

Electronic Supporting Information

Reactivity study of 4-hydroxythiocoumarin: a novel synthetic route to fused chromono-2-methylthiophene and -thiopyran through solvent-dependent thio-Claisen rearrangement

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Content	Page No
1. General Information and Methods	S1
2. Crystal Data and Structure Refinement for Compound	S2
3. Computational Details	S3-S18
4. Copies of ¹ H NMR, ¹³ C NMR and HRMS spectra of all Compounds	S19-S257
5. References	S258

Experimental

General Information:

¹H and ¹³C NMR spectra were recorded on 400 MHz, 500 MHz and 100 MHz, 125 MHz NMR spectrometer (Bruker), respectively. TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). ¹H NMR Spectra are reported in the order: multiplicity, coupling constant (*J* value) in Hertz (Hz) and no. of protons; signals were characterized as s (singlet), d (doublet), t (triplet), and m (multiplet). IR spectra were recorded on IR spectrophotometer (PerkinElmer). HRMS spectra were recorded using mass analyzer type ESI. Melting points were determined on a melting point apparatus (Buchi- 540). The crystal structure was determined using a single crystal XRD diffractometer.

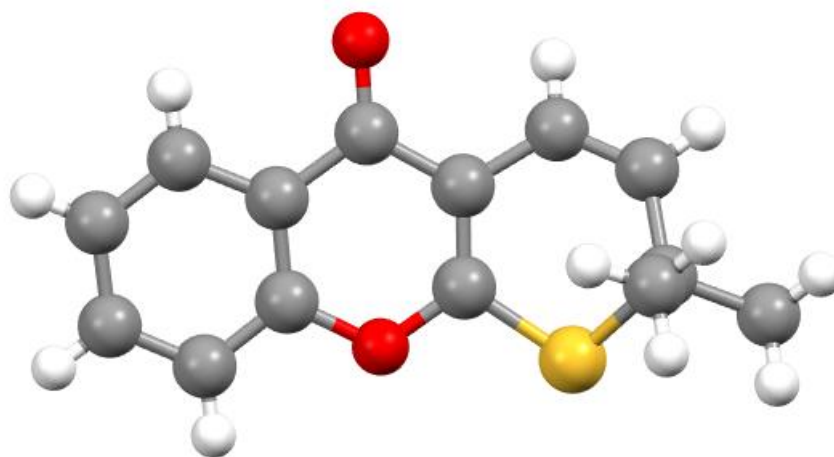


Figure S1. ORTEP Diagrams of compound 10a.

Table S1. Crystal data and structure refinement for compound 10a.

Entry	Identification Code	Compound 10a
01	Empirical formula	C ₁₄ H ₁₂ O ₂ S
02	Formula weight	244.30
03	Temperature	297 K
04	Wavelength	0.71073
05	Radiation type	Mo K α
06	Radiation system	Fine-focus sealed tube
07	Crystal system	Monoclinic
08	Space group	P 2 ₁ /n
09	Cell length	a 12.9925 (10) b 5.6889 (4) c 16.3926 (12)
10	Cell angle	α 90 β 102.803 (2) γ 90
11	Cell volume	1181.50 (15)
12	Density	1.373
13	Completeness to theta	99.9
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F ²
16	Index ranges	-15 $\leq$ h $\leq$ 15, -6 $\leq$ k $\leq$ 6, -20 $\leq$ l $\leq$ 19
17	Reflection number	2236
18	Theta range	2.6- 25.6
19	Cell formula units Z	4
20	CCDC no	2266735

Computational details:

In work, Gaussian G16^{S1} software was utilized for density functional theory (DFT) computations. During the geometry calculations, B3LYP, augmented with atom-pairwise dispersion corrections (EmpiricalDispersion=D3), was applied. The Def2-SVP^{S2} basis set was employed for all calculations, unless specified otherwise. An implicit solvation model, specifically the SMD^{S3} solvation model, was incorporated to account for the impact of *N,N*-dimethylformamide and chlorobenzene solvents. Following the geometry optimizations, frequency calculations were performed to verify the absence of a saddle point for the intermediate structure and the presence of one imaginary frequency for the transition state.

➤ I:

C	-1.180939000	-0.196069000	-0.491392000
C	1.312486000	-0.585893000	-0.364002000
C	1.390168000	0.670302000	0.259494000
C	-0.871743000	1.270563000	-0.264874000
H	2.386988000	-2.369618000	-0.892595000
H	-1.968362000	-0.285174000	-1.247888000
C	2.459290000	-1.397429000	-0.400192000
C	2.572737000	1.113646000	0.852557000
C	3.694638000	0.284038000	0.820858000
C	3.644109000	-0.970437000	0.192199000
H	2.600887000	2.100216000	1.318722000
H	4.622614000	0.623603000	1.287483000
H	4.530496000	-1.608218000	0.171322000
O	0.333095000	1.559066000	0.265102000
C	0.027717000	-1.026355000	-0.941285000
O	-0.102839000	-1.999247000	-1.655573000
C	-1.677913000	-0.791989000	0.829471000
H	-0.995998000	-0.732652000	1.687279000
C	-4.022343000	-1.932787000	1.080701000
C	-2.850654000	-1.364300000	0.956422000
H	-4.907474000	-1.354886000	1.375339000
H	-4.158060000	-3.005752000	0.894840000
S	-1.933653000	2.482138000	-0.540654000

➤ I^{DMF}:

C	0.174758000	-0.046465000	-0.130833000
C	2.623031000	-0.678702000	-0.323822000
C	2.906461000	0.609665000	0.154365000
C	0.648999000	1.392280000	-0.097946000

H	3.424377000	-2.594579000	-0.842496000
H	-0.726004000	-0.133230000	-0.753573000
C	3.672275000	-1.602232000	-0.459157000
C	4.207530000	0.976001000	0.510766000
C	5.232441000	0.038679000	0.385429000
C	4.971116000	-1.251950000	-0.102991000
H	4.390642000	1.990970000	0.867138000
H	6.250856000	0.319646000	0.665152000
H	5.783669000	-1.975043000	-0.201142000
O	1.948230000	1.591732000	0.246264000
C	1.224606000	-1.040554000	-0.651693000
O	0.912253000	-2.066737000	-1.212072000
C	-0.152982000	-0.474035000	1.301891000
H	0.619959000	-0.297978000	2.061004000
C	-2.386096000	-1.649994000	1.999355000
C	-1.272242000	-1.061240000	1.647034000
H	-3.253143000	-1.073722000	2.340486000
H	-2.489039000	-2.740406000	1.959614000
S	-0.297797000	2.693886000	-0.348067000
N	-4.363834000	-0.054221000	-0.264215000
C	-3.833824000	1.211376000	0.207373000
H	-3.623134000	1.170622000	1.290788000
H	-2.897993000	1.435116000	-0.319621000
H	-4.557882000	2.024628000	0.026723000
C	-5.627615000	-0.495473000	0.280474000
H	-5.913325000	-1.462254000	-0.159878000
H	-5.568742000	-0.620962000	1.377408000
H	-6.430287000	0.233214000	0.068358000
C	-3.666138000	-0.807225000	-1.160116000
O	-2.589066000	-0.521003000	-1.646833000
H	-4.203621000	-1.751372000	-1.421026000

➤ TS I:

C	-0.049498000	-0.073234000	-0.826152000
C	-2.295854000	-0.700756000	0.014887000
C	-2.627969000	0.658801000	-0.058918000
C	-0.421555000	1.294563000	-0.748529000
H	-2.989865000	-2.672844000	0.463726000
H	0.907486000	0.695396000	1.190861000
C	-3.279808000	-1.621075000	0.413547000
C	-3.920383000	1.106325000	0.249148000
C	-4.882513000	0.177639000	0.636214000
C	-4.565682000	-1.190292000	0.721383000
H	-4.137411000	2.173712000	0.179746000
H	-5.892520000	0.519546000	0.876801000
H	-5.329596000	-1.909239000	1.026880000
O	-1.711552000	1.604496000	-0.403776000
C	-0.926282000	-1.135828000	-0.342483000
O	-0.565080000	-2.307572000	-0.229913000
C	1.265180000	-0.428996000	-1.323442000
H	1.811744000	0.402755000	-1.789344000

C	2.590786000	-2.706627000	-1.362522000
C	1.895982000	-1.599177000	-1.265692000
H	3.289360000	-3.040769000	-0.583970000
H	2.451232000	-3.393755000	-2.206695000
S	0.576442000	2.645094000	-0.985227000
N	3.412446000	0.206141000	1.096426000
C	3.295149000	1.663942000	1.043317000
H	2.662308000	1.981621000	0.185184000
H	2.823411000	2.028295000	1.967769000
H	4.298657000	2.096425000	0.956159000
C	4.606554000	-0.417024000	0.533099000
H	4.637371000	-1.482096000	0.797559000
H	4.581257000	-0.335733000	-0.565376000
H	5.502505000	0.082047000	0.926662000
C	2.370757000	-0.540135000	1.385966000
O	1.208104000	-0.073867000	1.729011000
H	2.492909000	-1.623047000	1.481187000

➤ II:

C	-0.281974000	0.314017000	0.935664000
C	1.819954000	-0.728685000	0.196536000
C	2.386944000	0.554888000	0.126395000
C	0.315122000	1.620955000	0.706585000
H	2.179720000	-2.838620000	-0.048815000
H	-1.049342000	-2.056184000	0.272405000
C	2.629730000	-1.846244000	-0.093770000
C	3.734112000	0.739886000	-0.204115000
C	4.520282000	-0.377277000	-0.472099000
C	3.969066000	-1.670899000	-0.420088000
H	4.129280000	1.755927000	-0.248434000
H	5.573660000	-0.243936000	-0.730067000
H	4.595544000	-2.538677000	-0.637762000
O	1.631959000	1.660035000	0.338519000
C	0.423187000	-0.828315000	0.563218000
O	-0.088354000	-2.053562000	0.513040000
C	-1.633387000	0.277105000	1.514488000
H	-2.120822000	1.257829000	1.575027000
C	-2.943016000	-1.801056000	2.439259000
C	-2.266733000	-0.770088000	2.004825000
H	-3.571656000	-2.377799000	1.749736000
H	-2.880900000	-2.137644000	3.480778000
S	-0.456506000	3.086955000	0.804666000
N	-2.201453000	0.040174000	-1.902388000
C	-0.872051000	-0.253049000	-2.410926000
H	-0.591764000	-1.273103000	-2.123610000
H	-0.859570000	-0.165413000	-3.510378000
H	-0.135523000	0.453512000	-1.996887000
C	-2.715948000	1.379000000	-2.138755000
H	-3.746996000	1.455925000	-1.765254000
H	-2.098851000	2.124882000	-1.608932000
H	-2.713751000	1.610588000	-3.216984000

C	-2.878365000	-0.853736000	-1.152365000
O	-2.461165000	-1.949089000	-0.781571000
H	-3.895814000	-0.497865000	-0.877775000

➤ **TS II:**

C	0.884228000	0.633327000	-0.076939000
C	-1.575478000	0.577367000	-0.023388000
C	-1.499830000	-0.830256000	-0.003666000
C	0.842574000	-0.760065000	-0.094781000
H	-2.897885000	2.265181000	-0.031390000
C	-2.853247000	1.173818000	-0.016289000
C	-2.657550000	-1.622820000	0.020512000
C	-3.904283000	-1.006328000	0.029225000
C	-4.005751000	0.399124000	0.009123000
H	-2.554102000	-2.710001000	0.032583000
H	-4.808424000	-1.620279000	0.051063000
H	-4.989736000	0.874801000	0.013645000
O	-0.305732000	-1.481789000	-0.016004000
C	-0.345305000	1.406520000	-0.035692000
O	-0.384521000	2.643209000	-0.011101000
C	2.201050000	1.190689000	0.075803000
H	2.301758000	2.244715000	0.349604000
C	4.659476000	0.434018000	-0.022168000
C	3.302030000	0.365478000	0.070128000
H	5.129813000	1.171032000	-0.684925000
H	5.314249000	-0.314434000	0.436649000
S	2.346998000	-1.582819000	-0.072384000

➤ **7a:**

C	0.784560000	-0.689744000	-0.000118000
C	-1.529544000	-0.808248000	0.000049000
C	-1.627151000	0.597970000	-0.000182000
C	-0.413596000	1.459475000	-0.000084000
C	0.828101000	0.691663000	-0.000100000
H	-2.546029000	-2.707862000	0.000063000
C	-2.667896000	-1.622969000	-0.000004000
C	-2.913101000	1.172429000	-0.000143000
C	-4.050933000	0.375775000	-0.000185000
C	-3.924359000	-1.025802000	0.000264000
H	-2.979906000	2.262456000	-0.000068000
H	-5.042923000	0.833504000	-0.000120000
H	-4.817574000	-1.655443000	0.000581000
O	-0.316115000	-1.450335000	-0.000099000
S	2.360793000	-1.417950000	0.000064000
C	3.120860000	0.184661000	0.000066000
O	-0.463417000	2.686138000	0.000306000
C	2.181487000	1.175754000	-0.000009000
H	2.432681000	2.237152000	-0.000090000
C	4.611910000	0.295524000	-0.000025000
H	5.057446000	-0.182338000	0.888798000

H	5.057275000	-0.182754000	-0.888714000
H	4.900568000	1.357126000	-0.000310000

➤ TS III:

