3.73 3.73 3.71 3.69 3.55 3.53 3.25 3.23 3.07 3.06 3.05 3.04 3.03 3.03 3.02 3.01 3.00 2.99 2.98 2.97 2.97 2.96 2.95 2.74 2.73 2.72 2.71 2.52 2.52 2.51 2.50 2.50 2.49 2.49 2.48 2.19 2.18 2.18 2.17 2.17 2.16 2.16 2.15 1.73 1.72 1.71 1.57 1.56 1.56 1.55 1.46 1.32 1.14 1.10
O
S+
O
O
O
O
O
O
1.02 2.04 0.96 0.97 1.15 1.03 2.05 0.99 0.97 2.03 1.00 0.93 0.95 1.09 1.05 3.16 3.08 3.05 3.05
f1 (ppm)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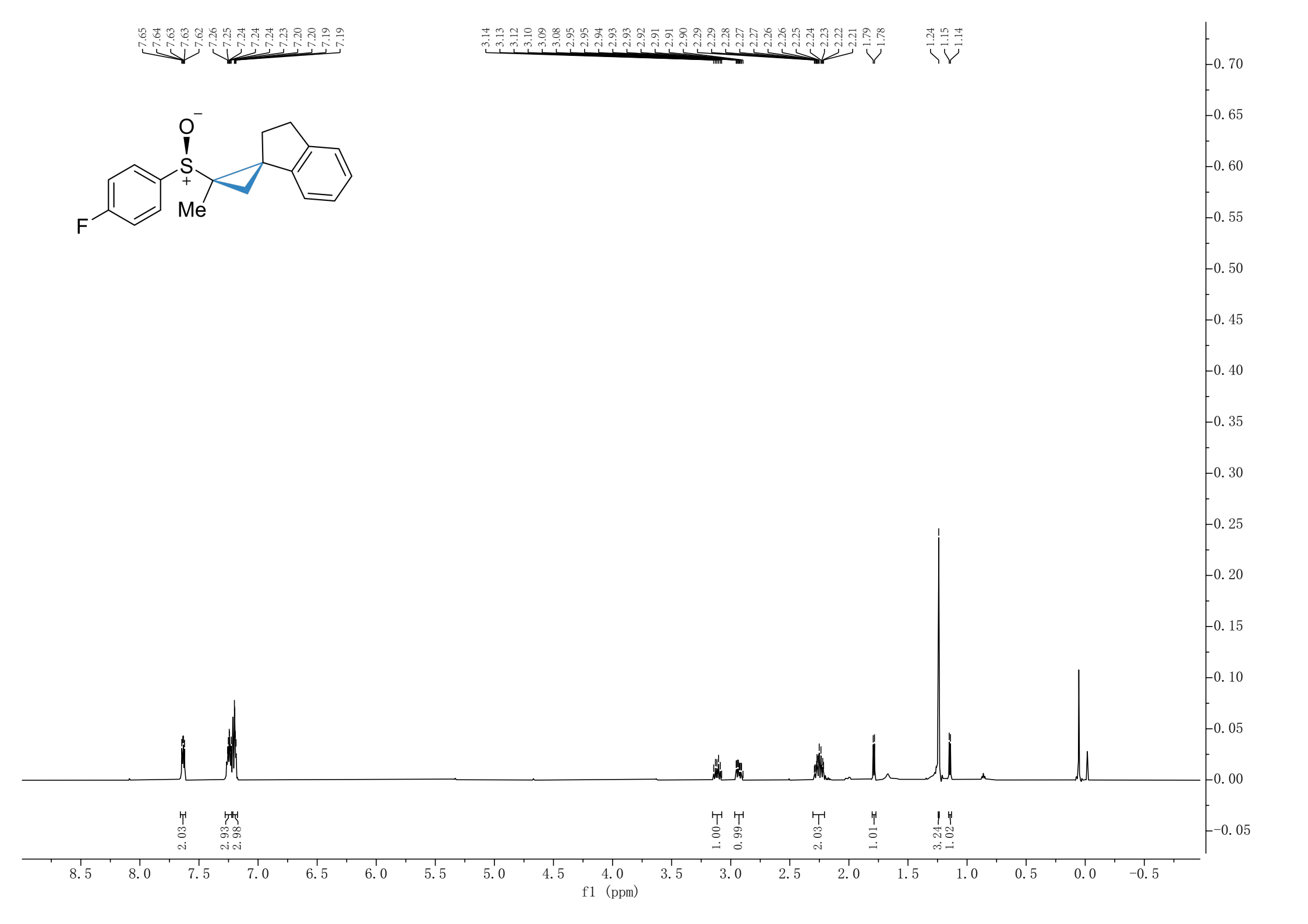
126.88
126.71
124.60
118.68
109.48
109.00
101.43
73.18
70.43
70.28
65.80
61.57
46.77
34.75
31.08
29.75
25.96
25.60
24.63
24.23
20.02
O
S+
O
O
O
O
O
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.65
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7.63
7.63
7.62
7.26
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7.24
7.24
7.24
7.23
7.20
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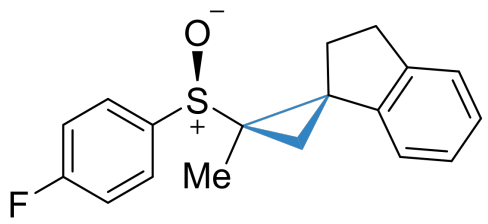
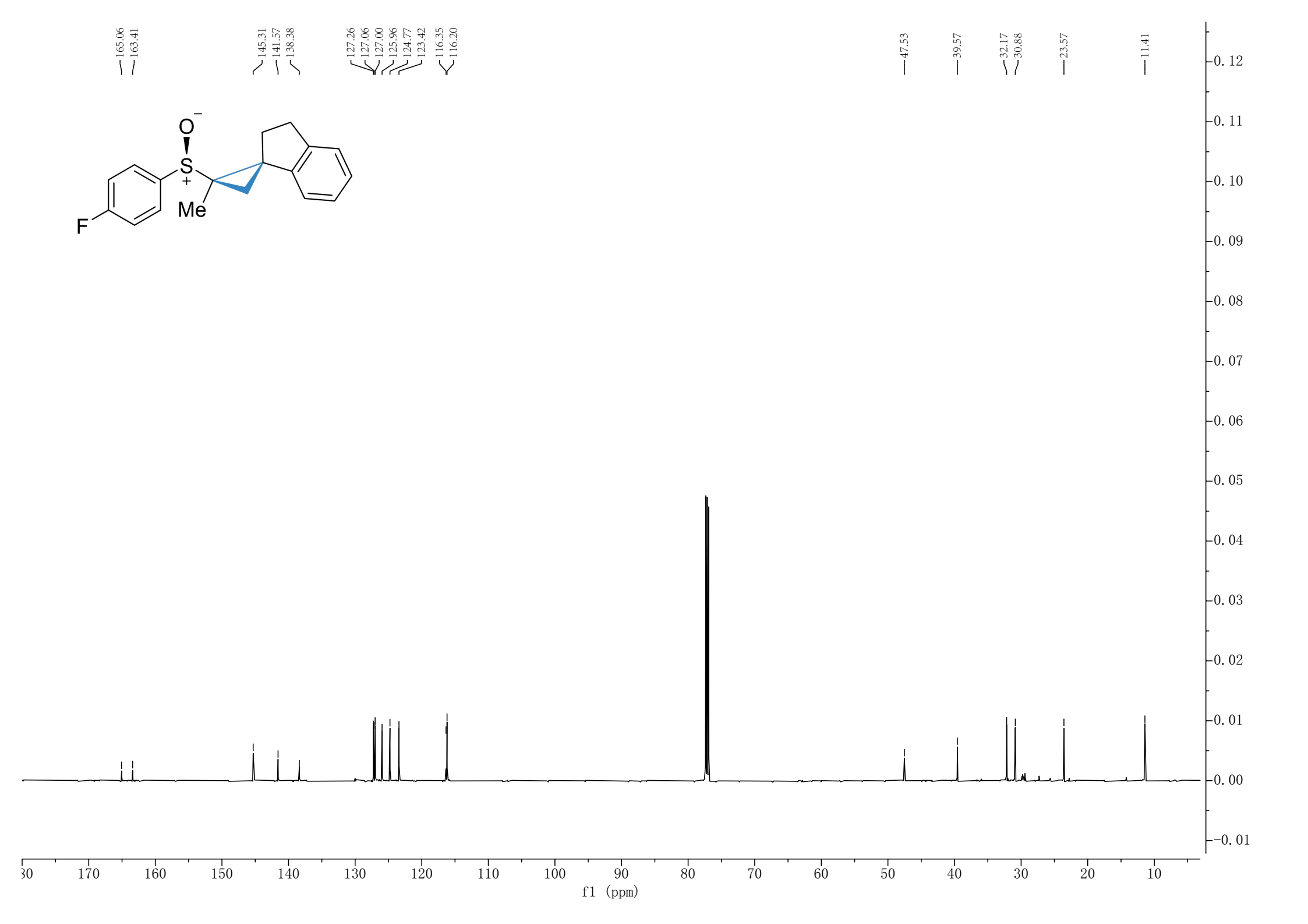
7.19
7.19
3.14
3.13
3.12
3.10
3.09
3.08
2.95
2.95
2.94
2.93
2.93
2.92
2.91
2.91
2.90
2.29
2.29
2.28
2.27
2.27
2.26
2.26
2.25
2.24
2.23
2.22
2.21
1.79
1.78
1.24
1.15
1.14
O
S
+
Me
F
2.03
2.93
2.98
1.00
0.99
2.03
1.01
3.24
1.02
f1 (ppm)



