Chloride Induced S-C bond Selective Cleavage of Disulfides to Access Unsymmetrical β-Fluorodisulfides

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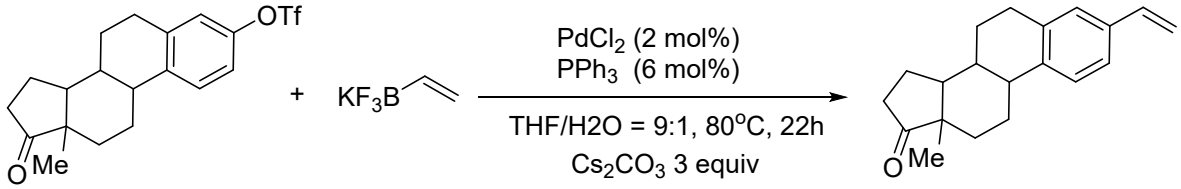
1. General Methods

All chemicals were commercially available and used without further purification. Analytical thin-layer chromatography were performed on glass plates precoated with silica gel impregnated with a fluorescent indicator (254 nm). The plates were visualized by exposure to ultraviolet light. ^{1}H NMR spectra were recorded on Bruker DRX400 (400 MHz) and ^{13}C NMR spectra on BrukerDRX400 (101 MHz) spectrometer. HRMS were taken on a Bruker microtof II in the electrospray ionization (ESI) mode.

2. Experimental Section

Preparation of vinylestrone B47[1]



A 2-neck 100 mL round-bottom flask was charged with 3-(trifluoromethanesulfonyl)estrone (1.5g, 3.72 mmol), potassium vinyltrifluoroborate (600 mg, 4.47 mmol), $PdCl_2$ (12.8 mg, 0.074 mmol), PPh_3 (60 mg, 0.221 mmol) and Cs_2CO_3 (3.75 g, 11.3 mmol), then THF (6.8 mL) and H2O (0.8 mL) was added to the mixture under N_2. The reaction mixture was stirred at 80 oC for 22 h. After cooling to room temperature, the resulting reaction mixture was washed with H_2O, dried (Na_2SO_4), and filtered. The filtrate was concentrated in vacuo and the residue was purified by flash column chromatography on silica gel (hexane/AcOEt = 4/1) to afford the title compound as a white solid.

Preparation of β-fluorinated disulfides **4**

A 25 mL reaction vessel with a magnetic stirring bar was equipped with disulfides (0.5 mmol), alkynes (0.6 mmol), LiCl (2 mmol), Selectfluor (1 mmol), MeCN: H_2O = 3:1 (3 mL). The mixture was stirred under at r.t. in a nitrogen atmosphere for 2 h.

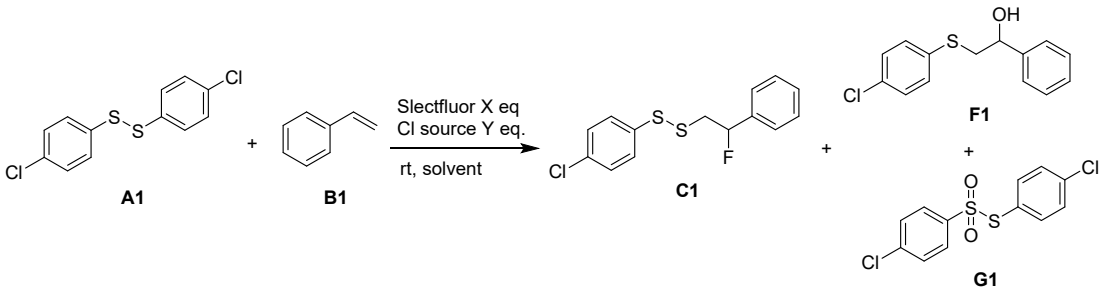
After the reaction, the solvent was removed under reduced pressure. Purification of the crude product was achieved by flash column chromatography using petrol n-hexane /ethyl acetate (9:1~15:1) as eluent.

References:

[1] Yasu, Y., Koike, T., & Akita, M. (2013). Intermolecular aminotrifluoromethylation of alkenes by visible-light-driven photoredox catalysis. *Organic letters*, *15*(9), 2136-2139.

3. Optimization of reaction conditions

Table S1. Optimization of reaction conditions for preparation of β-fluorinated disulfides [a]



Entry	solvent	Cl source	X (equiv)	Y (equiv)	Yield (%)[b]		
					C1	**F1**	**G1**
1	MeCN	NaCl	2	4	trace	trace	trace
2	DMF	NaCl	2	4	trace	trace	trace
3	THF	NaCl	2	4	trace	trace	trace
4	MeOH	NaCl	2	4	trace	trace	trace
5	MeCN/H_2O (3:1)	NaCl	2	4	32	21	28
6	THF/H_2O (3:1)	NaCl	2	4	24	20	33
7	DMF/H_2O (3:1)	NaCl	2	4	18	14	28
8	MeOH/H_2O (3:1)	NaCl	2	4	25	27	24
9	H_2O	NaCl	2	4	trace	trace	trace
10	MeCN/H_2O (3:1)	NaBr	2	4	trace	trace	14

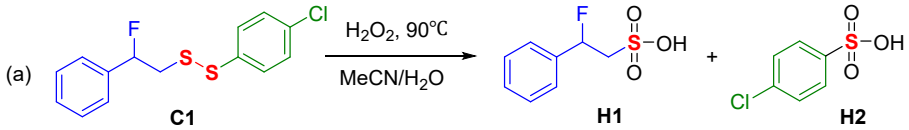
11	MeCN/H_2O (3:1)	NaI	2	4	trace	62	17
12	MeCN/H_2O (3:1)	HCl (aq)	2	4	22	15	21
13	**MeCN/H_2O (3:1)**	**LiCl**	**2**	**4**	**73**	**trace**	**trace**
14	MeCN/H_2O (3:1)	KCl	2	4	36	19	25
15	MeCN/H_2O (3:1)	$ZnCl_2$	2	4	45	22	14
16	MeCN/H_2O (3:1)	$CuCl_2$	2	4	34	26	28
17	MeCN/H_2O (3:1)	$MgCl_2$	2	4	38	13	22
18	MeCN/H_2O (3:1)	$CuCl_2$	2	4	36	16	18
19	MeCN/H_2O (3:1)	NaF	2	4	NR	NR	NR
20	MeCN/H_2O (3:1)	TBAC	2	4	trace	trace	trace
21	MeCN/H_2O (3:1)	NH_4Cl	2	4	21	16	23
22	MeCN/H_2O (5:1)	LiCl	2	4	52	trace	trace
23	MeCN/H_2O (10:1)	LiCl	2	4	trace	trace	trace
24	MeCN/H_2O (2:1)	LiCl	2	4	68	trace	trace
25	MeCN/H_2O (1:1)	LiCl	2	4	46	trace	trace
26[c]	MeCN/H_2O (3:1)	LiCl	1	4	trace	trace	trace
27	MeCN/H_2O (3:1)	LiCl	2	2	trace	12	22
28	MeCN/H_2O (3:1)	LiCl	3	6	70	trace	trace
29[c]	MeCN/H_2O (3:1)	LiCl	2	4	73	trace	trace

[a] Reaction conditions: **A1** (0.5 mmol), **B1** (1.2 equiv), selectfluor (2 equiv), catalyst (4 equiv), and solvent (3 mL), under N_2 atmosphere at r.t. for 6 h. [b] Isolated yields. [c] Reaction temperature 60°C.

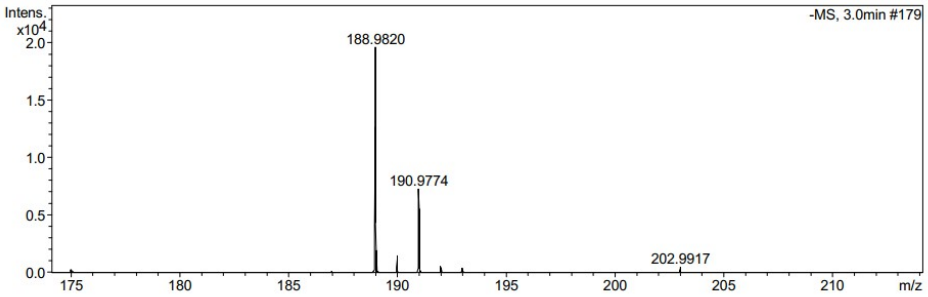
4. Additional evidence for the structure of product.

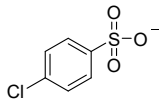
Although the desired products have been identified by ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR and HRMS, further studies were performed to provide additional evidence for the structure. First, the product was treated with H_2O_2, as was expected, oxidative cleavage of S-S bond products sulfonic acid **H1** and **H2** have been detected (Figure S3). Then the product could be selectively oxidized by oxone/KI, and corresponding disulfoxide **I1** and **K1** was obtained (Figure S4). These results confirmed the structure is consistent with our expectation.

4.1 General procedure for Oxidative Cleavage of β-fluorodisulfides

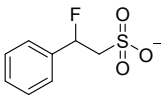


H_2O_2 (2.0 mmol) was added in aqueous acetonitrile (3mL, 50:50, v/v), followed by substrate (0.5 mmol) was added. Resulting mixture was stirred for 2h at 90°C. After complete consumption of the starting material as observed by TLC. Then the mixture was characterized by HRMS.

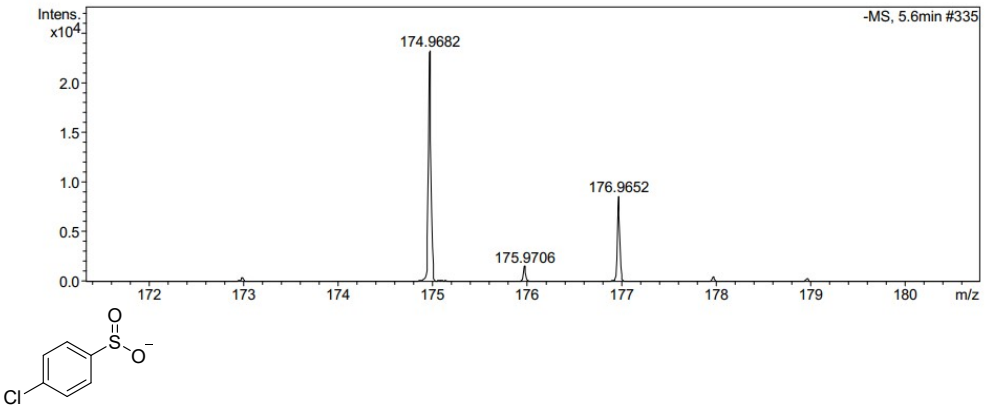




HRMS calcd for $C_6H_4ClSO_3$ {[M]$^-$}:190.9575, found:190.9774.



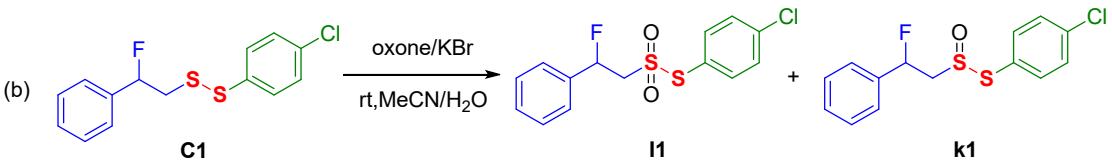
HRMS calcd for $C_8H_8FSO_3$ {[M]$^-$}: 203.0184, found:202.9917.



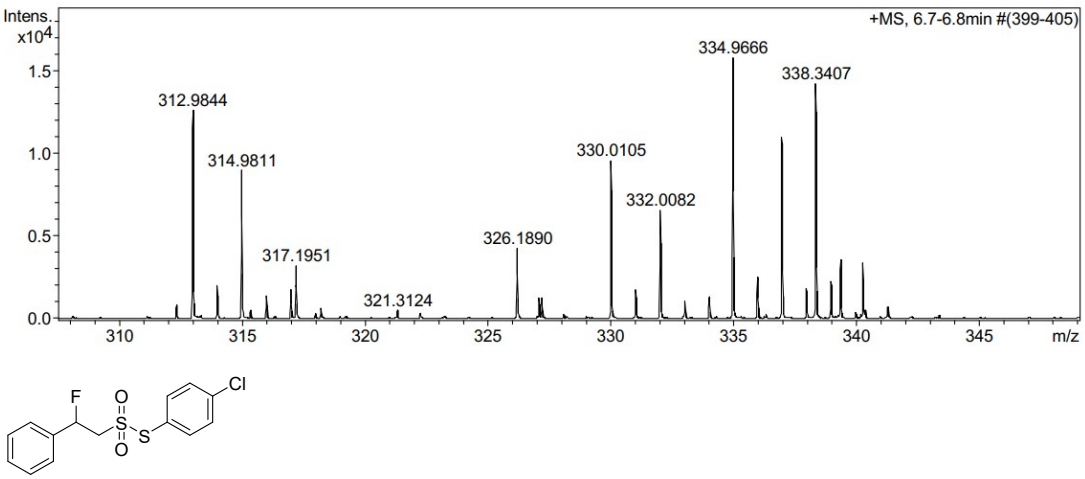
HRMS calcd for C8H8FSO2 {[M]-}: 174.9626, found:174.9682.

Figure S3. LC-MS spectrums result of oxidative cleavage of β-fluorodisulfides

4.2 General procedure for the selectively oxidation of β-fluorodisulfides



oxone (1.0 mmol) was added to a well-stirred solution of KBr 0.25 mmol in aqueous acetonitrile (50:50, v/v), followed by substrate (0.5 mmol) was added. Resulting mixture was stirred for 1h at room temperature. After complete consumption of the starting material as observed by TLC, water (25 mL) was added and the mixture was extracted with ethyl acetate. The extract was washed with brine, dried over anhydrous sodium sulfate and evaporated to afford the corresponding thiosulfonate as the sole product. Then the mixture was characterized by HRMS.



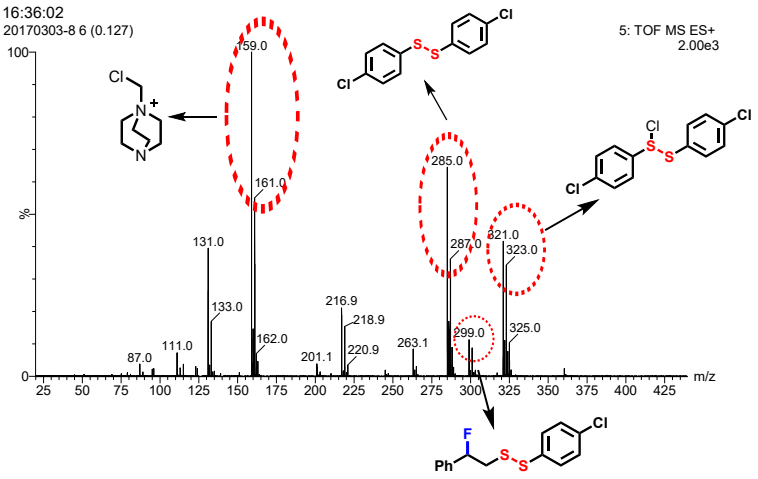
HRMS calcd for $C_{14}H_{13}ClFO_2S_2$ {[M+1]+}: 331.0030, found:331.0068.

HRMS calcd for $C_{14}H_{13}ClFO_1S_2$ {[M+1]+}: 315.0080, found:314.9811.

Figure S4. LC-MS spectrums result of the selectively oxidation of β-

fluorodisulfides

5. MS study of the module reaction



6. Density functional theory (DFT) calculations.

6.1 Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

6.2 Computational Methods

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. Density functional theory B3LYP[1] with a 6-31G(d) basis set was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. Intrinsic Reaction Coordinate (IRC) calculations were performed to ensure that the saddle points found were true transition states connecting the reactants and the products. M11[2] functional with the 6-311+G(d,p) basis set was employed to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with a SMD continuum solvation model[3].

6.3 Calculated results of competing pathway

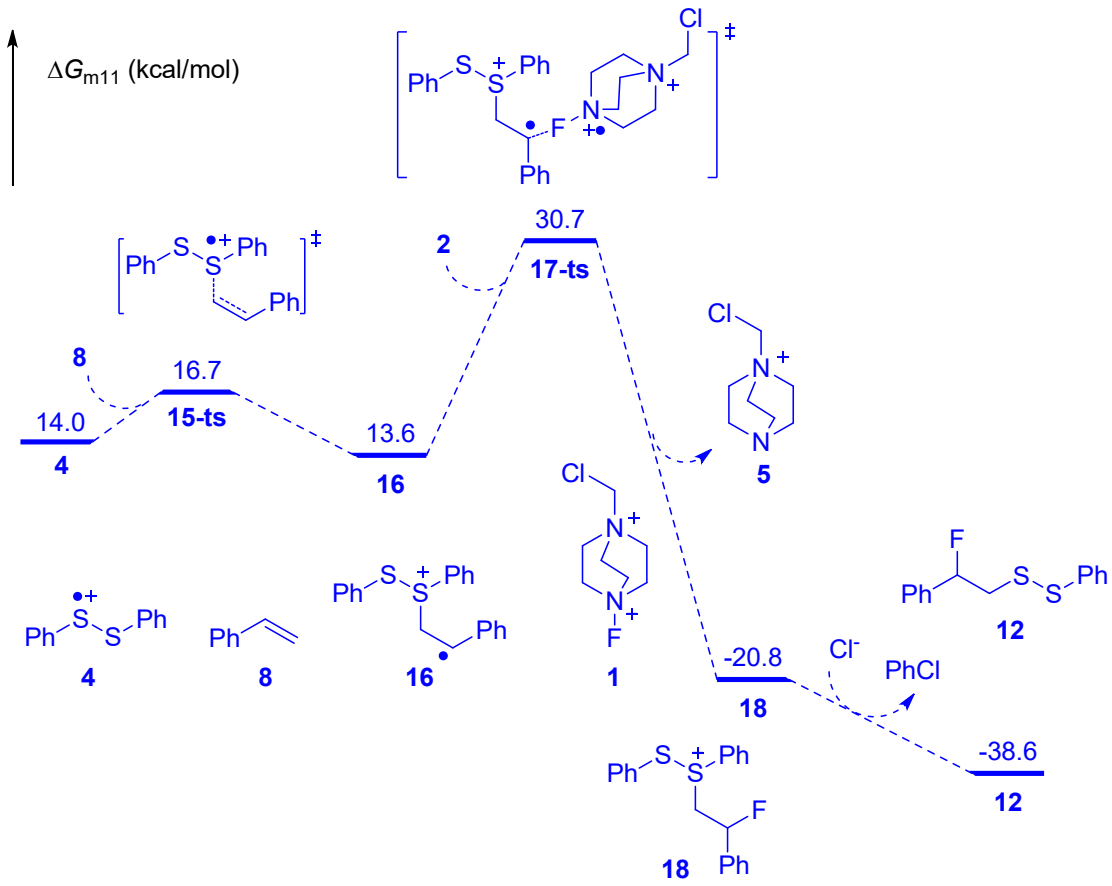


Figure S7. Energy profiles for the competing pathway. Calculations were performed at the M11/6-311+G(d,p)/SMD(acetonitrile)//B3LYP/6-31G(d) level of theory.

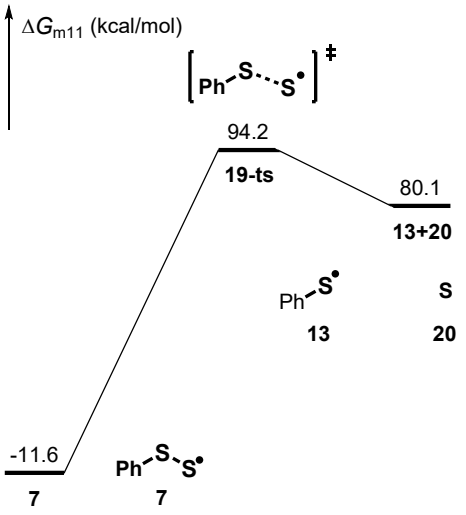


Figure S8 Energy profiles for the S-S bond cleavage process from compound **7**.

6.4 Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{(\text{elec-B3LYP})}$[1]	$G_{(\text{corr-B3LYP})}$[2]	$H_{(\text{corr-B3LYP})}$[3]	$E_{(\text{solv, M11})}$[4]	IF[5]
1	-943.964122	0.187432	0.233099	-944.199571	-
2	-944.342892	0.179242	0.231521	-944.384662	-
3	-1259.662823	0.141701	0.197713	-1259.508279	-
4	-1259.387954	0.141287	0.197658	-1259.274512	-
5	-844.599284	0.183843	0.228251	-844.588093	-
6	-1719.823514	0.138608	0.200764	-1719.676061	-
7	-1028.003816	0.059208	0.101023	-1027.927096	-
8	-309.641799	0.102289	0.140539	-309.523403	-
9-ts	-1337.637157	0.179085	0.243046	-1337.441334	-294.05
10	-1337.644598	0.180173	0.243973	-1337.458079	-
11-ts	-2281.712239	0.386129	0.478788	-2281.66628	-67.61
12	-1437.520114	0.186725	0.250642	-1437.359125	-
13	-629.802334	0.060415	0.097385	-629.719787	-
14	-1090.012695	0.059071	0.101014	-1089.942012	-
15-ts	-1569.046259	0.265766	0.340858	-1568.815847	-109.99

16	-1569.046702	0.266525	0.341776	-1568.82152	-
17-ts	-2512.942889	0.467603	0.575757	-2513.007469	-35.66
18	-1668.909204	0.272145	0.348147	-1668.722328	-
19-ts	-1027.905534	0.057213	0.098333	-1027.756514	-34.4
20	-398.039559	-0.014896	0.00236	-398.047472	-
Cl^-	-460.248732	-0.01502	0.00236	-460.378934	-
PhCl	-691.836755	0.061475	0.097693	-691.761631	-
Cl_2	-920.342921	-0.02068	0.00469	-920.357068	-
F^-	-99.752968	-0.01416	0.00236	-100.00983	-

[1]The electronic energy calculated by B3LYP in gas phase. [2]The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. [3]The thermal correction to enthalpy calculated by B3LYP in gas phase. [4]The electronic energy calculated by M11 in acetonitrile solvent. [5]The B3LYP calculated imaginary frequencies for the transition states.

6.5 B3LYP Geometries for All the Optimized Compounds and Transition State

1

C	1.27155200	-0.67911800	-1.30065600
C	-0.26326000	-0.48806400	-1.19236200
C	0.28717300	1.66637000	-0.10072400
C	1.77248400	1.28583000	0.13071400
H	-0.66086100	-0.01428100	-2.09243500
H	-0.78669000	-1.43165500	-1.03682900
H	1.55008600	-1.72749300	-1.42727800
H	1.72950100	-0.08695600	-2.09550700
H	0.12553200	2.09838000	-1.09073800
H	-0.04927900	2.38104000	0.65366000
H	2.43367000	1.72101100	-0.62172400
H	2.13867300	1.54699800	1.12556200
N	-0.57776100	0.41318900	-0.00030700
N	1.86719200	-0.21170300	0.00088900
C	-0.22010900	-0.32114000	1.28854300
H	-0.30443300	0.39958300	2.10495800
H	-0.95217600	-1.11551700	1.44256200
C	1.21114000	-0.90017600	1.16927200
H	1.81717300	-0.69235500	2.05379500
H	1.23142000	-1.97208400	0.96279600
F	3.21263400	-0.55419100	0.00280200
C	-2.06131600	0.84659400	0.00159500
H	-2.21060400	1.44628900	0.90115900
H	-2.21162700	1.45011300	-0.89523700
Cl	-3.16330000	-0.52279600	0.00045100

2

C	1.24694000	-0.66825400	-1.24723200
C	-0.29797200	-0.50088300	-1.19476900
C	0.18282400	1.67263200	-0.09466800
C	1.68306200	1.30661100	0.08003700
H	-0.69787000	0.00029600	-2.08979800
H	-0.81279700	-1.45916000	-1.03918700
H	1.51877100	-1.73957400	-1.33981200
H	1.68667800	-0.09575500	-2.08920100
H	-0.03682000	2.10295800	-1.08385800
H	-0.17746600	2.34551900	0.69872900
H	2.28997800	1.76134000	-0.72962300
H	2.06596500	1.63594700	1.06731600
N	-0.64261900	0.38321200	0.00082600
N	1.79419800	-0.14601300	0.00139900
C	-0.26270600	-0.33637400	1.29109300
H	-0.41685400	0.39161400	2.10255500
H	-0.94895000	-1.18603600	1.41405800

C	1.21582200	-0.80126000	1.17089500
H	1.79053200	-0.50597600	2.07272800
H	1.28329300	-1.89882300	1.02697400
F	3.76239100	-0.57419100	-0.00244500
C	-2.08274000	0.81145600	-0.00615200
H	-2.25998400	1.40864300	0.90110200
H	-2.25468100	1.39286200	-0.92460100
Cl	-3.23904300	-0.56177100	0.00140100

3

C	-3.92249700	-0.31759500	-0.70344300
C	-2.97910600	0.67407600	-0.42958700
C	-1.88217900	0.38256400	0.39567100
C	-1.73729800	-0.89865400	0.94897200
C	-2.68813300	-1.88443500	0.67317900
C	-3.77827300	-1.59574000	-0.15291900
H	-4.77396200	-0.09090700	-1.34420000
H	-3.08945000	1.67149700	-0.85230600
H	-0.88730300	-1.11786500	1.59286600
H	-2.57578700	-2.87862000	1.10429600
H	-4.51832700	-2.36627400	-0.36648800
S	-0.69361600	1.66391900	0.80432200
S	0.69369600	1.66400400	-0.80411200
C	1.88221200	0.38254600	-0.39563800
C	2.97945700	0.67404700	0.42921600
C	1.73696000	-0.89877700	-0.94864600
C	3.92279200	-0.31772100	0.70293900
H	3.09007700	1.67153600	0.85170500
C	2.68771800	-1.88464700	-0.67293900
H	0.88672500	-1.11796300	-1.59223300
C	3.77817700	-1.59594500	0.15273300
H	4.77450400	-0.09103100	1.34336500
H	2.57507300	-2.87890200	-1.10381200
H	4.51818000	-2.36654900	0.36621600

4

C	2.31685200	1.35193400	-1.44612100
C	1.59924000	0.18733600	-1.20878700
C	1.70656900	-0.43418500	0.05185200
C	2.52543600	0.10671800	1.06421800
C	3.24416900	1.26872100	0.80292000
C	3.13757800	1.89365600	-0.44538600
H	2.25569000	1.83188400	-2.41777800
H	0.98870800	-0.25151800	-1.99095700
H	2.59513400	-0.37793300	2.03331900
H	3.88186900	1.69091000	1.57292800
H	3.69997400	2.80083700	-0.64379700
S	0.96302400	-1.99635300	0.40304400
S	-0.96313800	-1.99639000	-0.40274100
C	-1.70658900	-0.43412300	-0.05183300
C	-1.59884000	0.18781200	1.20856200
C	-2.52581100	0.10643300	-1.06408900
C	-2.31639200	1.35247200	1.44576700
H	-0.98802300	-0.25076800	1.99066500
C	-3.24448300	1.26850300	-0.80292300
H	-2.59583700	-0.37853100	-2.03300700
C	-3.13747800	1.89384900	0.44514200
H	-2.25490200	1.83274200	2.41724600
H	-3.88245900	1.69042800	-1.57284700
H	-3.69982800	2.80108000	0.64345200

5

C	1.53522600	-0.94768400	-1.19722200
C	0.04854600	-0.47475800	-1.24570300
C	0.72833600	1.55751800	-0.00002300
C	2.19333000	1.01602100	0.00011400
H	-0.16942900	0.16500500	-2.10484200
H	-0.66378300	-1.30021700	-1.23690900
H	1.58209900	-2.03958700	-1.19612000
H	2.07157600	-0.59300800	-2.08118600
H	0.49443200	2.14905600	-0.88852500
H	0.49432100	2.14917500	0.88837200
H	2.72614900	1.37828500	-0.88276700
H	2.72594500	1.37814700	0.88317900
N	-0.22829400	0.36448500	-0.00000700
N	2.20796100	-0.44433700	0.00000300
C	0.04854200	-0.47472500	1.24570000
H	-0.16926400	0.16511500	2.10483000
H	-0.66389100	-1.30009500	1.23702400
C	1.53515100	-0.94784600	1.19713200
H	2.07154600	-0.59342100	2.08116800
H	1.58189900	-2.03975600	1.19580200
C	-1.63751700	0.91279200	-0.00000900
H	-1.75333200	1.52251600	0.89626400
H	-1.75333900	1.52251400	-0.89628000
Cl	-2.89072200	-0.34427500	0.00000500

6

C	3.52945200	1.35019400	-0.47519300
C	2.75935200	0.28330300	-0.93494800
C	1.74278200	-0.23425900	-0.11838800
C	1.49735200	0.30380400	1.15029800

C	2.27929700	1.37006700	1.59885300
C	3.28998500	1.89343100	0.79065700
H	4.31985300	1.75254900	-1.10255400
H	2.94224300	-0.14608400	-1.91524800
H	0.72103100	-0.12524100	1.77406200
H	2.09653900	1.78891800	2.58433900
H	3.89573700	2.72196400	1.14728800
S	0.79690200	-1.63450800	-0.71665700
S	-0.74401600	-0.78439000	-1.91018100
C	-1.65859200	0.28184600	-0.80526400
C	-2.62495100	-0.25564200	0.05813900
C	-1.44838400	1.66713500	-0.86326300
C	-3.37927100	0.60061600	0.85903800
H	-2.76661100	-1.32946700	0.10807000
C	-2.21708500	2.51515900	-0.06511400
H	-0.69504500	2.07025600	-1.53246500
C	-3.18001400	1.98276900	0.79495000
H	-4.12495400	0.18716600	1.53195500
H	-2.06054000	3.58917800	-0.11301600
H	-3.77600100	2.64502300	1.41703200
Cl	-0.29046900	-2.64720200	1.54066800

7

C	-1.90594600	1.45124300	0.00016900
C	-0.56362500	1.07449200	0.00030500
C	-0.23519900	-0.28399200	0.00008500
C	-1.24054900	-1.26270500	-0.00020800
C	-2.57877700	-0.87301800	-0.00027700
C	-2.91465600	0.48333300	-0.00013500
H	-2.16494800	2.50646900	0.00042100
H	0.22633600	1.81928700	0.00057900
H	-0.97763500	-2.31762300	-0.00031900
H	-3.35842900	-1.62954100	-0.00046000
H	-3.95816800	0.78512900	-0.00022400
S	1.44922000	-0.90718200	0.00039400
S	2.72986500	0.61344200	-0.00037100

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C	-0.51530900	-0.22055300	-0.00079800
C	-0.00910700	1.09267500	-0.00114100
C	1.36231100	1.32994200	-0.00035900
C	2.26571900	0.26200000	0.00067800
C	1.78129900	-1.04637200	0.00081600
C	0.40657600	-1.28171800	0.00001500
H	-0.69422400	1.93550100	-0.00227600
H	1.73044300	2.35265500	-0.00067800
H	3.33579100	0.45078000	0.00125400
H	2.47255800	-1.88506000	0.00151500
H	0.03502400	-2.30411700	0.00014500
C	-1.95513700	-0.52969400	-0.00130600
C	-2.97773300	0.33518300	0.00177600
H	-2.18641400	-1.59505800	-0.00431900
H	-4.00487900	-0.01657300	0.00097200
H	-2.84000900	1.41309400	0.00530200

9-ts

C	4.18868500	1.77438400	-0.57365200
C	3.11117800	0.89357700	-0.67881200
C	3.19888900	-0.37569900	-0.10075500
C	4.36440800	-0.76133400	0.57663900
C	5.43842400	0.12366600	0.66817800
C	5.35432200	1.39518400	0.09591400
H	4.11633000	2.76126900	-1.02351800
H	2.20576700	1.18515800	-1.20210200
H	4.42920300	-1.74630800	1.03227800
H	6.33909800	-0.18016200	1.19503000
H	6.19005100	2.08508100	0.17244100
S	1.89689400	-1.61807200	-0.19902000
S	0.19038400	-0.69442100	-0.81363900
C	-3.26280700	0.51346800	0.40444800
C	-4.19048300	1.53524200	0.09396200
C	-3.70787500	-0.82801800	0.32847300
C	-5.50053100	1.23520100	-0.26191000
H	-3.86544600	2.57197300	0.14053100
C	-5.01691600	-1.12372000	-0.03205000
H	-3.01609200	-1.63808400	0.53766400
C	-5.92184700	-0.09673600	-0.32627100
H	-6.19514800	2.03828500	-0.49296600
H	-5.33651800	-2.16074900	-0.08939300
H	-6.94410700	-0.33391900	-0.60737200
C	-1.91599300	0.87750400	0.78098900
C	-0.89495800	0.01180500	1.15568800
H	-1.67028700	1.93477000	0.69574800
H	0.00707600	0.43508200	1.58493300
H	-1.12337000	-0.99964000	1.47422500

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C	4.68142000	-1.50000700	-0.48670000
C	3.45704800	-1.40828200	0.17947400
C	2.89665700	-0.15164400	0.44120400
C	3.55843200	1.00932900	0.02313600
C	4.76884200	0.90759400	-0.66147100

C	5.33721200	-0.34467000	-0.91322200
H	5.11197000	-2.47793800	-0.68514200
H	2.93548700	-2.30850400	0.49252100
H	3.12083100	1.98212600	0.22470000
H	5.27605200	1.81130200	-0.98903200
H	6.28401500	-0.41764400	-1.44109100
S	1.37449700	-0.11311400	1.40643700
S	0.19798600	1.35510400	0.51714600
C	-2.95526100	-0.36906900	-0.39782000
C	-3.58995800	0.90129200	-0.50197300
C	-3.77863500	-1.48126000	-0.05871200
C	-4.95440400	1.03893400	-0.28719600
H	-3.00010200	1.78043100	-0.74222700
C	-5.14100600	-1.33418700	0.15172500
H	-3.31739200	-2.46173500	0.03226900
C	-5.74222600	-0.07286500	0.03856800
H	-5.41288100	2.02097500	-0.36994600
H	-5.74359000	-2.20170900	0.40793400
H	-6.80940700	0.04248300	0.20520900
C	-1.56733900	-0.57170900	-0.62007500
C	-0.58182400	0.46956500	-0.97067300
H	-1.17794700	-1.57237800	-0.45077500
H	0.25328700	0.06671000	-1.54869300
H	-1.01379000	1.30593000	-1.53065200

11-ts

S	-1.03811100	0.79916000	0.41324200
C	-2.23457200	-4.88164100	-0.37846700
C	-1.64206200	-3.99955500	0.50615300
C	-1.98618800	-2.61320700	0.48837800
C	-2.93185700	-2.14615700	-0.47474100
C	-3.51241600	-3.03615000	-1.35843400
C	-3.16997000	-4.40002800	-1.30854100
H	-1.98679600	-5.93765800	-0.35341100
H	-0.91990600	-4.35369100	1.23607700
H	-3.19070300	-1.09351400	-0.51507400
H	-4.23698000	-2.68859300	-2.08747800
H	-3.63975900	-5.09283500	-2.00112400
C	-1.41172200	-1.77502600	1.46179200
C	-1.77786800	-0.36846300	1.71990500
H	-0.75308400	-2.24718000	2.18167500
H	-2.85860300	-0.22205200	1.63766300
H	-1.43320900	-0.03885100	2.70000300
C	2.43781600	-0.23018900	-1.04869400
C	3.87957700	0.24083600	-1.41204900
C	4.84417300	-1.33225300	0.25067500
C	3.39750900	-1.89002900	0.42796700
H	4.34817900	-0.38827600	-2.17240500
H	3.90875100	1.27776300	-1.74727000
H	1.72356000	0.59393800	-1.07500600
H	2.09094900	-1.00795100	-1.73105000
H	5.39807400	-1.85784600	-0.53017900
H	5.42102200	-1.36801400	1.17740100
H	3.15554500	-2.63053800	-0.33603300
H	3.27245000	-2.35278400	1.40835000
N	4.75314200	0.13922300	-0.16084400
N	2.47132100	-0.77106700	0.30648000
C	4.09611100	0.92295600	0.97732300
H	4.78489000	0.89905100	1.82470200
H	3.99670900	1.95372000	0.63741600
C	2.72141000	0.26308700	1.30611400
H	2.72731800	-0.19964800	2.29475100
H	1.90921900	0.99161900	1.26766200
F	0.66063600	-1.58430400	0.61525300
C	6.16906800	0.63139600	-0.43217000
H	6.74865900	0.46741600	0.47695700
H	6.56778900	0.03499800	-1.25351200
Cl	6.24215300	2.34359400	-0.86798600
S	-2.00653100	2.59178600	0.81565300
C	-3.63717900	2.42265500	0.09156300
C	-3.81641200	2.24916700	-1.29001700
C	-4.74372100	2.55805000	0.94388800
C	-5.10753000	2.19463000	-1.81004300
H	-2.95479100	2.17425300	-1.94651200
C	-6.03269500	2.51794500	0.40776100
H	-4.59619500	2.70557700	2.00957600
C	-6.21480900	2.33205000	-0.96374100
H	-5.25308400	2.07044600	-2.87913800
H	-6.89110500	2.63099200	1.06286400
H	-7.21817500	2.30461900	-1.37793100

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F	-0.67318600	-0.83642700	0.58455600
C	-2.85552100	-0.29369100	-0.18126300
C	-3.38272700	-0.68125300	1.05572400
C	-4.75884600	-0.85701100	1.20794200
C	-5.61923100	-0.64393800	0.12898400
C	-5.09707700	-0.25972600	-1.10819300
C	-3.72102100	-0.08860000	-1.26252300
H	-2.71057900	-0.85869000	1.88884600

H	-5.15876600	-1.16334600	2.17086400
H	-6.69025400	-0.78218800	0.24924800
H	-5.75928000	-0.10133300	-1.95506300
H	-3.31789800	0.19977600	-2.23143800
C	-1.36993800	-0.04910400	-0.34352000
C	-1.00969400	1.41642600	-0.09491300
H	-1.03532100	-0.35270600	-1.34233700
H	-1.68605000	2.05483300	-0.67505000
H	-1.15640100	1.65581700	0.96251600
C	3.31069300	-2.19784000	-0.32930700
C	2.46143400	-1.17562600	0.09376900
C	2.97702200	0.11117300	0.29953900
C	4.33990600	0.36257600	0.09095600
C	5.18608100	-0.67183200	-0.31375900
C	4.67215400	-1.95129700	-0.52911900
H	2.90927300	-3.19466300	-0.49243800
H	1.40823900	-1.36589200	0.26054500
H	4.72931400	1.36452700	0.24386300
H	6.24269200	-0.47280100	-0.47170100
H	5.32901600	-2.75471800	-0.85167500
S	1.97355300	1.46650700	0.92661700
S	0.66115300	1.98209800	-0.63306100

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C	1.53821100	1.21553700	-0.00003300
C	0.14987600	1.22029400	0.00022900
C	-0.57875900	-0.00005200	0.00025500
C	0.14995100	-1.22034000	0.00019500
C	1.53827100	-1.21549500	0.00000000
C	2.23642700	0.00004200	-0.00024700
H	2.08440700	2.15473200	-0.00000100
H	-0.40346300	2.15400300	0.00052200
H	-0.40332900	-2.15408800	0.00054200
H	2.08450600	-2.15466800	-0.00001500
H	3.32302700	0.00008100	-0.00059100
S	-2.30556300	0.00000100	-0.00017800

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C	-2.24365500	1.21143900	-0.20553000
C	-0.90434200	1.21701700	0.18097500
C	-0.22995200	0.00134100	0.37824800
C	-0.90302300	-1.21586800	0.18583300
C	-2.24225100	-1.21334100	-0.20090200
C	-2.91099700	-0.00169100	-0.39677800
H	-2.76675800	2.15140100	-0.35696300
H	-0.37465400	2.15226700	0.33219400
H	-0.37231100	-2.14990900	0.34088700
H	-2.76429500	-2.15445400	-0.34877000
H	-3.95513100	-0.00286300	-0.69766800
S	1.44999300	0.00346200	0.95789200
Cl	2.56697500	-0.00265900	-0.83806100

15-ts

C	0.35242300	3.84020600	0.76100100
C	0.04394400	2.56651000	1.23785900
C	0.39855600	1.44586400	0.47172000
C	1.05511100	1.58731000	-0.75978900
C	1.35396300	2.86823900	-1.22265200
C	1.00500700	3.99039700	-0.46507000
H	0.08012600	4.71260700	1.34684500
H	-0.46482100	2.44169600	2.18855600
H	1.33436600	0.71923000	-1.34683400
H	1.86036500	2.98958300	-2.17536500
H	1.24089700	4.98429000	-0.83324800
S	-0.04949400	-0.14828600	1.13765700
S	1.71553800	-1.12538900	1.87148100
C	2.86356500	-1.18672900	0.51221600
C	2.86734300	-2.29499900	-0.35316000
C	3.82706300	-0.17307500	0.37642200
C	3.82651100	-2.37536100	-1.36106600
H	2.14151400	-3.09121600	-0.21869000
C	4.78576300	-0.26900200	-0.63216400
H	3.82909500	0.66729000	1.06276500
C	4.78293300	-1.36388500	-1.50049900
H	3.83850900	-3.23267700	-2.02732000
H	5.53868700	0.50663200	-0.73451100
H	5.53476100	-1.43644600	-2.28079700
C	-0.86884200	-1.24222000	-0.58723500
C	-1.96573300	-0.51308800	-1.11317100
H	-1.06257000	-2.15710300	-0.03183500
H	0.03083900	-1.29172200	-1.19490100
H	-1.74462300	0.21481100	-1.89012100
C	-3.32285800	-0.60006700	-0.68616900
C	-4.29544500	0.20385600	-1.34526600
C	-3.76135800	-1.46002700	0.36029300
C	-5.63139600	0.14680900	-0.98240600
H	-3.97588900	0.86439700	-2.14680300
C	-5.09792100	-1.50733900	0.71968700
H	-3.04858500	-2.08686000	0.88699500
C	-6.03908200	-0.70809800	0.05133700
H	-6.36114700	0.76339100	-1.49777800

H	-5.41960300	-2.16713700	1.51951100
H	-7.08591200	-0.75377000	0.33600400

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C	0.48508900	3.86052000	0.78146400
C	0.09305600	2.59164700	1.20662000
C	0.41807600	1.47893500	0.41733200
C	1.13151700	1.61749600	-0.78190400
C	1.50968600	2.89451500	-1.19409700
C	1.18938600	4.01108300	-0.41549400
H	0.23457900	4.72871200	1.38285100
H	-0.46134300	2.46661600	2.13151800
H	1.39115600	0.75486000	-1.38543800
H	2.05716000	3.01687900	-2.12355100
H	1.48872400	5.00142400	-0.74491200
S	-0.12191200	-0.10457000	1.04126000
S	1.59158200	-1.17792200	1.83275500
C	2.78061700	-1.26018300	0.51536900
C	2.77185700	-2.35308700	-0.37085700
C	3.78781000	-0.28234900	0.43073600
C	3.76191000	-2.45417800	-1.34591100
H	2.01133100	-3.12207400	-0.27632800
C	4.77603900	-0.39887700	-0.54589400
H	3.79924900	0.54494500	1.13272600
C	4.76075900	-1.47833800	-1.43385900
H	3.76408000	-3.29960800	-2.02718100
H	5.56206100	0.34756700	-0.60823400
H	5.53586400	-1.56693500	-2.18932300
C	-0.81253700	-1.05193900	-0.54972600
C	-1.96218900	-0.33379700	-1.07728300
H	-1.01626400	-2.03196500	-0.11490600
H	0.04209800	-1.10596900	-1.22425200
H	-1.75924200	0.43050900	-1.82225200
C	-3.30977300	-0.50573700	-0.66601100
C	-4.32124800	0.27920900	-1.29348100
C	-3.71556700	-1.43404700	0.33638600
C	-5.65404300	0.13895100	-0.94380400
H	-4.03135200	0.99202400	-2.06090000
C	-5.05101200	-1.56411900	0.68118300
H	-2.97822300	-2.05088600	0.84148200
C	-6.02767900	-0.78244500	0.04513400
H	-6.40954500	0.74349100	-1.43620900
H	-5.34304200	-2.27677900	1.44652400
H	-7.07254400	-0.89250600	0.31872400

17-ts

C	2.00928500	0.78423000	3.80323900
C	1.63193400	0.39277500	2.51782800
C	2.57115700	0.49742800	1.47928100
C	3.87047800	0.97172000	1.70241500
C	4.22724800	1.35357600	2.99532800
C	3.30277800	1.25725600	4.04164900
H	1.29909900	0.70792800	4.62074100
H	0.62807900	0.03666600	2.30902300
H	4.59684300	1.02075300	0.89765200
H	5.23189400	1.71714900	3.18743600
H	3.59536900	1.54588500	5.04652500
S	2.00989100	-0.06555100	-0.13271500
S	3.81699800	-0.60731800	-1.34417300
C	4.04499500	-2.32992100	-1.14364900
C	4.89344000	-2.80523600	-0.11758700
C	3.51132600	-3.21635800	-2.10684900
C	5.20303100	-4.15880100	-0.06414300
H	5.31476500	-2.11363600	0.60472800
C	3.83690000	-4.56560900	-2.04235100
H	2.88064300	-2.83611200	-2.90405200
C	4.67795200	-5.03507700	-1.02385500
H	5.86450900	-4.53318900	0.71058500
H	3.45204100	-5.25271500	-2.78922800
H	4.93590700	-6.08926800	-0.98486800
C	1.68795900	1.51835400	-1.04467700
C	0.80728100	2.47797900	-0.32003700
H	1.29432400	1.23040400	-2.02373100
H	2.66523400	1.99719300	-1.20635300
C	0.28514700	3.64023600	-0.87881400
C	-0.32895600	4.59171500	0.00873700
C	0.42631400	3.98178800	-2.26827800
C	-0.74542000	5.82080000	-0.46075500
H	-0.43384000	4.33941200	1.06017000
C	0.00266800	5.21102700	-2.72415100
H	0.87918500	3.28054800	-2.96188700
C	-0.57637600	6.13149000	-1.82299600
H	-1.18729200	6.54949400	0.21095000
H	0.11868000	5.48085900	-3.76880500
H	-0.89608900	7.10296800	-2.19119900
H	0.70881400	2.34826300	0.75314200
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C	-3.18048100	-0.26142700	-1.09362800
C	-4.63765600	-0.81845000	-1.05087200
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H	-5.37855600	-0.07148700	-1.34468800
H	-4.76366300	-1.70182400	-1.67755100
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H	-3.14922000	0.71790100	-1.57387200
H	-5.77658200	0.66610700	0.95287800
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18

C	-0.19177200	3.93055600	-0.36049700
C	0.17022400	2.68361700	-0.86736900
C	-0.27229600	1.52824600	-0.20566100
C	-1.07640800	1.60036300	0.94080400
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H	5.39781100	-2.57837000	-0.79664200
H	6.36832100	-0.34368300	-1.28539400
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19-ts

C	-0.87264900	-1.77207700	-0.00015400
C	-0.14050400	-0.59299600	-0.00018500
C	-0.79826000	0.66730600	-0.00004400
C	-2.21948800	0.68966400	0.00012300
C	-2.94279200	-0.49508600	0.00015600
C	-2.27380800	-1.72757600	0.00002100
H	-0.35902600	-2.72942100	-0.00026600
H	0.94493500	-0.60056400	-0.00031500
H	-2.72436200	1.65039900	0.00023000
H	-4.02892600	-0.46789300	0.00028800
H	-2.84474800	-2.65213900	0.00005000
S	0.11384600	2.13280000	-0.00006000
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20

S	0.00000000	0.00000000	0.00000000

Cl-

Cl	0.00000000	0.00000000	0.00000000

PhCl

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C	-0.17824700	1.21641800	0.00001400
C	-1.57444000	1.20780400	-0.00001200
C	-2.27509300	0.00000500	0.00000000
C	-1.57446600	-1.20779000	0.00001000
C	-0.17825400	-1.21642000	-0.00000800

H 0.37488000 2.14968600 0.00001000

H -2.11247300 2.15180800 -0.00001700

H -3.36124500 0.00002600 -0.00000700

H -2.11248200 -2.15180300 0.00001000

H 0.37483100 -2.14971400 -0.00001700

Cl 2.26435700 0.00000000 -0.00000200

Cl2

Cl 0.00000000 0.00000000 1.02240700

Cl 0.00000000 0.00000000 -1.02240700

F-

F 0.00000000 0.00000000 0.00000000

6.6 Energy profiles for the competing pathway

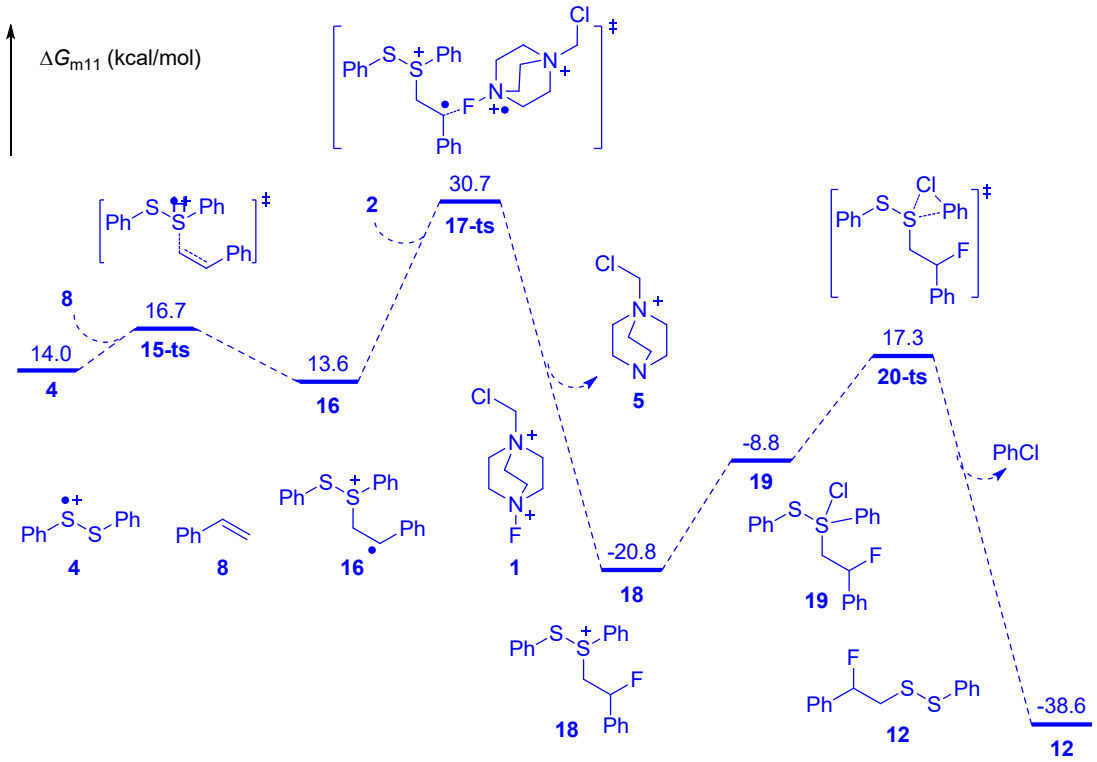


Figure S9. Energy profiles for the competing pathway. Calculations were performed at the M11/6-311+G(d,p)/SMD(acetonitrile)//B3LYP/6-31G(d) level of theory.

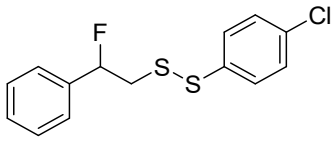
6.7 Reference

1. a) A. D. Becke, *J. Chem. Phys*. **1993**, *98*, 5648; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785.

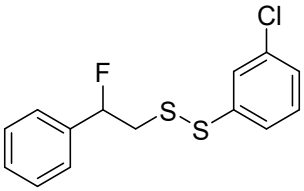
2. Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2011**, *2*, 2810.

3. a) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378; b) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys*. **2006**, *125*, 194101.

