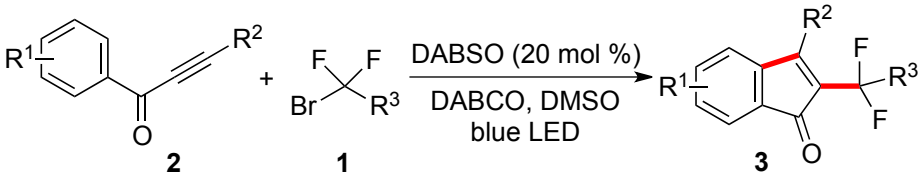
Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

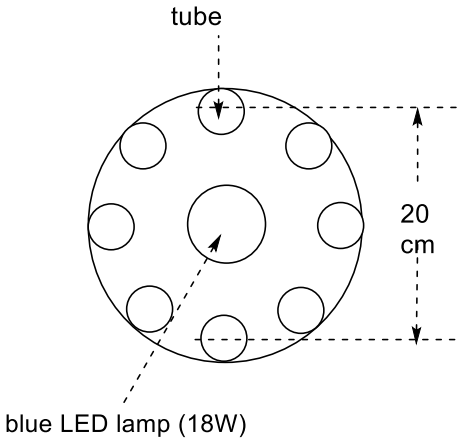
General experimental methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32-63 μm, standard grade). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25 mm 230-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25-35 °C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H NMR, ^{19}F NRM and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX - 400 Spectrometer operating at 400 MHz、376 MHz and 100 MHz respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

*General experimental procedure for the DABCO·$(SO_2)_2$-catalyzed radical cyclization of 1,3-diarylprop-2-yn-1-ones **2** with difluoroalkyl halides **1**:*



In a glass tube, 1,3-Diarylprop-2-yn-1-one **2** (0.2 mmol) was combined with DABCO·$(SO_2)_2$ (0.04 mmol, 20 mol %). The tube was evacuated and backfilled with N_2 three times before the addition of DMSO (3.0 mL). Subsequently, the difluoroalkyl halide **1** (0.26 mmol) was added to the solution. Then, the mixture was stirred under blue LED irradiation (18 W) for 18 hours at room temperature. After completion of reaction as indicated by TLC, the mixture was washed with EtOAc and brine. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate three times. The combined organic phases were dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo, and the residue was purified by flash column chromatography (EtOAc/*n*-hexane, 1:16) to provide the desired product **3**.

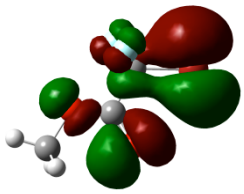
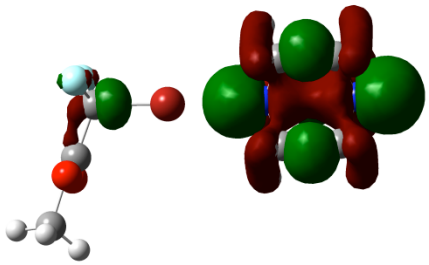
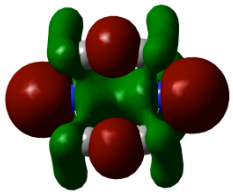
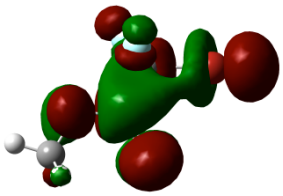
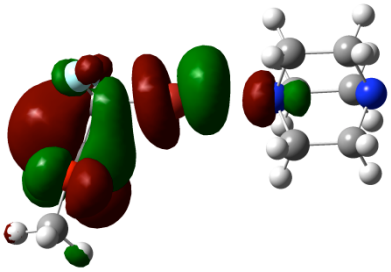
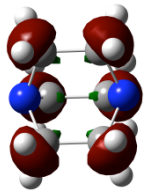


Computational details

The B3LYP density functional theory calculations were performed with the Gaussian09 package using 6-31+G(d,p) basis set.[1-2] Structures were optimized with Truhlar and coworkers' SMD solvation model[3] in dimethylsulfoxide solution. The geometry optimizations were performed without symmetry constraints, and the nature of the extrema was checked by analytical frequency calculations. The intrinsic reaction coordinate (IRC)[4] pathways have been traced to verify two desired minima connected by the transition states.

In this study, for the reaction is a two-state reaction,[5] the minimum energy crossing point (MECP) between potential energy surface (PES) of different spin states must be located to calculate the reaction barrier. In the present work, the MECPs were located with the code developed by Harvey and co-workers[6] at B3LYP/6-31+g(d,p) level in dimethylsulfoxide solution.

Table S1. HOMO, LUMO energies calculated for **R1**, **R2'** and **COM'**

R1	COM'	R2'
		
HOMO (-8.45 eV)	HOMO(-5.33 eV)	HOMO (-5.12 eV)
		
LUMO(-1.36 eV)	LUMO (-1.33 eV)	LUMO(0.37 eV)

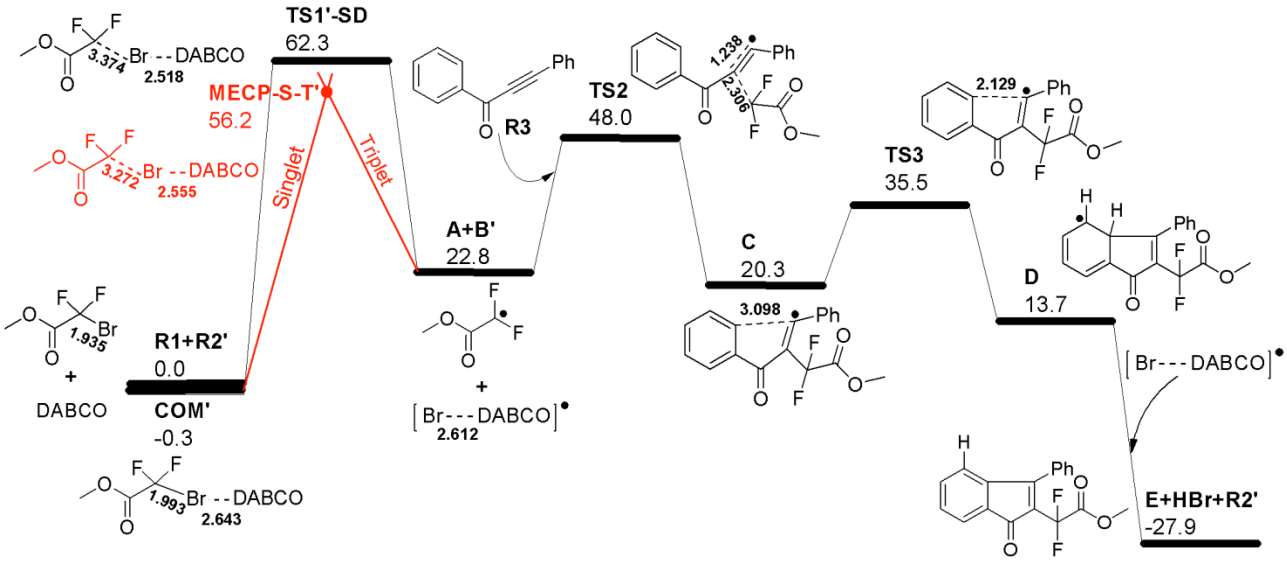


Figure S1. Free-energy reaction profile (kcal mol^{-1}) for the title reaction promoted by DABCO, calculated at the SMD (Dimethylsulfoxide) B3LYP/6-31+G(d, p) level.

Table S2. Coordinate data sets and absolute energies for DFT optimized complexes at B3LYP/6-311++G(d,p).

R1 **-7782.9605851 a.u.**

Br	-1.896432	-2.184014	1.237699
C	-0.348021	-1.038740	1.051631
C	-0.375593	-0.192118	-0.253206
F	-0.290182	-0.197281	2.118042
F	0.773266	-1.801682	1.081801
O	-1.317391	-0.154600	-1.010131
O	0.767735	0.462565	-0.365470
C	0.905323	1.328201	-1.527058
H	1.895329	1.769778	-1.433378
H	0.133812	2.099354	-1.505879
H	0.829926	0.735696	-2.440029

R2 **-893.83956 a.u.**

S	-3.488283	-0.093061	-0.444590
O	-3.872851	-0.854430	0.780823
O	-3.706172	1.379797	-0.333266
N	1.260357	-0.142107	0.194450
C	0.753048	-1.522258	0.128046
C	-0.795789	-1.527663	-0.100602
N	-1.264137	-0.120841	-0.161631
C	-0.950858	0.570056	1.110947
C	0.602548	0.557533	1.309588
C	-0.610240	0.584585	-1.291512
C	0.938652	0.550149	-1.063456
H	1.005792	-2.031310	1.062327
H	1.262864	-2.043815	-0.686810
H	-1.328734	-2.023871	0.713702
H	-1.068879	-2.016421	-1.039789
H	-1.347879	1.586137	1.048225
H	-1.470724	0.043954	1.915438
H	0.991268	1.578429	1.358724
H	0.865697	0.052678	2.243209
H	-0.997424	1.605785	-1.318482
H	-0.897913	0.081946	-2.218784
H	1.436684	0.028104	-1.885216
H	1.342337	1.565341	-1.016615

COM **-1660.8057727 a.u.**

Br	0.372970	3.013116	2.190117
C	0.078920	4.947167	1.860480
C	1.400704	5.716319	2.033242
F	-0.443573	5.123000	0.618282
F	-0.831913	5.417457	2.748204
O	1.726488	6.203365	3.094084
O	2.100199	5.713910	0.909044
C	3.409699	6.340943	0.958652
H	3.830207	6.197403	-0.034703
H	4.027433	5.852491	1.714132
H	3.304240	7.403992	1.181123
S	1.683408	-4.239828	3.692827
O	3.044746	-4.074062	4.280013
O	0.607003	-4.438130	4.706436
N	1.271363	-2.077280	3.200934
C	2.249958	-1.606288	2.191289
C	1.960371	-0.099428	1.889157
N	0.810650	0.367544	2.684183
C	-0.373174	-0.442574	2.345949
C	-0.108030	-1.948594	2.673122
C	1.112942	0.211217	4.118191
C	1.412534	-1.288294	4.446845
H	2.142732	-2.227092	1.298206
H	3.252730	-1.753942	2.598097
H	1.733505	0.047834	0.829978
H	2.827058	0.519387	2.136272
H	-1.227406	-0.067430	2.915596
H	-0.592122	-0.309161	1.283309
H	-0.795499	-2.328054	3.432236

H	-0.193287	-2.578544	1.783910
H	0.256332	0.571218	4.694019
H	1.972125	0.840977	4.363708
H	2.429976	-1.427573	4.819750
H	0.713806	-1.692196	5.183489

R3 -652.678729 a.u.

C	-4.228605	2.825463	1.045979
C	-3.594000	3.932703	0.469439
C	-2.361702	3.780110	-0.160254
C	-1.749123	2.516006	-0.219070
C	-2.390359	1.409658	0.363098
C	-3.625774	1.565514	0.991834
C	-0.432016	2.384561	-0.902374
C	0.188859	1.082518	-0.940835
O	0.133880	3.349623	-1.431718
C	0.766162	0.011385	-1.011625
C	1.436287	-1.242217	-1.093425
C	2.675379	-1.341646	-1.761190
C	3.326560	-2.570193	-1.843001
C	2.755748	-3.708509	-1.263573
C	1.527972	-3.617908	-0.598843
C	0.867395	-2.394807	-0.511058
H	-5.190172	2.945940	1.536112
H	-4.062408	4.911191	0.512568
H	-1.861378	4.630503	-0.610435
H	-1.923875	0.430786	0.322195
H	-4.116713	0.706352	1.438277
H	3.113192	-0.455439	-2.208759
H	4.279255	-2.640836	-2.358497
H	3.266660	-4.664271	-1.329826
H	1.085578	-4.501472	-0.149400
H	-0.085138	-2.319635	0.003086

A -466.194617 a.u.

Br	-1.896432	-2.184014	1.237699
C	-0.348021	-1.038740	1.051631
C	-0.375593	-0.192118	-0.253206
F	-0.290182	-0.197281	2.118042
F	0.773266	-1.801682	1.081801
O	-1.317391	-0.154600	-1.010131
O	0.767735	0.462565	-0.365470
C	0.905323	1.328201	-1.527058
H	1.895329	1.769778	-1.433378
H	0.133812	2.099354	-1.505879
H	0.829926	0.735696	-2.440029

B -3465.567547 a.u.

S	-3.471290	0.139665	-0.451161
O	-3.831543	-0.628413	0.769802
O	-3.663937	1.609092	-0.332715
N	1.328022	0.078841	0.175655
C	0.869900	-1.318057	0.112134
C	-0.683265	-1.304051	-0.112648
N	-1.144527	0.098505	-0.175829
C	-0.838793	0.791346	1.090802
C	0.714108	0.783187	1.312586
C	-0.496812	0.796134	-1.306061
C	1.057373	0.781344	-1.088195
H	1.135073	-1.813750	1.046857
H	1.386800	-1.818217	-0.707827
H	-1.204573	-1.802693	0.706595
H	-0.948001	-1.798580	-1.049810
H	-1.222862	1.811518	1.027480
H	-1.354521	0.271727	1.901065
H	1.117265	1.795718	1.353790
H	0.983170	0.261929	2.232028
H	-0.878211	1.818217	-1.344944
H	-0.768305	0.284578	-2.232028
H	1.569255	0.255321	-1.895071
H	1.460397	1.792398	-1.018881
Br	3.831543	0.071597	0.550065

C **-1118.888735 a.u.**

C	7.159859	-0.670288	0.234528
C	6.183759	-0.069026	1.037487
C	4.843235	-0.412167	0.879395
C	4.460882	-1.344712	-0.101246
C	5.446118	-1.946148	-0.902847
C	6.790164	-1.613396	-0.727969
C	3.018638	-1.695755	-0.211644
C	2.430464	-2.090889	-1.536403
O	2.266800	-1.636227	0.762877
C	1.087388	-2.812784	-1.440851
C	2.947284	-1.763357	-2.698533
C	3.167495	-1.532607	-4.040952
C	3.871597	-2.481920	-4.847462
C	4.107831	-2.215060	-6.187327
C	3.669971	-1.014556	-6.768074
C	2.982584	-0.071448	-5.987963
C	2.731025	-0.310805	-4.645955
C	-0.041071	-1.981646	-0.784005
F	1.259382	-4.011134	-0.791667
F	0.631462	-3.126461	-2.702814
O	-0.748012	-2.681759	0.090065
O	-0.254413	-0.838192	-1.131988
C	-1.861050	-1.991261	0.715267
H	8.205608	-0.407302	0.362877
H	6.469491	0.664552	1.785048
H	4.080765	0.046689	1.499861
H	5.173600	-2.697034	-1.635245
H	7.547162	-2.093447	-1.340239
H	4.208789	-3.411964	-4.402678
H	4.636794	-2.946878	-6.790287
H	3.862598	-0.816070	-7.817475
H	2.641325	0.856810	-6.436064
H	2.201223	0.419025	-4.043250
H	-2.291844	-2.712307	1.407557
H	-2.592374	-1.700117	-0.040664
H	-1.500529	-1.111714	1.251442

D **-1118.899273 a.u.**

C	7.159859	-0.670288	0.234528
C	6.183759	-0.069026	1.037487
C	4.843235	-0.412167	0.879395
C	4.460882	-1.344712	-0.101246
C	5.446118	-1.946148	-0.902847
C	6.790164	-1.613396	-0.727969
C	3.018638	-1.695755	-0.211644
C	2.430464	-2.090889	-1.536403
O	2.266800	-1.636227	0.762877
C	1.087388	-2.812784	-1.440851
C	2.947284	-1.763357	-2.698533
C	3.167495	-1.532607	-4.040952
C	3.871597	-2.481920	-4.847462
C	4.107831	-2.215060	-6.187327
C	3.669971	-1.014556	-6.768074
C	2.982584	-0.071448	-5.987963
C	2.731025	-0.310805	-4.645955
C	-0.041071	-1.981646	-0.784005
F	1.259382	-4.011134	-0.791667
F	0.631462	-3.126461	-2.702814
O	-0.748012	-2.681759	0.090065
O	-0.254413	-0.838192	-1.131988
C	-1.861050	-1.991261	0.715267
H	8.205608	-0.407302	0.362877
H	6.469491	0.664552	1.785048
H	4.080765	0.046689	1.499861
H	5.173600	-2.697034	-1.635245
H	7.547162	-2.093447	-1.340239
H	4.208789	-3.411964	-4.402678
H	4.636794	-2.946878	-6.790287
H	3.862598	-0.816070	-7.817475
H	2.641325	0.856810	-6.436064

H	2.201223	0.419025	-4.043250
H	-2.291844	-2.712307	1.407557
H	-2.592374	-1.700117	-0.040664
H	-1.500529	-1.111714	1.251442

E -1118.355704 a.u.

C	6.924910	-0.631806	-0.166122
C	6.394932	-0.659665	1.163206
C	5.025734	-0.876048	1.380221
C	4.171006	-0.931495	0.294944
C	4.630403	-0.576806	-1.086525
C	6.116741	-0.674811	-1.265952
C	2.848707	-1.535839	0.205281
C	2.594723	-1.750805	-1.243245
O	2.082260	-1.859025	1.126487
C	1.297171	-2.372492	-1.662404
C	3.634239	-1.299835	-2.002436
C	3.861171	-1.378979	-3.452171
C	3.662322	-2.584687	-4.151912
C	3.927520	-2.662339	-5.518307
C	4.386833	-1.538731	-6.212043
C	4.592393	-0.337227	-5.527768
C	4.346669	-0.260041	-4.157435
C	0.067212	-1.815380	-0.894673
F	1.364120	-3.745677	-1.532399
F	1.010078	-2.134957	-2.992421
O	-0.718085	-2.771135	-0.424406
O	-0.141127	-0.620589	-0.844097
C	-1.927648	-2.336167	0.250228
H	8.002967	-0.603019	-0.294346
H	7.075481	-0.617778	2.007137
H	4.657749	-1.098044	2.377947
H	4.396714	0.499056	-1.250418
H	6.534520	-0.659932	-2.267335
H	3.321780	-3.466528	-3.619970
H	3.777616	-3.602189	-6.040889
H	4.588180	-1.600218	-7.277231
H	4.948274	0.539967	-6.059355
H	4.506313	0.681747	-3.641670
H	-2.421019	-3.252306	0.569499
H	-2.562071	-1.779654	-0.441875
H	-1.672855	-1.716647	1.111909

HBr -2572.337889 a.u.

Br	0.624426	0.360513	0.000000
H	-0.606003	-0.349876	0.000000

TS1-SD -3931.723102 a.u.

Br	-1.097602	1.509344	-0.628805
C	-1.229377	4.397099	-0.068701
C	0.191155	4.697485	-0.219246
F	-2.111810	4.750390	-0.998645
F	-1.759139	4.443536	1.146980
O	0.967044	4.685520	0.726866
O	0.514989	4.898309	-1.503573
C	1.928072	5.050897	-1.782494
H	1.996758	5.143374	-2.865783
H	2.475979	4.170787	-1.437698
H	2.316704	5.949822	-1.298484
S	0.568740	-5.250609	1.804602
O	0.664138	-5.949822	0.494718
O	-0.685076	-5.518913	2.559356
N	0.058917	-3.136511	1.035413
C	1.222433	-2.594960	0.299341
C	0.858973	-1.166368	-0.241904
N	-0.501831	-0.850316	0.209456
C	-1.477047	-1.787751	-0.363115
C	-1.112312	-3.230139	0.141409
C	-0.581836	-0.828971	1.675291
C	-0.258348	-2.274417	2.194374
H	1.459631	-3.271980	-0.523310
H	2.071478	-2.547971	0.985009

H	0.880561	-1.141608	-1.332332
H	1.543881	-0.412605	0.149227
H	-2.475979	-1.496782	-0.034915
H	-1.422616	-1.728708	-1.451155
H	-1.941556	-3.666739	0.702156
H	-0.857413	-3.884709	-0.694327
H	-1.586050	-0.519757	1.968018
H	0.141527	-0.104616	2.052060
H	0.603512	-2.263051	2.865783
H	-1.117050	-2.702561	2.714657

TS2 -1118.844654 a.u.

C	6.70738900	-1.67687600	1.40361500
C	5.82789400	-0.73169400	1.94615400
C	4.66641400	-0.38676900	1.26099100
C	4.37291400	-0.98373800	0.02157800
C	5.25908300	-1.93205900	-0.51662000
C	6.42121800	-2.27631800	0.17391200
C	3.12458300	-0.58883500	-0.68467100
C	2.84877700	-1.19300000	-1.99487000
O	2.32601200	0.22343000	-0.21682800
C	1.45969100	-2.95489500	-1.46326200
C	2.96266000	-1.14551800	-3.22645300
C	3.01444900	-1.17646200	-4.63578900
C	4.03423600	-1.90035600	-5.29970300
C	4.08298700	-1.91675700	-6.68949600
C	3.12750800	-1.21730300	-7.43693900
C	2.11611400	-0.49687400	-6.78969400
C	2.05372700	-0.47137200	-5.40055200
C	0.21261300	-2.38272700	-0.89936200
F	2.21269700	-3.72219900	-0.66406400
F	1.32691600	-3.52449700	-2.66265500
O	0.26014000	-2.32429600	0.43376000
O	-0.69012700	-1.96698700	-1.60775200
C	-0.85071700	-1.66169600	1.08586100
H	7.61309000	-1.94464600	1.93962000
H	6.05054400	-0.26727100	2.90182200
H	3.97785200	0.34270900	1.67313900
H	5.04019800	-2.39862200	-1.47117000
H	7.10170300	-3.00978700	-0.24706500
H	4.77305300	-2.43843900	-4.71522100
H	4.86642900	-2.47380900	-7.19360400
H	3.17103900	-1.23322600	-8.52160800
H	1.37609200	0.04396500	-7.37115800
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H	-0.60741500	-1.67454700	2.14694300
H	-1.77724600	-2.20887500	0.90138500
H	-0.94075800	-0.63528400	0.72554700

TS3 -1118.844654 a.u.

C	6.70738900	-1.67687600	1.40361500
C	5.82789400	-0.73169400	1.94615400
C	4.66641400	-0.38676900	1.26099100
C	4.37291400	-0.98373800	0.02157800

MECP-S-T -1118.844654 a.u.

C	6.70738900	-1.67687600	1.40361500
C	5.82789400	-0.73169400	1.94615400
C	4.66641400	-0.38676900	1.26099100
C	4.37291400	-0.98373800	0.02157800

R2' -345.207616 a.u.

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C	-0.770916	-1.298293	-0.128914
N	-1.271591	0.089556	-0.207286
C	-0.965188	0.780322	1.061615
C	0.577908	0.784906	1.310680
C	-0.577930	0.785663	-1.310338
C	0.965168	0.781080	-1.061285
H	1.020476	-1.805099	1.066816
H	1.309854	-1.810956	-0.676704

H	-1.309572	-1.811531	0.675423
H	-1.020193	-1.804548	-1.068093
H	-1.363693	1.799160	1.001308
H	-1.498485	0.264948	1.868141
H	0.970081	1.806194	1.371007
H	0.833150	0.278379	2.248116
H	-0.970204	1.806950	-1.370002
H	-0.833128	0.279715	-2.248098
H	1.498510	0.266247	-1.868128
H	1.363575	1.799920	-1.000369

B' -2916.944057 a.u.

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C	0.54069800	0.55756200	1.31197600
C	-0.63699900	0.55213000	-1.31192200
C	0.92517700	0.55794800	-1.07512900
H	0.98732500	-2.02565800	1.06271200
H	1.27500500	-2.02878000	-0.69328700
H	-1.33789800	-2.04426800	0.67465200
H	-1.04988300	-2.03353100	-1.07894900
H	-1.39981400	1.56516200	0.99578800
H	-1.52936400	0.02100800	1.86569300
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H	0.79723300	0.03544800	2.23557000
H	-1.01311800	1.57732000	-1.36535800
H	-0.87260400	0.04328100	-2.25059700
H	1.45329100	0.03193700	-1.87244200
H	1.31500800	1.57442800	-0.99735100
Br	3.75595400	-0.11920300	0.59447800

TS1'-SD -3383.078694 a.u.

Br	-1.83413800	1.54564900	0.90300000
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C	-4.20229100	-0.23384300	-0.30781900
F	-2.91535200	-1.64835500	1.19953100
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O	-3.27833900	-0.59937900	-1.22124600
C	-3.22266700	0.21837300	-2.40157700
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C	-0.09377500	0.73632600	5.22247700
C	-0.44752600	0.61809500	3.69594900
N	-1.14948000	1.84916900	3.30734300
C	-2.40524100	1.99290500	4.05863300
C	-2.03504800	2.09039400	5.58245200
C	-0.29125400	3.02433400	3.49071300
C	0.05547200	3.11807100	5.02340200
H	-0.55334600	-0.07692900	5.79381100
H	0.98886600	0.68055200	5.37764400
H	-1.10496000	-0.22681300	3.47589600
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H	-3.03806100	1.13248100	3.82575800
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F	-2.75464411	-0.98962982	0.77624956

F	-4.38949652	0.30407310	1.46483885
O	-5.22030417	0.61670146	-1.15138921
O	-3.45397863	-0.70282775	-1.76008249
C	-3.93493427	-0.73303008	-3.12098074
H	-3.23612225	-1.37348488	-3.65912978
H	-3.93685010	0.27235892	-3.55020850
H	-4.94042510	-1.15820250	-3.16552327
N	-0.48388424	1.82215866	6.06453524
C	-0.12855775	0.60475246	5.35807439
C	-0.47187392	0.80713813	3.79548263
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C	-1.90210815	2.09992422	5.92491717
C	0.00953590	3.13956739	4.01508062
C	0.30843143	2.94026142	5.58991143
H	-0.70351960	-0.23547018	5.75257348
H	0.93942228	0.40981303	5.47233226
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H	-2.48157259	1.24944181	6.28985754
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H	0.03112520	3.84630333	6.13203292

COM'' -4480.497344 a.u.

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F	-3.63626800	2.16853900	3.83112500
F	-5.25022300	3.36425900	2.97236400
O	-3.60065000	4.00048300	0.95594500
O	-1.84824000	3.24037200	2.18597400

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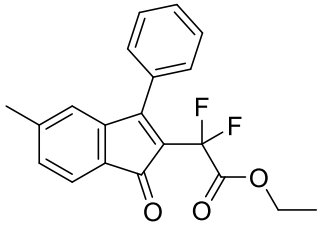
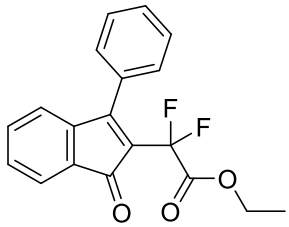


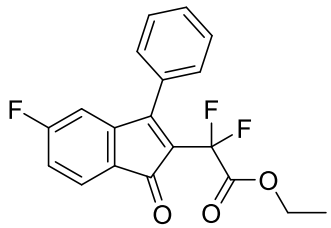
Ethyl 2,2-difluoro-2-(5-methyl-1-oxo-3-phenyl-1*H*-inden-2-yl)acetate (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 5H), 7.45 (d, *J* = 7.3 Hz, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.88 (s, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 2.34 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.11 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.3, 162.8, 162.6 (t, *J* = 3.7 Hz), 145.0, 144.3, 133.0, 130.8, 130.7, 130.2, 128.4, 128.0 (t, *J* = 2.2 Hz), 124.5, 123.4, 111.1 (t, *J* = 248.8 Hz), 63.2, 22.0, 13.8 ppm; HRMS calcd for $C_{20}H_{16}F_2O_3Na$ ($M+Na^+$): 365.0960, found: 365.0951.



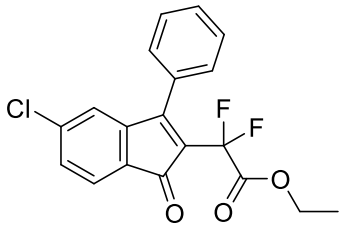
Ethyl 2,2-difluoro-2-(1-oxo-3-phenyl-1*H*-inden-2-yl)acetate (**3b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 6.9 Hz, 1H), 7.53 (s, 5H), 7.43 – 7.36 (m, 2H), 7.11 (d, *J* = 6.8 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.13 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 162.9 (d, *J* = 27.1 Hz), 143.8, 133.8, 130.7, 130.7, 130.4, 130.0, 129.3, 128.9, 128.4, 128.1 (t, *J* = 2.2 Hz), 123.4, 123.3, 111.1 (t, *J* = 249.0 Hz), 63.2, 13.8 ppm; HRMS calcd for $C_{19}H_{15}F_2O_3$ ($M+H^+$): 329.0984, found: 329.0983.



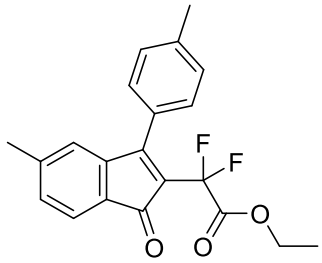
Ethyl 2,2-difluoro-2-(5-fluoro-1-oxo-3-phenyl-1*H*-inden-2-yl)acetate (**3c**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.0, 5.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 2H), 7.02 (td, *J* = 8.5, 2.2 Hz, 1H), 6.86 (dd, *J* = 8.2, 2.1 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 166.4 (d, *J* = 256.0 Hz), 162.5, 160.8, 130.4 (d, *J* = 51.9 Hz), 130.1, 128.6, 128.0 (t, *J* = 2.2 Hz), 125. 8 (d, *J* = 1.9 Hz), 125.3 (d, *J* = 9.8 Hz), 116.5 (d, *J* = 23.1 Hz), 112.1 (d, *J* = 26.0 Hz), 110.8 (t, *J* = 249.0 Hz), 63.4, 13.8 ppm; HRMS calcd for $C_{19}H_{14}F_3O_3$ ($M+H^+$): 347.0890, found: 347.0880.



Ethyl 2-(5-chloro-1-oxo-3-phenyl-1*H*-inden-2-yl)-2,2-difluoroacetate (**3d**)

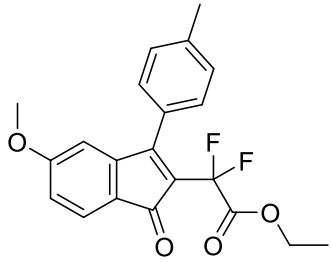
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 6H), 7.37 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.08 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.50 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.1, 162.6, 161.7, 145.8, 140.3, 130.9, 130.7, 130.4, 130.1, 129.8, 128.7, 128.0, 124.4, 123.9, 110.8 (t, *J* = 249.0 Hz), 63.4, 13.8 ppm; HRMS calcd for $C_{19}H_{14}ClF_2O_3$ ($M+H^+$): 363.0594, found: 363.0590.



Ethyl 2,2-difluoro-2-(5-methyl-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)acetate (**3e**)

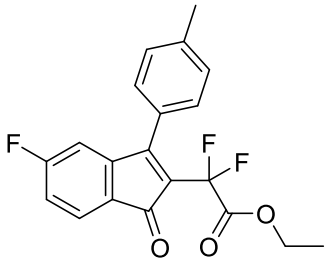
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.42 (m, 3H), 7.33 (d, *J* = 8.0 Hz, 3H), 7.15 (d, *J* = 7.3 Hz, 1H), 6.92 (s, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 2.34 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.96 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.4, 162.9, 144.9, 144.3, 140.7, 130.6, 129.1, 128.2, 127.9, 127.7, 124.5, 123.3,

111.1 (t, *J* = 249.0 Hz), 109.9, 63.2, 22.0, 21.5, 13.8 ppm; HRMS calcd for $C_{21}H_{19}F_2O_3$ ($M+H^+$): 357.1297, found: 357.1299.