-109.89

f1 (ppm)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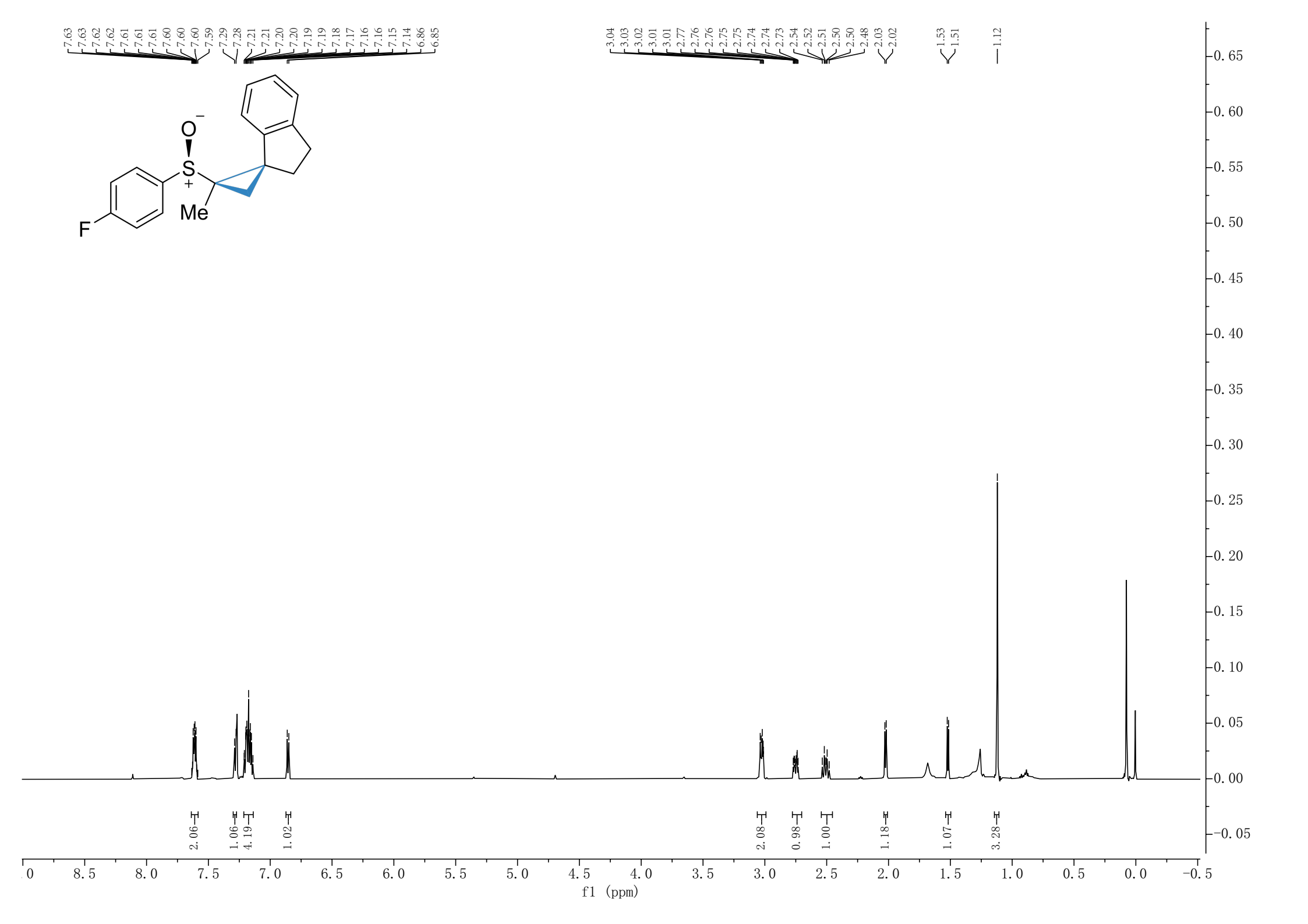
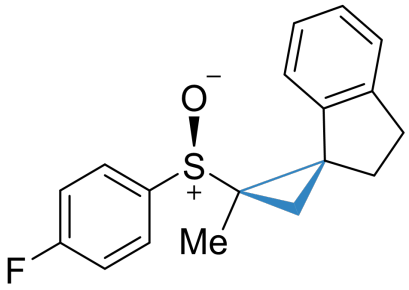
163.41
145.31
141.57
138.38
127.26
127.06
127.00
125.96
124.77
123.42
116.35
116.20
47.53
39.57
32.17
30.88
23.57
11.41
O
S
+
Me
F
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.63 7.63 7.62 7.62 7.61 7.61 7.61 7.60 7.60 7.60 7.59 7.29 7.28 7.21 7.21 7.20 7.20 7.19 7.19 7.18 7.17 7.16 7.16 7.15 7.14 6.86 6.85
3.04 3.03 3.02 3.01 3.01 2.77 2.76 2.76 2.75 2.75 2.74 2.74 2.73 2.54 2.52 2.51 2.50 2.50 2.48 2.03 2.02
1.53 1.51
1.12
O
S
+
Me
F
2.06 1.06 4.19 1.02 2.08 0.98 1.00 1.18 1.07 3.28
f1 (ppm)