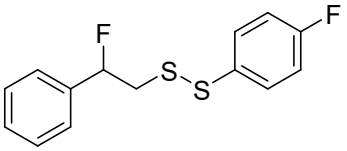
7. Characterization data



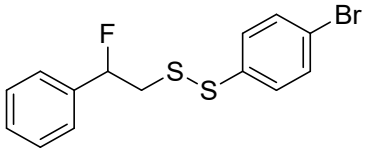
1-(4-chlorophenyl)-2-(2-fluoro-2-phenylethyl)disulfane (C1). White solid (108.8 mg, 73%). Mp: 96-97°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.58 (m, 2H), 7.57-7.49 (m, 2H), 7.49-7.46 (m, 1H), 7.46-7.30 (m, 4H), 5.46-5.17 (m, 1H), 3.70-3.24 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9 (d, J = 26.4 Hz), 138.5 (dd, J = 93.6, 40.8 Hz), 129.8 (d, J = 5.6 Hz), 129.1 (d, J = 11.8 Hz), 127.3, 127.0, 125.6, 125.3, 67.6 (d, J = 80.0 Hz), 56.0 (d, J = 14.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.5 ppm. HRMS calcd for $C_{14}H_{13}ClFS_2$ {$[M+H]^+$}:299.0131, found 299.0126.



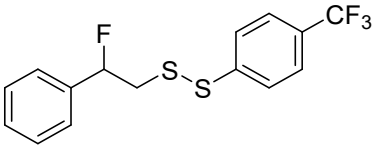
1-(3-chlorophenyl)-2-(2-fluoro-2-phenylethyl)disulfane (C2). White solid (99.8 mg, 67%). Mp: 60-61°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 14.1 Hz, 1H), 7.51-7.33 (m, 8H), 5.47-5.21 (m, 1H), 3.71-3.26 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6 (d, *J* = 21.3 Hz), 138.6 (d, *J* = 58.2 Hz), 135.9 (d, *J* = 2.5 Hz), 131.6 (d, *J* = 23.9 Hz), 130.7 (d, *J* = 2.9 Hz), 129.1 (d, *J* = 14.6 Hz), 127.5, 127.0, 124.0 (d, *J* = 14.6 Hz), 122.1 (d, *J* = 21.0 Hz), 67.5 (d, *J* = 69.1 Hz), 56.0 (d, *J* = 14.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.5. HRMS calcd for $C_{14}H_{13}ClFS_2$ {$[M+H]^+$}: 299.0131, found 299.0126.



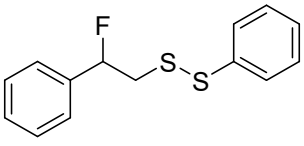
1-(2-fluoro-2-phenylethyl)-2-(4-fluorophenyl)disulfane (C3). Colorless viscous oil (91.6 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.63 (m, 2H), 7.61-7.50 (m, 2H), 7.49-7.46 (m, 1H), 7.45-7.32 (m, 4H), 5.46-5.17 (m, 1H), 3.70-3.24 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5 (d, *J* = 26.4 Hz), 138.7 (d, *J* = 56.6 Hz), 132.7 (d, *J* = 5.9 Hz), 129.1 (d, *J* = 12.2 Hz), 127.3, 127.0, 125.7, 125.5, 67.5 (d, *J* = 79.0 Hz), 56.0 (d, *J* = 14.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.5 (d, J = 353.1 Hz), -220.6. HRMS calcd for $C_{14}H_{13}F_2S_2$ {$[M+H]^+$}: 283.0427, found 283.0423.



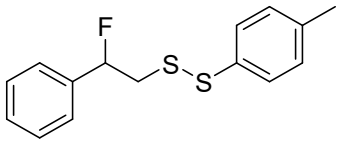
1-(4-bromophenyl)-2-(2-fluoro-2-phenylethyl)disulfane (C4). White solid (116.3 mg, 68%). Mp: 115-116°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.67 (m, 2H), 7.57-7.52 (m, 2H), 7.49-7.36 (m, 5H), 5.46-5.17 (m, 1H), 3.70-3.24 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9 (d, *J* = 13.9 Hz), 163.4 (d, *J* = 13.5 Hz), 138.8 (d, *J* = 59.2 Hz), 129.1 (d, *J* = 11.3 Hz), 127.3, 127.0, 126.4 (dd, *J* = 24.1, 8.9 Hz), 116.9 (dd, *J* = 22.6, 5.7 Hz), 67.6 (d, *J* = 80.5 Hz), 56.1 (d, *J* = 10.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{14}H_{13}BrFS_2$ {$[M+H]^+$}:342.9626, found 342.9621.



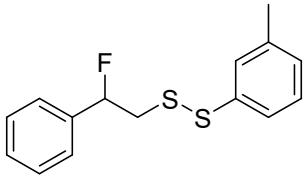
1-(2-fluoro-2-phenylethyl)-2-(4-(trifluoromethyl)phenyl)disulfane (C5). White solid (116.2 mg, 70%). Mp: 81-82°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.72 (m, 3H), 7.64-7.28 (m, 6H), 5.49-5.24 (m, 1H), 3.80-3.26 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5 (d, *J* = 53.5 Hz), 129.5, 129.2, 129.1, 127.3, 127.0, 126.5, 124.6, 124.3, 67.4 (d, *J* = 67.7 Hz), 55.8 (d, *J* = 18.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.87 (d, *J* = 10.4 Hz), -220.4. HRMS calcd for $C_{15}H_{13}F_4S_2$ {$[M+H]^+$}: 333.0395, found 333.0387.



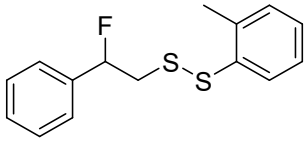
1-(2-fluoro-2-phenylethyl)-2-phenyldisulfane (C6). Colorless viscous oil, (72.6 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.63 (m, 2H), 7.56-7.40 (m, 6H), 7.38-7.32 (m, 2H), 5.47-5.18 (m, 1H), 3.73-3.24 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4 (d, *J* = 23.1 Hz), 138.9 (d, *J* = 59.8 Hz), 131.5 (d, *J* = 22.8 Hz), 129.5 (d, *J* = 3.7 Hz), 129.1 (d, *J* = 11.6 Hz), 127.3, 127.0, 124.0 (d, *J* = 19.2 Hz), 67.6 (d, *J* = 78.0 Hz), 56.2 (d, *J* = 5.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.7. HRMS calcd for $C_{14}H_{14}FS_2$ {$[M+H]^+$}:265.0521, found 265.0514.



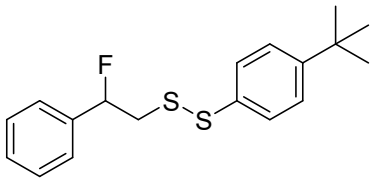
1-(2-fluoro-2-phenylethyl)-2-(p-tolyl)disulfane (C7). White solid (98.7 mg, 71%). Mp: 85-86°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.5-7.54 (m, 2H), 7.49-7.33 (m, 6H), 5.45-5.14 (m, 1H), 3.75-3.18 (m, 2H), 2.44 (d, *J* = 8.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1 (d, *J* = 25.1 Hz), 139.6 (dd, *J* = 123.5, 43.3 Hz), 130.2 (d, *J* = 4.5 Hz), 129.1, 128.97, 127.3, 127.0, 124.9 (d, *J* = 19.7 Hz), 67.6 (d, *J* = 82.3 Hz), 56.2, 21.4 (d, *J* = 5.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{15}H_{16}FS_2$ {$[M+H]^+$}: 279.0677, found 279.0672.



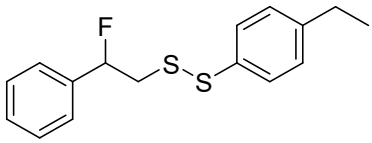
1-(2-fluoro-2-phenylethyl)-2-(m-tolyl)disulfane (C8). White solid (86.2 mg, 62%). Mp: 71-72°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.87 (m, 1H), 7.52 (d, *J* = 6.6 Hz, 1H), 7.49-7.32 (m, 6H), 7.24-7.19 (m, 1H), 5.53-5.31 (m, 1H), 3.53-3.09 (m, 2H), 2.32 (d, *J* = 106.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7 (d, *J* = 2.1 Hz), 139.0 (d, *J* = 58.0 Hz), 134.4 (d, *J* = 6.6 Hz), 131.1 (d, *J* = 11.4 Hz), 130.9 (d, *J* = 1.7 Hz), 129.4, 129.0 (d, *J* = 13.6 Hz), 127.3, 127.0, 123.6 (d, *J* = 21.4 Hz), 66.2 (d, *J* = 70.1 Hz), 56.5 (d, *J* = 26.5 Hz), 18.0 (d, *J* = 18.0 Hz). δ -220.6. HRMS calcd for $C_{15}H_{16}FS_2$ {$[M+H]^+$}: 279.0677, found 279.0671.



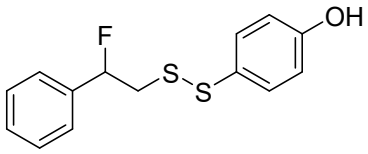
1-(2-fluoro-2-phenylethyl)-2-(o-tolyl)disulfane (C9). White solid (87.6 mg, 63%). Mp: 78-79°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 10.0 Hz, 2H), 7.44-7.42 (m, 4H), 7.40-7.25 (m, 3H), 5.47-5.18 (m, 1H), 3.71-3.26 (m, 2H), 2.44 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3 (d, *J* = 18.5 Hz), 139.8 (d, *J* = 5.3 Hz), 138.9 (d, *J* = 63.0 Hz), 132.3 (d, *J* = 24.0 Hz), 129.3 (d, *J* = 1.6 Hz), 129.0 (d, *J* = 12.4 Hz), 127.4, 127.0, 124.2 (d, *J* = 15.8 Hz), 121.1 (d, *J* = 20.1 Hz), 67.6 (d, *J* = 72.8 Hz), 56.3, 21.4 (d, *J* = 3.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.3. HRMS calcd for $C_{15}H_{16}FS_2$ {$[M+H]^+$}: 279.0677, found 279.0672.



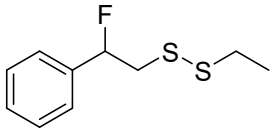
1-(4-(tert-butyl)phenyl)-2-(2-fluoro-2-phenylethyl)disulfane (C10). White solid (115.2 mg, 72%). Mp: 97-98°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.54 (m, 4H), 7.50-7.34 (m, 5H), 5.47-5.18 (m, 1H), 3.75-3.24 (m, 2H), 1.36 (d, *J* = 7.5 Hz, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3 (d, *J* = 26.7 Hz), 139.5 (dd, *J* = 109.7, 40.7 Hz), 129.3, 129.0 (d, *J* = 12.4 Hz), 127.4, 127.0, 126.6 (d, *J* = 5.0 Hz), 123.9 (d, *J* = 20.8 Hz), 67.5 (d, *J* = 70.3 Hz), 56.3 (d, *J* = 7.4 Hz), 35.1 (d, *J* = 4.7 Hz), 31.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.5. HRMS calcd for $C_{18}H_{22}FS_2$ {$[M+H]^+$}:321.1147, found 321.1142.



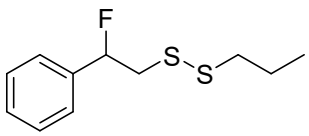
1-(4-ethylphenyl)-2-(2-fluoro-2-phenylethyl)disulfane (C11). White solid (99.3 mg, 68%). Mp: 93-94°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.56 (m, 2H), 7.50-7.30 (m, 7H), 5.46-5.16 (m, 1H), 3.73-3.26 (m, 2H), 2.78-2.67 (m, 2H), 1.27 (dd, *J* = 16.0, 7.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4 (d, *J* = 24.2 Hz), 139.7 (dd, *J* = 137.1, 41.9 Hz), 129.3, 129.08, 129.0 (d, *J* = 6.2 Hz), 127.3, 127.02, 124.2 (d, *J* = 20.0 Hz), 67.6 (d, *J* = 76.2 Hz), 56.3 (d, *J* = 3.0 Hz), 28.8 (d, *J* = 2.8 Hz), 15.4 (d, *J* = 3.9 Hz). HRMS calcd for $C_{16}H_{18}FS_2$ {$[M+H]^+$}: 293.0834, found 293.0831.



4-((2-fluoro-2-phenylethyl)disulfanyl)phenol (C12). Colorless viscous oil (78.4 mg, 56%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.53 (m, 1H), 7.51-7.30 (m, 5H), 7.00-6.96 (m, 2H), 6.83-6.77 (m, 1H), 5.38-5.01 (m, 1H), 3.83-3.29 (m, 2H), 2.97 (d, *J* = 30.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2 (dd, *J* = 104.8, 81.5 Hz), 138.6, 130.2, 129.1, 127.0 (dd, *J* = 24.2, 15.4 Hz), 117.0 (d, *J* = 5.9 Hz), 116.7, 115.6, 56.1, 29.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{14}H_{14}FOS_2$ {$[M+H]^+$}:281.0470, found 281.0459.

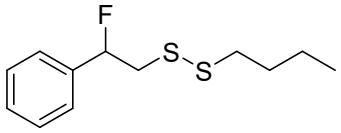


1-ethyl-2-(2-fluoro-2-phenylethyl)disulfane (C13). White solid (68.0 mg, 63%). Mp: 78-79°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.34 (m, 5H), 5.44-5.36 (m, 1H), 3.55-3.15 (m, 2H), 2.81-2.75 (m, 2H), 1.41-1.31 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2 (d, *J* = 84.0 Hz), 129.3, 129.1, 127.1 (d, *J* = 37.7 Hz), 61.6 (d, *J* = 63.1 Hz), 56.1 (d, *J* = 15.5 Hz), 46.3 (d, *J* = 5.7 Hz), 6.7 (d, *J* = 11.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -227.0. HRMS calcd for $C_{10}H_{14}FS_2$ {$[M+H]^+$}: 217.0521, found 217.0512.

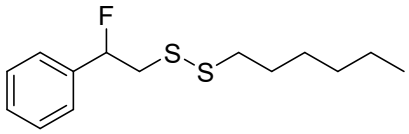


1-(2-fluoro-2-phenylethyl)-2-propyldisulfane (C14). White solid (73.6 mg, 64%). Mp: 81-82°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.38 (m, 5H), 5.45-5.36 (m, 1H), 3.55-3.16 (m, 2H), 2.83-2.57 (m, 2H), 1.90-1.76 (m, 2H), 1.14-1.03 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2 (d, *J* = 83.9 Hz), 129.3, 129.1, 127.1 (d, *J* = 38.1 Hz), 62.3 (d, *J* = 64.8 Hz), 56.1 (d, *J* = 18.9 Hz), 54.9, 16.3 (d, *J* = 11.2

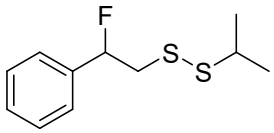
Hz), 13.4 (d, J = 7.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -227.4. HRMS calcd for $C_{11}H_{16}FS_2$ {[M+H]$^+$}: 231.0677, found 231.0674.



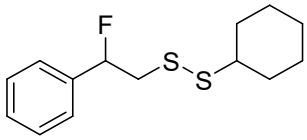
1-butyl-2-(2-fluoro-2-phenylethyl)disulfane (C15). White solid (73.2 mg, 60%). Mp: 86-87°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.31 (m, 5H), 5.44-5.36 (m, 1H), 3.55-3.13 (m, 2H), 2.82-2.61 (m, 2H), 1.83-1.65 (m, 2H), 1.58-1.39 (m, 2H), 1.00-0.92 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2 (d, J = 84.5 Hz), 129.3, 129.1, 127.2 (d, J = 37.7 Hz), 62.2 (d, J = 62.2 Hz), 56.1 (d, J = 17.6 Hz), 52.7 (d, J = 4.2 Hz), 24.5 (d, J = 10.6 Hz), 22.0 (d, J = 7.4 Hz), 13.7 (d, J = 3.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{12}H_{18}FS_2$ {[M+H]$^+$}: 245.0834, found 245.0830.



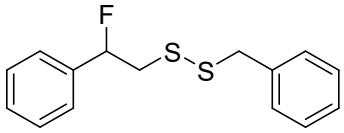
1-(2-fluoro-2-phenylethyl)-2-hexyldisulfane (C16). White solid (74.8 mg, 55%). Mp: 92-93°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.33 (m, 5H), 5.43-5.35 (m, 1H), 3.54-3.14 (m, 2H), 2.75-2.63 (m, 2H), 1.82-1.71 (m, 2H), 1.50-142 (m, 1H), 1.39-1.21 (m, 5H), 0.93-0.84 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2 (d, J = 83.4 Hz), 129.3, 129.0, 127.1 (d, J = 37.5 Hz), 62.2 (d, J = 60.8 Hz), 56.1 (d, J = 18.0 Hz), 53.0 (d, J = 4.4 Hz), 31.3 (d, J = 3.4 Hz), 28.4 (d, J = 7.7 Hz), 22.5 (d, J = 10.2 Hz), 22.4 (d, J = 3.4 Hz), 13.9 (d, J = 2.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.0. HRMS calcd for $C_{14}H_{22}FS_2$ {[M+H]$^+$}: 273.1147, found 273.1141.



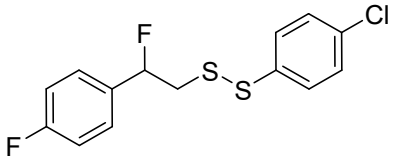
1-(2-fluoro-2-phenylethyl)-2-isopropyldisulfane (C17). White solid (67.9 mg, 59%). Mp: 76-76°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.34 (m, 5H), 5.47-5.31 (m, 1H), 3.45-3.05 (m, 2H), 2.87-2.82 (m, 1H), 1.37-1.23 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3 (d, J = 99.9 Hz), 129.3, 129.0, 127.2 (d, J = 41.9 Hz), 58.9 (d, J = 64.8 Hz), 56.4 (d, J = 8.3 Hz), 51.1 (d, J = 12.0 Hz), 15.3 (dd, J = 104.4, 15.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -226.8. HRMS calcd for $C_{11}H_{16}FS_2$ {[M+H]$^+$}:231.0677, found 231.0687.



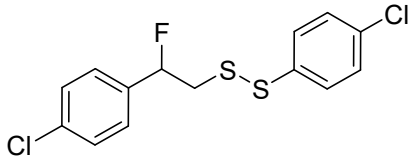
1-cyclohexyl-2-(2-fluoro-2-phenylethyl)disulfane (C18). White solid (86.4 mg, 64%). Mp: 68-69°C .^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.36 (m, 5H), 5.46-5.36 (m, 1H), 3.49-3.11 (m, 2H), 2.62 (s, 1H), 2.12 (s, 1H), 1.93-1.83 (m, 4H), 1.73-169 (m, 1H), 1.35-1.27 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3 (d, J = 99.3 Hz), 129.2, 128.99, 127.2 (d, J = 40.9 Hz), 59.5 (dd, J = 67.0, 39.4 Hz), 56.4 (d, J = 10.8 Hz), 26.2 (d, J = 6.8 Hz), 25.4 (dd, J = 10.1, 4.2 Hz), 25.2 (d, J = 3.0 Hz), 24.8.^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{14}H_{20}FS_2$ {[M+H]$^+$}:271.0990, found 271.0996.



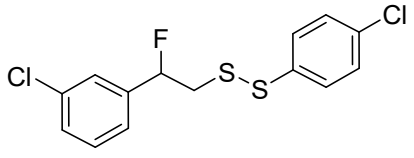
1-benzyl-2-(2-fluoro-2-phenylethyl)disulfane (C19). White solid (100.0 mg, 72%). Mp: 103-104°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.37 (m, 8H), 7.32-7.26 (m, 2H), 5.39-5.28 (m, 1H), 4.13-4.02 (m, 2H), 3.44-3.07 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.0 (d, *J* = 88.0 Hz), 130.1 (d, *J* = 1.6 Hz), 129.3 (d, *J* = 4.4 Hz), 129.1 (d, *J* = 3.4 Hz), 129.0 (d, *J* = 2.2 Hz), 128.7, 127.3, 127.0, 60.7 (d, *J* = 80.9 Hz), 58.7, 56.0.^{19}F NMR (376 MHz, $CDCl_3$) δ -220.5. HRMS calcd for $C_{15}H_{16}FS_2$ {$[M+H]^+$}: 279.0677, found 279.0692.



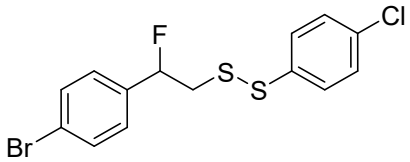
1-(4-chlorophenyl)-2-(2-fluoro-2-(4-fluorophenyl)ethyl)disulfane (C20). White solid (110.6 mg, 70%). Mp: 93-94°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.45 (m, 4H), 7.40-7.36 (m, 1H), 7.15-7.02 (m, 2H), 5.45-5.18 (m, 1H), 3.72-3.16 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0 (dd, *J* = 249.2, 20.7 Hz), 141.7 (d, *J* = 28.9 Hz), 137.9 (d, *J* = 25.1 Hz), 134.6 (dd, *J* = 61.9, 3.3 Hz), 129.8 (d, *J* = 6.3 Hz), 129.1 (dd, *J* = 35.6, 8.5 Hz), 125.4 (d, *J* = 20.0 Hz), 116.1 (dd, *J* = 21.9, 15.9 Hz), 67.4 (d, *J* = 79.9 Hz), 55.2 (d, *J* = 15.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.6 (d, *J* = 136.8 Hz), -220.7. HRMS calcd for $C_{14}H_{12}ClF_2S_2$ {$[M+H]^+$}: 317.0037, found 317.0029.



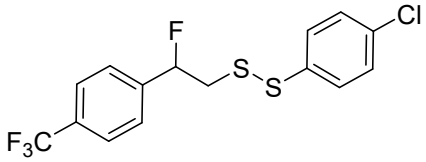
1-(4-chlorophenyl)-2-(2-fluoro-2-(4-fluorophenyl)ethyl)disulfane (C21). White solid (119.5 mg, 72%). Mp: 116-118°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.48 (m, 4H), 7.42 (s, 2H), 7.34 (s, 2H), 5.43-5.16 (m, 1H), 3.67-3.19 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7 (d, *J* = 27.8 Hz), 137.6 (dd, *J* = 68.1, 41.1 Hz), 135.2 (d, *J* = 28.6 Hz), 129.9 (d, *J* = 6.6 Hz), 129.3 (d, *J* = 15.3 Hz), 128.7, 128.4, 125.4 (d, *J* = 20.7 Hz), 67.3 (d, *J* = 78.8 Hz), 55.2 (d, *J* = 17.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -221.1. HRMS calcd for $C_{14}H_{12}Cl_2FS_2$ {$[M+H]^+$}: 332.9742, found 332.9736.



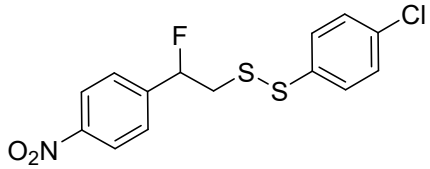
1-(4-chlorophenyl)-2-(2-(3-chlorophenyl)-2-fluoroethyl)disulfane (C22). White solid (111.2 mg, 67%). Mp: 104-106°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.48 (m, 4H), 7.49-7.19 (m, 4H), 5.42-5.14 (m, 1H), 3.66-3.21 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6 (d, *J* = 23.9 Hz), 140.6 (d, *J* = 51.1 Hz), 137.9 (d, *J* = 27.8 Hz), 135.0 (d, *J* = 17.4 Hz), 130.4 (d, *J* = 10.0 Hz), 129.9 (d, *J* = 8.4 Hz), 129.44 (d, *J* = 33.9 Hz), 127.35 (d, *J* = 24.7 Hz), 125.57 (d, *J* = 7.0 Hz), 125.27 (d, *J* = 4.5 Hz), 67.07 (d, *J* = 81.2 Hz), 55.0 (d, *J* = 19.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -218.5. HRMS calcd for $C_{14}H_{12}Cl_2FS_2$ (M+H): 332.9742, found 332.9736.



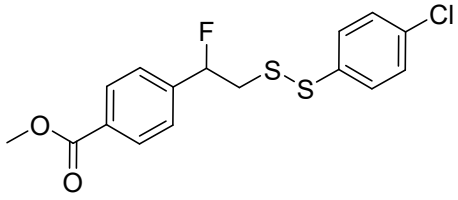
1-(2-(4-bromophenyl)-2-fluoroethyl)-2-(4-chlorophenyl)disulfane (C23). Light yellow solid (131.6 mg, 70%). Mp: 126-128°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.49 (m, 5H), 7.37 (d, *J* = 8.5 Hz, 1H), 7.29-7.27 (m, 2H), 5.42-5.15 (m, 1H), 3.66-3.17 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7 (d, *J* = 26.6 Hz), 137.9 (d, *J* = 23.7 Hz), 137.5, 132.3 (d, *J* = 15.1 Hz), 129.9 (d, *J* = 6.7 Hz), 128.8 (d, *J* = 33.4 Hz), 125.4 (d, *J* = 21.2 Hz), 123.4 (d, *J* = 32.2 Hz), 67.2 (d, *J* = 76.1 Hz), 55.2 (d, *J* = 17.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -221.1. HRMS calcd for $C_{14}H_{12}BrClFS_2$ {$[M+H]^+$}: 376.9236, found 376.9240.



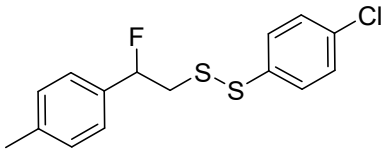
1-(4-chlorophenyl)-2-(2-fluoro-2-(4-(trifluoromethyl)phenyl)ethyl)disulfane(C24). White solid (124.4 mg, 68%). Mp: 114-116°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.3 Hz, 1H), 7.67-7.31 (m, 7H), 5.51-5.23 (m, 1H), 3.68-3.22 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5 (d, *J* = 49.6 Hz), 141.5 (d, *J* = 26.5 Hz), 138.0 (d, *J* = 28.3 Hz), 129.9 (d, *J* = 8.9 Hz), 127.8, 127.5, 126.1 (dd, *J* = 13.9, 3.7 Hz), 125.5, 125.2, 67.0 (d, *J* = 87.7 Hz), 54.9 (d, *J* = 26.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.81 (d, *J* = 15.4 Hz), -221.8. HRMS calcd for $C_{15}H_{12}ClF_4S_2$ {$[M+H]^+$}: 367.0005, found 366.9997.



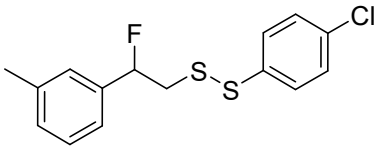
1-(4-chlorophenyl)-2-(2-fluoro-2-(4-nitrophenyl)ethyl)disulfane (C25). White solid (108.0 mg, 63%). Mp: 132-134°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33-8.23 (m, 2H), 7.72-7.51 (m, 6H), 5.55-5.29 (m, 1H), 3.70-3.20 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2 (d, *J* = 24.8 Hz), 145.5 (d, *J* = 44.6 Hz), 141.4 (d, *J* = 39.9 Hz), 138.1 (d, *J* = 25.1 Hz), 130.0 (d, *J* = 7.8 Hz), 128.3 (d, *J* = 37.1 Hz), 125.4 (d, *J* = 20.5 Hz), 124.3 (d, *J* = 10.5 Hz), 66.8 (d, *J* = 118.7 Hz), 54.4 (d, *J* = 41.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -222.5. HRMS calcd for $C_{14}H_{12}ClFNO_2S_2$ {$[M+H]^+$}: 343.9982, found 343.9972.



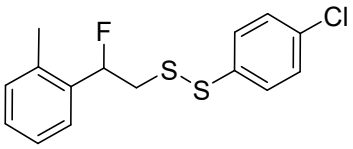
methyl 4-(2-((4-chlorophenyl)disulfanyl)-1-fluoroethyl)benzoate (C26). White solid (126.4 mg, 71%). Mp: 106-108°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-7.99 (m, 2H), 7.63-7.47 (m, 6H), 5.50-5.21 (m, H), 3.95 (d, *J* = 9.6 Hz, 3H), 3.68-3.22 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3 (d, *J* = 5.6 Hz), 143.3 (d, *J* = 48.5 Hz), 141.6 (d, *J* = 29.4 Hz), 138.0 (d, *J* = 25.4 Hz), 131.0 (d, *J* = 30.2 Hz), 130.4 (d, *J* = 11.2 Hz), 129.9 (d, *J* = 6.5 Hz), 127.2 (d, *J* = 33.8 Hz), 125.4 (d, *J* = 20.3 Hz), 67.1 (d, *J* = 87.2 Hz), 55.2 (d, *J* = 27.6 Hz), 52.3 (d, *J* = 3.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -221.6. HRMS calcd for $C_{16}H_{15}ClFO_2S_2$ {$[M+H]^+$}:357.0186, found 357.0182.



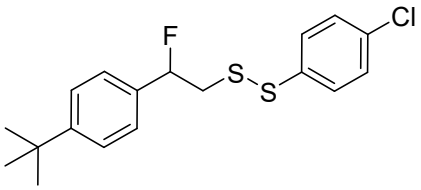
1-(4-chlorophenyl)-2-(2-fluoro-2-(p-tolyl)ethyl)disulfane (C27). White solid (115.4 mg, 74%). Mp: 112-114°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.50 (m, 4H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.29-7.23 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 1H), 5.43-5.15 (m, 1H), 3.69-3.24 (m, 2H), 2.38 (d, *J* = 18.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0 (d, *J* = 22.3 Hz), 139.4 (d, *J* = 28.3 Hz), 137.7 (d, *J* = 24.0 Hz), 135.8 (d, *J* = 61.7 Hz), 129.8 (d, *J* = 1.1 Hz), 129.7 (d, *J* = 7.4 Hz), 127.1 (d, *J* = 32.2 Hz), 125. 5 (d, *J* = 19.7 Hz), 67.5 (d, *J* = 64.2 Hz), 56.0 (d, *J* = 6.1 Hz), 21.2 (d, *J* = 9.1 Hz).^{19}F NMR (376 MHz, $CDCl_3$) δ -220.3. HRMS calcd for $C_{15}H_{15}ClFS_2$ {$[M+H]^+$}: 313.0288, found 313.0283.



1-(4-chlorophenyl)-2-(2-fluoro-2-(m-tolyl)ethyl)disulfane (C28). White solid (106.1 mg, 68%). Mp: 96-97°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.50 (m, 4H), 7.33-7.13 (m, 4H), 5.42-5.13 (m, 1H), 3.71-3.15 (m, 2H), 2.38 (d, *J* = 21.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9 (d, *J* = 22.8 Hz), 139.0 (d, *J* = 12.9 Hz), 138.3, 137.7 (d, *J* = 26.3 Hz), 130.1 (d, *J* = 32.5 Hz), 129.8 (d, *J* = 7.4 Hz), 129.0 (d, *J* = 12.0 Hz), 127.8 (d, *J* = 38.1 Hz), 125.5 (d, *J* = 23.3 Hz), 124.2 (d, *J* = 23.2 Hz), 67.5 (d, *J* = 75.7 Hz), 56.1 (d, *J* = 7.8 Hz), 21.4 (d, *J* = 9.1 Hz).^{19}F NMR (376 MHz, $CDCl_3$) δ -220.3. HRMS calcd for $C_{15}H_{15}ClFS_2$ {$[M+H]^+$}: 313.0288, found 313.0282.

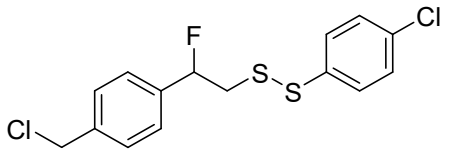


1-(4-chlorophenyl)-2-(2-fluoro-2-(o-tolyl)ethyl)disulfane (C29). White solid (99.8 mg, 64%). Mp: 106-108°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.51 (m, 4H), 7.44-7.12 (m, 4H), 5.77-5.42 (m, 1H), 3.78-3.18 (m, 2H), 2.43 (d, *J* = 26.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0 (d, *J* = 22.1 Hz), 137.8 (d, *J* = 29.9 Hz), 136.7 (d, *J* = 46.1 Hz), 135.8 (d, *J* = 46.0 Hz), 131.1 (d, *J* = 9.5 Hz), 129.8 (d, *J* = 6.2 Hz), 129.1 (d, *J* = 22.4 Hz), 126.9 (d, *J* = 22.8 Hz), 126.5, 125.4 (d, *J* = 23.0 Hz), 66.7 (d, *J* = 73.8 Hz), 52.2 (d, *J* = 48.2 Hz), 19.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -219.2. HRMS calcd for $C_{15}H_{15}ClFS_2$ {$[M+H]^+$}: 313.0288, found 313.0283.

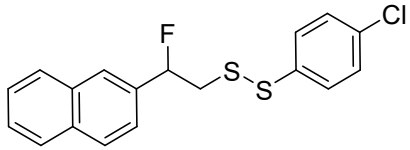


1-(2-(4-(tert-butyl)phenyl)-2-fluoroethyl)-2-(4-chlorophenyl)disulfane (C30). White solid (118.6 mg, 67%). Mp: 134-136°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.48 (m, 4H), 7.45-7.31 (m, 4H), 5.46-5.14 (m, 1H), 3.72-3.24 (m, 2H), 1.33 (d, *J* = 15.1 Hz, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5 (d, *J* = 24.0 Hz), 142.0 (d, *J* = 16.9 Hz), 137.7 (d, *J* = 30.1 Hz), 135.6 (d, *J* = 64.4 Hz), 129.8 (d, *J* = 8.6 Hz), 126.8 (d, *J* = 29.1 Hz), 126.0 (d, *J* = 13.9 Hz), 125.5 (d, *J* = 26.6 Hz), 67.4 (d, *J* = 71.9 Hz), 55.9 (d, *J* =

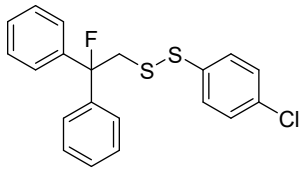
5.1 Hz), 34.7 (d, *J* = 7.0 Hz), 31.2 (d, *J* = 3.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.4. HRMS calcd for $C_{18}H_{21}ClF_4S_2$ {[M+H]$^+$}: 355.0757, found 355.0752.



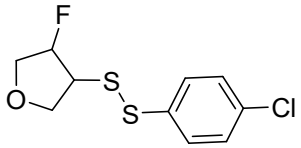
1-(2-(4-(chloromethyl)phenyl)-2-fluoroethyl)-2-(4-chlorophenyl)disulfane. (C31) White solid (110.7 mg, 64%). Mp: 122-124°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.47 (m, 5H), 7.40 (s, 2H), 7.28 (s, 1H), 5.47-5.16 (m, 1H), 4.62 (s, 1H), 4.58 (s, 1H), 3.69-3.23 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8 (d, *J* = 22.9 Hz), 139.0 (d, *J* = 40.1 Hz), 138.6 (d, *J* = 5.5 Hz), 137.9 (d, *J* = 26.8 Hz), 129.8 (d, *J* = 7.0 Hz), 129.3 (d, *J* = 11.3 Hz), 127.6 (d, *J* = 32.4 Hz), 125.4 (d, *J* = 23.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.9. HRMS calcd for $C_{15}H_{14}Cl_2FS_2$ (M+H): 346.9898, found 346.9893.



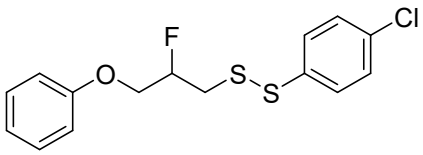
1-(4-chlorophenyl)-2-(2-fluoro-2-(naphthalen-2-yl)ethyl)disulfane. (C32) White solid (114.8 mg, 66%). Mp: 108-110°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.82 (m, 4H), 7.77-7.31 (m, 7H), 5.64-5.37 (m, 1H), 3.78-3.34 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8 (d, *J* = 18.3 Hz), 137.8 (d, *J* = 25.4 Hz), 135.8 (d, *J* = 65.4 Hz), 133.5 (d, *J* = 20.2 Hz), 133.0, 129.8 (d, *J* = 8.2 Hz), 129.3 (d, *J* = 29.8 Hz), 128.2 (d, *J* = 18.3 Hz), 127.8 (d, *J* = 6.8 Hz), 127.1 (d, *J* = 2.0 Hz), 127.0-126.8 (m), 126.3, 125.4 (d, *J* = 20.4 Hz), 124.1 (d, *J* = 18.0 Hz), 67.4 (d, *J* = 51.9 Hz), 56.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.1. HRMS calcd for $C_{18}H_{15}ClFS_2$ (M+H): 349.0288, found 349.0280.



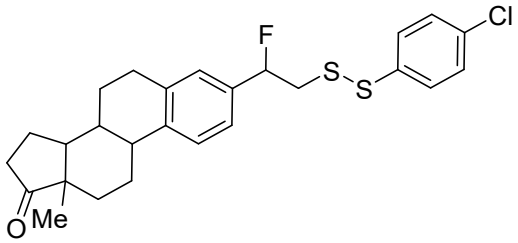
1-(4-chlorophenyl)-2-(2-fluoro-2,2-diphenylethyl)disulfane (C33). White solid (87.9 mg, 47%). Mp: 88-90°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.58 (m, 3H), 7.56-7.45 (m, 3H), 7.43-7.35 (m, 3H), 7.32-7.22 (m, 7H), 3.70-3.57 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 143.9, 142.3, 137.2, 129.9, 128.6, 128.4, 127.8, 127.6, 126.6, 125.62, 125.4, 78.4, 66.9.^{19}F NMR (376 MHz, $CDCl_3$) δ -220.3. HRMS calcd for $C_{20}H_{17}ClFS_2$ {[M+H]$^+$}: 375.0444, found 375.0439.



3-((4-chlorophenyl)disulfanyl)-4-fluorotetrahydrofuran (C34). Colorless viscous oil, (60.7 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (q, *J* = 3.0 Hz, 4H), 4.48-4.43 (m, 1H), 4.42-4.21 (m, 2H), 4.06-4.03 (m, 1H), 3.93-3.91 (m, 1H), 3.84-3.81 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.7, 131.1, 128.7 (d, *J* = 45.6 Hz), 128.1 (d, *J* = 42.2 Hz), 73.7, 70.4, 60.7, 53.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{10}H_{11}ClFOS_2$ {[M+H]$^+$}:264.9924, found 264.9935.



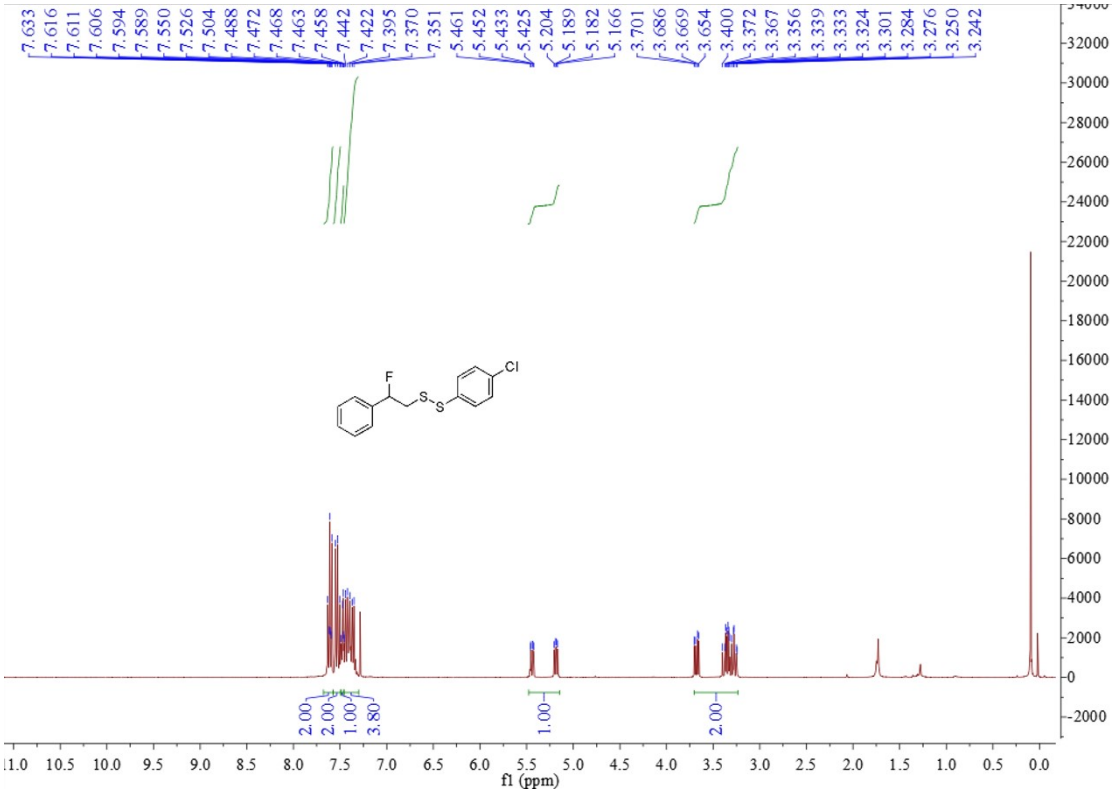
1-(4-chlorophenyl)-2-(2-fluoro-3-phenoxypropyl)disulfane (C35). Colorless viscous oil, (100.0 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.53 (m, 4H), 7.34-7.28 (m, 2H), 7.06-6.81 (m, 3H), 4.45-4.22 (m, 2H), 4.02-3.88 (m, 2H), 3.45-3.29 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6 (d, *J* = 6.7 Hz), 139.7, 139.0, 138.2, 129.7 (dd, *J* = 10.9, 5.1 Hz), 126.3 (d, *J* = 10.0 Hz), 121.8 (d, *J* = 9.9 Hz), 114.6 (d, *J* = 6.2 Hz), 66.1 (d, *J* = 66.8 Hz), 62.4 (d, *J* = 81.7 Hz), 38.7 (d, *J* = 21.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.5. HRMS calcd for $C_{15}H_{15}ClFOS_2$ {$[M+H]^+$}:329.0237, found 329.0231.

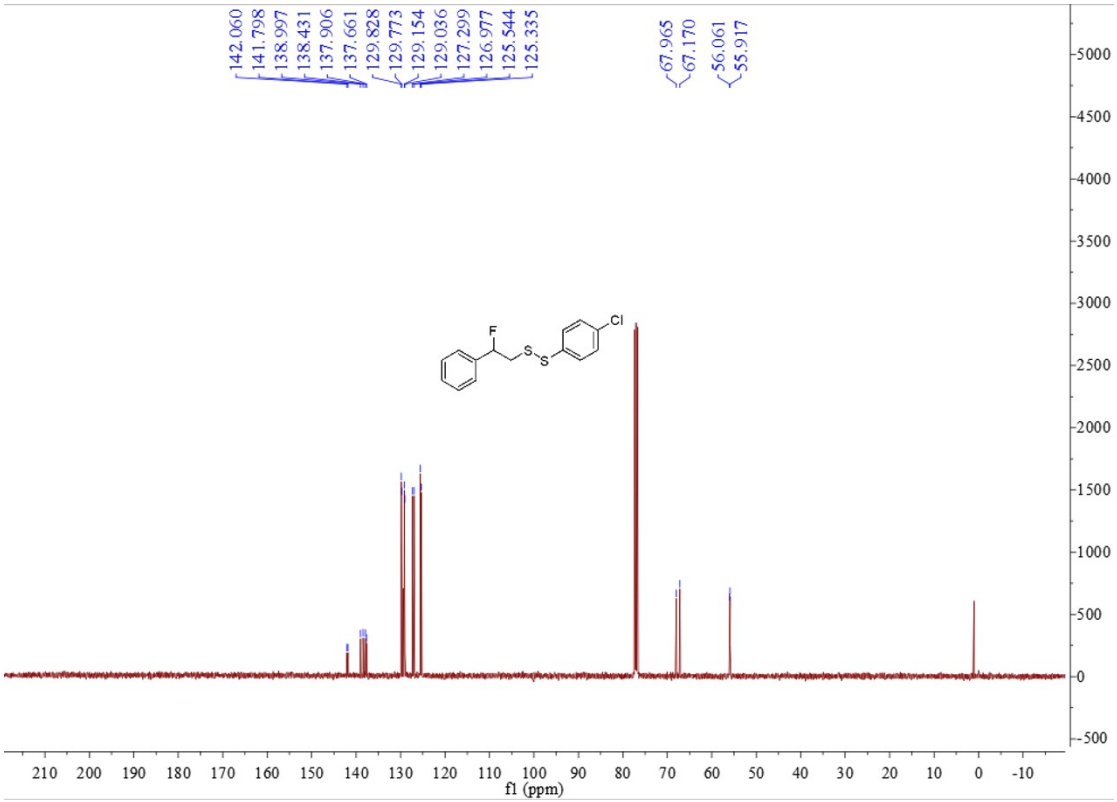


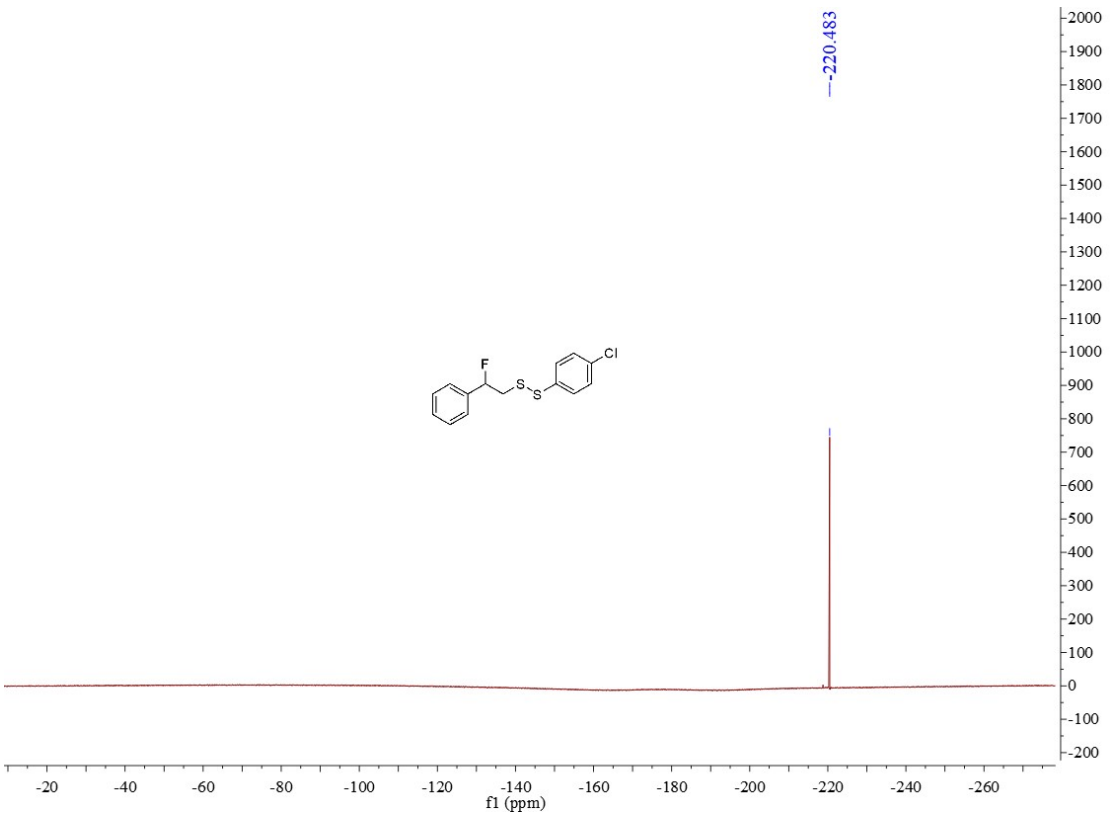
3-(2-((4-chlorophenyl)disulfanyl)-1-fluoroethyl)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (C36). White solid (106.7 mg, 45%). Mp: 116-1118°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.59 (m, 2H), 7.55-7.49 (m, 2H), 7.29-7.24 (m, 2H), 7.17 (d, *J* = 7.7 Hz, 1H), 5.41-5.10 (m, 1H), 3.43-3.24 (m, 2H), 2.96-2.89 (m, 2H), 2.53 (d, *J* = 10.2 Hz, 1H), 2.42 (d, *J* = 10.1 Hz, 1H), 2.30 (d, *J* = 10.1 Hz, 1H), 2.19-1.98 (m, 4H), 1.66-1.46 (m, 6H), 0.93 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9 (d, *J* = 15.3 Hz), 141.0, 137.5 (d, *J* = 16.4 Hz), 136.4, 129.8, 129.7, 127.5, 126.1, 125.6, 125.3, 124.4, 67.5 (d, *J* = 9.0 Hz), 55.8, 50.5, 44.4, 38.0, 35.8, 31.6, 29.3, 26.3, 25.6, 21.6, 13.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -220.6. HRMS calcd for $C_{26}H_{29}ClFOS_2$ {$[M+H]^+$}: 475.1332, found 475.1261.