Ethyl 2,2-difluoro-2-(5-methoxy-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)acetate (**3f**)

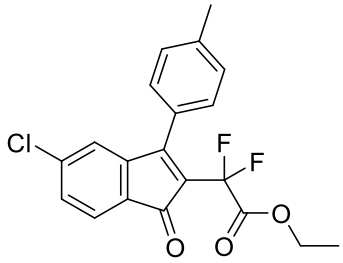
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 6.75 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.67 (d, *J* = 2.0 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 3.82 (s, 3H), 2.44 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.15 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.3, 164.6, 162.9 (t, *J* = 33.1 Hz), 161.0, 146.5, 140.7, 129.1, 128.2, 127.7, 125.3, 122.7, 113.9, 112.3, 112.1, 111.1 (t, *J* = 249.0 Hz), 63.2, 55.8, 21.5, 13.8 ppm; HRMS calcd for $C_{21}H_{19}F_2O_4$ ($M+H^+$): 373.1246, found: 373.1233.



Ethyl 2,2-difluoro-2-(5-fluoro-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)acetate (**3g**)

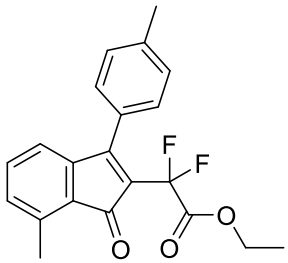
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 8.0, 5.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.02 (td, *J* = 8.4, 2.0 Hz, 1H), 6.86 (dd, *J* = 8.2, 2.0 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.34 (s, 2F), -102.85 (td, *J* = 8.5, 5.1 Hz, 1F) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.9, 166.4 (d, *J* = 255.8 Hz), 162.7 (t, *J* = 33.0 Hz), 161.1, 147.1 (d, *J* = 9.4 Hz), 141.2, 129.3, 128.1 (t, *J* = 2.2 Hz), 127.2, 125.9 (d, *J* = 2.2 Hz), 125.2 (d, *J* = 9.8 Hz), 116.4 (d, *J* = 23.2

Hz), 112.2 (d, *J* = 25.9 Hz), 110.9 (t, *J* = 249.0 Hz), 63.3, 21.6, 13.8 ppm; HRMS calcd for $C_{20}H_{16}F_3O_3$ ($M+H^+$): 361.1046, found: 361.1046.



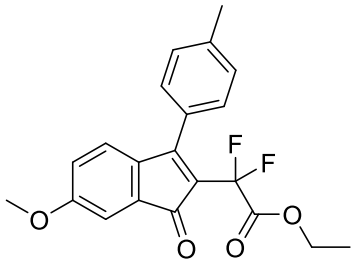
Ethyl 2-(5-chloro-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)-2,2-difluoroacetate (**3h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.7 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.37 – 7.33 (m, 3H), 7.11 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 2.46 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.49 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.2, 162.6, 161.9 (t, *J* = 3.5 Hz), 145.8, 141.3, 140.1, 130.3, 129.3, 128.2 (t, *J* = 1.9 Hz), 128.1 (t, *J* = 2.2 Hz), 127.2, 124.2, 124.0, 110.9 (t, *J* = 249.3 Hz), 63.3, 21.6, 13.8 ppm; HRMS calcd for $C_{20}H_{16}ClF_2O_3$ ($M+H^+$): 377.0751, found: 377.0750.



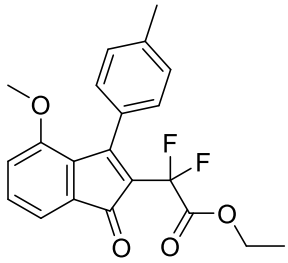
Ethyl 2,2-difluoro-2-(7-methyl-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)acetate (**3i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.9 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.94 (d, *J* = 7.2 Hz, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 2.56 (s, 3H), 2.44 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.13 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 163.0, 162.1, 144.3, 140.5, 138.5, 133.8, 132.8, 129.0, 128.2 (t, *J* = 2.1 Hz), 127.9, 126.6, 123.9, 121.3, 111.3 (t, *J* = 248.6 Hz), 63.1, 21.5, 17.2, 13.8 ppm; HRMS calcd for $C_{21}H_{19}F_2O_3$ ($M+H^+$): 357.1297, found: 357.1287.



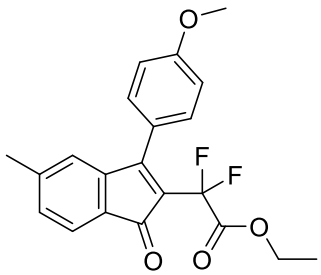
Ethyl 2,2-difluoro-2-(6-methoxy-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)acetate (**3j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.9 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 7.13 (d, *J* = 2.2 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 6.81 (dd, *J* = 8.1, 2.2 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 3.84 (s, 3H), 2.44 (s, 3H), 1.30 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.40 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.4, 164.6, 163.0, 162.4, 140.9, 135.3, 133.2, 132.5, 129.1, 128.1, 124.6, 116.6, 111.2, 110.7, 63.1, 55.9, 21.5, 13.8 ppm; HRMS calcd for $C_{21}H_{19}F_2O_4$ ($M+H^+$): 373.1246, found: 373.1237.



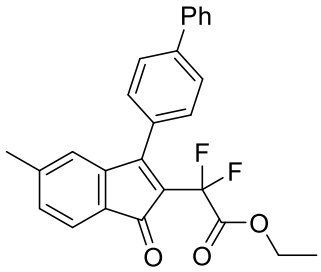
Ethyl 2,2-difluoro-2-(4-methoxy-1-oxo-3-(*p*-tolyl)-1*H*-inden-2-yl)acetate (**3j'**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.32 (m, 3H), 7.22 – 7.19 (m, 3H), 6.98 (d, *J* = 8.4 Hz, 1H), 4.20 (q, *J* = 7.1 Hz, 2H), 3.57 (s, 3H), 2.41 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.34 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 165.5, 162.9 (t, *J* = 32.6 Hz), 155.3, 133.0, 132.0, 130.0, 127.9, 127.6 (t, *J* = 2.1 Hz), 125.0, 123.5, 119.6, 116.1, 111.1 (t, *J* = 248.5 Hz), 63.0, 55.6, 21.5, 13.8 ppm; HRMS calcd for $C_{21}H_{19}F_2O_4$ ($M+H^+$): 373.1246, found: 373.1222.



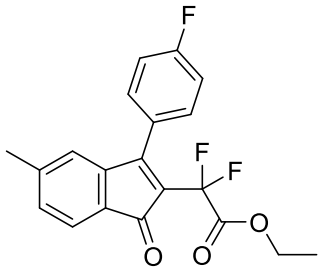
Ethyl 2,2-difluoro-2-(3-(4-methoxyphenyl)-5-methyl-1-oxo-1*H*-inden-2-yl)acetate (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.6 Hz, 2H), 7.44 (d, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 7.3 Hz, 1H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.97 (s, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 2.35 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.67 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.4, 163.0, 162.6 (t, *J* = 3.3 Hz), 161.4 (s), 144.7, 144.2, 130.6, 130.2 (t, *J* = 2.4 Hz), 127.9, 124.5, 123.3, 123.0, 113.9, 111.2 (t, *J* = 248.3 Hz), 63.1, 55.4, 22.0, 13.8 ppm; HRMS calcd for $C_{21}H_{19}F_2O_4$ ($M+H^+$): 373.1246, found: 373.1244.



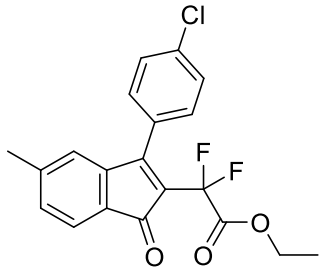
Ethyl 2-(3-([1,1'-biphenyl]-4-yl)-5-methyl-1-oxo-1*H*-inden-2-yl)-2,2-difluoroacetate (**3l**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.66 (d, *J* = 7.4 Hz, 2H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.51 – 7.46 (m, 3H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.17 (d, *J* = 7.3 Hz, 1H), 6.97 (s, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 2.36 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.91 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.3 (t, *J* = 3.7 Hz), 162.9, 162.4 (t, *J* = 3.5 Hz), 145.0, 144.2, 143.2, 140.0, 130.7, 129.6, 128.9, 128.7, 128.0, 127.7, 127.1, 127.0, 124.5, 123.5, 111.1 (t, *J* = 248.8 Hz), 63.2, 22.0, 13.8 ppm; HRMS calcd for $C_{26}H_{21}F_2O_3$ ($M+H^+$): 419.1453, found: 419.1458.



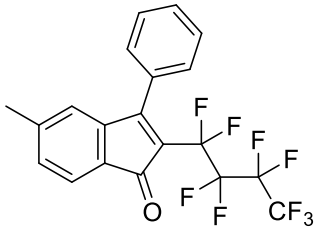
Ethyl 2,2-difluoro-2-(3-(4-fluorophenyl)-5-methyl-1-oxo-1*H*-inden-2-yl)acetate **(3m**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 5.5 Hz, 2H), 7.53 (d, *J* = 5.4 Hz, 1H), 7.46 (d, *J* = 7.3 Hz, 2H), 7.22 (t, *J* = 8.6 Hz, 1H), 7.17 (d, *J* = 7.3 Hz, 1H), 6.87 (s, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 2.36 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.17, -109.37 – -109.44 (m) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.1, 163.8 (d, *J* = 251.1 Hz), 161.6 (t, *J* = 3.3 Hz), 145.1, 144.1, 130.8, 130.3 (dt, *J* = 8.5, 2.2 Hz), 127.5, 126.7 (d, *J* = 3.3 Hz), 124.3, 123.5, 115.8, 115.6, 111.0 (t, *J* = 249.0 Hz), 63.3, 22.0, 13.8 ppm; HRMS calcd for $C_{20}H_{16}F_3O_3$ ($M+H^+$): 361.1046, found: 361.1043.



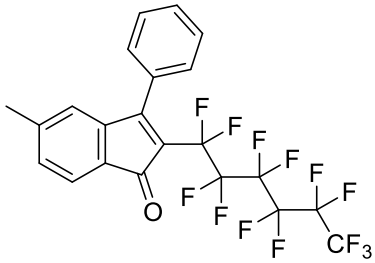
Ethyl 2-(3-(4-chlorophenyl)-5-methyl-1-oxo-1*H*-inden-2-yl)-2,2-difluoroacetate (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 5H), 7.17 (d, *J* = 7.3 Hz, 1H), 6.85 (s, 1H), 4.32 (q, *J* = 7.1 Hz, 2H), 2.35 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.25 ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.0, 162.7, 161.3, 145.2, 144.0, 136.4, 134.2, 130.9, 129.5 (t, *J* = 2.3 Hz), 129.2, 128.8, 127.5, 124.2, 123.6, 111.0 (t, *J* = 249.3 Hz), 63.3, 22.0, 13.8 ppm; HRMS calcd for $C_{20}H_{16}ClF_2O_3$ ($M+H^+$): 377.0751, found: 377.0753.



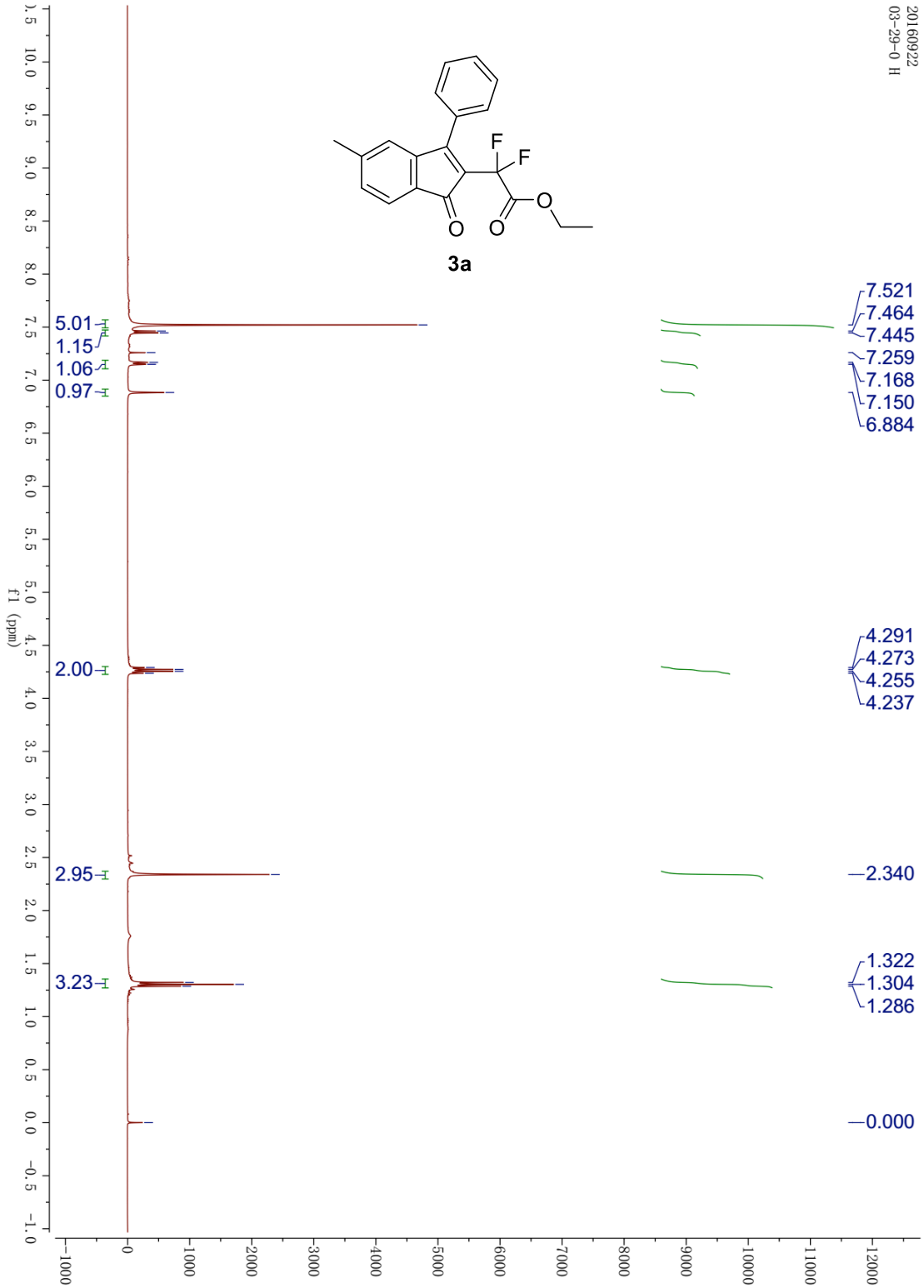
5-Methyl-2-(perfluorobutyl)-3-phenyl-1*H*-inden-1-one (**3p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.50 (m, 4H), 7.38 (d, *J* = 3.2 Hz, 2H), 7.21 (d, *J* = 7.3 Hz, 1H), 6.74 (s, 1H), 2.33 (s, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.97 (t, *J* = 9.8 Hz, 3F), -106.18 (t, *J* = 12.8 Hz, 2F), -121.49 – -121.62 (m, 2F), -125.91 – -126.04 (m, 2F) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 145.2, 144.3, 132.9, 131.4, 130.8, 129.8, 129.5, 128.4, 127.5, 127.3, 124.7, 123.6, 120.8, 118.8, 117.5, 116.0 (t, *J* = 33.8 Hz), 114.9 (t, *J* = 34.1 Hz), 21.9 ppm; HRMS calcd for $C_{20}H_{12}F_9O$ ($M+H^+$): 439.0739, found: 439.0751.



5-Methyl-2-(perfluorohexyl)-3-phenyl-1*H*-inden-1-one (**3q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.51 (m, 4H), 7.40 – 7.38 (m, 2H), 7.22 (d, *J* = 7.4 Hz, 1H), 6.74 (s, 1H), 2.34 (s, 3H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.82 (t, *J* = 10.0 Hz, 3F), -105.92 – -106.03 (m, 2F), -120.59 – -120.71 (m, 2F), -121.83 (s, 2F), -122.75 (s, 2F), -126.11 – -126.21 (m, 2F) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.2, 166.7, 145.2, 144.3, 131.4, 130.7, 129.8, 128.4, 127.5, 127.3, 124.7, 123.6, 21.9 ppm; HRMS calcd for $C_{22}H_{12}F_{13}O$ ($M+H^+$): 539.0675, found: 539.0665.


20160922
03-29-0 H
3a
F
F
O
O
O
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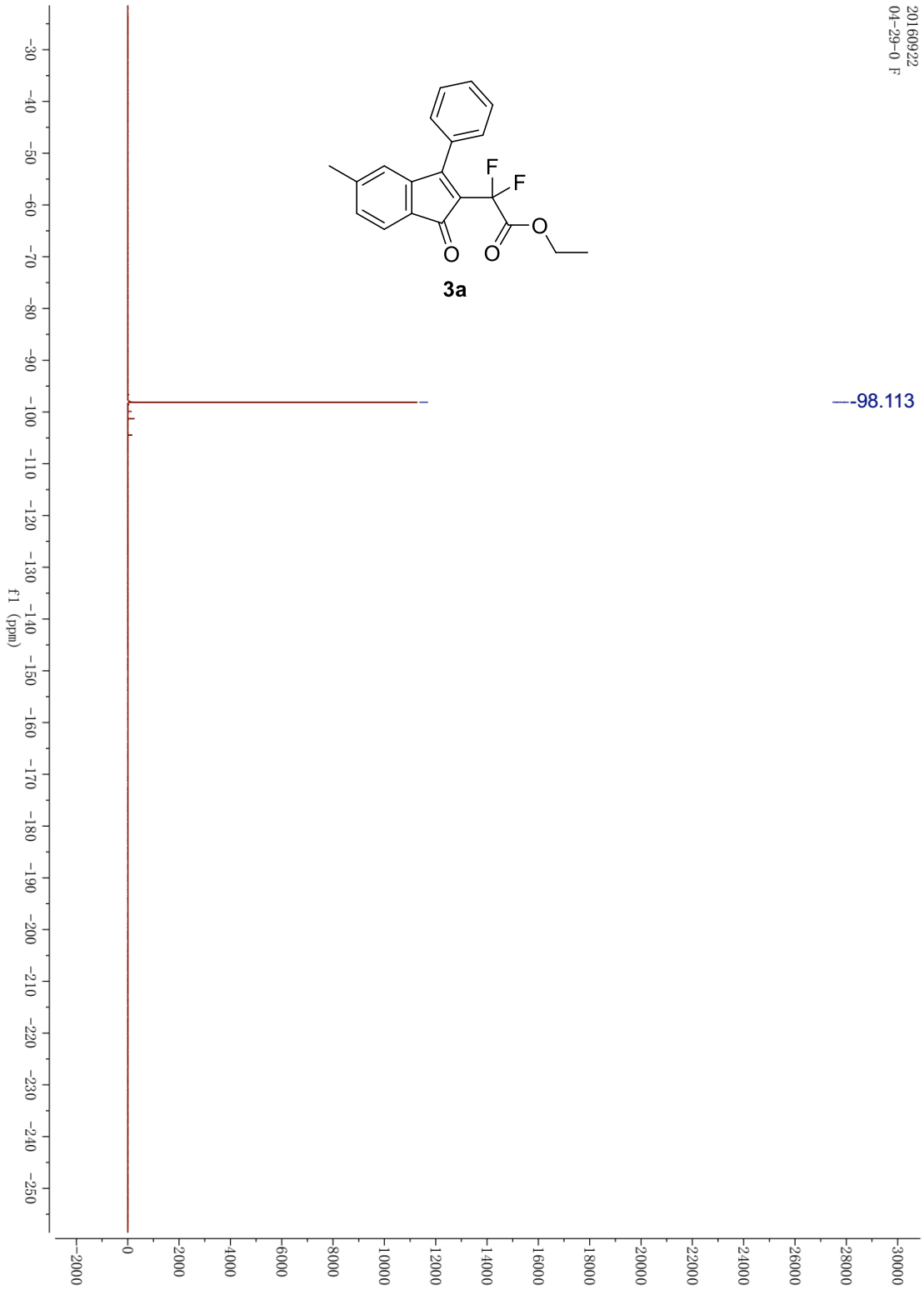
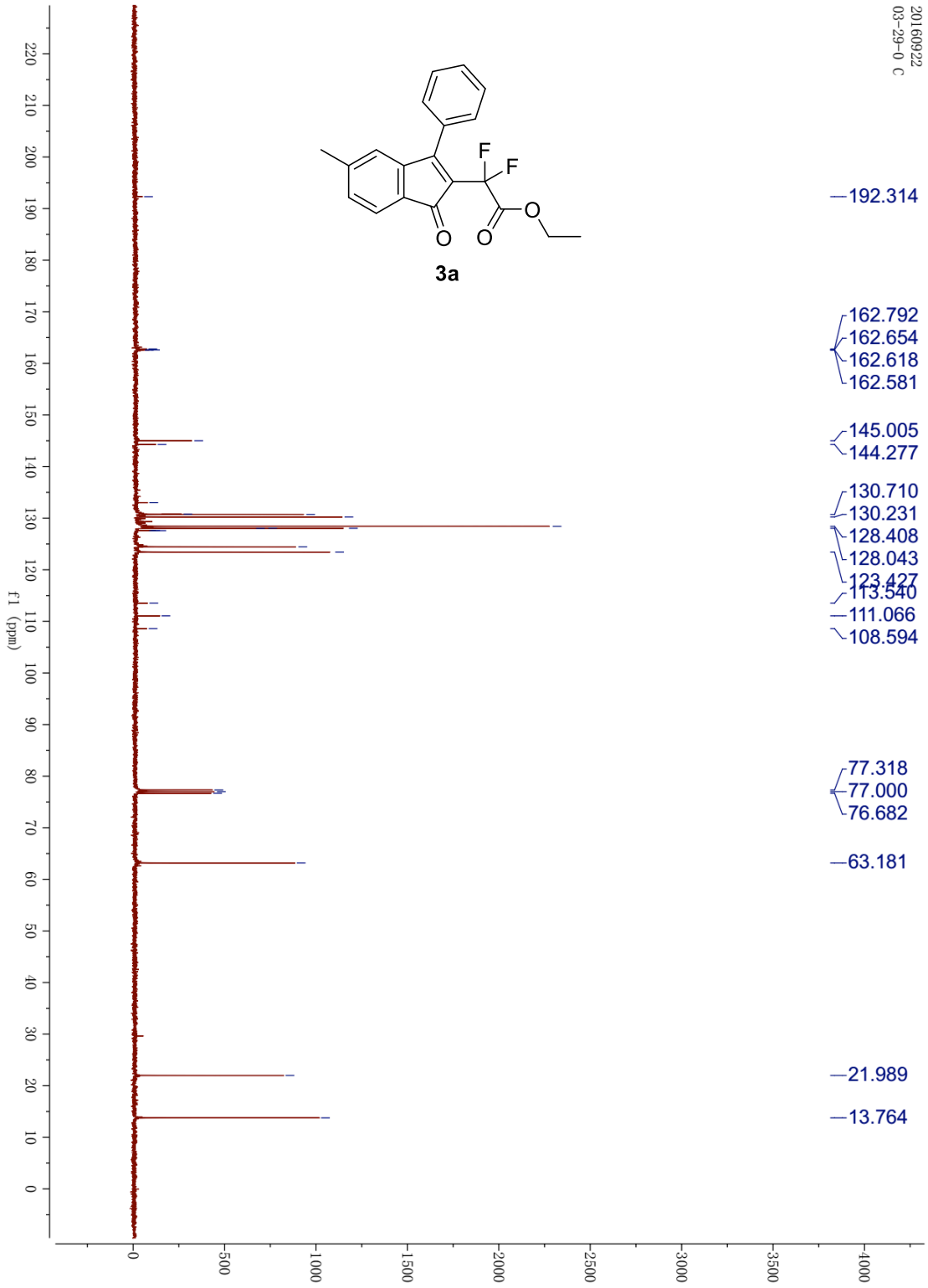
7.464
7.445
7.259
7.168
7.150
6.884
4.291
4.273
4.255
4.237
2.340
1.322
1.304
1.286
0.000
5.01
1.15
1.06
0.97
2.00
2.95
3.23
f1 (ppm)


20160922
04-29-0 F
F
F
O
O
O
3a
-98.113
f1 (ppm)


20160922
03-29-0 C
F
F
O
O
O
3a
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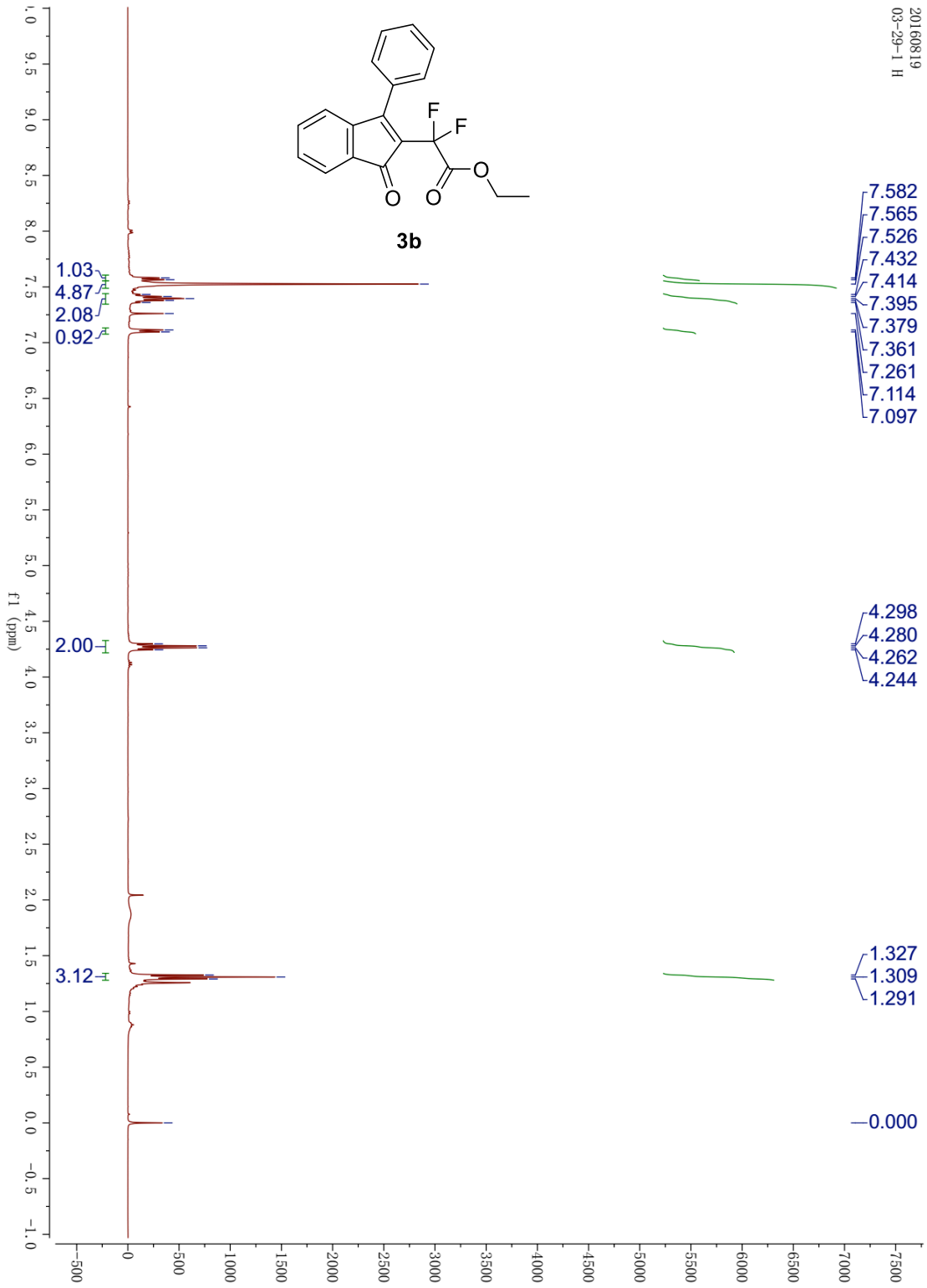
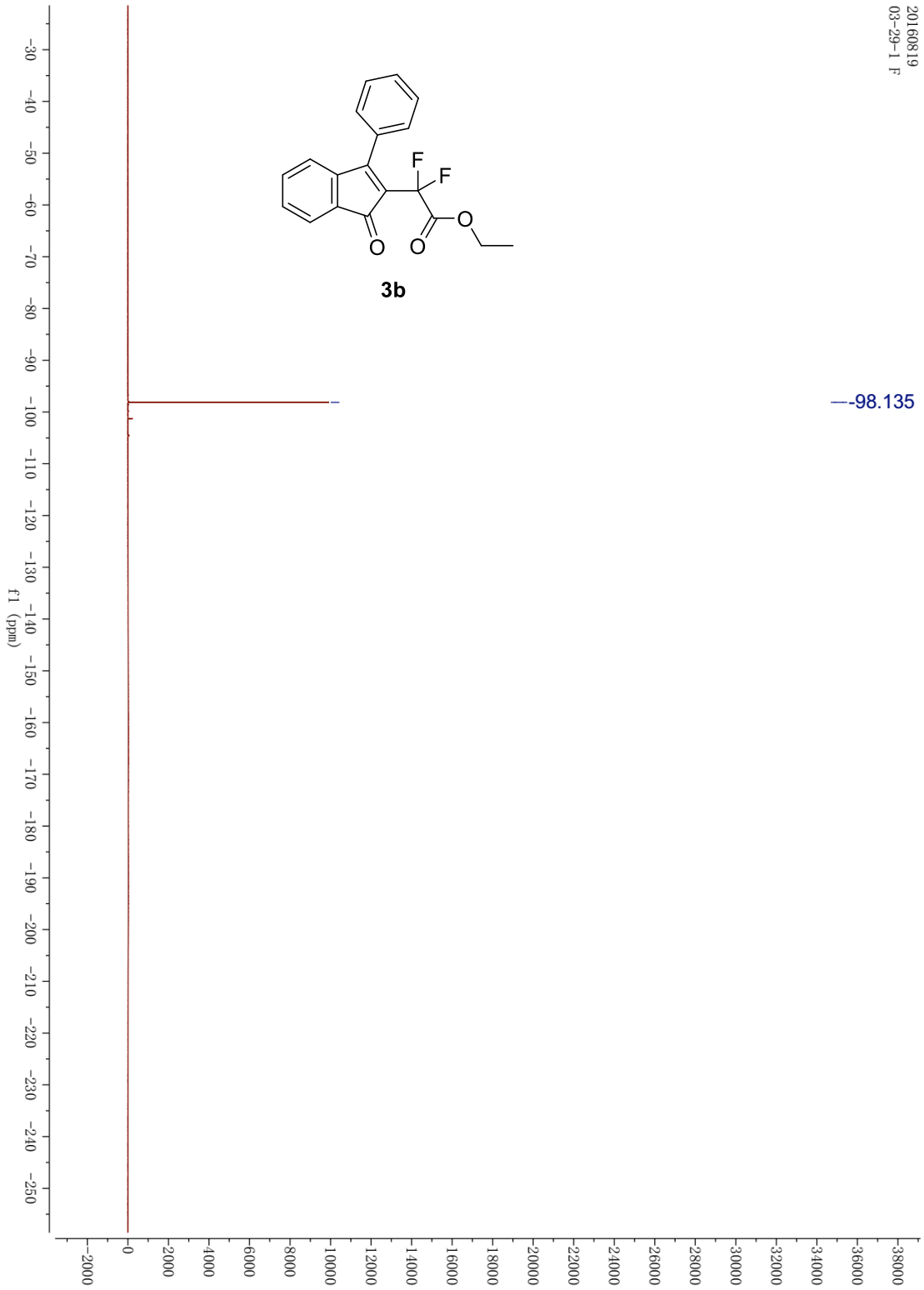
162.654
162.618
162.581
145.005
144.277
130.710
130.231
128.408
128.043
123.427
113.540
111.066
108.594
77.318
77.000
76.682
63.181
21.989
13.764
f1 (ppm)