C	1.086471000	-0.221583000	-0.218893000
C	-1.377595000	-0.578850000	-0.183701000
C	-1.495048000	0.777841000	0.155691000
C	0.840230000	1.205051000	-0.111255000
H	-2.430697000	-2.422016000	-0.492062000
H	1.528357000	-1.104382000	0.960430000
C	-2.538790000	-1.370001000	-0.219833000
C	-2.735033000	1.343746000	0.467227000
C	-3.872067000	0.537939000	0.436752000
C	-3.778698000	-0.820778000	0.091699000
H	-2.786382000	2.404173000	0.720923000
H	-4.844074000	0.974061000	0.680225000
H	-4.676650000	-1.442336000	0.069138000
O	-0.415410000	1.624742000	0.169467000
C	-0.047906000	-1.155329000	-0.493478000
O	0.103058000	-2.294085000	-0.908569000
C	2.468201000	-0.661878000	-0.539438000
H	2.997810000	-0.536630000	-1.489244000
C	3.625808000	-1.798473000	1.529364000
C	2.819276000	-1.371189000	0.544465000
H	4.490704000	-1.203184000	1.847973000
H	3.373880000	-2.688903000	2.114103000
S	2.032330000	2.342456000	-0.281098000

➤ I^H:

C	-0.904491000	0.205976000	-0.262357000
C	1.462408000	0.636205000	-0.076604000
C	1.661721000	-0.754644000	0.062538000
C	-0.590373000	-1.106132000	-0.108746000
H	2.424468000	2.539911000	-0.155024000
H	-2.867739000	0.570862000	1.702482000
C	2.595621000	1.466580000	-0.045718000
C	2.936527000	-1.302520000	0.226445000
C	4.039271000	-0.452440000	0.252817000
C	3.870699000	0.935380000	0.116745000
H	3.036709000	-2.384326000	0.330035000
H	5.039442000	-0.873499000	0.380501000
H	4.741158000	1.595070000	0.138517000
O	0.604630000	-1.655672000	0.046328000
C	0.096474000	1.247870000	-0.257231000
O	-0.084425000	2.450905000	-0.378014000
C	-2.405507000	0.081584000	-0.386223000
H	-2.798326000	0.269830000	-1.396885000
C	-4.371456000	1.367830000	0.442912000
C	-3.242916000	0.691360000	0.680029000
H	-4.754282000	1.504033000	-0.573796000
H	-4.945145000	1.820980000	1.255462000

S	-2.182862000	-1.844189000	-0.180966000
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➤ **TS IV:**

C	-0.968940000	0.678077000	0.054519000
C	1.550367000	0.611982000	0.070294000
C	1.444499000	-0.776865000	-0.051863000
C	-0.964521000	-0.772361000	0.049649000
H	2.895069000	2.280010000	0.204706000
H	-4.016164000	1.611855000	-1.186774000
C	2.830122000	1.194405000	0.108458000
C	2.577277000	-1.593704000	-0.137962000
C	3.835615000	-0.997099000	-0.102119000
C	3.966593000	0.397921000	0.022715000
H	2.451356000	-2.673971000	-0.229998000
H	4.727908000	-1.624307000	-0.170877000
H	4.959747000	0.851777000	0.051392000
O	0.230630000	-1.402726000	-0.073201000
C	0.321778000	1.423968000	0.124249000
O	0.359730000	2.647090000	0.211024000
C	-2.071131000	1.478625000	-0.295627000
H	-1.789937000	2.485092000	-0.624955000
C	-3.996822000	0.120852000	0.349155000
C	-3.420784000	1.107707000	-0.416967000
H	-5.005813000	-0.244627000	0.131566000
H	-3.601254000	-0.118420000	1.333017000
S	-2.244280000	-1.868023000	0.062475000

➤ **8a:**

C	0.936045000	-0.605736000	-0.052014000
C	-1.405600000	-0.804454000	-0.007349000
C	-1.561391000	0.589951000	0.022333000
C	-0.372900000	1.474438000	-0.005641000
C	0.914831000	0.768626000	-0.051629000
H	-2.335358000	-2.748788000	-0.024726000
C	-2.504736000	-1.670656000	-0.000535000
C	-2.866383000	1.115484000	0.059866000
C	-3.968849000	0.269654000	0.069052000
C	-3.784504000	-1.125374000	0.038456000
H	-2.975258000	2.201746000	0.080012000
H	-4.979184000	0.684076000	0.099450000
H	-4.651499000	-1.790563000	0.044802000
O	-0.162810000	-1.378359000	-0.034679000
S	2.391928000	-1.583247000	-0.179135000
C	3.620983000	-0.368720000	0.467351000
H	3.610214000	-0.416796000	1.571176000
H	4.593145000	-0.757605000	0.130695000
C	3.379148000	1.035128000	-0.018514000
O	-0.463640000	2.699881000	-0.011278000
C	2.147787000	1.543321000	-0.193863000
H	2.010645000	2.592732000	-0.464436000
H	4.261456000	1.665015000	-0.168247000

➤ **4a:**

C	1.572926000000	-0.745815000000	0.042750000000
C	1.800693000000	0.632988000000	-0.077263000000
C	3.120590000000	1.106823000000	0.011310000000
C	4.175459000000	0.224270000000	0.212990000000
C	3.922706000000	-1.154550000000	0.330383000000
C	2.623879000000	-1.647843000000	0.246427000000
H	3.271824000000	2.184225000000	-0.084182000000
H	5.199878000000	0.597509000000	0.280803000000
H	4.751088000000	-1.849458000000	0.489000000000
H	2.400220000000	-2.712456000000	0.333422000000
C	0.657823000000	1.562202000000	-0.286256000000
C	-0.641933000000	0.896048000000	-0.338864000000
H	-1.521563000000	1.527212000000	-0.443654000000
O	0.802688000000	2.772718000000	-0.394617000000
C	-0.751504000000	-0.454703000000	-0.223831000000
O	0.310305000000	-1.271937000000	-0.039654000000
S	-2.203905000000	-1.457670000000	-0.282997000000
C	-3.494786000000	-0.257189000000	-0.769852000000
H	-3.120422000000	0.318026000000	-1.633837000000
H	-4.301918000000	-0.898998000000	-1.163510000000
C	-4.043343000000	0.662676000000	0.290925000000
H	-4.824645000000	1.337582000000	-0.082891000000
C	-3.682208000000	0.725477000000	1.573028000000
H	-2.904207000000	0.073722000000	1.980829000000
H	-4.153539000000	1.436801000000	2.255673000000

➤ **DABCO:**

C	0.783092000000	0.683913000000	1.200952000000
C	-0.783340000000	0.684017000000	1.200733000000
H	1.188260000000	0.167851000000	2.086838000000
H	1.188525000000	1.709017000000	1.209601000000
H	-1.188848000000	0.168503000000	2.086784000000
H	-1.188617000000	1.709186000000	1.208698000000
C	0.783442000000	-1.381852000000	-0.008279000000
H	1.188671000000	-1.890878000000	-0.898196000000
H	1.189068000000	-1.901808000000	0.875120000000
C	-0.783038000000	-1.382080000000	-0.007935000000
H	-1.188528000000	-1.891715000000	-0.897386000000
H	-1.188099000000	-1.901675000000	0.875936000000
C	-0.783313000000	0.697733000000	-1.192858000000
H	-1.188342000000	0.191958000000	-2.084715000000
H	-1.189031000000	1.722753000000	-1.189465000000
C	0.783156000000	0.698276000000	-1.192642000000
H	1.188807000000	0.193279000000	-2.084659000000
H	1.188135000000	1.723584000000	-1.188573000000
N	-1.276758000000	-0.000192000000	-0.000012000000
N	1.276758000000	0.000178000000	0.000038000000

➤ **IM:**

C	3.456966000000	-1.047363000000	-0.032077000000
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C	4.287261000000	0.081991000000	0.020395000000
C	5.667831000000	-0.105343000000	0.202372000000
C	6.196881000000	-1.384882000000	0.326520000000
C	5.345243000000	-2.503079000000	0.270670000000
C	3.974280000000	-2.342683000000	0.091697000000
H	6.291829000000	0.790197000000	0.241017000000
H	7.271095000000	-1.525161000000	0.467347000000
H	5.759449000000	-3.509742000000	0.367960000000
H	3.291691000000	-3.192912000000	0.043881000000
C	2.251176000000	1.447287000000	-0.274306000000
H	1.757810000000	2.415619000000	-0.323946000000
O	4.382959000000	2.460540000000	-0.063656000000
C	1.535071000000	0.290409000000	-0.328025000000
O	2.104802000000	-0.933545000000	-0.213274000000
S	-0.205487000000	0.063348000000	-0.525074000000
C	-0.757032000000	1.745798000000	-0.972421000000
H	-0.057494000000	2.152404000000	-1.721947000000
H	-1.709366000000	1.556229000000	-1.488689000000
C	-0.978079000000	2.731014000000	0.144382000000
H	-1.339192000000	3.708116000000	-0.203695000000
C	-0.788291000000	2.533632000000	1.450218000000
H	-0.423573000000	1.576318000000	1.833227000000
H	-0.985706000000	3.327162000000	2.175288000000
C	-4.610298000000	-1.017137000000	1.590628000000
C	-3.229391000000	-0.426749000000	1.150232000000
H	-5.085694000000	-0.394474000000	2.366138000000
H	-4.500517000000	-2.030614000000	2.009975000000
H	-2.991225000000	0.507259000000	1.682645000000
H	-2.400405000000	-1.125796000000	1.342658000000
C	-5.700952000000	0.257755000000	-0.116124000000
H	-6.404197000000	0.195042000000	-0.962658000000
H	-6.174091000000	0.887749000000	0.654683000000
C	-4.318558000000	0.845168000000	-0.563378000000
H	-4.309385000000	1.078897000000	-1.641433000000
H	-4.074991000000	1.775012000000	-0.023876000000
C	-3.531925000000	-1.371308000000	-1.035432000000
H	-3.515480000000	-1.138945000000	-2.113030000000
H	-2.707943000000	-2.077202000000	-0.844051000000
C	-4.916269000000	-1.953631000000	-0.590789000000
H	-5.615882000000	-2.022700000000	-1.439900000000
H	-4.810544000000	-2.968189000000	-0.173151000000
N	-3.259096000000	-0.134941000000	-0.290649000000
N	-5.511227000000	-1.088301000000	0.433907000000
C	3.701380000000	1.443937000000	-0.106999000000

➤ TS:

C	-1.406460000000	1.174044000000	-0.734244000000
C	-2.526466000000	1.186944000000	0.113950000000
C	-2.976668000000	2.416479000000	0.628007000000
C	-2.319640000000	3.598622000000	0.310459000000
C	-1.198342000000	3.566025000000	-0.539323000000

C	-0.739747000000	2.362573000000	-1.065670000000
H	-3.851308000000	2.395834000000	1.281843000000
H	-2.669005000000	4.550319000000	0.716783000000
H	-0.678881000000	4.493653000000	-0.792429000000
H	0.125237000000	2.314438000000	-1.729087000000
C	-2.555705000000	-1.285237000000	-0.110857000000
H	-3.159278000000	-2.191387000000	-0.123597000000
O	-4.192847000000	-0.143669000000	1.173524000000
C	-1.509410000000	-1.192994000000	-1.051663000000
O	-0.902225000000	0.022614000000	-1.261337000000
S	-0.768086000000	-2.533541000000	-1.729749000000
C	0.223729000000	-3.224771000000	0.478664000000
H	0.581534000000	-4.199885000000	0.136182000000
H	0.947811000000	-2.398291000000	0.447785000000
C	-0.914794000000	-3.148505000000	1.270065000000
H	-1.538346000000	-4.041818000000	1.386875000000
C	-1.445890000000	-1.919731000000	1.671153000000
H	-0.793720000000	-1.043050000000	1.701239000000
H	-2.329872000000	-1.874016000000	2.311806000000
C	2.516938000000	1.702609000000	0.902879000000
C	1.722060000000	0.367621000000	1.086668000000
H	2.837462000000	2.119399000000	1.871657000000
H	1.896491000000	2.467040000000	0.407975000000
H	1.625605000000	0.091880000000	2.150167000000
H	0.707534000000	0.451088000000	0.674208000000
C	4.560218000000	0.469025000000	0.748426000000
H	5.463273000000	0.315480000000	0.135294000000
H	4.889828000000	0.885444000000	1.714452000000
C	3.767459000000	-0.869081000000	0.942937000000
H	4.263146000000	-1.711525000000	0.433867000000
H	3.678243000000	-1.137558000000	2.008426000000
C	2.512769000000	-0.403005000000	-1.049662000000
H	3.021767000000	-1.240764000000	-1.552544000000
H	1.495895000000	-0.352660000000	-1.462468000000
C	3.295398000000	0.940249000000	-1.229065000000
H	4.196154000000	0.805144000000	-1.849986000000
H	2.673404000000	1.704269000000	-1.724548000000
N	2.416464000000	-0.721726000000	0.385090000000
N	3.707446000000	1.458911000000	0.081601000000
C	-3.205514000000	-0.083905000000	0.455236000000

➤ A:

C	1.383091000000	1.192626000000	0.688598000000
C	2.449965000000	1.236390000000	-0.221536000000
C	2.838064000000	2.475722000000	-0.758401000000
C	2.162196000000	3.639778000000	-0.407164000000
C	1.093057000000	3.574331000000	0.502061000000
C	0.703044000000	2.357137000000	1.058392000000
H	3.675345000000	2.482082000000	-1.459776000000
H	2.459623000000	4.600010000000	-0.833765000000
H	0.560024000000	4.485701000000	0.783955000000