8. Compound data

C1



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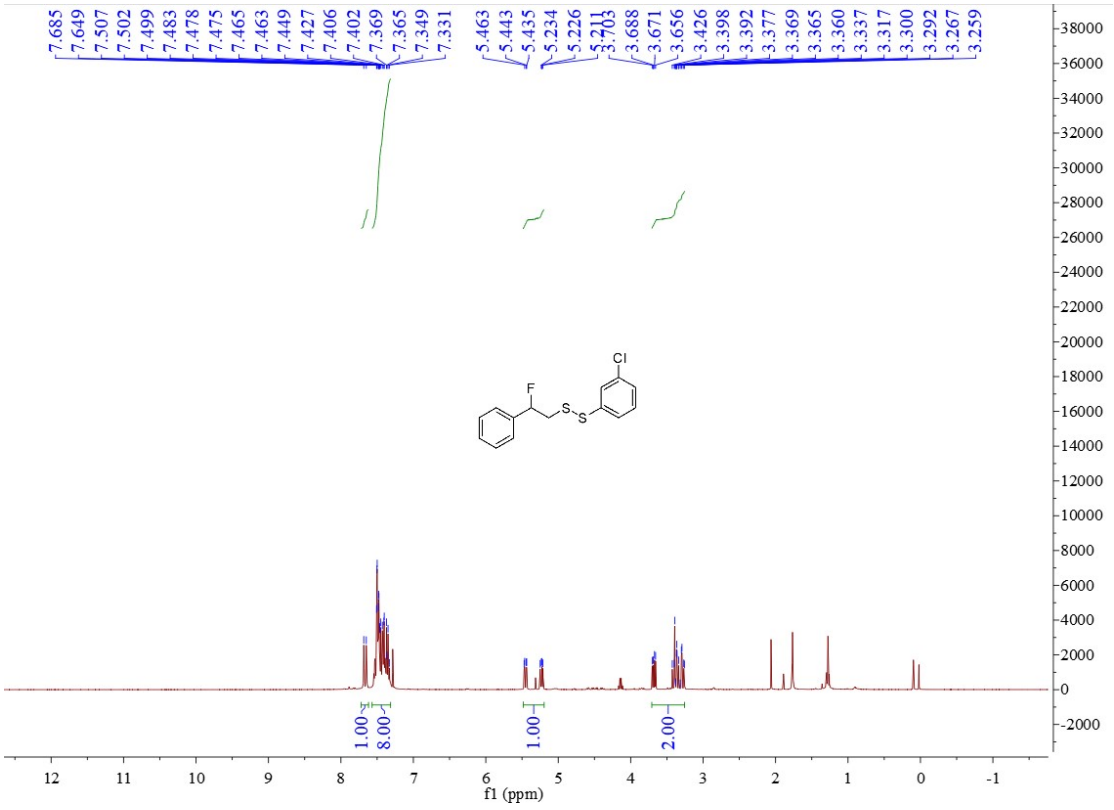
S
Cl
f1 (ppm)

C2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S
S
Cl
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8.00
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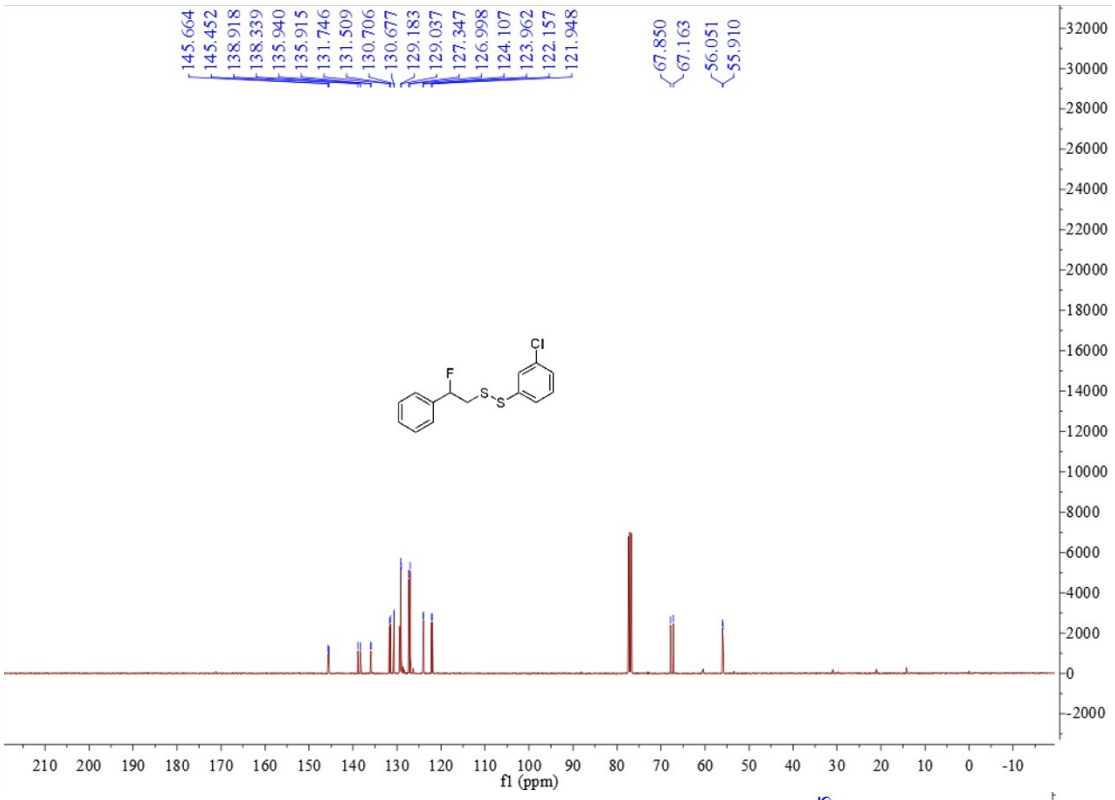
2.00
f1 (ppm)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Cl
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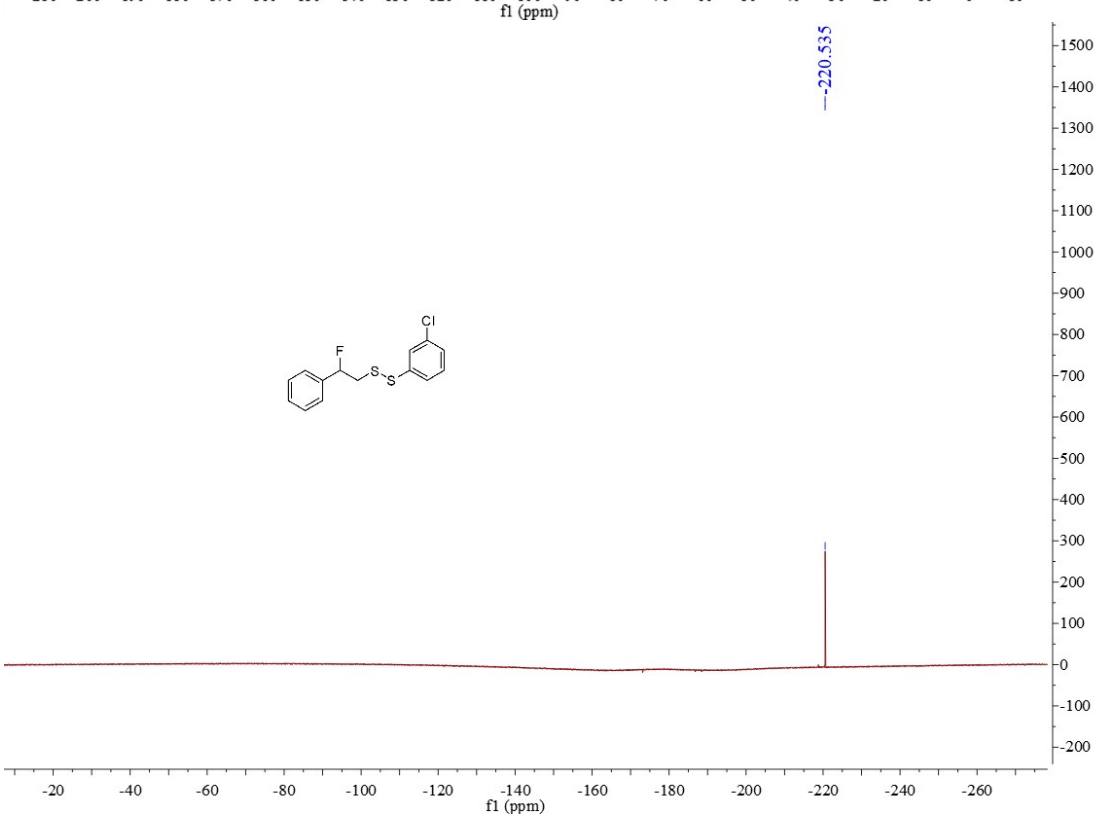
S
S
f1 (ppm)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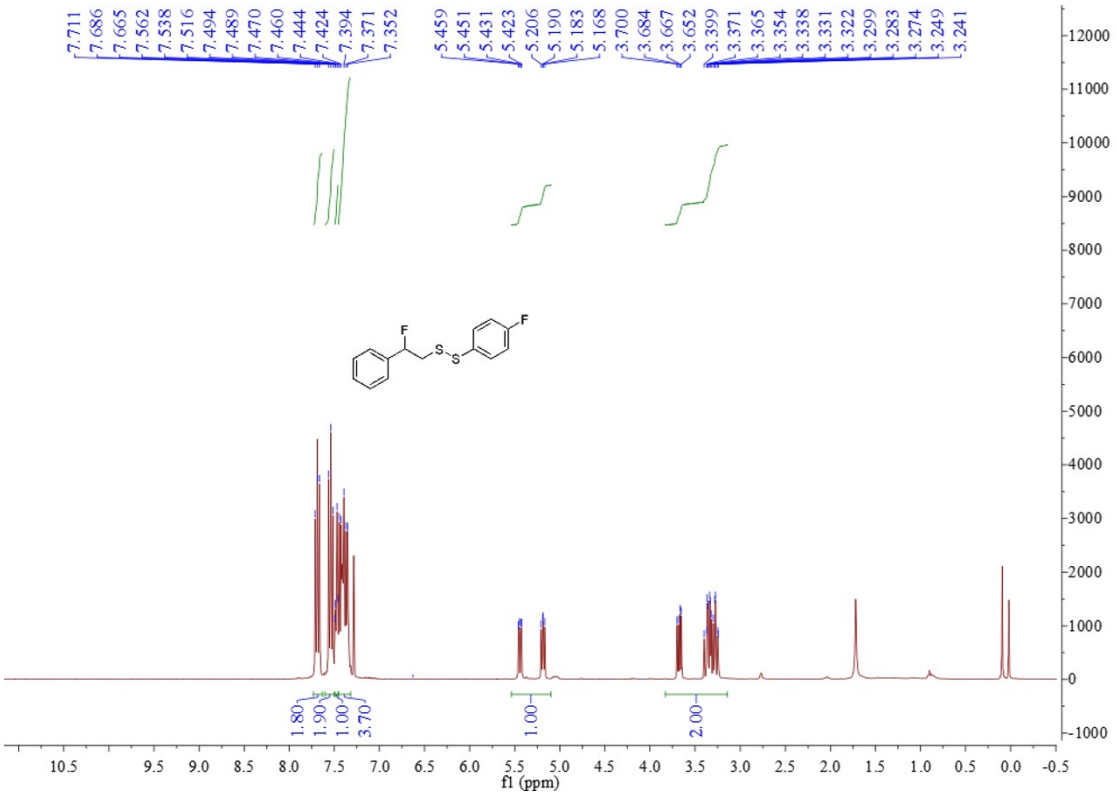
C3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3.274
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S
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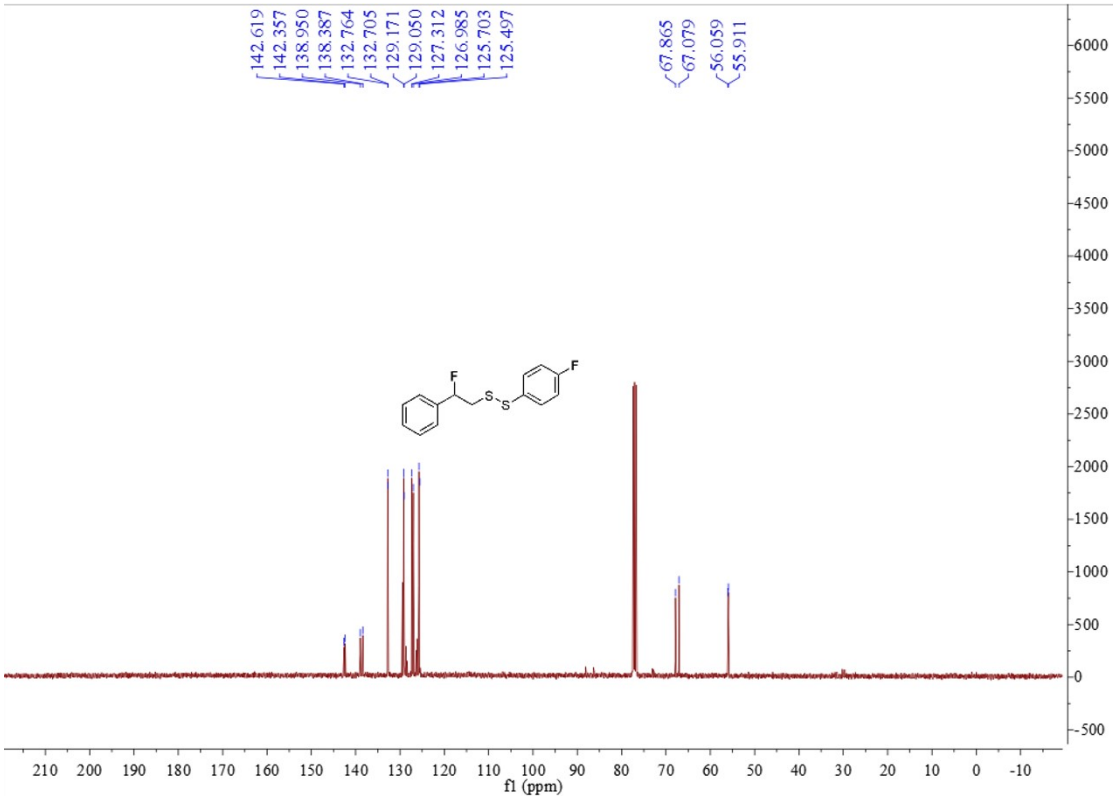
2.00
f1 (ppm)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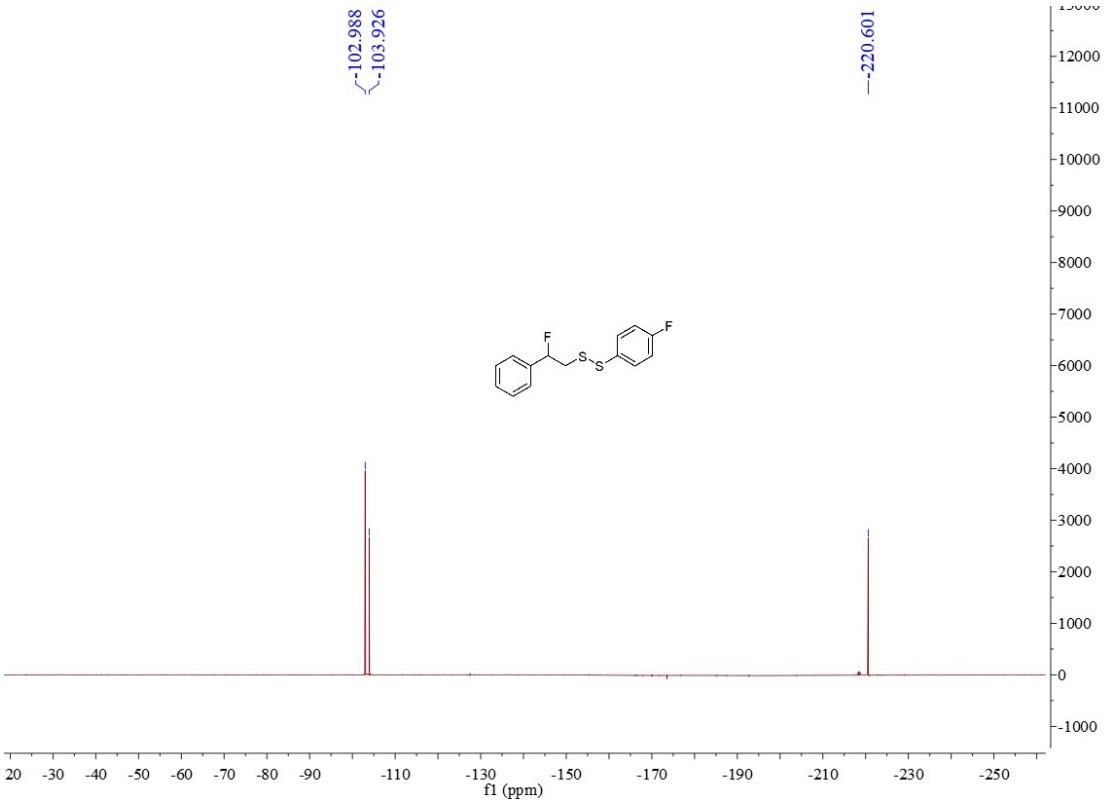
55.911
F
S
S
F
f1 (ppm)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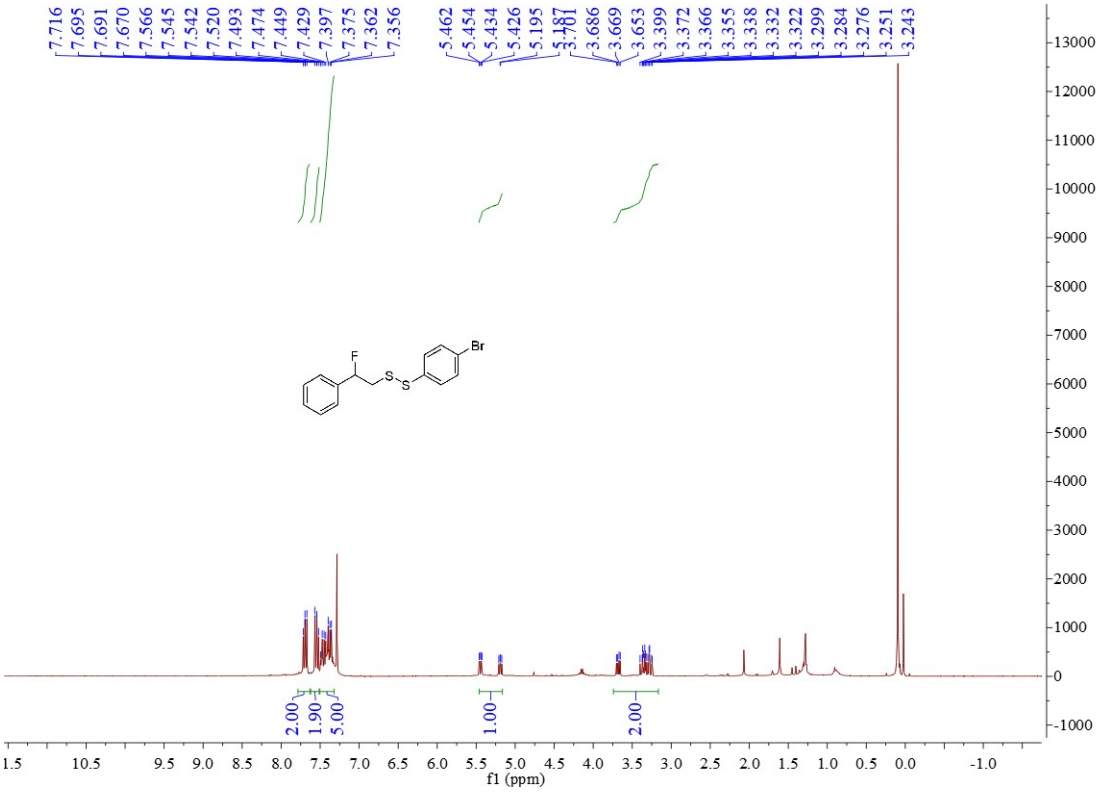
S
S
F
f1 (ppm)

C4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S
S
Br
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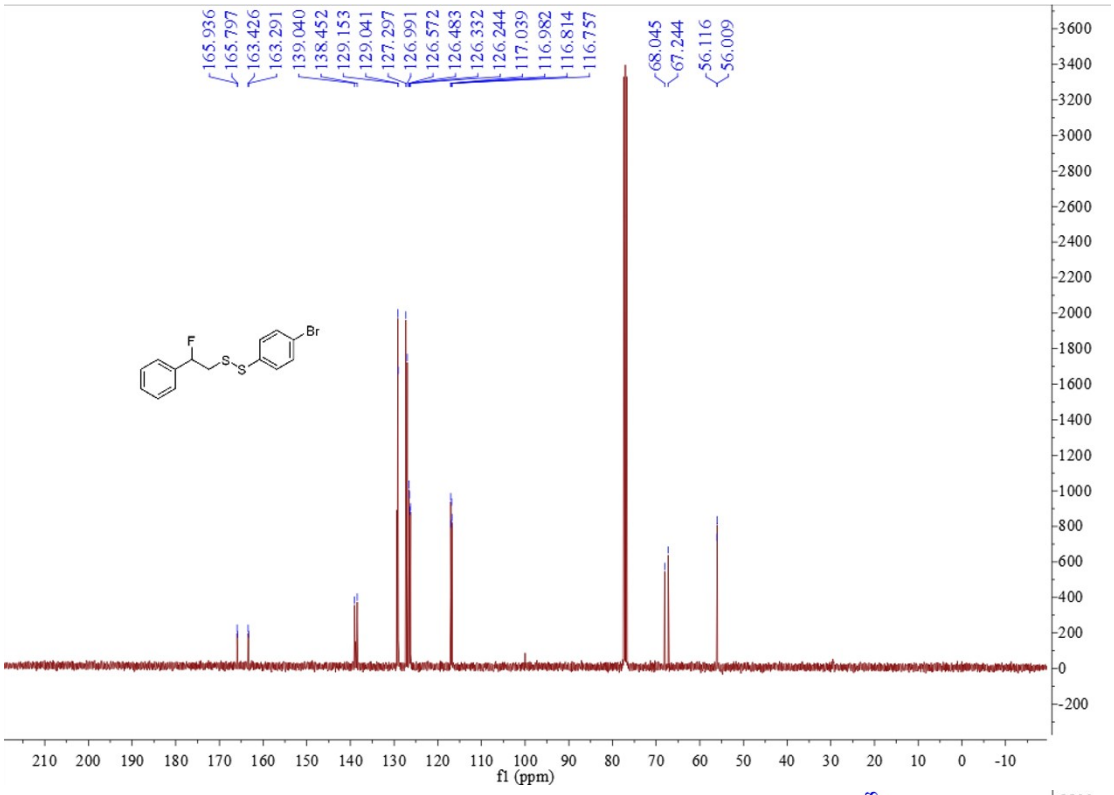
2.00
f1 (ppm)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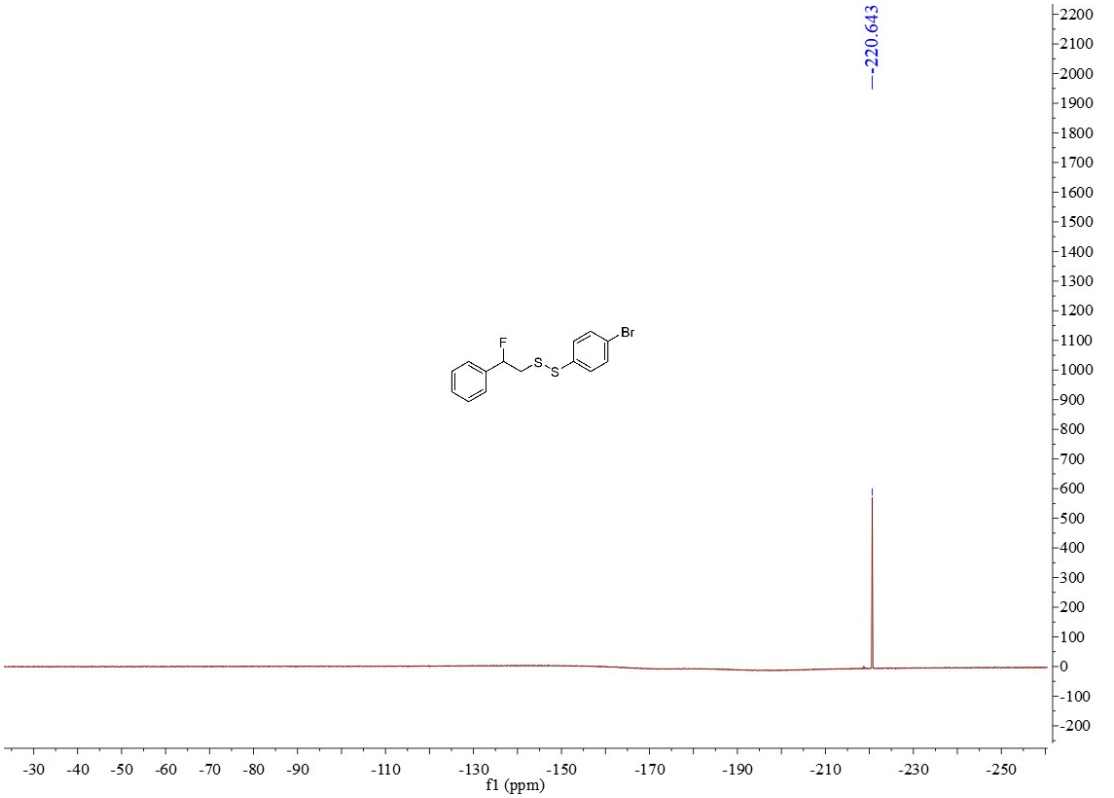
S
S
Br
f1 (ppm)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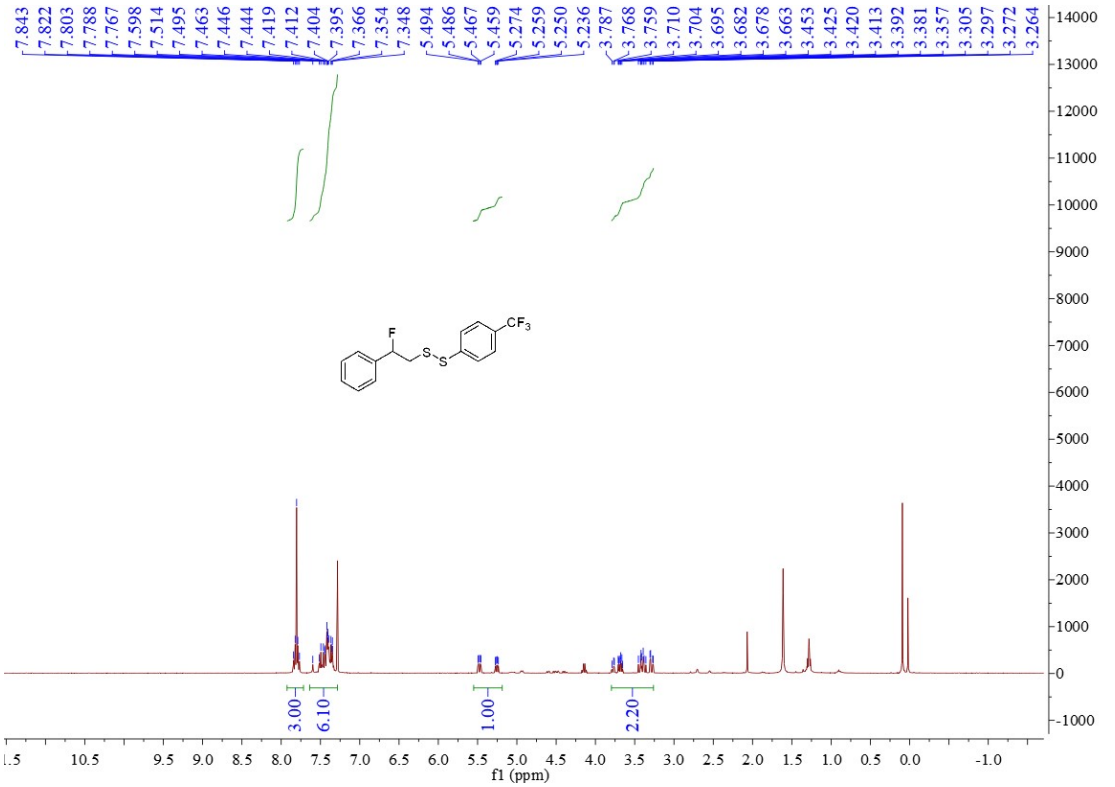
Br
f1 (ppm)

C5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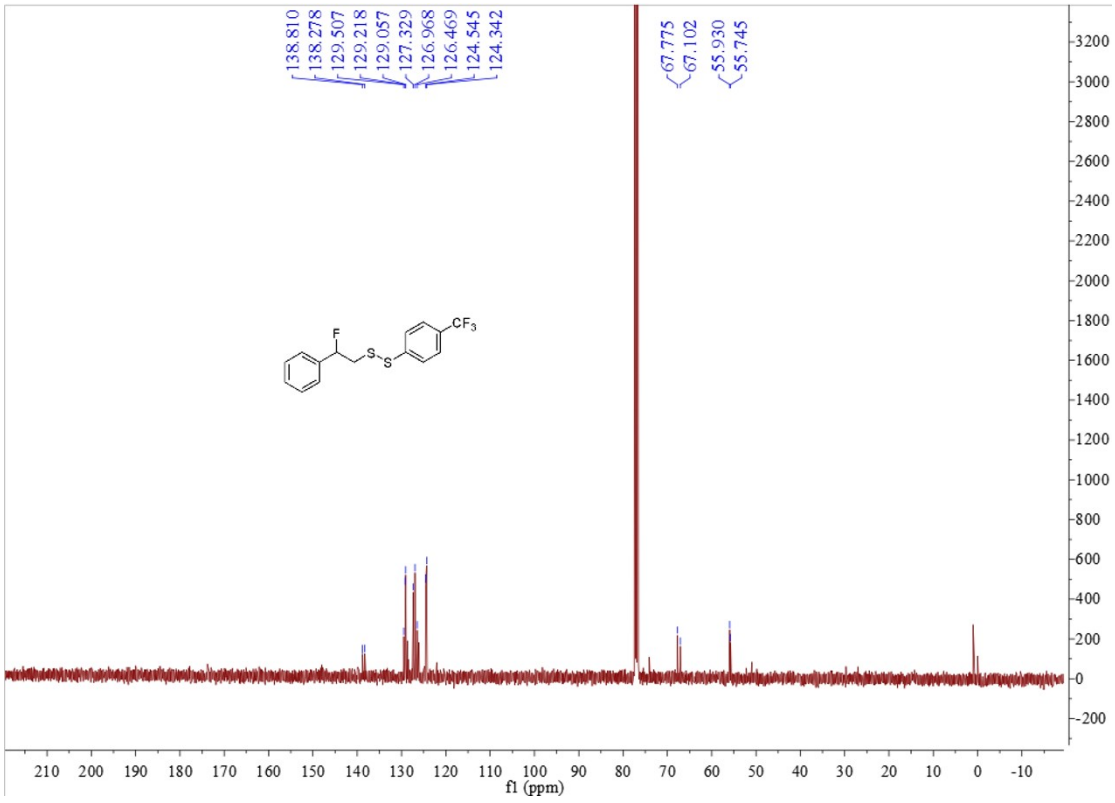
1.00
2.20
f1 (ppm)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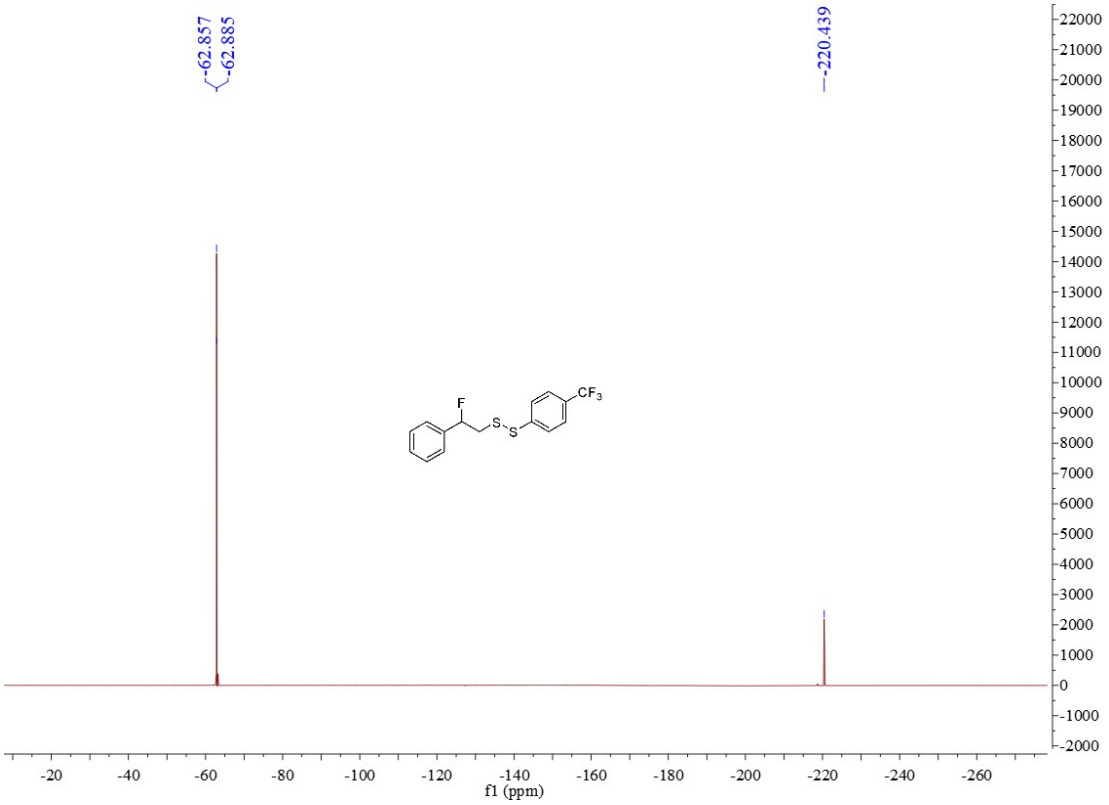
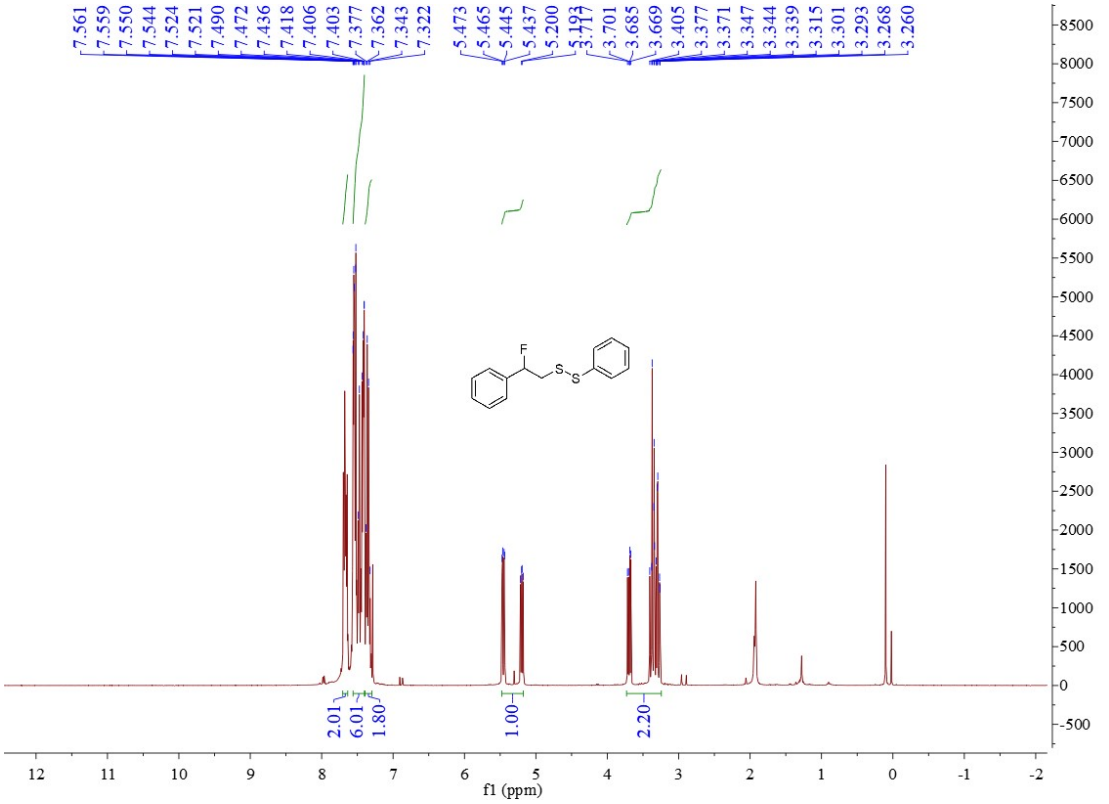
138.278
129.507
129.218
129.057
127.329
126.968
126.469
124.545
124.342
67.775
67.102
55.930
55.745
F
S
S
CF3
f1 (ppm)


-62.857
-62.885
-220.439
F
S
S
CF3
f1 (ppm)

C6


7.561
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7.550
7.544
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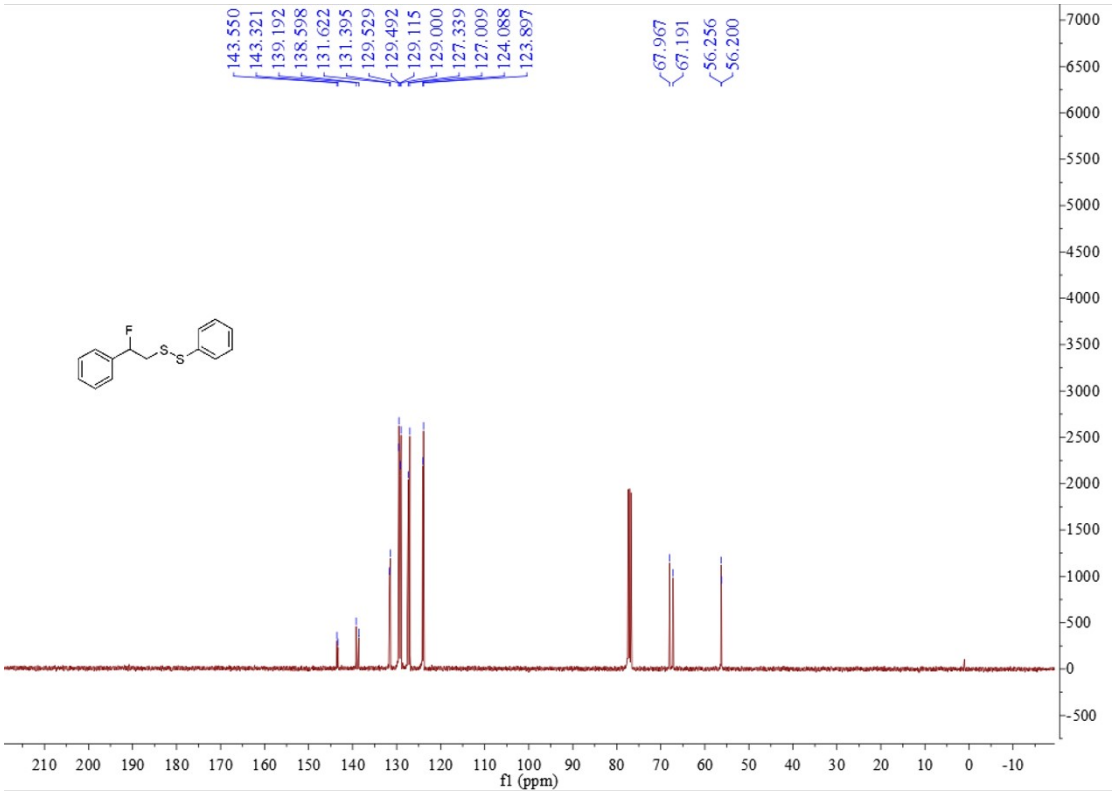
7.521
7.490
7.472
7.436
7.418
7.406
7.403
7.377
7.362
7.343
7.322
5.473
5.465
5.445
5.437
5.200
3.717
3.701
3.685
3.669
3.405
3.377
3.371
3.347
3.344
3.339
3.315
3.301
3.293
3.268
3.260
F
S
S
2.01
6.01
1.80
1.00
2.20
f1 (ppm)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143.321
139.192
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131.395
129.529
129.492
129.115
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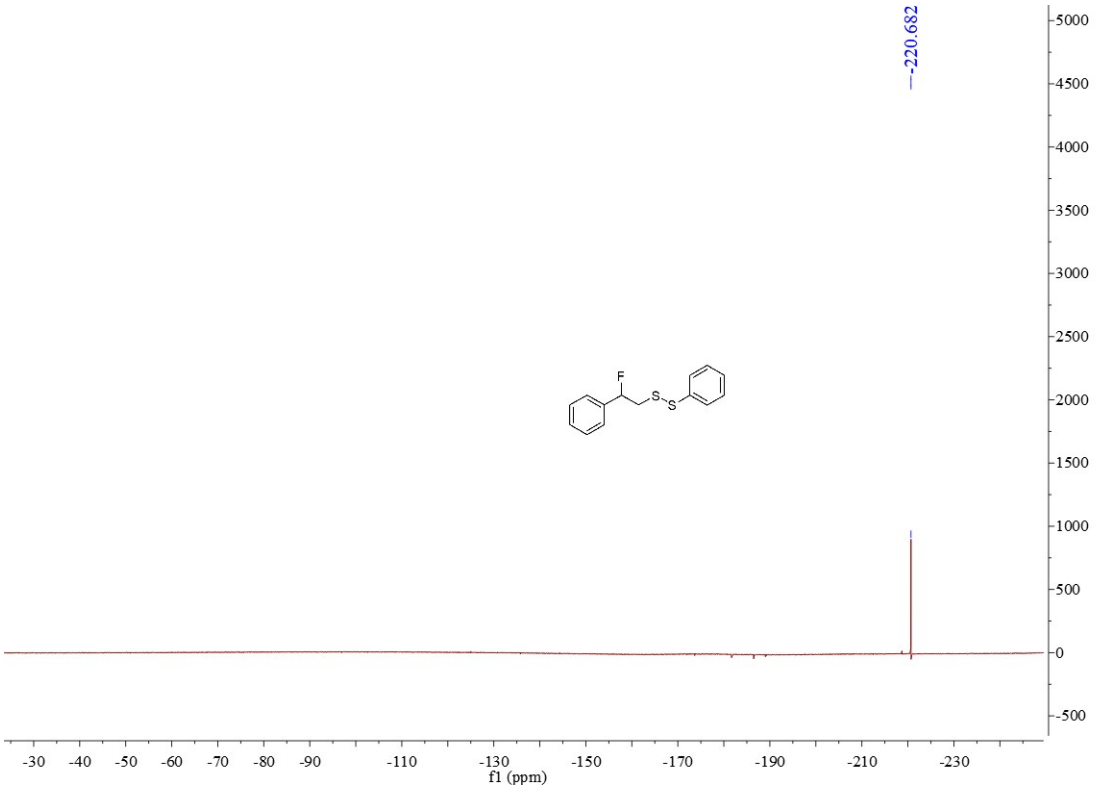
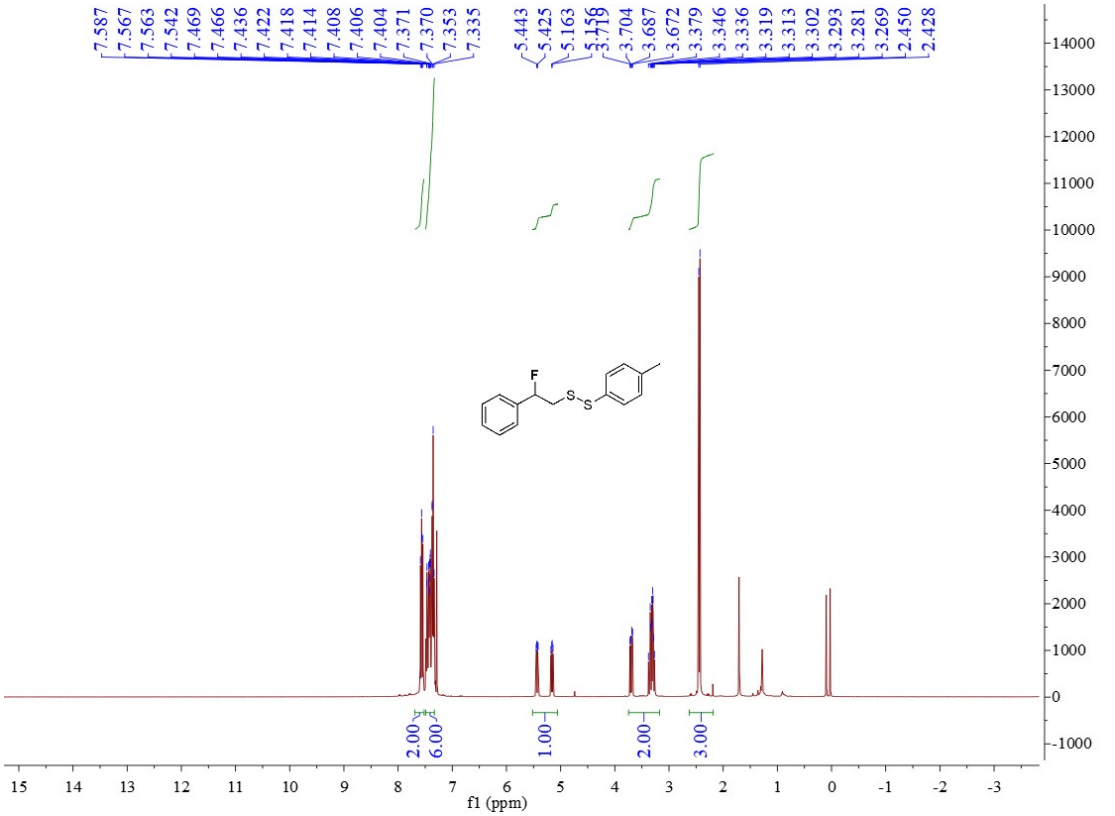
127.339
127.009
124.088
123.897
67.967
67.191
56.256
56.200
F
S
S
f1 (ppm)


-220.682
F
S
S
f1 (ppm)

C7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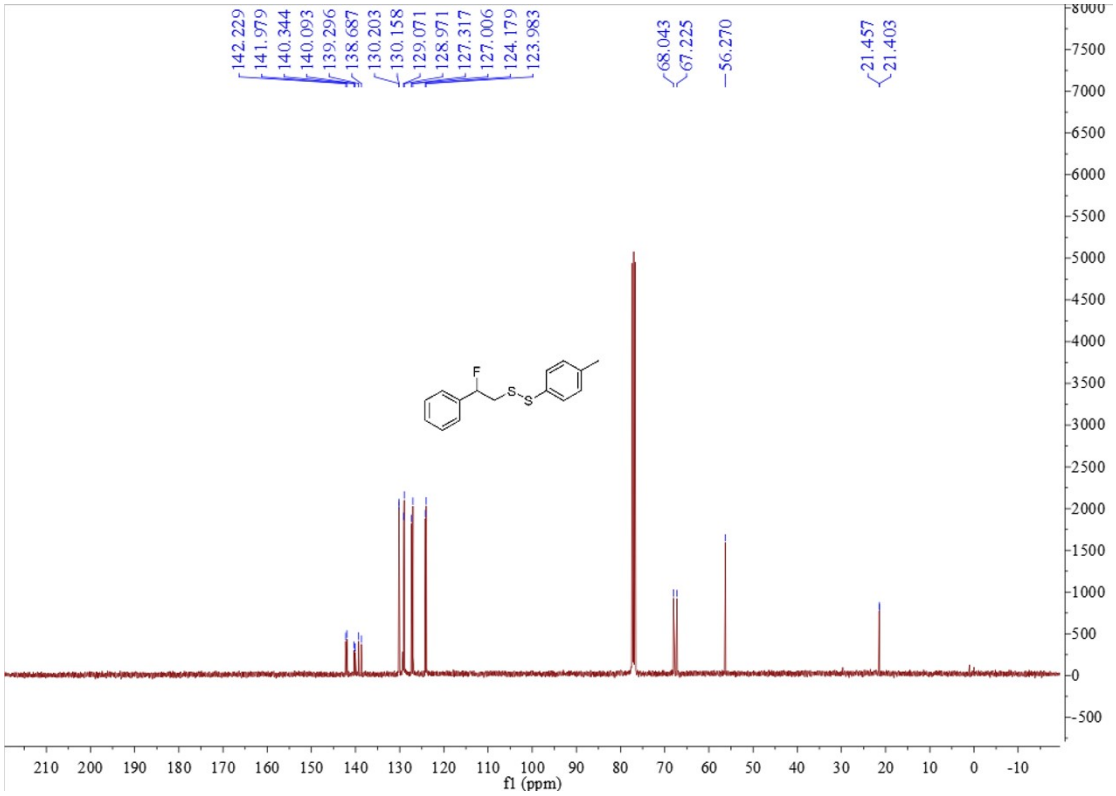
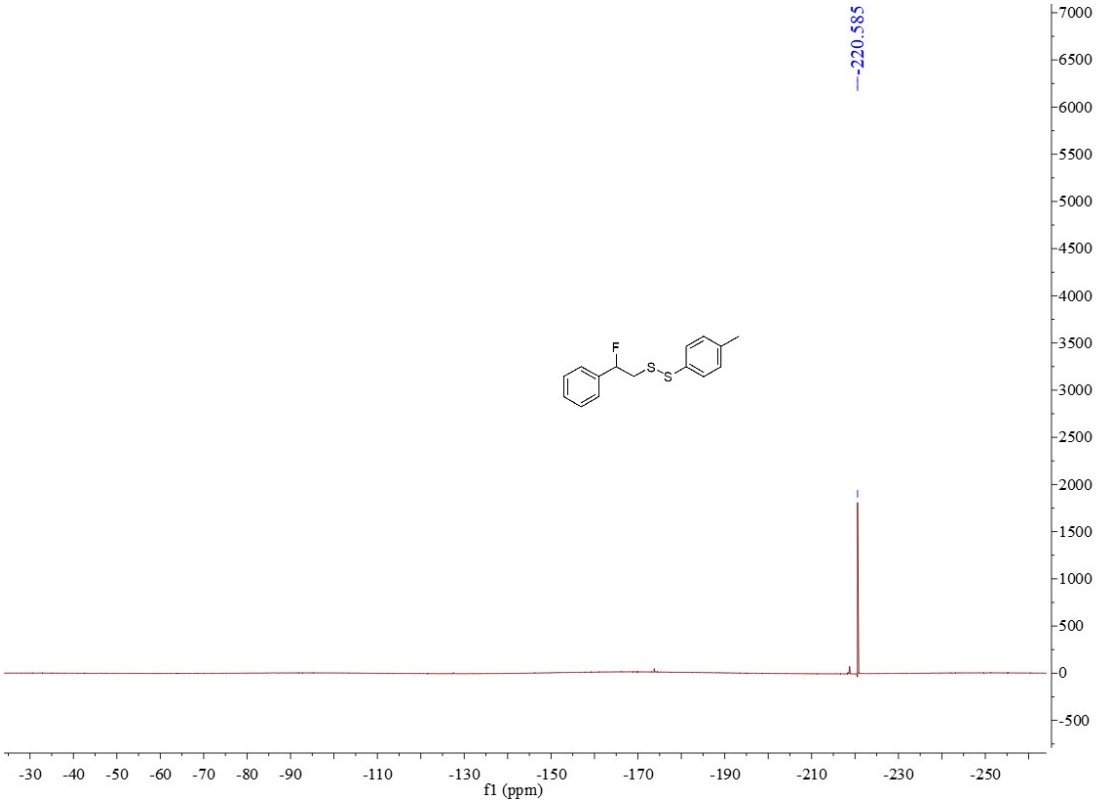
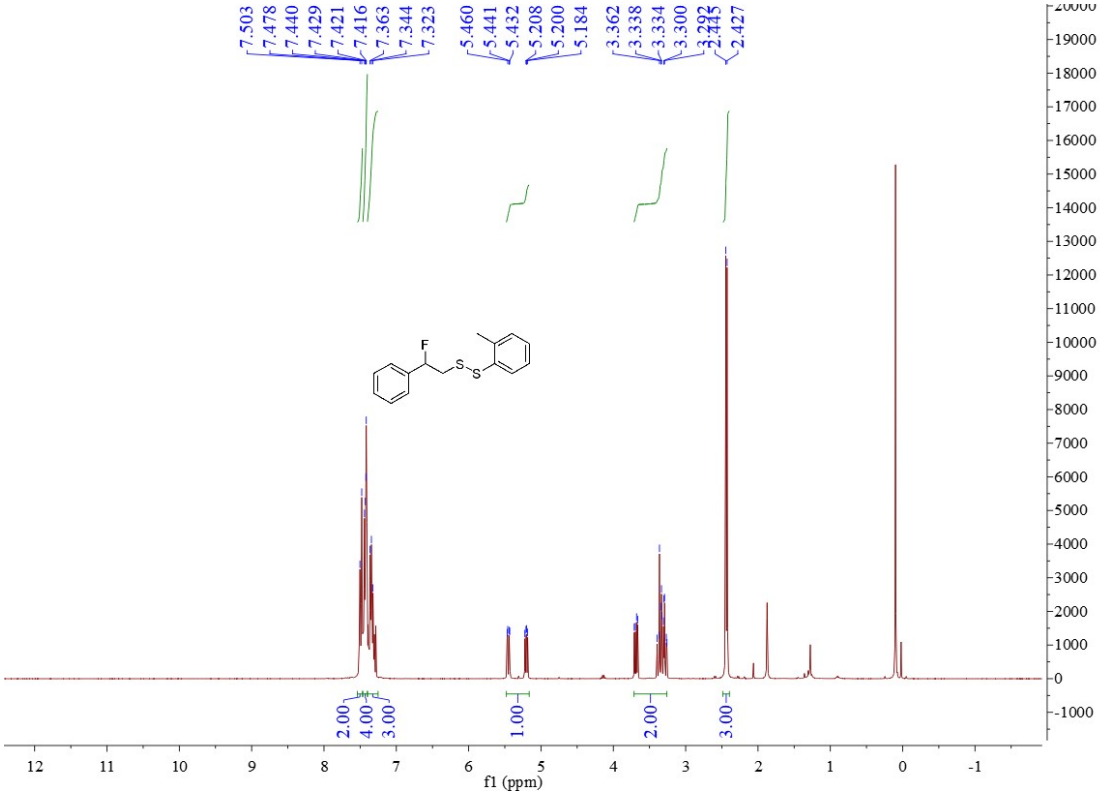
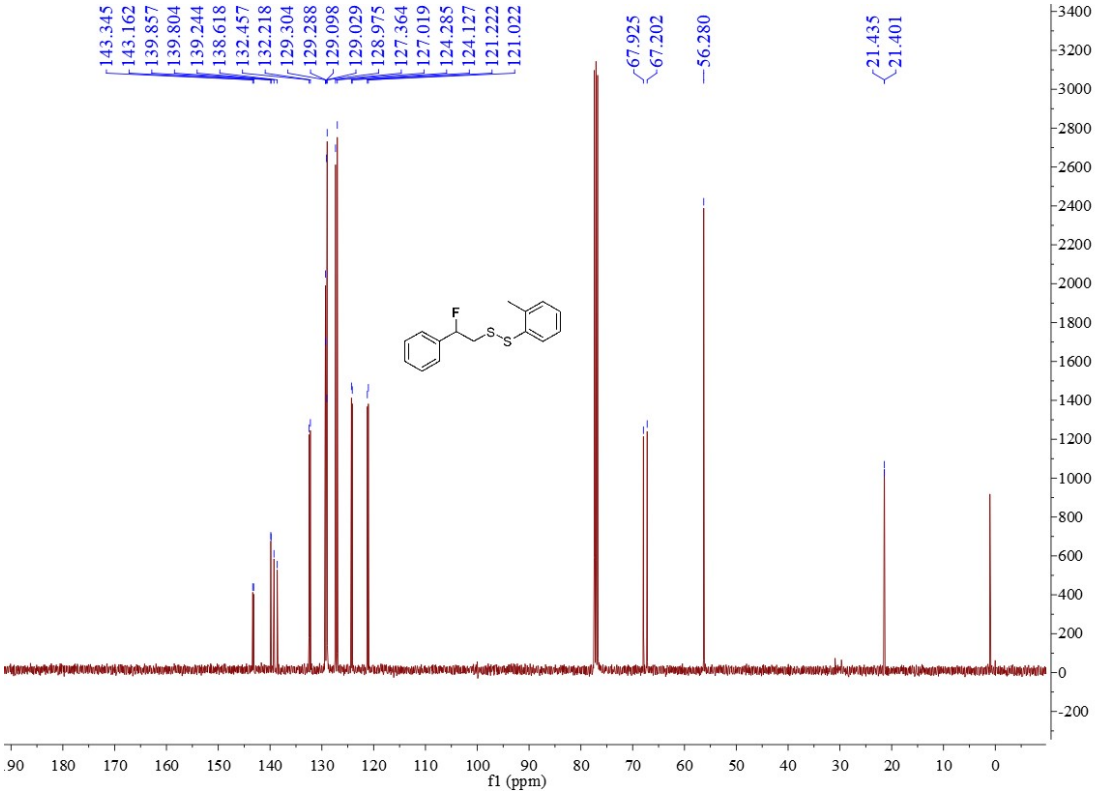
7.567
7.563
7.542
7.469
7.466
7.436
7.422
7.418
7.414
7.408
7.406
7.404
7.371
7.370
7.353
7.335
5.443
5.425
5.163
3.704
3.687
3.672
3.379
3.346
3.336
3.319
3.313
3.302
3.293
3.281
3.269
2.450
2.428
F
S
S
2.00
6.00
1.00
2.00
3.00
f1 (ppm)