20160819
03-29-1 H
3b
F
F
O
O
O
1.03
4.87
2.08
0.92
2.00
3.12
7.582
7.565
7.526
7.432
7.414
7.395
7.379
7.361
7.261
7.114
7.097
4.298
4.280
4.262
4.244
1.327
1.309
1.291
0.000
f1 (ppm)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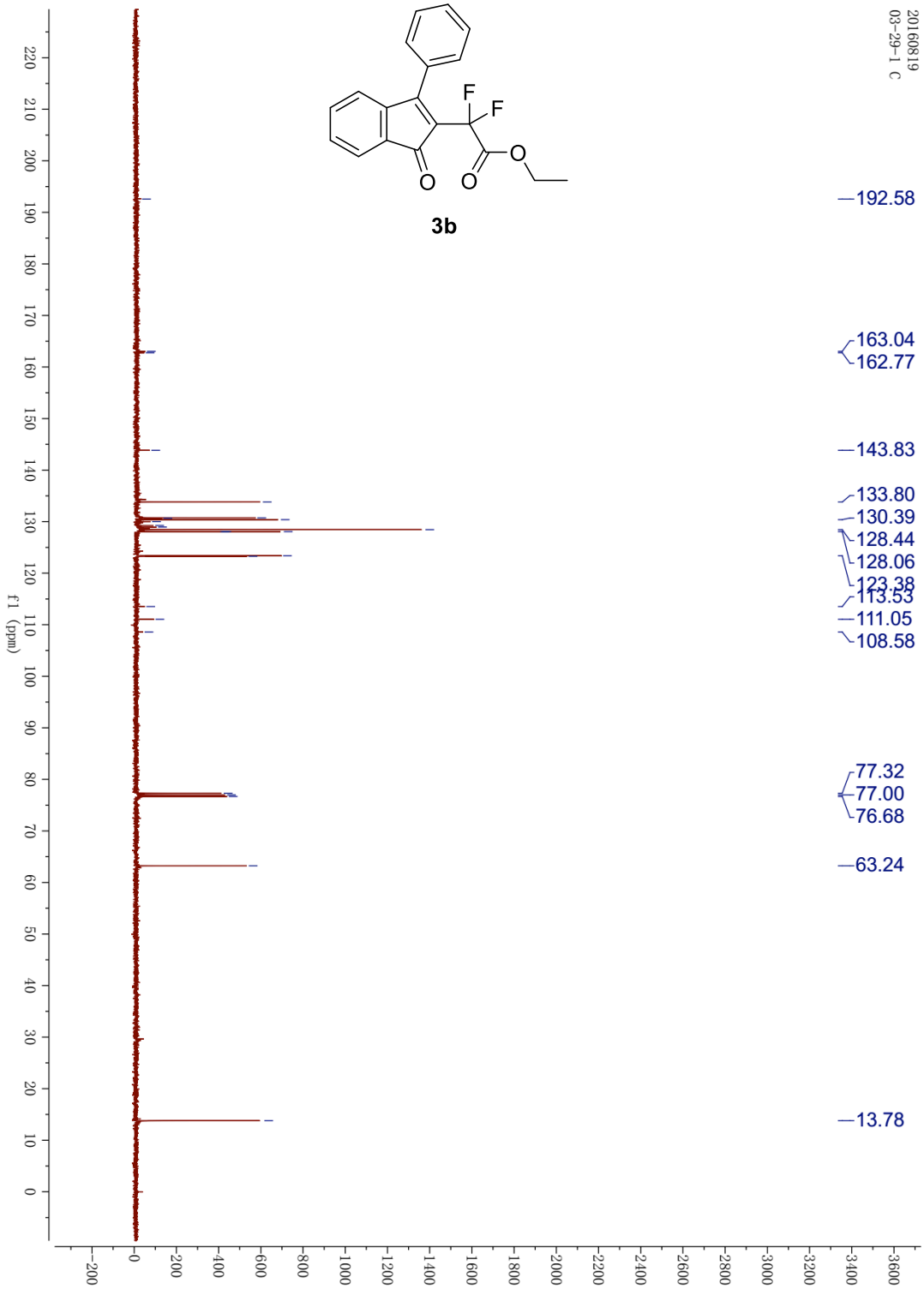
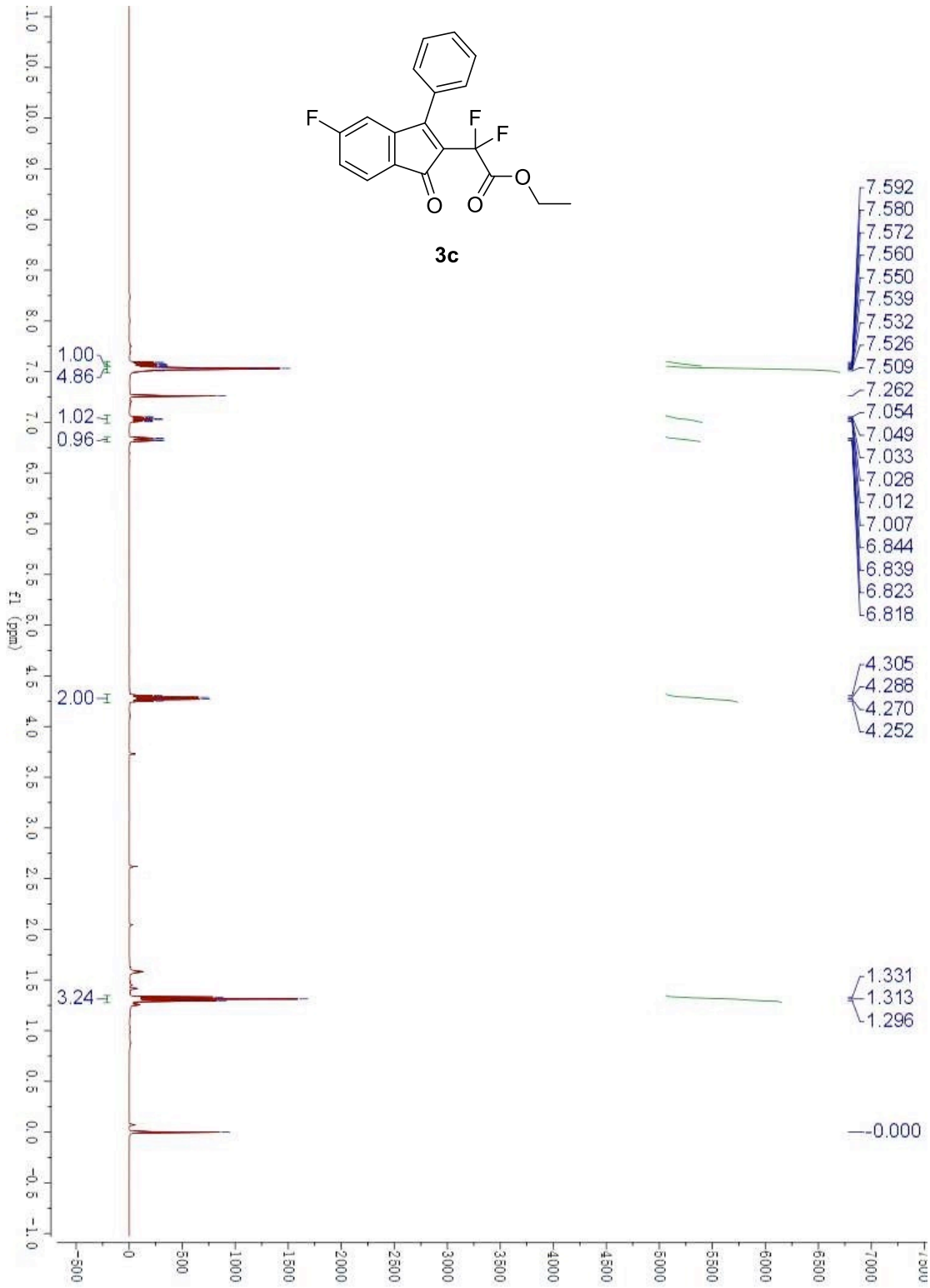
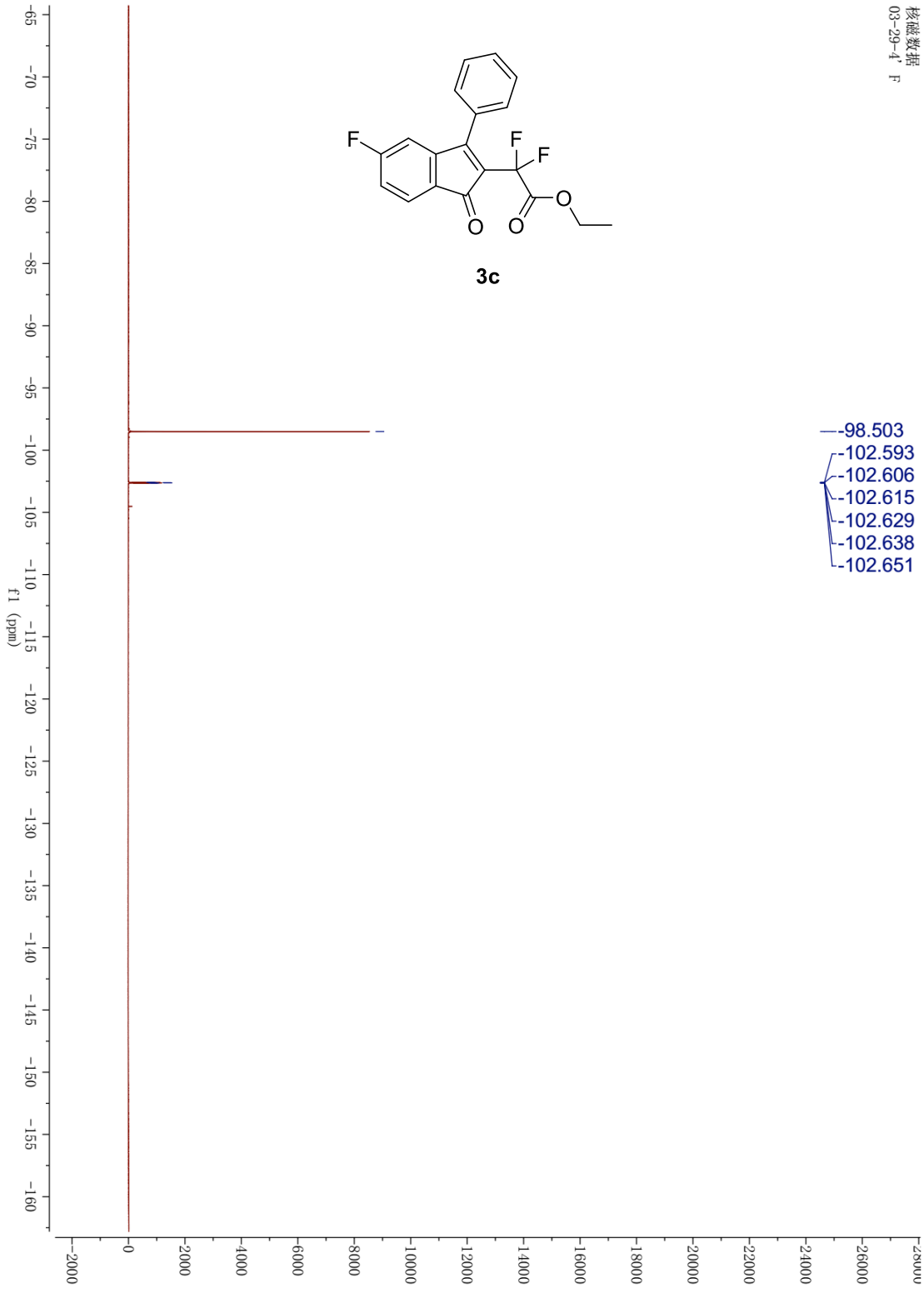
F
F
O
O
O
3b
-98.135
f1 (ppm)


20160819
03-29-1 C
F
F
O
O
O
3b
192.58
163.04
162.77
143.83
133.80
130.39
128.44
128.06
123.38
113.53
111.05
108.58
77.32
77.00
76.68
63.24
13.78
f1 (ppm)


F
F
F
O
O
O
3c
7.592
7.580
7.572
7.560
7.550
7.539
7.532
7.526
7.509
7.262
7.054
7.049
7.033
7.028
7.012
7.007
6.844
6.839
6.823
6.818
4.305
4.288
4.270
4.252
1.331
1.313
1.296
-0.000
1.00
4.86
1.02
0.96
2.00
3.24
f1 (ppm)


核磁数据
03-29-4' F
F
F
F
O
O
O
3c
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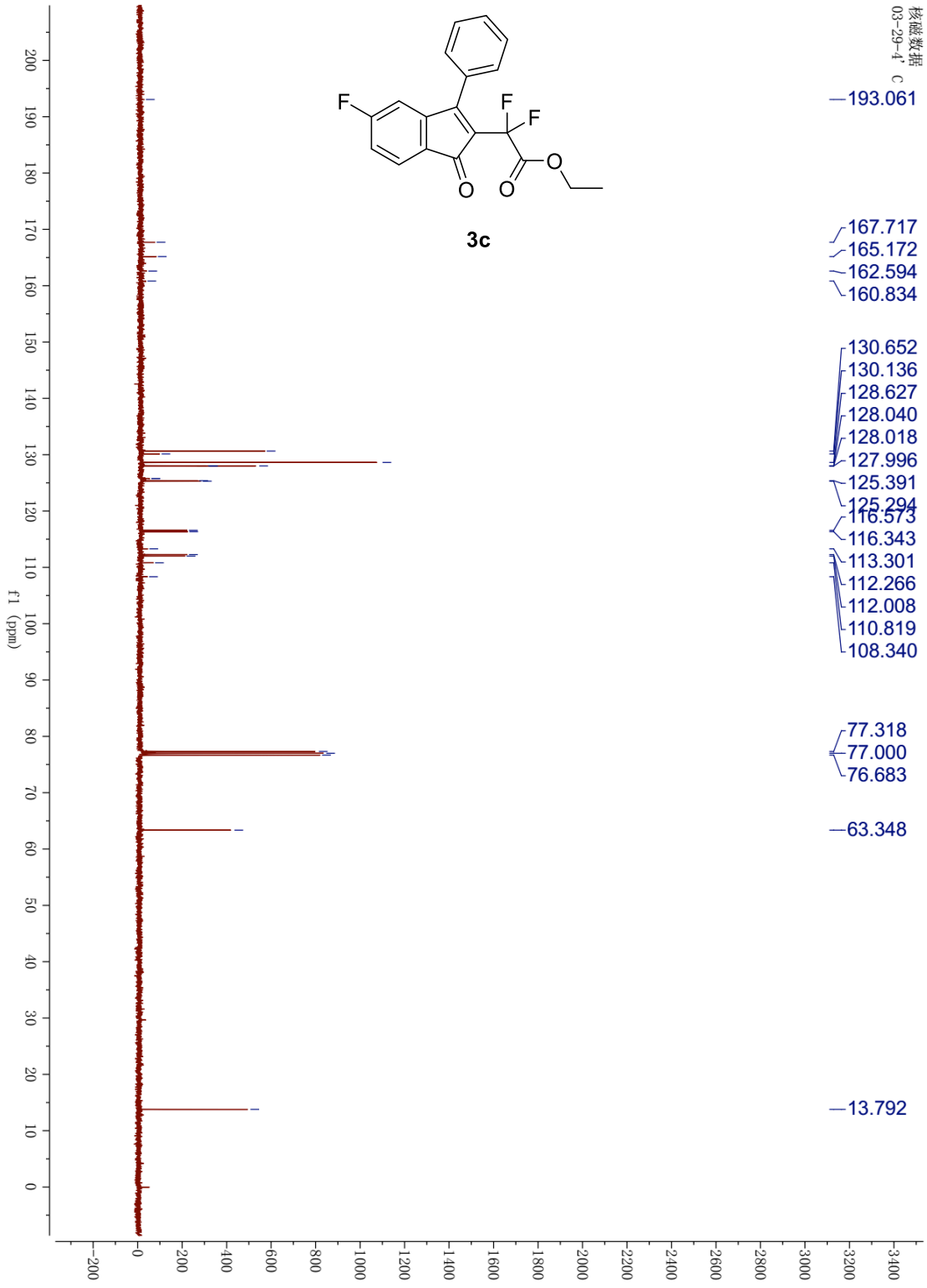
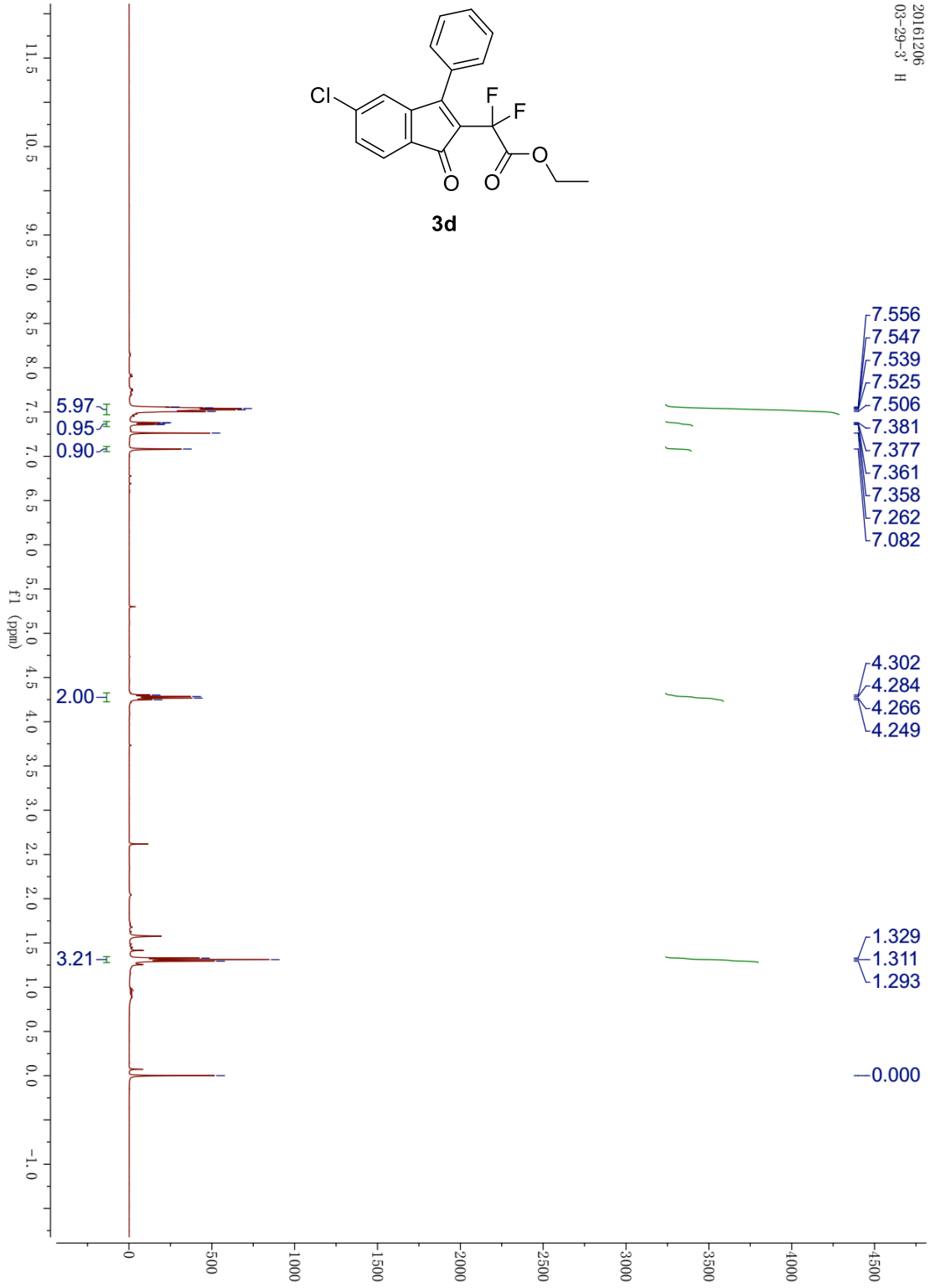
-102.593
-102.606
-102.615
-102.629
-102.638
-102.651
f1 (ppm)


核磁数据
03-29-4' C
F
F
F
O
O
O
3c
193.061
167.717
165.172
162.594
160.834
130.652
130.136
128.627
128.040
128.018
127.996
125.391
125.294
116.573
116.343
113.301
112.266
112.008
110.819
108.340
77.318
77.000
76.683
63.348
13.792
f1 (ppm)


20161206
03-29-3' H
Cl
F
F
O
O
O
3d
7.556
7.547
7.539
7.525
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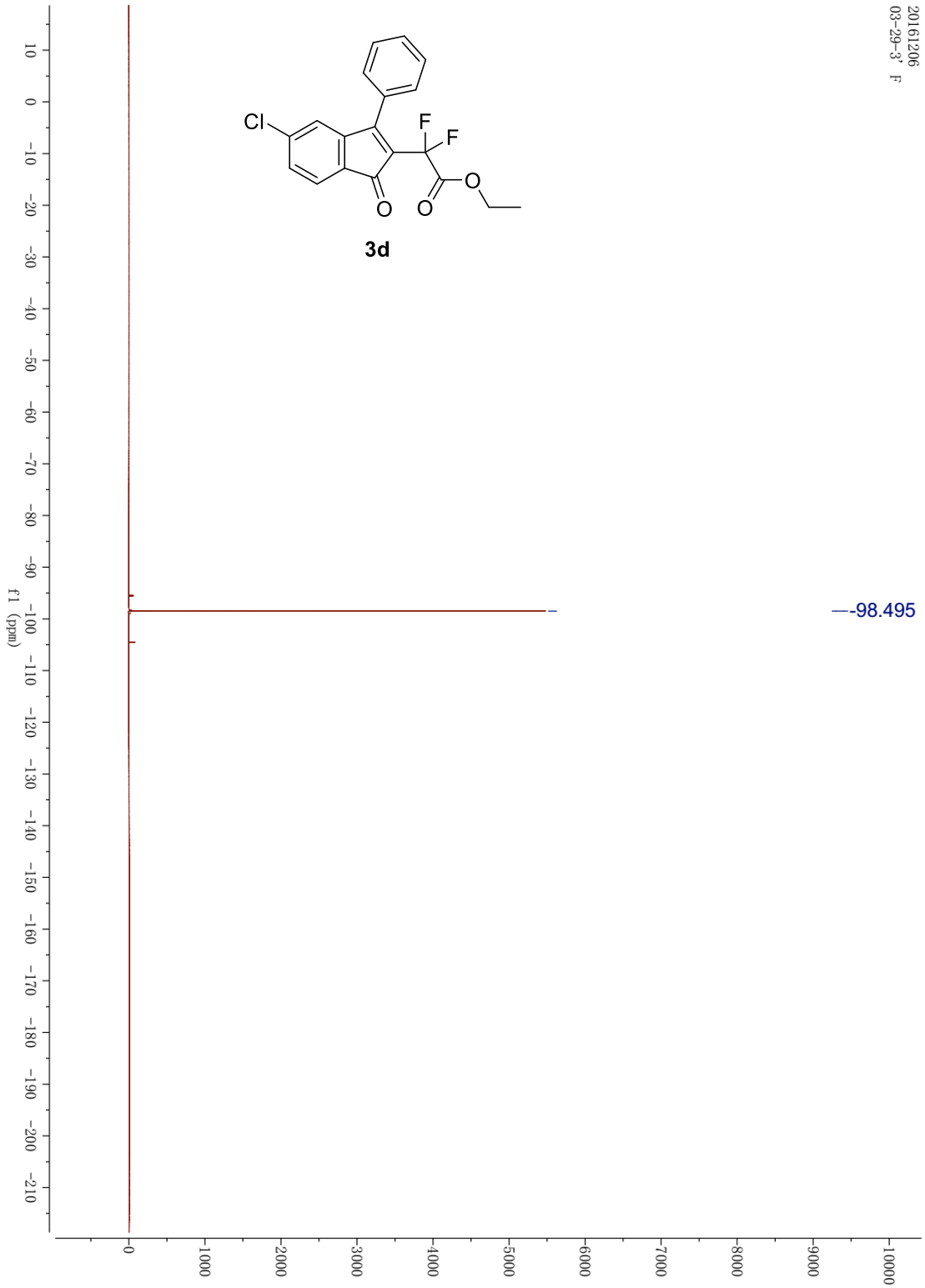
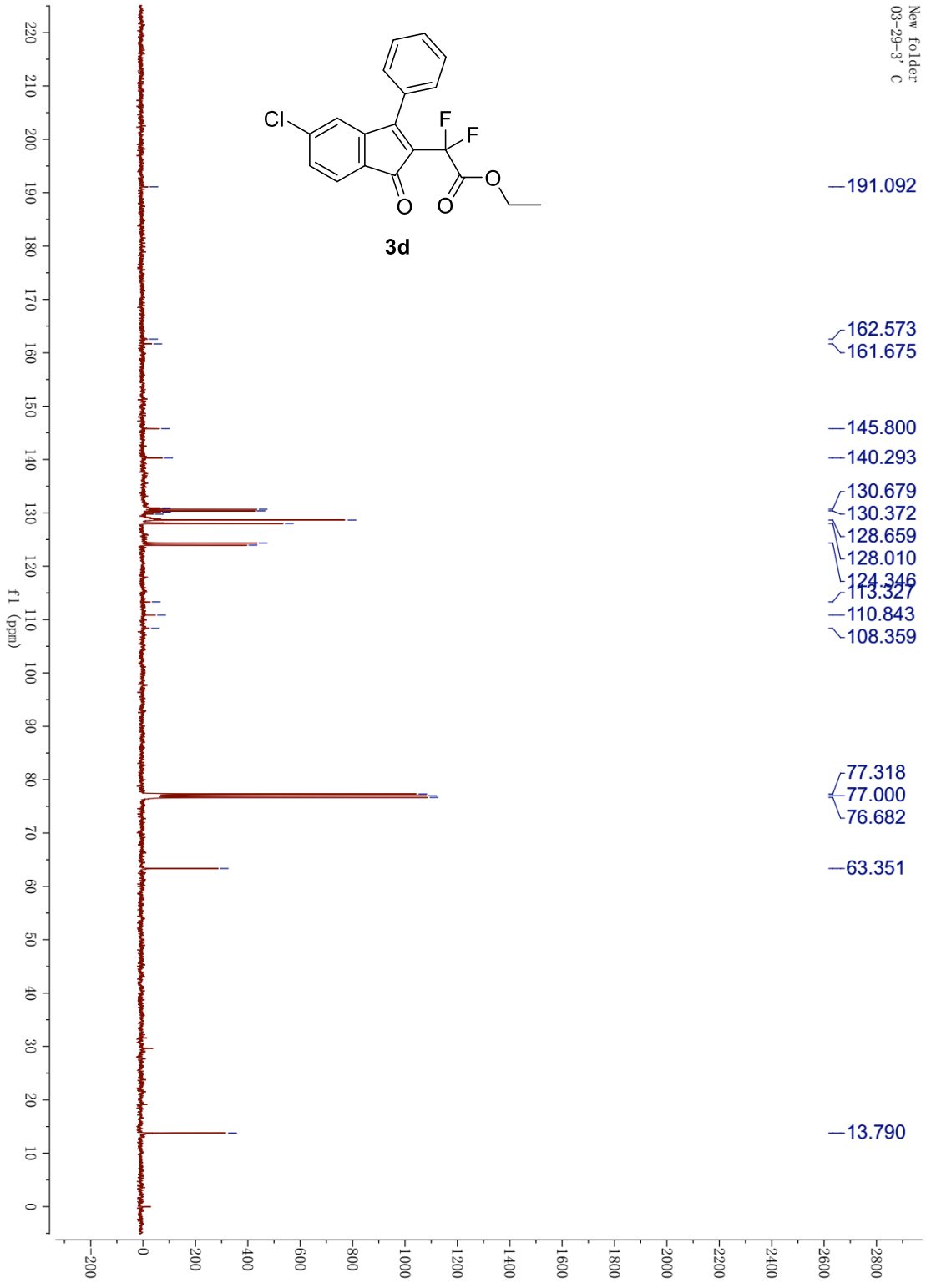
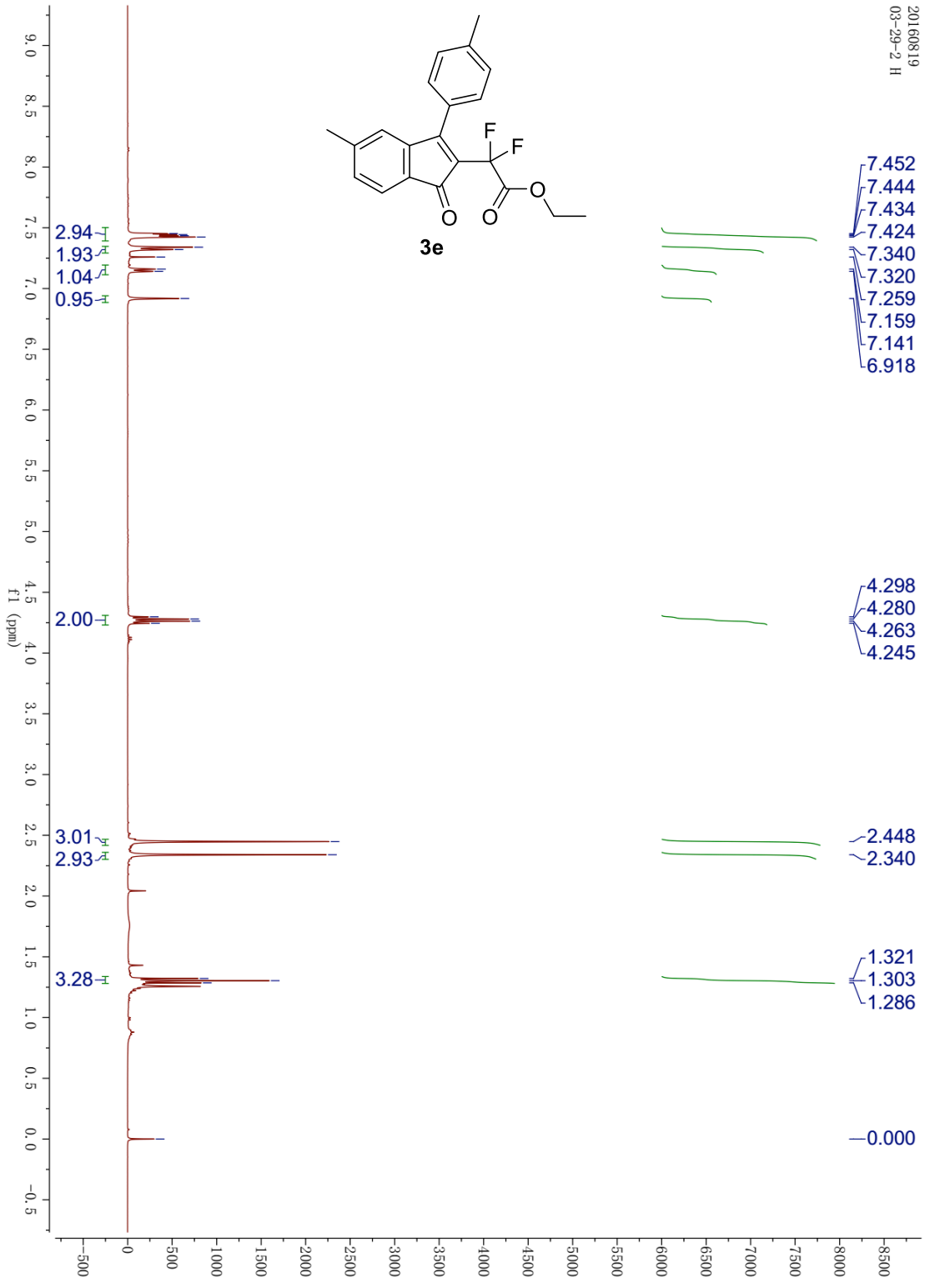
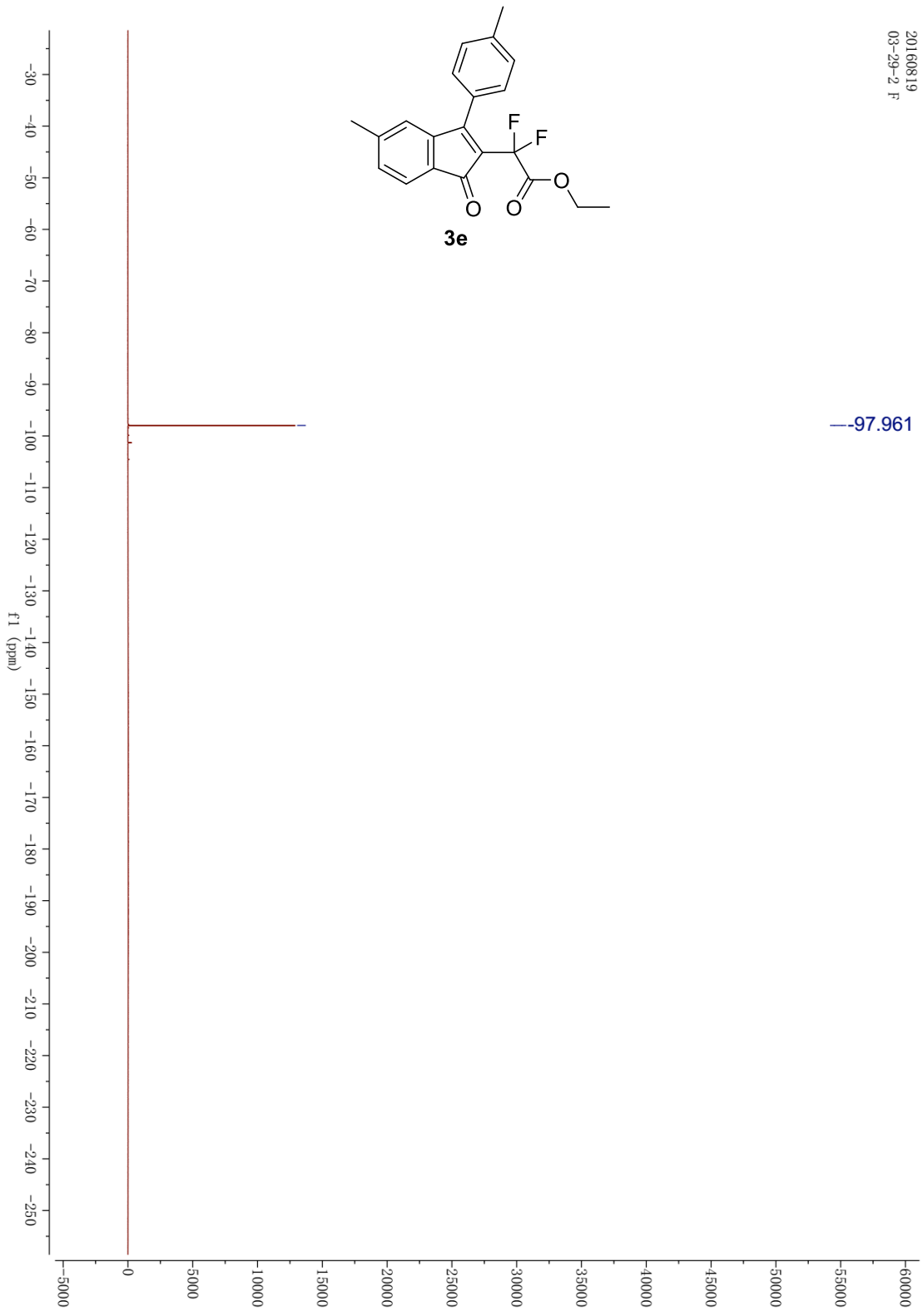
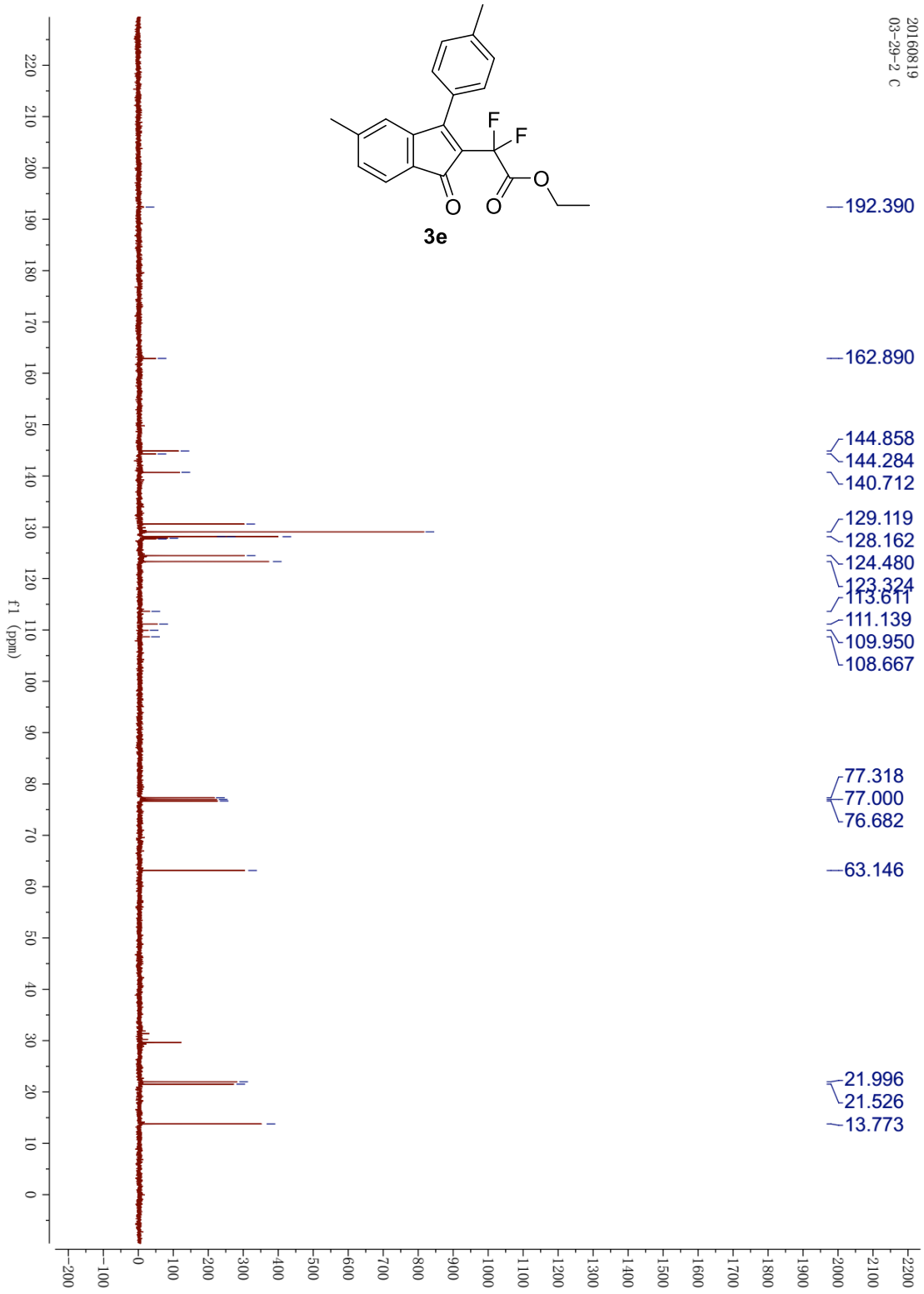
7.381
7.377
7.361
7.358
7.262
7.082
4.302
4.284
4.266
4.249
1.329
1.311
1.293
0.000
5.97
0.95
0.90
2.00
3.21
f1 (ppm)