H	-0.112774000000	2.285560000000	1.779087000000
C	2.406079000000	-1.296647000000	-0.183552000000
H	3.161486000000	-2.079547000000	-0.035914000000
O	4.125770000000	-0.058995000000	-1.295610000000
C	1.580977000000	-1.172393000000	1.071468000000
O	0.971624000000	0.029512000000	1.287368000000
S	1.266062000000	-2.398091000000	2.091589000000
C	-0.376657000000	-3.394420000000	-1.151982000000
H	-0.722711000000	-4.428276000000	-1.057929000000
H	-1.132492000000	-2.598255000000	-1.151458000000
C	0.927793000000	-3.118964000000	-1.247682000000
H	1.664503000000	-3.931384000000	-1.214072000000
C	1.492968000000	-1.738571000000	-1.392661000000
H	0.687010000000	-1.000749000000	-1.530790000000
H	2.148292000000	-1.688340000000	-2.278760000000
C	-2.665331000000	1.769499000000	-0.557934000000
C	-1.852953000000	0.555007000000	-1.118968000000
H	-3.108738000000	2.368351000000	-1.370252000000
H	-2.019783000000	2.443956000000	0.027235000000
H	-1.841903000000	0.544129000000	-2.221194000000
H	-0.806317000000	0.589733000000	-0.782316000000
C	-4.649229000000	0.436549000000	-0.480562000000
H	-5.462438000000	0.088848000000	0.177322000000
H	-5.110263000000	1.052950000000	-1.269833000000
C	-3.849669000000	-0.767087000000	-1.087116000000
H	-4.269067000000	-1.735175000000	-0.768436000000
H	-3.866657000000	-0.751021000000	-2.189202000000
C	-2.403443000000	-0.740089000000	0.826083000000
H	-2.851084000000	-1.690616000000	1.157618000000
H	-1.352792000000	-0.750273000000	1.148613000000
C	-3.173698000000	0.493851000000	1.403814000000
H	-3.990418000000	0.184232000000	2.076239000000
H	-2.503384000000	1.145409000000	1.988756000000
N	-2.451035000000	-0.699074000000	-0.644042000000
N	-3.746314000000	1.284297000000	0.306458000000
C	3.123718000000	-0.020813000000	-0.611446000000

➤ Et₃N:

N	-0.000078000000	-0.387536000000	0.224063000000
C	-1.206196000000	-0.825285000000	-0.470198000000
H	-1.090259000000	-1.905662000000	-0.663658000000
H	-1.310278000000	-0.354722000000	-1.476767000000
C	1.205968000000	-0.825604000000	-0.470211000000
H	1.089816000000	-1.905969000000	-0.663537000000
H	1.310092000000	-0.355116000000	-1.476773000000
C	0.000144000000	1.010853000000	0.648225000000
H	-0.873124000000	1.171819000000	1.299687000000
H	0.873258000000	1.171521000000	1.299989000000
C	-2.496750000000	-0.611594000000	0.318040000000
H	-2.769601000000	0.452067000000	0.401054000000
H	-3.333691000000	-1.123914000000	-0.182018000000

H	-2.396799000000	-1.019948000000	1.336482000000
C	2.496507000000	-0.611996000000	0.318070000000
H	3.333471000000	-1.124305000000	-0.181955000000
H	2.769341000000	0.451668000000	0.401113000000
H	2.396471000000	-1.020350000000	1.336499000000
C	0.000406000000	2.068318000000	-0.467224000000
H	0.000569000000	3.081718000000	-0.034154000000
H	0.889717000000	1.982770000000	-1.112285000000
H	-0.888905000000	1.983021000000	-1.112331000000

➤ IM':

C	-3.210627000000	0.280784000000	-0.229579000000
C	-2.716323000000	-0.938287000000	0.259667000000
C	-3.629731000000	-1.965842000000	0.552973000000
C	-4.993082000000	-1.773189000000	0.364403000000
C	-5.465734000000	-0.542217000000	-0.126544000000
C	-4.581104000000	0.489227000000	-0.426750000000
H	-3.220644000000	-2.906074000000	0.928733000000
H	-5.699089000000	-2.574220000000	0.595147000000
H	-6.537570000000	-0.390017000000	-0.275831000000
H	-4.920943000000	1.452897000000	-0.809920000000
C	-0.457829000000	0.048984000000	0.114816000000
H	0.625412000000	-0.022430000000	0.216182000000
O	-0.773049000000	-2.187419000000	0.830678000000
C	-1.039111000000	1.182145000000	-0.362079000000
O	-2.373878000000	1.319615000000	-0.535993000000
S	-0.254173000000	2.671984000000	-0.891587000000
C	1.480550000000	2.404899000000	-0.375633000000
H	1.797994000000	1.395747000000	-0.684292000000
H	2.047473000000	3.113423000000	-1.002984000000
C	1.809793000000	2.616573000000	1.077936000000
H	2.873199000000	2.462935000000	1.302143000000
C	0.973582000000	2.934631000000	2.066950000000
H	-0.094253000000	3.088381000000	1.887390000000
H	1.334477000000	3.048869000000	3.092140000000
C	-1.254778000000	-1.122714000000	0.445837000000
N	2.690340000000	-0.970353000000	-0.168023000000
C	2.640427000000	-1.674772000000	1.119541000000
H	1.610455000000	-2.046717000000	1.234510000000
H	3.296784000000	-2.573909000000	1.116919000000
C	2.980538000000	-0.800810000000	2.323333000000
H	2.356392000000	0.106456000000	2.335909000000
H	2.787952000000	-1.360078000000	3.252195000000
H	4.037867000000	-0.490945000000	2.343657000000
C	2.143011000000	-1.808107000000	-1.239227000000
H	1.195958000000	-2.221633000000	-0.858656000000
H	2.793805000000	-2.686641000000	-1.449026000000
C	1.863902000000	-1.061870000000	-2.542199000000
H	2.781920000000	-0.708037000000	-3.037528000000
H	1.351111000000	-1.730796000000	-3.251111000000
H	1.209527000000	-0.192653000000	-2.368492000000

C	3.972399000000	-0.334336000000	-0.473352000000
H	4.178822000000	0.410131000000	0.312707000000
H	3.852634000000	0.250661000000	-1.399461000000
C	5.188064000000	-1.261032000000	-0.619778000000
H	5.046011000000	-1.998104000000	-1.425937000000
H	6.087857000000	-0.672583000000	-0.861468000000
H	5.392968000000	-1.815901000000	0.309263000000

➤ TS':

C	-1.720984000000	0.863242000000	-0.842285000000
C	-2.815272000000	0.553878000000	-0.016855000000
C	-3.682358000000	1.587797000000	0.380468000000
C	-3.455482000000	2.895818000000	-0.028192000000
C	-2.350936000000	3.187240000000	-0.850283000000
C	-1.483992000000	2.180159000000	-1.261755000000
H	-4.525842000000	1.316621000000	1.019140000000
H	-4.128168000000	3.696711000000	0.286482000000
H	-2.168638000000	4.215426000000	-1.172876000000
H	-0.622754000000	2.383515000000	-1.900145000000
C	-1.977231000000	-1.780680000000	-0.015727000000
H	-2.215994000000	-2.839720000000	0.069219000000
O	-3.965658000000	-1.184579000000	1.134948000000
C	-0.998384000000	-1.411014000000	-0.959005000000
O	-0.834049000000	-0.082566000000	-1.265641000000
S	0.180615000000	-2.468433000000	-1.508743000000
C	1.301325000000	-2.499557000000	0.732468000000
H	1.996569000000	-3.312663000000	0.504455000000
H	1.682767000000	-1.480680000000	0.576257000000
C	0.200050000000	-2.744933000000	1.543782000000
H	-0.051781000000	-3.782086000000	1.791105000000
C	-0.753233000000	-1.758057000000	1.806899000000
H	-0.474186000000	-0.705593000000	1.712289000000
H	-1.603260000000	-1.963738000000	2.461928000000
C	1.661973000000	1.435774000000	0.830773000000
H	0.689720000000	1.185393000000	0.379779000000
C	3.983312000000	0.596075000000	0.823843000000
H	4.577218000000	-0.231698000000	0.406436000000
H	3.899330000000	0.373331000000	1.899111000000
C	2.596411000000	0.593631000000	-1.224067000000
H	1.548887000000	0.424515000000	-1.515049000000
N	2.643793000000	0.529193000000	0.239393000000
C	-3.029348000000	-0.841411000000	0.428190000000
H	1.851054000000	2.497348000000	0.548144000000
H	2.864999000000	1.609383000000	-1.596697000000
C	1.540907000000	1.338158000000	2.349629000000
H	2.411670000000	1.764758000000	2.870881000000
H	0.652342000000	1.893081000000	2.689257000000
H	1.435474000000	0.289997000000	2.671934000000
C	4.745648000000	1.915336000000	0.635001000000
H	5.736439000000	1.856253000000	1.113580000000
H	4.904090000000	2.146591000000	-0.430419000000

H	4.209151000000	2.765899000000	1.085603000000
C	3.458326000000	-0.447851000000	-1.930261000000
H	3.241685000000	-0.434096000000	-3.009502000000
H	4.537332000000	-0.264157000000	-1.808027000000
H	3.228786000000	-1.458288000000	-1.558936000000

➤ A':

C	-1.744439000000	0.822162000000	-0.836776000000
C	-2.801066000000	0.546579000000	0.044146000000
C	-3.673101000000	1.585602000000	0.410635000000
C	-3.476495000000	2.874446000000	-0.074308000000
C	-2.403700000000	3.132850000000	-0.944109000000
C	-1.537998000000	2.112285000000	-1.334482000000
H	-4.491687000000	1.341843000000	1.091471000000
H	-4.149292000000	3.682755000000	0.219870000000
H	-2.244343000000	4.143985000000	-1.326832000000
H	-0.707920000000	2.288191000000	-2.020246000000
C	-1.747575000000	-1.729729000000	0.363665000000
H	-2.100799000000	-2.768760000000	0.356509000000
O	-3.902239000000	-1.178608000000	1.251364000000
C	-0.983342000000	-1.457246000000	-0.905185000000
O	-0.885179000000	-0.150761000000	-1.283400000000
S	-0.171079000000	-2.581294000000	-1.754413000000
C	1.568831000000	-2.407866000000	1.524990000000
H	2.281214000000	-3.233755000000	1.614407000000
H	1.967528000000	-1.420503000000	1.258179000000
C	0.260769000000	-2.614191000000	1.706802000000
H	-0.108651000000	-3.622972000000	1.930361000000
C	-0.790425000000	-1.550470000000	1.607126000000
H	-0.334712000000	-0.548404000000	1.570220000000
H	-1.448287000000	-1.586585000000	2.491562000000
C	1.707904000000	1.571494000000	0.569116000000
H	0.744615000000	1.222111000000	0.168767000000
C	4.040171000000	0.786749000000	0.750839000000
H	4.641564000000	-0.113489000000	0.549974000000
H	3.968569000000	0.843441000000	1.848649000000
C	2.637507000000	0.226727000000	-1.206038000000
H	1.581195000000	0.035594000000	-1.448419000000
N	2.697721000000	0.558844000000	0.218365000000
C	-2.949794000000	-0.818996000000	0.590571000000
H	1.900193000000	2.544834000000	0.059430000000
H	2.943780000000	1.088523000000	-1.843789000000
C	1.551955000000	1.812938000000	2.068526000000
H	2.420802000000	2.327817000000	2.506780000000
H	0.668966000000	2.444252000000	2.255434000000
H	1.416100000000	0.860988000000	2.606649000000
C	4.784840000000	2.023133000000	0.225632000000
H	5.781307000000	2.094687000000	0.690592000000
H	4.929519000000	1.980544000000	-0.865693000000
H	4.243765000000	2.955287000000	0.455359000000
C	3.443797000000	-1.007409000000	-1.600285000000

H	3.212151000000	-1.281449000000	-2.640939000000
H	4.531392000000	-0.846150000000	-1.534366000000
H	3.178556000000	-1.863401000000	-0.960774000000

➤ **Imidazole:**

C	-0.583209000000	1.001950000000	0.000101000000
C	-1.144210000000	-0.256711000000	-0.000061000000
C	0.972723000000	-0.567249000000	-0.000160000000
H	-1.015310000000	1.999493000000	-0.001177000000
H	-2.203260000000	-0.513020000000	0.000606000000
H	1.968812000000	-1.011192000000	-0.000101000000
N	-0.166254000000	-1.220727000000	-0.000013000000
N	0.777784000000	0.786137000000	0.000205000000
H	1.497226000000	1.498915000000	0.000049000000

➤ **IM'':**

C	-2.910192000000	0.198680000000	-0.188821000000
C	-2.340043000000	-1.050291000000	0.103384000000
C	-3.194097000000	-2.146280000000	0.317404000000
C	-4.573158000000	-1.992382000000	0.241951000000
C	-5.122354000000	-0.730801000000	-0.052358000000
C	-4.297931000000	0.368874000000	-0.269417000000
H	-2.726954000000	-3.107561000000	0.541389000000
H	-5.232378000000	-2.847193000000	0.409672000000
H	-6.206687000000	-0.608547000000	-0.112357000000
H	-4.697417000000	1.357959000000	-0.499846000000
C	-0.134825000000	0.044407000000	-0.060189000000
H	0.952552000000	0.021815000000	-0.017492000000
O	-0.323136000000	-2.272787000000	0.408905000000
C	-0.787354000000	1.206421000000	-0.339649000000
O	-2.135589000000	1.304090000000	-0.408272000000
S	-0.090082000000	2.787343000000	-0.683265000000
C	1.698161000000	2.469922000000	-0.449035000000
H	1.984720000000	1.562652000000	-1.005180000000
H	2.175711000000	3.319811000000	-0.966925000000
C	2.201926000000	2.370443000000	0.967317000000
H	3.248227000000	2.047219000000	1.024777000000
C	1.524050000000	2.607930000000	2.090807000000
H	0.472040000000	2.907642000000	2.073738000000
H	2.001379000000	2.499249000000	3.067973000000
C	-0.863920000000	-1.190729000000	0.174930000000
C	5.062136000000	-1.881291000000	-0.304239000000
C	4.555274000000	-0.625060000000	-0.550455000000
C	2.860311000000	-1.853926000000	-0.049840000000
N	3.964062000000	-2.651738000000	0.013628000000
H	3.969858000000	-3.635773000000	0.253334000000
H	6.071993000000	-2.282662000000	-0.327788000000
H	5.103678000000	0.271996000000	-0.836189000000
H	1.847526000000	-2.210772000000	0.161471000000
N	3.190074000000	-0.622439000000	-0.389364000000