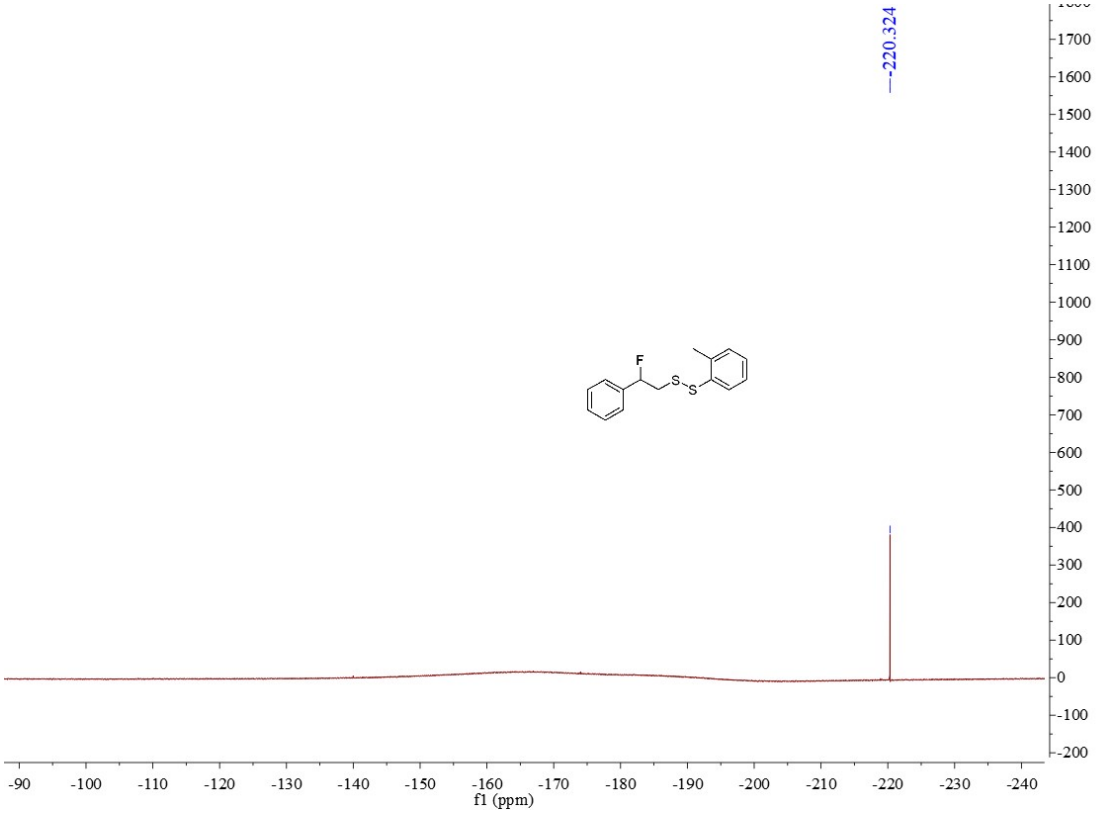

142.229
141.979
140.344
140.093
139.296
138.687
130.203
130.158
129.071
128.971
127.317
127.006
124.179
123.983
68.043
67.225
56.270
21.457
21.403
F
S
S
f1 (ppm)


-220.585
F
S
S
f1 (ppm)

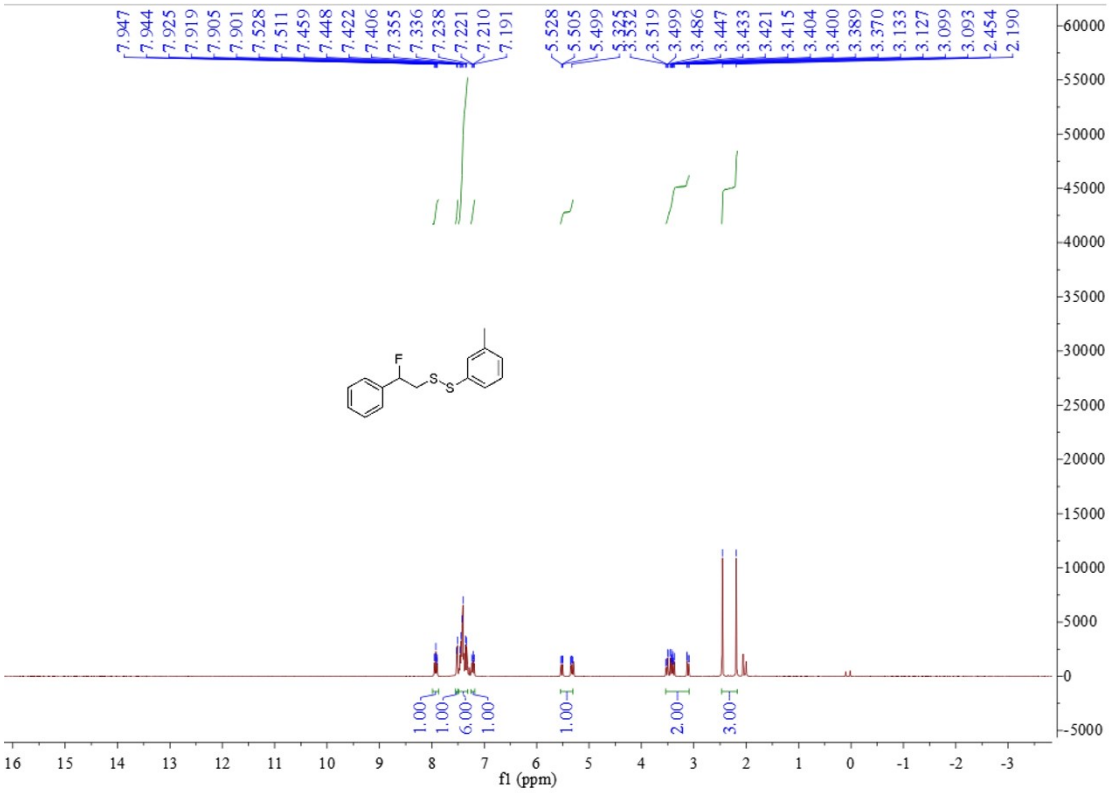
C8


7.503
7.478
7.440
7.429
7.421
7.416
7.363
7.344
7.323
5.460
5.441
5.432
5.208
5.200
5.184
3.362
3.338
3.334
3.300
2.427
F
S
S
2.00
4.00
3.00
1.00
2.00
3.00
f1 (ppm)


143.345
143.162
139.857
139.804
139.244
138.618
132.457
132.218
129.304
129.288
129.098
129.029
128.975
127.364
127.019
124.285
124.127
121.222
121.022
67.925
67.202
56.280
21.435
21.401
F
S
S
f1 (ppm)


-220.324
F
S
S
f1 (ppm)

C9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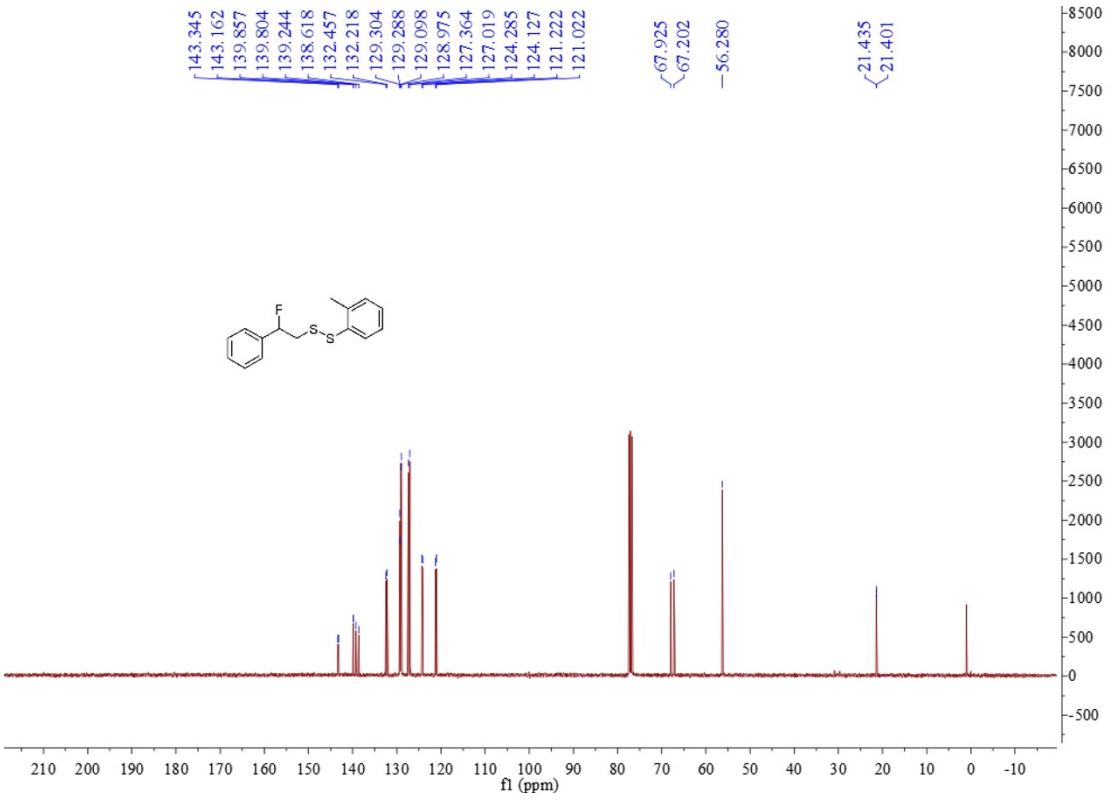
7.944
7.925
7.919
7.905
7.901
7.528
7.511
7.459
7.448
7.422
7.406
7.355
7.336
7.238
7.221
7.210
7.191
5.528
5.505
5.499
3.519
3.499
3.486
3.447
3.433
3.421
3.415
3.404
3.400
3.389
3.370
3.133
3.127
3.099
3.093
2.454
2.190
1.00
1.00
6.00
1.00
1.00
2.00
3.00
f1 (ppm)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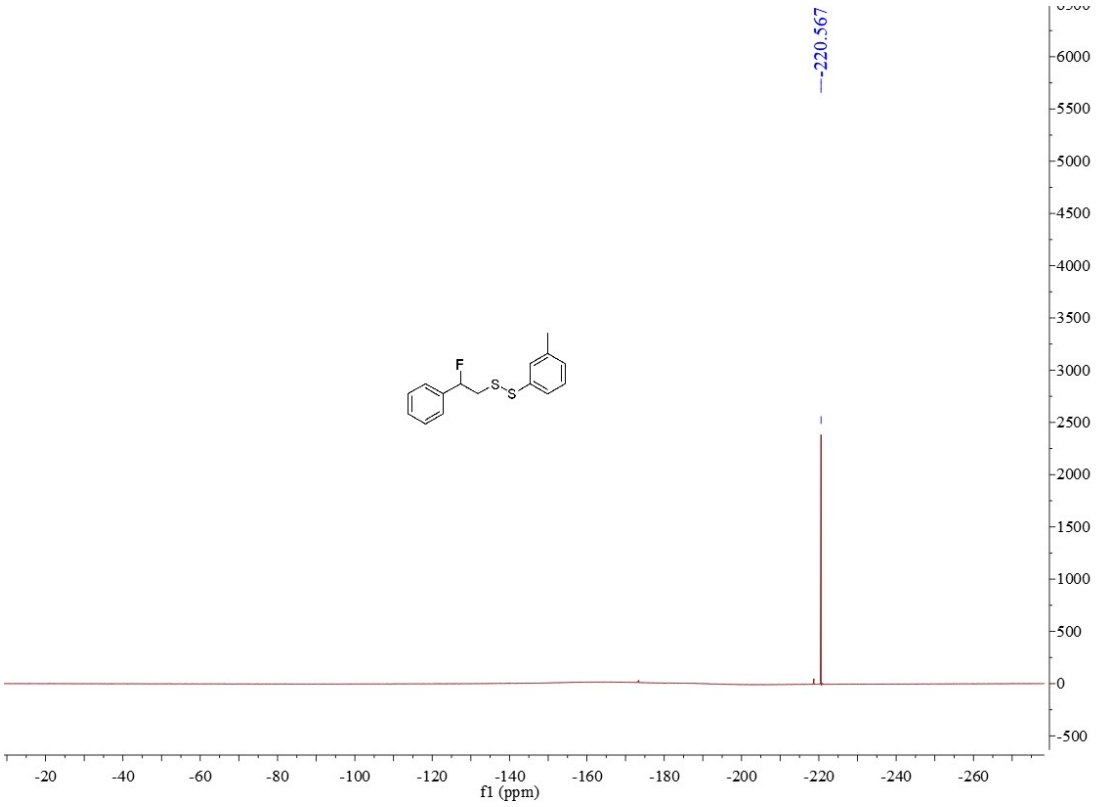
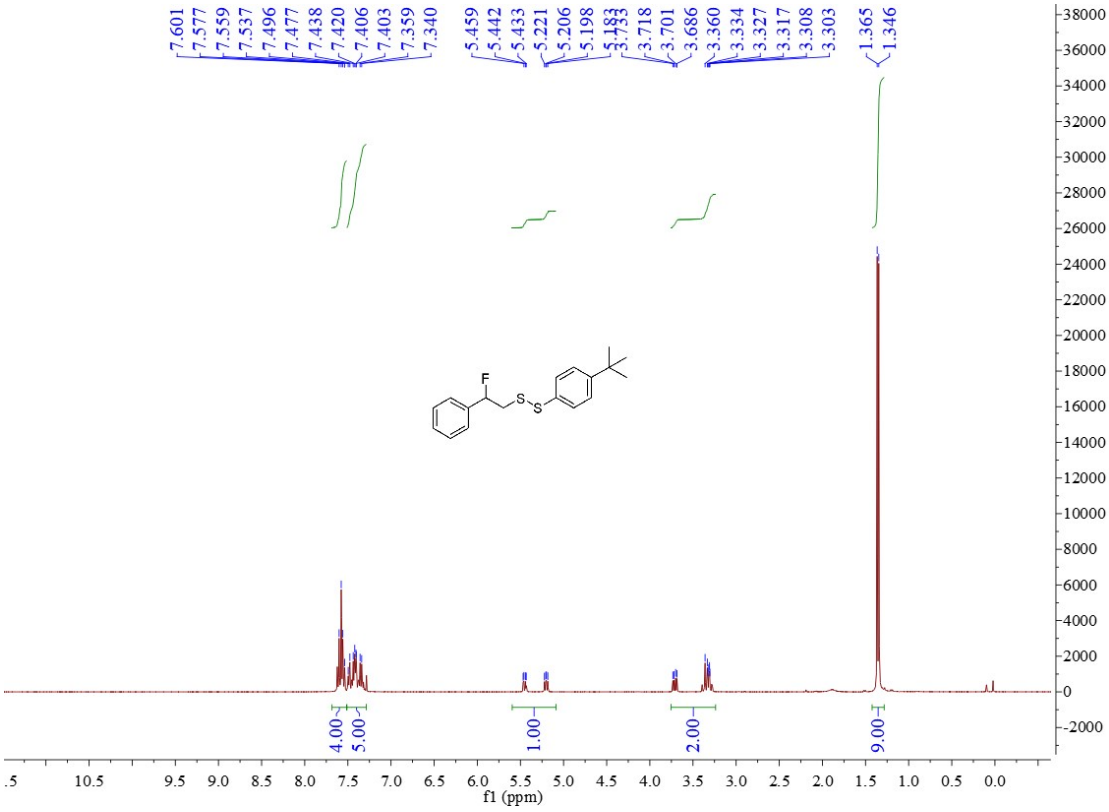
143.162
139.857
139.804
139.244
138.618
132.457
132.218
129.304
129.288
129.098
128.975
127.364
127.019
124.285
124.127
121.222
121.022
67.925
67.202
56.280
21.435
21.401
f1 (ppm)


-220.567
F
S
S
f1 (ppm)

C10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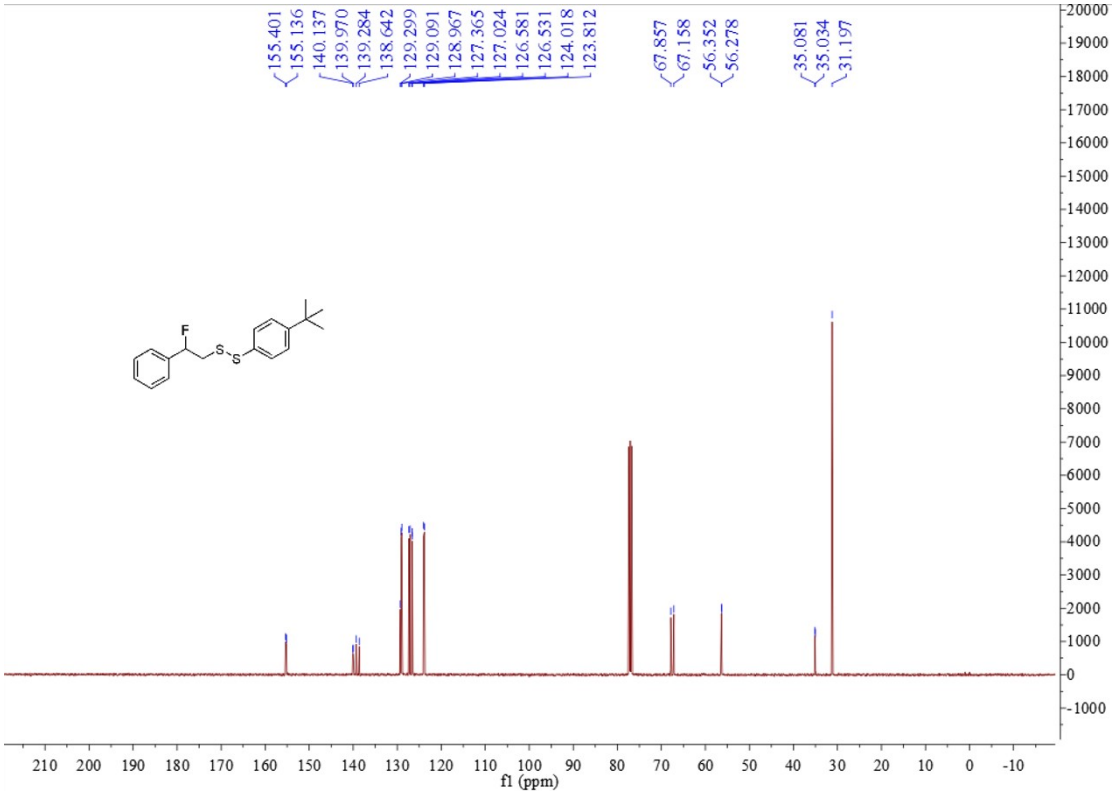
7.537
7.496
7.477
7.438
7.420
7.406
7.403
7.359
7.340
5.459
5.442
5.433
5.221
5.206
5.198
3.718
3.701
3.686
3.360
3.334
3.327
3.317
3.308
3.303
1.365
1.346
F
S
S
4.00
5.00
1.00
2.00
9.00
f1 (ppm)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140.137
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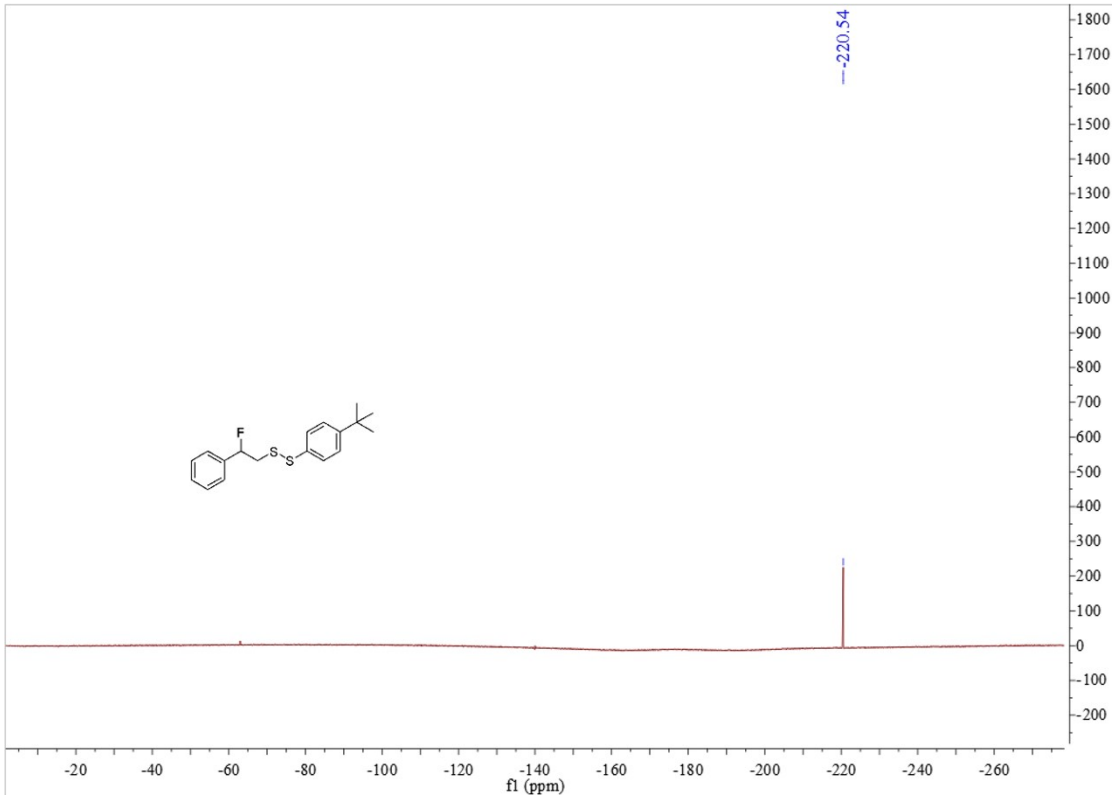
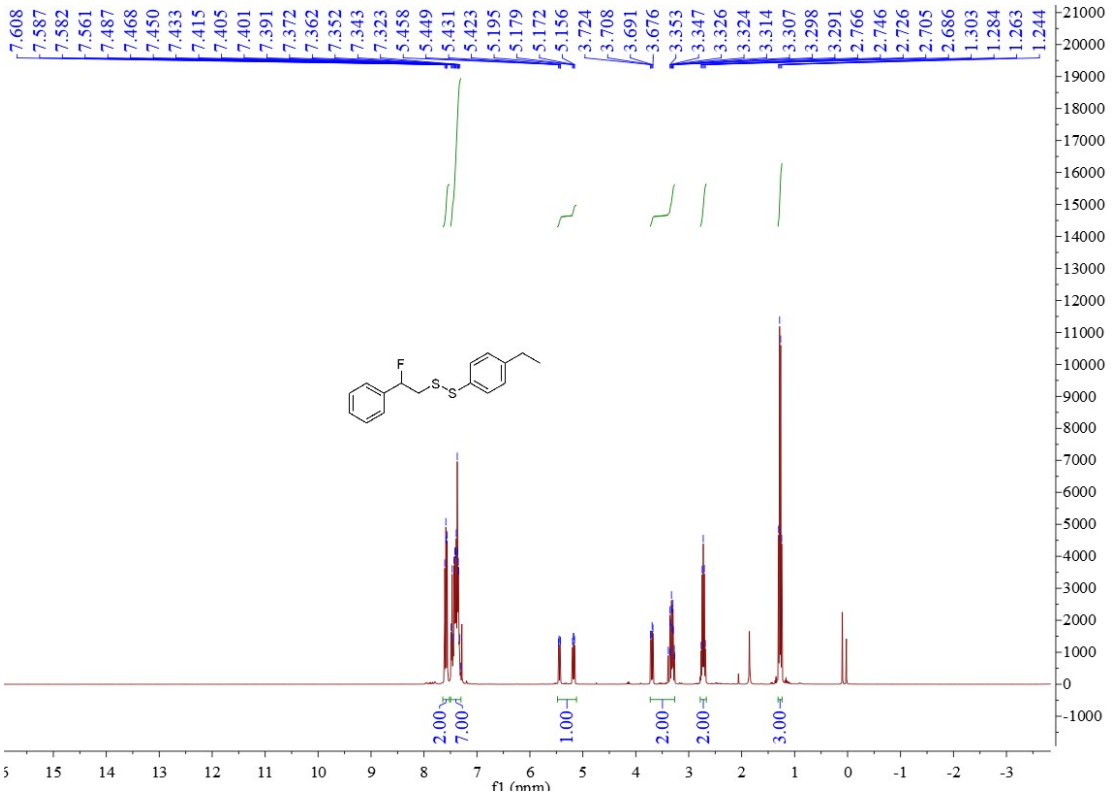
138.642
129.299
129.091
128.967
127.365
127.024
126.581
126.531
124.018
123.812
67.857
67.158
56.352
56.278
35.081
35.034
31.197
F
S
S
fl (ppm)


-220.54
F
S
S
fl (ppm)

C11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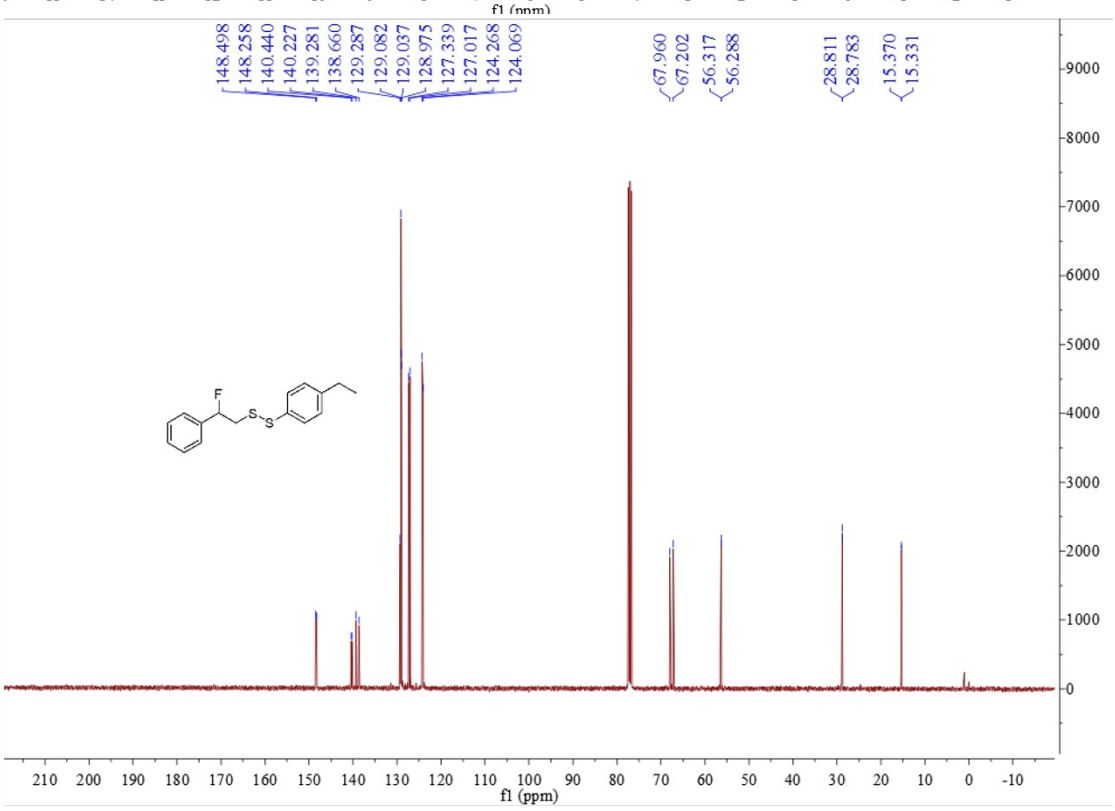
7.487
7.468
7.450
7.433
7.415
7.405
7.401
7.391
7.372
7.362
7.352
7.343
7.323
5.458
5.449
5.431
5.423
5.195
5.179
5.172
5.156
3.724
3.708
3.691
3.676
3.353
3.347
3.326
3.324
3.314
3.307
3.298
3.291
2.766
2.746
2.726
2.705
2.686
1.303
1.284
1.263
1.244
F
S
S
2.00
7.00
1.00
2.00
2.00
3.00
f1 (ppm)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140.227
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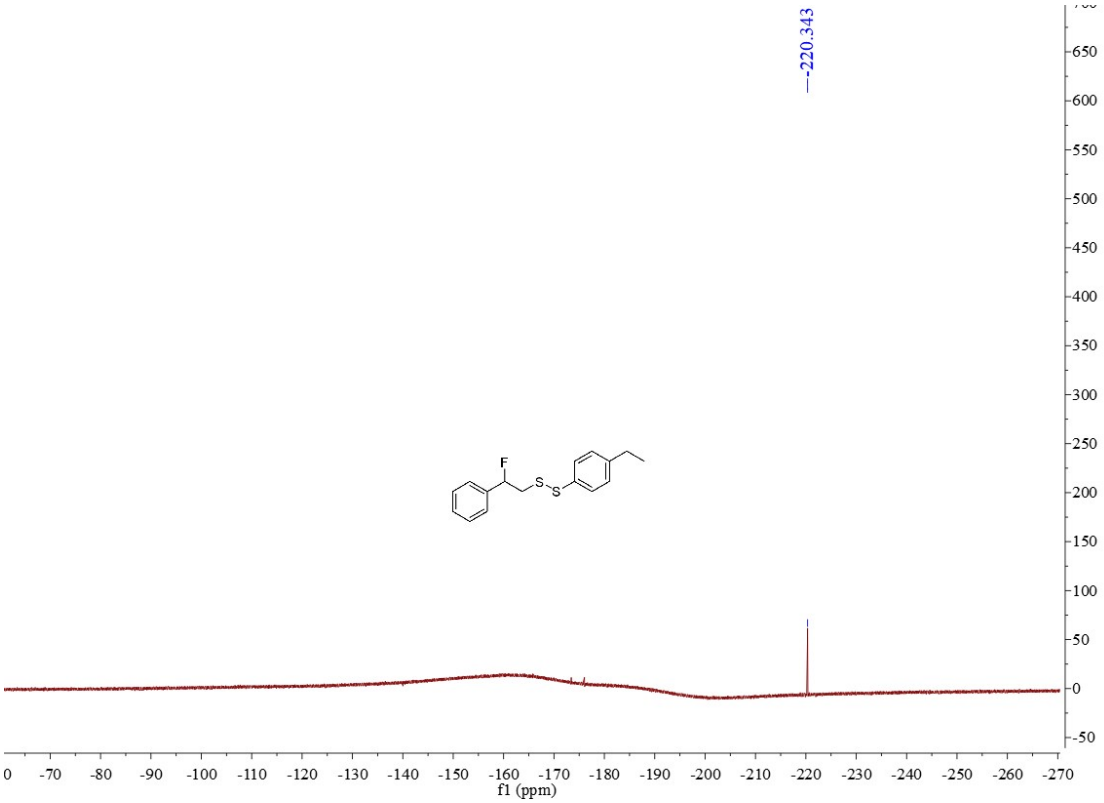
138.660
129.287
129.082
129.037
128.975
127.339
127.017
124.268
124.069
67.960
67.202
56.317
56.288
28.811
28.783
15.370
15.331
F
S
S
f1 (ppm)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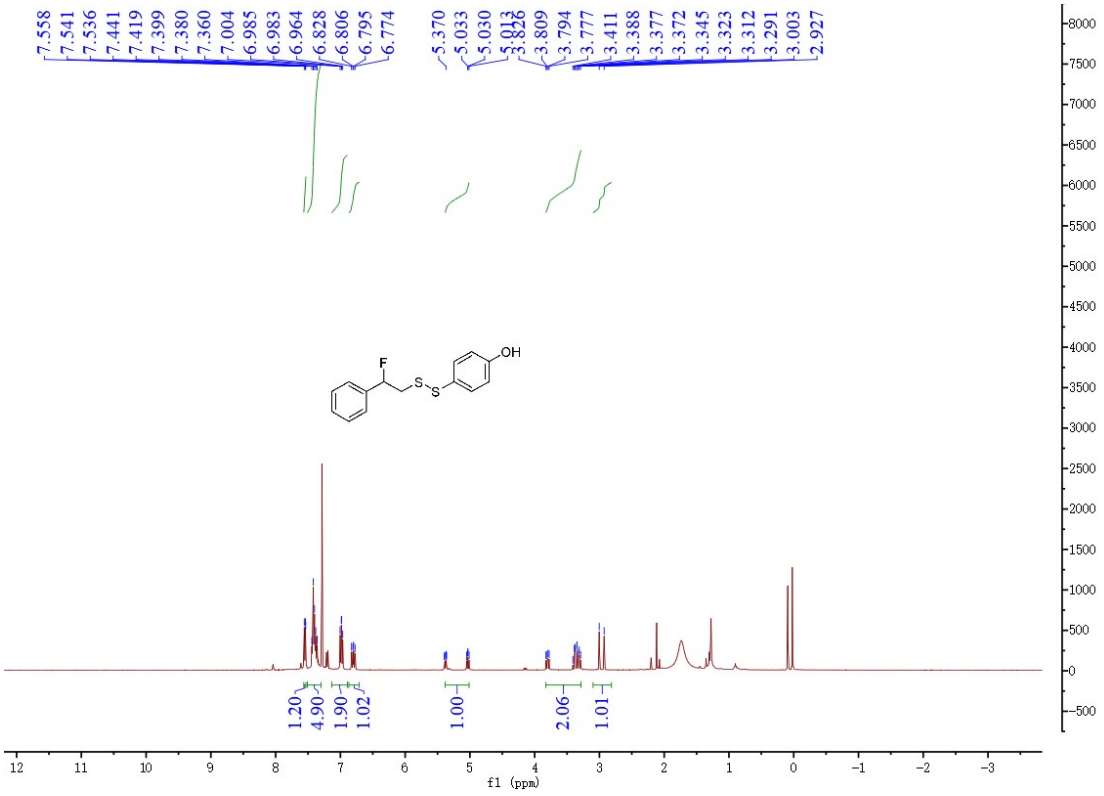
F
S
S
f1 (ppm)

C12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7.360
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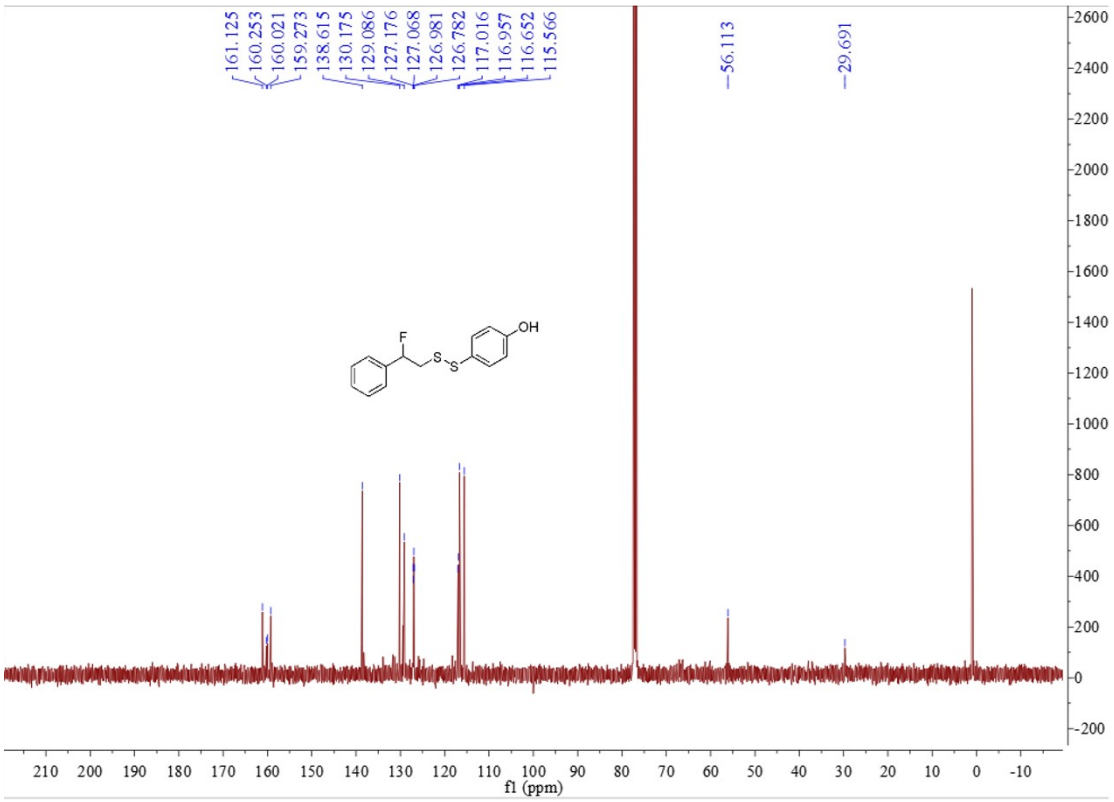
6.983
6.964
6.828
6.806
6.795
6.774
5.370
5.033
5.030
3.826
3.809
3.794
3.777
3.411
3.388
3.377
3.372
3.345
3.323
3.312
3.291
3.003
2.927
F
S
S
OH
1.20
4.90
1.90
1.02
1.00
2.06
1.01
f1 (ppm)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130.175
129.086
127.176
127.068
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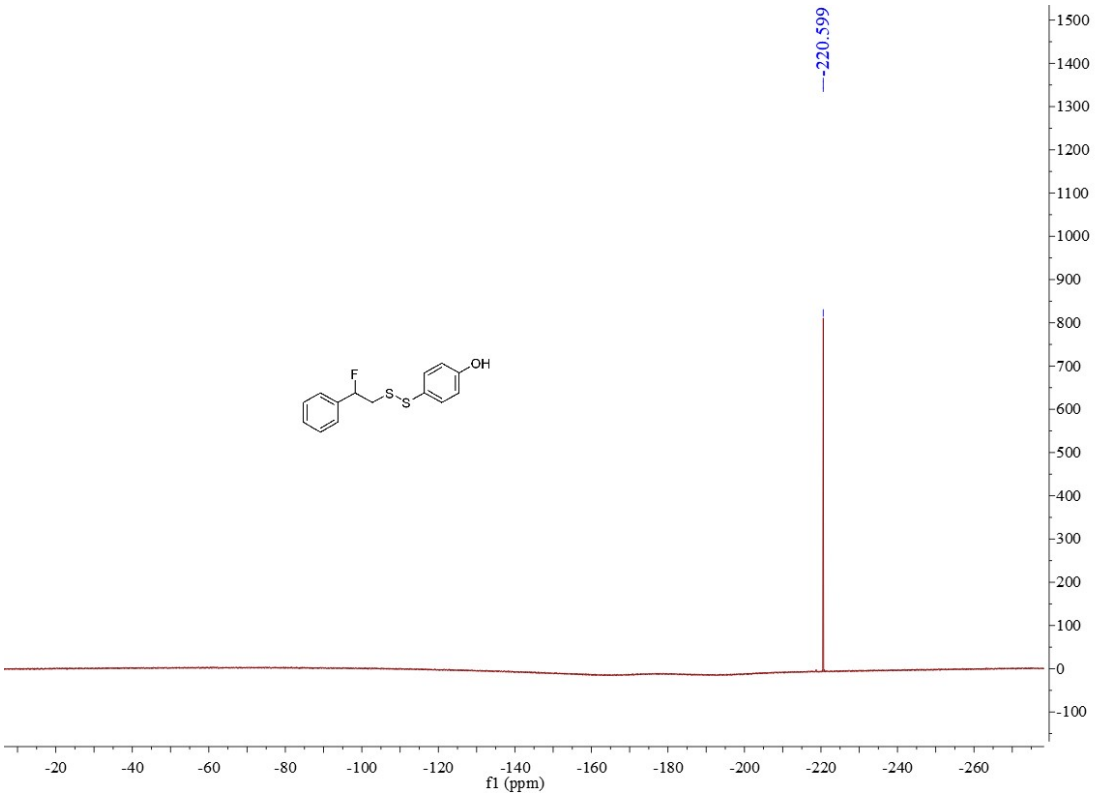
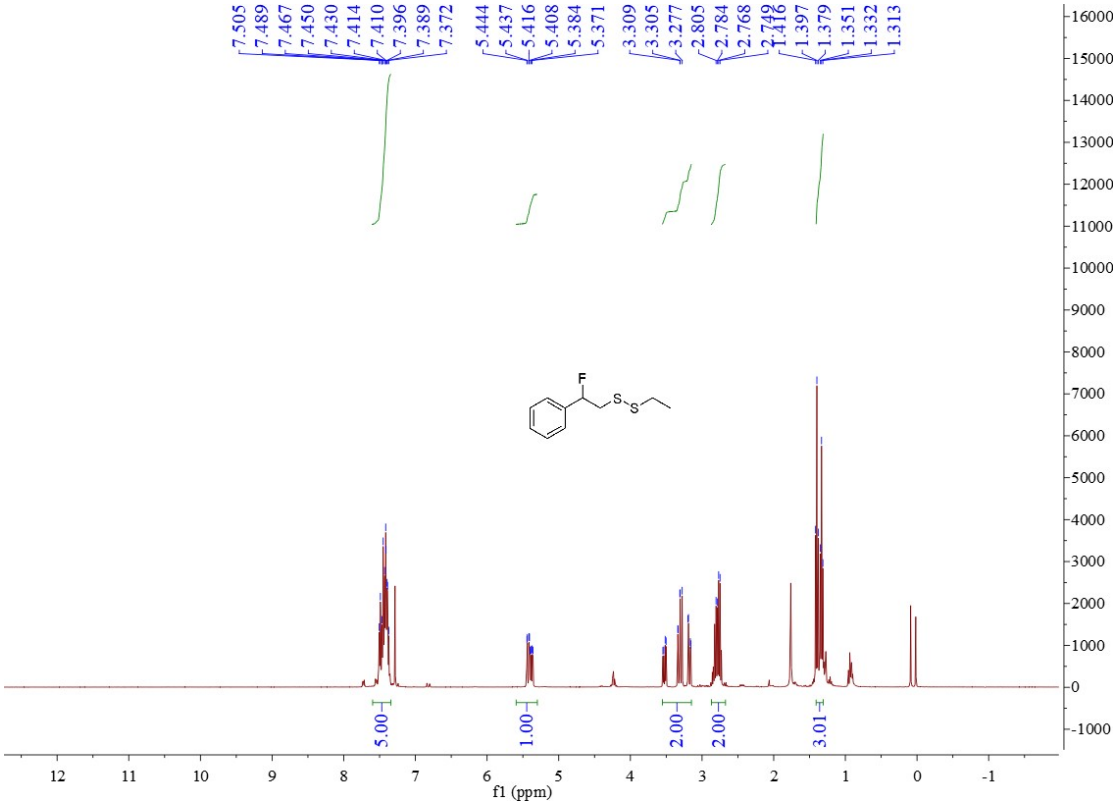
116.957
116.652
115.566
56.113
29.691
F
S
S
OH
f1 (ppm)


-220.599
F
S
S
OH
f1 (ppm)

C13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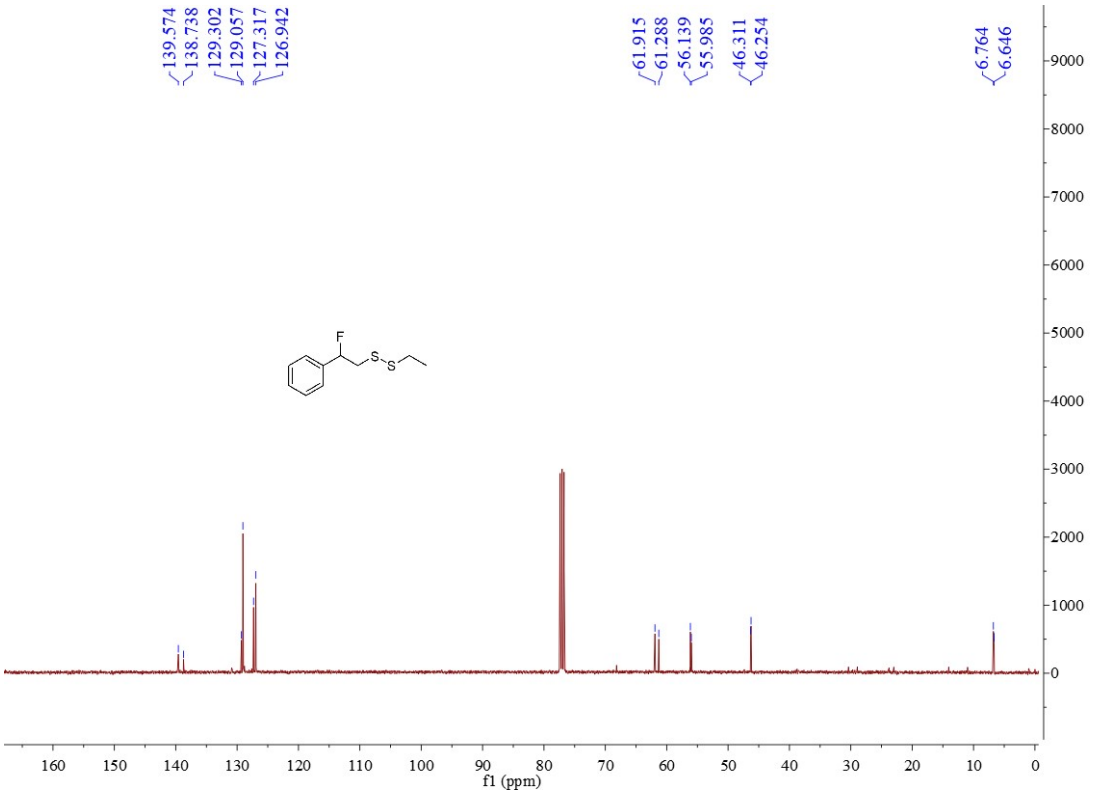
7.489
7.467
7.450
7.430
7.414
7.410
7.396
7.389
7.372
5.444
5.437
5.416
5.408
5.384
5.371
3.309
3.305
3.277
2.805
2.784
2.768
2.749
1.416
1.397
1.379
1.351
1.332
1.313
F
S
S
5.00
1.00
2.00
2.00
3.01
f1 (ppm)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129.302
129.057
127.317
126.942
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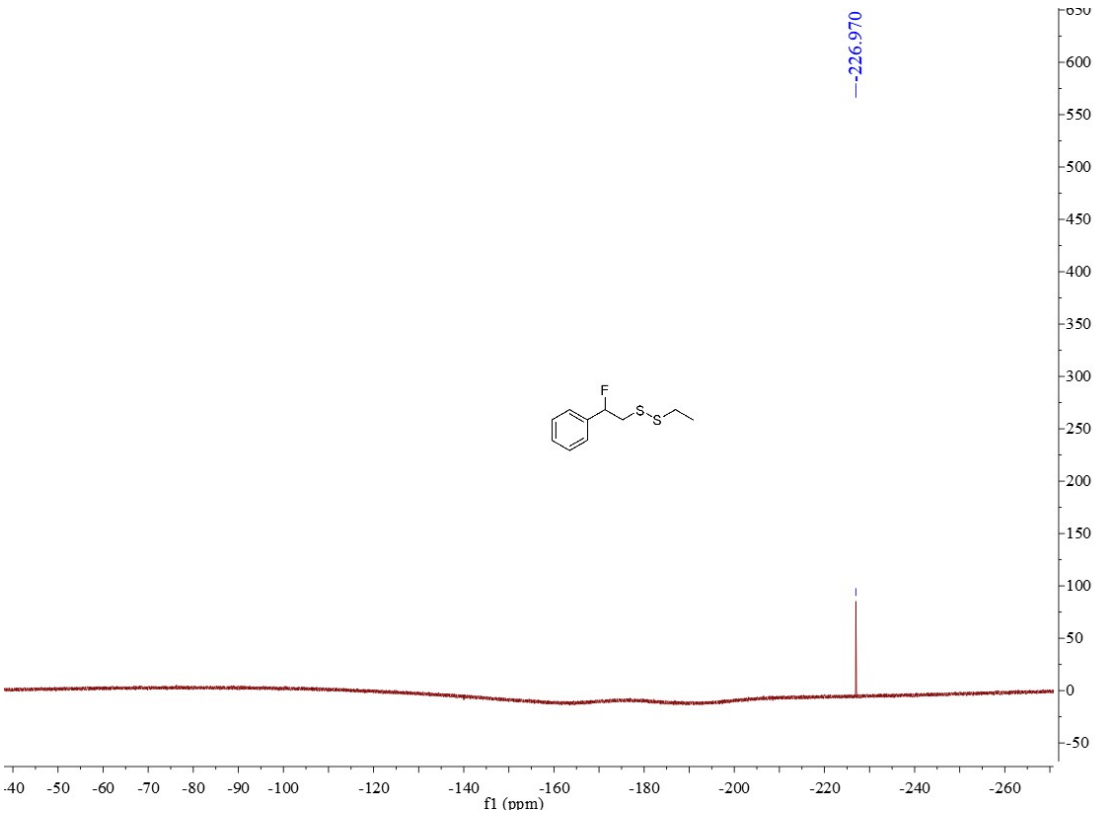
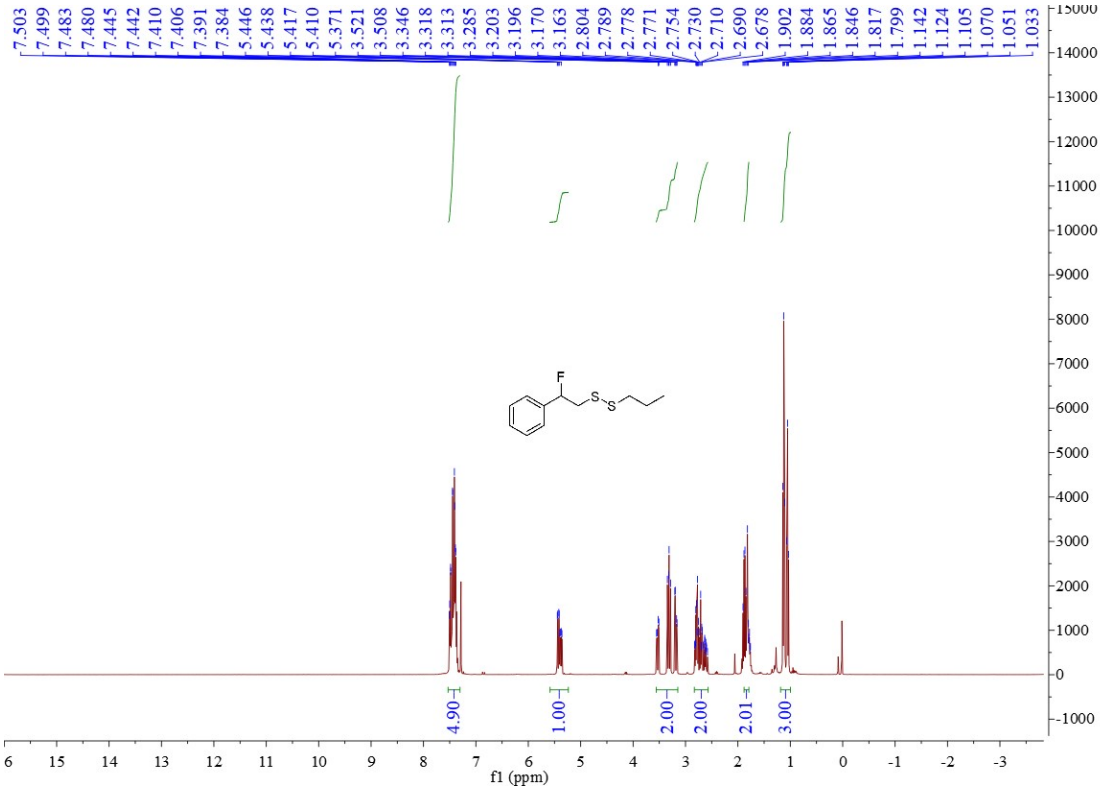
55.985
46.311
46.254
6.764
6.646
F
S
S
f1 (ppm)