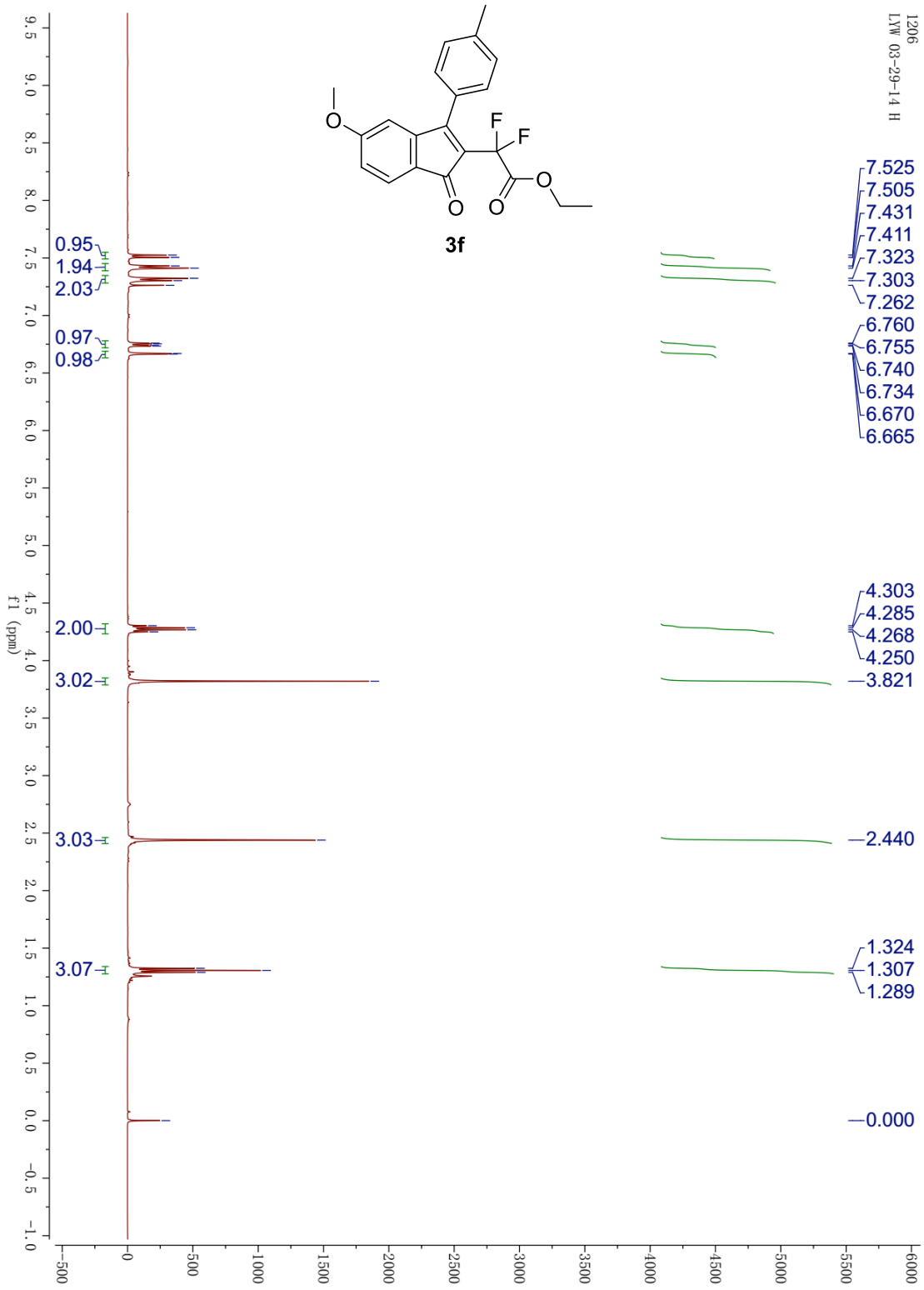

20161206
03-29-3' F
Cl
F
F
O
O
O
3d
-98.495
f1 (ppm)

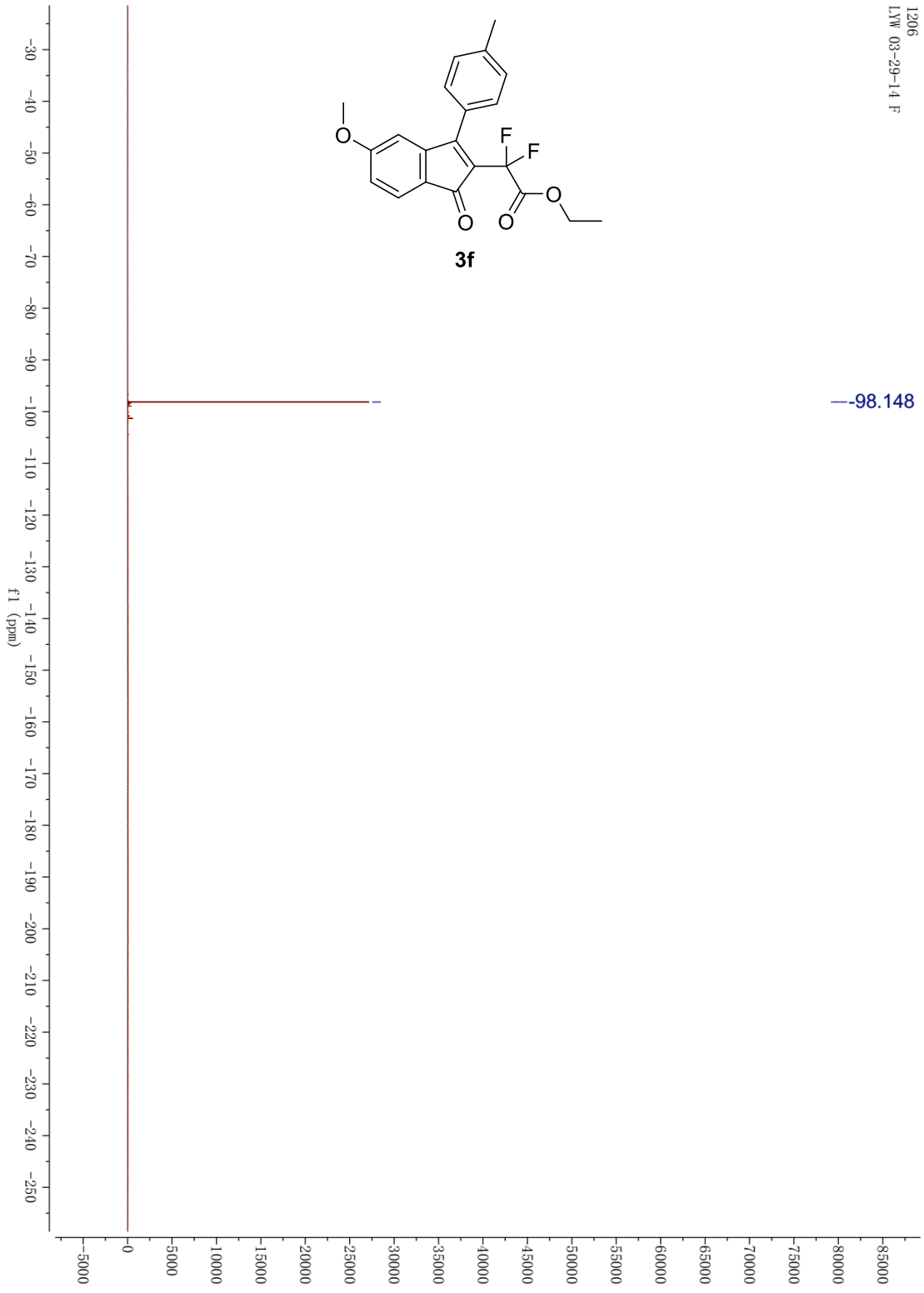

New folder
03-29-3' C
Cl
F
F
O
O
O
3d
f1 (ppm)
191.092
162.573
161.675
145.800
140.293
130.679
130.372
128.659
128.010
124.346
113.327
110.843
108.359
77.318
77.000
76.682
63.351
13.790

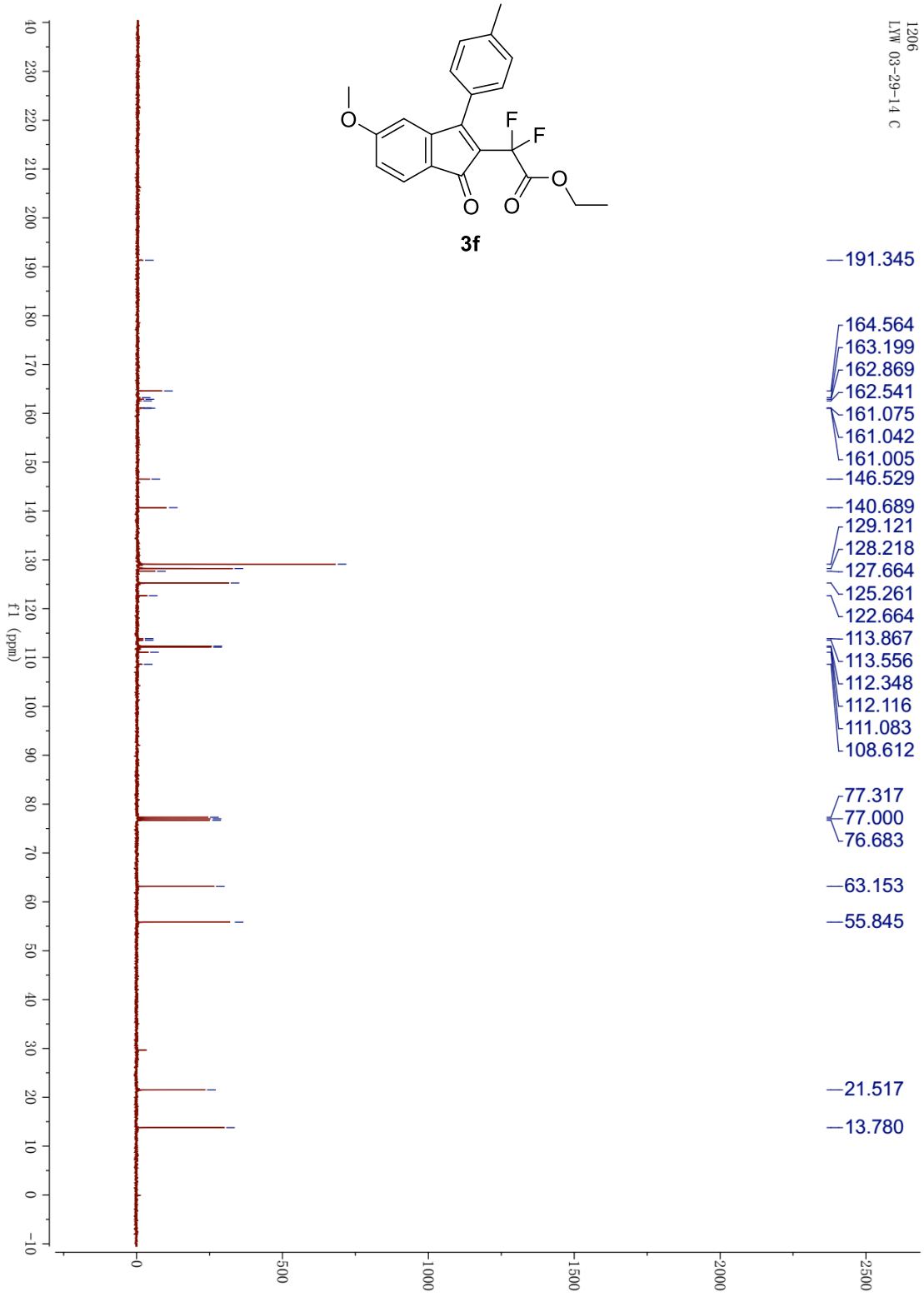

20160819
03-29-2 H
3e
F
F
O
O
O
7.452
7.444
7.434
7.424
7.340
7.320
7.259
7.159
7.141
6.918
4.298
4.280
4.263
4.245
2.448
2.340
1.321
1.303
1.286
0.000
2.94
1.93
1.04
0.95
2.00
3.01
2.93
3.28
f1 (ppm)

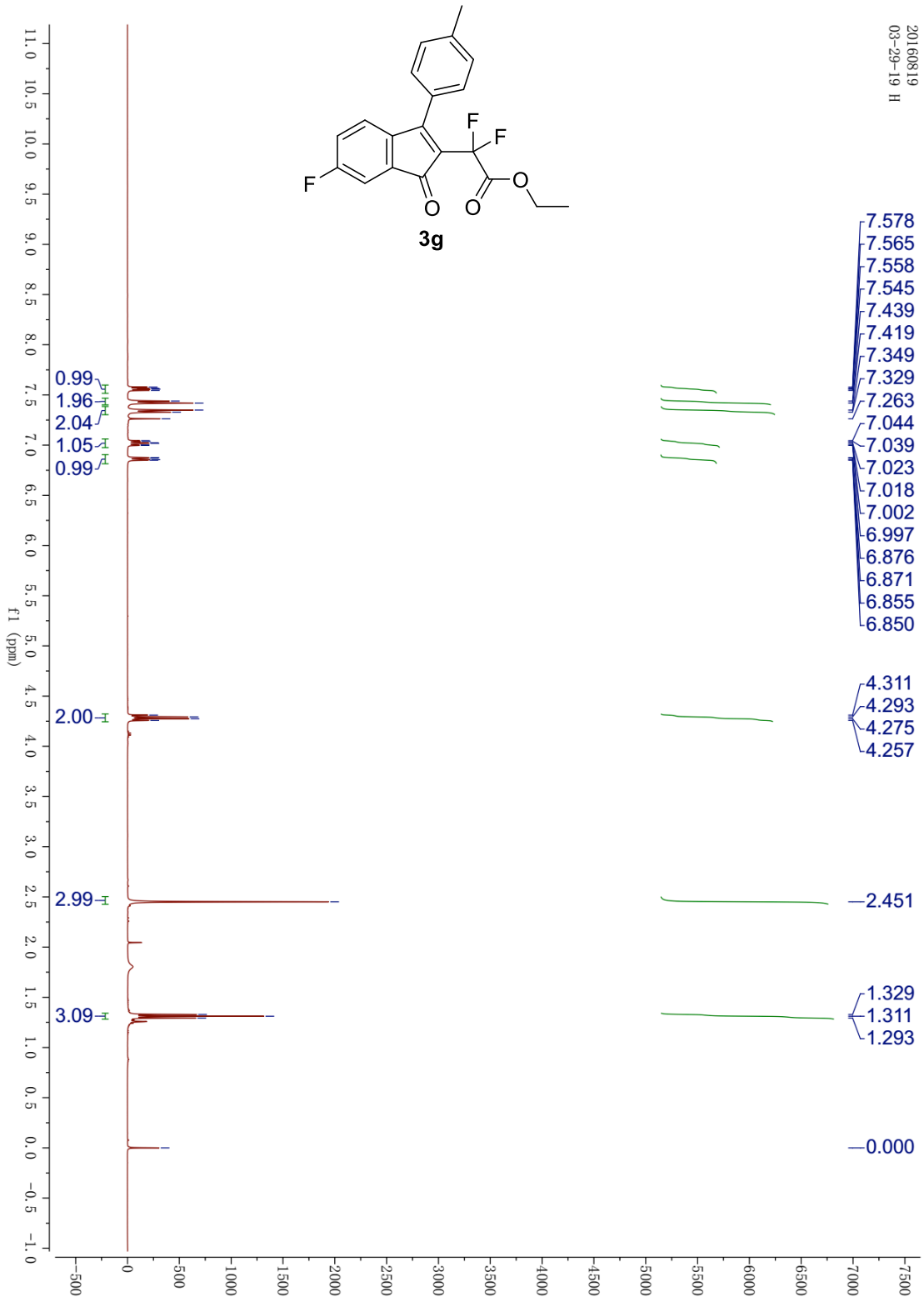

20160819
03-29-2 F
F
F
O
O
O
3e
-97.961
f1 (ppm)

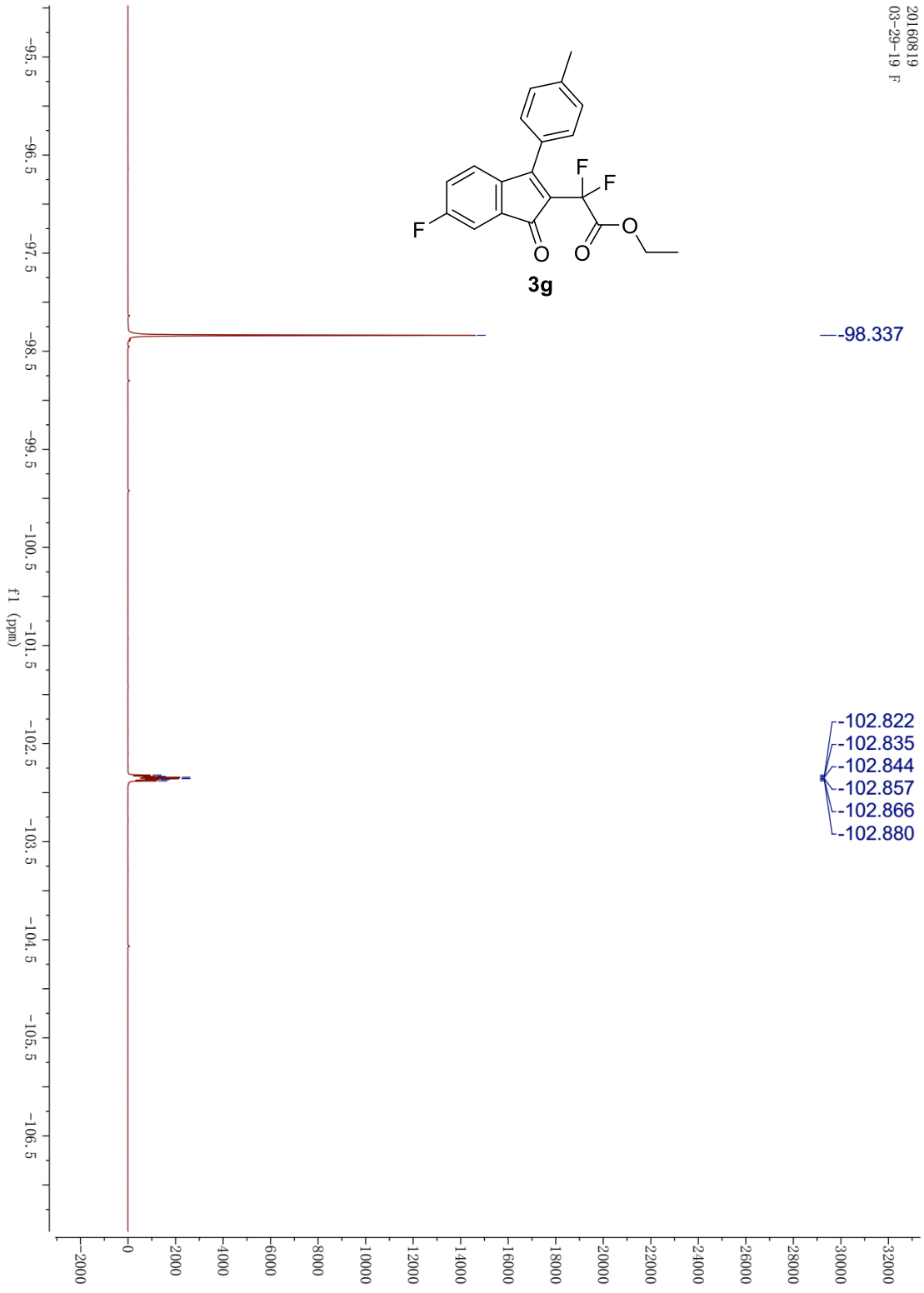

20160819
03-29-2 C
F
F
O
O
O
3e
192.390
162.890
144.858
144.284
140.712
129.119
128.162
124.480
123.324
113.611
111.139
109.950
108.667
77.318
77.000
76.682
63.146
21.996
21.526
13.773
f1 (ppm)

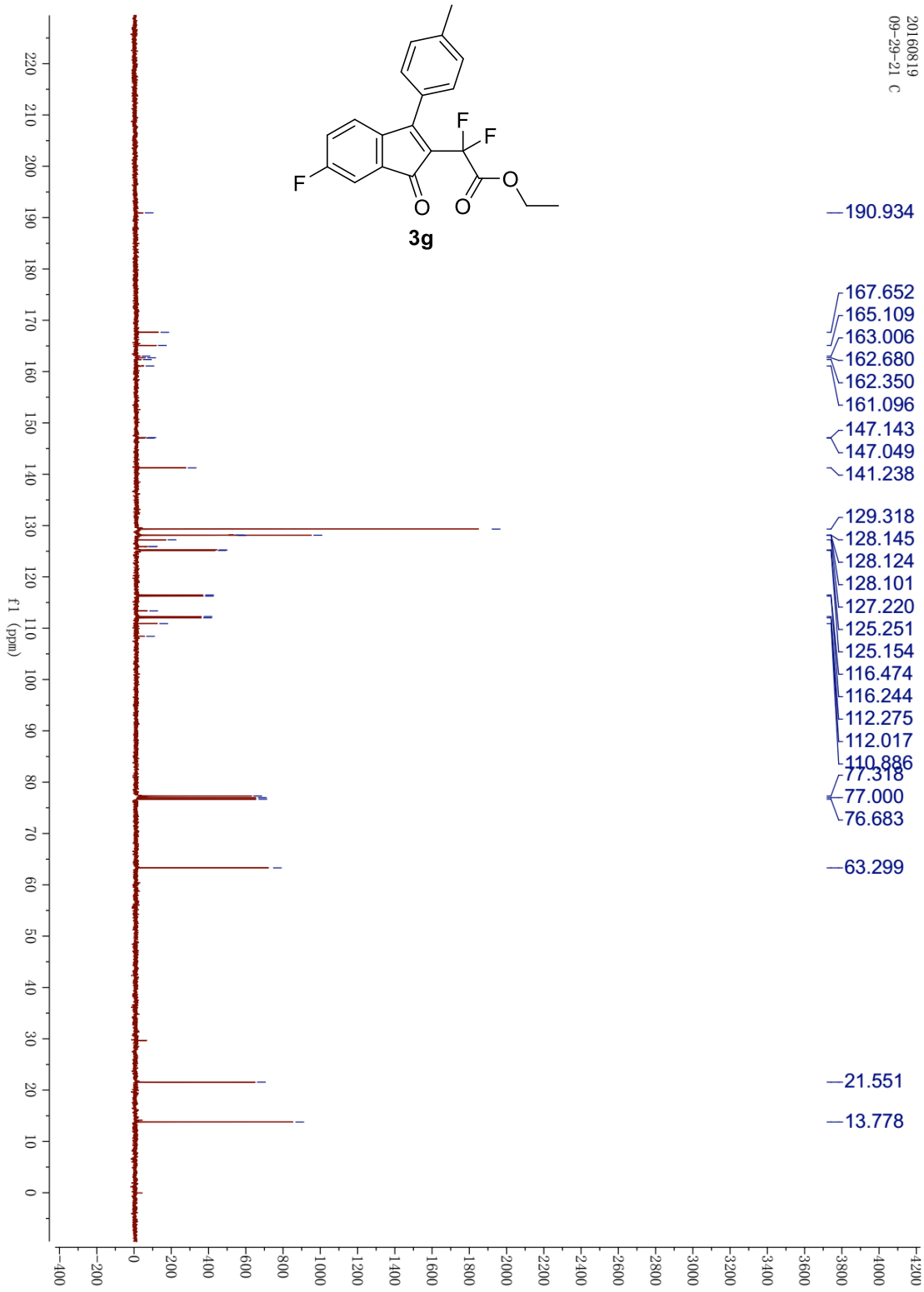

1206
LYW 03-29-14 H
3f
7.525
7.505
7.431
7.411
7.323
7.303
7.262
6.760
6.755
6.740
6.734
6.670
6.665
4.303
4.285
4.268
4.250
3.821
2.440
1.324
1.307
1.289
0.000
0.95
1.94
2.03
0.97
0.98
2.00
3.02
3.03
3.07
f1 (ppm)