➤ TS'':

C	-2.789889000000	0.040565000000	-0.223369000000
C	-2.052307000000	-1.148189000000	-0.077552000000
C	-2.734689000000	-2.342337000000	0.222166000000
C	-4.114197000000	-2.347479000000	0.378000000000
C	-4.836307000000	-1.147555000000	0.231232000000
C	-4.184833000000	0.043222000000	-0.070082000000
H	-2.135673000000	-3.249345000000	0.327394000000
H	-4.639635000000	-3.275451000000	0.614289000000
H	-5.922569000000	-1.148134000000	0.352336000000
H	-4.723626000000	0.983986000000	-0.195022000000
C	-0.021565000000	0.222103000000	-0.465496000000
H	1.016810000000	0.274199000000	-0.793476000000
O	0.107037000000	-2.132787000000	-0.137566000000
C	-0.853674000000	1.320989000000	-0.763347000000
O	-2.203550000000	1.230179000000	-0.523035000000
S	-0.254734000000	2.846709000000	-1.109338000000
C	0.464698000000	3.130181000000	1.271056000000
H	0.985685000000	4.078605000000	1.118974000000
H	-0.577586000000	3.202172000000	1.592867000000
C	1.173755000000	1.949383000000	1.436109000000
H	2.237175000000	1.918097000000	1.183341000000
C	0.530643000000	0.720927000000	1.601451000000
H	-0.492242000000	0.690068000000	1.989203000000
H	1.128973000000	-0.183465000000	1.726486000000
C	-0.583885000000	-1.121532000000	-0.231660000000
C	5.425577000000	-1.168326000000	-0.240934000000
C	4.772902000000	0.006502000000	0.058199000000
C	3.234068000000	-1.481979000000	-0.150235000000
N	4.425369000000	-2.108719000000	-0.370489000000
H	4.548411000000	-3.088769000000	-0.594276000000
H	6.477175000000	-1.411510000000	-0.369641000000
H	5.211943000000	0.987601000000	0.235622000000
H	2.265871000000	-1.986265000000	-0.197527000000
N	3.415393000000	-0.202299000000	0.111978000000

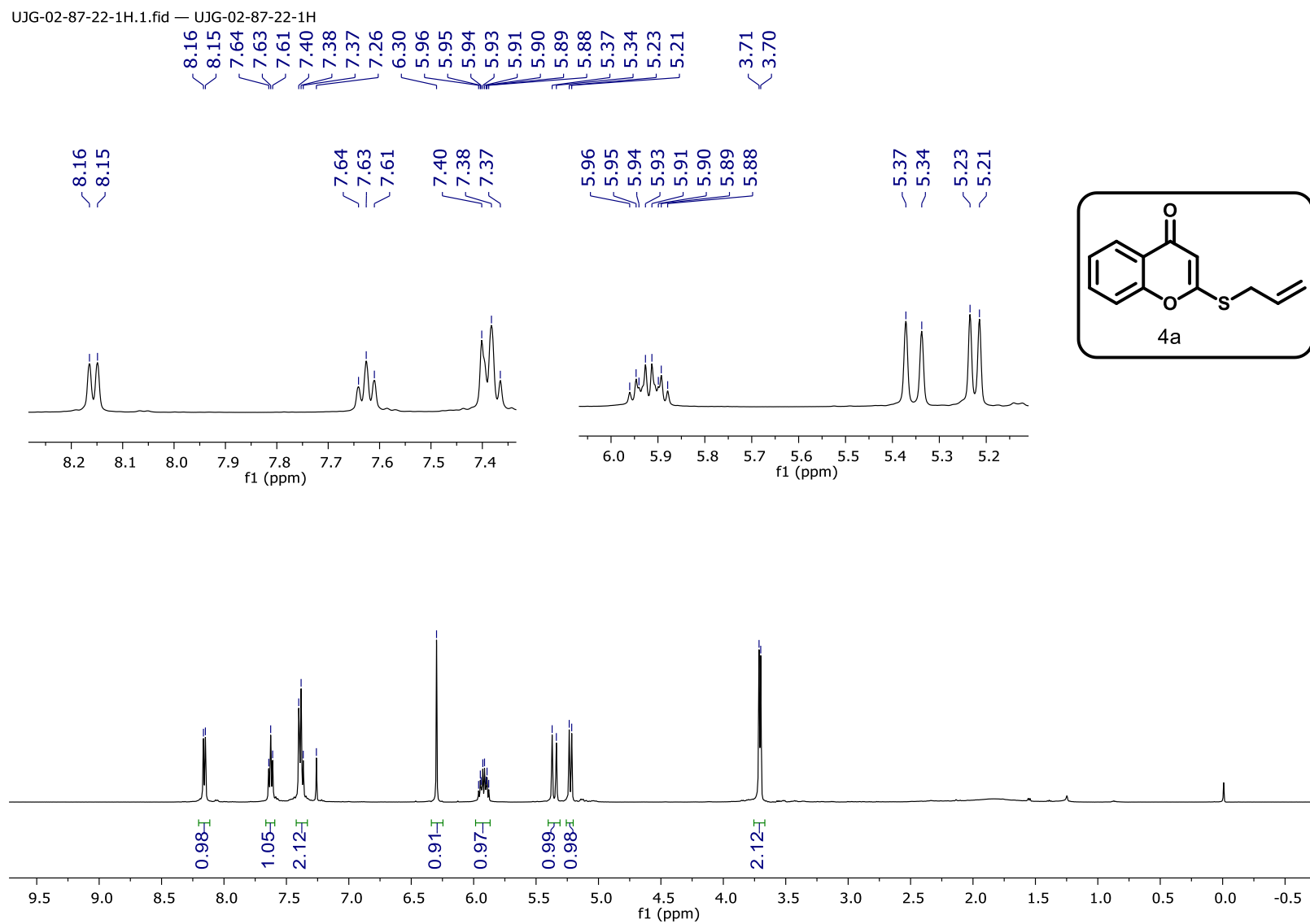
➤ A'':

C	-2.771291000000	0.094101000000	-0.199088000000
C	-2.060718000000	-1.109004000000	-0.052221000000
C	-2.766962000000	-2.290066000000	0.234147000000
C	-4.148629000000	-2.266286000000	0.389595000000
C	-4.840772000000	-1.051036000000	0.251469000000
C	-4.161612000000	0.128707000000	-0.047458000000
H	-2.189420000000	-3.211262000000	0.337699000000
H	-4.694017000000	-3.183972000000	0.619946000000
H	-5.926675000000	-1.026390000000	0.372687000000
H	-4.681006000000	1.079361000000	-0.178378000000
C	0.040146000000	0.289336000000	-0.156768000000
H	1.011746000000	0.256363000000	-0.666784000000
O	0.082428000000	-2.113517000000	-0.167790000000
C	-0.820966000000	1.356200000000	-0.782430000000

O	-2.162984000000	1.270408000000	-0.546082000000
S	-0.250615000000	2.639213000000	-1.600472000000
C	0.683598000000	2.995612000000	2.164532000000
H	1.297764000000	3.895832000000	2.255643000000
H	-0.303670000000	3.019061000000	2.639077000000
C	1.117657000000	1.919460000000	1.503091000000
H	2.099987000000	1.914582000000	1.020090000000
C	0.342039000000	0.647766000000	1.348124000000
H	-0.600762000000	0.683609000000	1.919427000000
H	0.942802000000	-0.195207000000	1.727044000000
C	-0.587947000000	-1.095915000000	-0.164076000000
C	5.422994000000	-1.064776000000	-0.202871000000
C	4.677861000000	0.086227000000	-0.076859000000
C	3.257102000000	-1.525113000000	-0.165580000000
N	4.497287000000	-2.085557000000	-0.258023000000
H	4.699167000000	-3.073234000000	-0.355133000000
H	6.493834000000	-1.243522000000	-0.256821000000
H	5.038162000000	1.111468000000	-0.001985000000
H	2.329076000000	-2.098431000000	-0.189037000000
N	3.337327000000	-0.214737000000	-0.054348000000

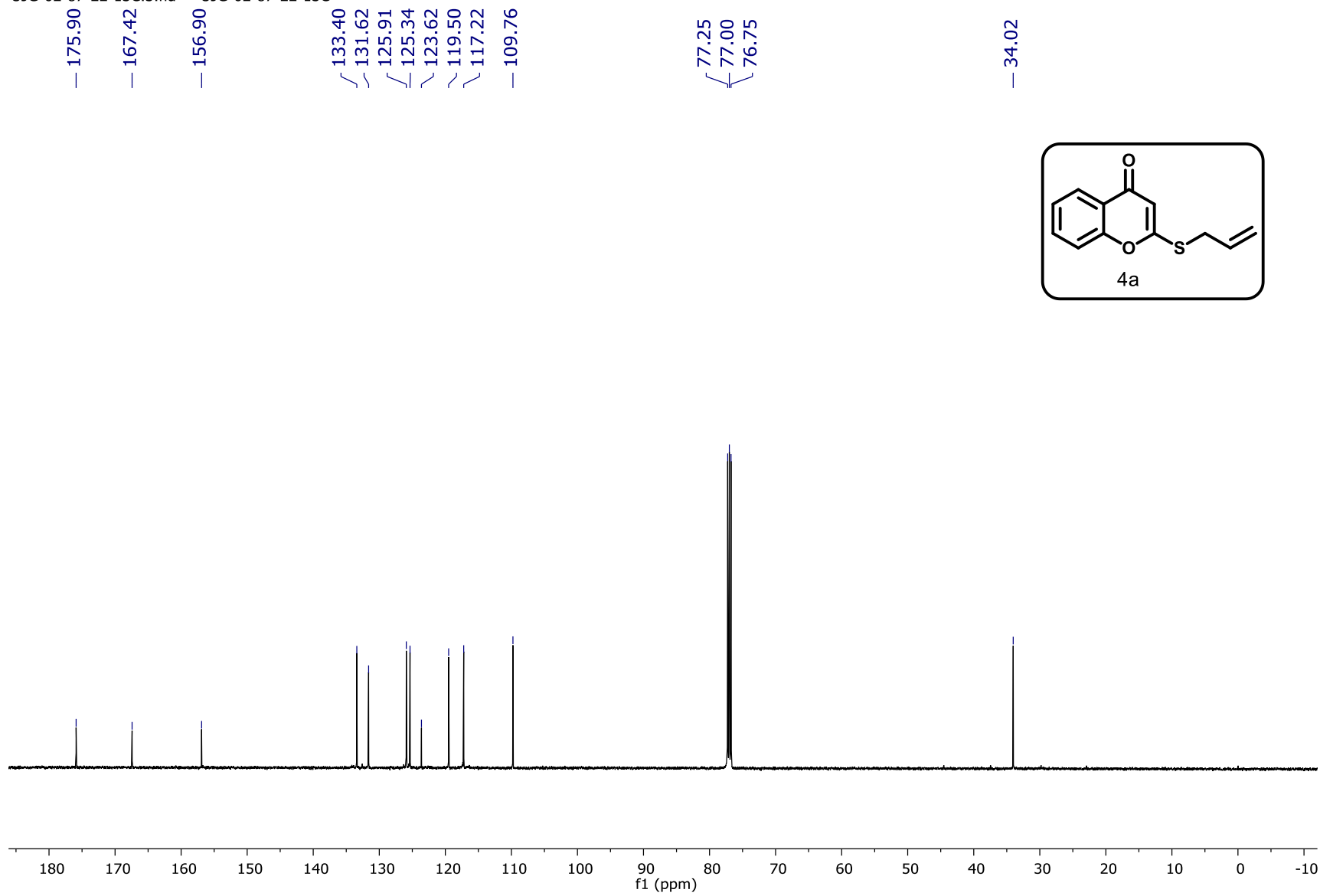
3. Copies of ^1H NMR, ^{13}C NMR and HRMS spectra of Compounds