-226.970
F
S
S
f1 (ppm)

C14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7.406
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5.417
5.410
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3.521
3.508
3.346
3.318
3.313
3.285
3.203
3.196
3.170
3.163
2.804
2.789
2.778
2.771
2.754
2.730
2.710
2.690
2.678
1.902
1.884
1.865
1.846
1.817
1.799
1.142
1.124
1.105
1.070
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F
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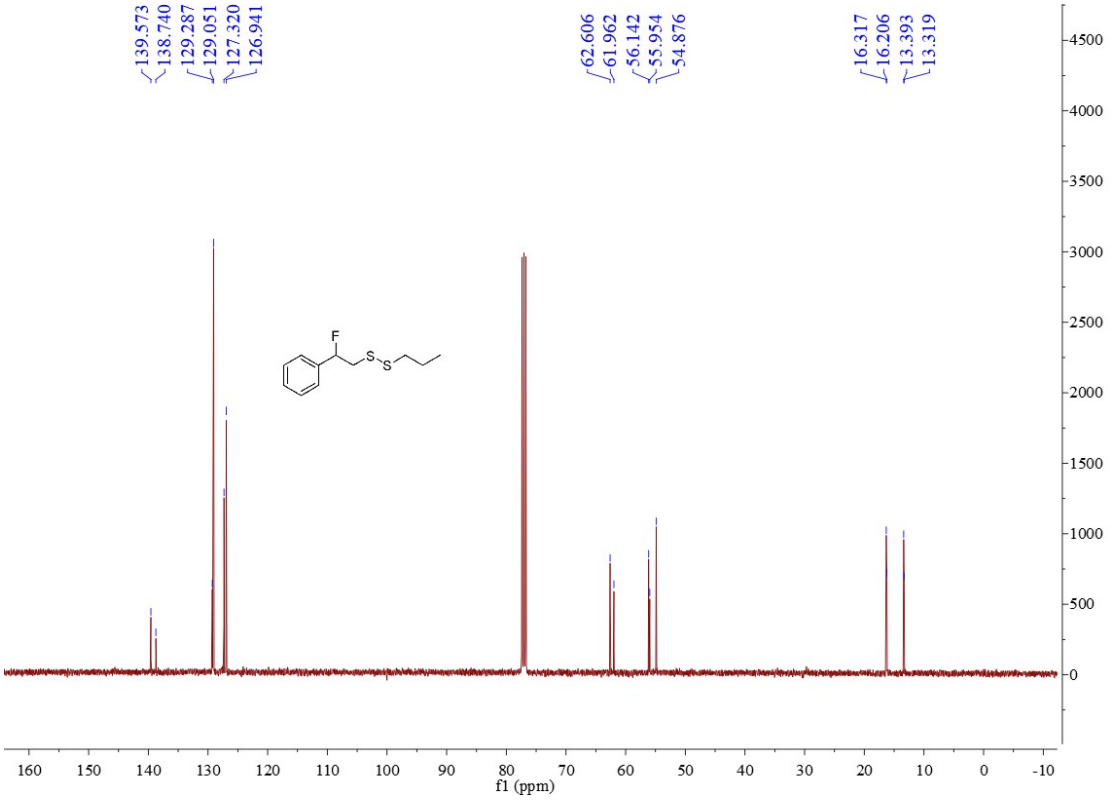
2.00
2.00
2.01
3.00
f1 (ppm)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129.051
127.320
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55.954
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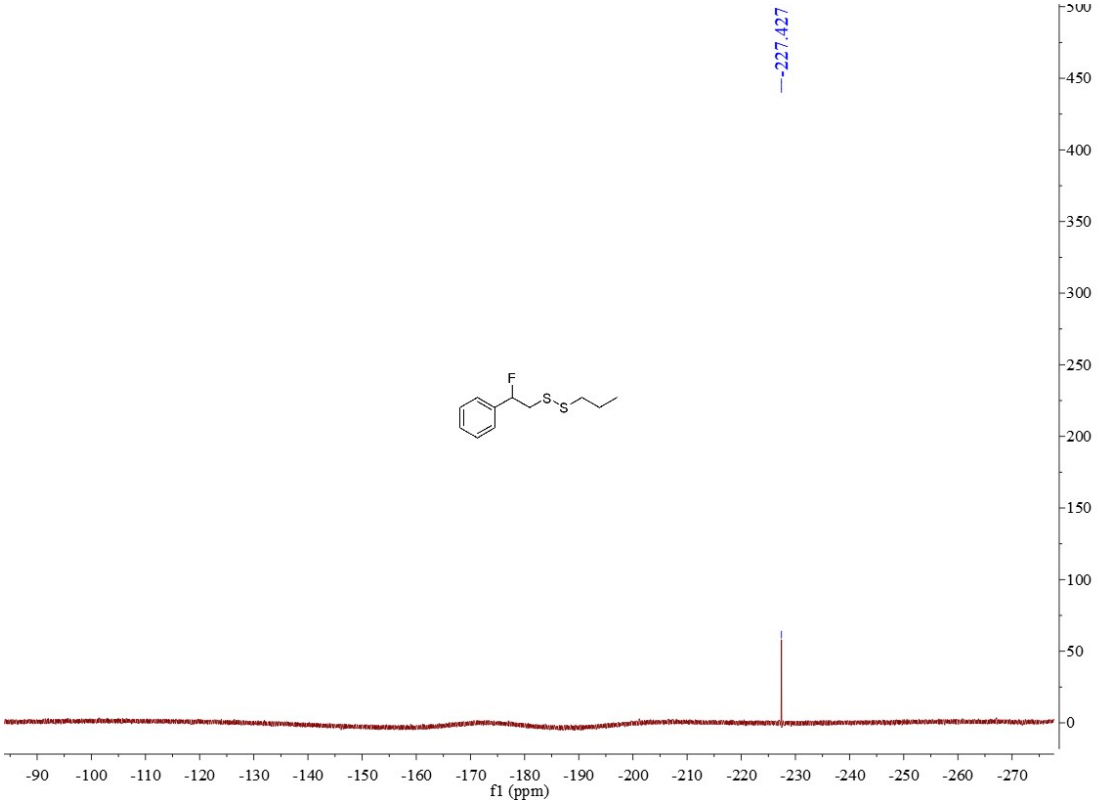
16.317
16.206
13.393
13.319
F
S
S
f1 (ppm)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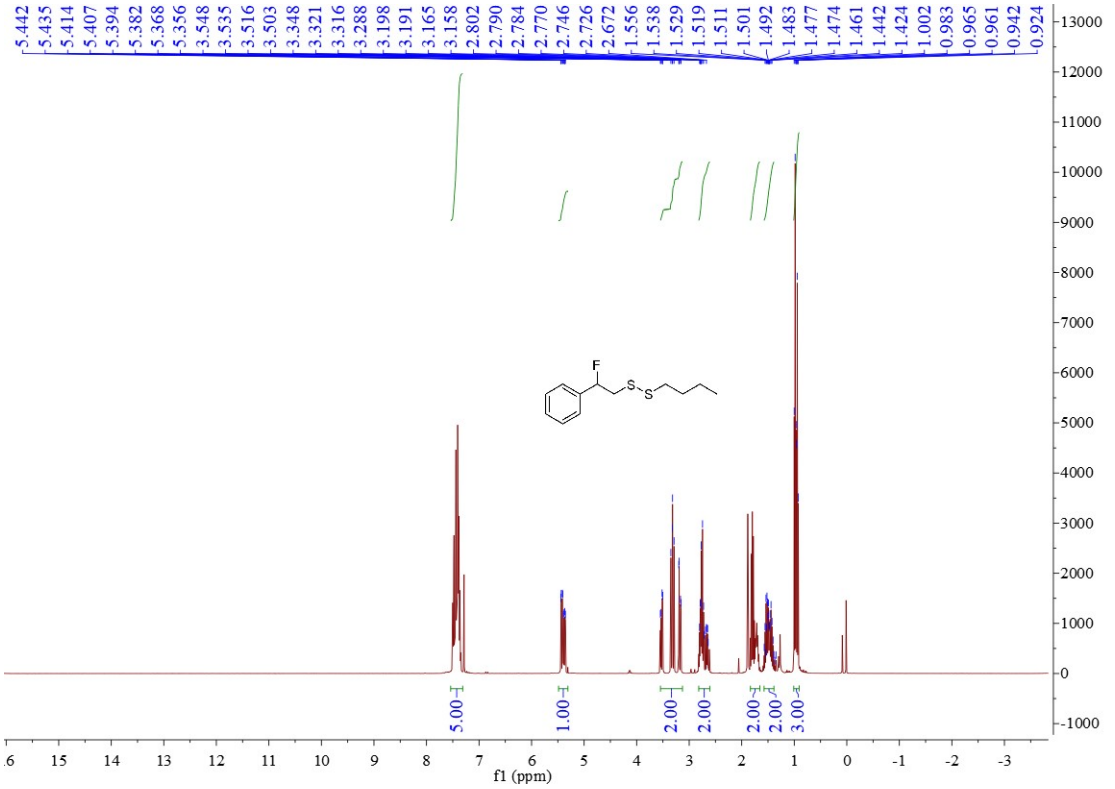
F
S
S
f1 (ppm)

C15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5.356
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3.516
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3.348
3.321
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3.191
3.165
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2.784
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2.746
2.726
2.672
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1.529
1.519
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1.501
1.492
1.483
1.477
1.474
1.461
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1.424
1.002
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0.965
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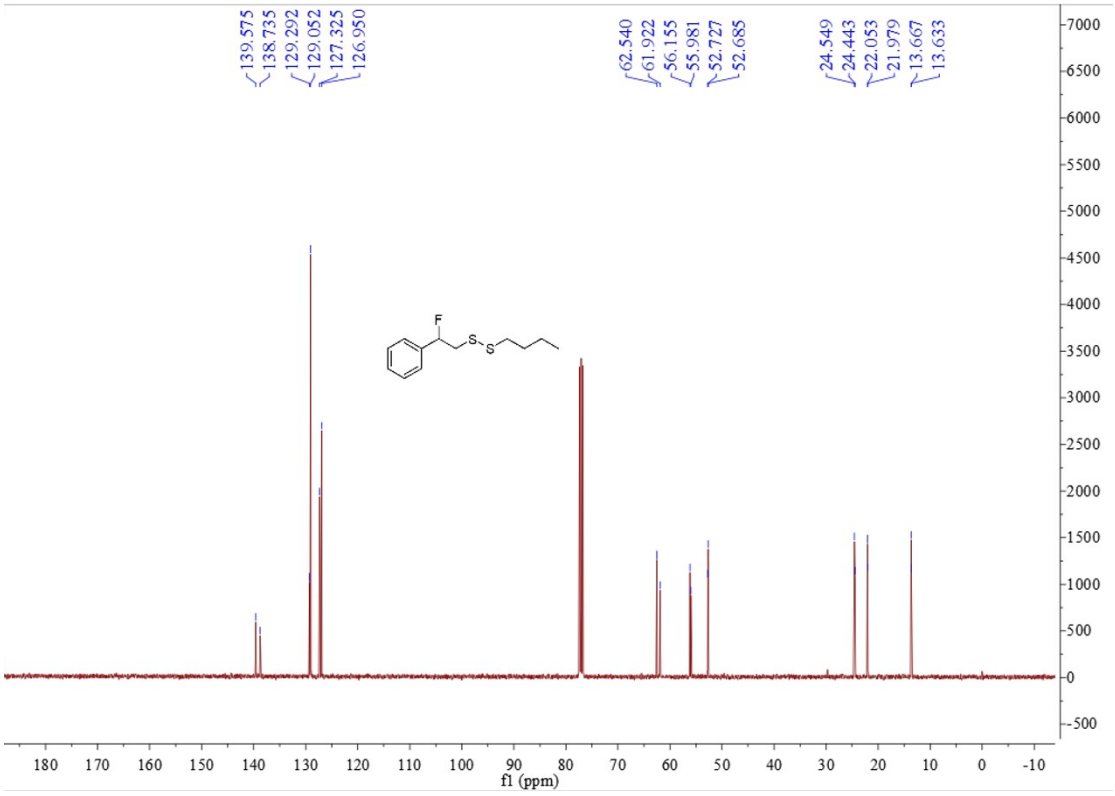
2.00
2.00
3.00
f1 (ppm)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127.325
126.950
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61.922
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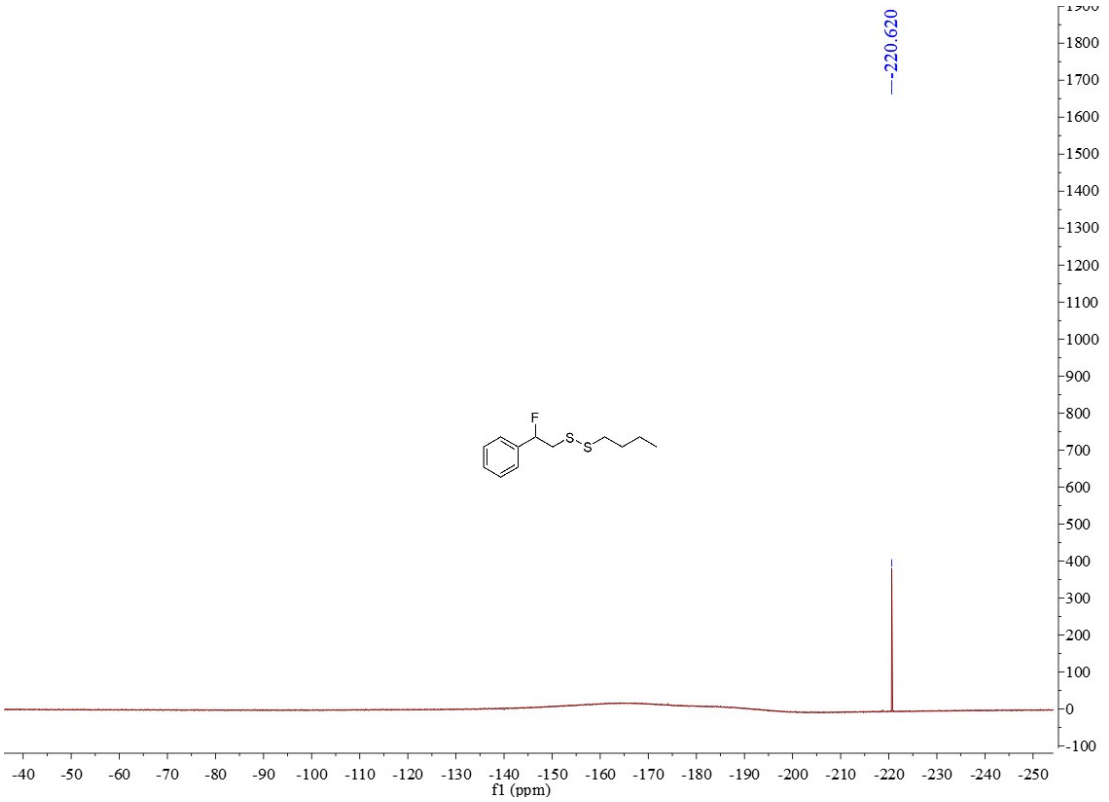
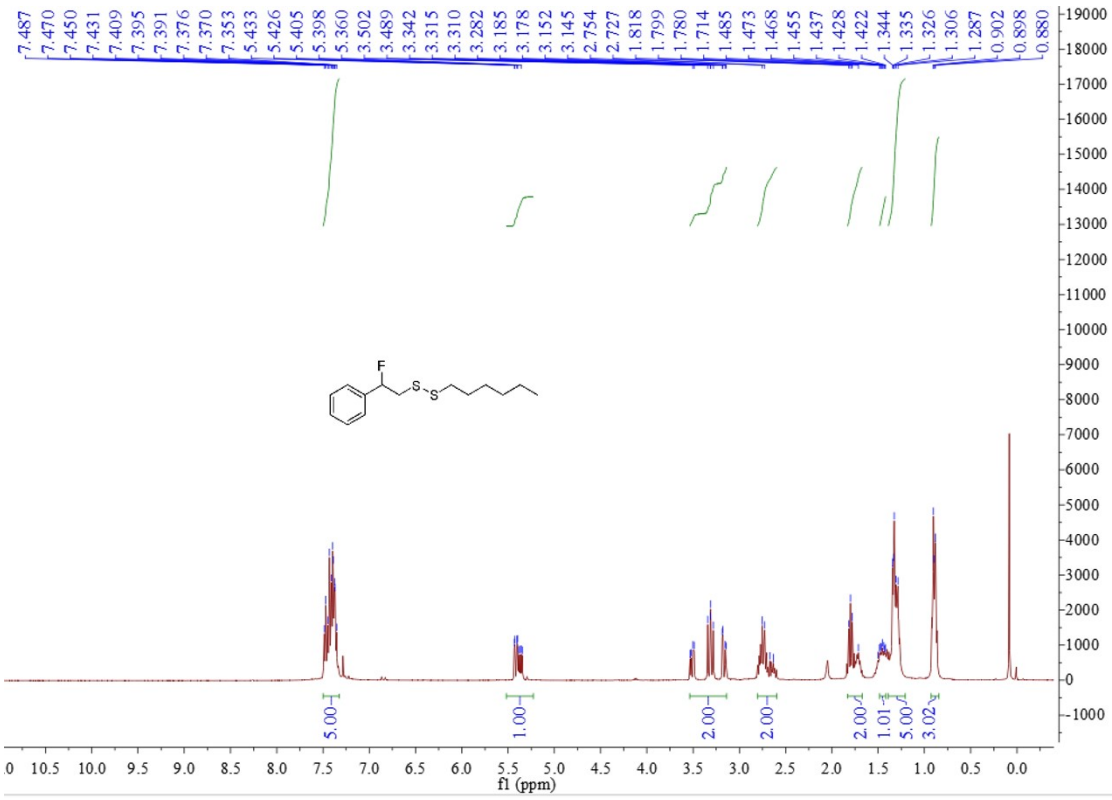
52.727
52.685
24.549
24.443
22.053
21.979
13.667
13.633
f1 (ppm)


-220.620
F
S
S
f1 (ppm)

C16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5.398
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3.178
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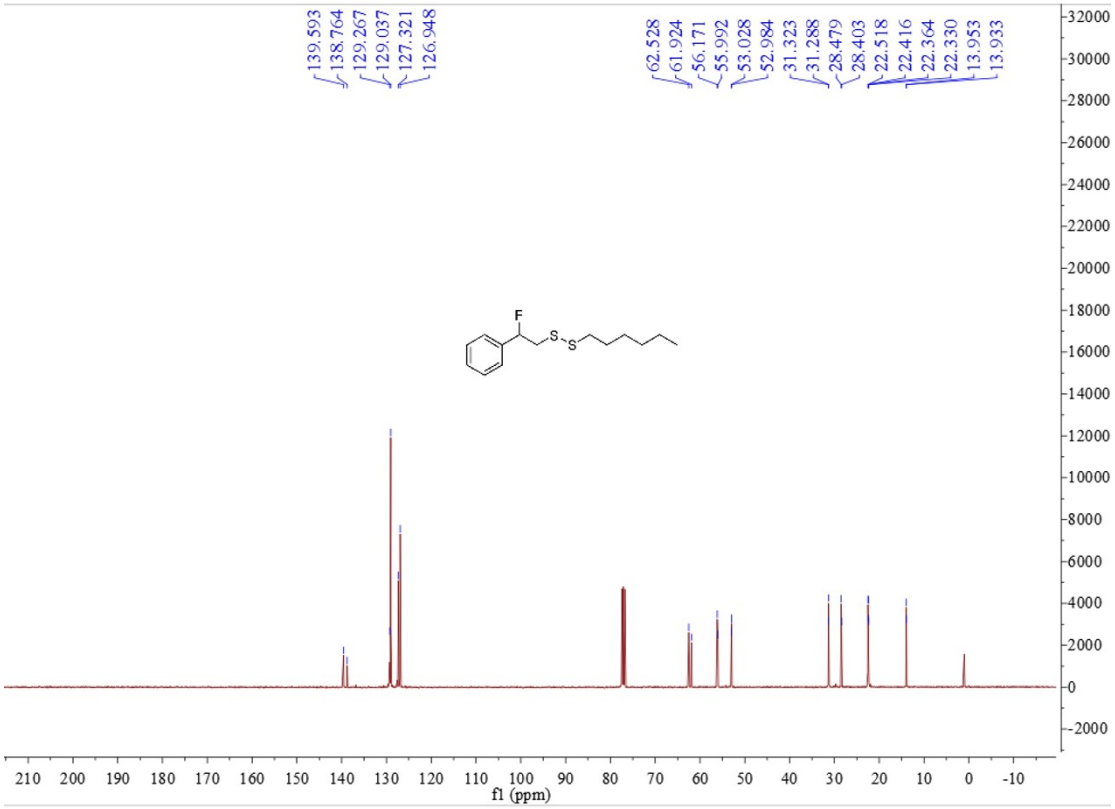
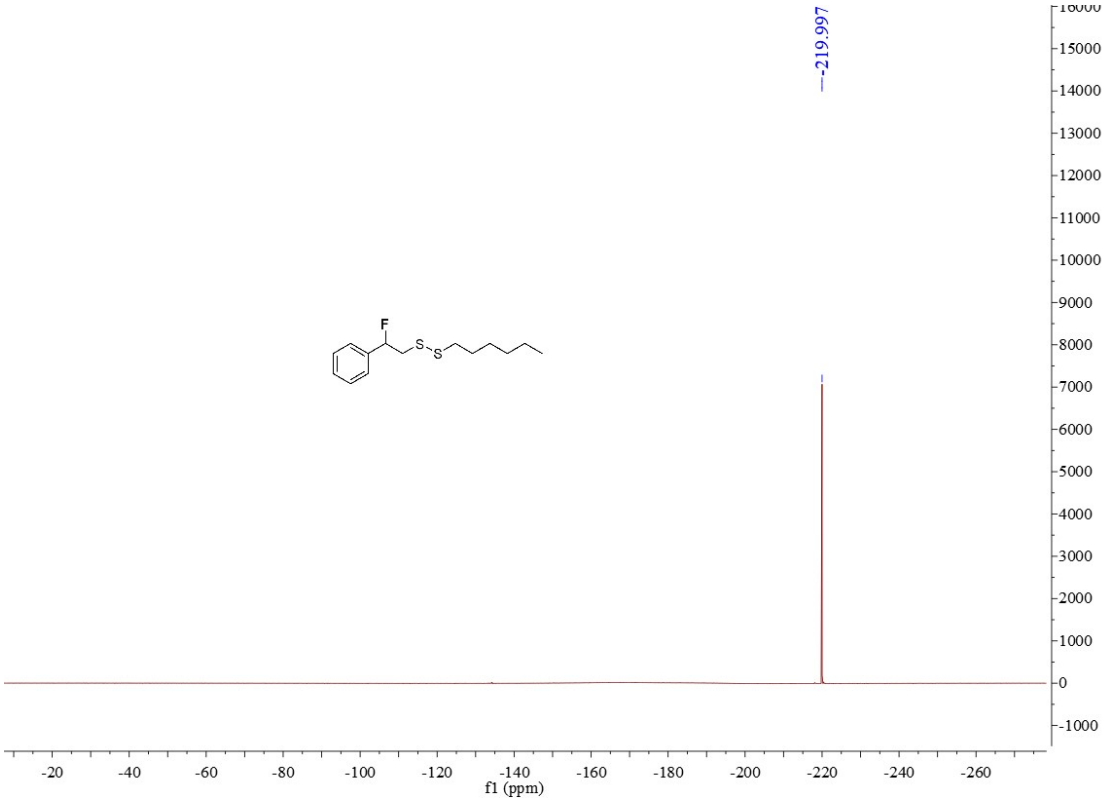
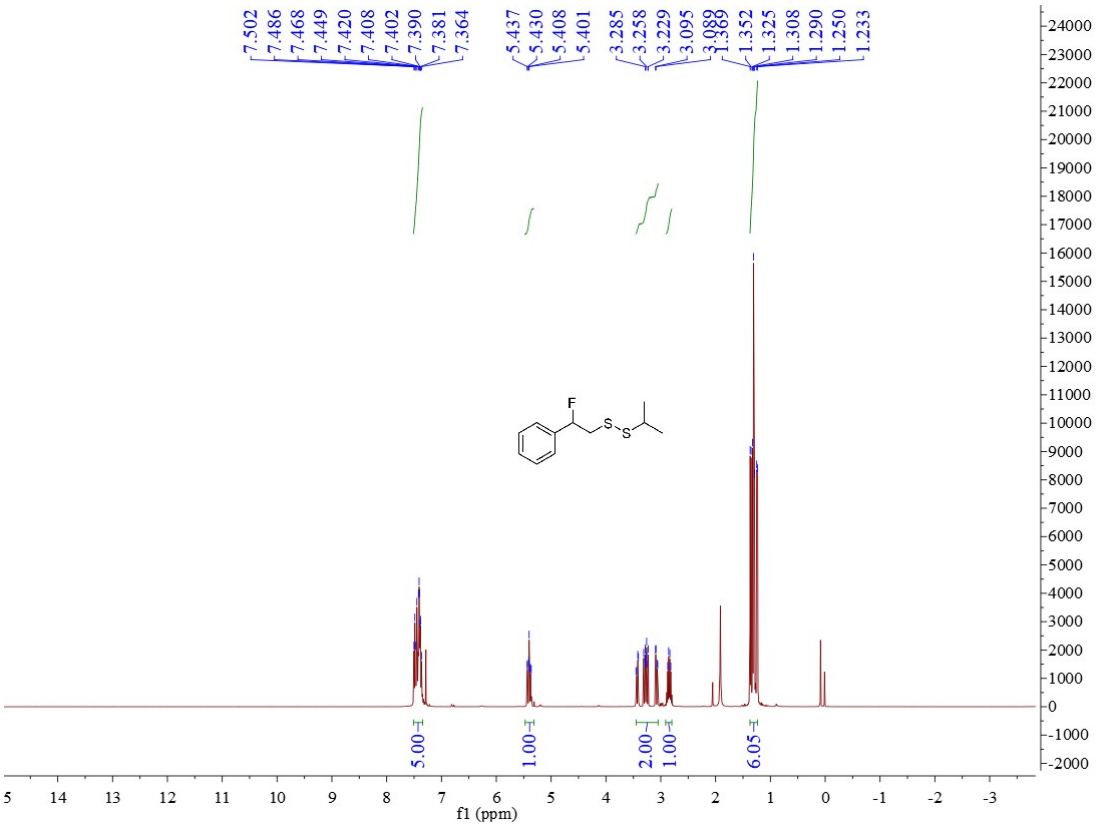
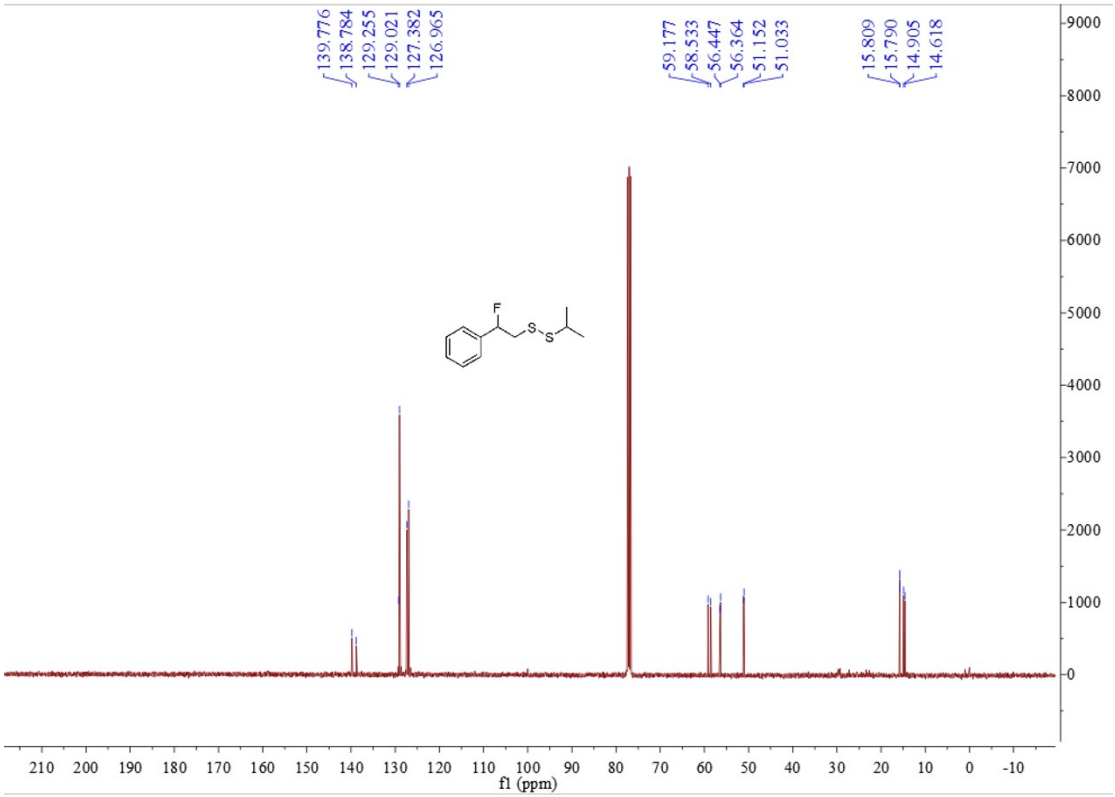
3.145
2.754
2.727
1.818
1.799
1.780
1.714
1.485
1.473
1.468
1.455
1.437
1.428
1.422
1.344
1.335
1.326
1.306
1.287
0.902
0.898
0.880
F
S
S
5.00
1.00
2.00
2.00
2.00
1.01
5.00
3.02
f1 (ppm)

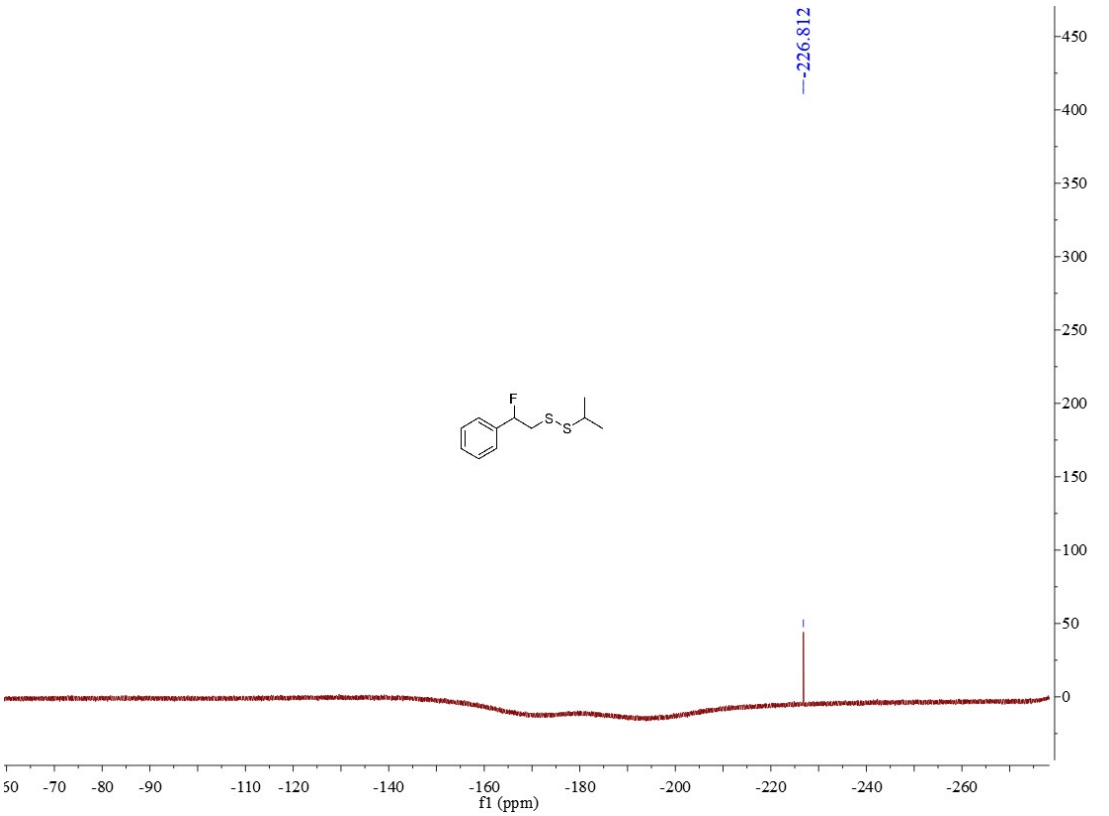

139.593
138.764
129.267
129.037
127.321
126.948
62.528
61.924
56.171
55.992
53.028
52.984
31.323
31.288
28.479
28.403
22.518
22.416
22.364
22.330
13.953
13.933
F
S
S
f1 (ppm)


-219.997
F
S
S
f1 (ppm)

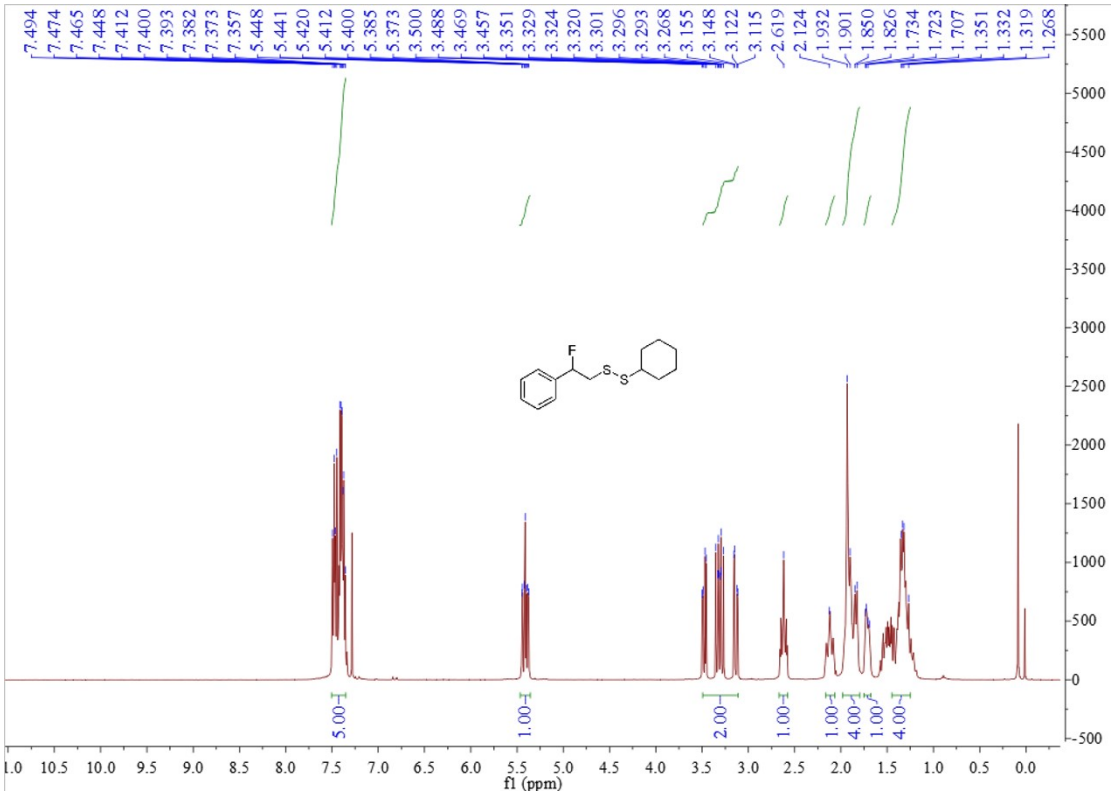
C17

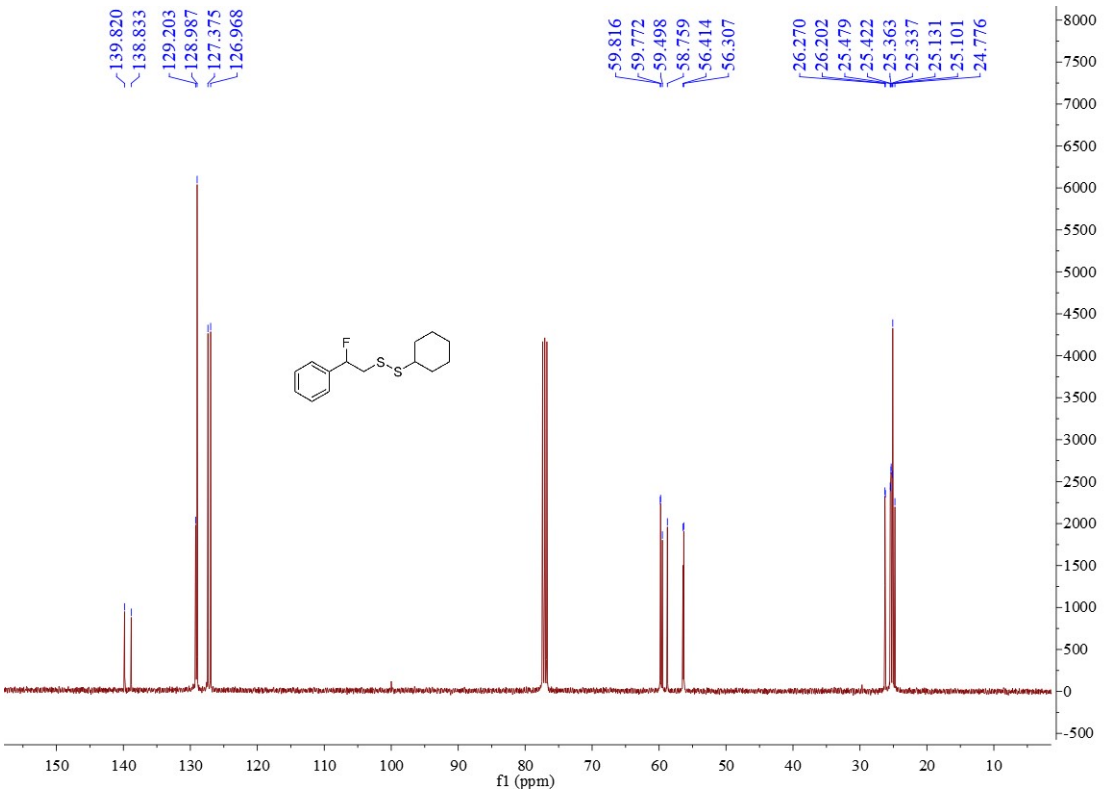

7.502
7.486
7.468
7.449
7.420
7.408
7.402
7.390
7.381
7.364
5.437
5.430
5.408
5.401
3.285
3.258
3.229
3.095
3.089
1.369
1.352
1.325
1.308
1.290
1.250
1.233
F
S
S
5.00
1.00
2.00
1.00
6.05
f1 (ppm)

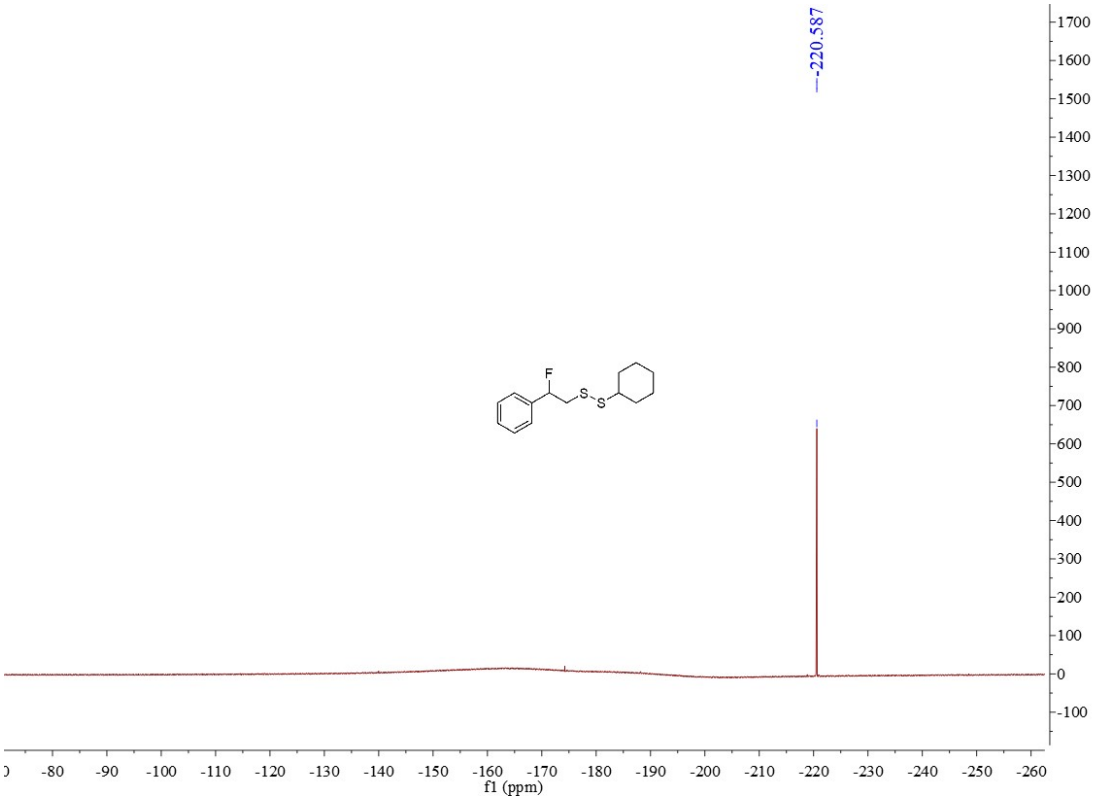

139.776
138.784
129.255
129.021
127.382
126.965
59.177
58.533
56.447
56.364
51.152
51.033
15.809
15.790
14.905
14.618
F
S
S
f1 (ppm)


-226.812
F
S
S
f1 (ppm)

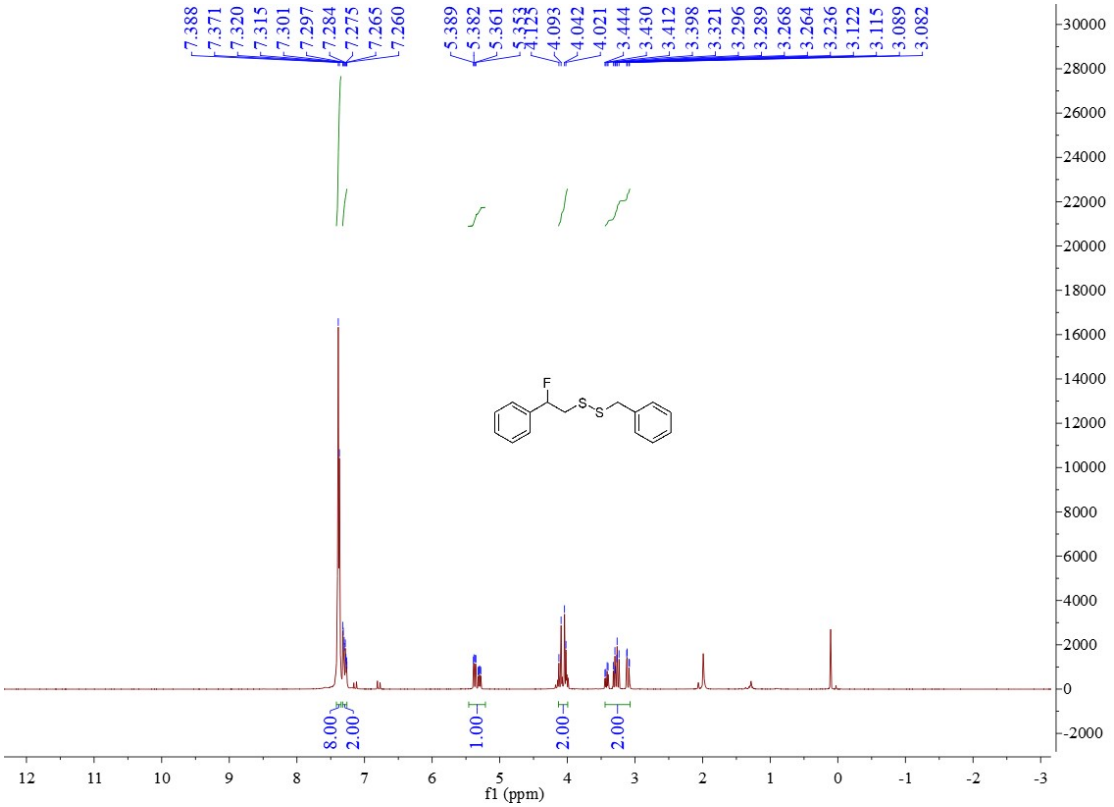
C18

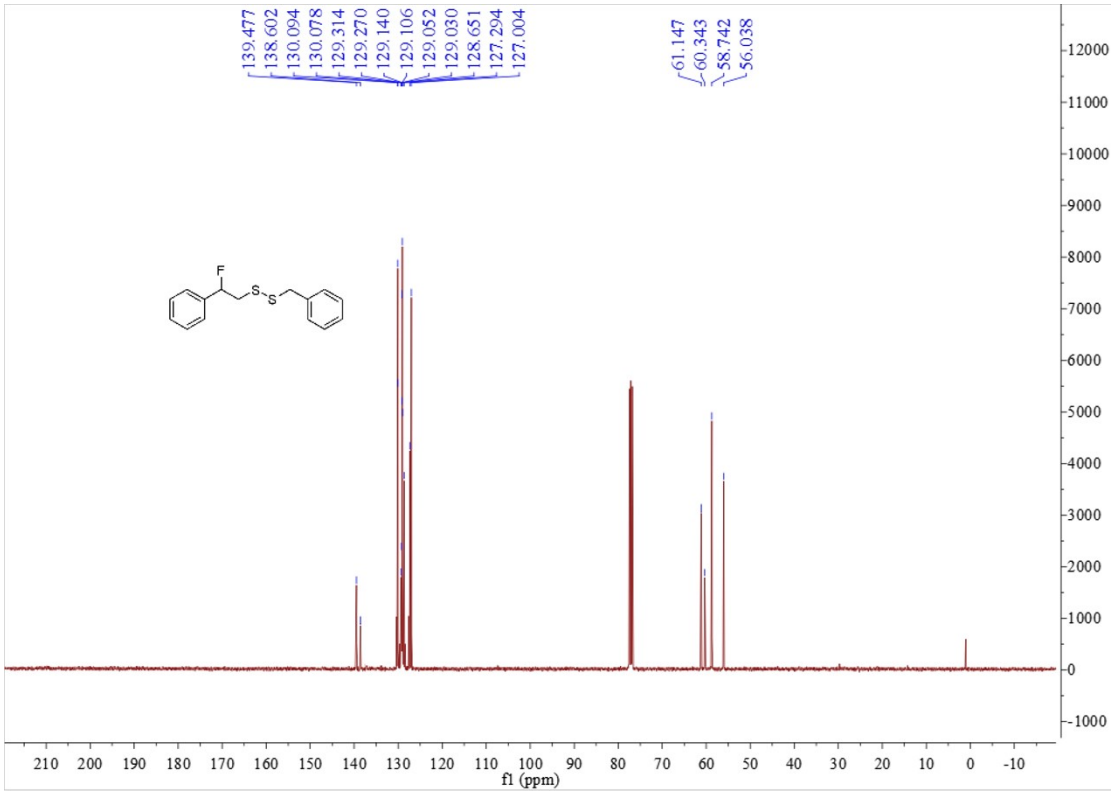

7.494
7.474
7.465
7.448
7.412
7.400
7.393
7.382
7.373
7.357
5.448
5.441
5.420
5.412
5.400
5.385
5.373
3.500
3.488
3.469
3.457
3.351
3.329
3.324
3.320
3.301
3.296
3.293
3.268
3.155
3.148
3.122
3.115
2.619
2.124
1.932
1.901
1.850
1.826
1.734
1.723
1.707
1.351
1.332
1.319
1.268
F
S
S
5.00
1.00
2.00
1.00
1.00
4.00
1.00
4.00
f1 (ppm)

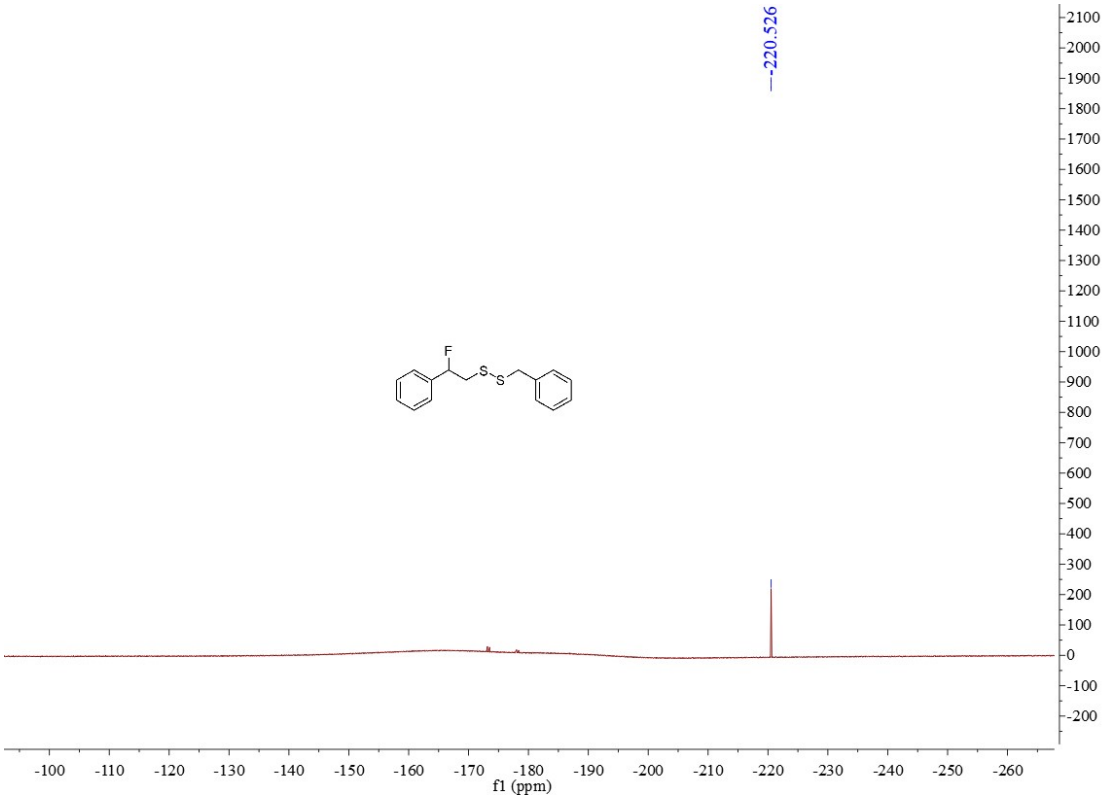

139.820
138.833
129.203
128.987
127.375
126.968
59.816
59.772
59.498
58.759
56.414
56.307
26.270
26.202
25.479
25.422
25.363
25.337
25.131
25.101
24.776
F
S
S
f1 (ppm)