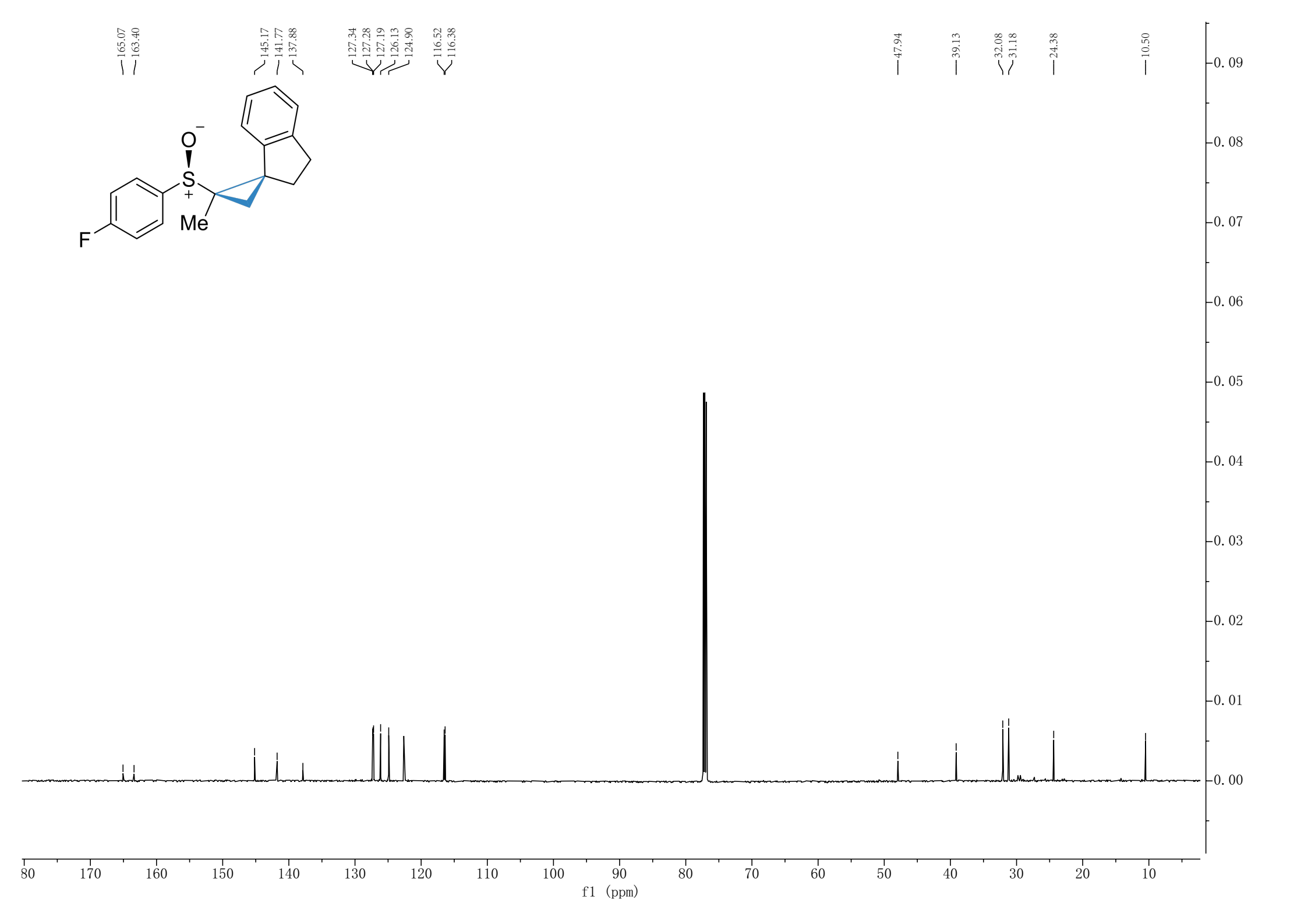


-108.81

30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0 -2

40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

f1 (ppm)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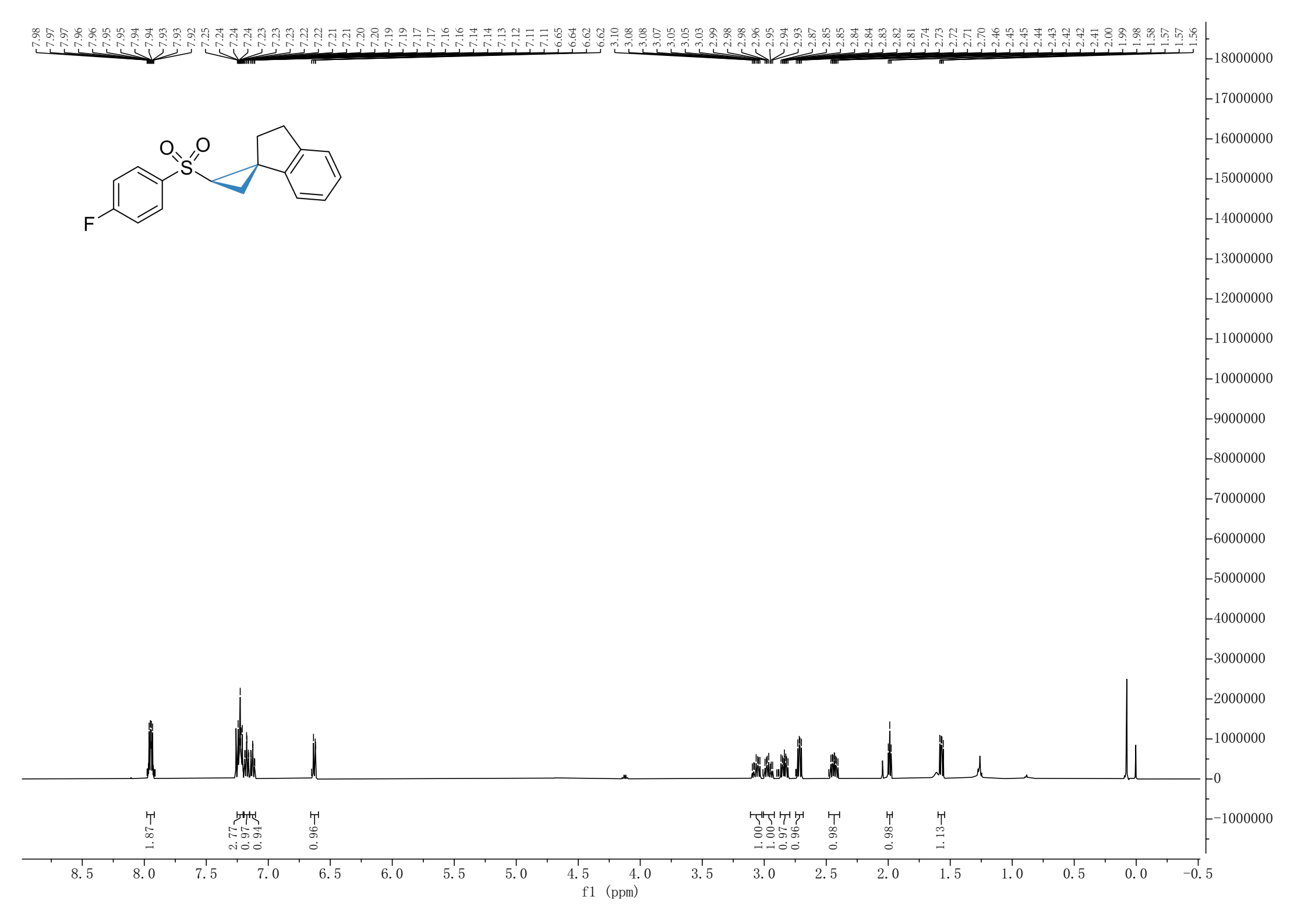
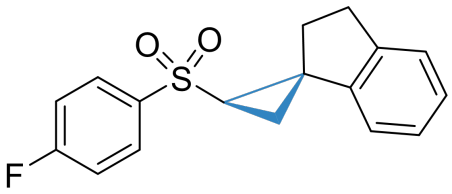
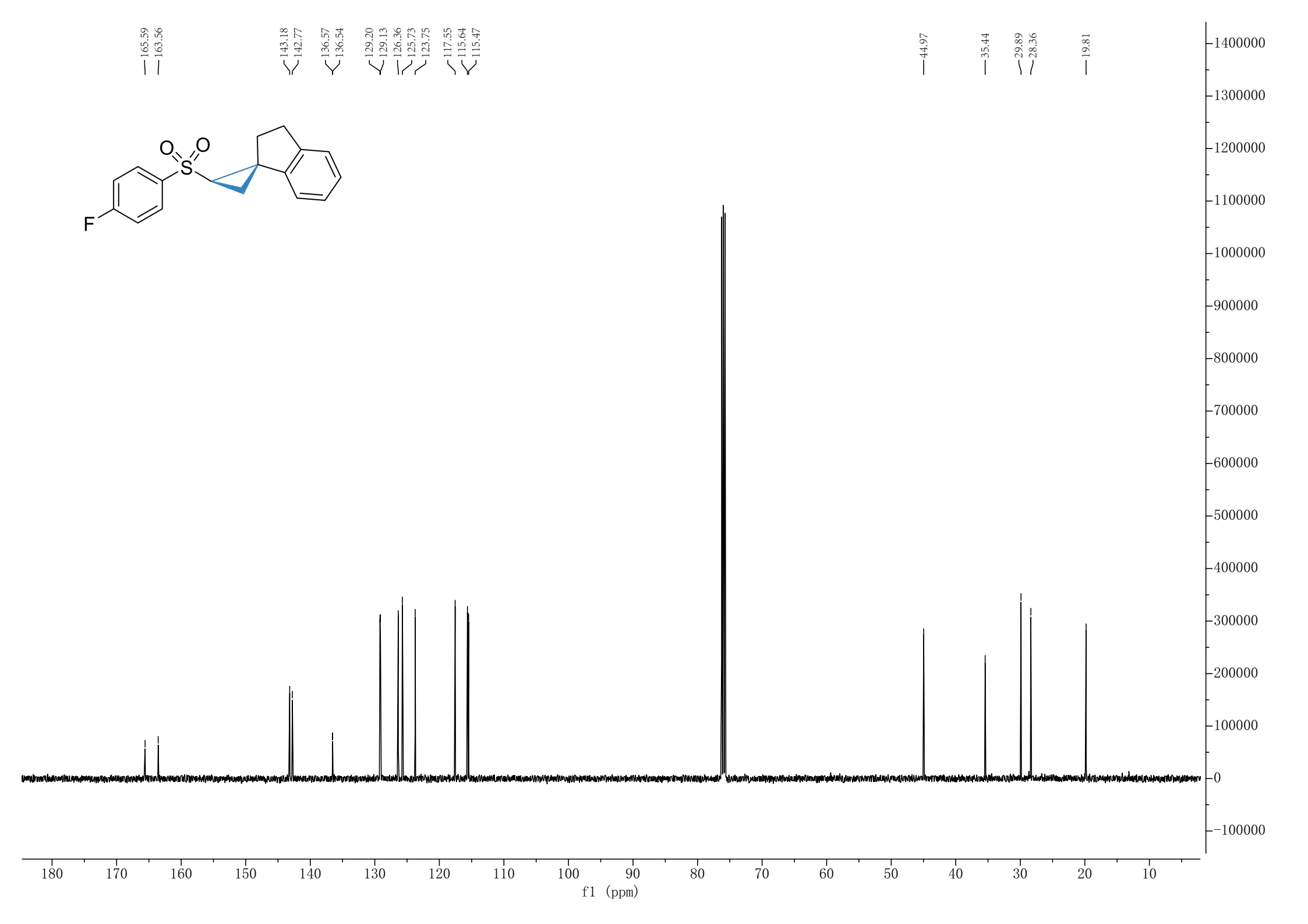
163.40
145.17
141.77
137.88
127.34
127.28
127.19
126.13
124.90
116.52
116.38
47.94
39.13
32.08
31.18
24.38
10.50
O
S
+
Me
F
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
O
S
F
f1 (ppm)


O
O
S
F

-104.09
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)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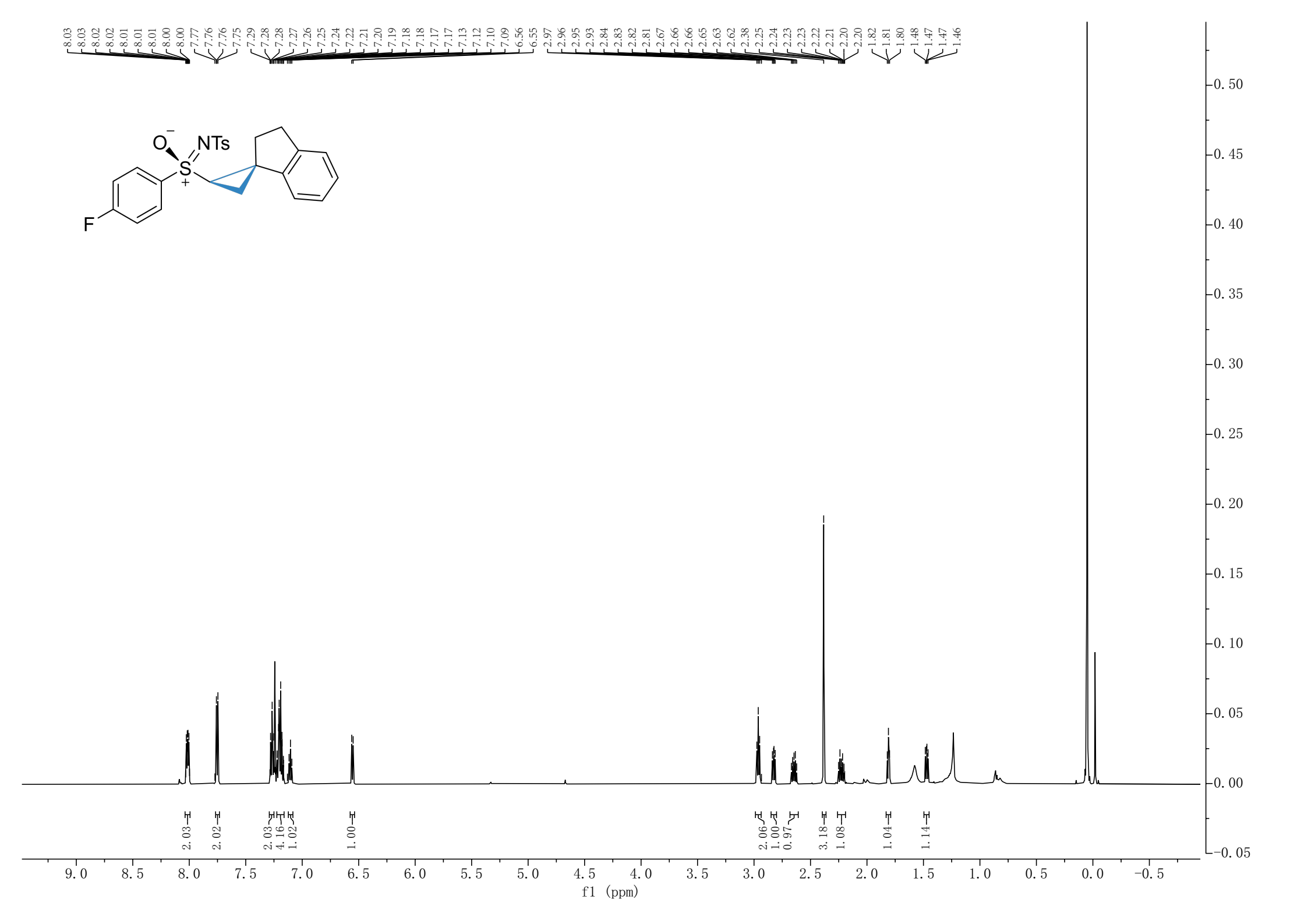
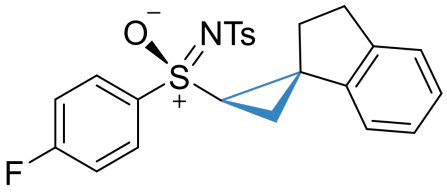
143.18
142.77
136.57
136.54
129.20
129.13
126.36
125.73
123.75
117.55
115.64
115.47
44.97
35.44
29.89
28.36
19.81
O
O
S
F
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.03 8.03 8.02 8.02 8.01 8.01 8.01 8.00 8.00 7.77 7.76 7.76 7.75 7.29 7.28 7.28 7.27 7.26 7.25 7.24 7.22 7.21 7.20 7.19 7.18 7.18 7.17 7.17 7.13 7.12 7.10 7.09 6.56 6.55 2.97 2.96 2.95 2.93 2.84 2.83 2.82 2.81 2.67 2.66 2.66 2.65 2.63 2.62 2.38 2.25 2.24 2.23 2.22 2.21 2.20 2.20 1.82 1.81 1.80 1.48 1.47 1.47 1.46
O
NTs
S
+
F
2.03 2.02 2.03 4.16 1.02 1.00 2.06 1.00 0.97 3.18 1.08 1.04 1.14
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
f1 (ppm)
0.50 0.45 0.40 0.35 0.30 0.25 0.20 0.15 0.10 0.05 0.00 -0.05