^1H NMR (500 MHz, CDCl_3) Spectrum of Compound 4a

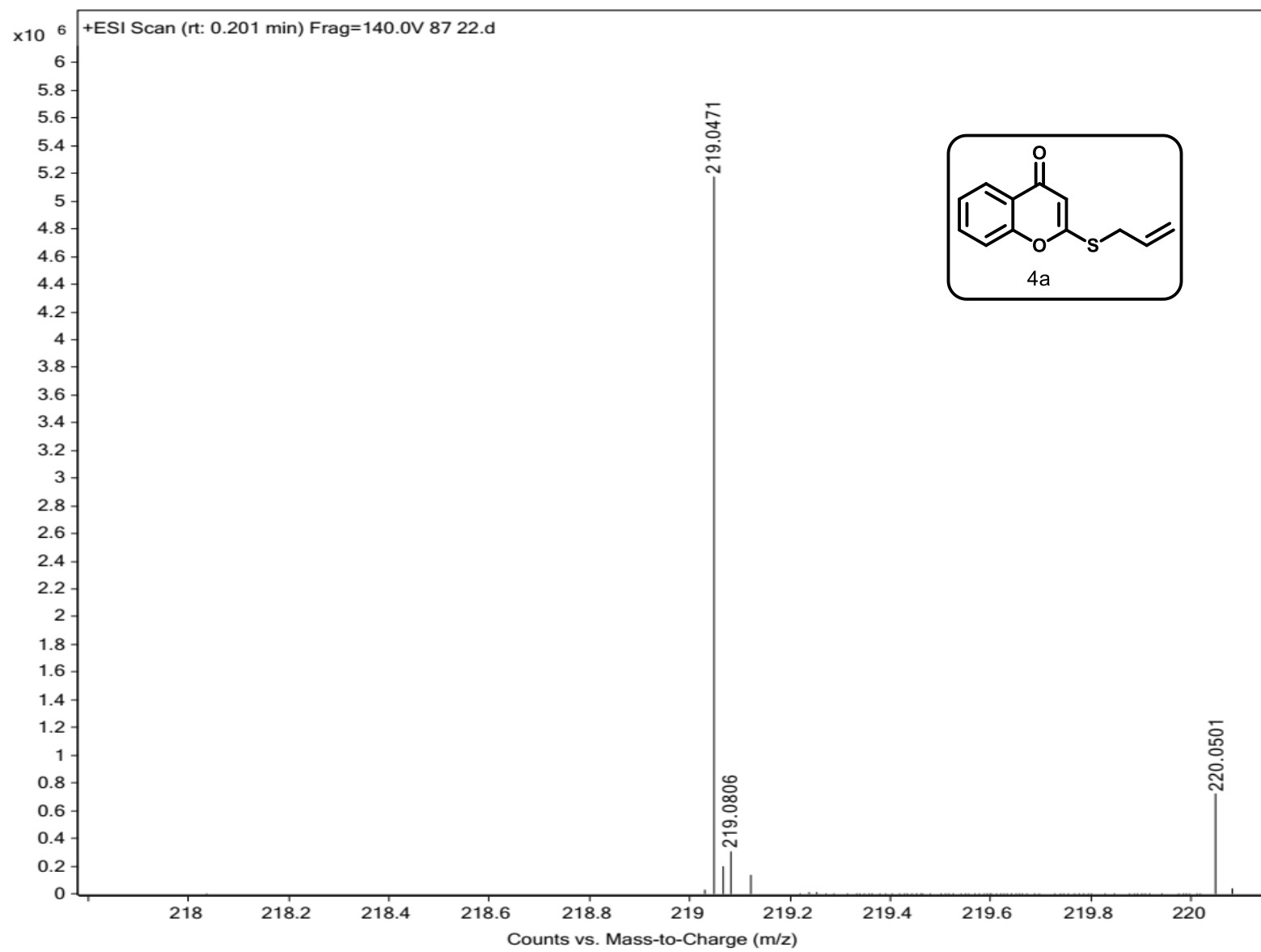


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4a

UJG-02-87-22-13C.3.fid — UJG-02-87-22-13C

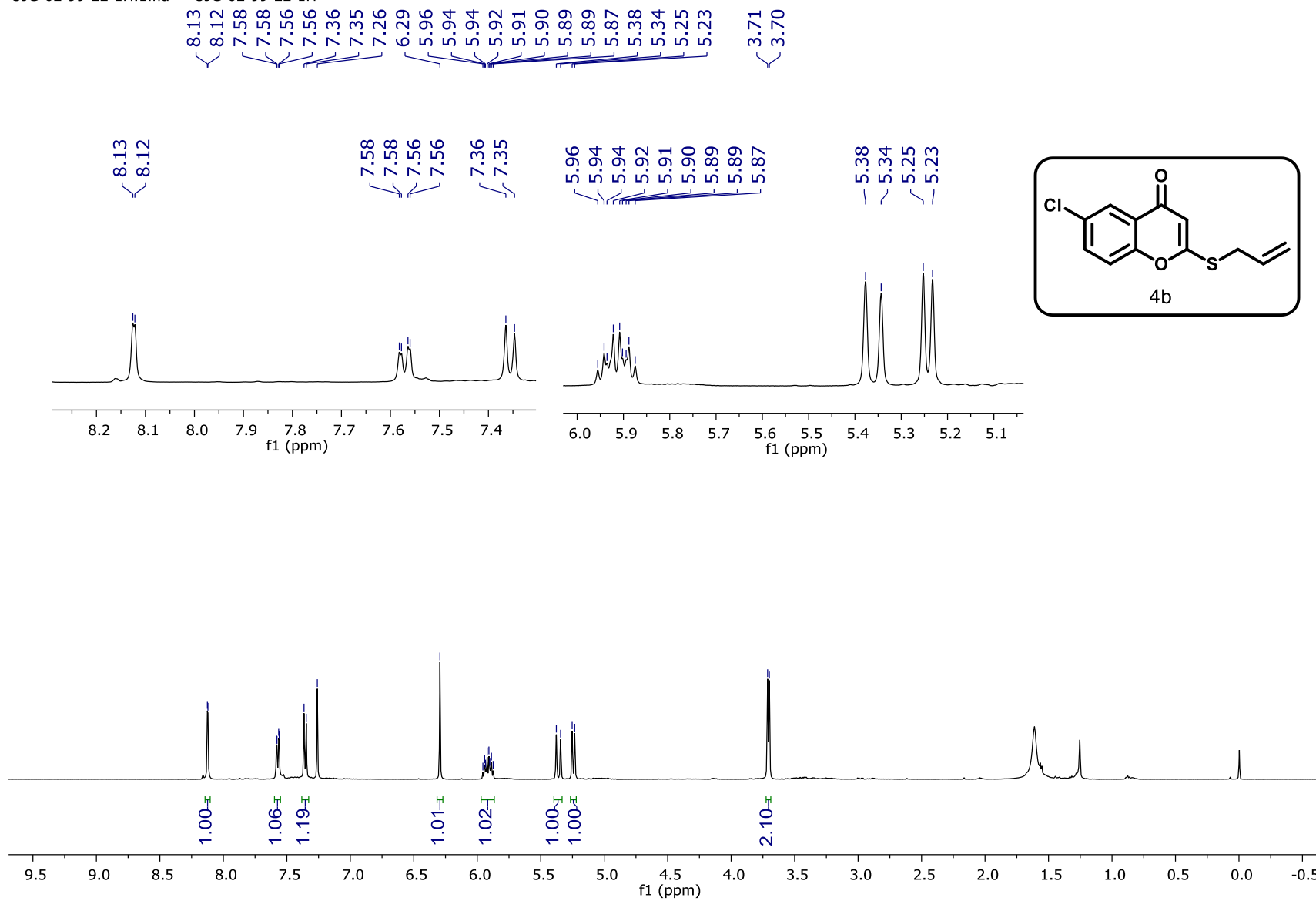


HRMS Spectrum of Compound 4a



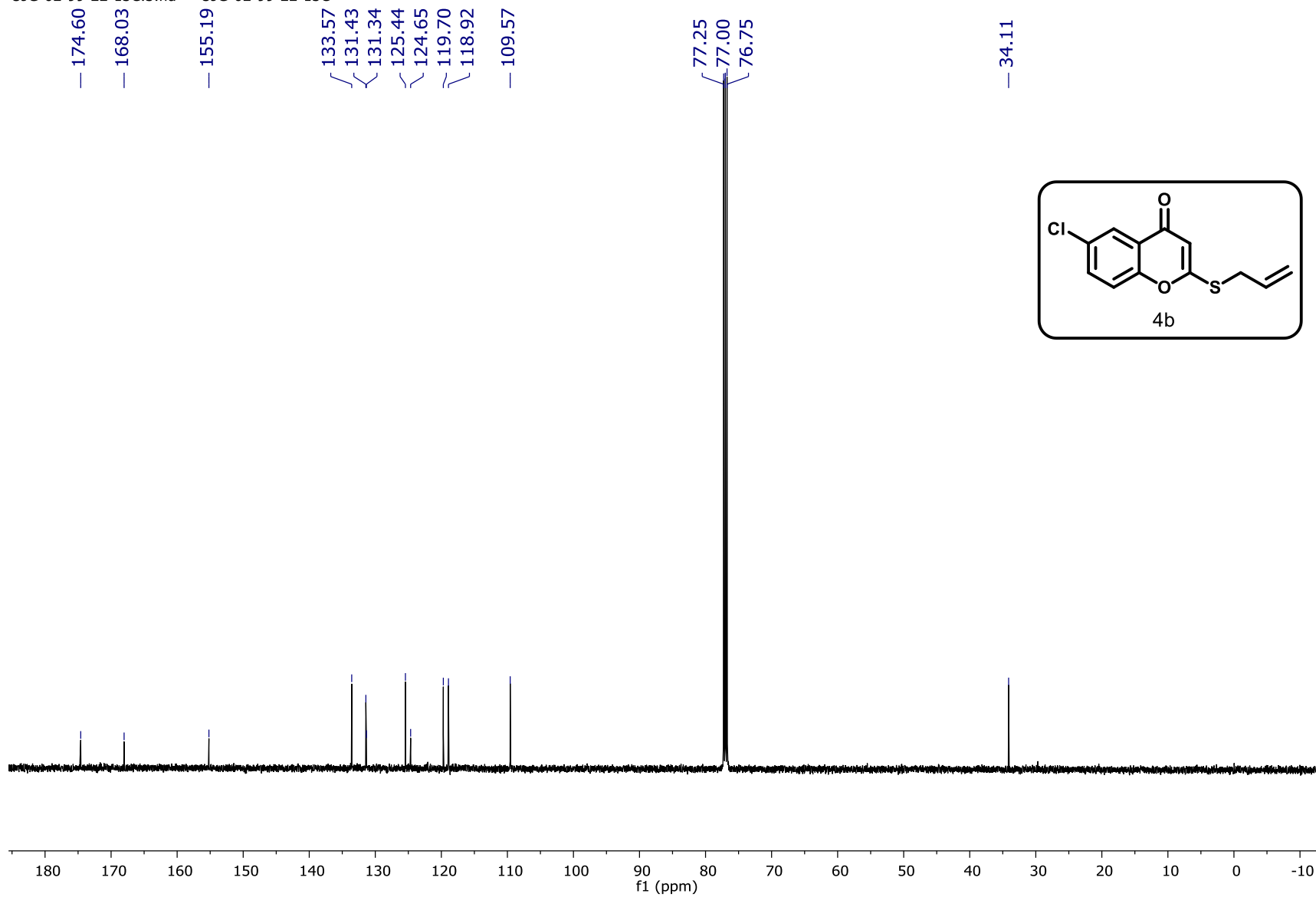
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4b