-220.587
F
S
S
f1 (ppm)

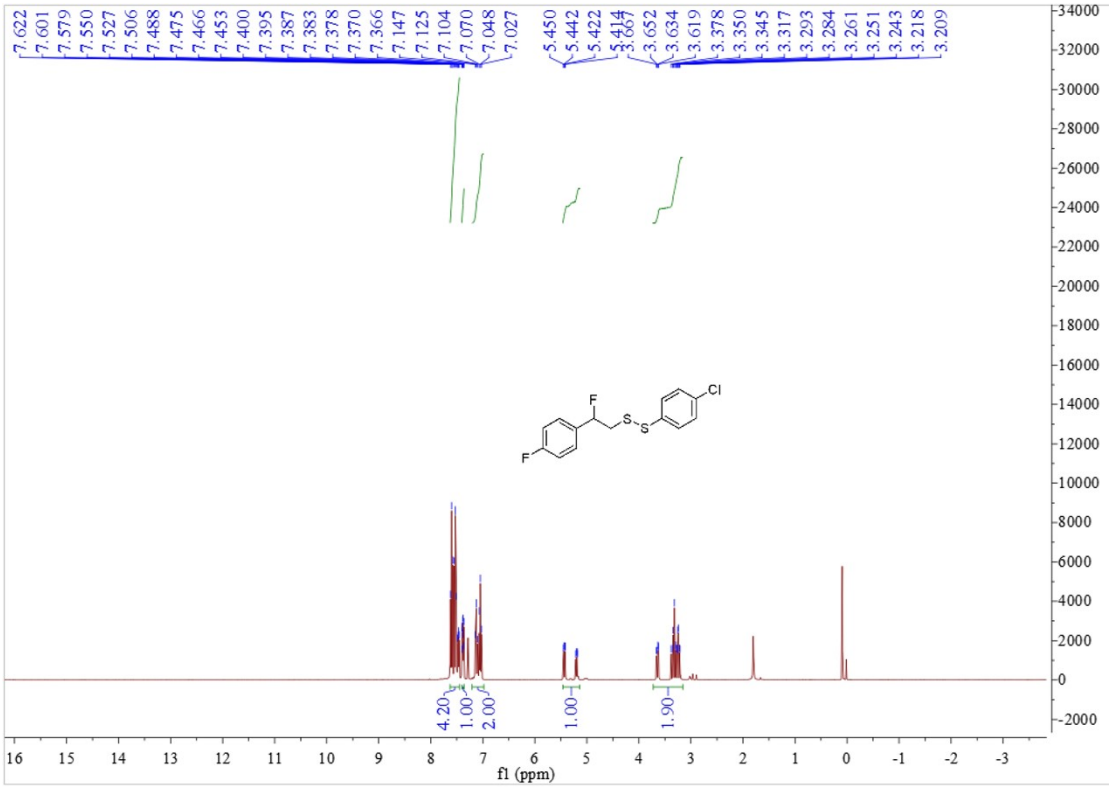
C19

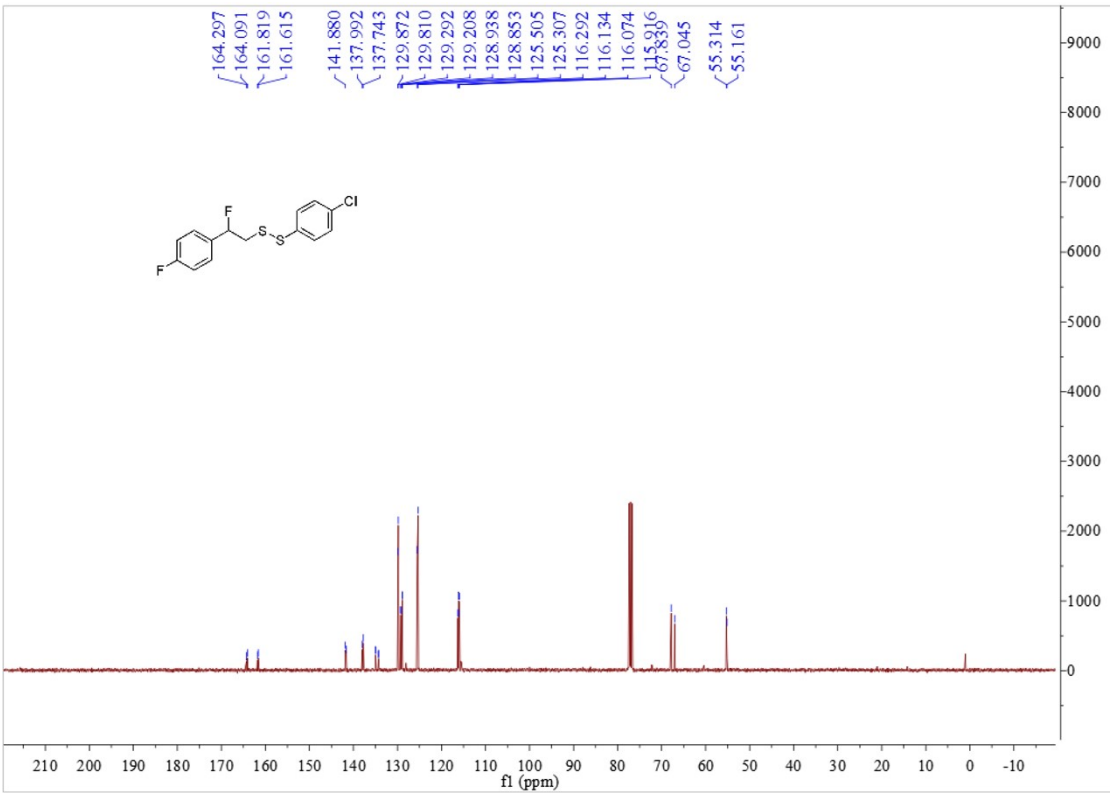

7.388
7.371
7.320
7.315
7.301
7.297
7.284
7.275
7.265
7.260
5.389
5.382
5.361
5.353
5.123
4.093
4.042
4.021
3.444
3.430
3.412
3.398
3.321
3.296
3.289
3.268
3.264
3.236
3.122
3.115
3.089
3.082
F
S
S
8.00
2.00
1.00
2.00
2.00
f1 (ppm)

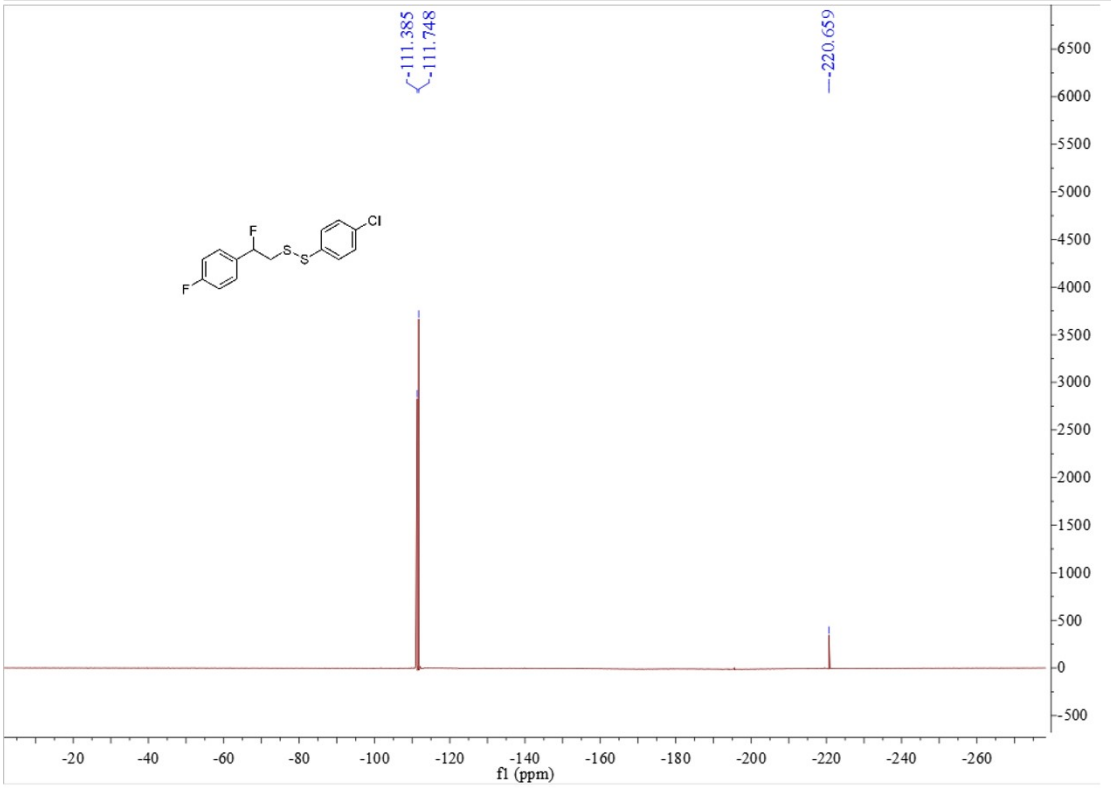

139.477
138.602
130.094
130.078
129.314
129.270
129.140
129.106
129.052
129.030
128.651
127.294
127.004
61.147
60.343
58.742
56.038
F
S
S
f1 (ppm)


-220.526
F
S
S
f1 (ppm)

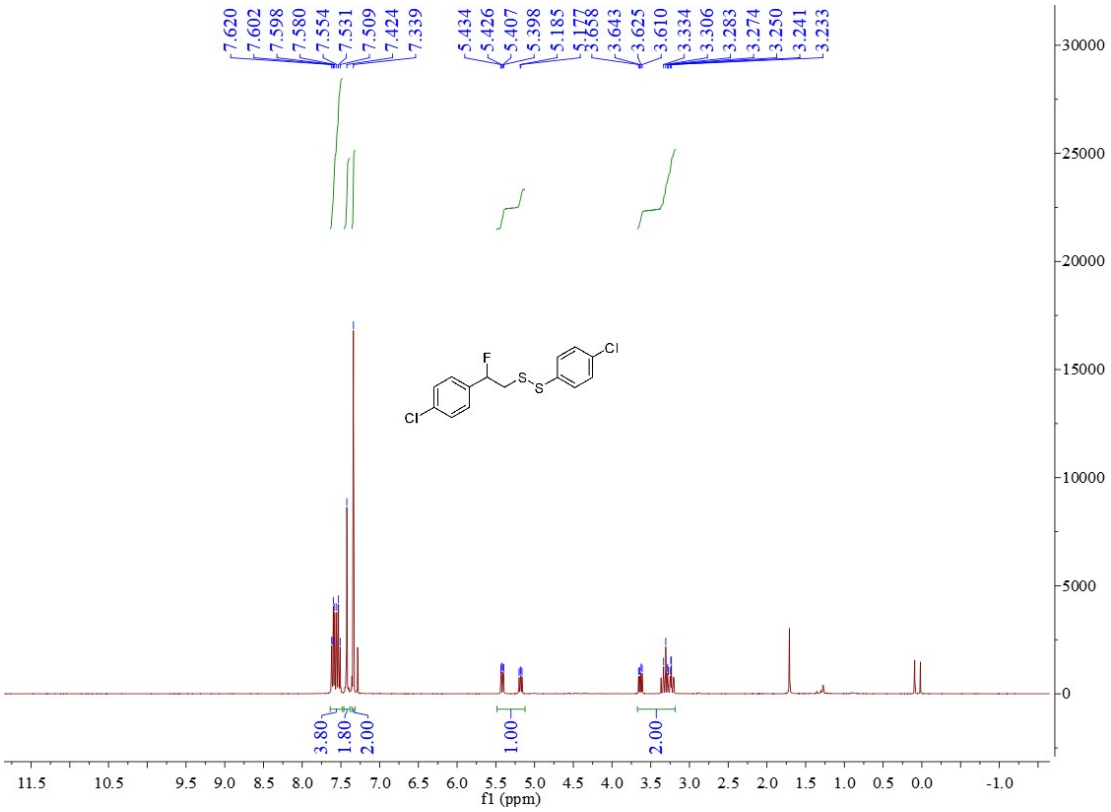
C20

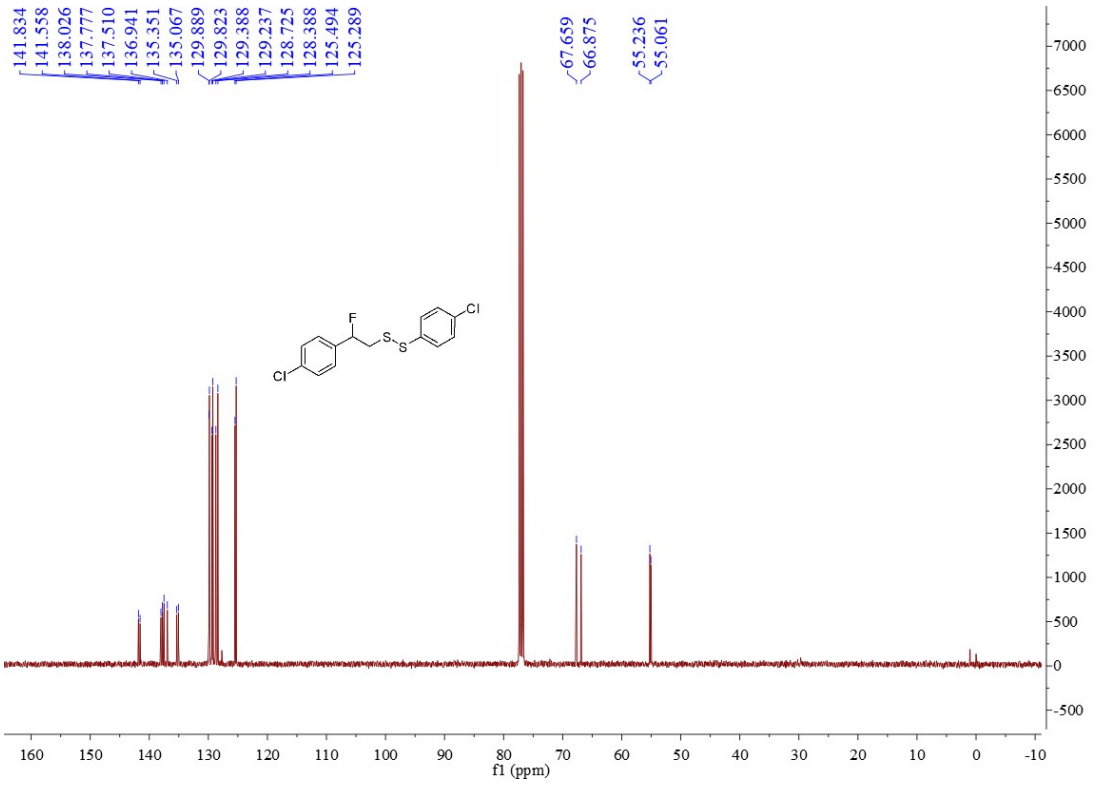

7.622
7.601
7.579
7.550
7.527
7.506
7.488
7.475
7.466
7.453
7.400
7.395
7.387
7.383
7.378
7.370
7.366
7.147
7.125
7.104
7.070
7.048
7.027
5.450
5.442
5.422
3.652
3.634
3.619
3.378
3.350
3.345
3.317
3.293
3.284
3.261
3.251
3.243
3.218
3.209
F
S
S
Cl
F
4.20
1.00
2.00
1.00
1.90
f1 (ppm)

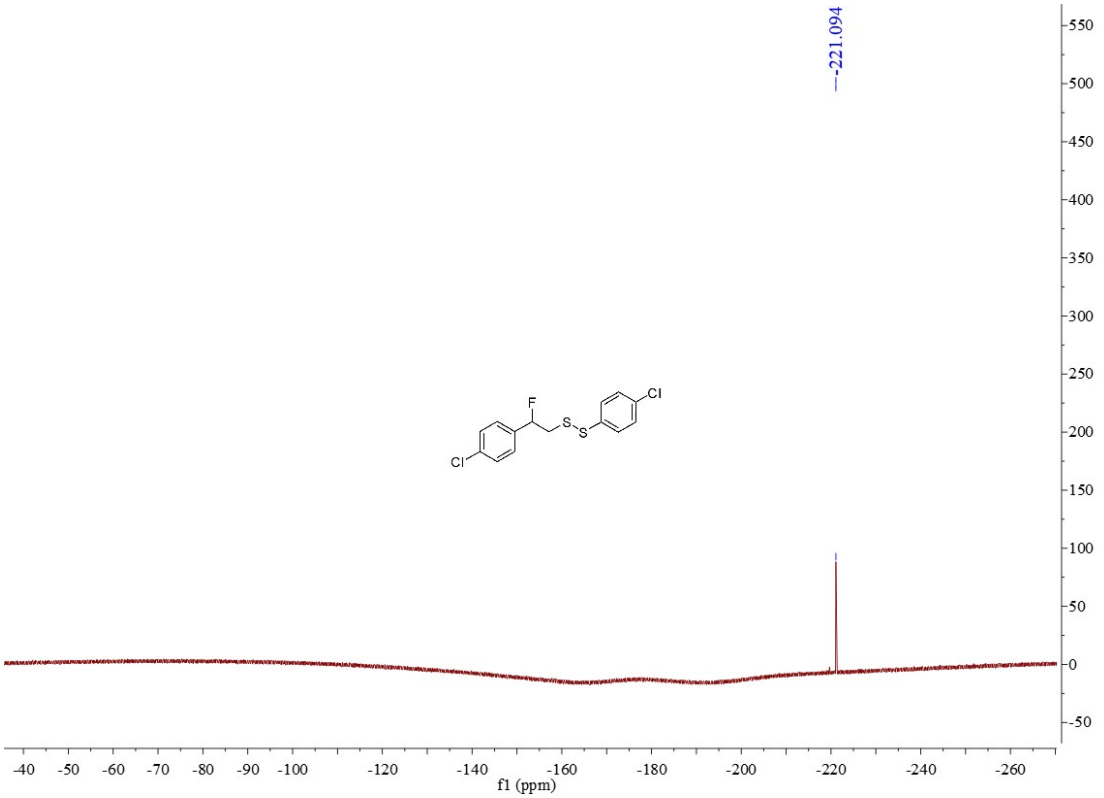

164.297
164.091
161.819
161.615
141.880
137.992
137.743
129.872
129.810
129.292
129.208
128.938
128.853
125.505
125.307
116.292
116.134
116.074
115.916
67.839
67.045
55.314
55.161
F
S
S
Cl
F
f1 (ppm)


-111.385
-111.748
-220.659
F
S
S
Cl
F
f1 (ppm)

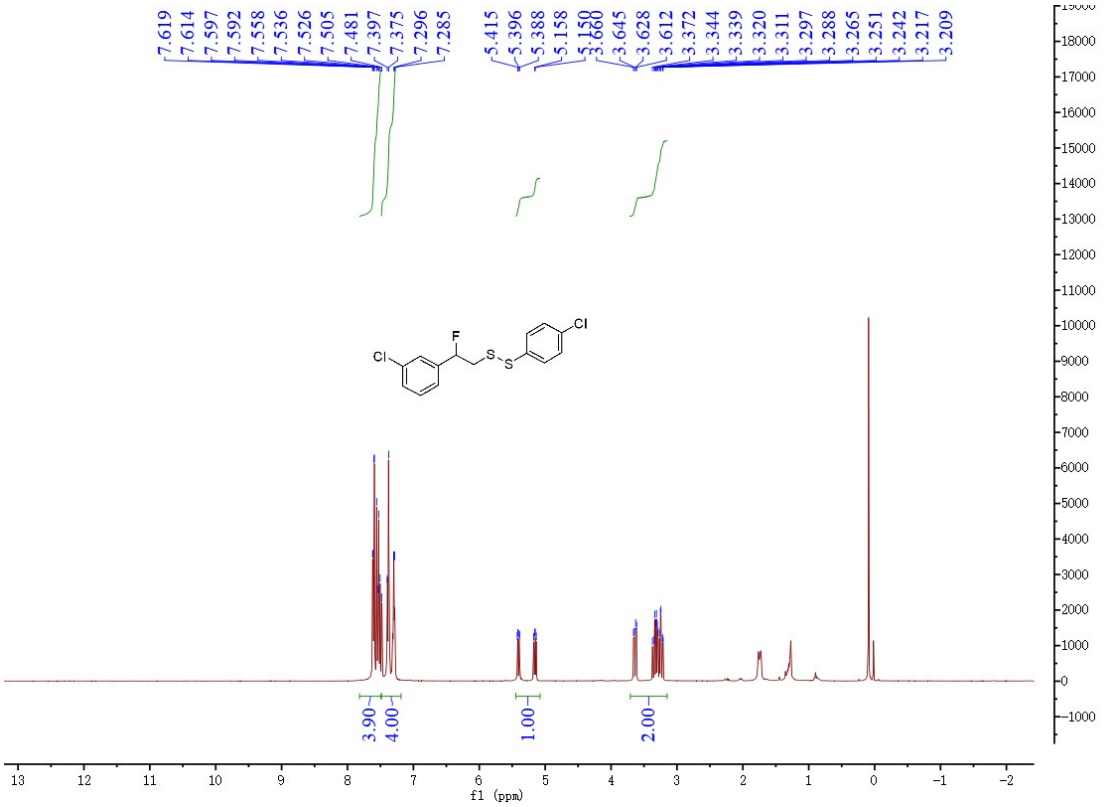
C21

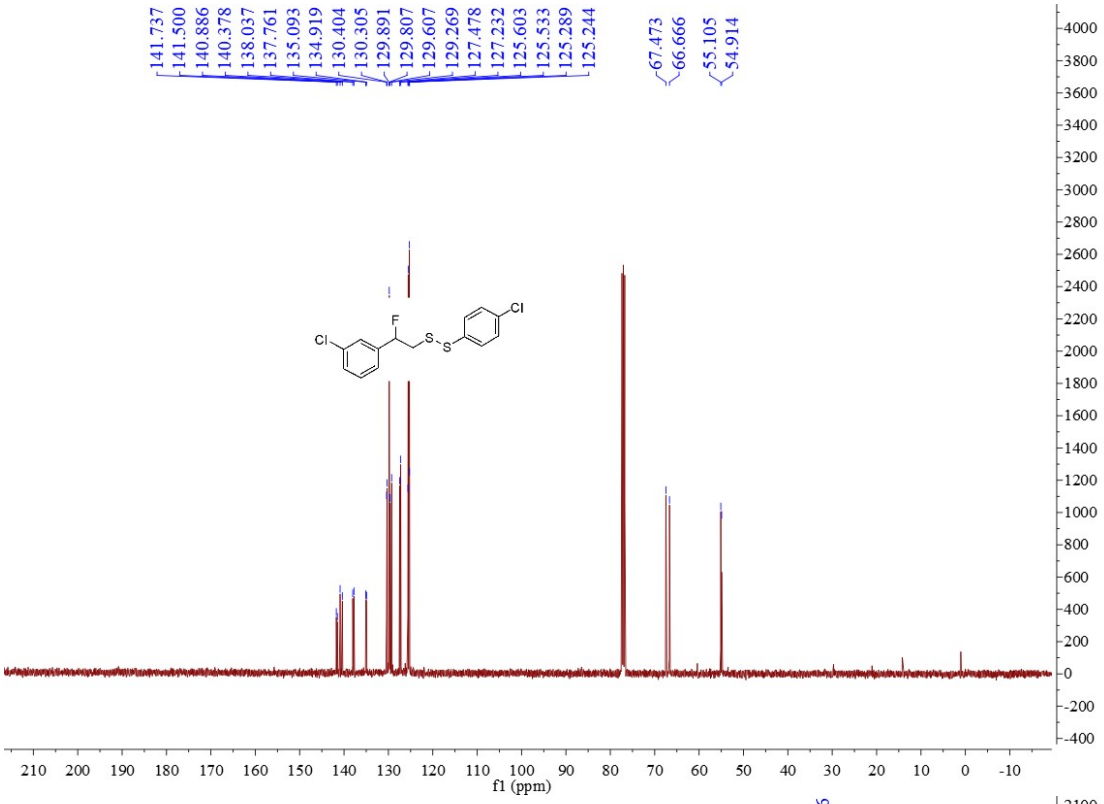

7.620
7.602
7.598
7.580
7.554
7.531
7.509
7.424
7.339
5.434
5.426
5.407
5.398
5.185
5.177
5.158
3.643
3.625
3.610
3.334
3.306
3.283
3.274
3.250
3.241
3.233
3.80
1.80
2.00
1.00
2.00
f1 (ppm)

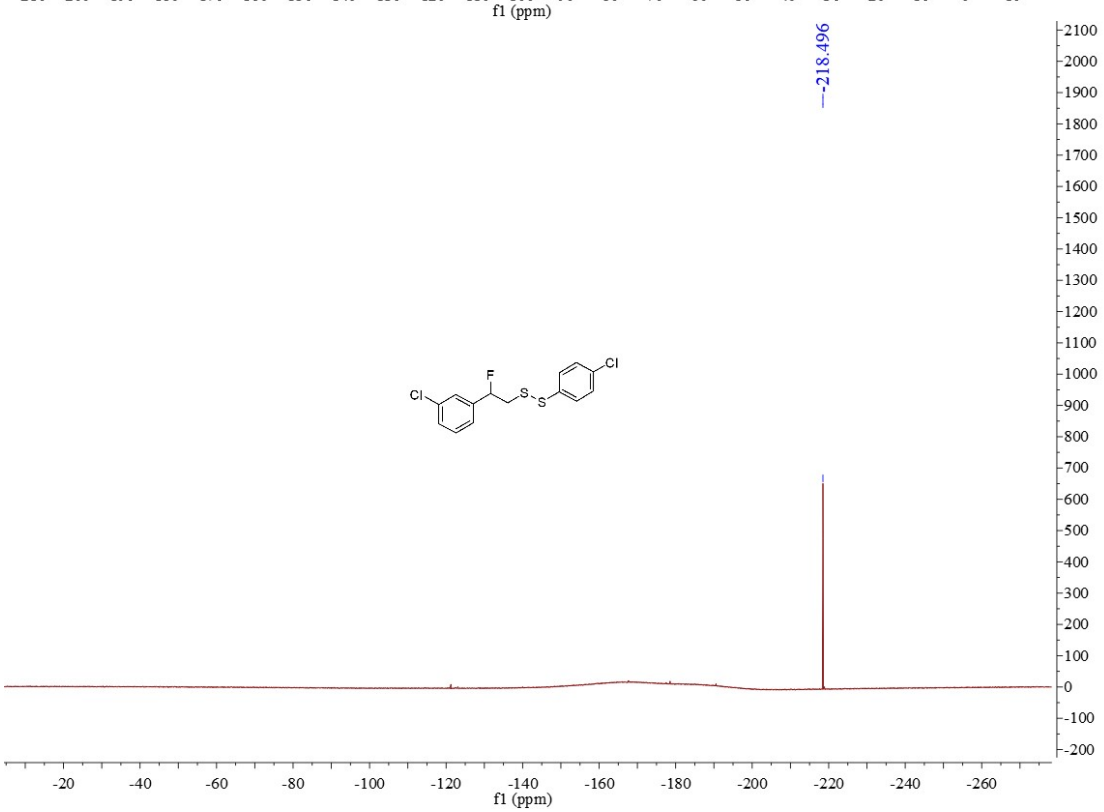

141.834
141.558
138.026
137.777
137.510
136.941
135.351
135.067
129.889
129.823
129.388
129.237
128.725
128.388
125.494
125.289
67.659
66.875
55.236
55.061
f1 (ppm)


-221.094
F
S
S
Cl
Cl
f1 (ppm)

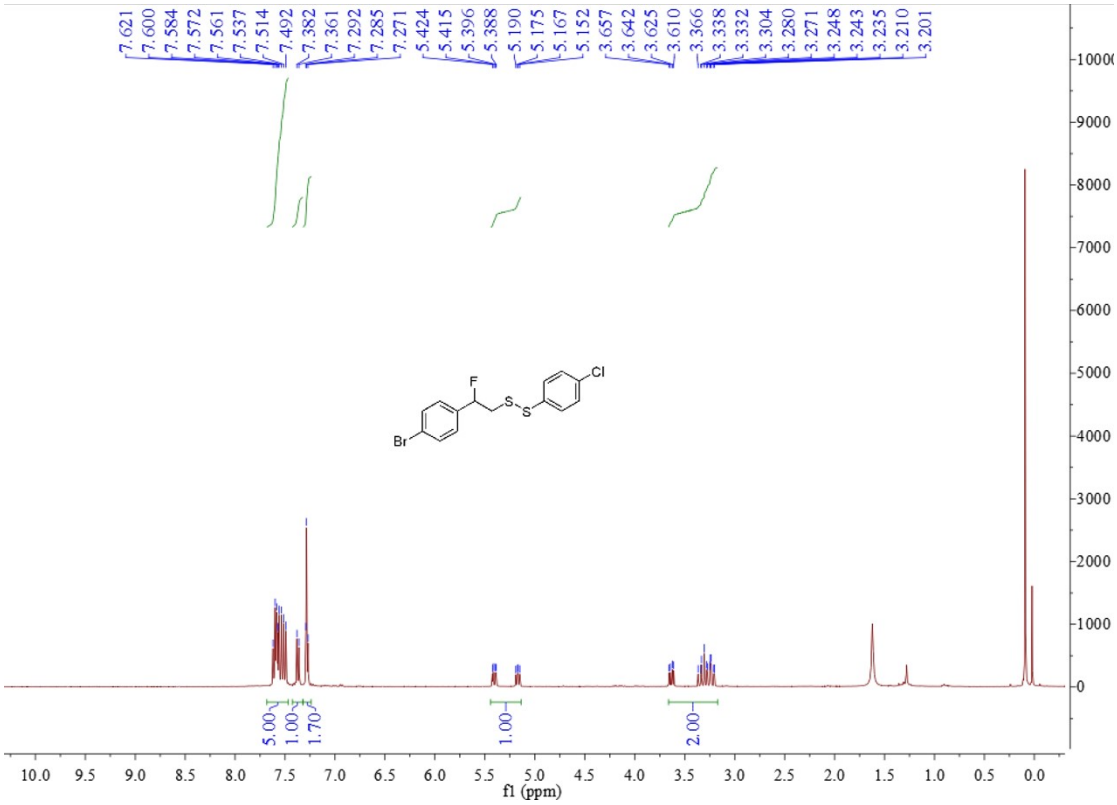
C22

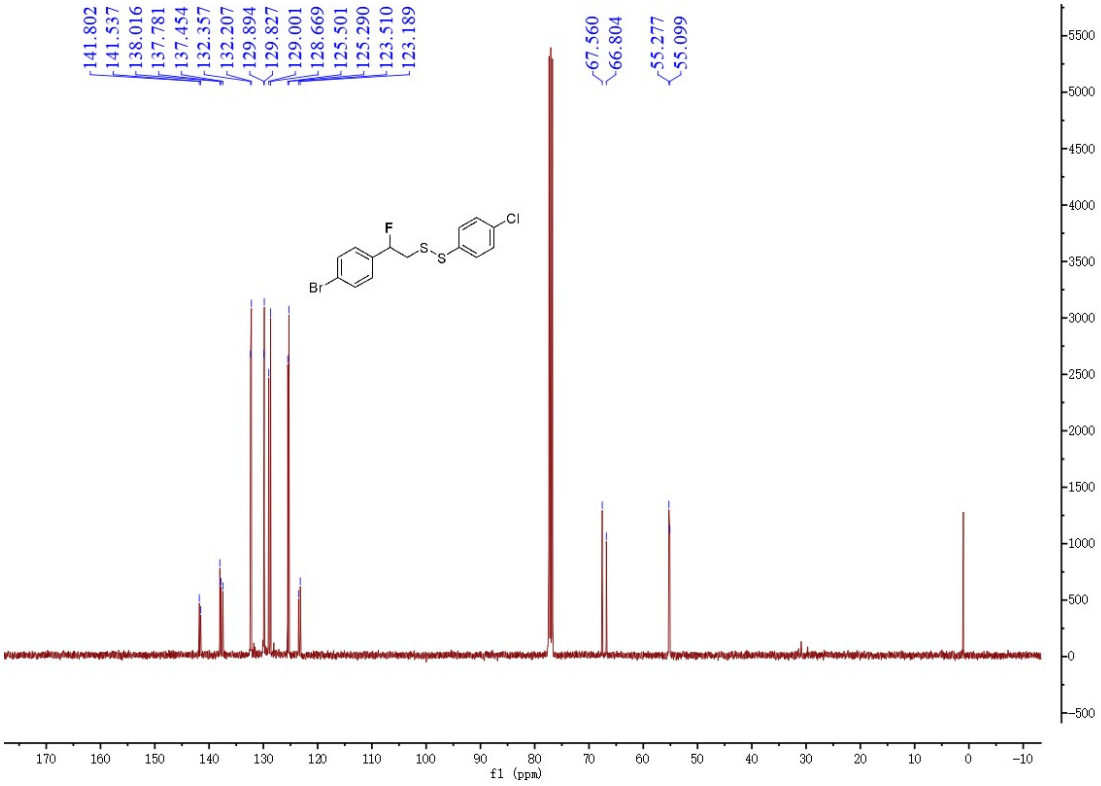

7.619
7.614
7.597
7.592
7.558
7.536
7.526
7.505
7.481
7.397
7.375
7.296
7.285
5.415
5.396
5.388
5.158
5.150
3.660
3.645
3.628
3.612
3.372
3.344
3.339
3.320
3.311
3.297
3.288
3.265
3.251
3.242
3.217
3.209
F
S
S
Cl
Cl
3.90
4.00
1.00
2.00
f1 (ppm)

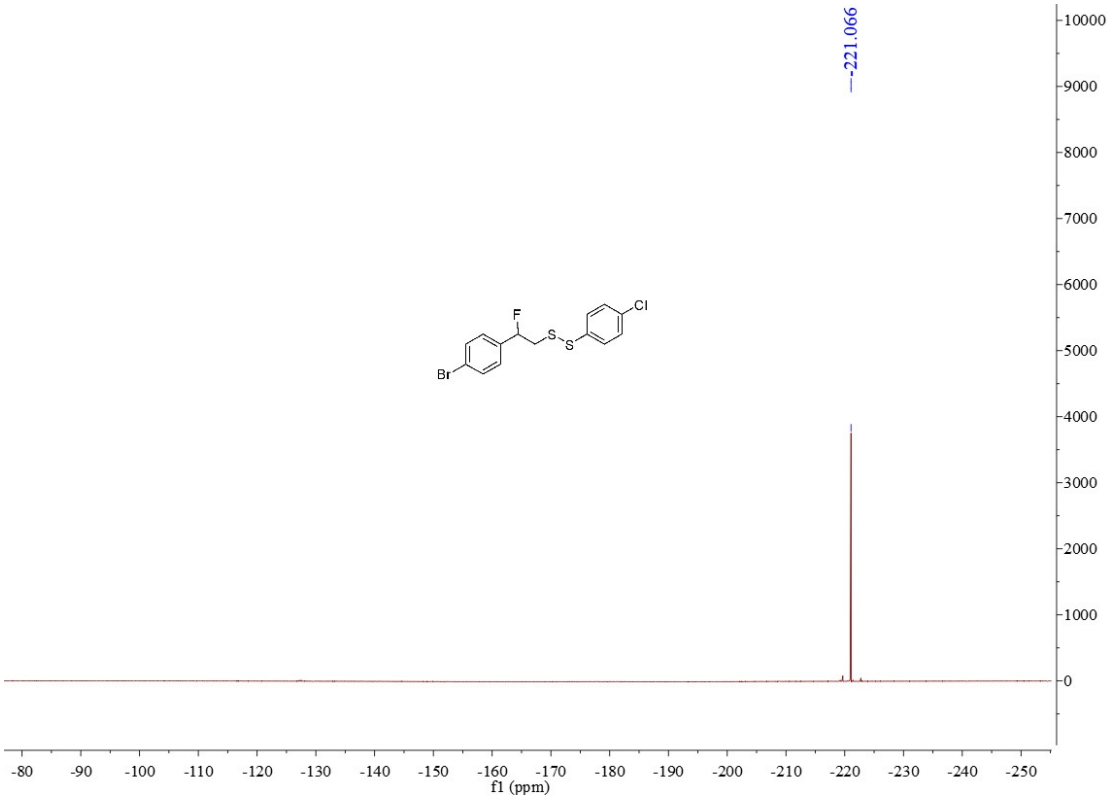

141.737
141.500
140.886
140.378
138.037
137.761
135.093
134.919
130.404
130.305
129.891
129.807
129.607
129.269
127.478
127.232
125.603
125.533
125.289
125.244
67.473
66.666
55.105
54.914
Cl
F
S
S
Cl
f1 (ppm)


-218.496
Cl
F
S
S
Cl
f1 (ppm)

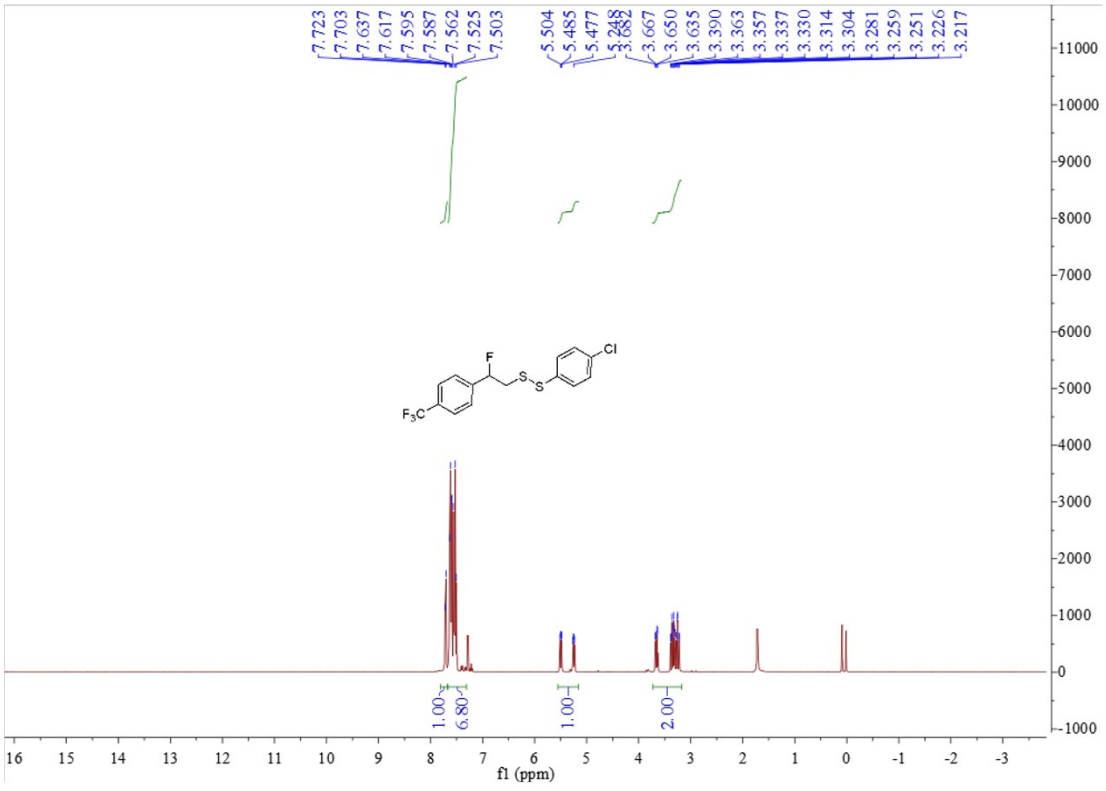
C23

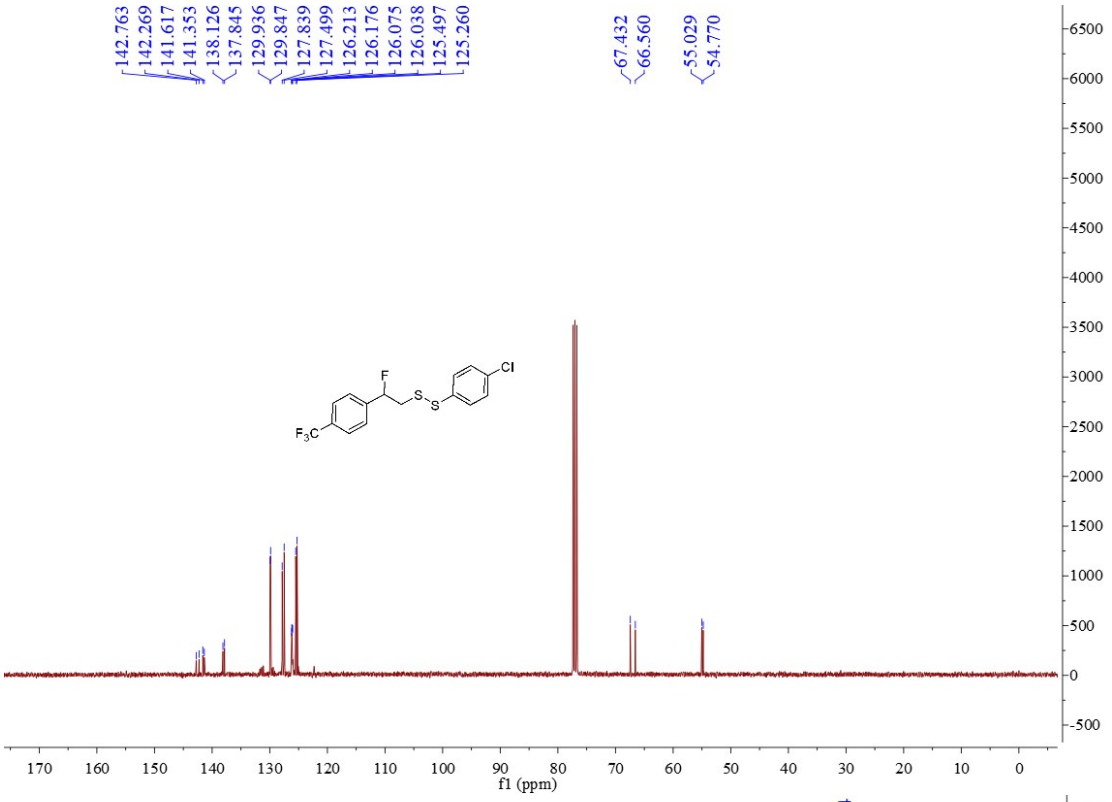

7.621
7.600
7.584
7.572
7.561
7.537
7.514
7.492
7.382
7.361
7.292
7.285
7.271
5.424
5.415
5.396
5.388
5.190
5.175
5.167
5.152
3.657
3.642
3.625
3.610
3.366
3.338
3.332
3.304
3.280
3.271
3.248
3.243
3.235
3.210
3.201
F
S
S
Cl
Br
5.00
1.00
1.70
1.00
2.00
f1 (ppm)


141.802
141.537
138.016
137.781
137.454
132.357
132.207
129.894
129.827
129.001
128.669
125.501
125.290
123.510
123.189
67.560
66.804
55.277
55.099
F
S
S
Cl
Br
f1 (ppm)


-221.066
F
S
S
Cl
Br
f1 (ppm)

C24


7.723
7.703
7.637
7.617
7.595
7.587
7.562
7.525
7.503
5.504
5.485
5.477
3.667
3.650
3.635
3.390
3.363
3.357
3.337
3.330
3.314
3.304
3.281
3.259
3.251
3.226
3.217
F
S
S
Cl
F3C
1.00
6.80
1.00
2.00
f1 (ppm)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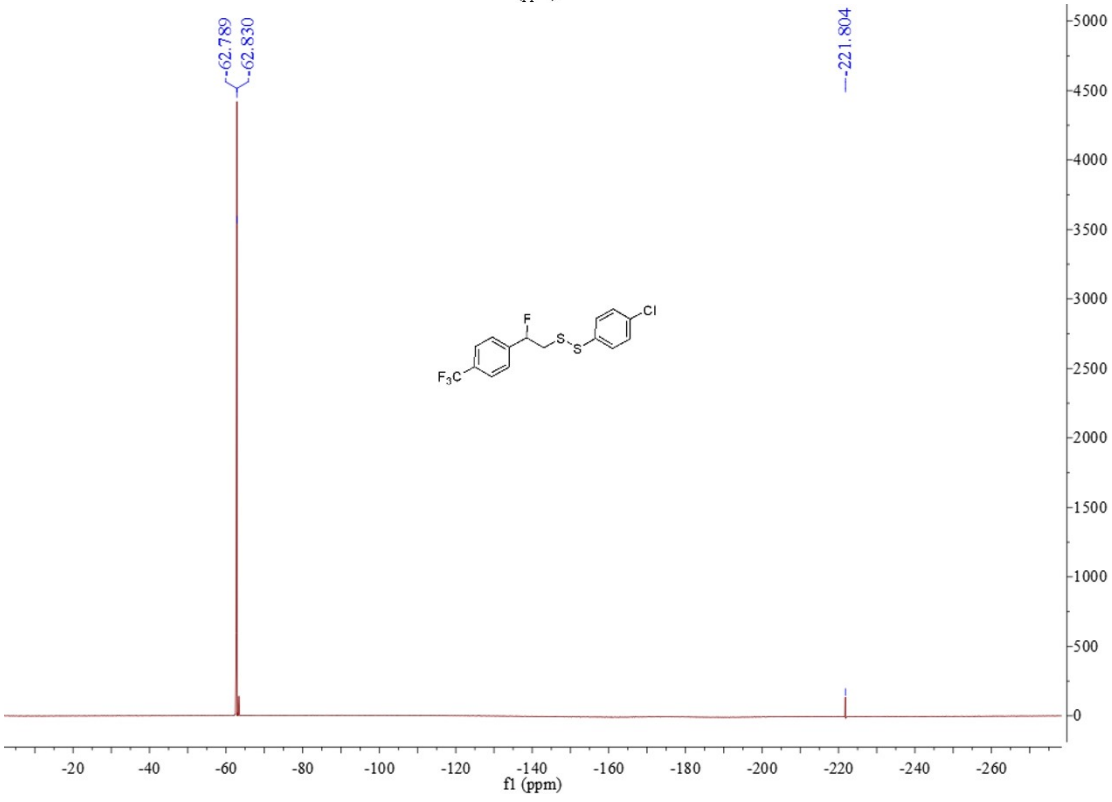
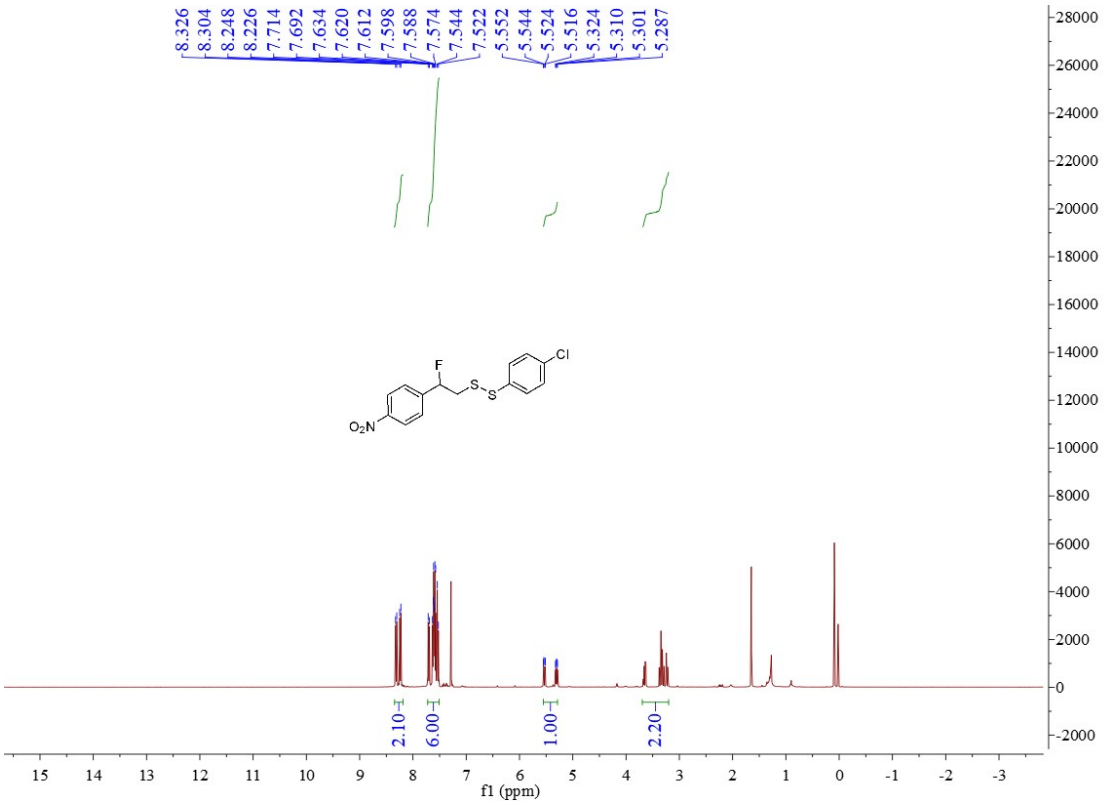
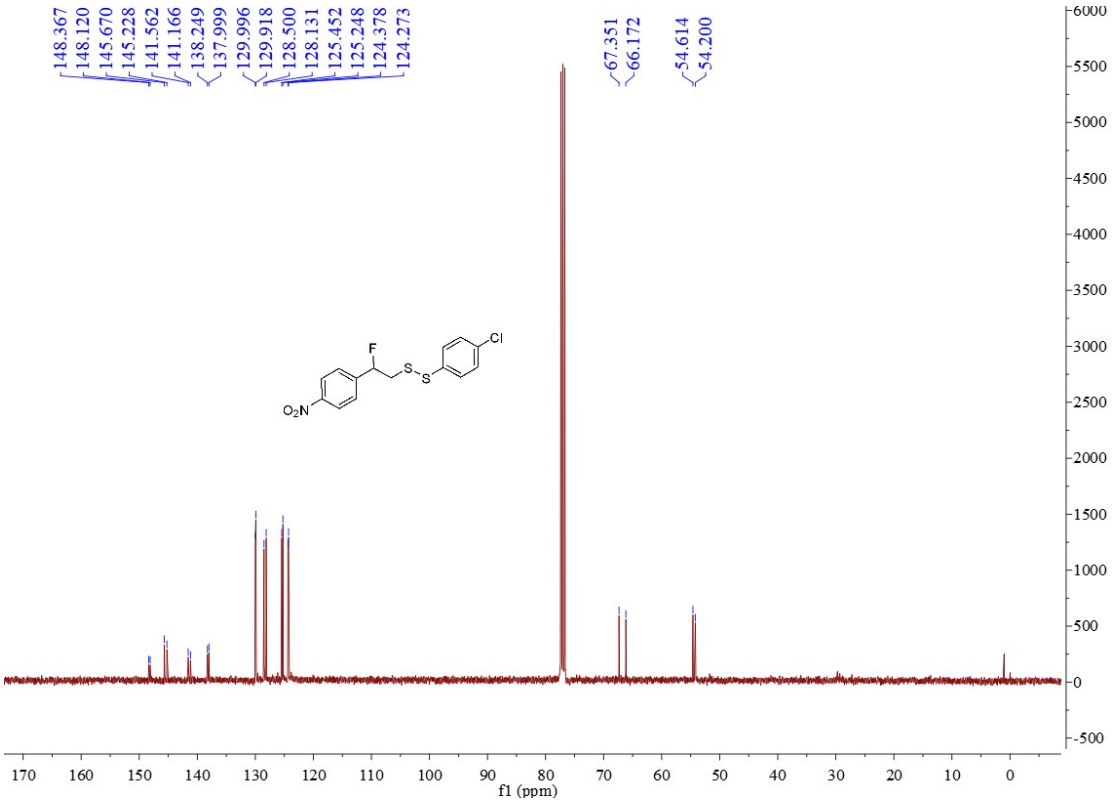
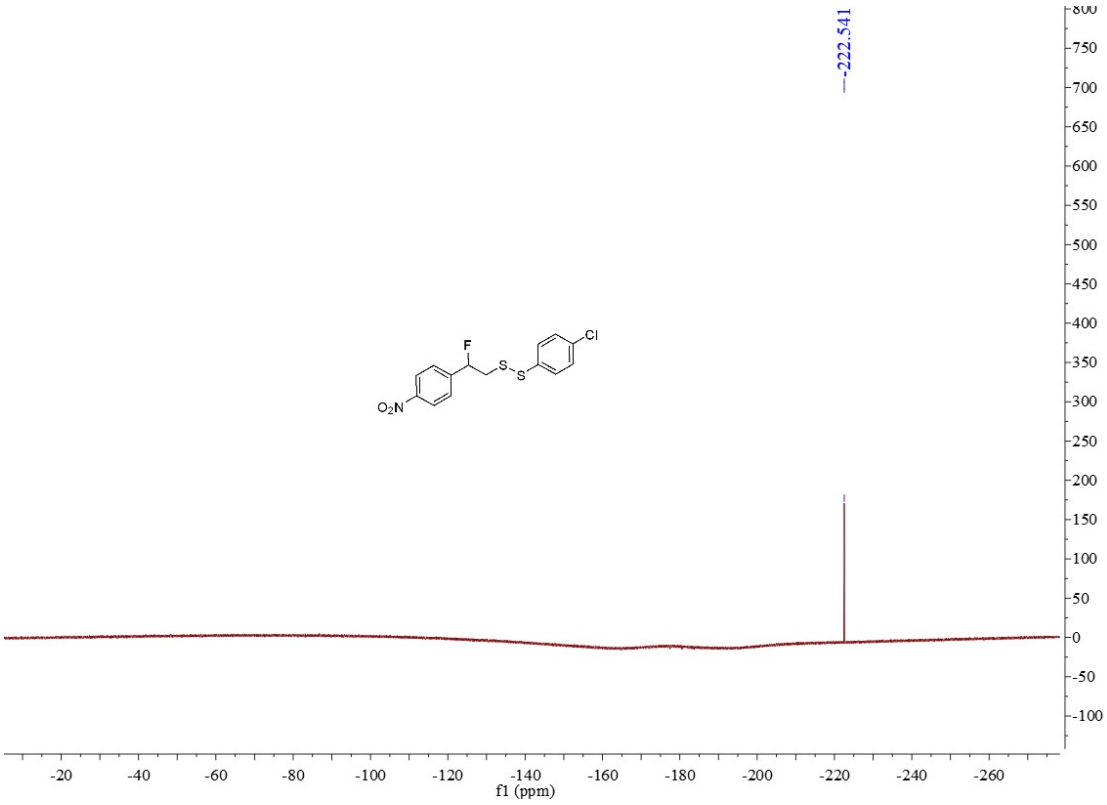
142.269
141.617
141.353
138.126
137.845
129.936
129.847
127.839
127.499
126.213
126.176
126.075
126.038
125.497
125.260
67.432
66.560
55.029
54.770
F
S
S
Cl
F3C
f1 (ppm)