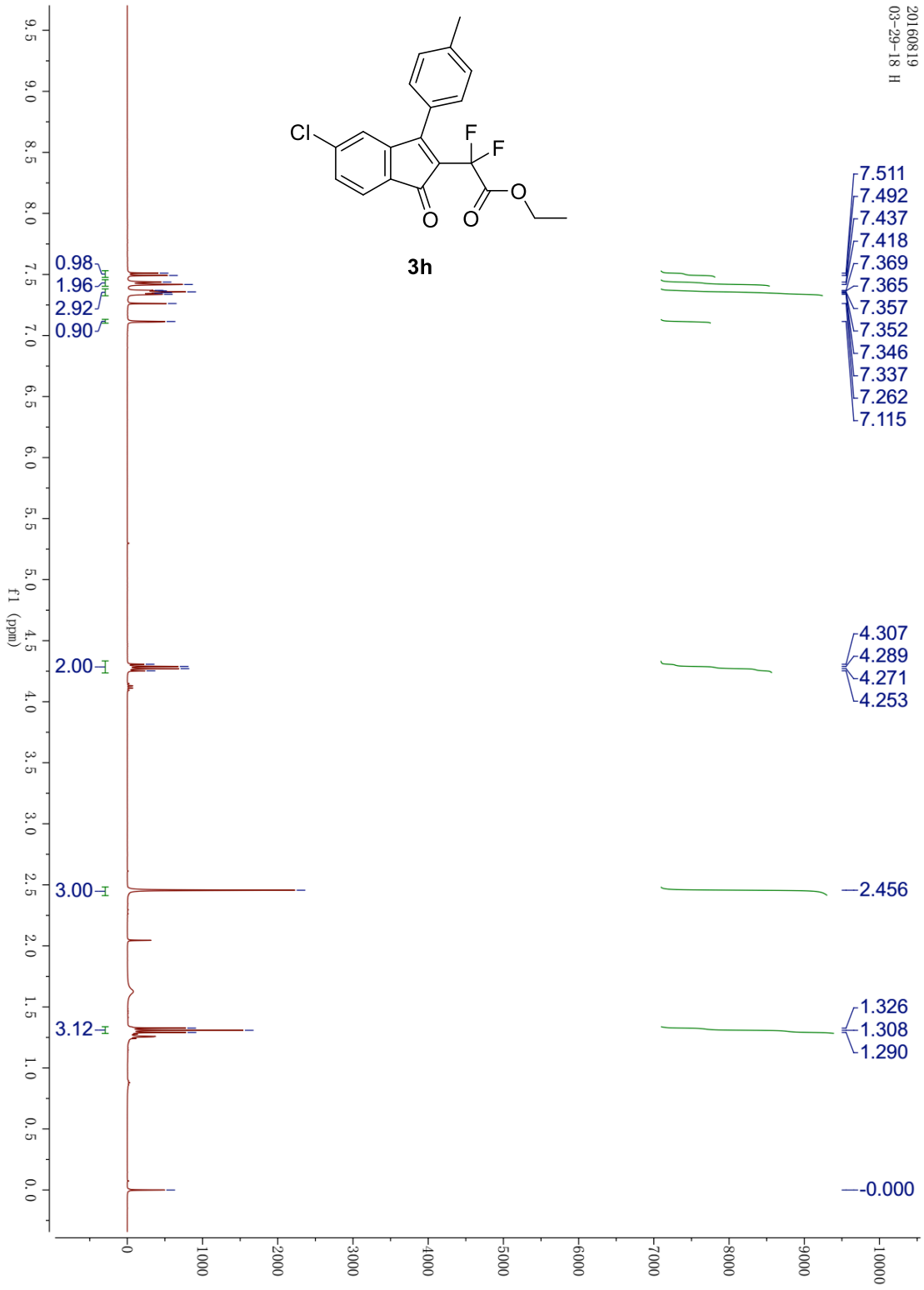

1206
LYW 03-29-14 F
-98.148
f1 (ppm)
3f

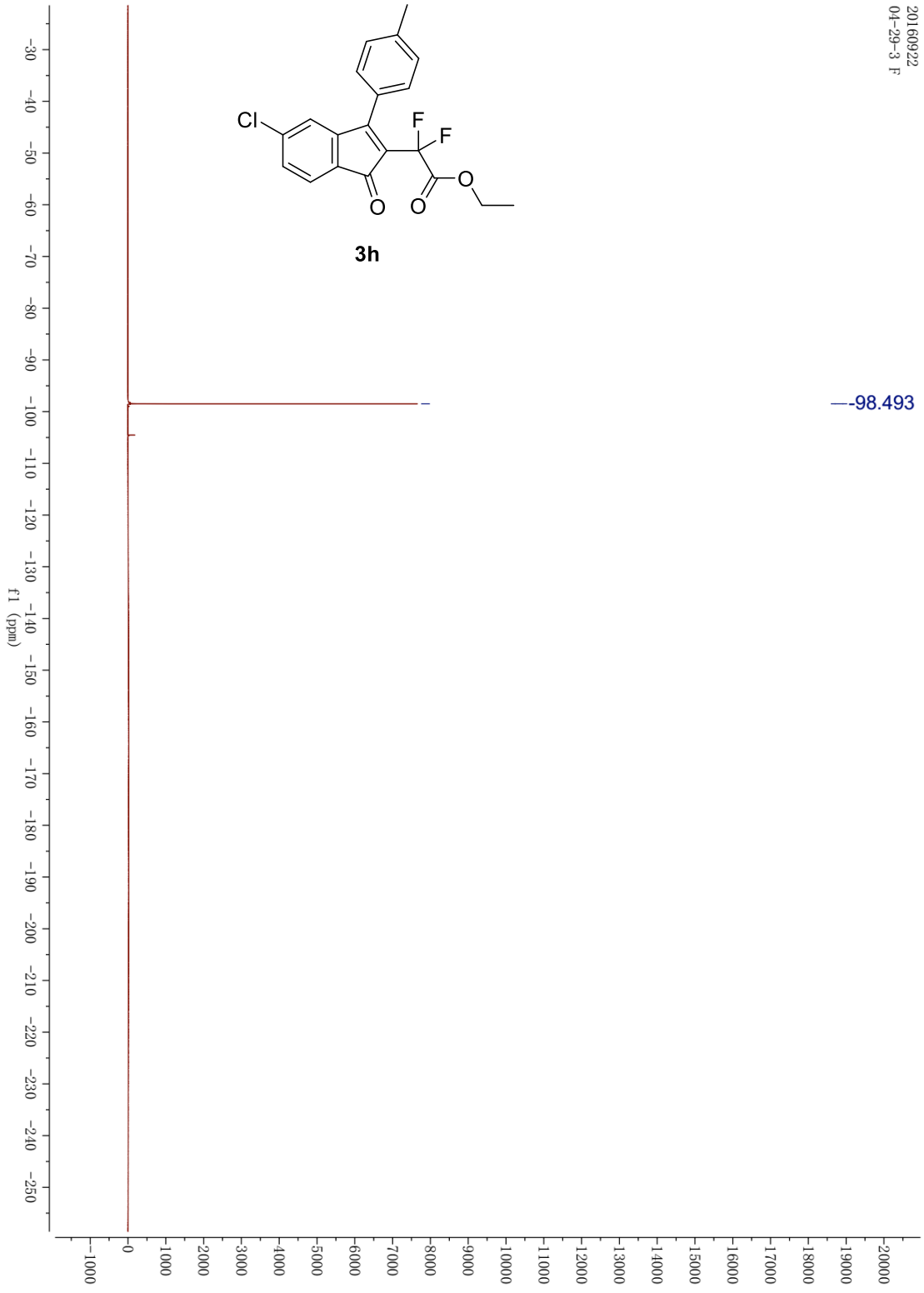

1206
LYW 03-29-14 C
3f
191.345
164.564
163.199
162.869
162.541
161.075
161.042
161.005
146.529
140.689
129.121
128.218
127.664
125.261
122.664
113.867
113.556
112.348
112.116
111.083
108.612
77.317
77.000
76.683
63.153
55.845
21.517
13.780
f1 (ppm)

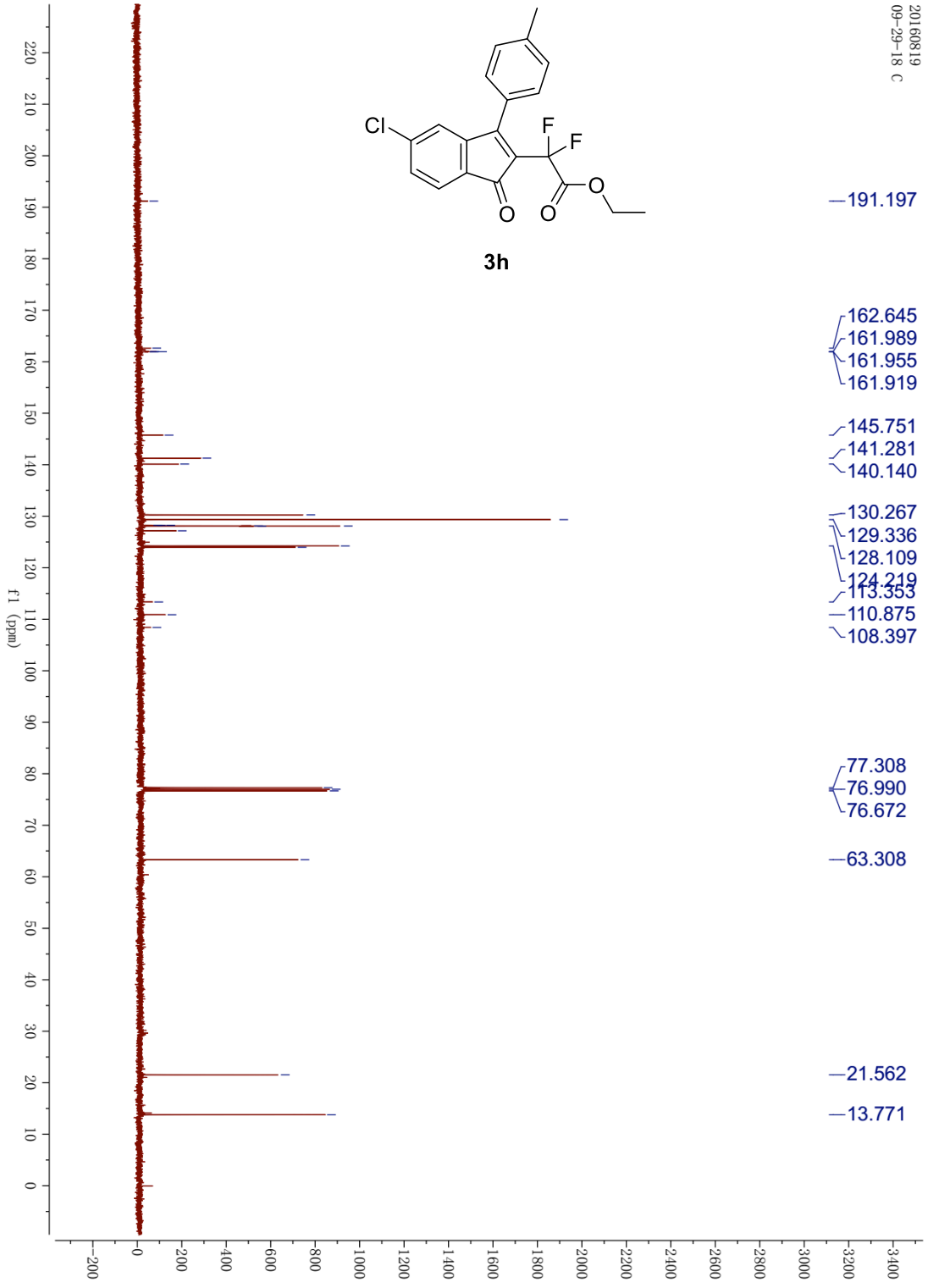

20160819
03-29-19 H
3g
F
F
F
O
O
O
7.578
7.565
7.558
7.545
7.439
7.419
7.349
7.329
7.263
7.044
7.039
7.023
7.018
7.002
6.997
6.876
6.871
6.855
6.850
4.311
4.293
4.275
4.257
2.451
1.329
1.311
1.293
0.000
0.99
1.96
2.04
1.05
0.99
2.00
2.99
3.09
f1 (ppm)

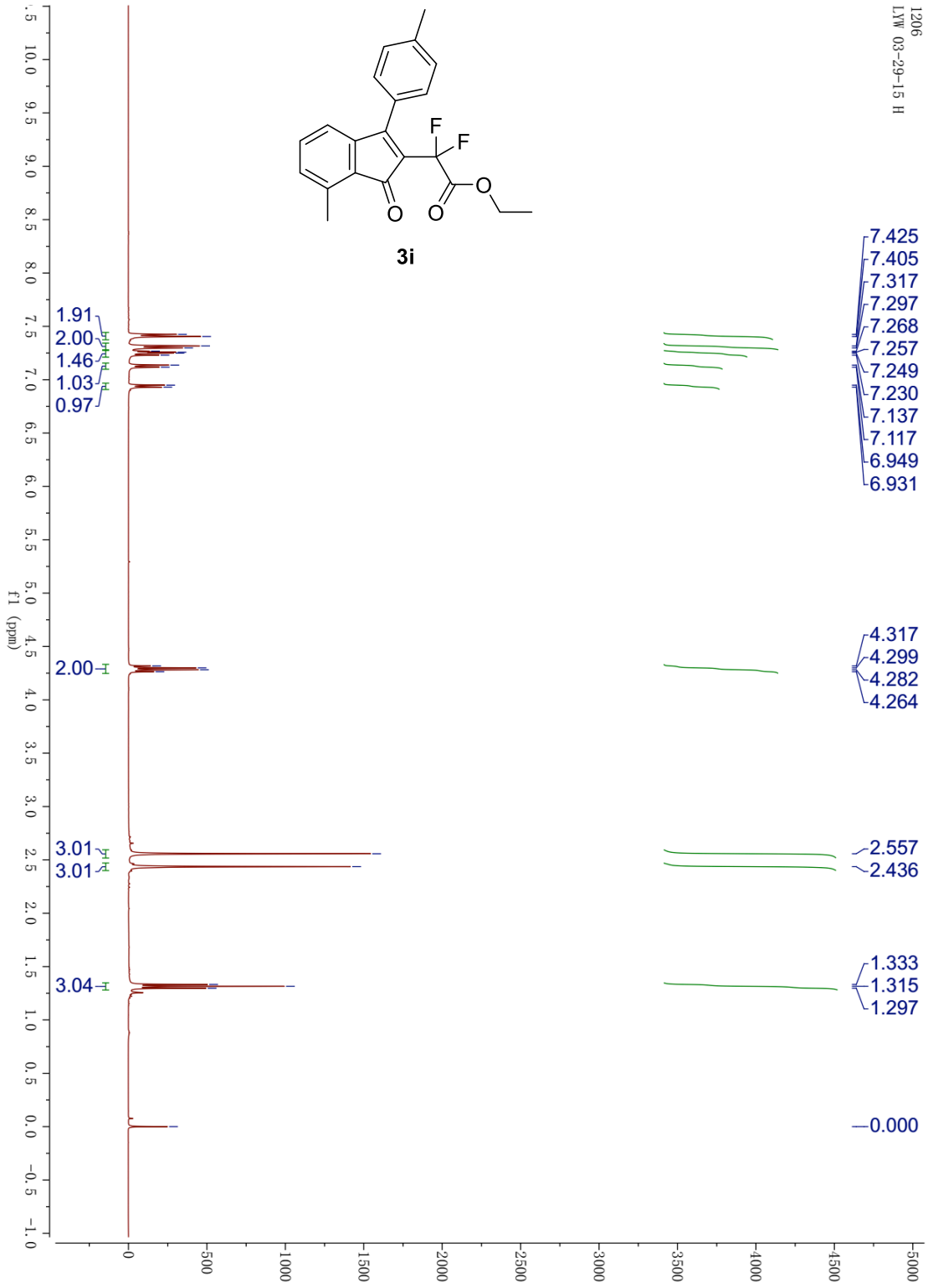

20160819
03-29-19 F
3g
-98.337
-102.822
-102.835
-102.844
-102.857
-102.866
-102.880
f1 (ppm)

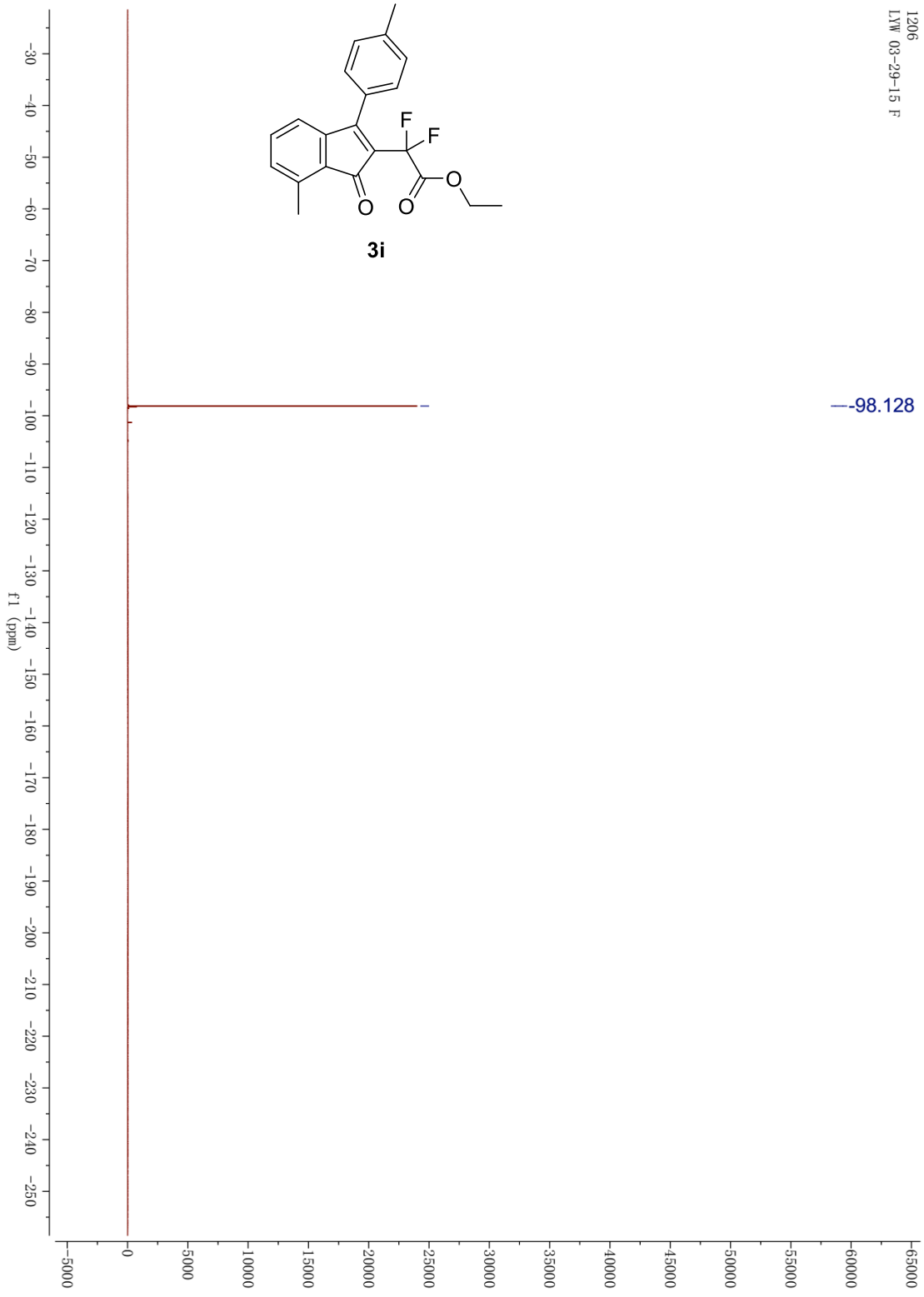

20160819
09-29-21 C
F
F
F
O
O
O
3g
190.934
167.652
165.109
163.006
162.680
162.350
161.096
147.143
147.049
141.238
129.318
128.145
128.124
128.101
127.220
125.251
125.154
116.474
116.244
112.275
112.017
110.886
77.318
77.000
76.683
63.299
21.551
13.778
f1 (ppm)

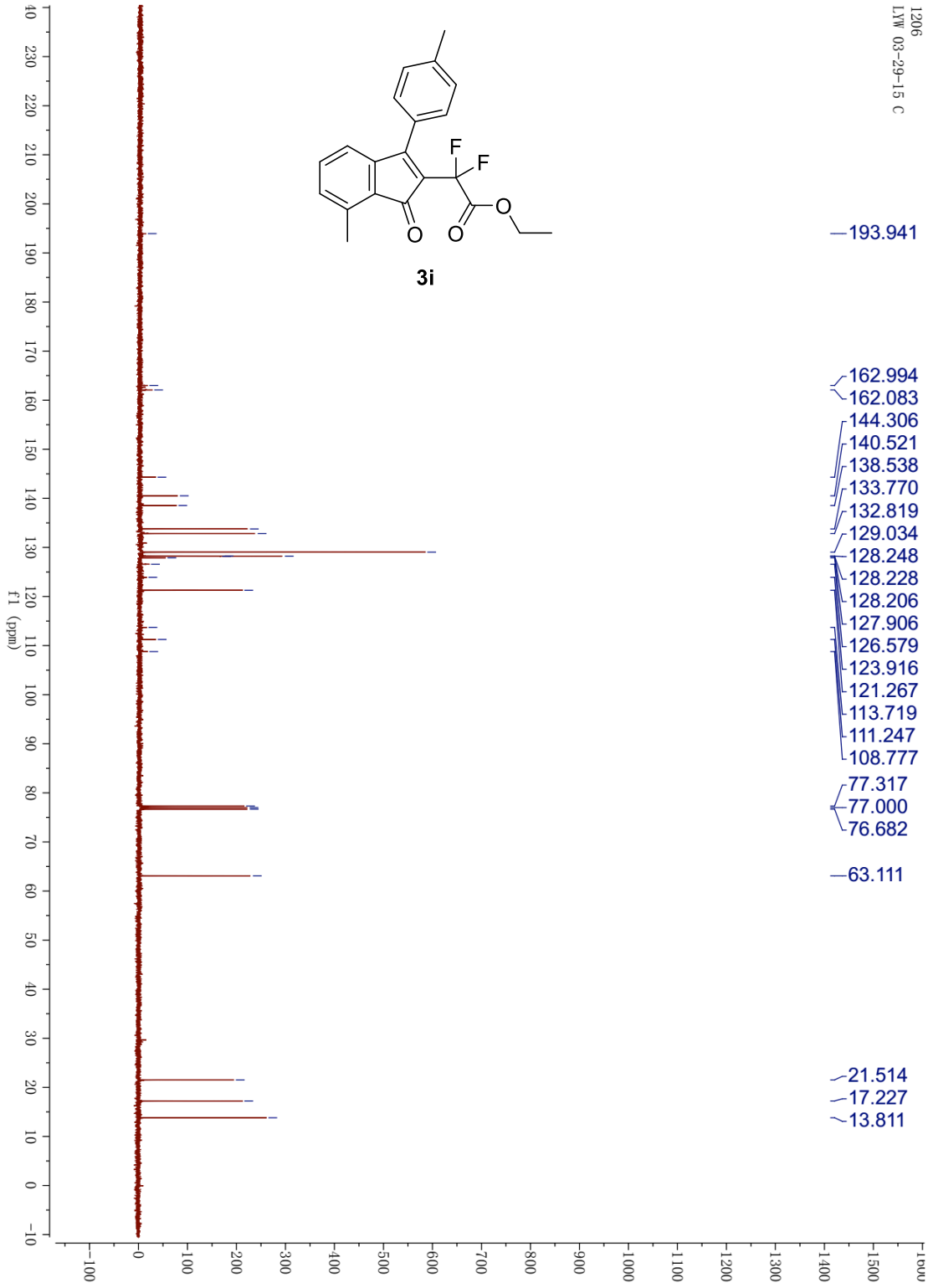

20160819
03-29-18 H
Cl
F
F
O
O
O
3h
0.98
1.96
2.92
0.90
2.00
3.00
3.12
7.511
7.492
7.437
7.418
7.369
7.365
7.357
7.352
7.346
7.337
7.262
7.115
4.307
4.289
4.271
4.253
2.456
1.326
1.308
1.290
0.000
f1 (ppm)

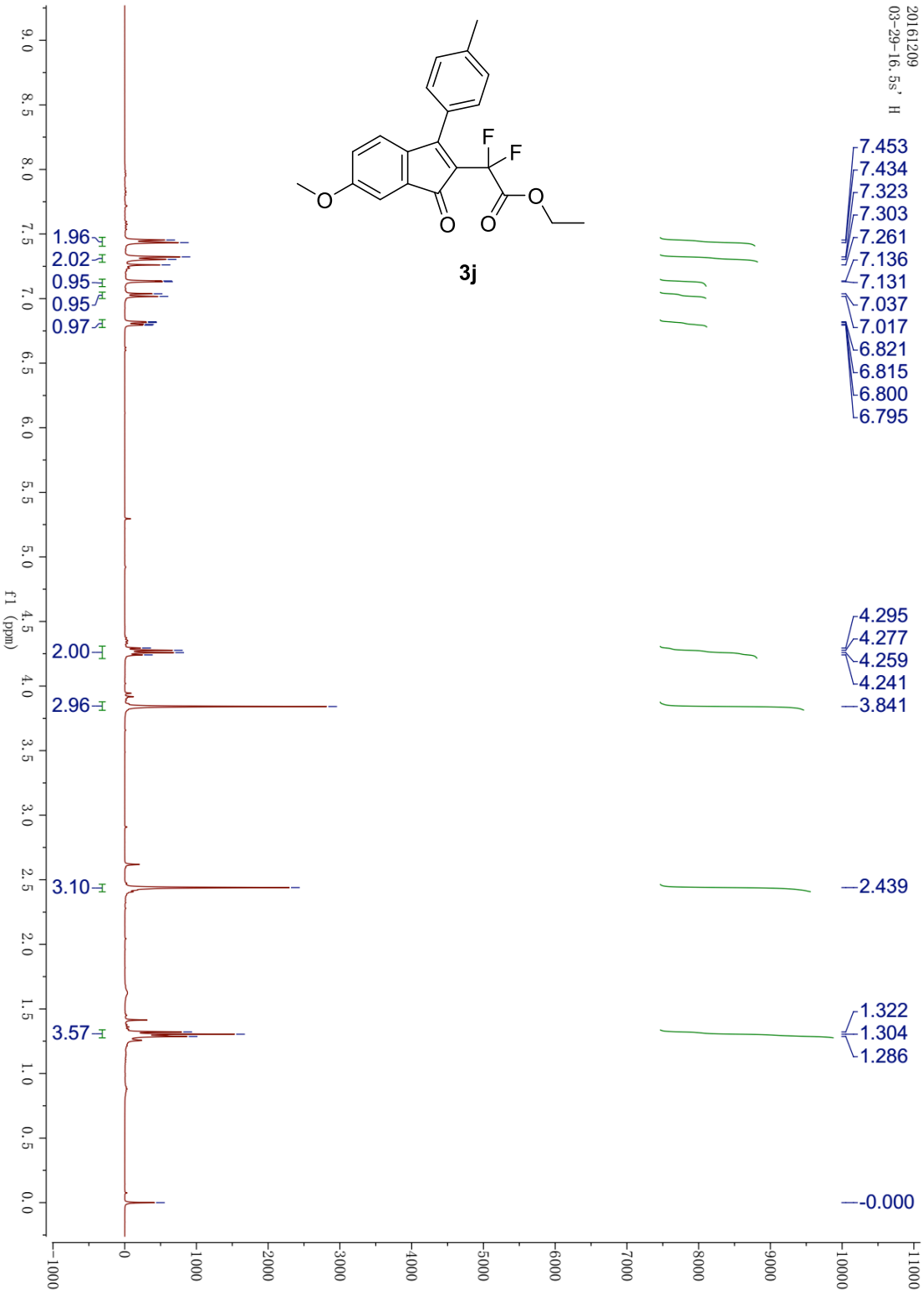

20160922
04-29-3 F
Cl
F
F
O
O
O
3h
-98.493
f1 (ppm)

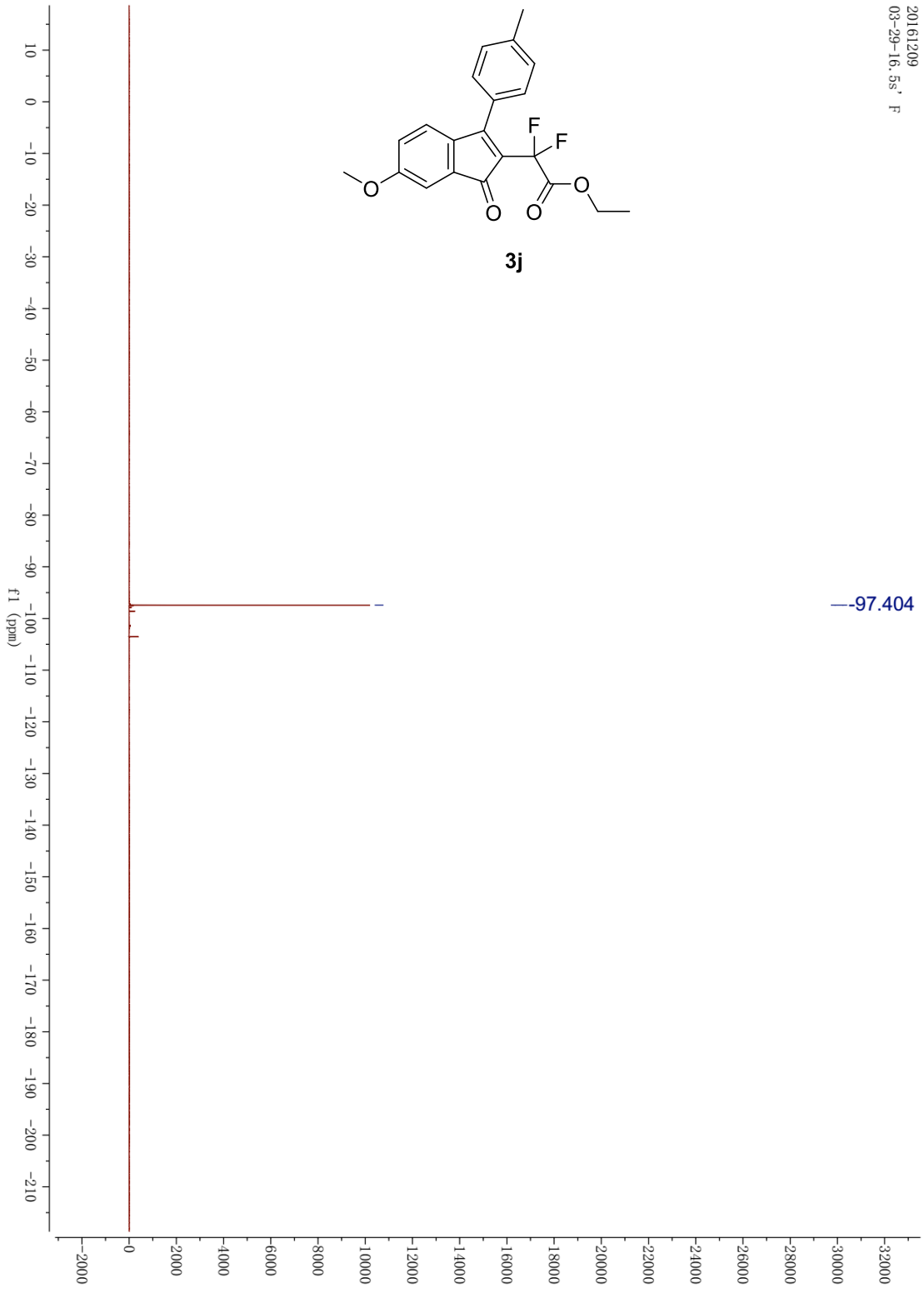

20160819
09-29-18 C
Cl
F
F
O
O
O
3h
191.197
162.645
161.989
161.955
161.919
145.751
141.281
140.140
130.267
129.336
128.109
124.219
113.353
110.875
108.397
77.308
76.990
76.672
63.308
21.562
13.771
f1 (ppm)