UJG-02-99-22-1H.1.fid — UJG-02-99-22-1H

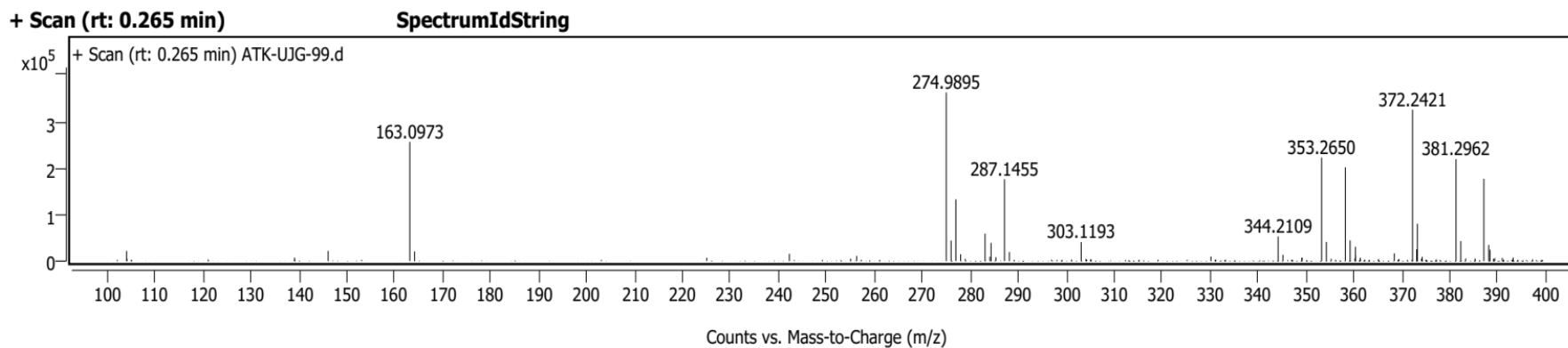


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4b

UJG-02-99-22-13C.3.fid — UJG-02-99-22-13C

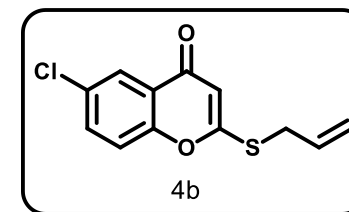


HRMS Spectrum of Compound 4b



SpectrumIdString

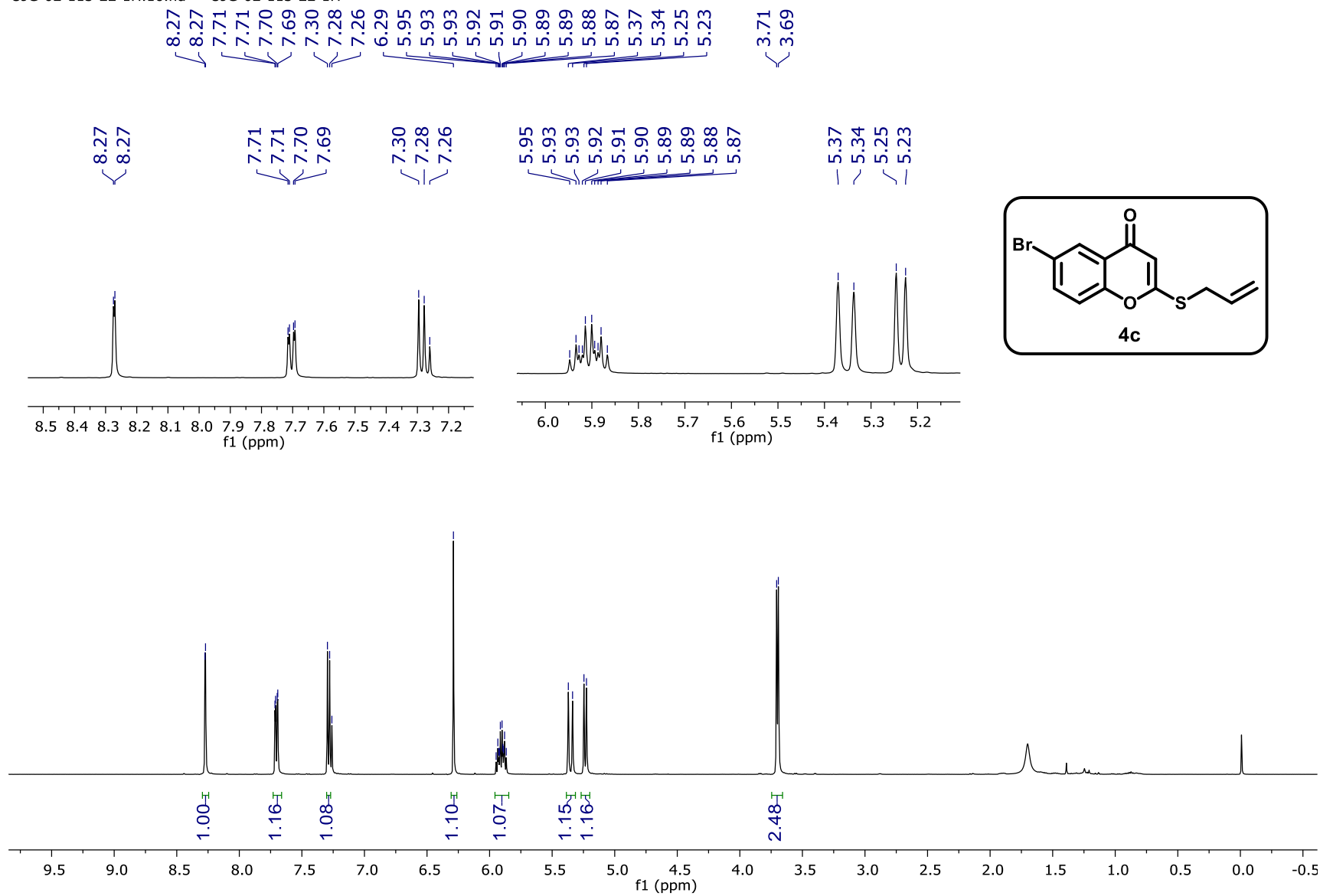
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
163.0973		256044	70.68					
274.9895	1	362256	100.00					
275.9926	1	44008	12.15					
276.9865	1	132665	36.62					
283.0850		58933	16.27					
284.3300		39135	10.80					
287.1455		175813	48.53					
303.1193		40754	11.25					
344.2109		52860	14.59					
353.2650	1	222227	61.35					
354.2680	1	40957	11.31					
358.2266	1	201370	55.59					
359.2297	1	44377	12.25					
360.3224		30614	8.45					
372.2421	1	325167	89.76					
373.2454	1	80073	22.10					
381.2962	1	218727	60.38					
382.2995	1	42817	11.82					
387.1107	1	176673	48.77					
388.1141	1	34812	9.61					



MassHunter Qual 10.0
(End of Report)

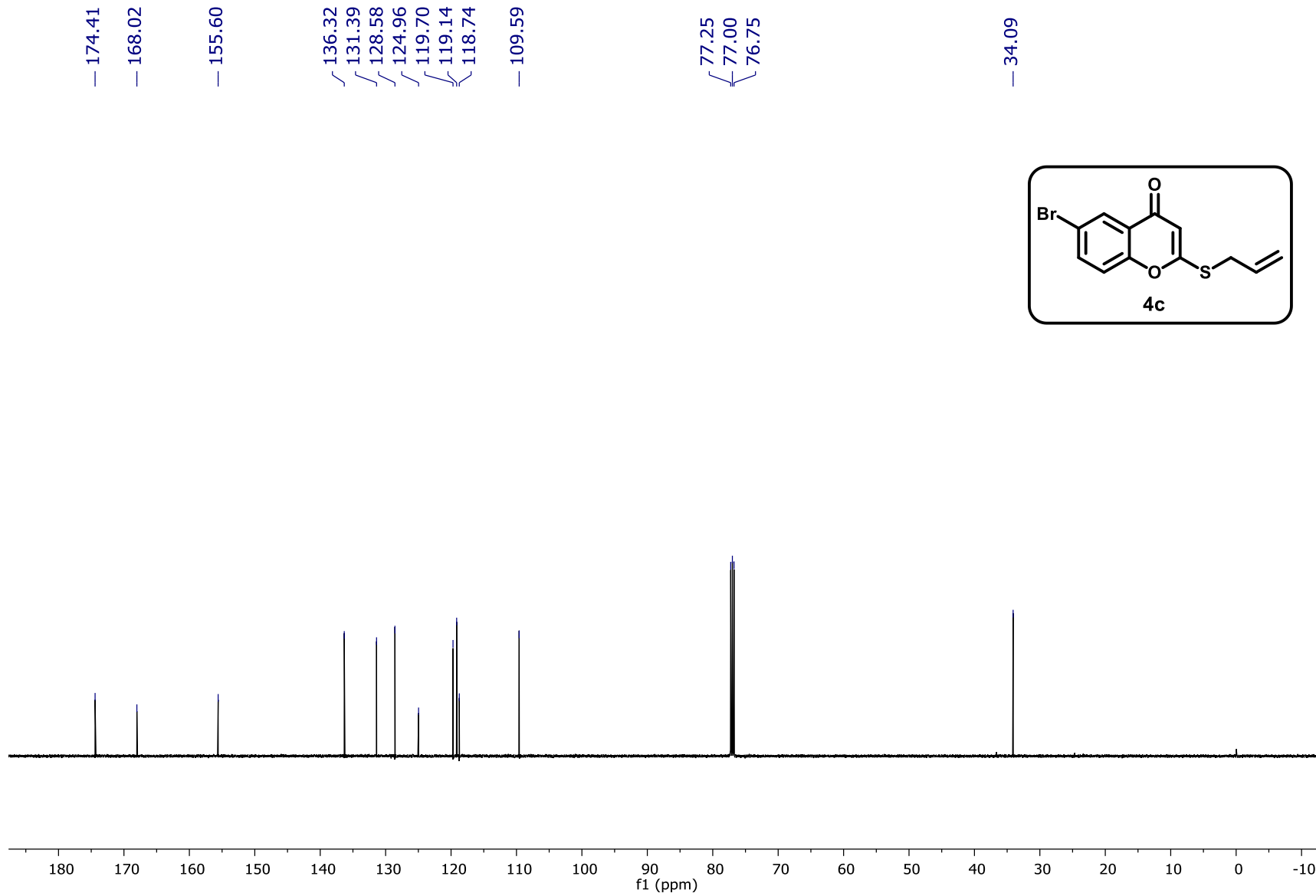
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4c

UJG-02-113-22-1H.16.fid — UJG-02-113-22-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4c

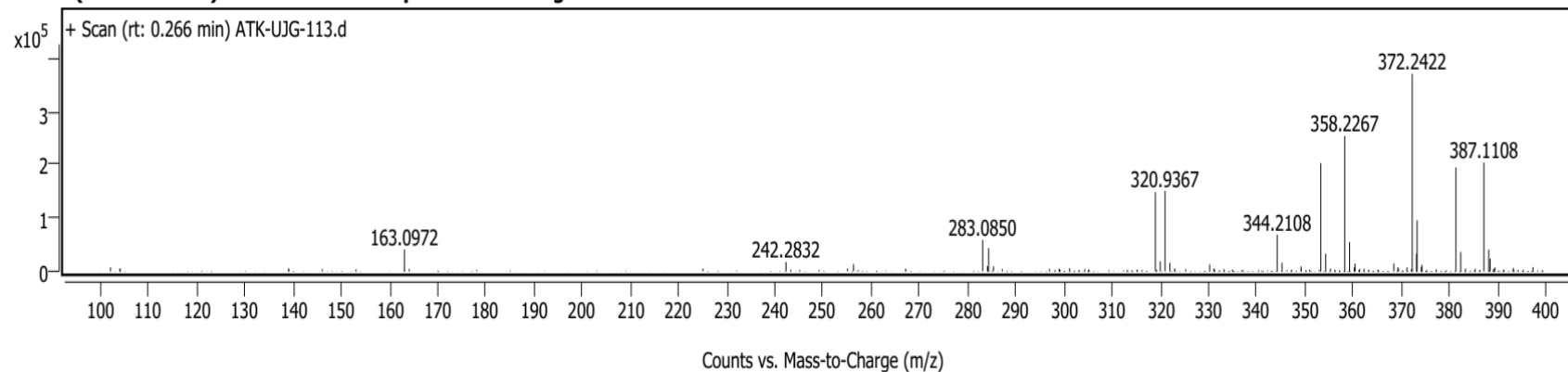
UJG-02-113-22-13C.18.fid —



HRMS Spectrum of Compound 4c

+ Scan (rt: 0.266 min)

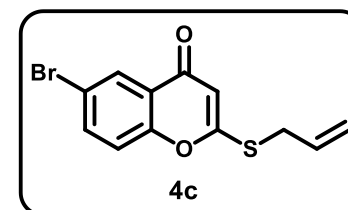
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SpectrumIdString

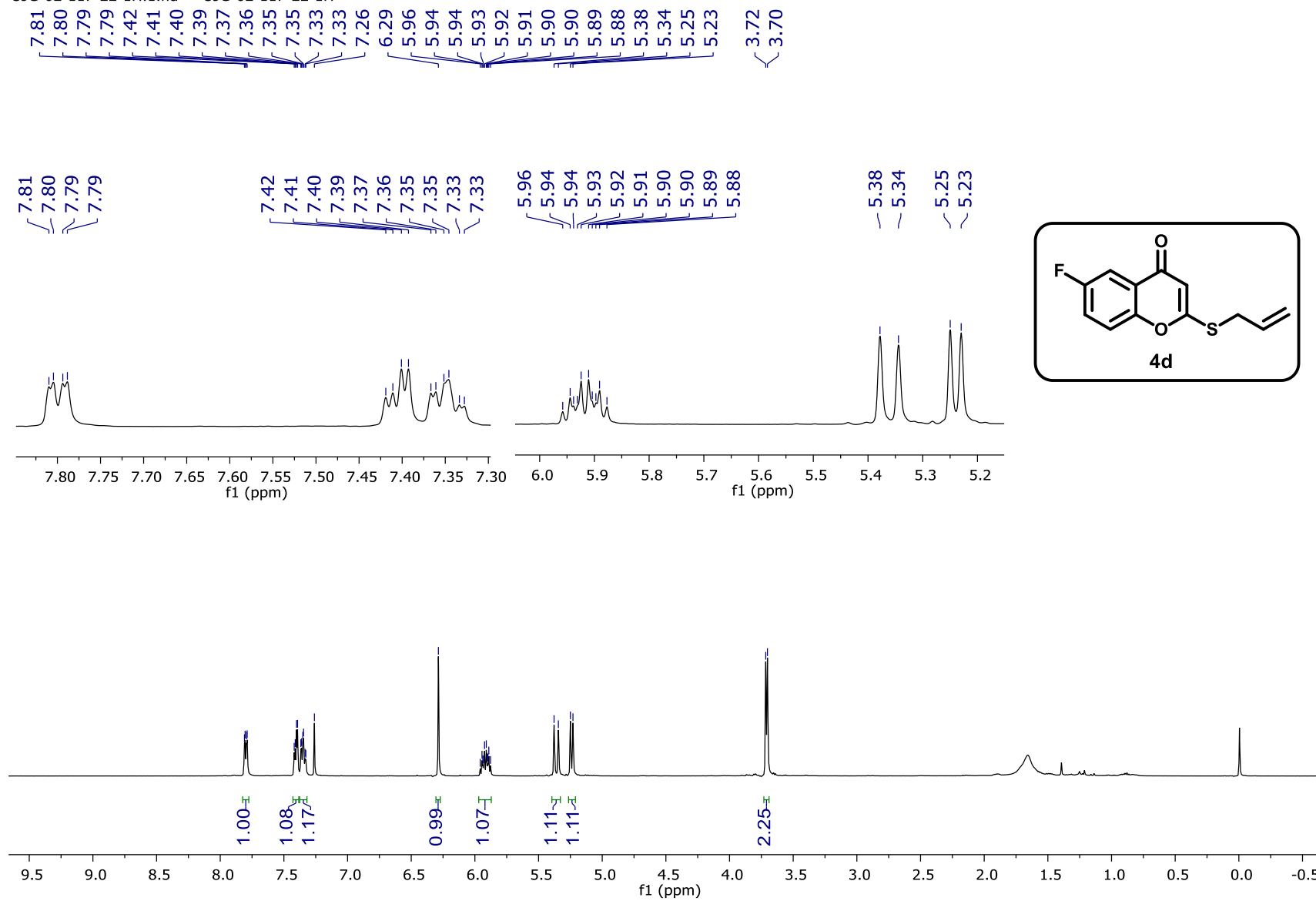
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula
163.0972		41148	11.10				
242.2832		17343	4.68				
283.0850		58976	15.90				
284.3302		43616	11.76				
318.9388	1	148520	40.05				
319.9420	1	18582	5.01				
320.9367	1	150906	40.70				
344.2108		68674	18.52				
353.2651	1	202940	54.73				
354.2686	1	33072	8.92				
358.2267	1	253746	68.43				
359.2299	1	54835	14.79				
372.2422	1	370815	100.00				
373.0953		32927	8.88				
373.2455	1	95801	25.84				
381.2963	1	195014	52.59				
382.2993	1	36145	9.75				
387.1108	1	204186	55.06				
388.1140	1	40659	10.96				
388.3924		23577	6.36				