-62.789
-62.830
-221.804
F
S
S
Cl
F3C
f1 (ppm)

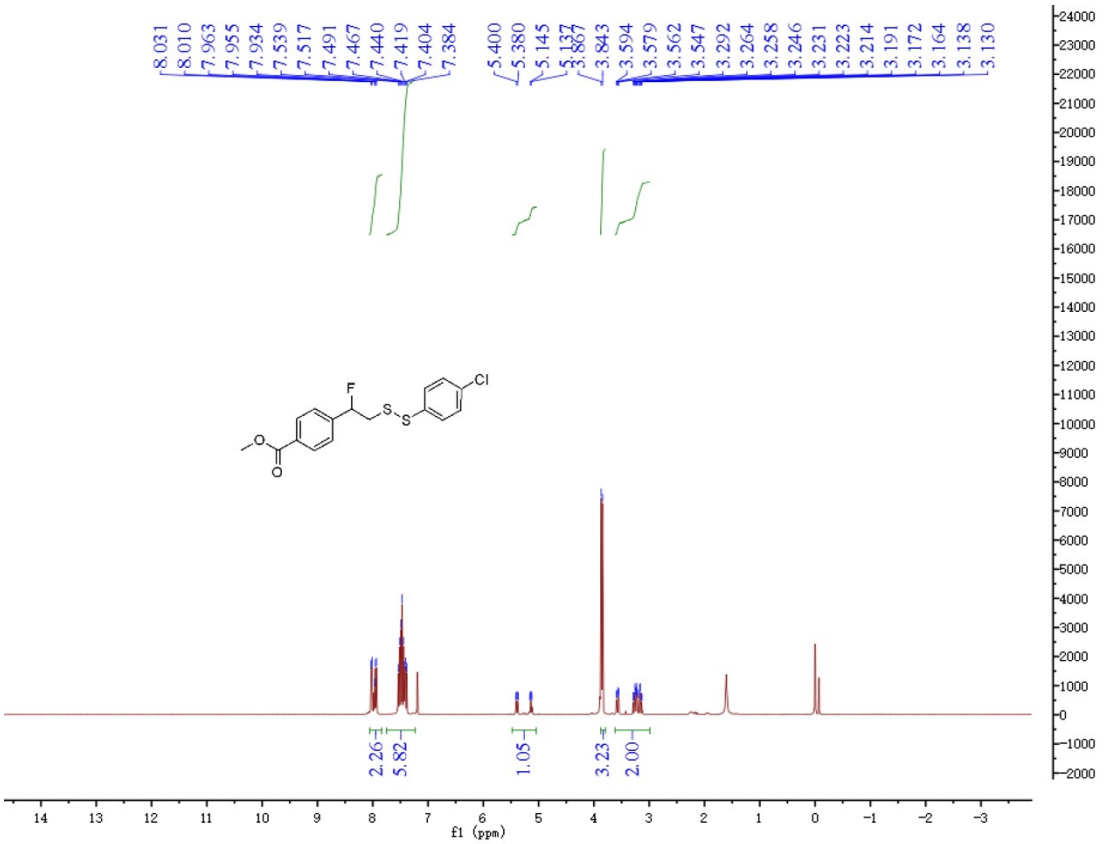
C25

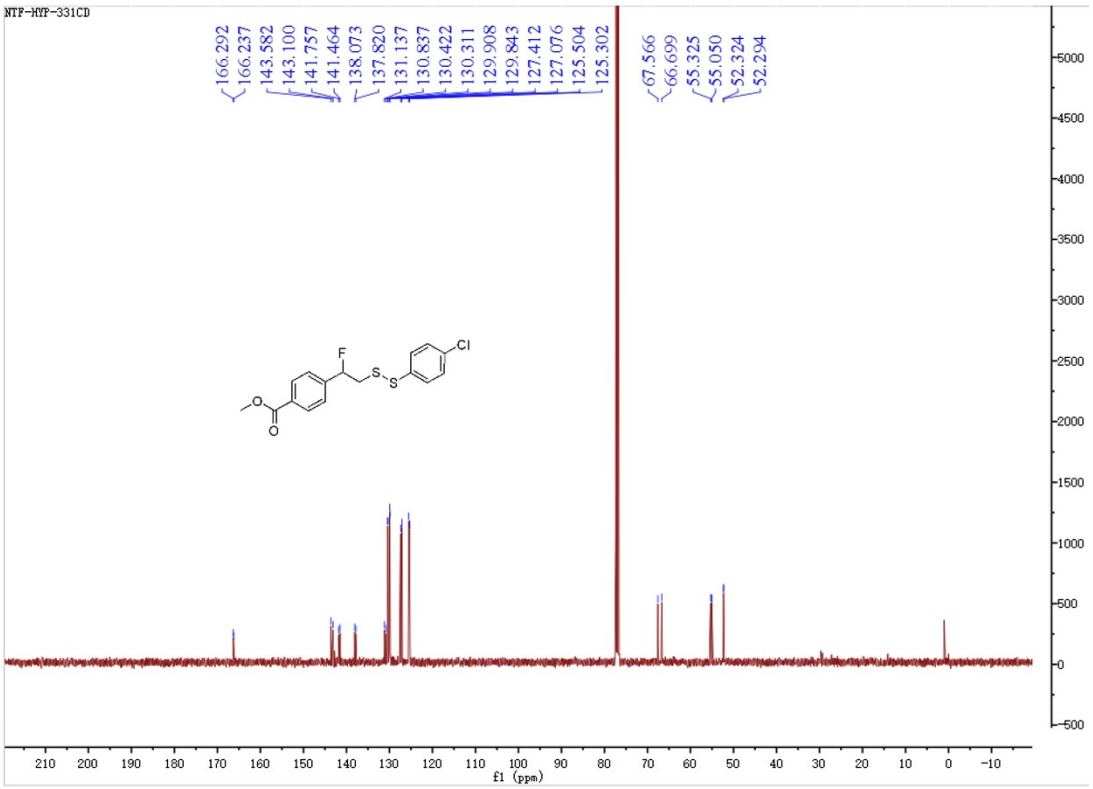

8.326
8.304
8.248
8.226
7.714
7.692
7.634
7.620
7.612
7.598
7.588
7.574
7.544
7.522
5.552
5.544
5.524
5.516
5.324
5.310
5.301
5.287
F
S
S
Cl
O2N
2.10
6.00
1.00
2.20
f1 (ppm)


148.367
148.120
145.670
145.228
141.562
141.166
138.249
137.999
129.996
129.918
128.500
128.131
125.452
125.248
124.378
124.273
67.351
66.172
54.614
54.200
F
S
S
Cl
O2N
f1 (ppm)


-222.541
F
S
S
Cl
O2N
f1 (ppm)

C26


8.031
8.010
7.963
7.955
7.934
7.539
7.517
7.491
7.467
7.440
7.419
7.404
7.384
5.400
5.380
5.145
3.867
3.843
3.594
3.579
3.562
3.547
3.292
3.264
3.258
3.246
3.231
3.223
3.214
3.191
3.172
3.164
3.138
3.130
F
S
S
Cl
O
O
2.26
5.82
1.05
3.23
2.00
f1 (ppm)


NTF-HYF-331CD
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166.237
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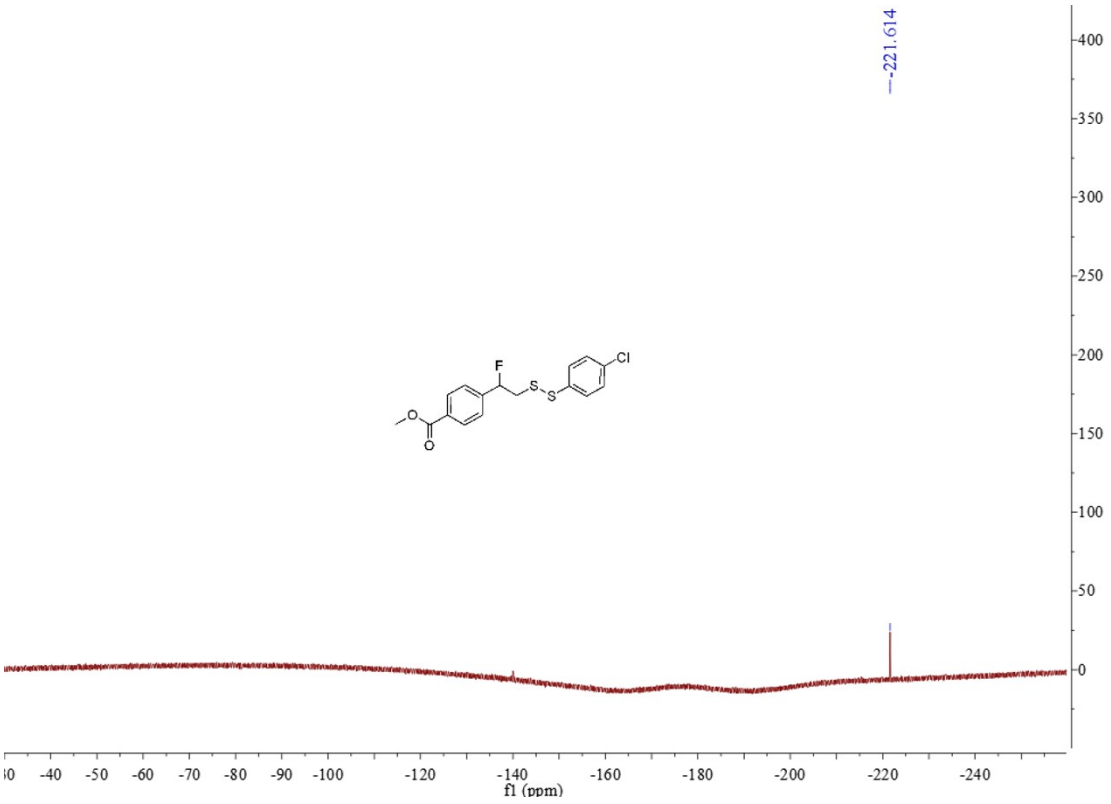
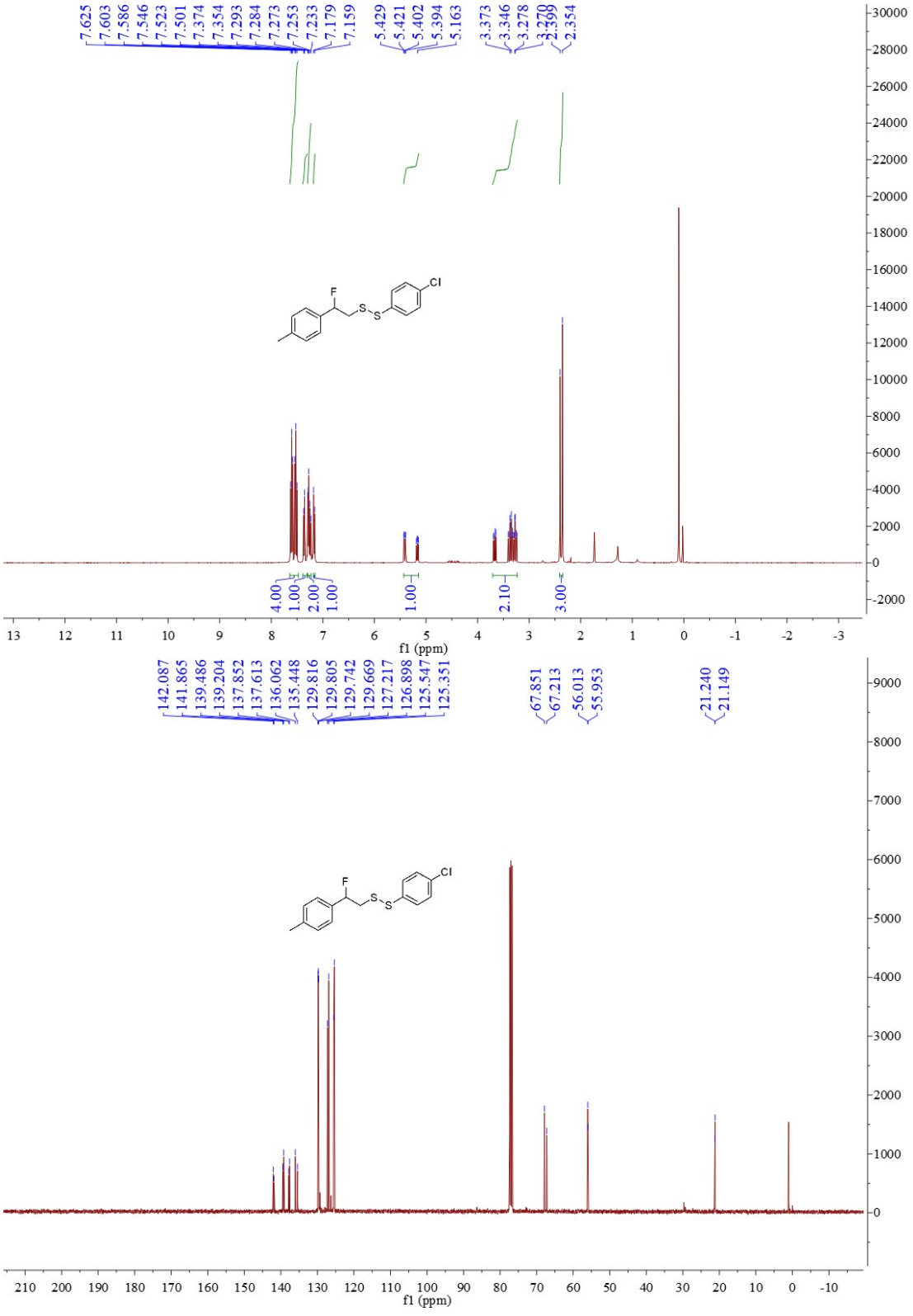
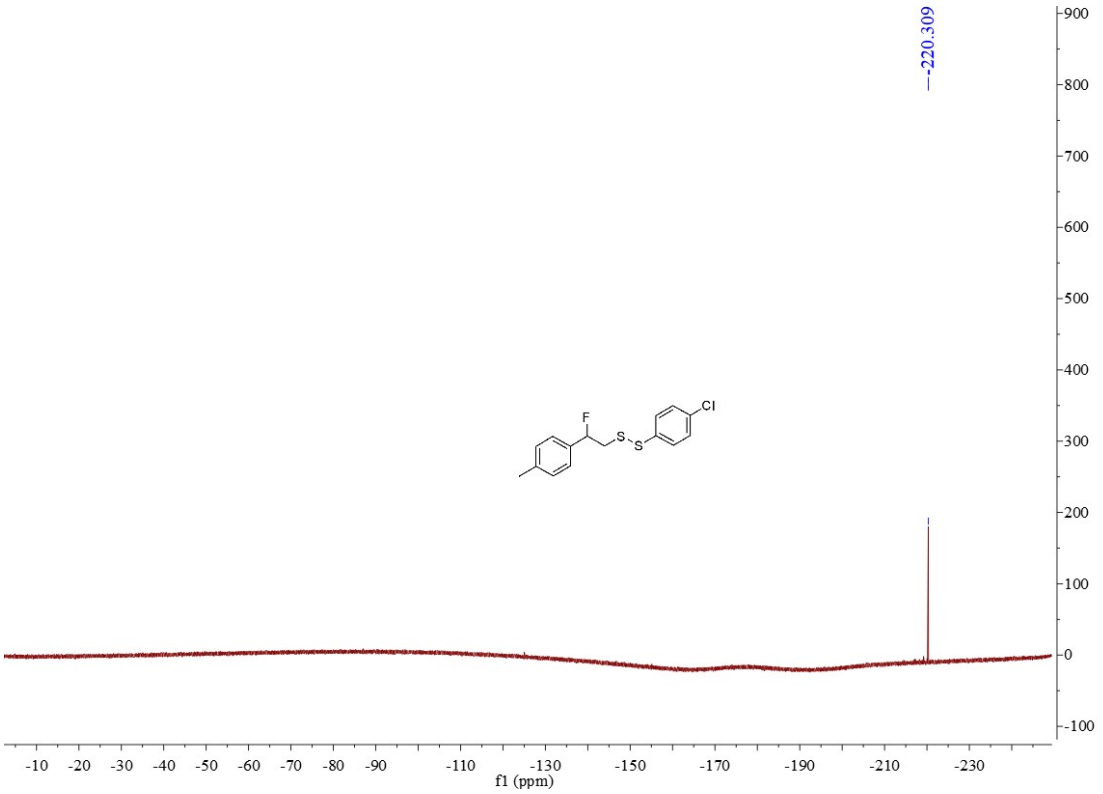
143.100
141.757
141.464
138.073
137.820
131.137
130.837
130.422
130.311
129.908
129.843
127.412
127.076
125.504
125.302
67.566
66.699
55.325
55.050
52.324
52.294
F
S
S
Cl
O
O
f1 (ppm)

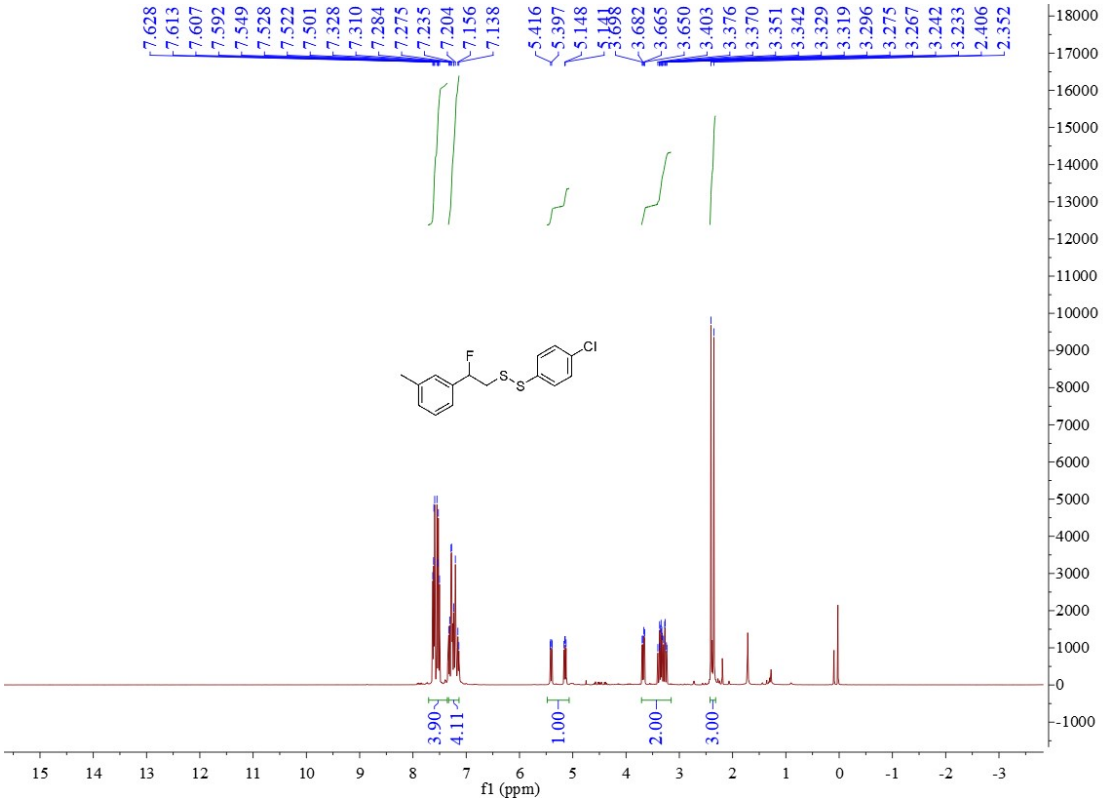

-221.614
F
S
S
Cl
O
O
f1 (ppm)

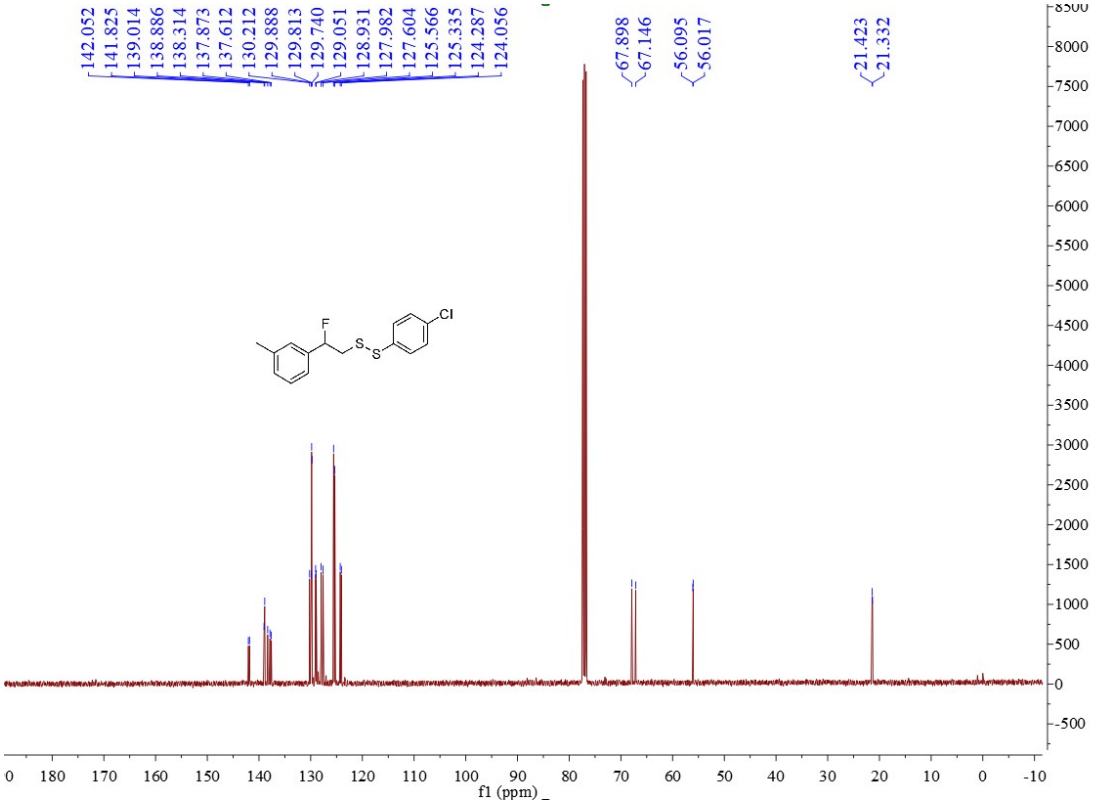
C27

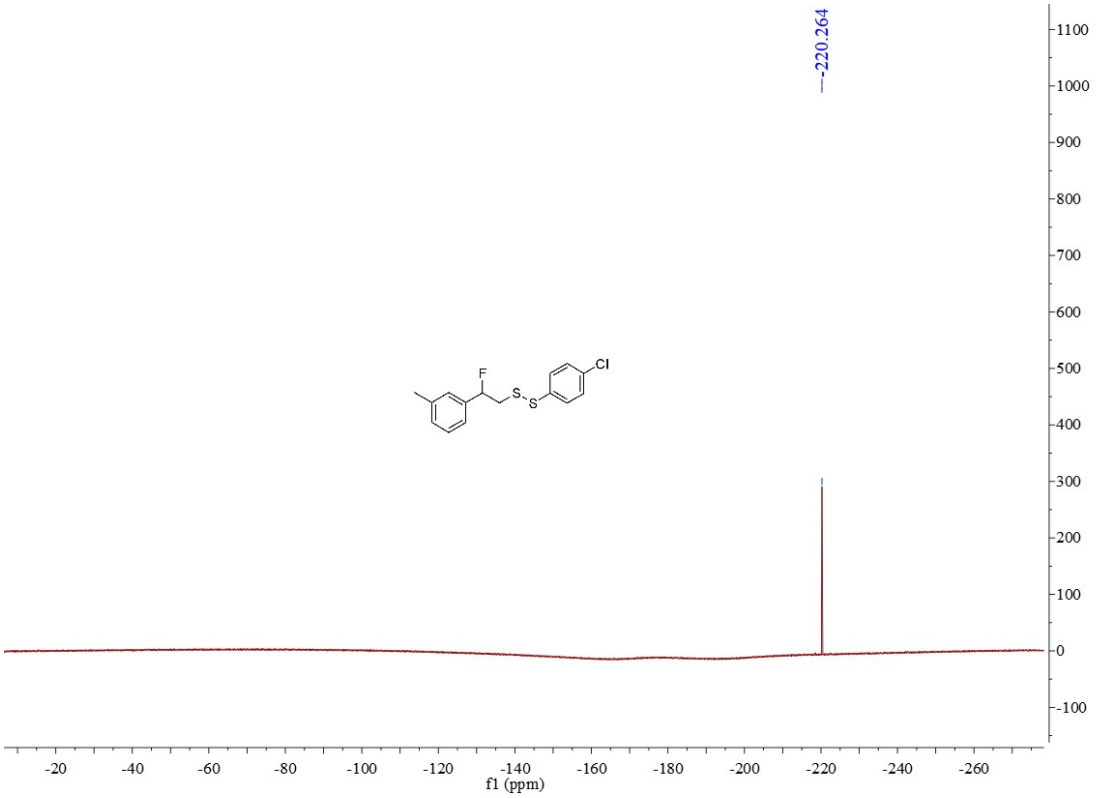

7.625
7.603
7.586
7.546
7.523
7.501
7.374
7.354
7.293
7.284
7.273
7.253
7.233
7.179
7.159
5.429
5.421
5.402
5.394
5.163
3.373
3.346
3.278
3.270
2.368
2.354
F
S
S
Cl
4.00
1.00
2.00
1.00
1.00
2.10
3.00
f1 (ppm)
142.087
141.865
139.486
139.204
137.852
137.613
136.062
135.448
129.816
129.805
129.742
129.669
127.217
126.898
125.547
125.351
67.851
67.213
56.013
55.953
21.240
21.149
f1 (ppm)


-220.309
F
S
S
Cl
f1 (ppm)

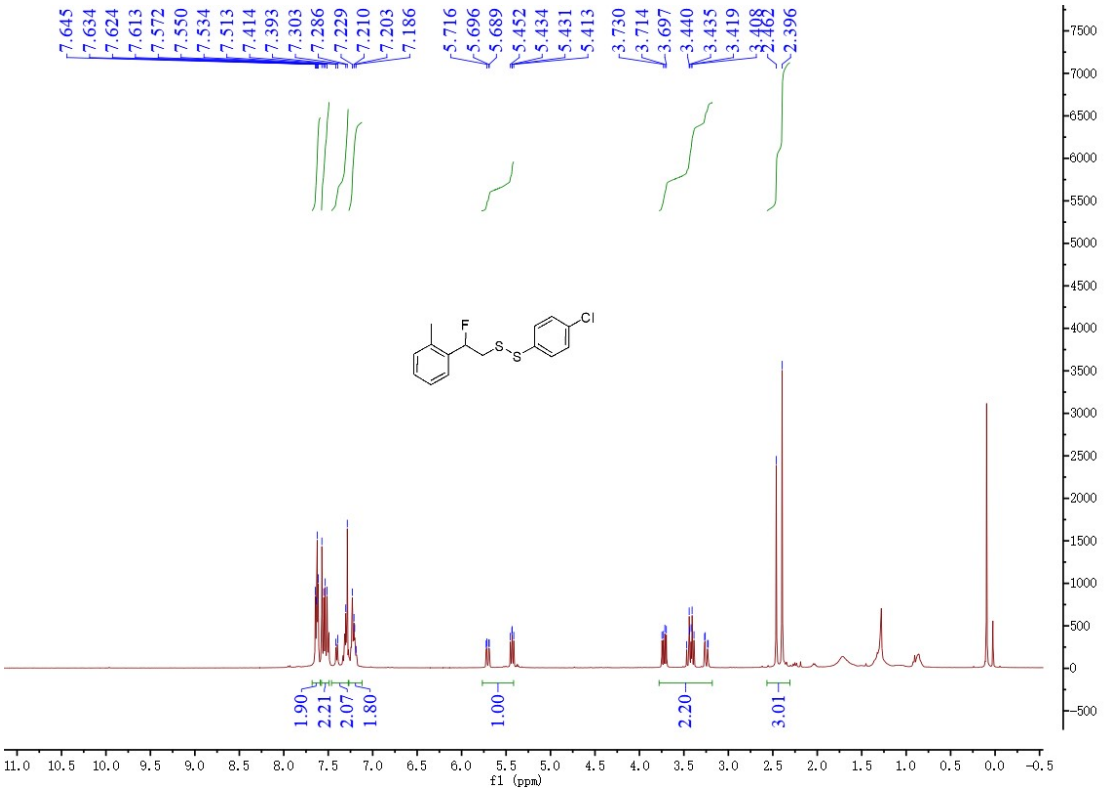
C28

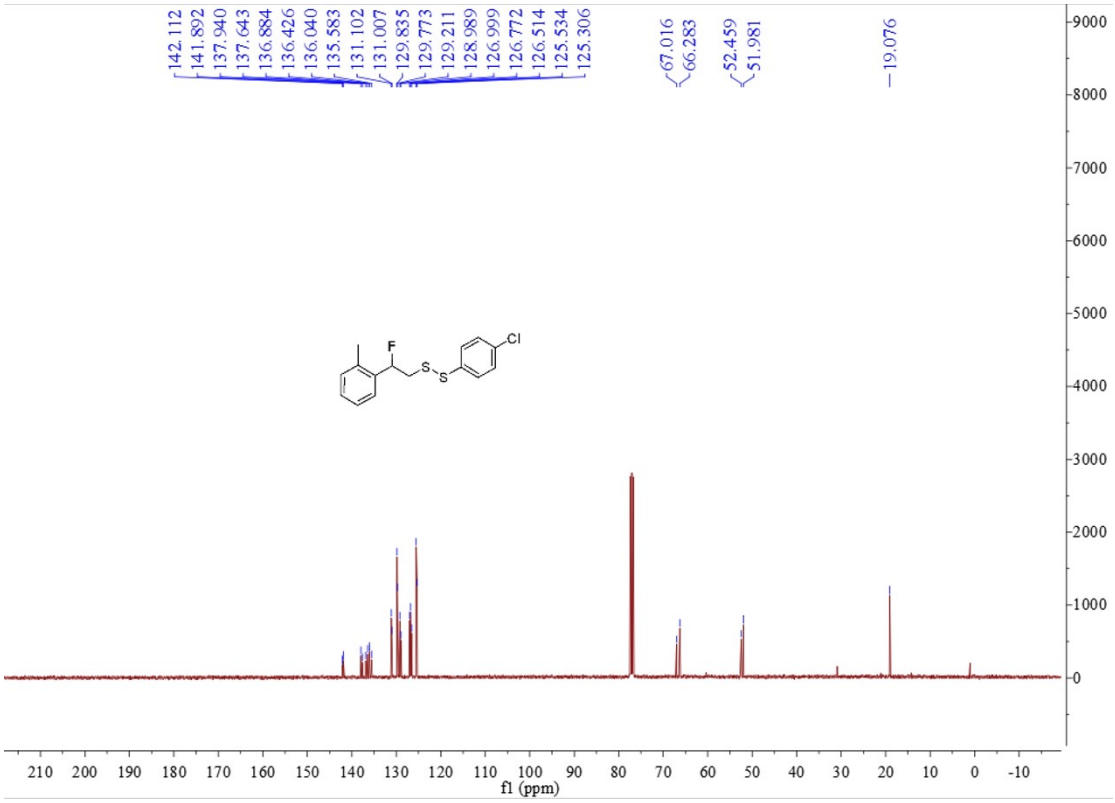

7.628
7.613
7.607
7.592
7.549
7.528
7.522
7.501
7.328
7.310
7.284
7.275
7.235
7.204
7.156
7.138
5.416
5.397
5.148
3.682
3.665
3.650
3.403
3.376
3.370
3.351
3.342
3.329
3.319
3.296
3.275
3.267
3.242
3.233
2.406
2.352
F
S
S
Cl
3.90
4.11
1.00
2.00
3.00
f1 (ppm)

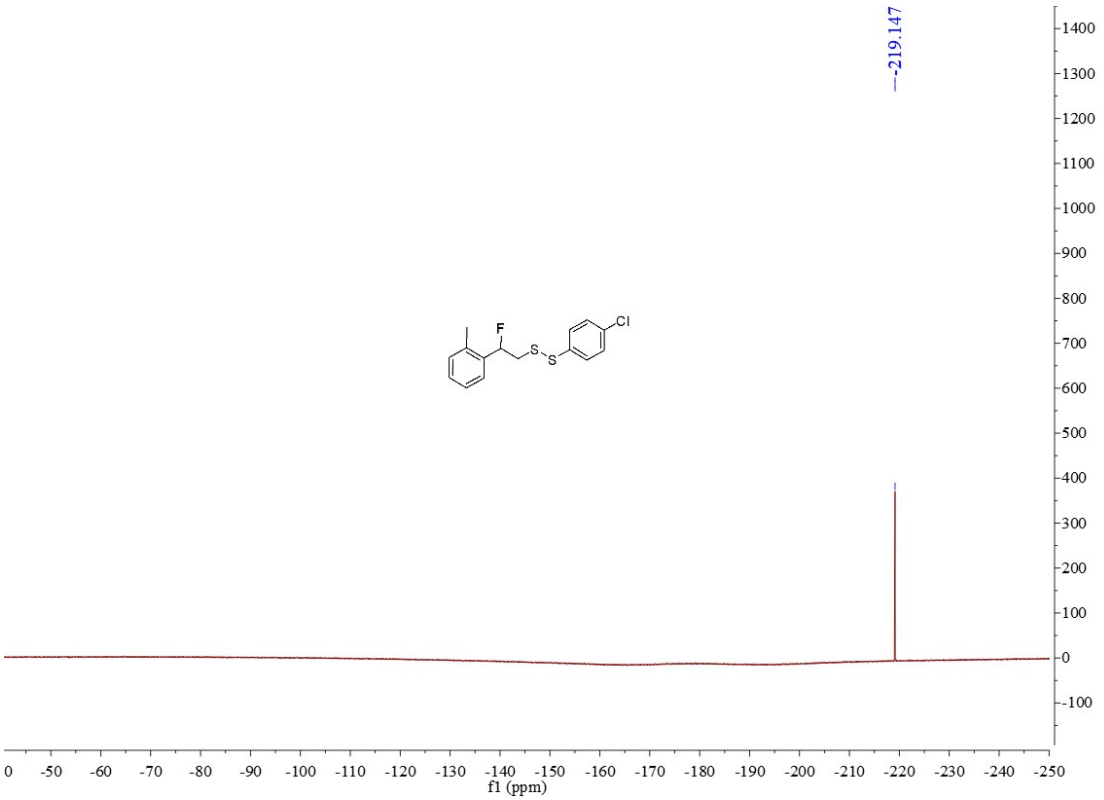

142.052
141.825
139.014
138.886
138.314
137.873
137.612
130.212
129.888
129.813
129.740
129.051
128.931
127.982
127.604
125.566
125.335
124.287
124.056
67.898
67.146
56.095
56.017
21.423
21.332
F
S
S
Cl
f1 (ppm)


-220.264
F
S
S
Cl
f1 (ppm)

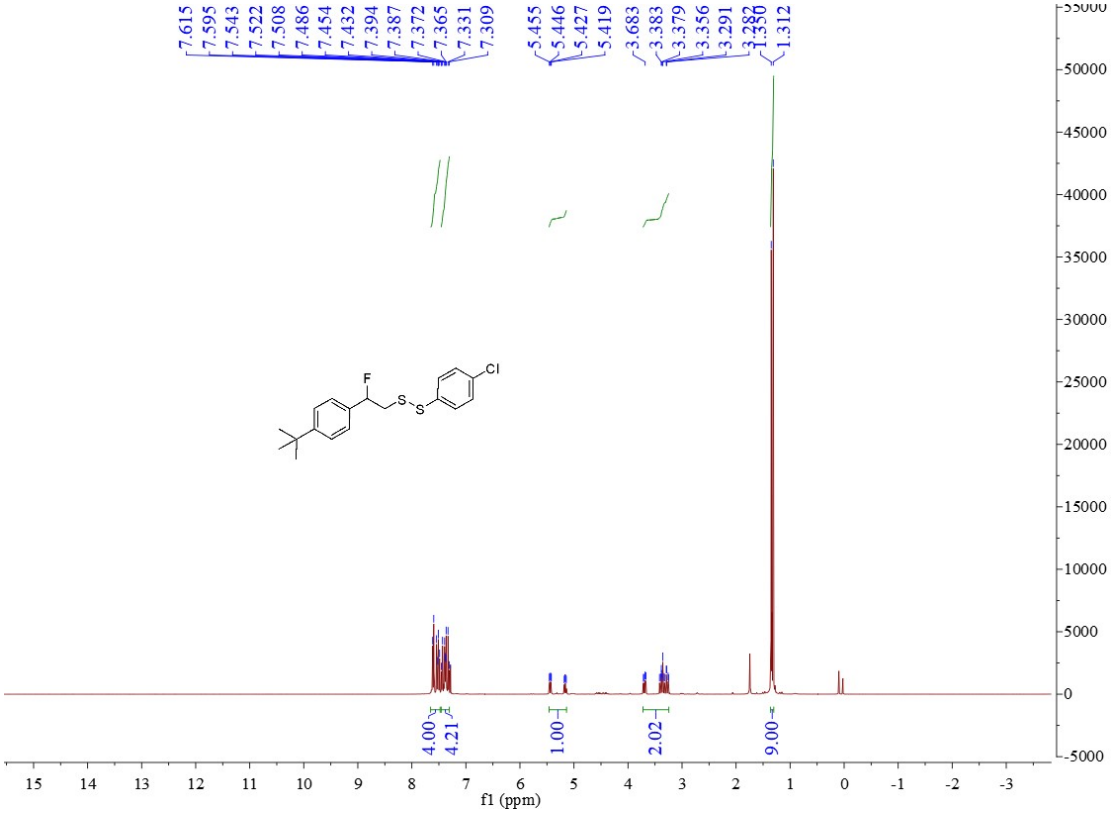
C29

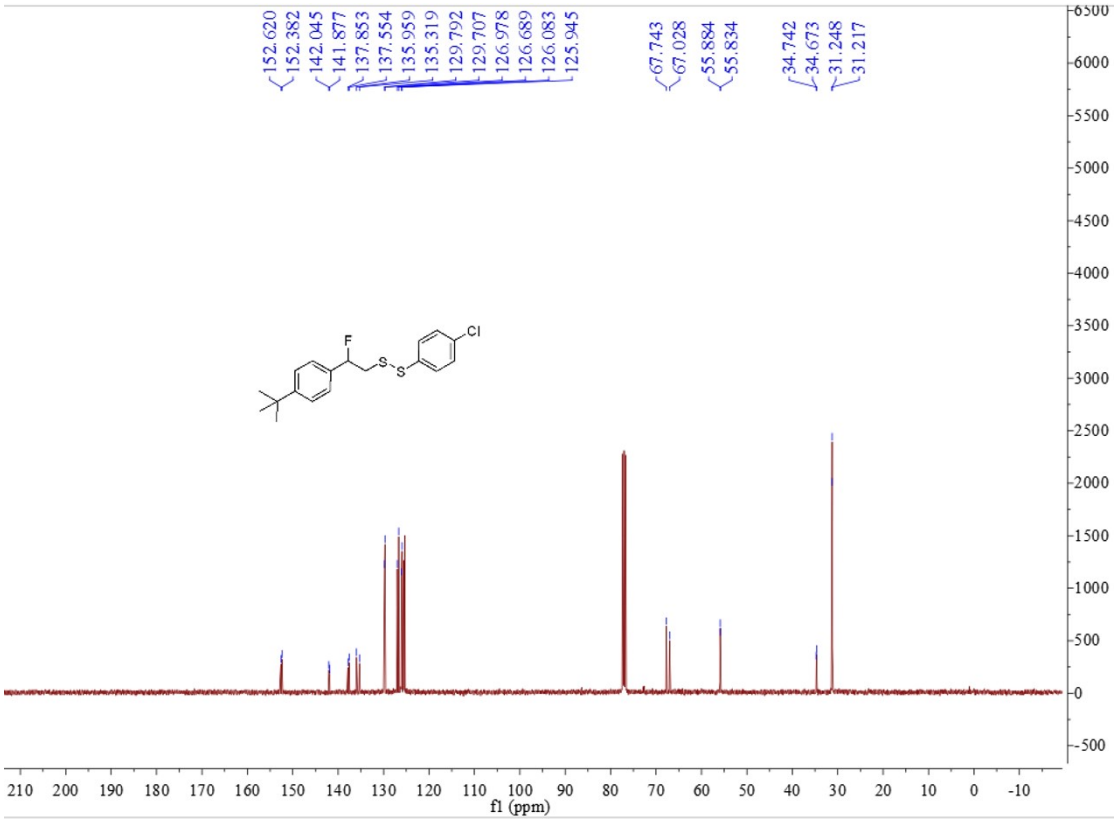

7.645
7.634
7.624
7.613
7.572
7.550
7.534
7.513
7.414
7.393
7.303
7.286
7.229
7.210
7.203
7.186
5.716
5.696
5.689
5.452
5.434
5.431
5.413
3.730
3.714
3.697
3.440
3.435
3.419
3.408
2.462
2.396
F
S
S
Cl
1.90
2.21
2.07
1.80
1.00
2.20
3.01
f1 (ppm)

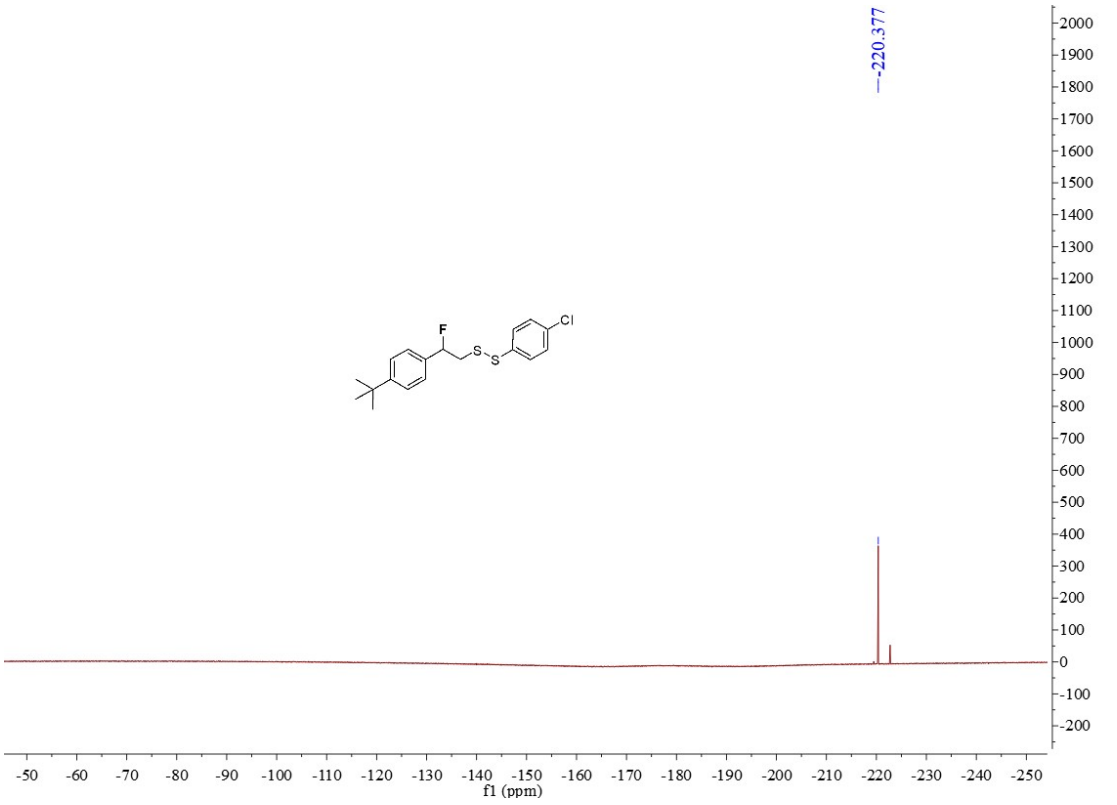

142.112
141.892
137.940
137.643
136.884
136.426
136.040
135.583
131.102
131.007
129.835
129.773
129.211
128.989
126.999
126.772
126.514
125.534
125.306
67.016
66.283
52.459
51.981
19.076
F
S
S
Cl
f1 (ppm)


-219.147
F
S
S
Cl
f1 (ppm)

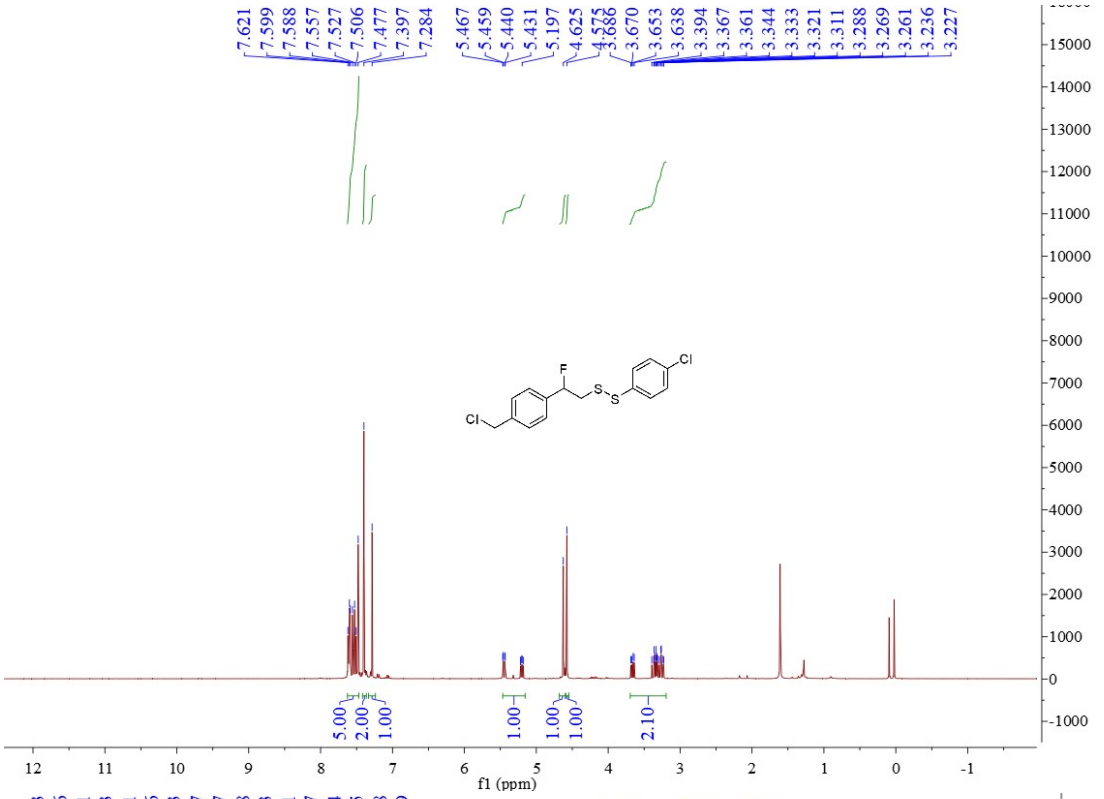
C30

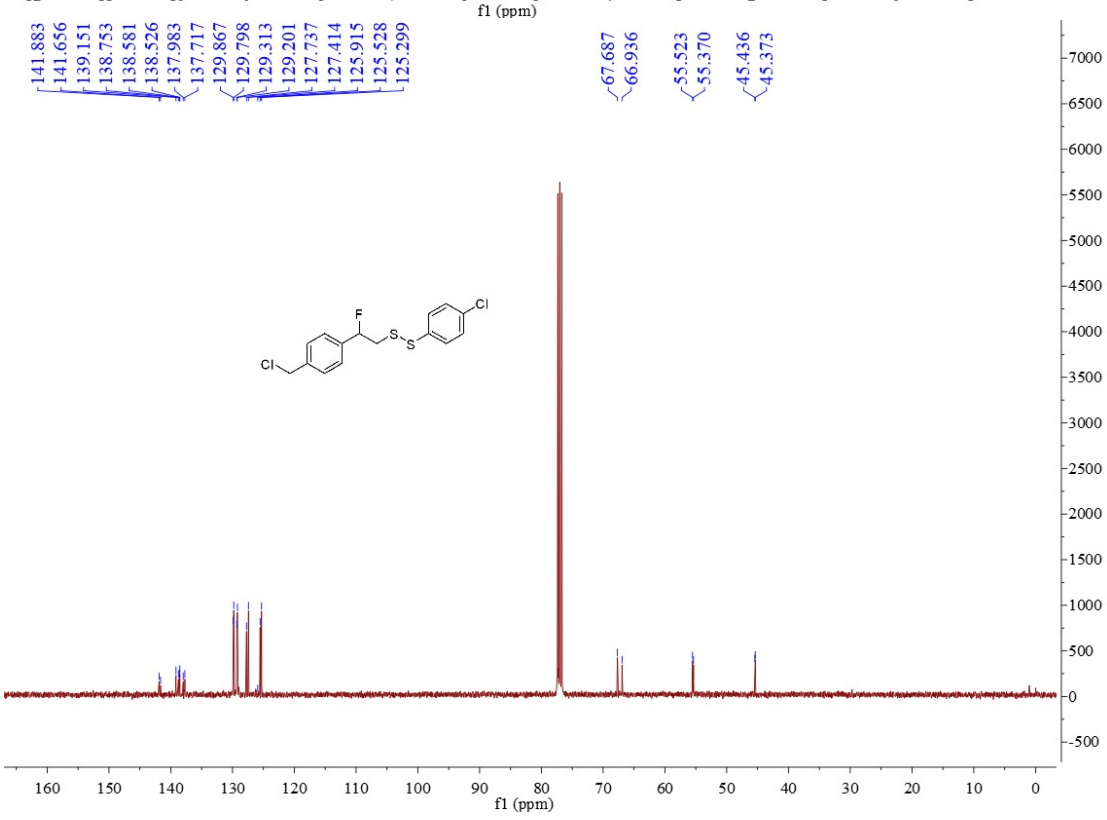

7.615
7.595
7.543
7.522
7.508
7.486
7.454
7.432
7.394
7.387
7.372
7.365
7.331
7.309
5.455
5.446
5.427
5.419
3.683
3.383
3.379
3.356
3.291
1.350
1.312
F
S
S
Cl
4.00
4.21
1.00
2.02
9.00
f1 (ppm)