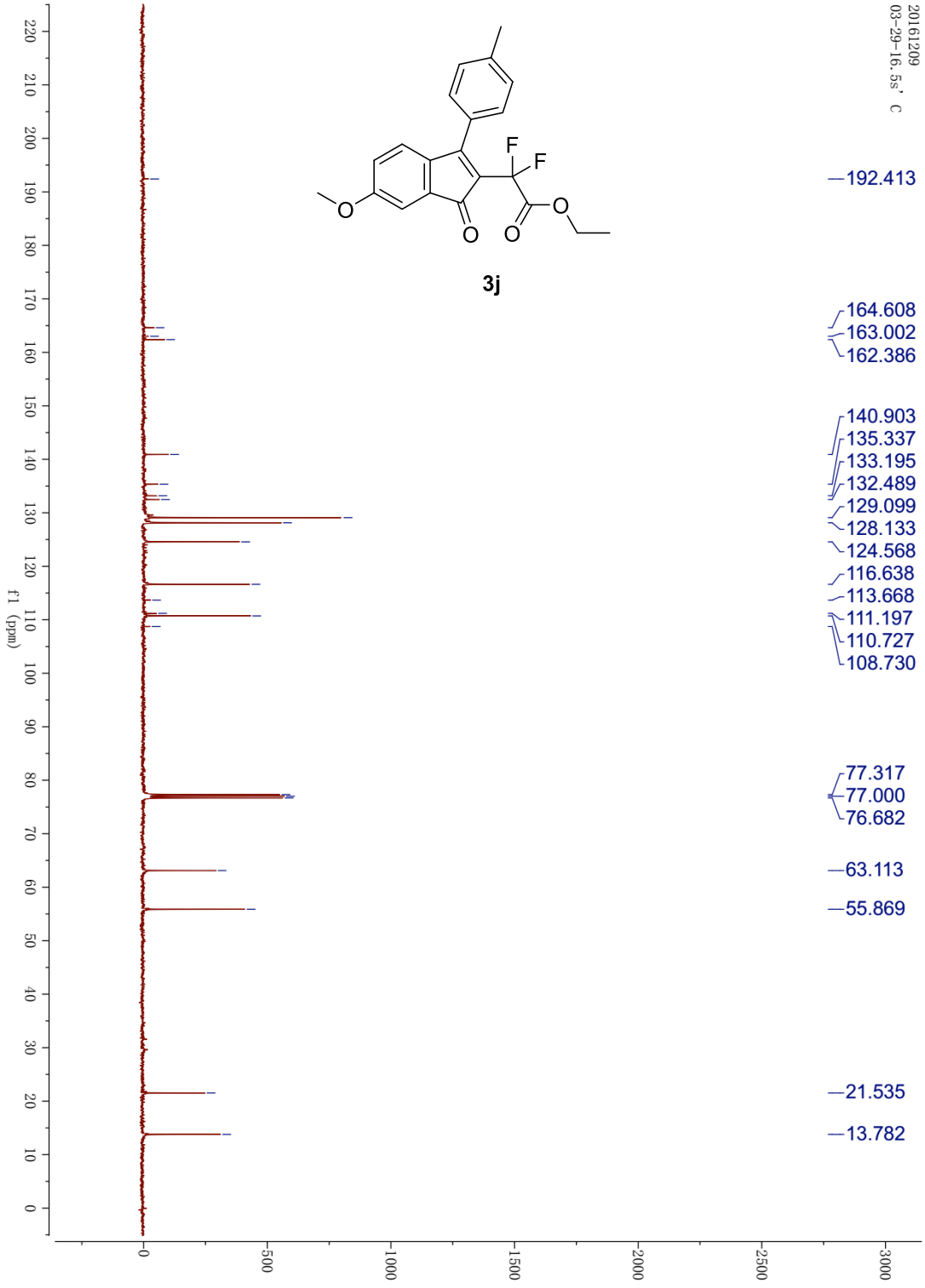

1206
LYW 03-29-15 H
3i
F
F
O
O
O
7.425
7.405
7.317
7.297
7.268
7.257
7.249
7.230
7.137
7.117
6.949
6.931
4.317
4.299
4.282
4.264
2.557
2.436
1.333
1.315
1.297
0.000
1.91
2.00
1.46
1.03
0.97
2.00
3.01
3.01
3.04
f1 (ppm)

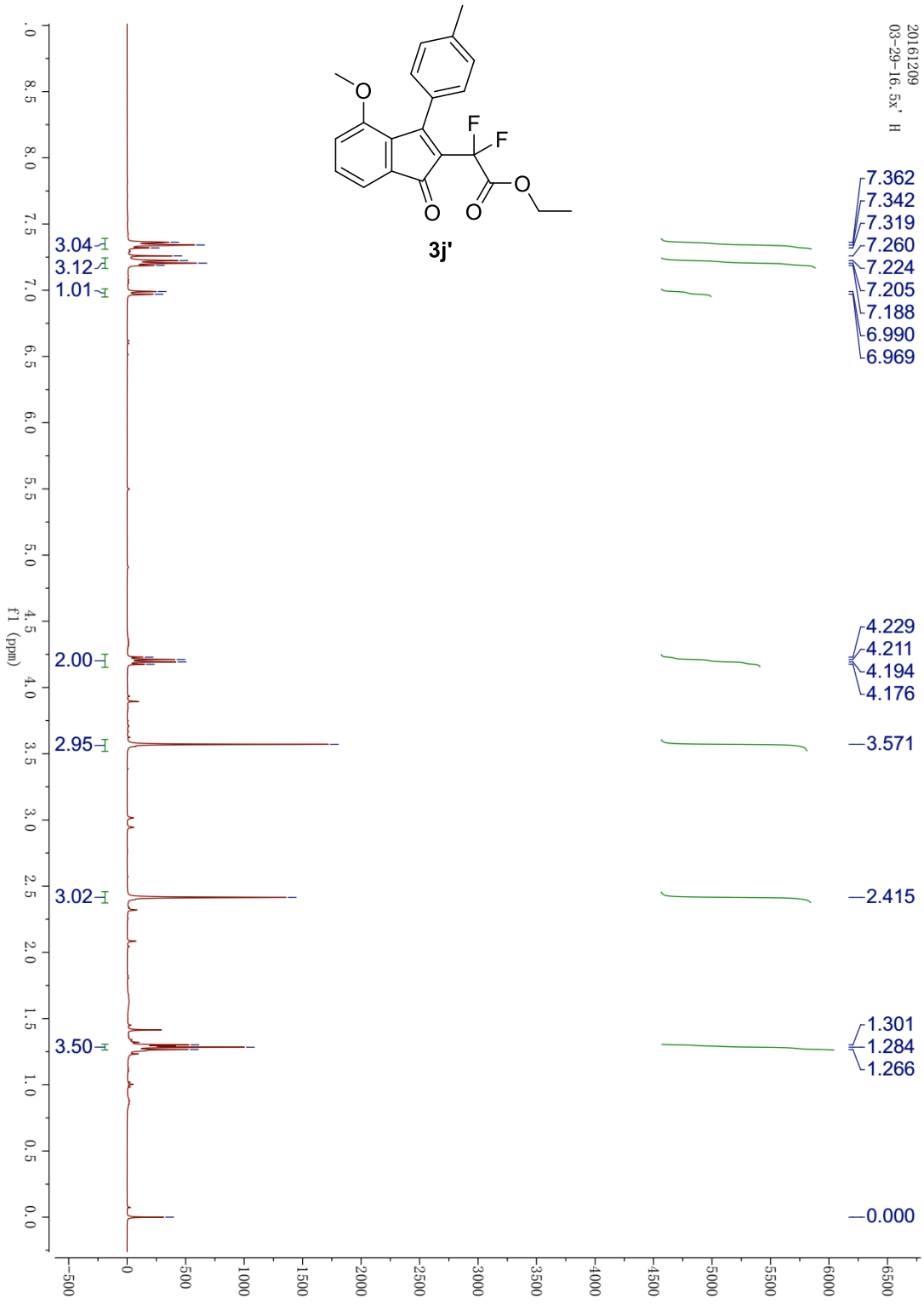

1206
LYW 03-29-15 F
F
F
O
O
O
3i
-98.128
f1 (ppm)
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
-250
-5000
0
5000
10000
15000
20000
25000
30000
35000
40000
45000
50000
55000
60000
65000

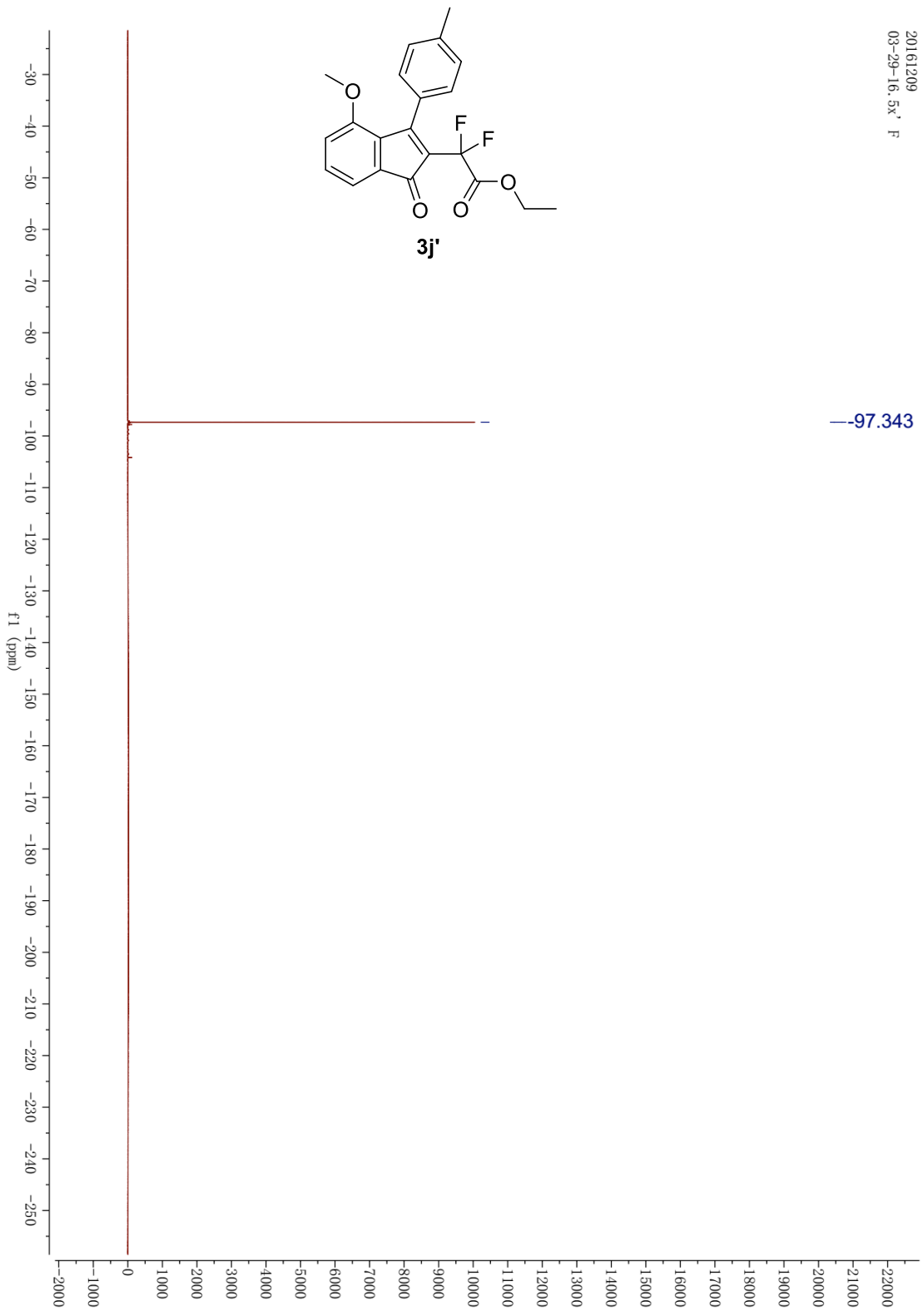

1206
LYW 03-29-15 C
F
F
O
O
O
3i
193.941
162.994
162.083
144.306
140.521
138.538
133.770
132.819
129.034
128.248
128.228
128.206
127.906
126.579
123.916
121.267
113.719
111.247
108.777
77.317
77.000
76.682
63.111
21.514
17.227
13.811
f1 (ppm)

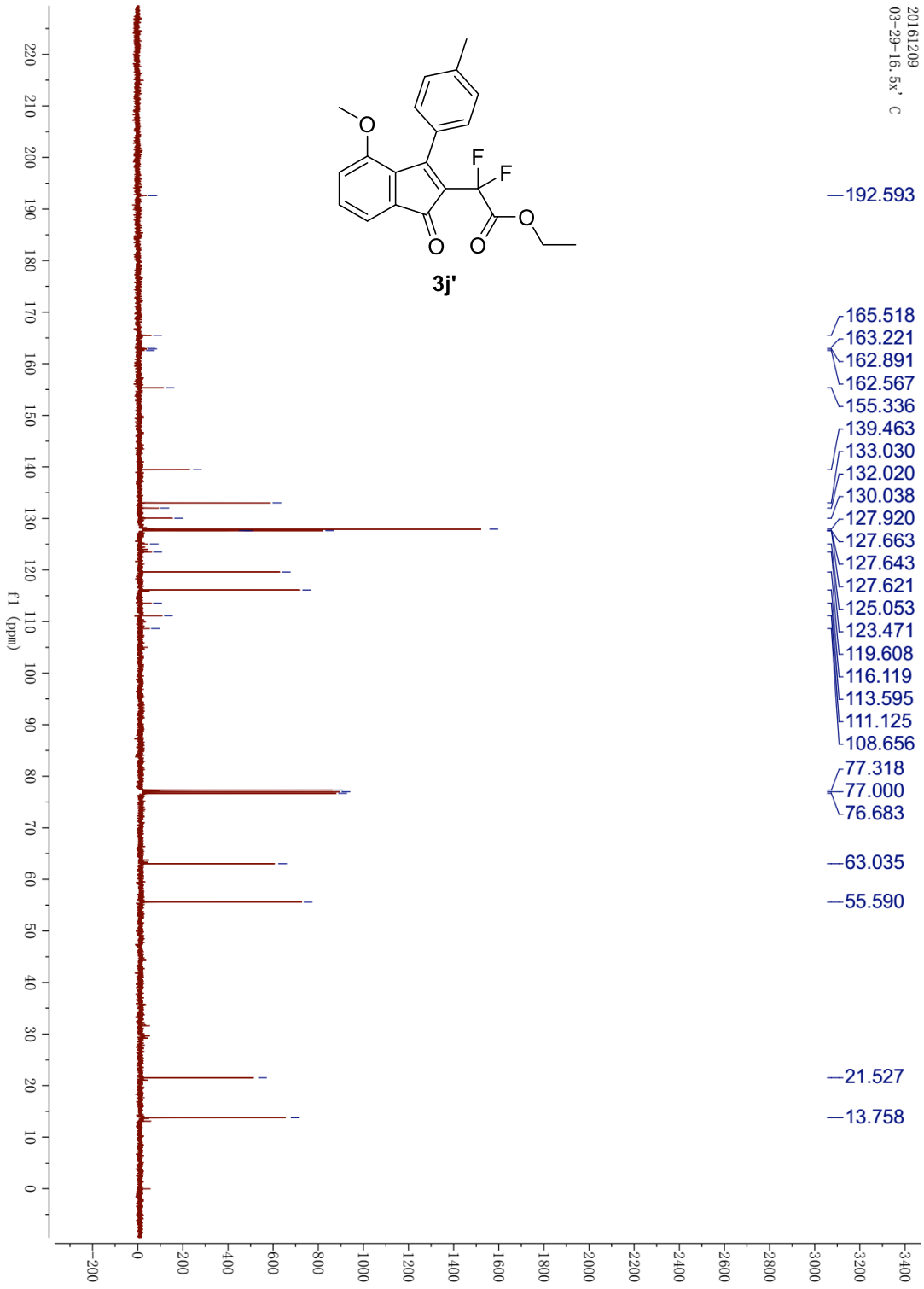

20161209
03-29-16.5s' H
3j
7.453
7.434
7.323
7.303
7.261
7.136
7.131
7.037
7.017
6.821
6.815
6.800
6.795
4.295
4.277
4.259
4.241
3.841
2.439
1.322
1.304
1.286
-0.000
1.96
2.02
0.95
0.95
0.97
2.00
2.96
3.10
3.57
f1 (ppm)

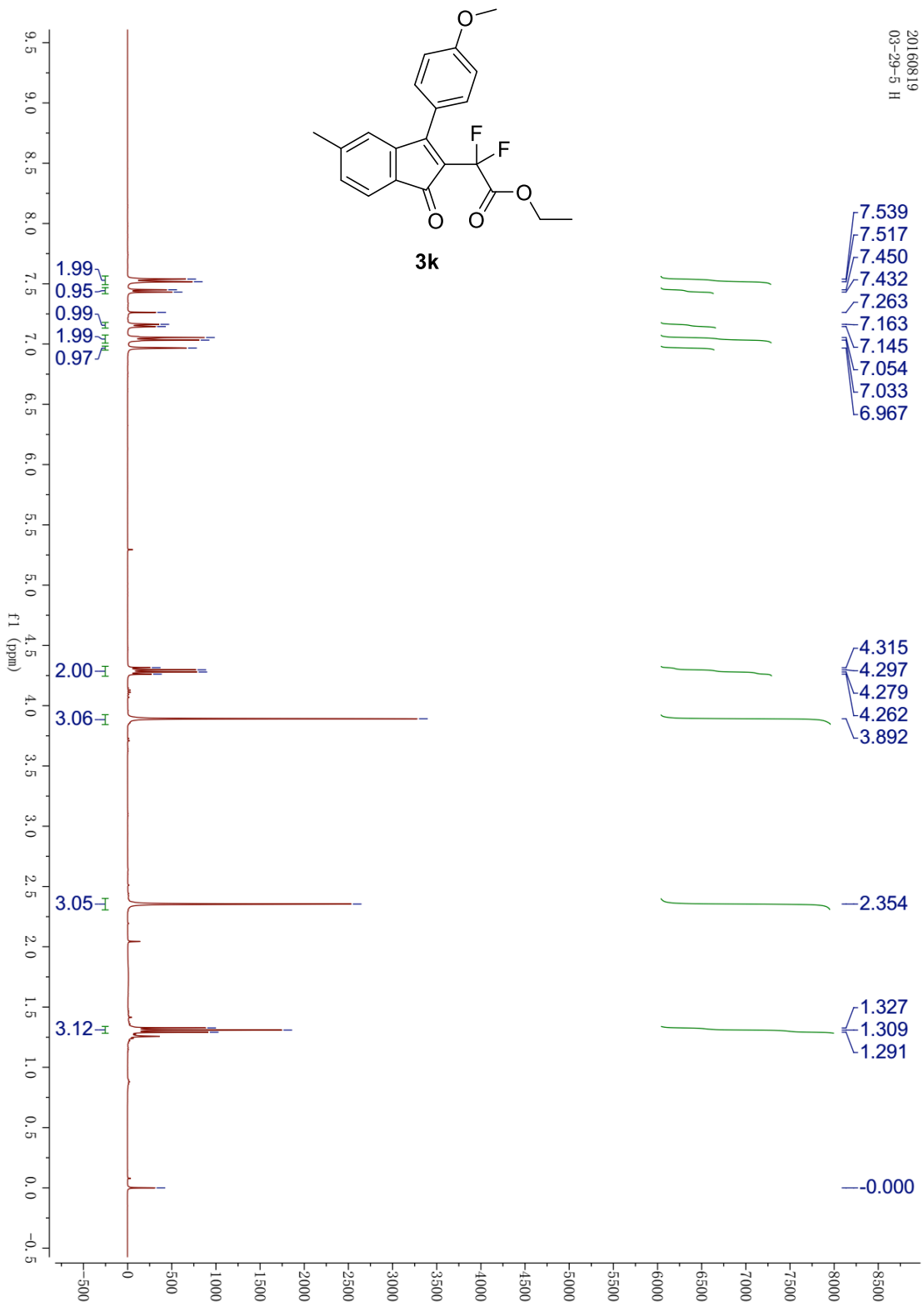

20161209
03-29-16.5s' F
F
F
O
O
O
O
3j
-97.404
f1 (ppm)

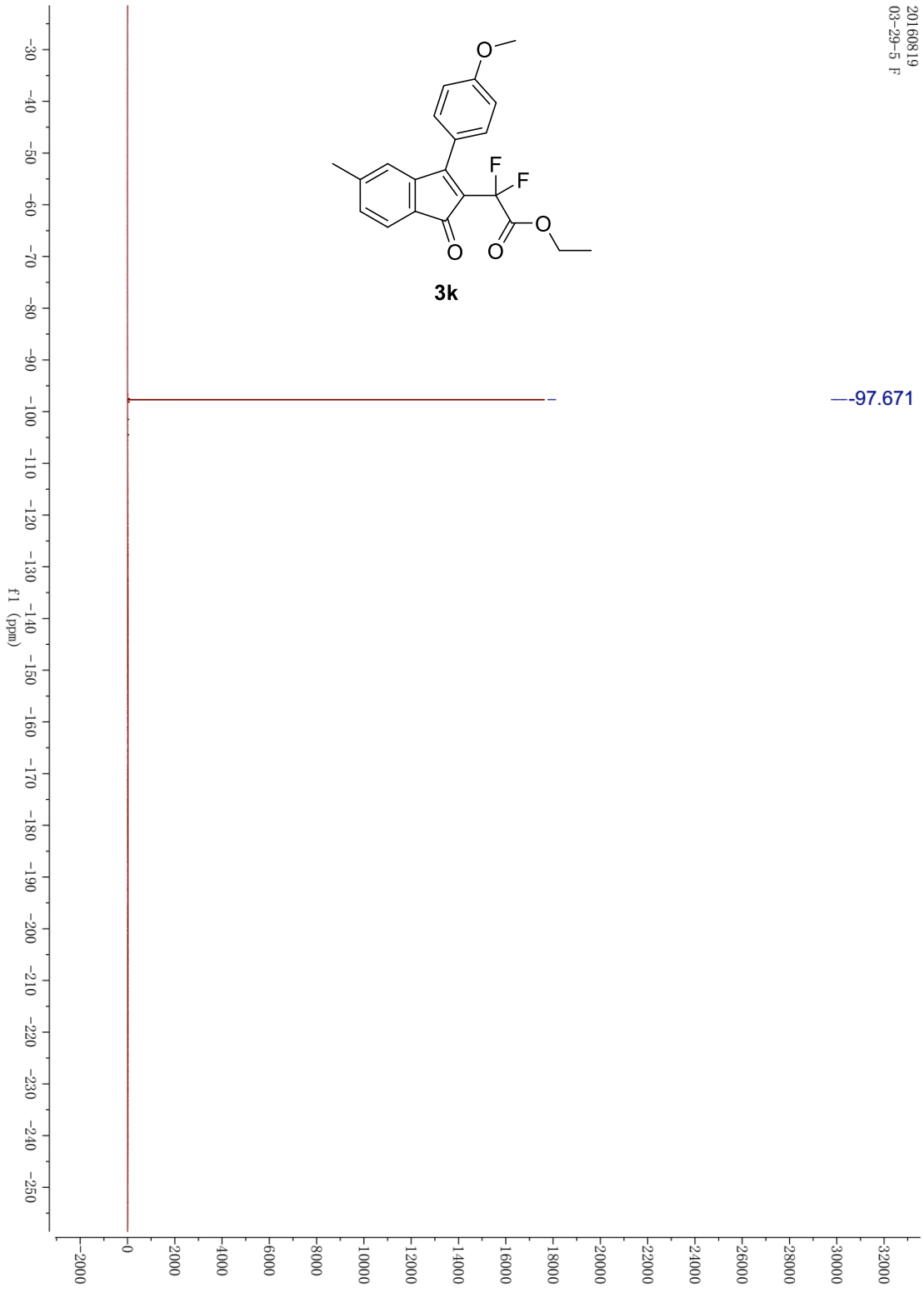

20161209
03-29-16.5s' C
F
F
O
O
O
O
3j
192.413
164.608
163.002
162.386
140.903
135.337
133.195
132.489
129.099
128.133
124.568
116.638
113.668
111.197
110.727
108.730
77.317
77.000
76.682
63.113
55.869
21.535
13.782
f1 (ppm)

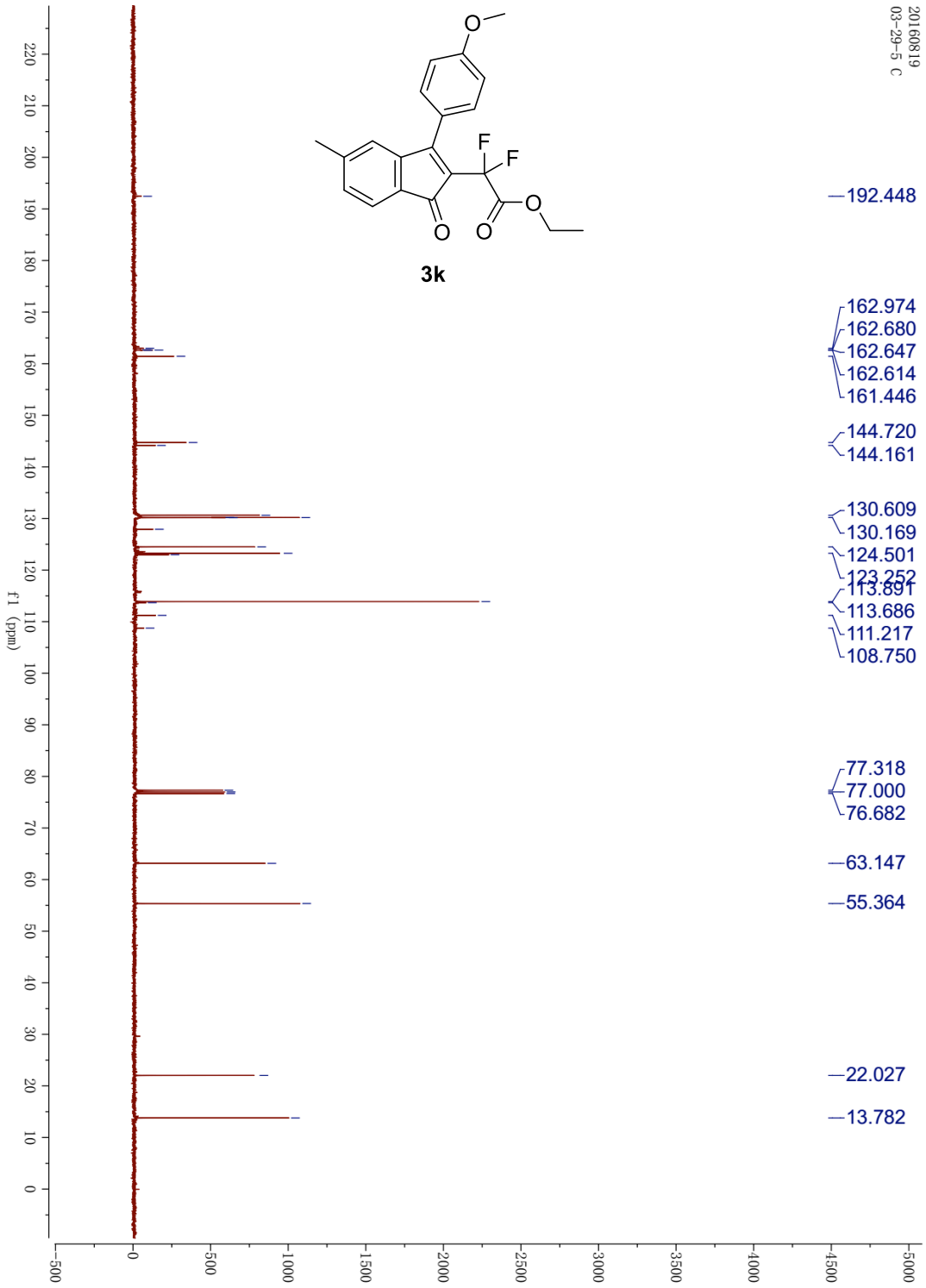

20161209
03-29-16.5x' H
3j'
7.362
7.342
7.319
7.260
7.224
7.205
7.188
6.990
6.969
4.229
4.211
4.194
4.176
3.571
2.415
1.301
1.284
1.266
0.000
3.04
3.12
1.01
2.00
2.95
3.02
3.50
f1 (ppm)