Ion Type



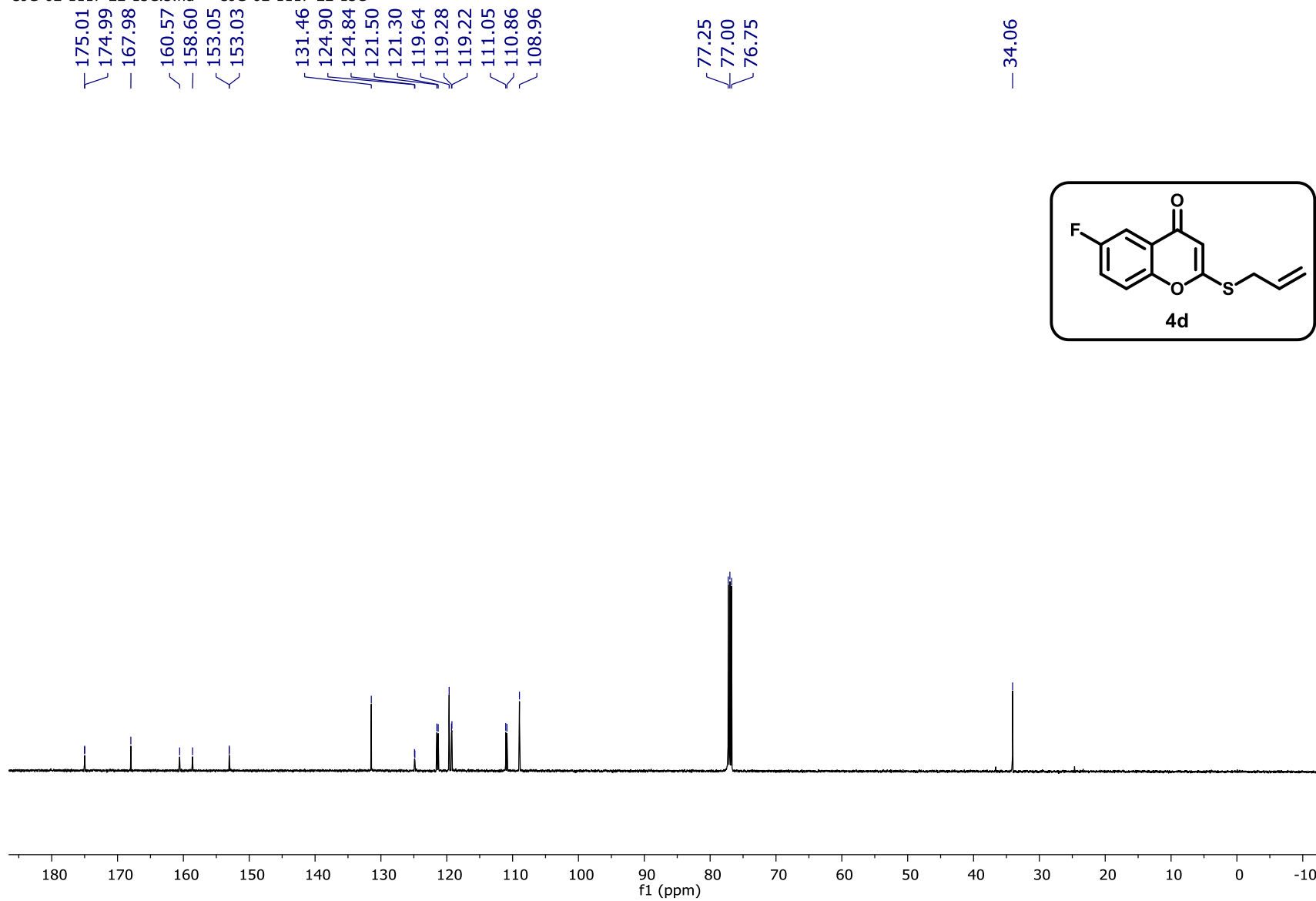
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4d

UJG-02-117-22-1H.1.fid — UJG-02-117-22-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4d

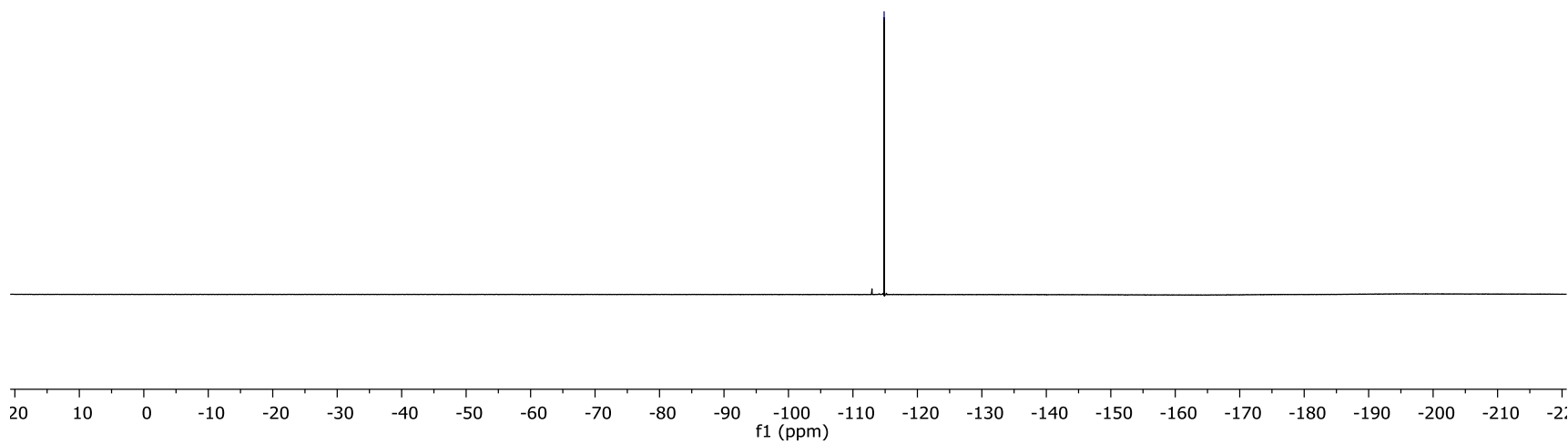
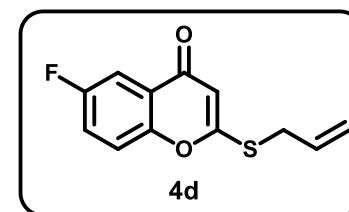
UJG-02-1117-22-13C.3.fid — UJG-02-1117-22-13C



¹⁹F NMR (471 MHz, CDCl₃) Spectrum of Compound 4d

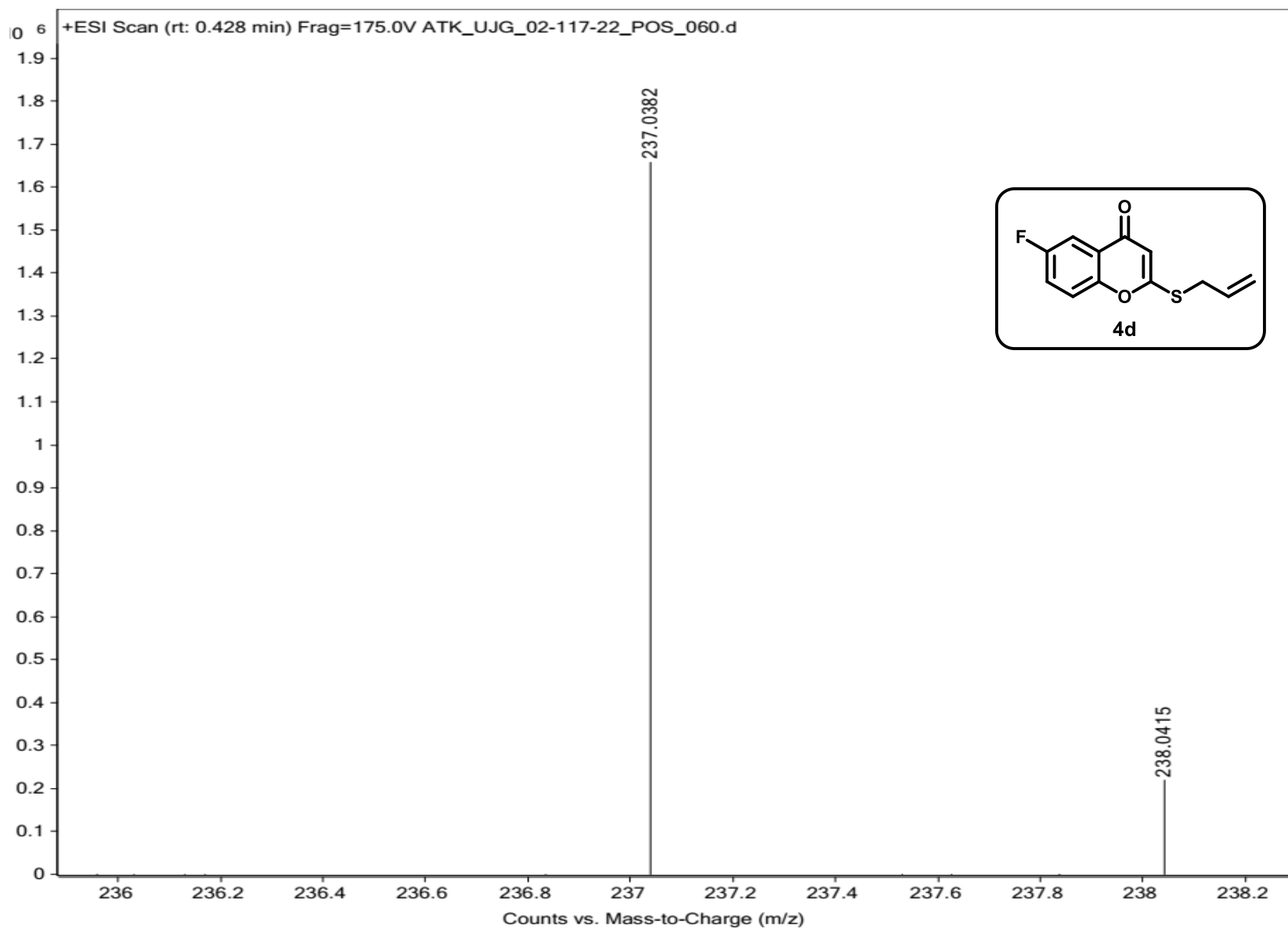
UJG-02-117-22-19F.3.fid — UJG-02-117-22-19F