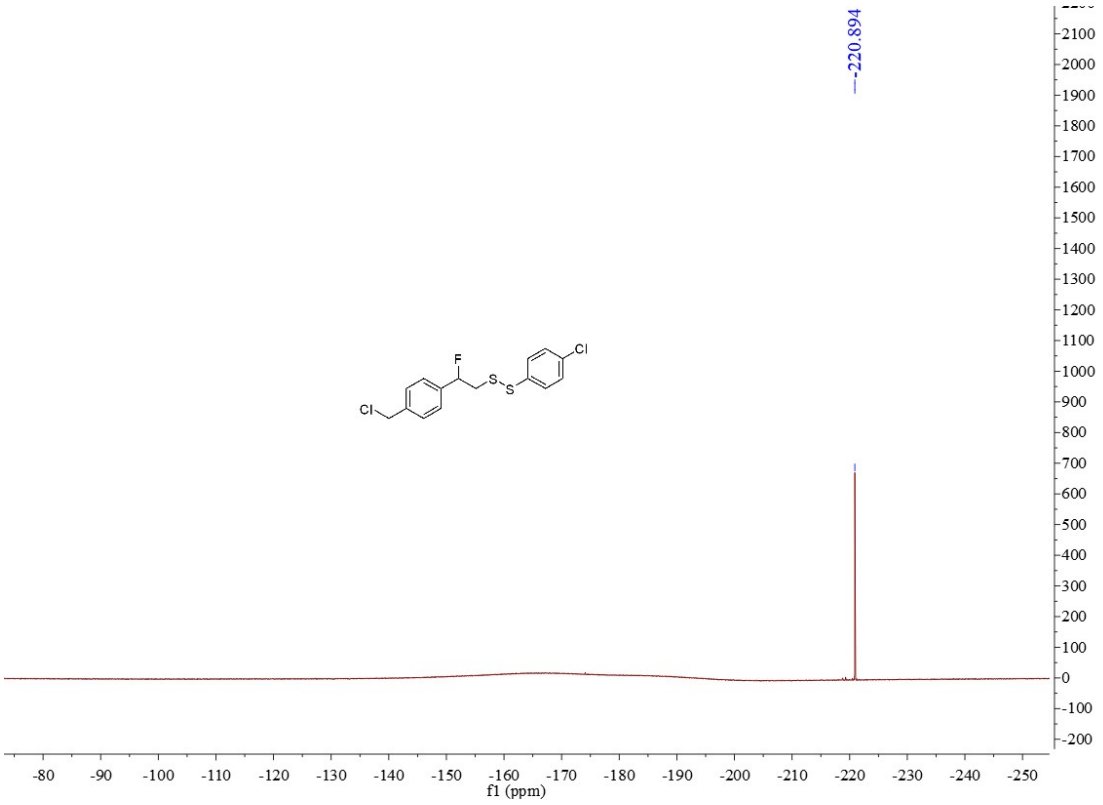

152.620
152.382
142.045
141.877
137.853
137.554
135.959
135.319
129.792
129.707
126.978
126.689
126.083
125.945
67.743
67.028
55.884
55.834
34.742
34.673
31.248
31.217
F
S
S
Cl
f1 (ppm)


-220.377
F
S
S
Cl
f1 (ppm)

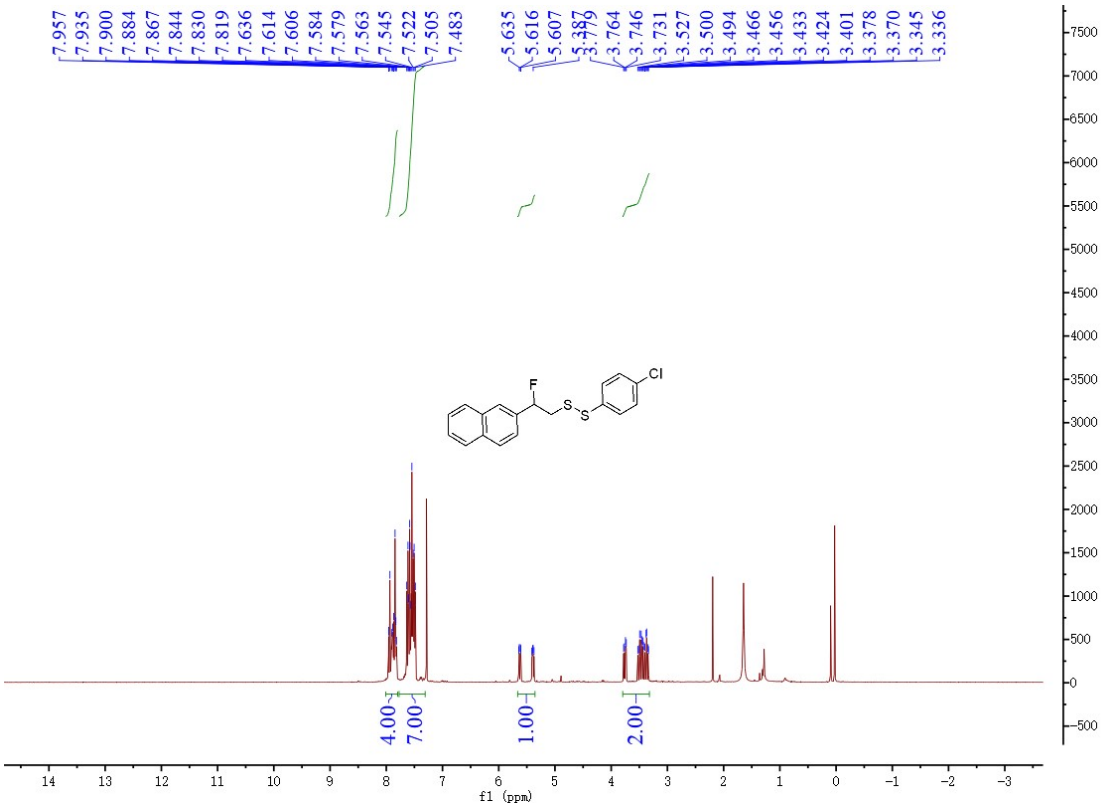
C31

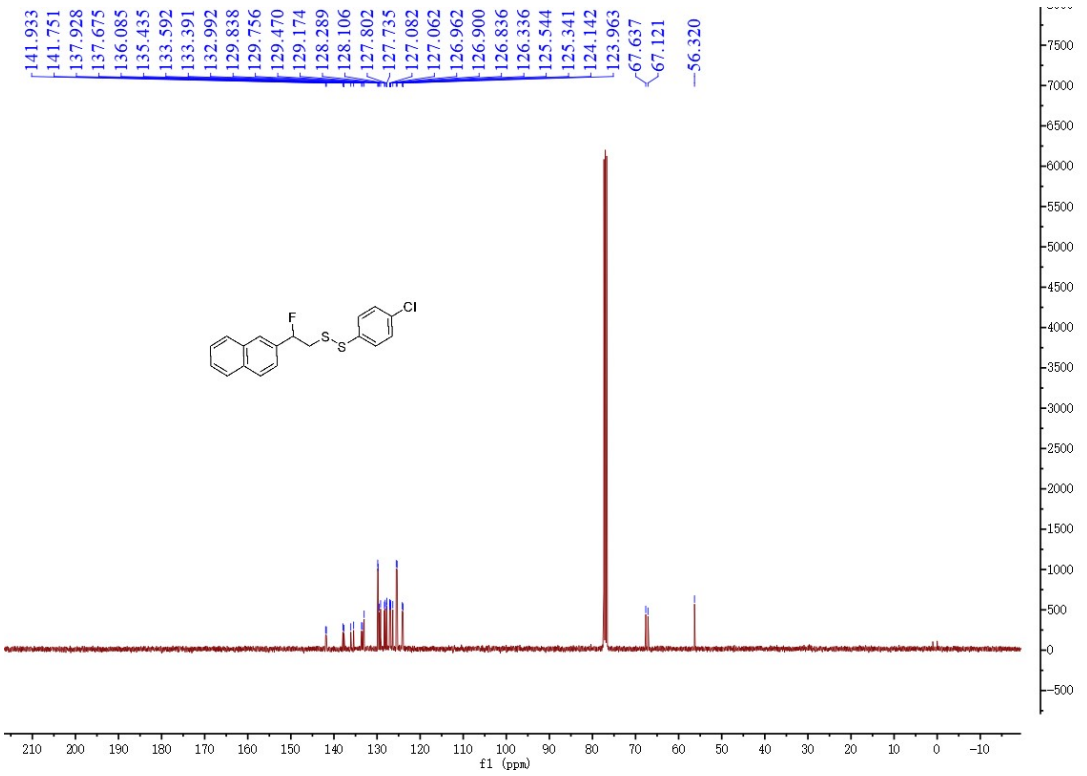

7.621
7.599
7.588
7.557
7.527
7.506
7.477
7.397
7.284
5.467
5.459
5.440
5.431
5.197
4.625
4.575
3.686
3.670
3.653
3.638
3.394
3.367
3.361
3.344
3.333
3.321
3.311
3.288
3.269
3.261
3.236
3.227
F
S
S
Cl
Cl
5.00
2.00
1.00
1.00
1.00
1.00
2.10
f1 (ppm)

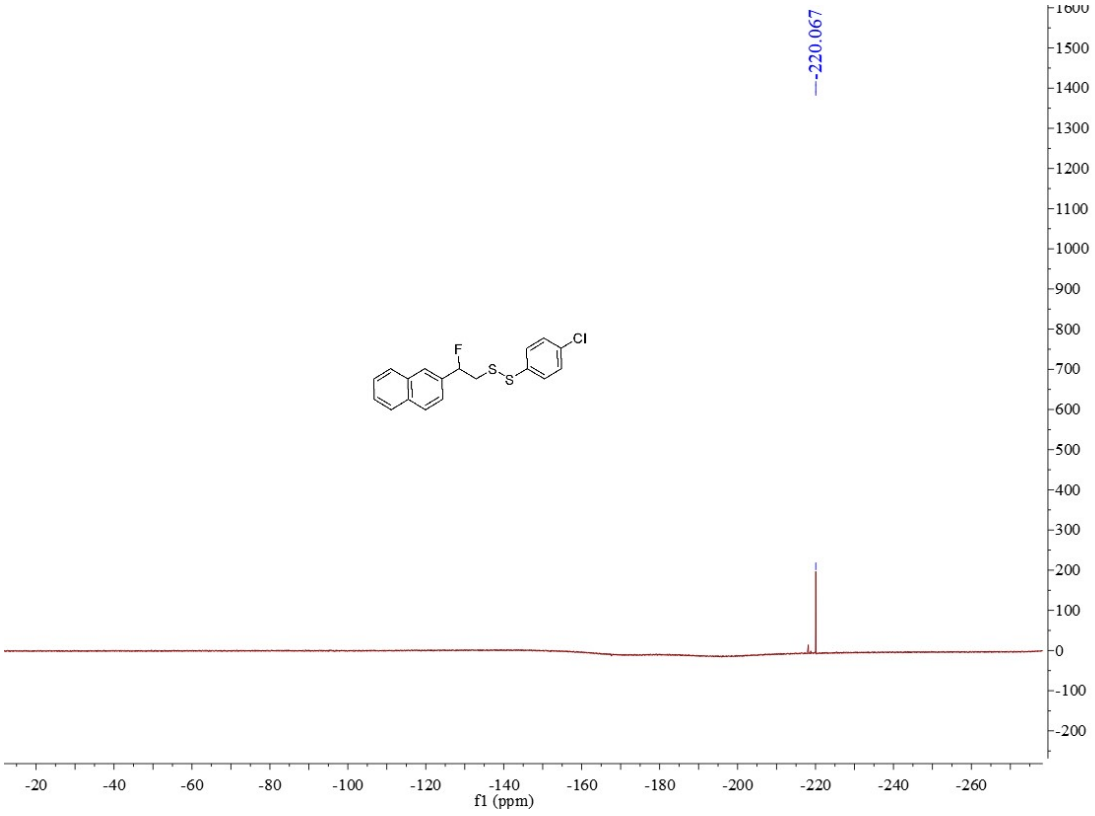

141.883
141.656
139.151
138.753
138.581
138.526
137.983
137.717
129.867
129.798
129.313
129.201
127.737
127.414
125.915
125.528
125.299
67.687
66.936
55.523
55.370
45.436
45.373
F
S
S
Cl
Cl
f1 (ppm)


-220.894
F
S
S
Cl
Cl
f1 (ppm)

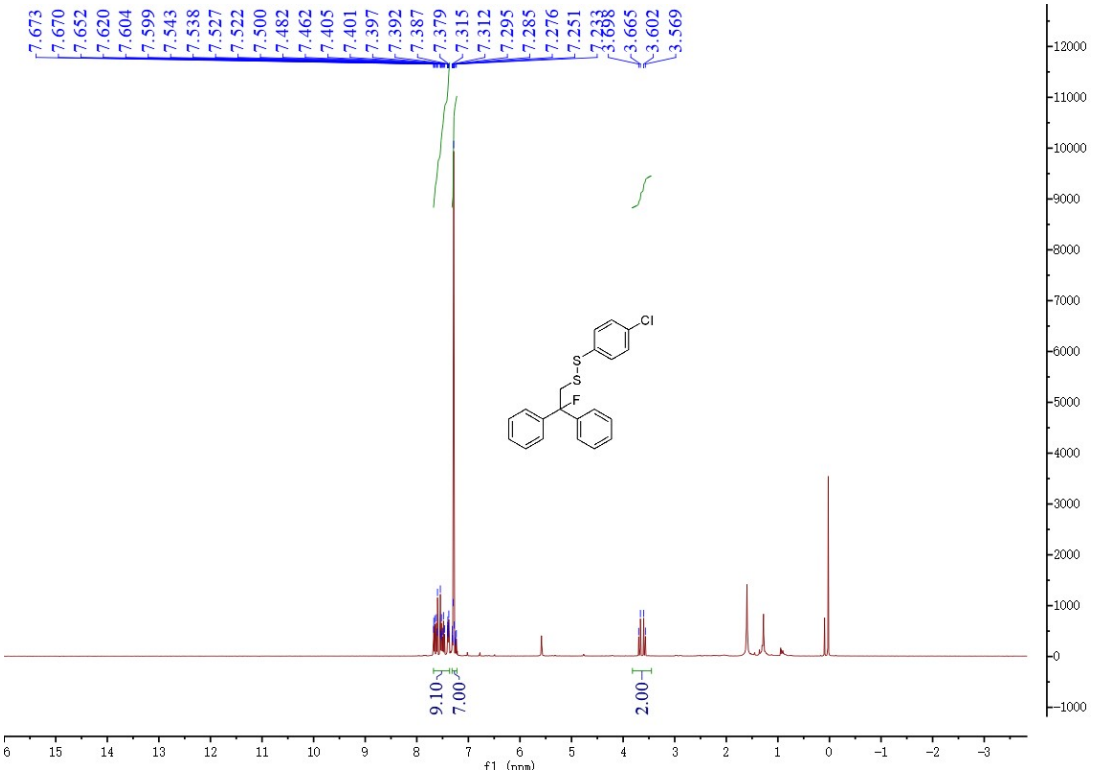
C32

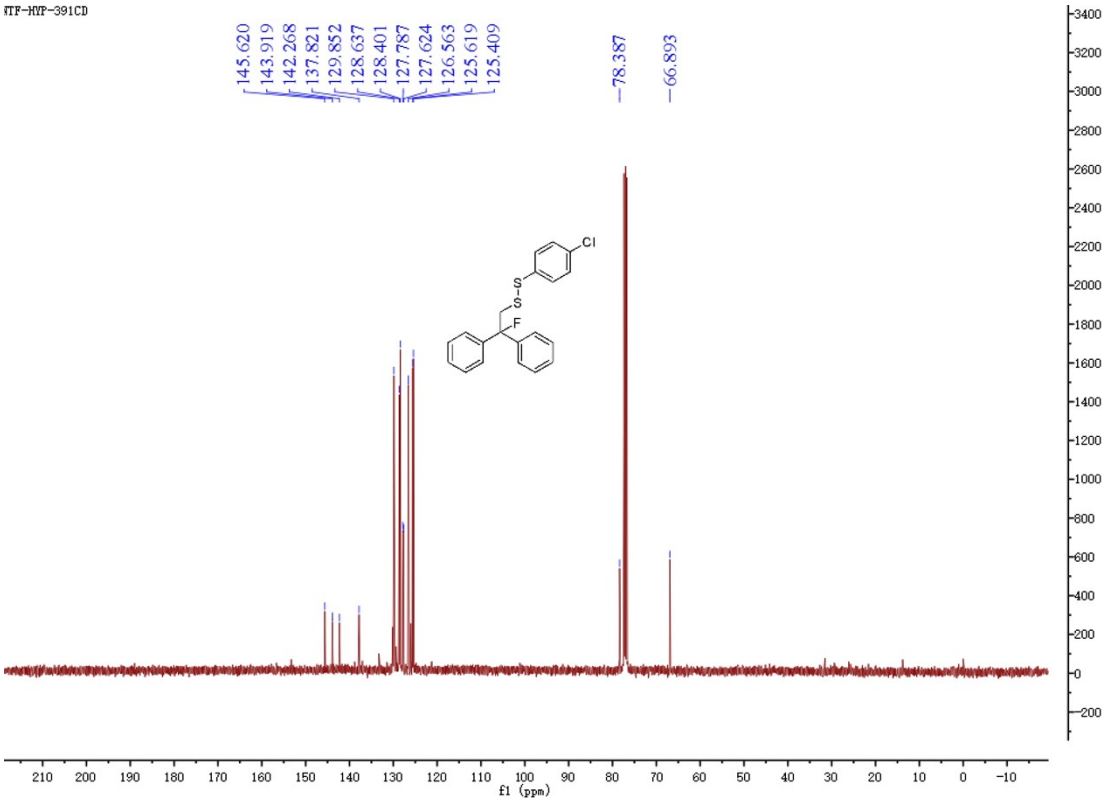

7.957
7.935
7.900
7.884
7.867
7.844
7.830
7.819
7.636
7.614
7.606
7.584
7.579
7.563
7.545
7.522
7.505
7.483
5.635
5.616
5.607
3.764
3.746
3.731
3.527
3.500
3.494
3.466
3.456
3.433
3.424
3.401
3.378
3.370
3.345
3.336
F
S
S
Cl
4.00
7.00
1.00
2.00
f1 (ppm)

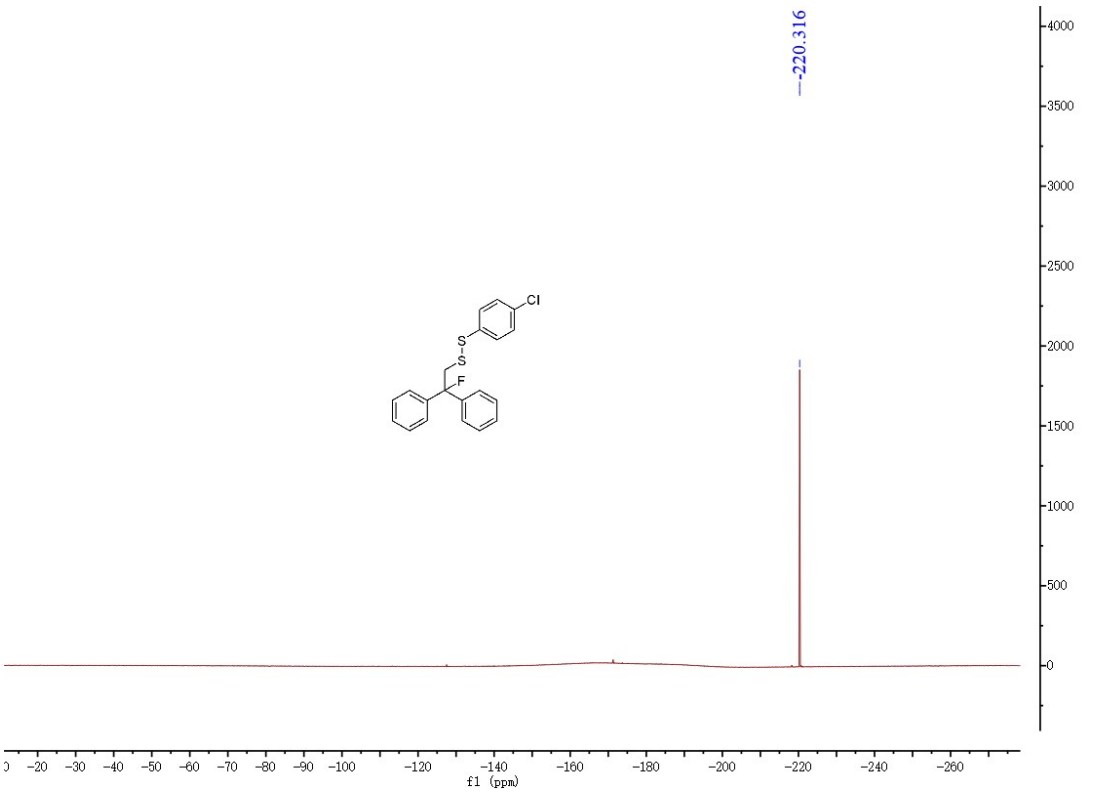

141.933
141.751
137.928
137.675
136.085
135.435
133.592
133.391
132.992
129.838
129.756
129.470
129.174
128.289
128.106
127.802
127.735
127.082
127.062
126.962
126.900
126.836
126.336
125.544
125.341
124.142
123.963
67.637
67.121
56.320
F
S
S
Cl
f1 (ppm)


-220.067
F
S
S
Cl
f1 (ppm)

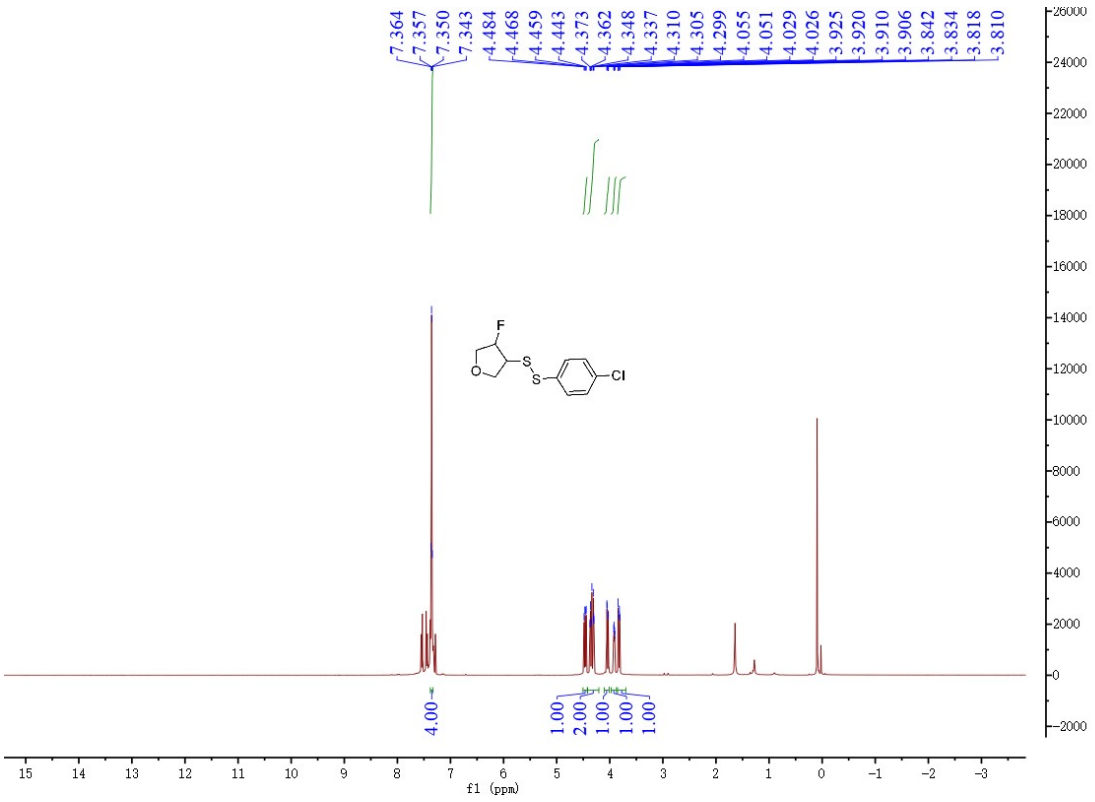
C33

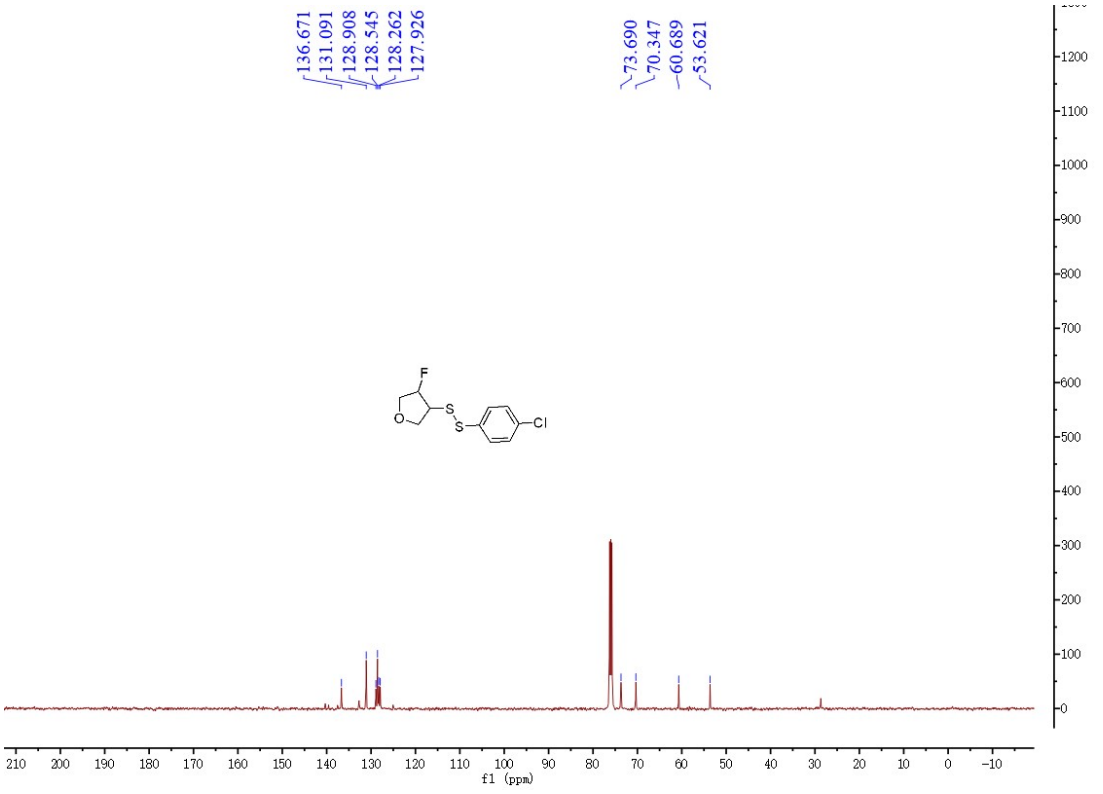

7.673
7.670
7.652
7.620
7.604
7.599
7.543
7.538
7.527
7.522
7.500
7.482
7.462
7.405
7.401
7.397
7.392
7.387
7.379
7.315
7.312
7.295
7.285
7.276
7.251
7.233
3.698
3.665
3.602
3.569
Cl
S
S
F
9.10
7.00
2.00
f1 (ppm)

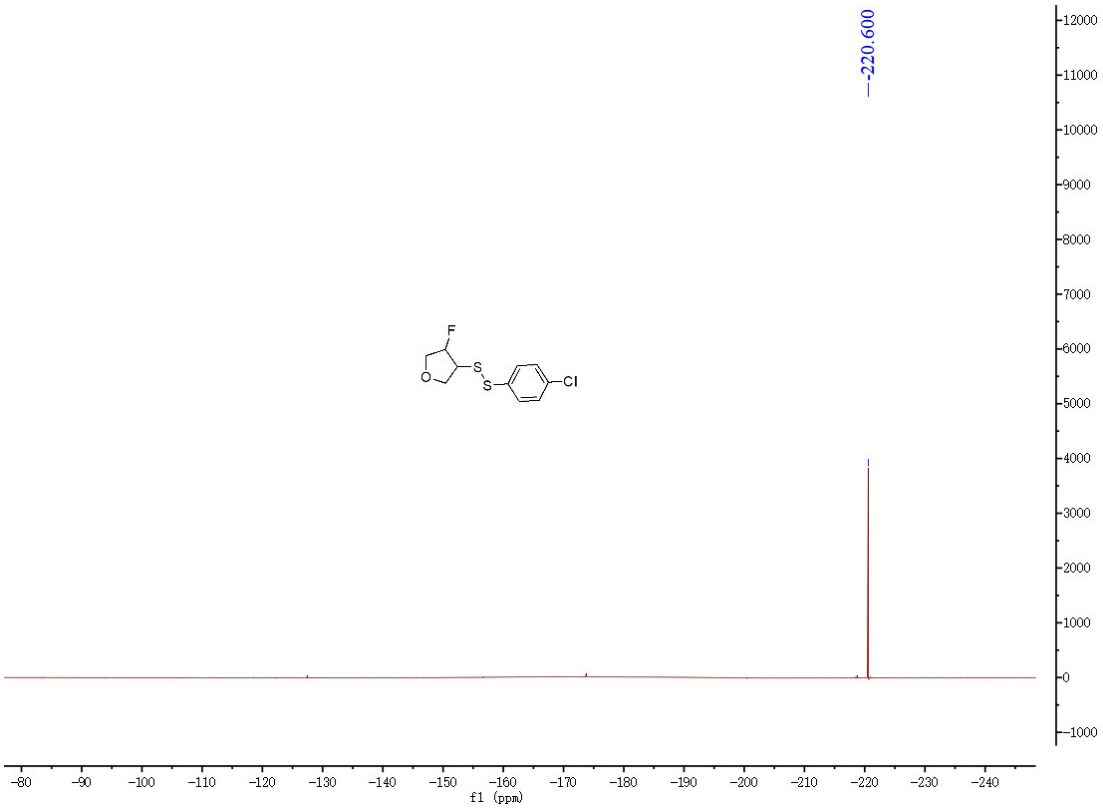

MTF-MYP-391CD
145.620
143.919
142.268
137.821
129.852
128.637
128.401
127.787
127.624
126.563
125.619
125.409
78.387
66.893
Cl
S
S
F
f1 (ppm)


-220.316
Cl
S
S
F
f1 (ppm)

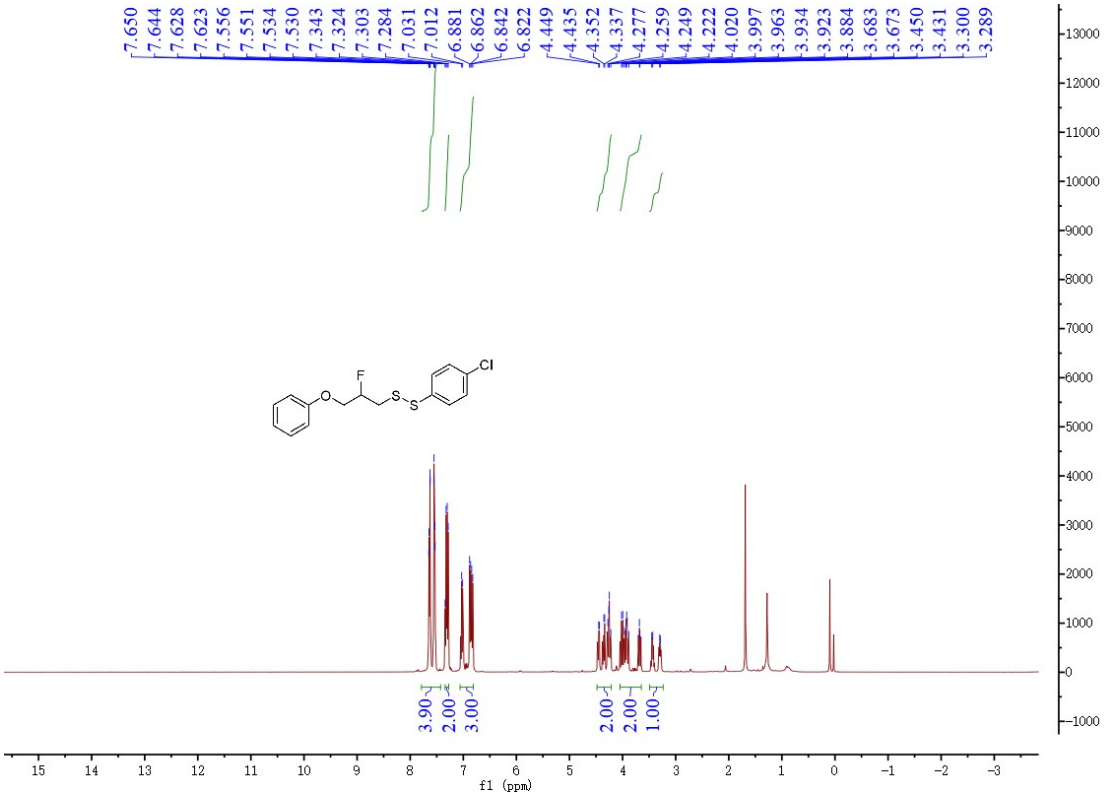
C34

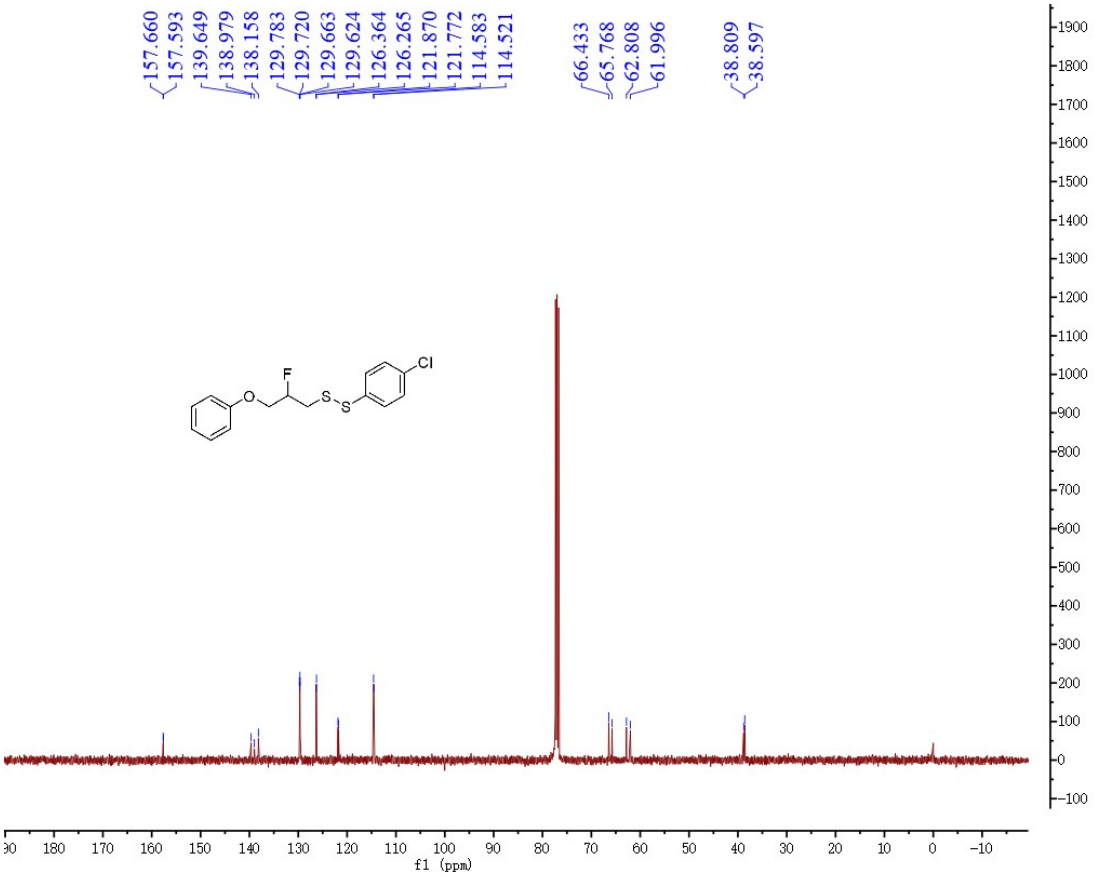

7.364
7.357
7.350
7.343
4.484
4.468
4.459
4.443
4.373
4.362
4.348
4.337
4.310
4.305
4.299
4.055
4.051
4.029
4.026
3.925
3.920
3.910
3.906
3.842
3.834
3.818
3.810
F
O
S
S
Cl
4.00
1.00
2.00
1.00
1.00
1.00
f1 (ppm)

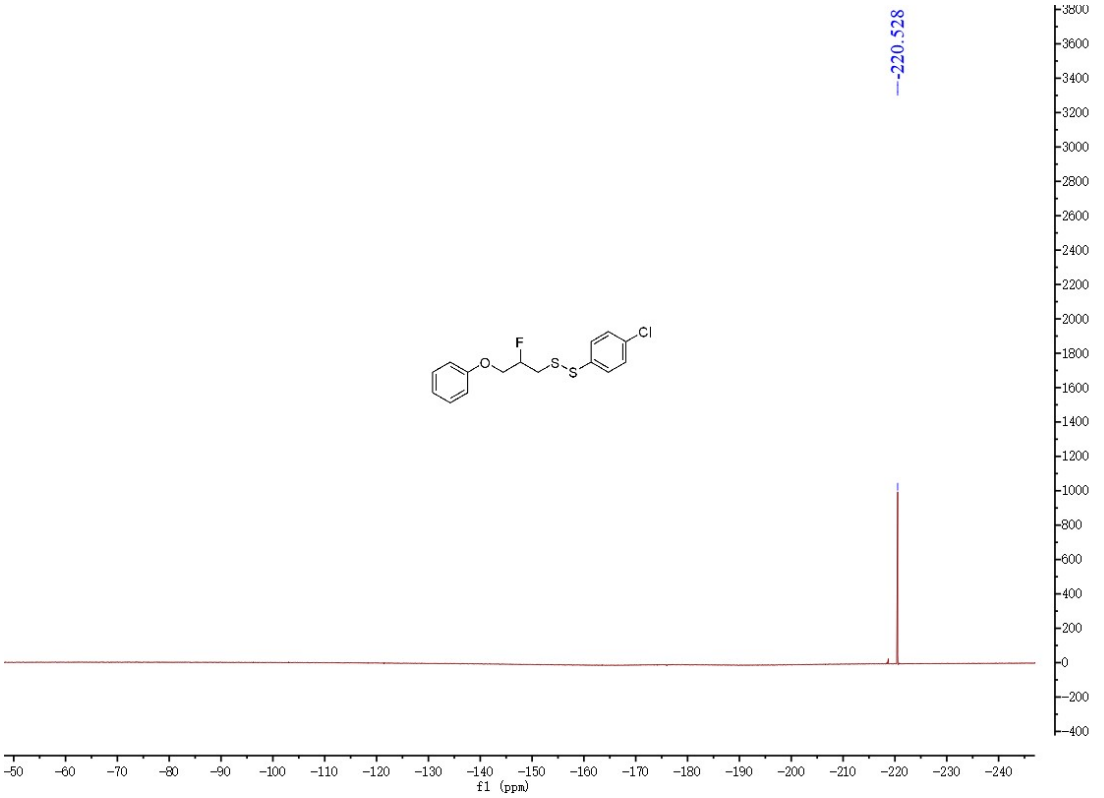

136.671
131.091
128.908
128.545
128.262
127.926
73.690
70.347
60.689
53.621
F
O
S
S
Cl
f1 (ppm)


-220.600
F
O
S
S
Cl
f1 (ppm)

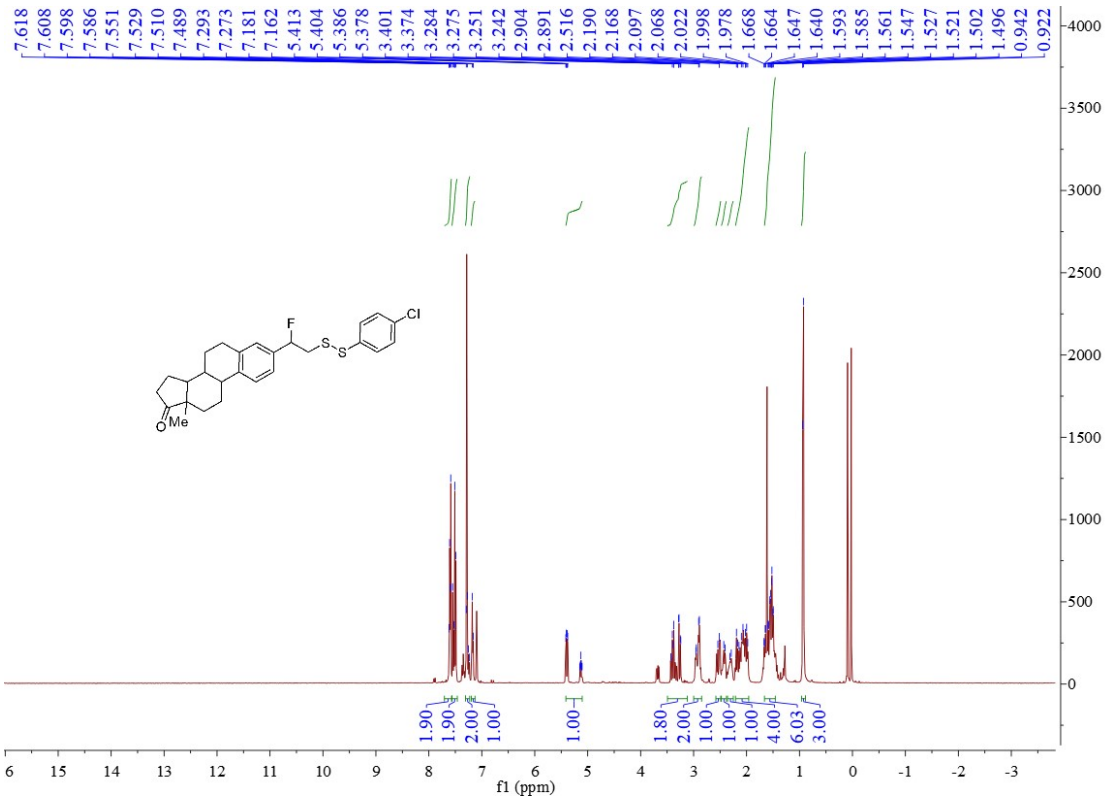
C35

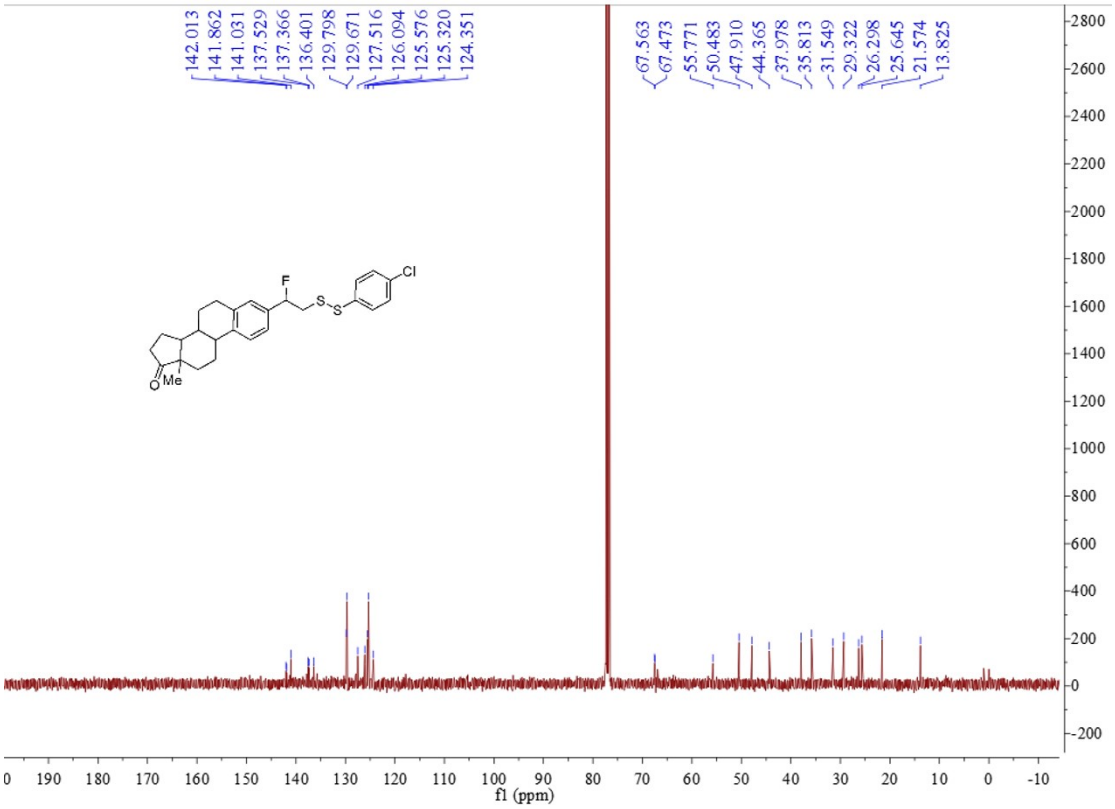

7.650
7.644
7.628
7.623
7.556
7.551
7.534
7.530
7.343
7.324
7.303
7.284
7.031
7.012
6.881
6.862
6.842
6.822
4.449
4.435
4.352
4.337
4.277
4.259
4.249
4.222
4.020
3.997
3.963
3.934
3.923
3.884
3.683
3.673
3.450
3.431
3.300
3.289
F
O
S
S
Cl
3.90
2.00
3.00
2.00
2.00
1.00
f1 (ppm)

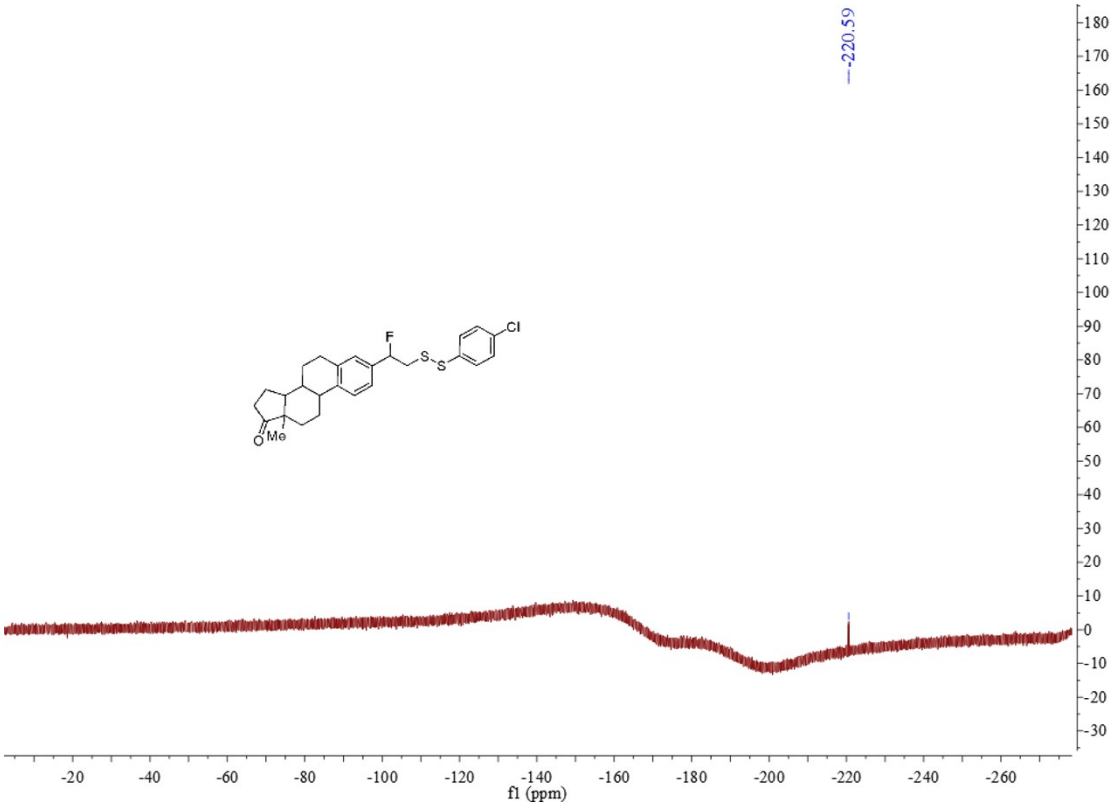

157.660
157.593
139.649
138.979
138.158
129.783
129.720
129.663
129.624
126.364
126.265
121.870
121.772
114.583
114.521
66.433
65.768
62.808
61.996
38.809
38.597
F
O
S
S
Cl
f1 (ppm)


-220.528
F
O
S
S
Cl
f1 (ppm)

C36


7.618
7.608
7.598
7.586
7.551
7.529
7.510
7.489
7.293
7.273
7.181
7.162
5.413
5.404
5.386
5.378
3.401
3.374
3.284
3.275
3.251
3.242
2.904
2.891
2.516
2.190
2.168
2.097
2.068
2.022
1.998
1.978
1.668
1.664
1.647
1.640
1.593
1.585
1.561
1.547
1.527
1.521
1.502
1.496
0.942
0.922
F
S
S
Cl
O
Me
1.90
1.90
2.00
1.00
1.00
1.80
2.00
1.00
1.00
1.00
4.00
6.03
3.00
f1 (ppm)


142.013
141.862
141.031
137.529
137.366
136.401
129.798
129.671
127.516
126.094
125.576
125.320
124.351
67.563
67.473
55.771
50.483
47.910
44.365
37.978
35.813
31.549
29.322
26.298
25.645
21.574
13.825
F
S
S
Cl
O
Me
fl (ppm)


-220.59
F
S
S
Cl
O
Me
fl (ppm)