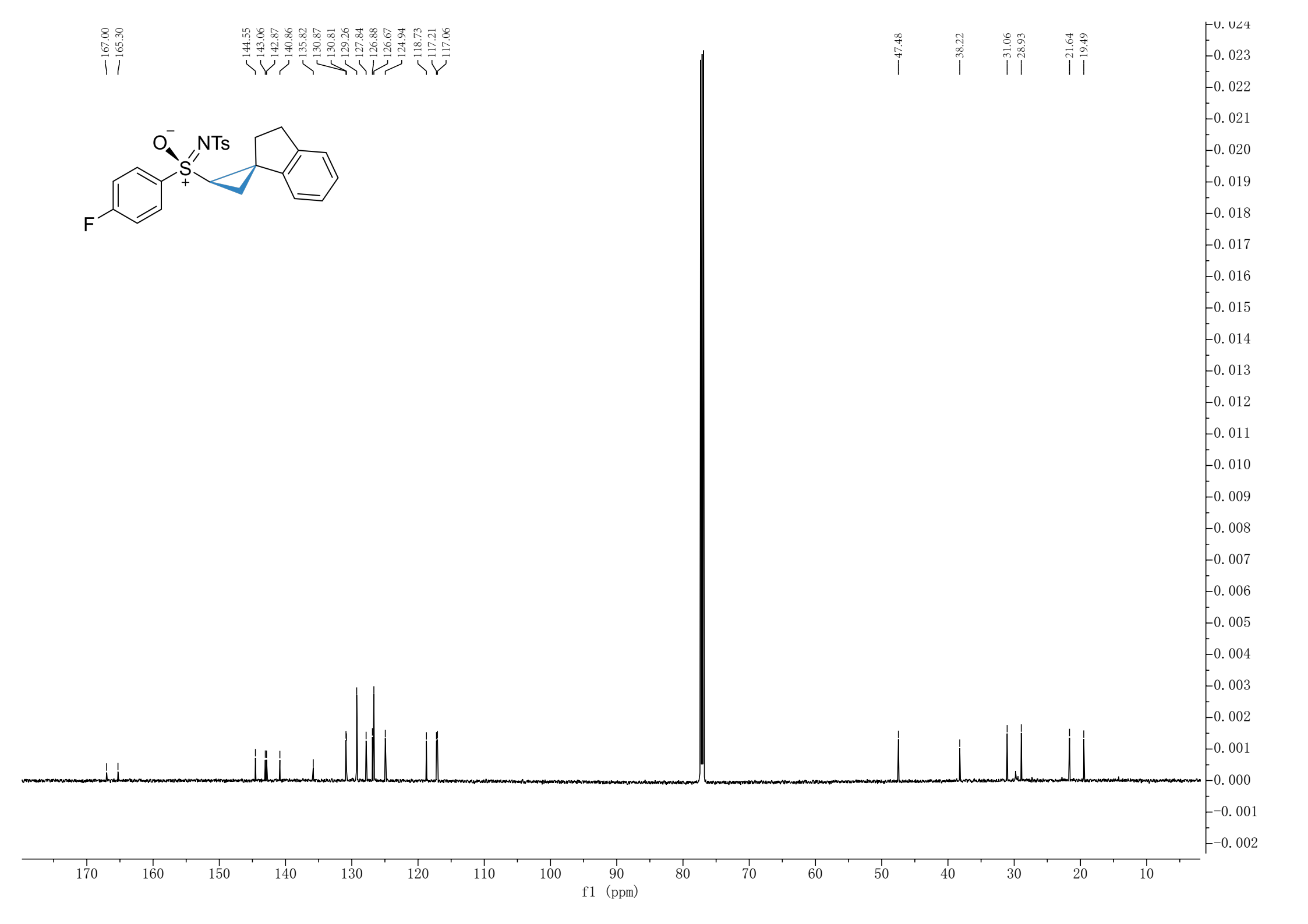


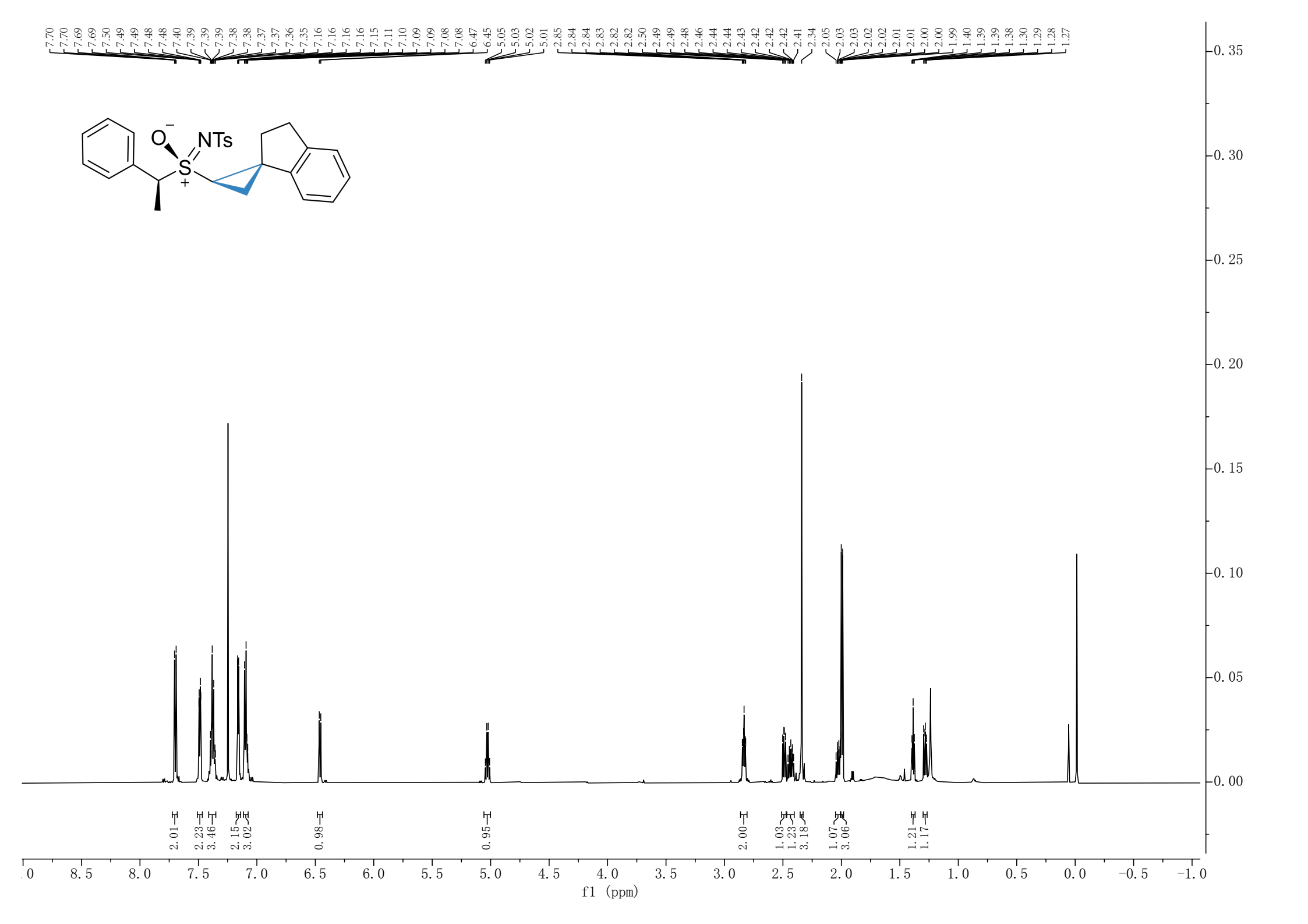
-102.70

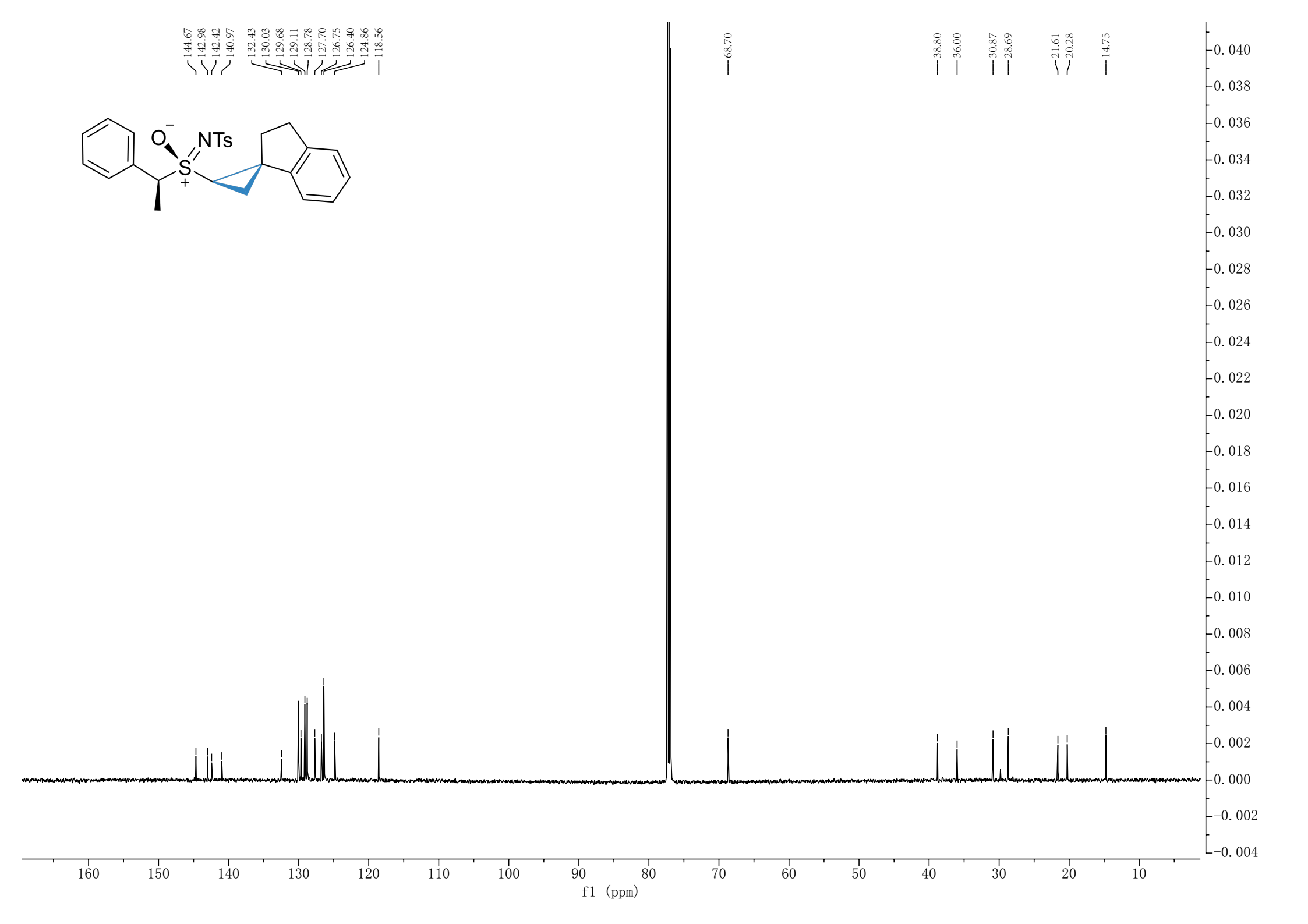
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