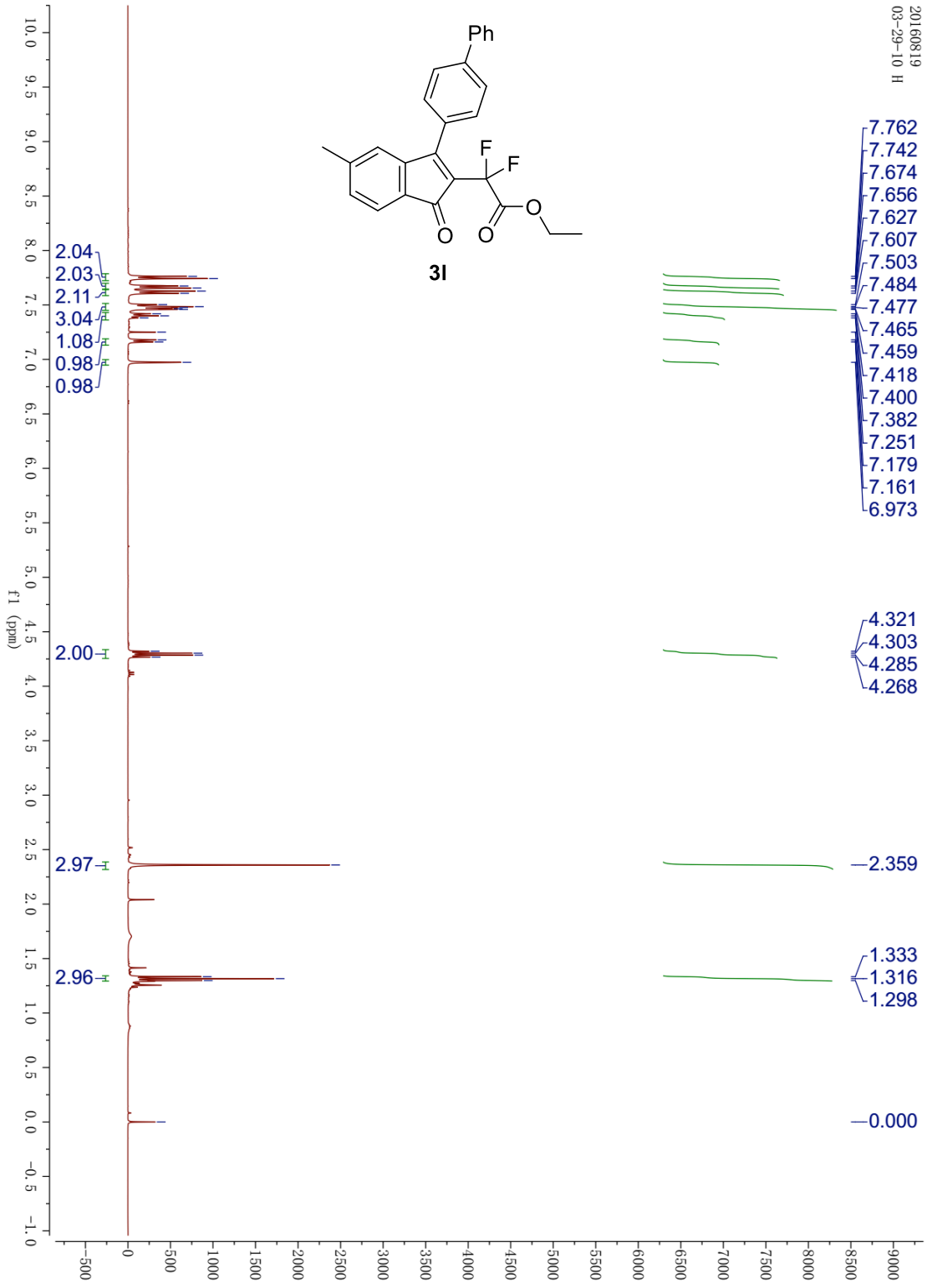

20161209
03-29-16.5x' F
3j'
-97.343
f1 (ppm)

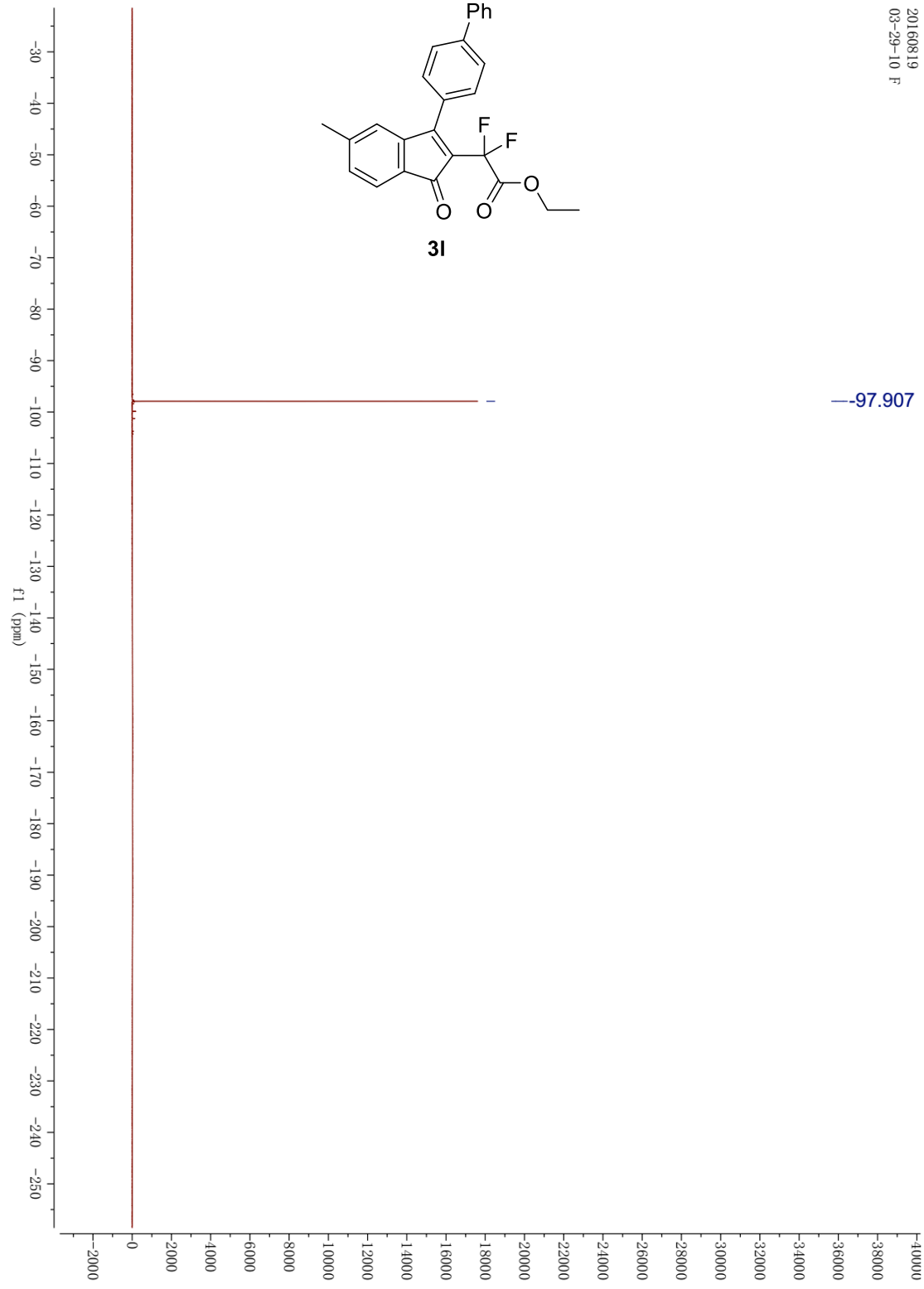

20161209
03-29-16.5x' C
3j'
192.593
165.518
163.221
162.891
162.567
155.336
139.463
133.030
132.020
130.038
127.920
127.663
127.643
127.621
125.053
123.471
119.608
116.119
113.595
111.125
108.656
77.318
77.000
76.683
63.035
55.590
21.527
13.758
f1 (ppm)

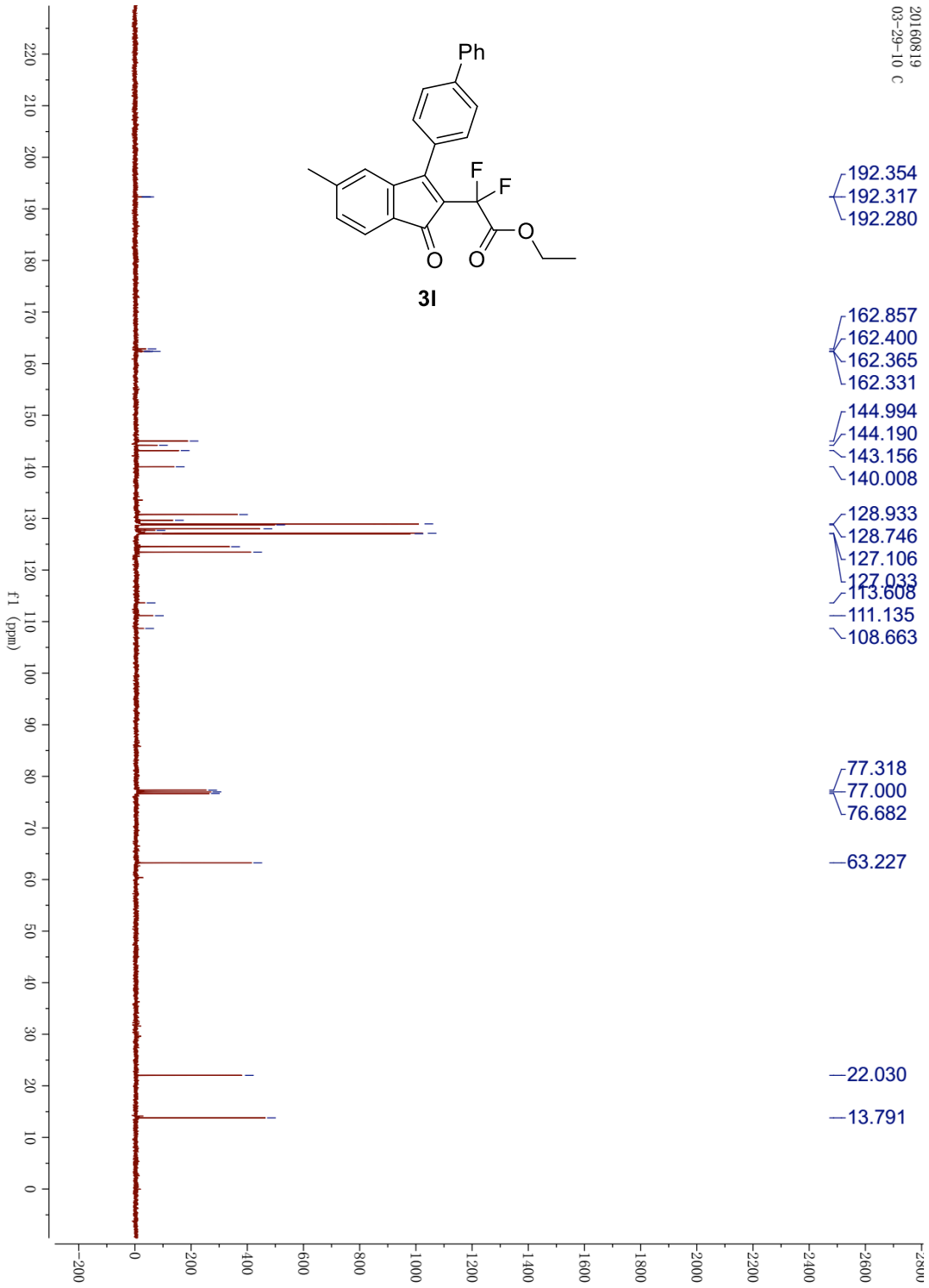

20160819
03-29-5 H
3k
F
F
O
O
O
O
7.539
7.517
7.450
7.432
7.263
7.163
7.145
7.054
7.033
6.967
4.315
4.297
4.279
4.262
3.892
2.354
1.327
1.309
1.291
-0.000
1.99
0.95
0.99
1.99
0.97
2.00
3.06
3.05
3.12
f1 (ppm)

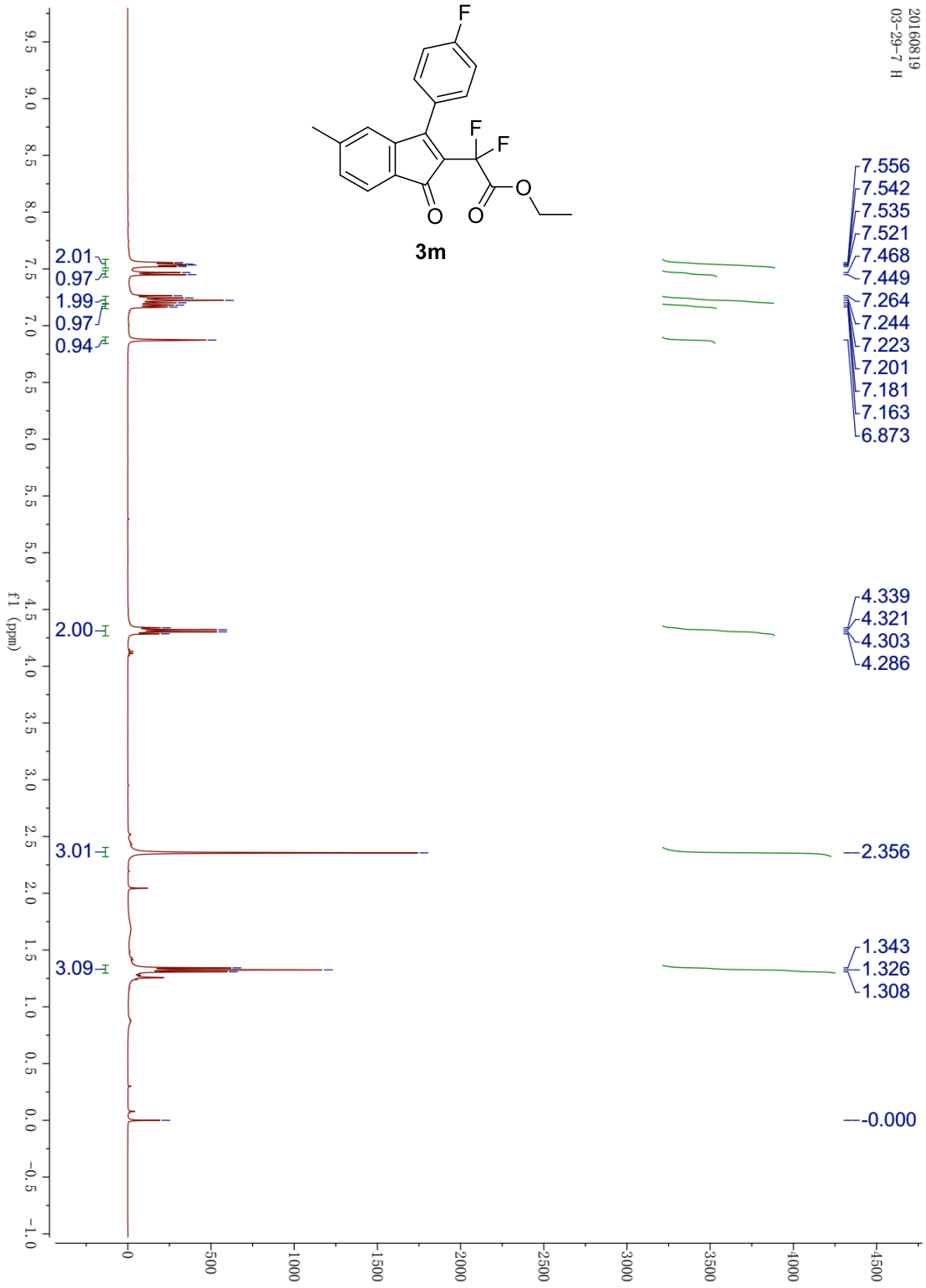

20160819
03-29-5 F
O
F
F
O
O
O
3k
-97.671
f1 (ppm)
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
-250
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000
32000

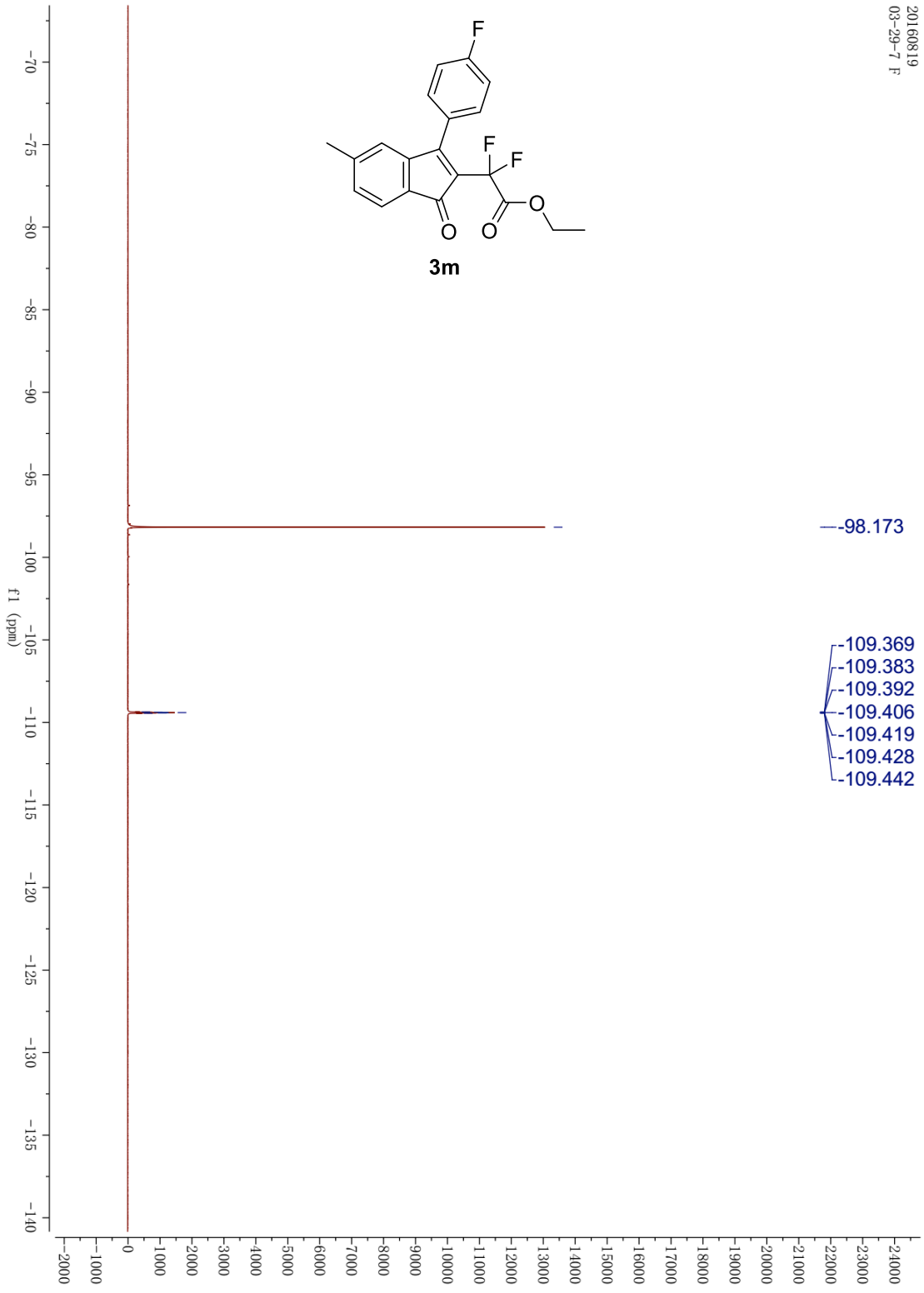

20160819
03-29-5 C
3k
192.448
162.974
162.680
162.647
162.614
161.446
144.720
144.161
130.609
130.169
124.501
123.252
113.891
113.686
111.217
108.750
77.318
77.000
76.682
63.147
55.364
22.027
13.782
f1 (ppm)

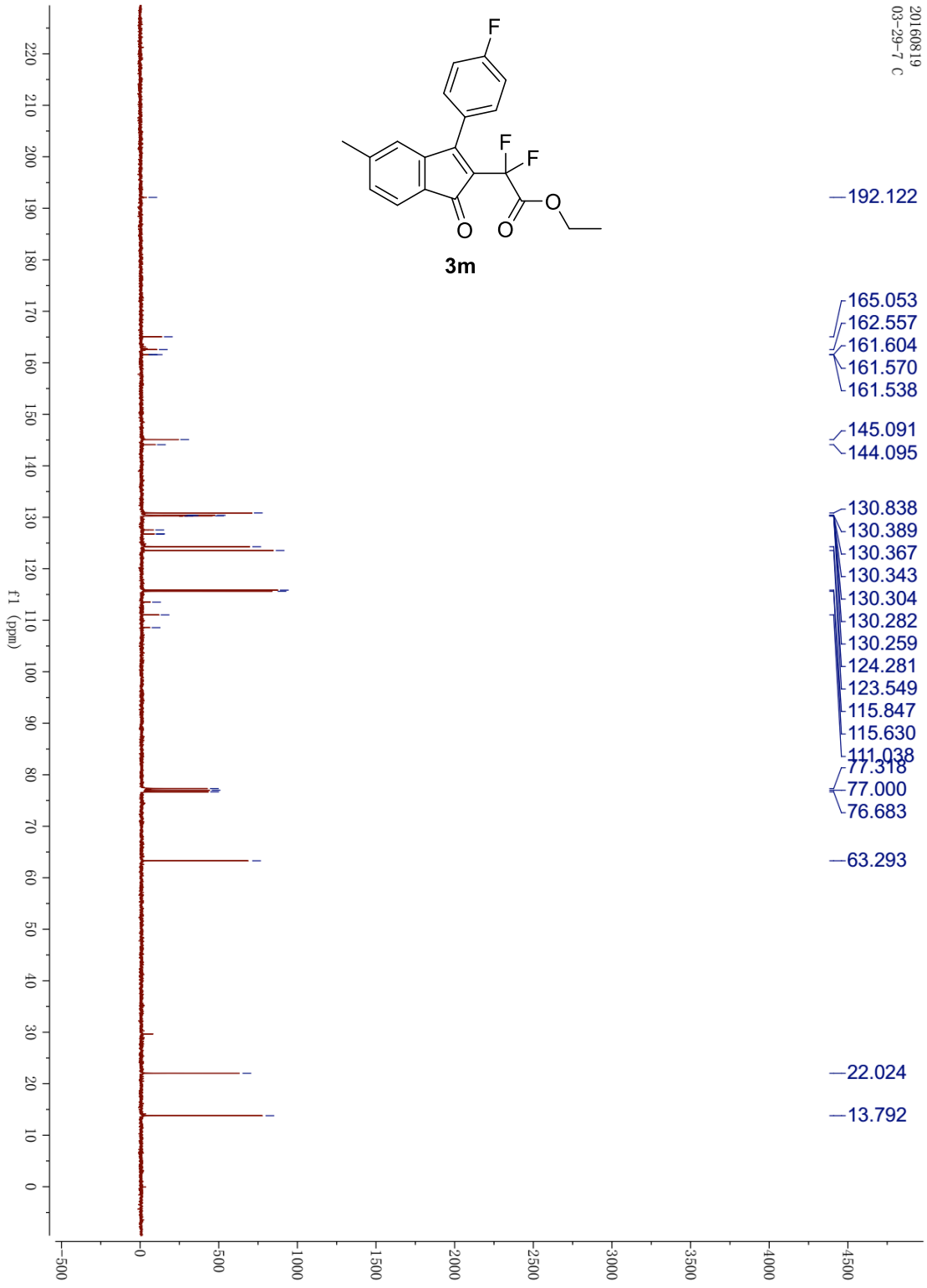

Ph
F
F
O
O
O
3l
20160819
03-29-10 H
7.762
7.742
7.674
7.656
7.627
7.607
7.503
7.484
7.477
7.465
7.459
7.418
7.400
7.382
7.251
7.179
7.161
6.973
4.321
4.303
4.285
4.268
2.359
1.333
1.316
1.298
0.000
2.04
2.03
2.11
3.04
1.08
0.98
0.98
2.00
2.97
2.96
f1 (ppm)

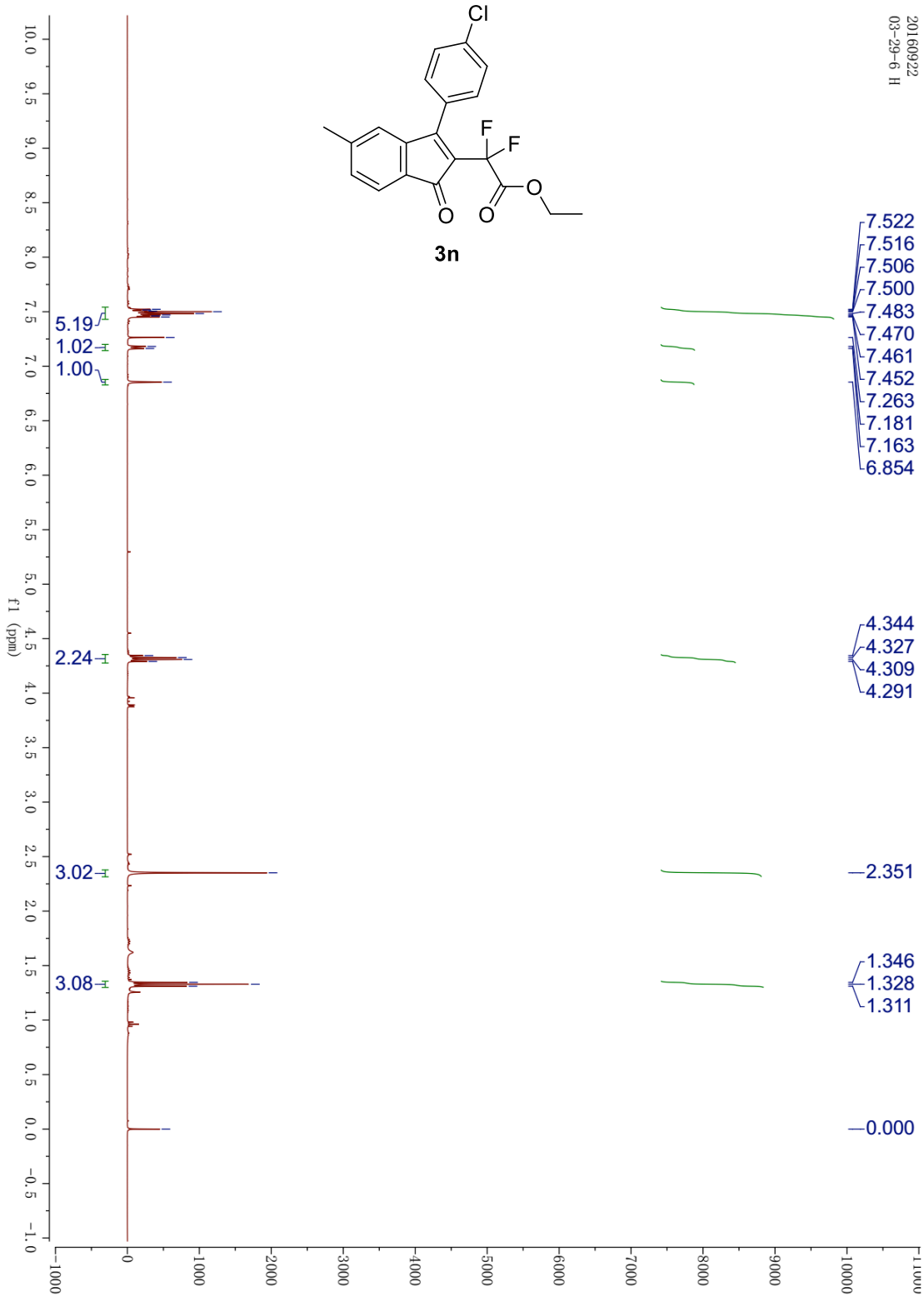

20160819
03-29-10 F
Ph
F
F
O
O
O
3l
-97.907
f1 (ppm)

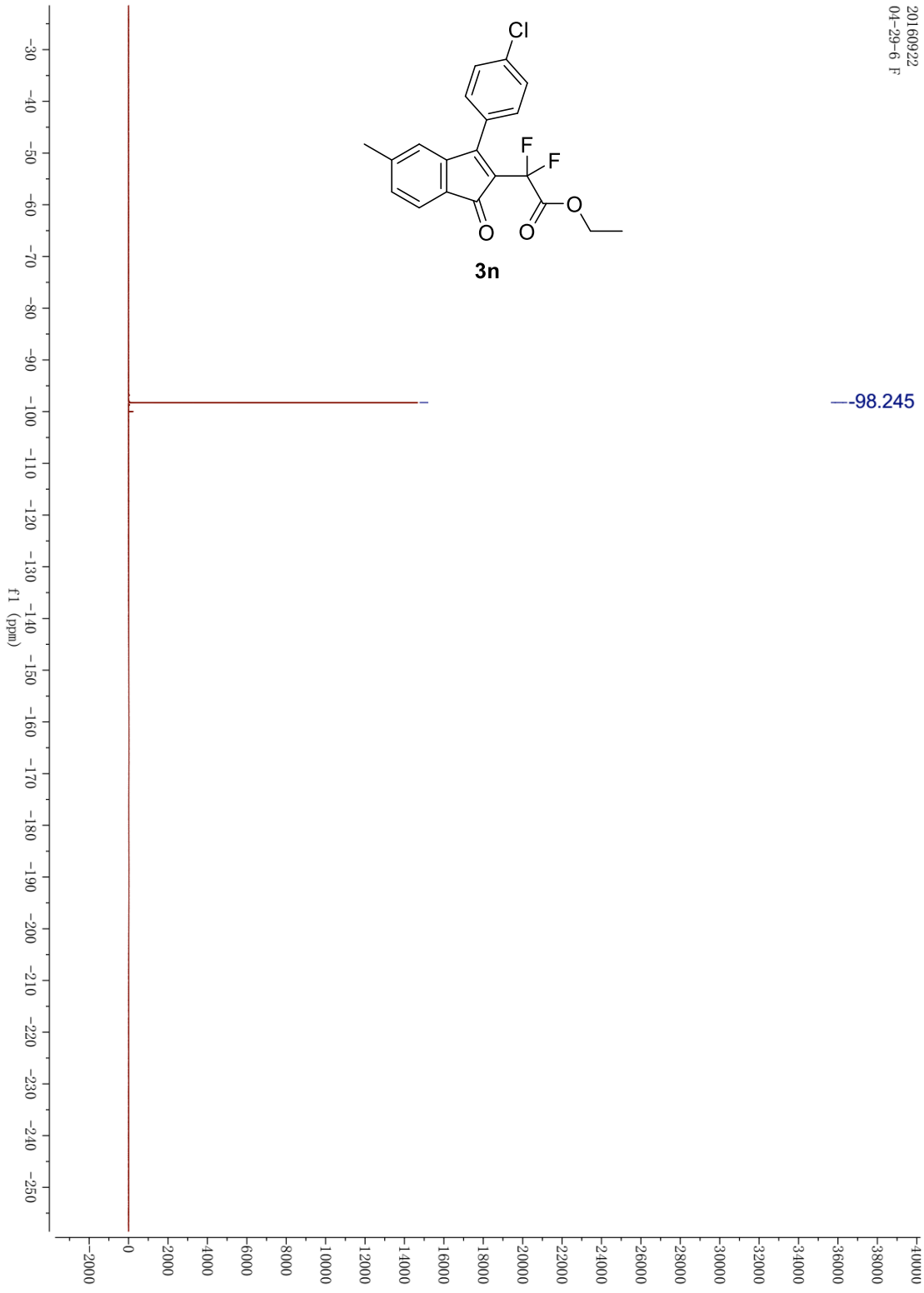

20160819
03-29-10 C
Ph
F
F
O
O
O
3l
192.354
192.317
192.280
162.857
162.400
162.365
162.331
144.994
144.190
143.156
140.008
128.933
128.746
127.106
127.033
113.608
111.135
108.663
77.318
77.000
76.682
63.227
22.030
13.791
f1 (ppm)