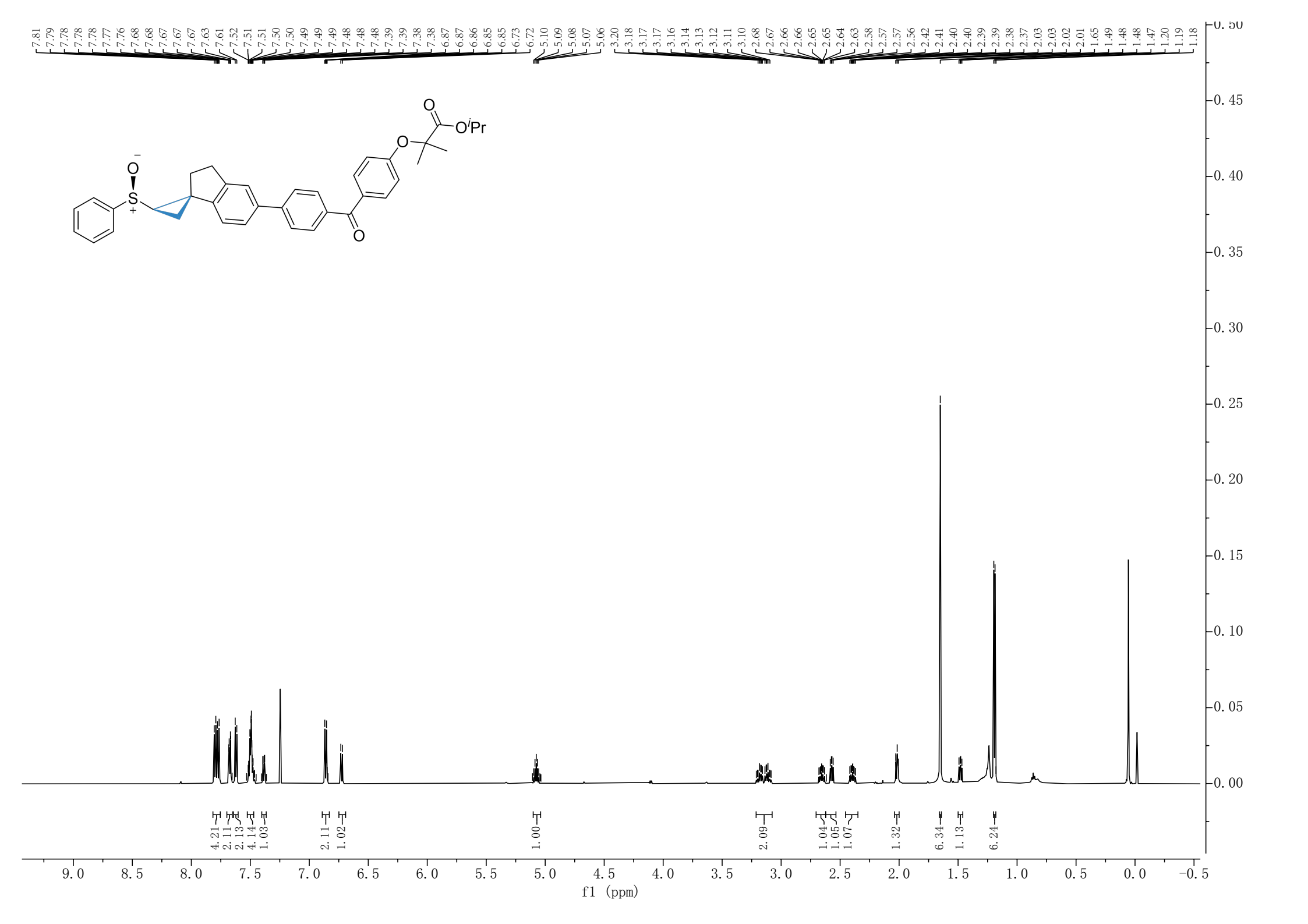
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240

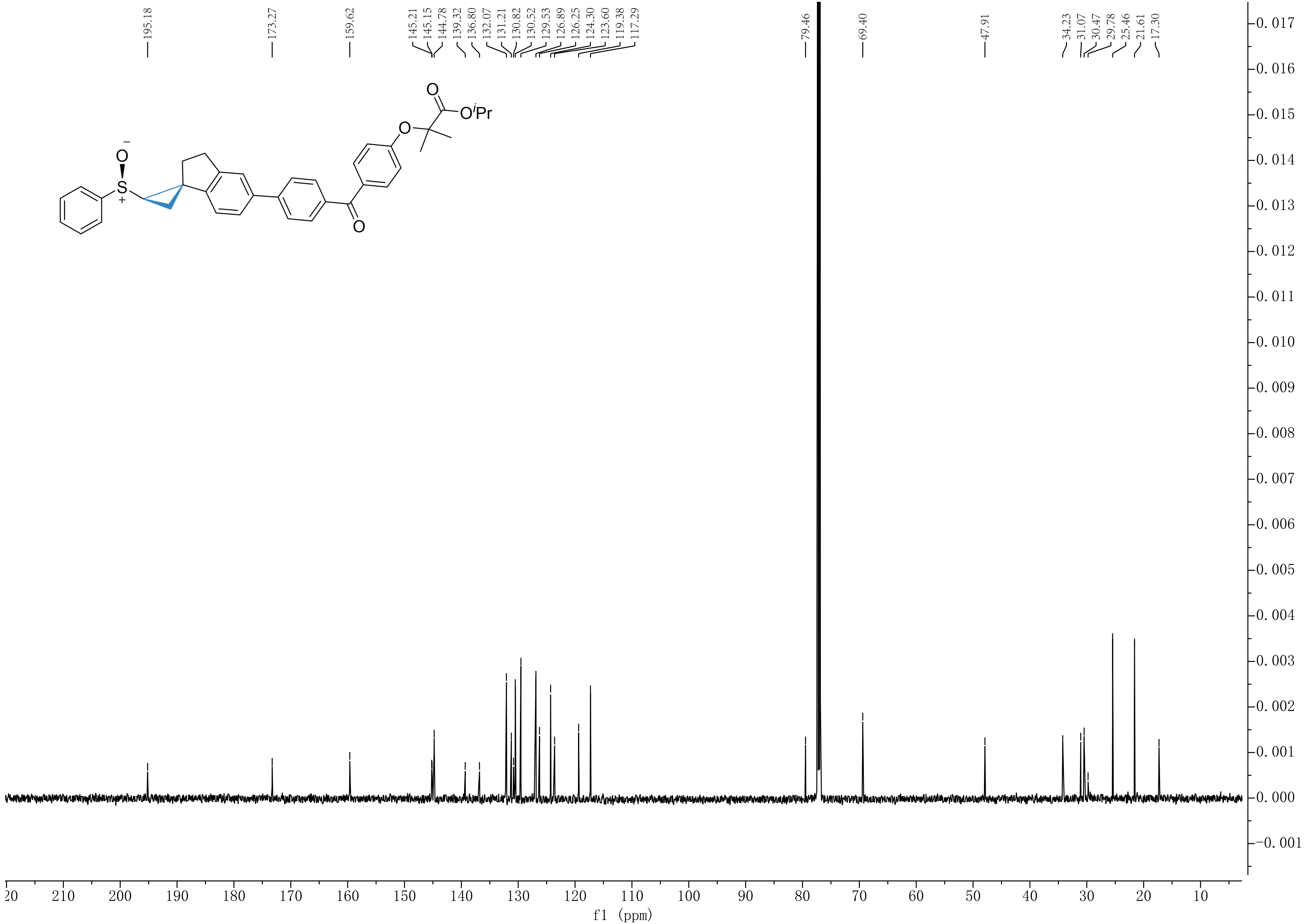
f1 (ppm)