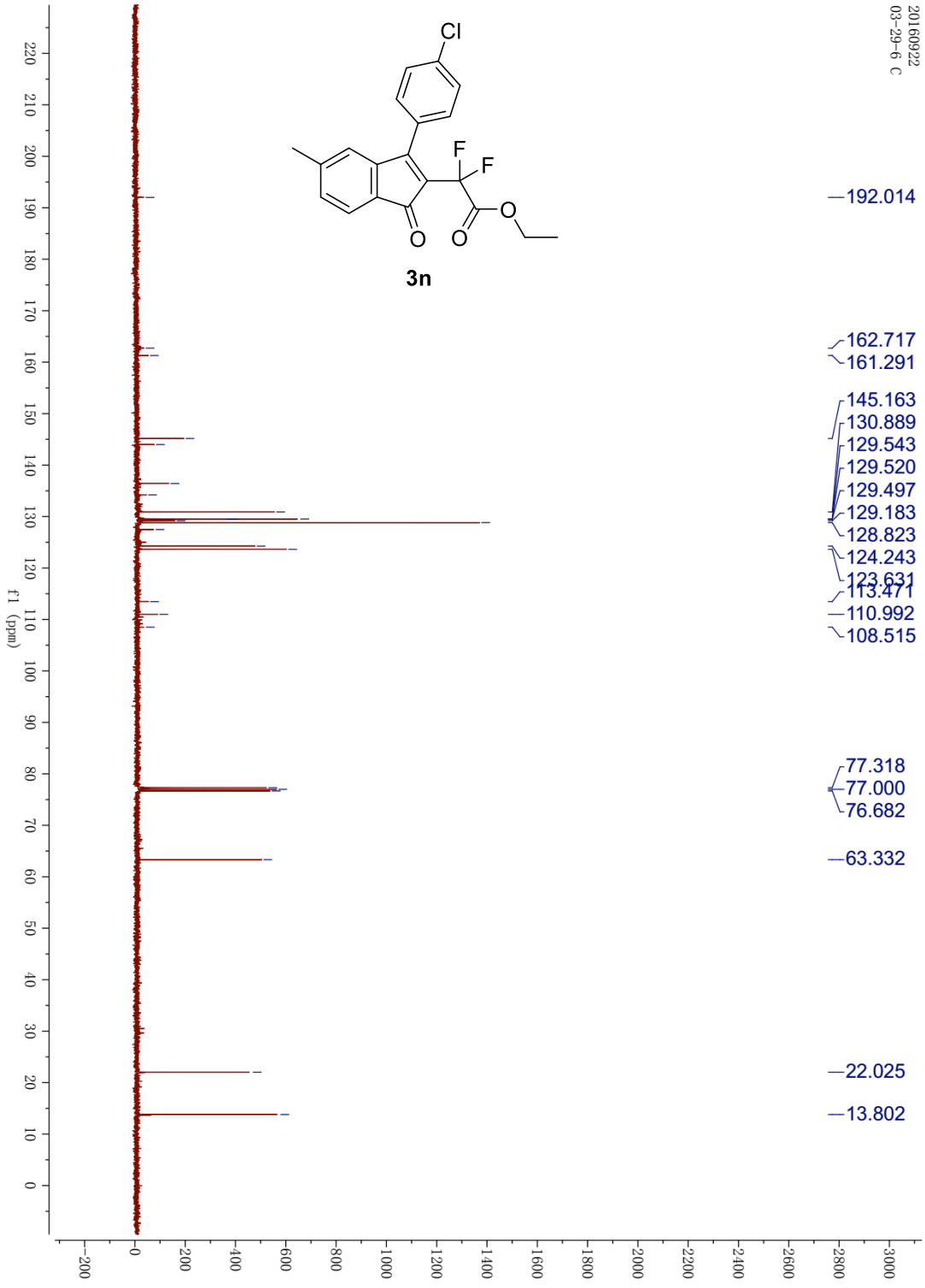

20160819
03-29-7 H
3m
F
F
F
O
O
O
2.01
0.97
1.99
0.97
0.94
2.00
3.01
3.09
7.556
7.542
7.535
7.521
7.468
7.449
7.264
7.244
7.223
7.201
7.181
7.163
6.873
4.339
4.321
4.303
4.286
2.356
1.343
1.326
1.308
-0.000
f1 (ppm)

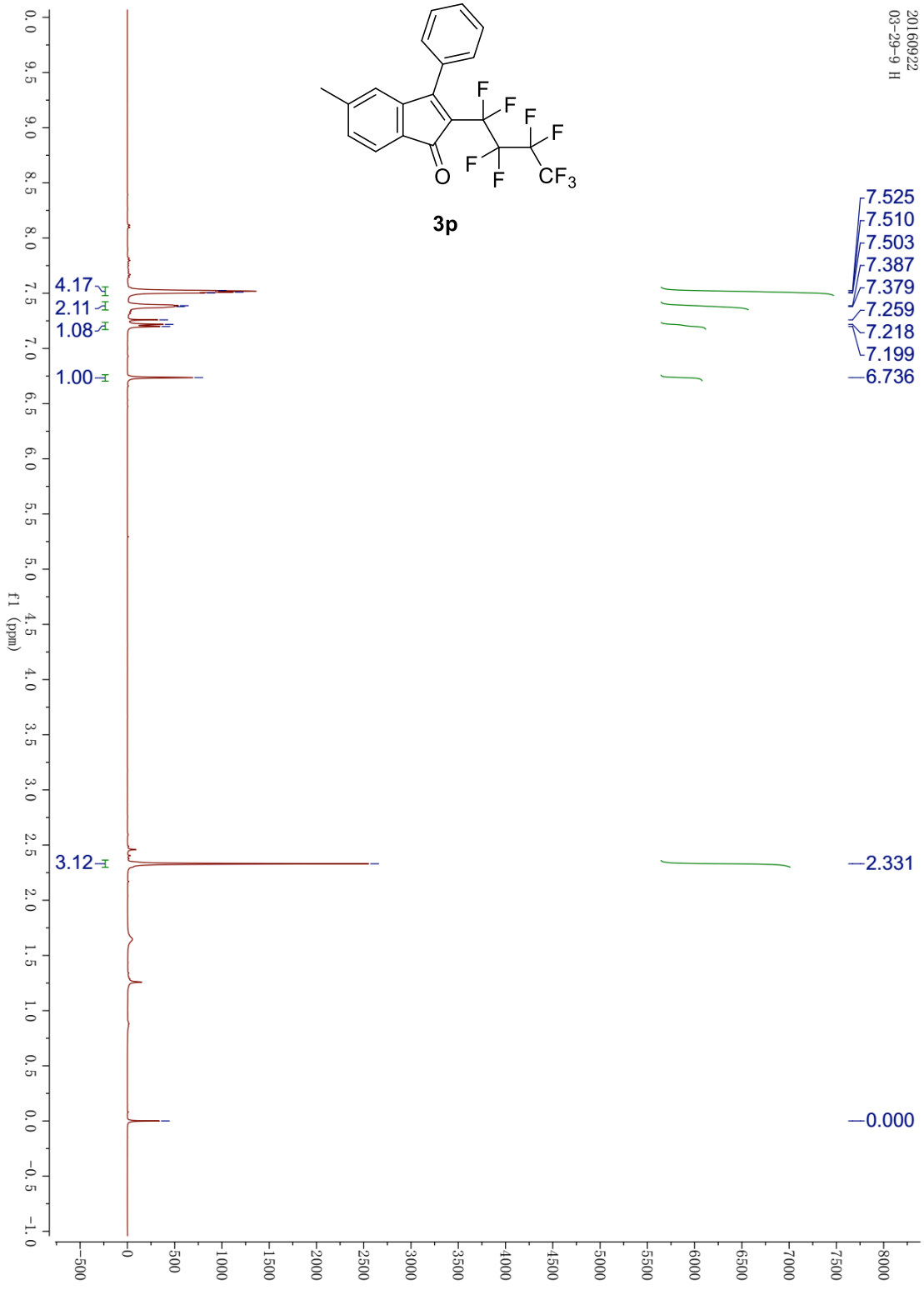

20160819
03-29-7 F
F
F
F
O
O
O
3m
-98.173
-109.369
-109.383
-109.392
-109.406
-109.419
-109.428
-109.442
f1 (ppm)

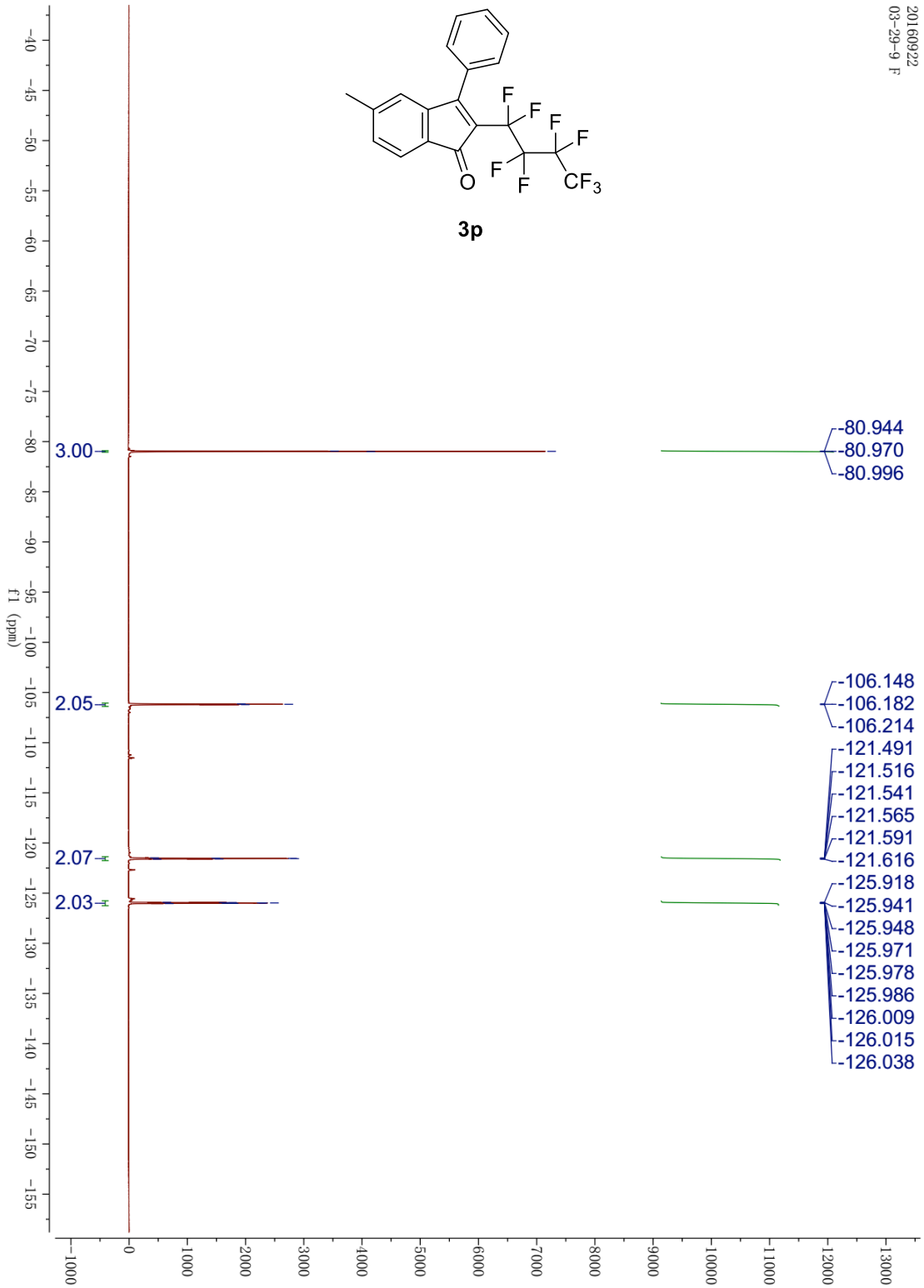

20160819
03-29-7 C
F
F
F
O
O
O
3m
192.122
165.053
162.557
161.604
161.570
161.538
145.091
144.095
130.838
130.389
130.367
130.343
130.304
130.282
130.259
124.281
123.549
115.847
115.630
111.038
77.318
77.000
76.683
63.293
22.024
13.792
f1 (ppm)

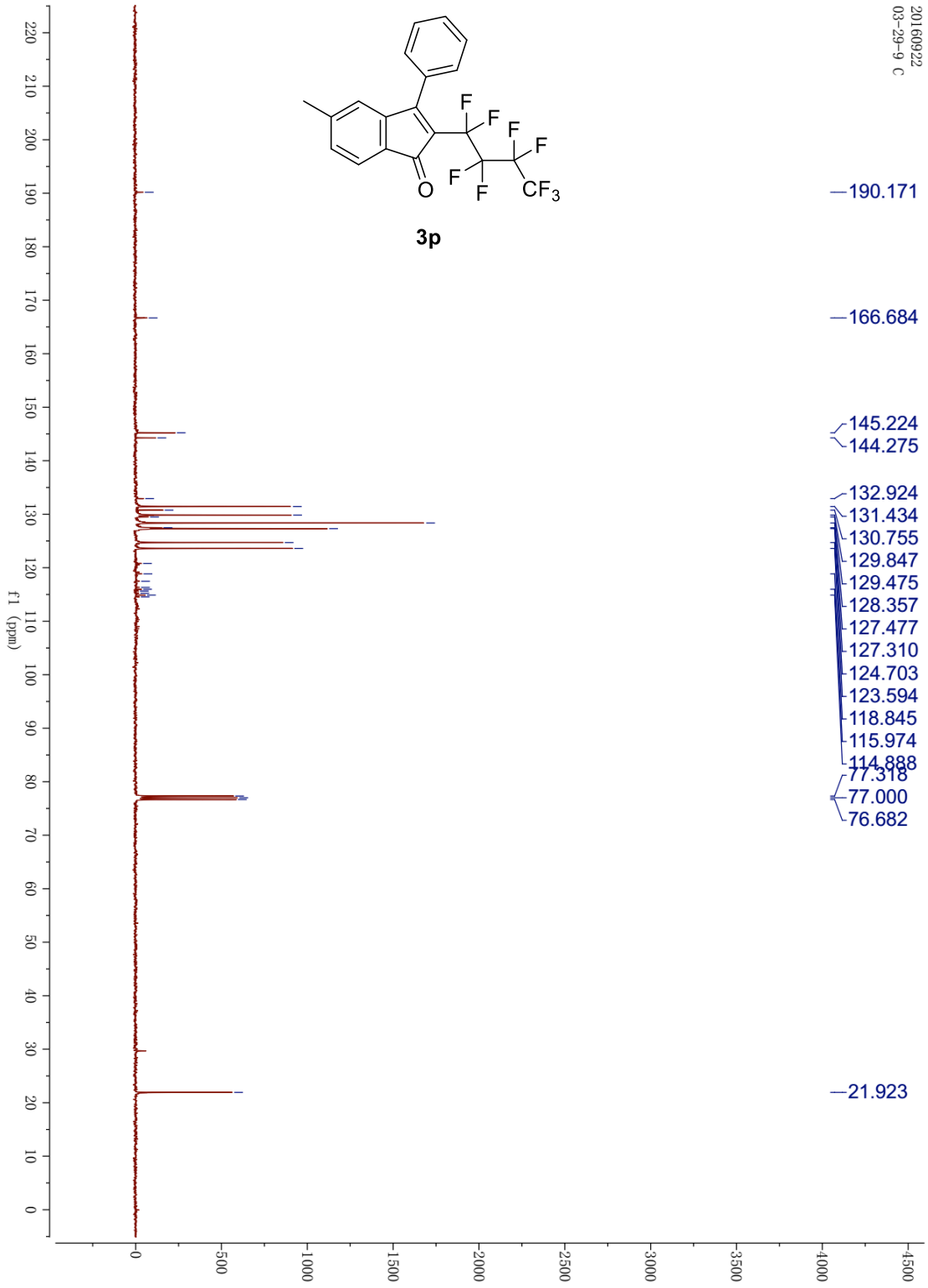

Cl
F
F
O
O
O
3n
20160922
03-29-6 H
7.522
7.516
7.506
7.500
7.483
7.470
7.461
7.452
7.263
7.181
7.163
6.854
4.344
4.327
4.309
4.291
2.351
1.346
1.328
1.311
0.000
5.19
1.02
1.00
2.24
3.02
3.08
f1 (ppm)

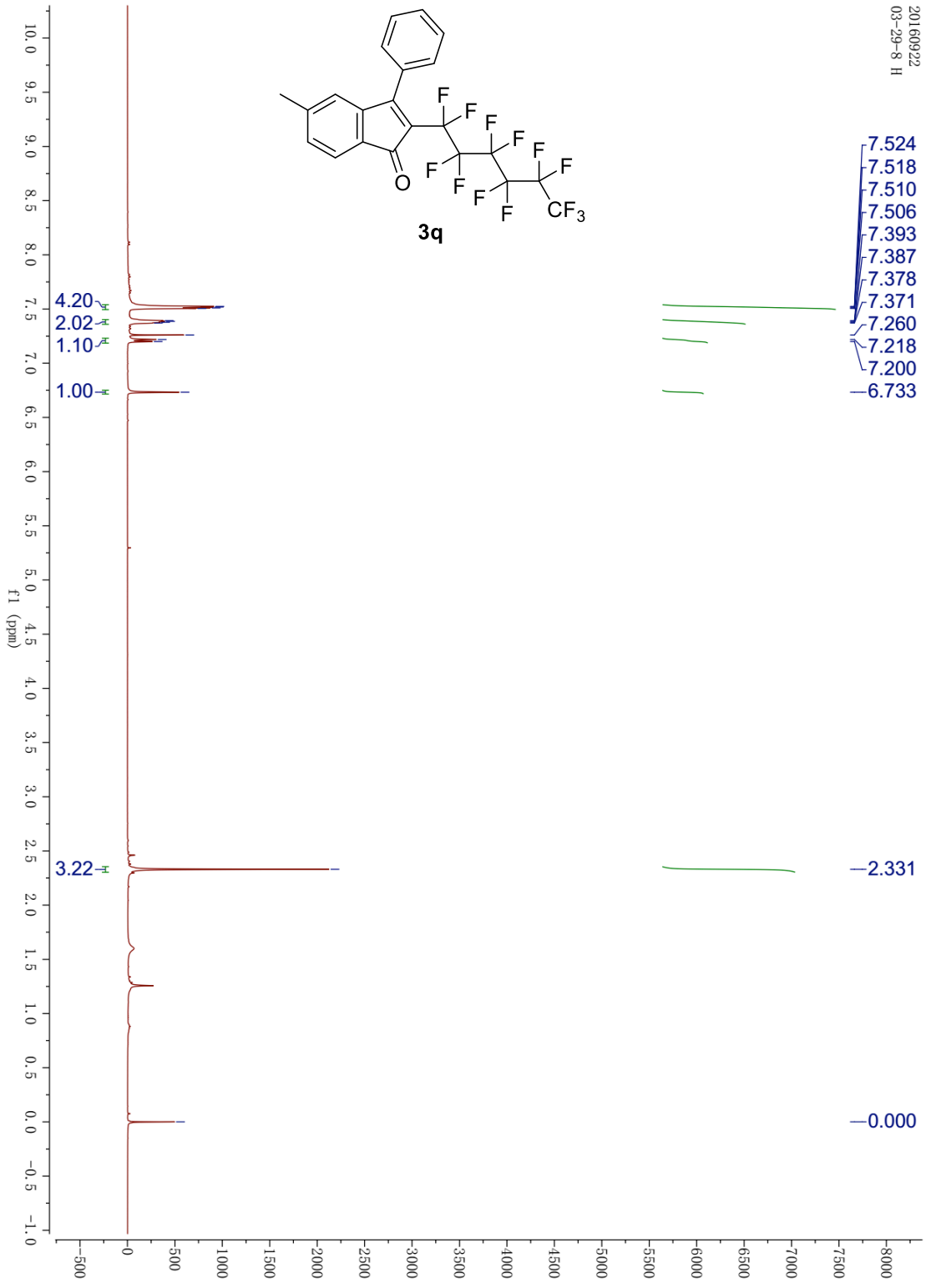

20160922
04-29-6 F
Cl
F
F
O
O
O
3n
-98.245
f1 (ppm)

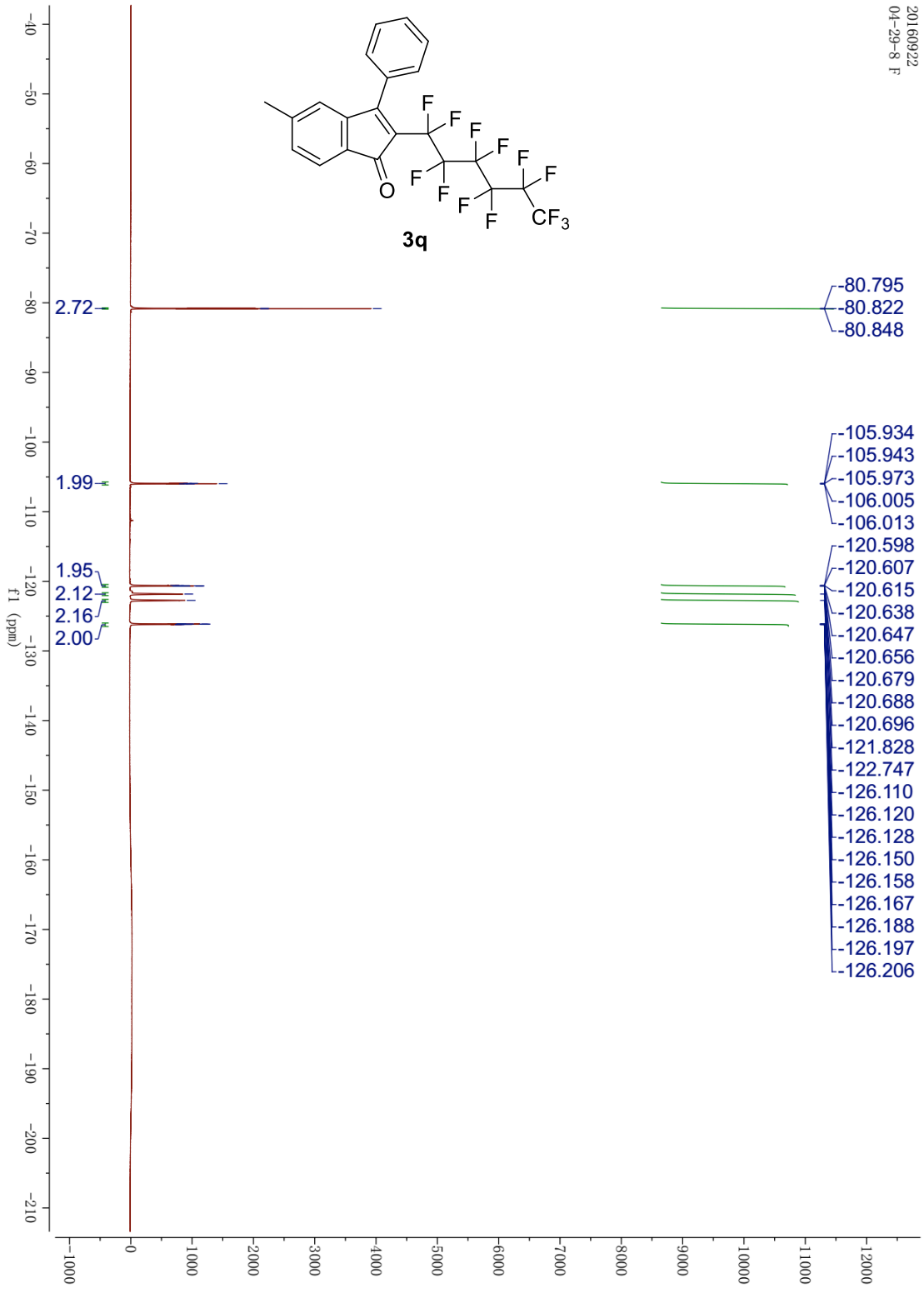

20160922
03-29-6 C
Cl
F
F
O
O
O
3n
192.014
162.717
161.291
145.163
130.889
129.543
129.520
129.497
129.183
128.823
124.243
123.631
113.471
110.992
108.515
77.318
77.000
76.682
63.332
22.025
13.802
f1 (ppm)

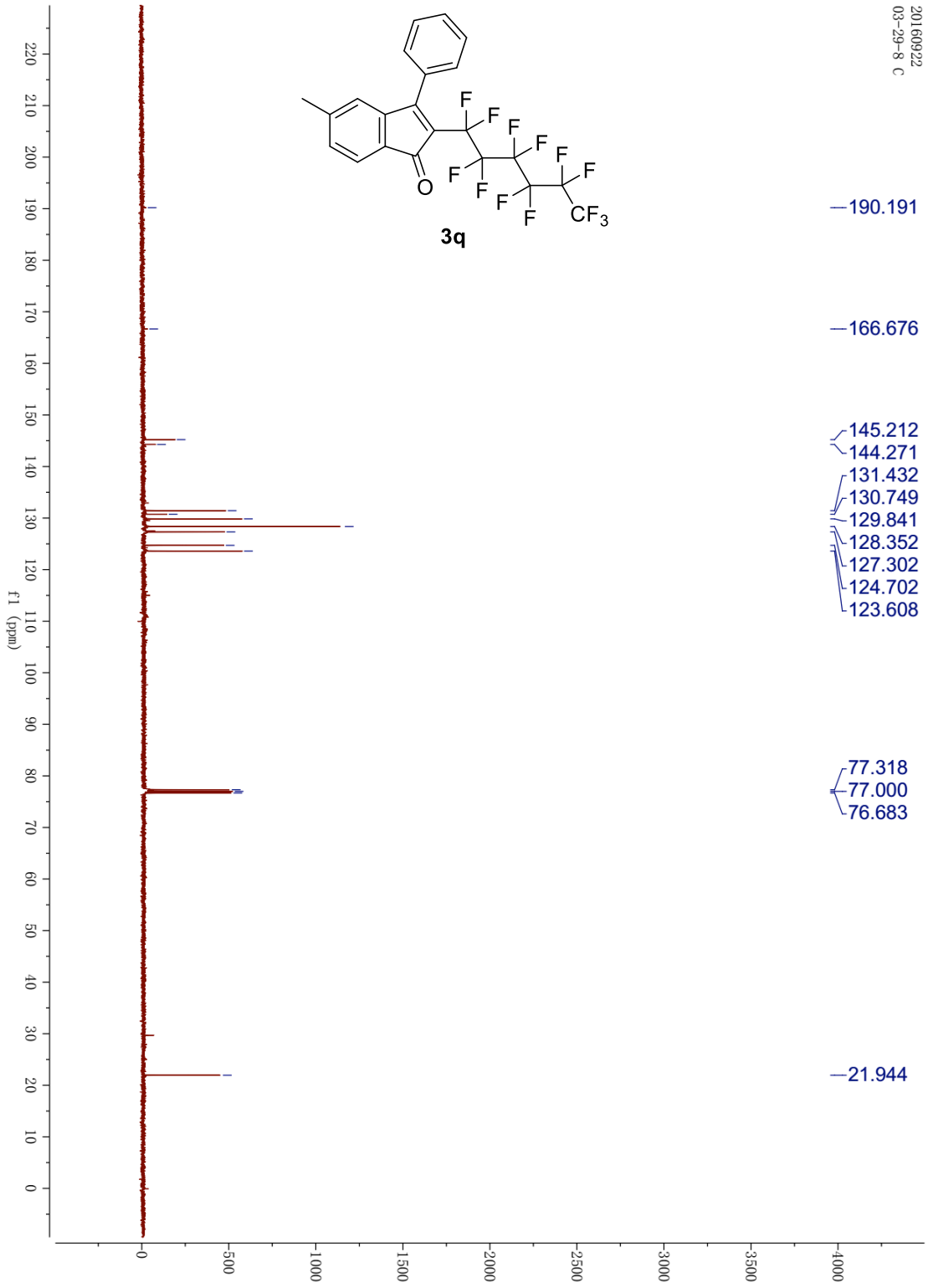

20160922
03-29-9 H
3p
F
F
F
F
F
F
CF3
O
7.525
7.510
7.503
7.387
7.379
7.259
7.218
7.199
6.736
4.17
2.11
1.08
1.00
3.12
2.331
0.000
f1 (ppm)

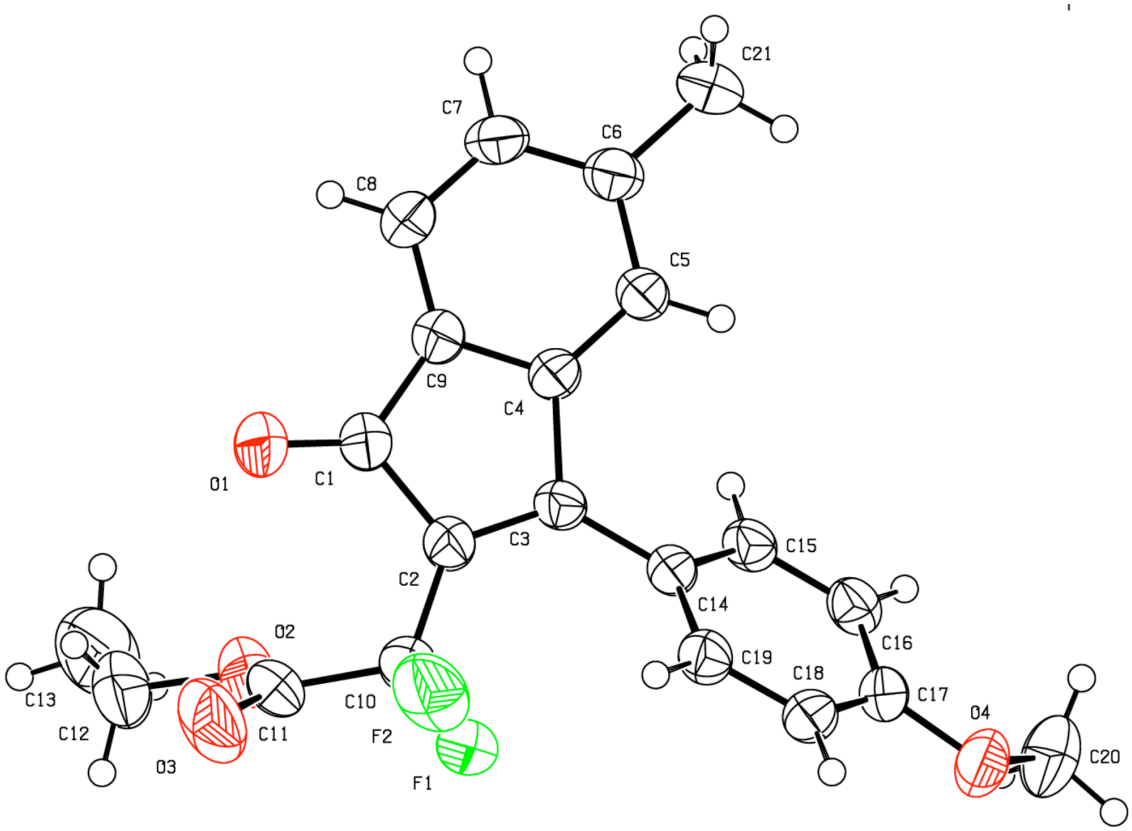

20160922
03-29-9 F
F
F
F
F
F
F
CF3
O
3p
-80.944
-80.970
-80.996
-106.148
-106.182
-106.214
-121.491
-121.516
-121.541
-121.565
-121.591
-121.616
-125.918
-125.941
-125.948
-125.971
-125.978
-125.986
-126.009
-126.015
-126.038
3.00
2.05
2.07
2.03
f1 (ppm)


20160922
03-29-9 C
3p
190.171
166.684
145.224
144.275
132.924
131.434
130.755
129.847
129.475
128.357
127.477
127.310
124.703
123.594
118.845
115.974
114.888
77.318
77.000
76.682
21.923
f1 (ppm)


20160922
03-29-8 H
3q
7.524
7.518
7.510
7.506
7.393
7.387
7.378
7.371
7.260
7.218
7.200
6.733
2.331
0.000
4.20
2.02
1.10
1.00
3.22
f1 (ppm)


20160922
04-29-8 F
3q
2.72
1.99
1.95
2.12
2.16
2.00
-80.795
-80.822
-80.848
-105.934
-105.943
-105.973
-106.005
-106.013
-120.598
-120.607
-120.615
-120.638
-120.647
-120.656
-120.679
-120.688
-120.696
-121.828
-122.747
-126.110
-126.120
-126.128
-126.150
-126.158
-126.167
-126.188
-126.197
-126.206
f1 (ppm)


20160922
03-29-8 C
3q
190.191
166.676
145.212
144.271
131.432
130.749
129.841
128.352
127.302
124.702
123.608
77.318
77.000
76.683
21.944
f1 (ppm)


C21
C7
C6
C8
C5
C9
C4
O1
C1
C3
C15
C2
C14
O2
C16
C19
C18
C13
C10
C17
O4
C12
C11
F2
C20
O3
F1