167.00
165.30
144.55
143.06
142.87
140.86
135.82
130.87
130.81
129.26
127.84
126.88
126.67
124.94
118.73
117.21
117.06
47.48
38.22
31.06
28.93
21.64
19.49
O
NTs
S
F
f1 (ppm)


7.70 7.70 7.69 7.69 7.50 7.49 7.49 7.48 7.48 7.40 7.39 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.35 7.16 7.16 7.16 7.15 7.11 7.10 7.09 7.09 7.08 7.08 6.47 6.45 5.05 5.03 5.02 5.01 2.85 2.84 2.84 2.83 2.82 2.82 2.50 2.49 2.49 2.48 2.46 2.44 2.44 2.43 2.42 2.42 2.42 2.41 2.34 2.05 2.03 2.03 2.02 2.02 2.01 2.01 2.00 2.00 1.99 1.40 1.39 1.39 1.38 1.30 1.29 1.28 1.27
O
NTs
S
+
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
2.01
2.23
3.46
2.15
3.02
0.98
0.95
2.00
1.03
1.23
3.18
1.07
3.06
1.21
1.17
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


144.67
142.98
142.42
140.97
132.43
130.03
129.68
129.11
128.78
127.70
126.75
126.40
124.86
118.56
68.70
38.80
36.00
30.87
28.69
21.61
20.28
14.75
O
NTs
S
+
0.040
0.038
0.036
0.034
0.032
0.030
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.81 7.79 7.78 7.78 7.78 7.77 7.76 7.68 7.68 7.67 7.67 7.67 7.63 7.61 7.52 7.51 7.51 7.50 7.50 7.49 7.49 7.49 7.48 7.48 7.48 7.39 7.39 7.38 7.38 6.87 6.87 6.86 6.85 6.85 6.73 6.72 5.10 5.09 5.08 5.07 5.06 3.20 3.18 3.17 3.17 3.16 3.14 3.13 3.12 3.11 3.10 2.68 2.67 2.66 2.66 2.65 2.65 2.64 2.63 2.58 2.57 2.57 2.56 2.42 2.41 2.40 2.40 2.39 2.39 2.38 2.37 2.03 2.03 2.02 2.01 1.65 1.49 1.48 1.48 1.47 1.20 1.19 1.18
O
O
O
O
O
O
iPr
S
+
−
4.21 2.11 2.13 4.14 1.03 2.11 1.02 1.00 2.09 1.04 1.05 1.07 1.32 6.34 1.13 6.24
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
f1 (ppm)
0.50 0.45 0.40 0.35 0.30 0.25 0.20 0.15 0.10 0.05 0.00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173.27
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145.15
144.78
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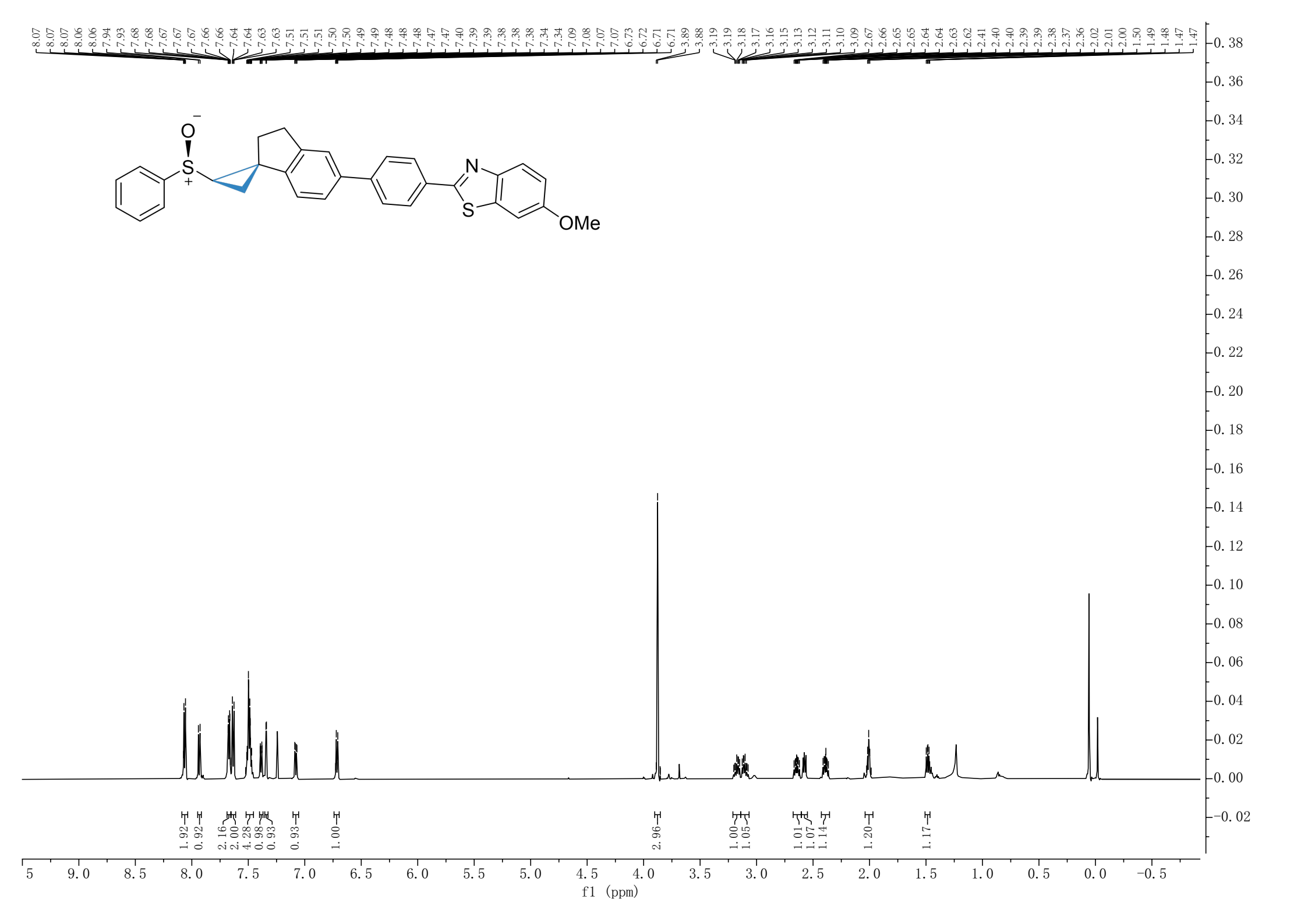
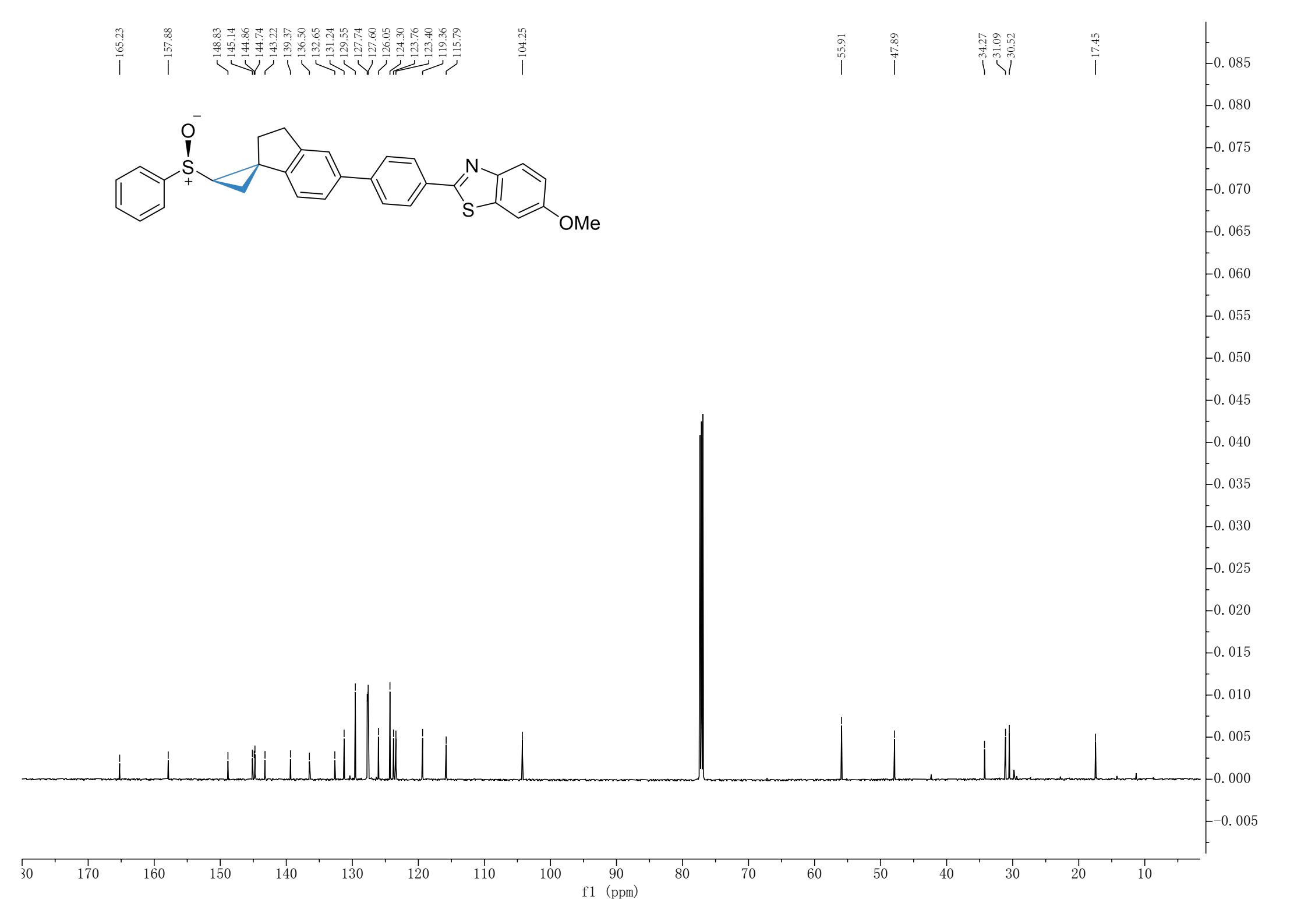
136.80
132.07
131.21
130.82
130.52
129.53
126.89
126.25
124.30
123.60
119.38
117.29
79.46
69.40
47.91
34.23
31.07
30.47
29.78
25.46
21.61
17.30
O
O^{i}Pr
S
f1 (ppm)


8.07 8.07 8.07 8.06 8.06 7.94 7.93 7.68 7.68 7.67 7.67 7.67 7.66 7.66 7.64 7.64 7.63 7.63 7.51 7.51 7.51 7.50 7.50 7.49 7.49 7.48 7.48 7.48 7.47 7.47 7.40 7.39 7.39 7.38 7.38 7.38 7.34 7.34 7.09 7.08 7.07 7.07 6.73 6.72 6.71 6.71 3.89 3.88
3.19 3.19 3.18 3.17 3.16 3.15 3.13 3.12 3.11 3.10 3.09 2.67 2.66 2.65 2.65 2.64 2.64 2.63 2.62 2.41 2.40 2.40 2.39 2.39 2.38 2.37 2.36 2.02 2.01 2.00 1.50 1.49 1.48 1.47 1.47
O
S
+
N
S
OMe
0.38 0.36 0.34 0.32 0.30 0.28 0.26 0.24 0.22 0.20 0.18 0.16 0.14 0.12 0.10 0.08 0.06 0.04 0.02 0.00 -0.02
1.92 0.92 2.16 2.00 4.28 0.98 0.93 0.93 1.00 2.96 1.00 1.05 1.01 1.07 1.14 1.20 1.17
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
f1 (ppm)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139.37
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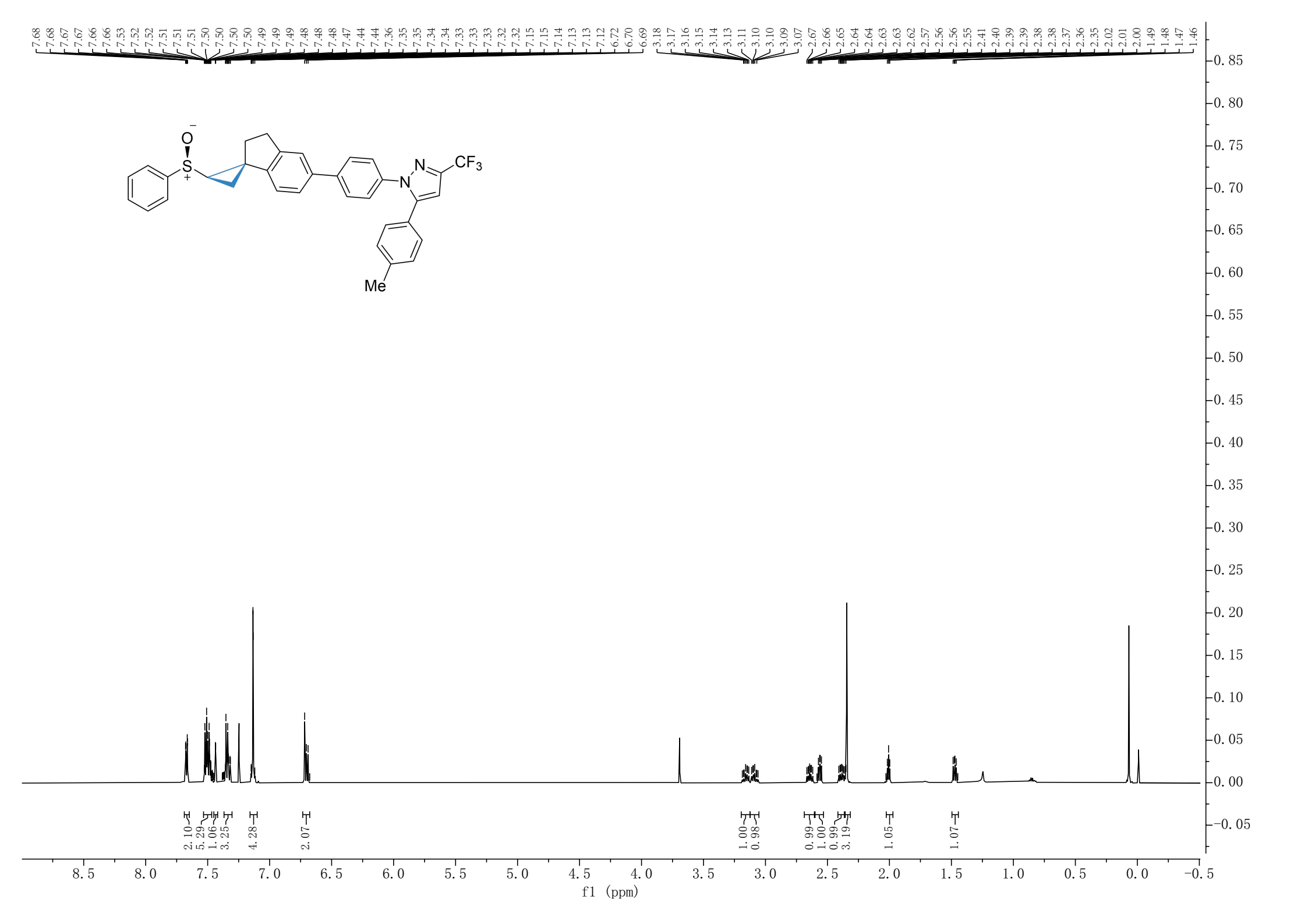
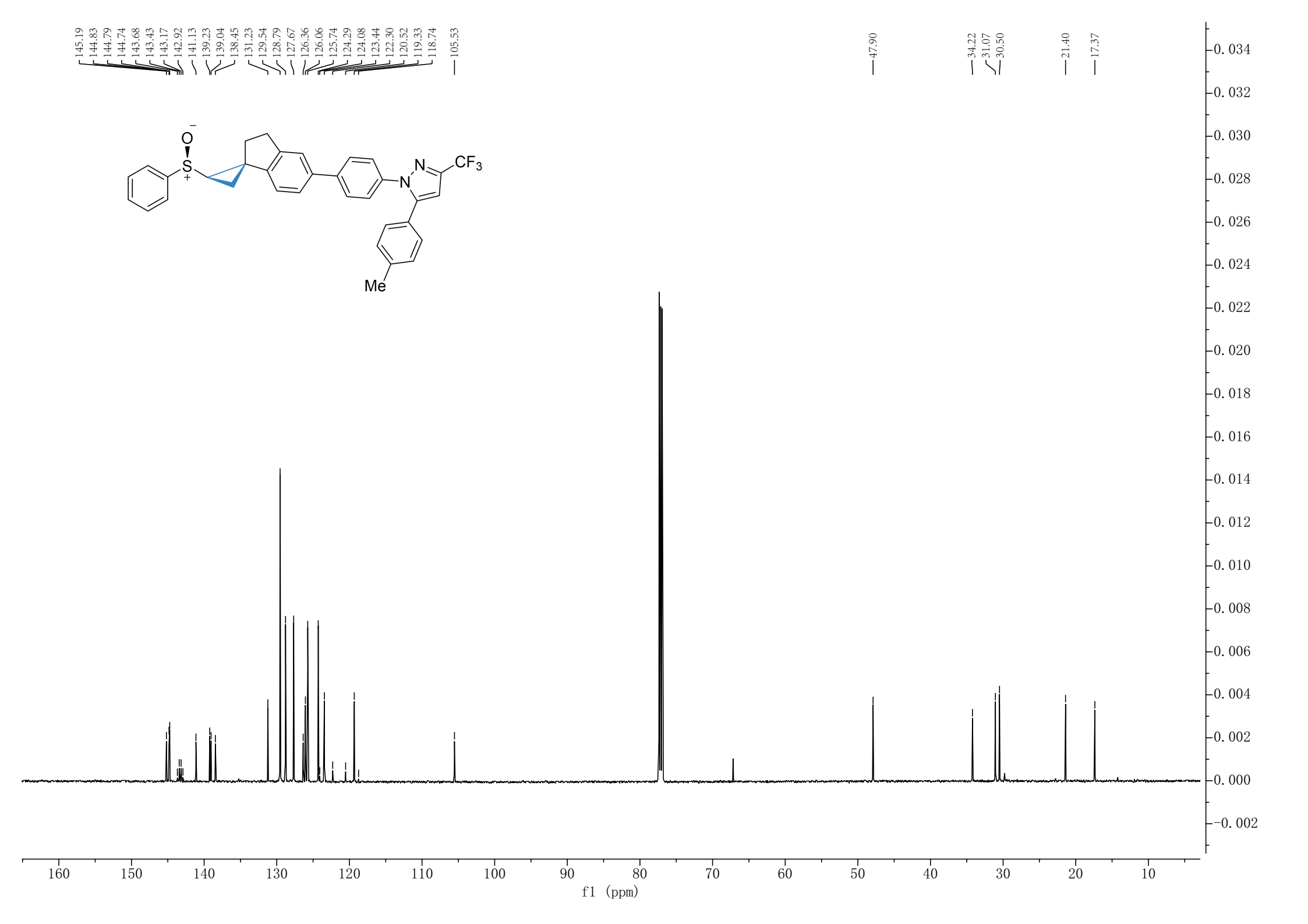
132.65
131.24
129.55
127.74
127.60
126.05
124.30
123.76
123.40
119.36
115.79
104.25
55.91
47.89
34.27
31.09
30.52
17.45
O
S
+
N
S
OMe
0.085
0.080
0.075
0.070
0.065
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.68 7.68 7.67 7.67 7.66 7.66 7.53 7.52 7.52 7.51 7.51 7.51 7.50 7.50 7.50 7.50 7.49 7.49 7.49 7.48 7.48 7.48 7.47 7.44 7.44 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.15 7.15 7.14 7.13 7.13 7.12 6.72 6.70 6.69
3.18 3.17 3.16 3.15 3.14 3.13 3.11 3.10 3.10 3.09 3.07
2.67 2.66 2.65 2.64 2.64 2.63 2.63 2.62 2.57 2.56 2.56 2.55 2.41 2.40 2.39 2.39 2.38 2.38 2.37 2.36 2.35 2.02 2.01 2.00 1.49 1.48 1.47 1.46
O
S
N
N
CF3
Me
2.10
5.29
1.06
3.25
4.28
2.07
1.00
0.98
0.99
1.00
0.99
3.19
1.05
1.07
f1 (ppm)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144.83
144.79
144.74
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143.43
143.17
142.92
141.13
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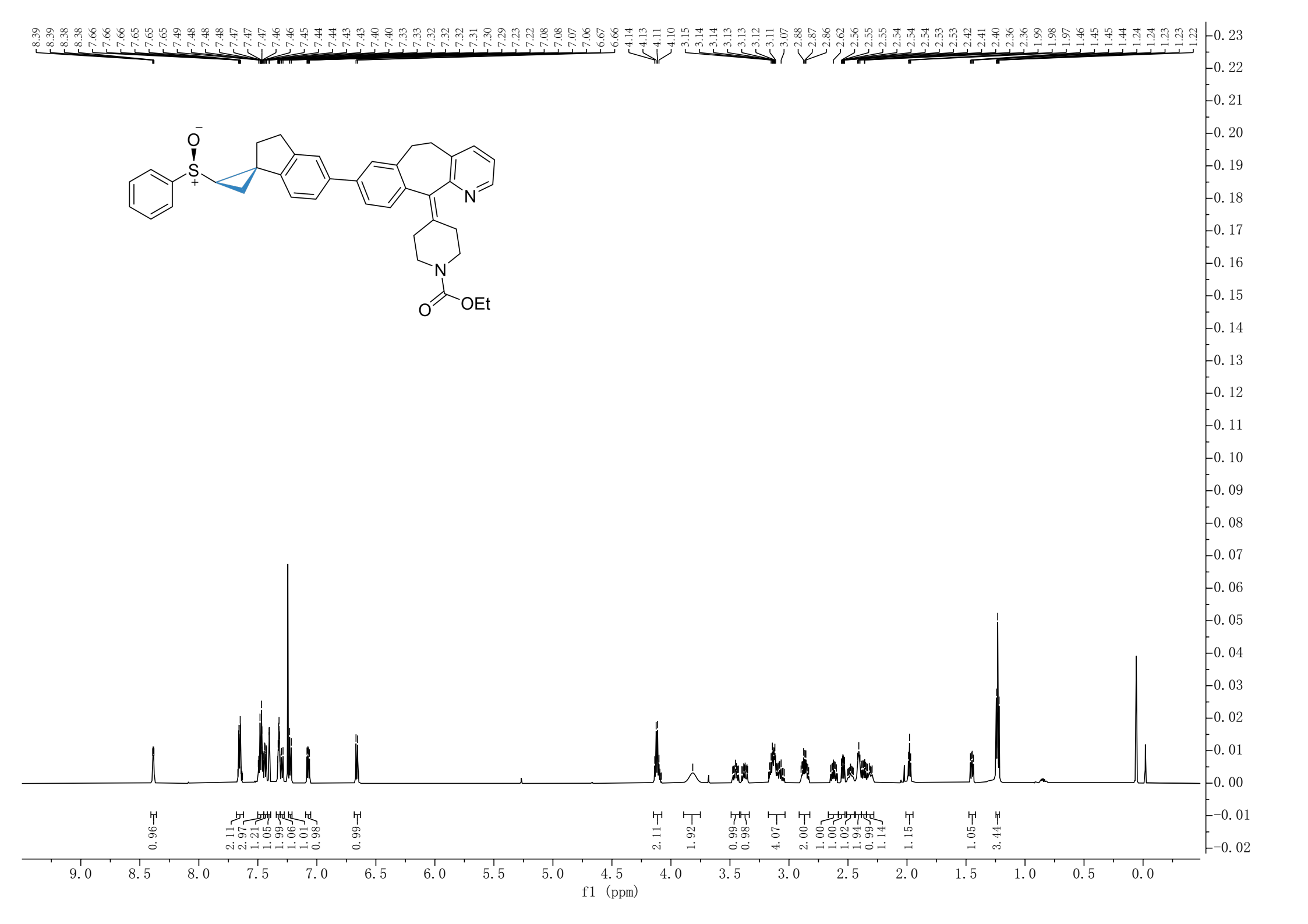
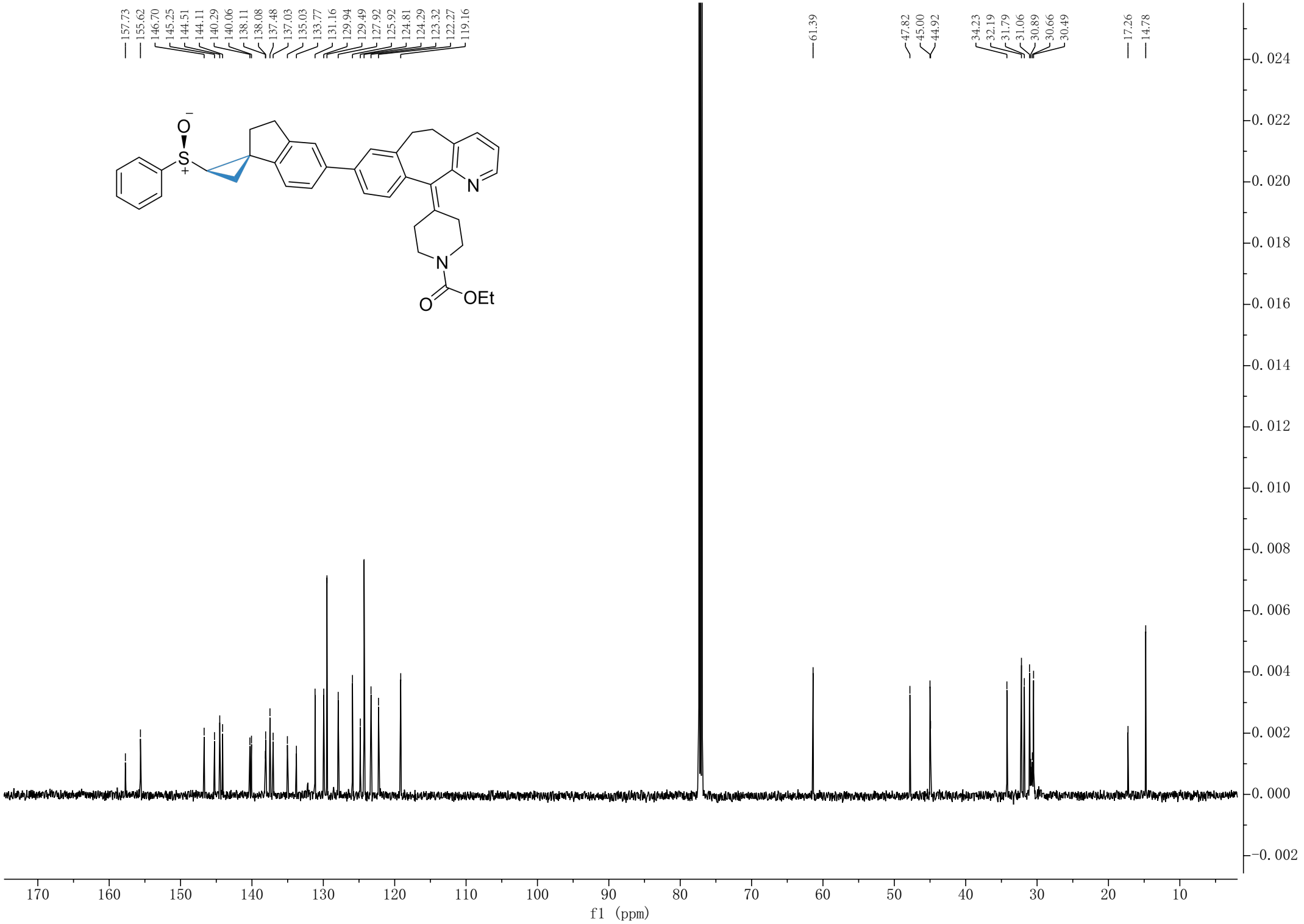
139.04
138.45
131.23
129.54
128.79
127.67
126.36
126.06
125.74
124.29
124.08
123.44
122.30
120.52
119.33
118.74
105.53
47.90
34.22
31.07
30.50
21.40
17.37
O
S
N
N
CF3
Me
0.034
0.032
0.030
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.39 8.39 8.38 8.38 7.66 7.66 7.66 7.65 7.65 7.65 7.49 7.48 7.48 7.48 7.47 7.47 7.47 7.46 7.46 7.45 7.44 7.44 7.43 7.43 7.40 7.40 7.33 7.33 7.32 7.32 7.32 7.31 7.30 7.29 7.23 7.22 7.08 7.08 7.07 7.06 6.67 6.66 4.14 4.13 4.11 4.10 3.15 3.14 3.14 3.13 3.13 3.12 3.11 3.07 2.88 2.87 2.86 2.62 2.56 2.55 2.55 2.54 2.54 2.54 2.53 2.53 2.42 2.41 2.40 2.36 2.36 1.99 1.98 1.97 1.46 1.45 1.45 1.44 1.24 1.24 1.23 1.23 1.22
O
S
+
N
N
O
OEt
0.96 2.11 2.97 1.21 1.05 1.99 1.06 1.01 0.98 0.99 2.11 1.92 0.99 0.98 4.07 2.00 1.00 1.00 1.02 1.94 0.99 1.14 1.15 1.05 3.44
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)
0.23 0.22 0.21 0.20 0.19 0.18 0.17 0.16 0.15 0.14 0.13 0.12 0.11 0.10 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0.00 -0.01 -0.02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145.25
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140.06
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138.08
137.48
137.03
135.03
133.77
131.16
129.94
129.49
127.92
125.92
124.81
124.29
123.32
122.27
119.16
61.39
47.82
45.00
44.92
34.23
32.19
31.79
31.06
30.89
30.66
30.49
17.26
14.78
O
S
+
N
N
O
OEt
0.024
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)