— -114.84



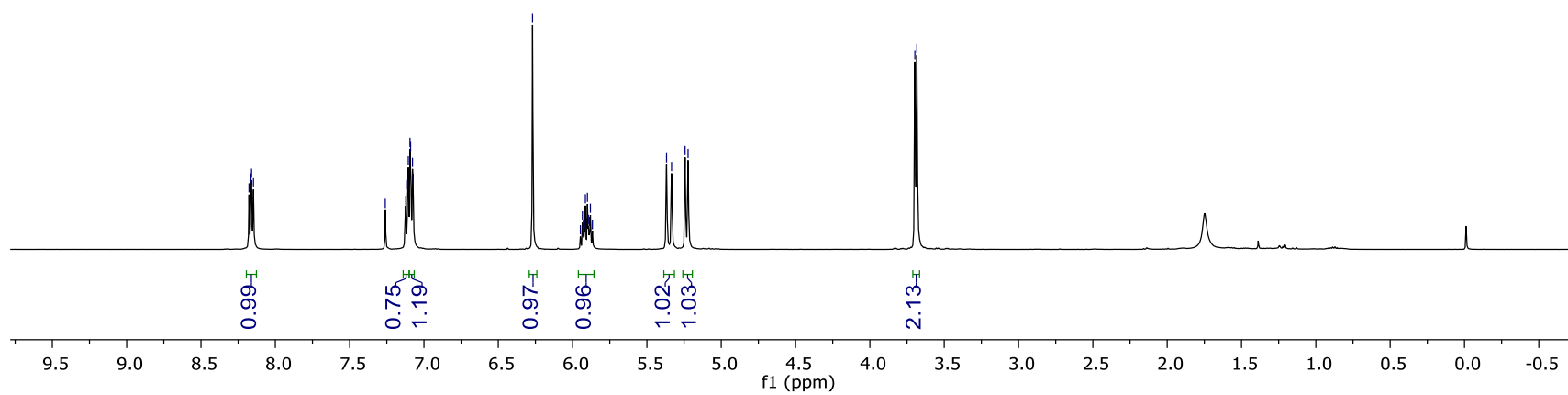
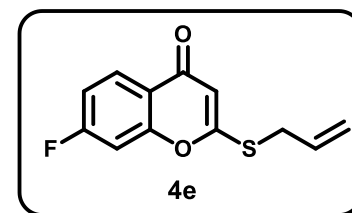
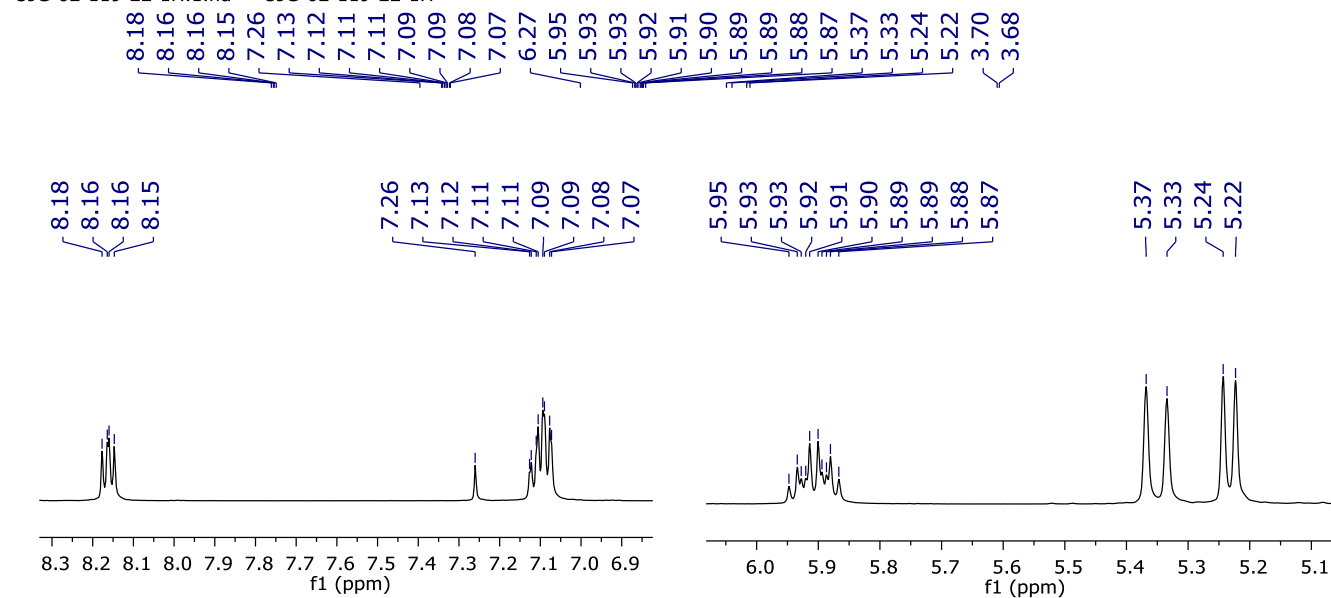
S30

HRMS Spectrum of Compound 4d



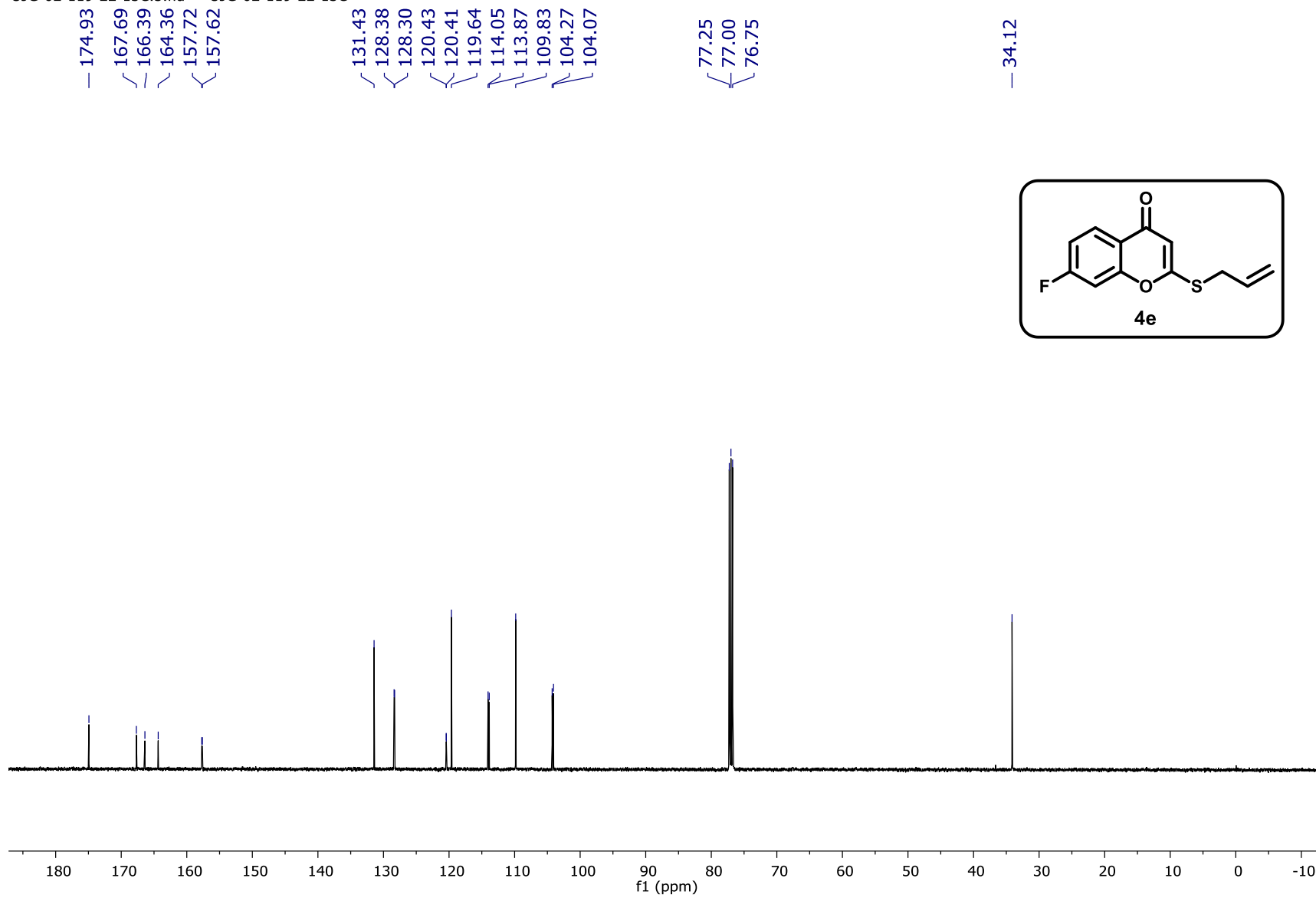
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4e

UJG-02-119-22-1H.1.fid — UJG-02-119-22-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4e

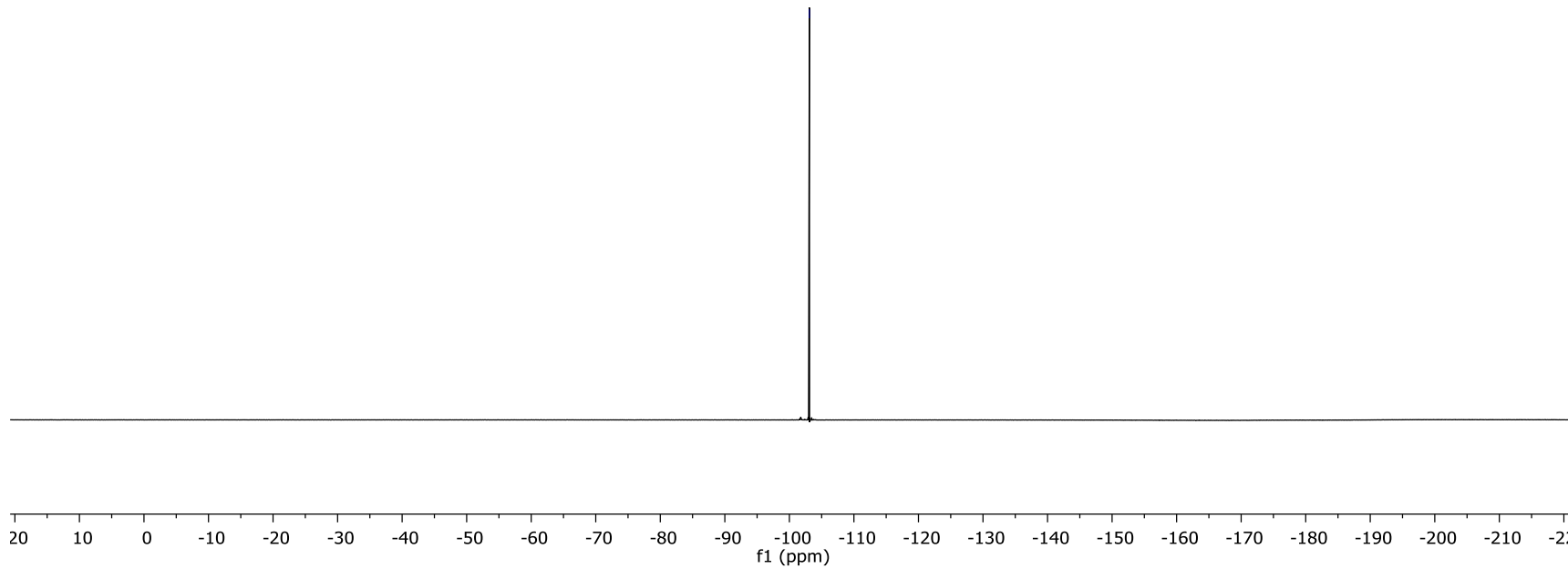
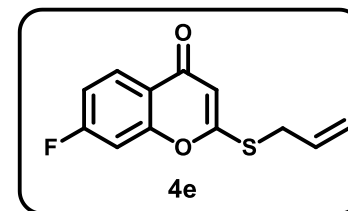
UJG-02-119-22-13C.5.fid — UJG-02-119-22-13C



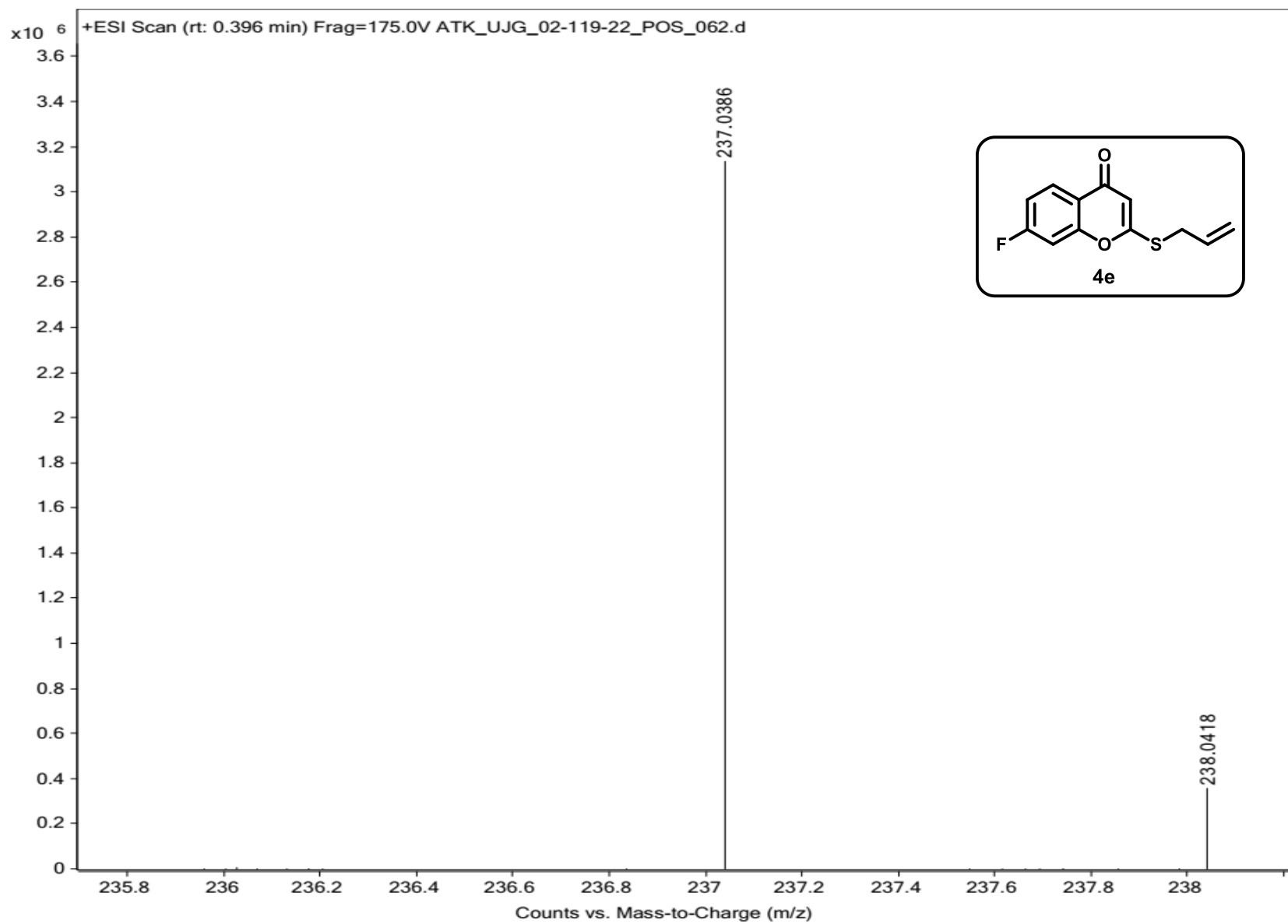
^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 4e

UJG-02-119-22-19F.3.fid — UJG-02-119-22-19F

— -103.09

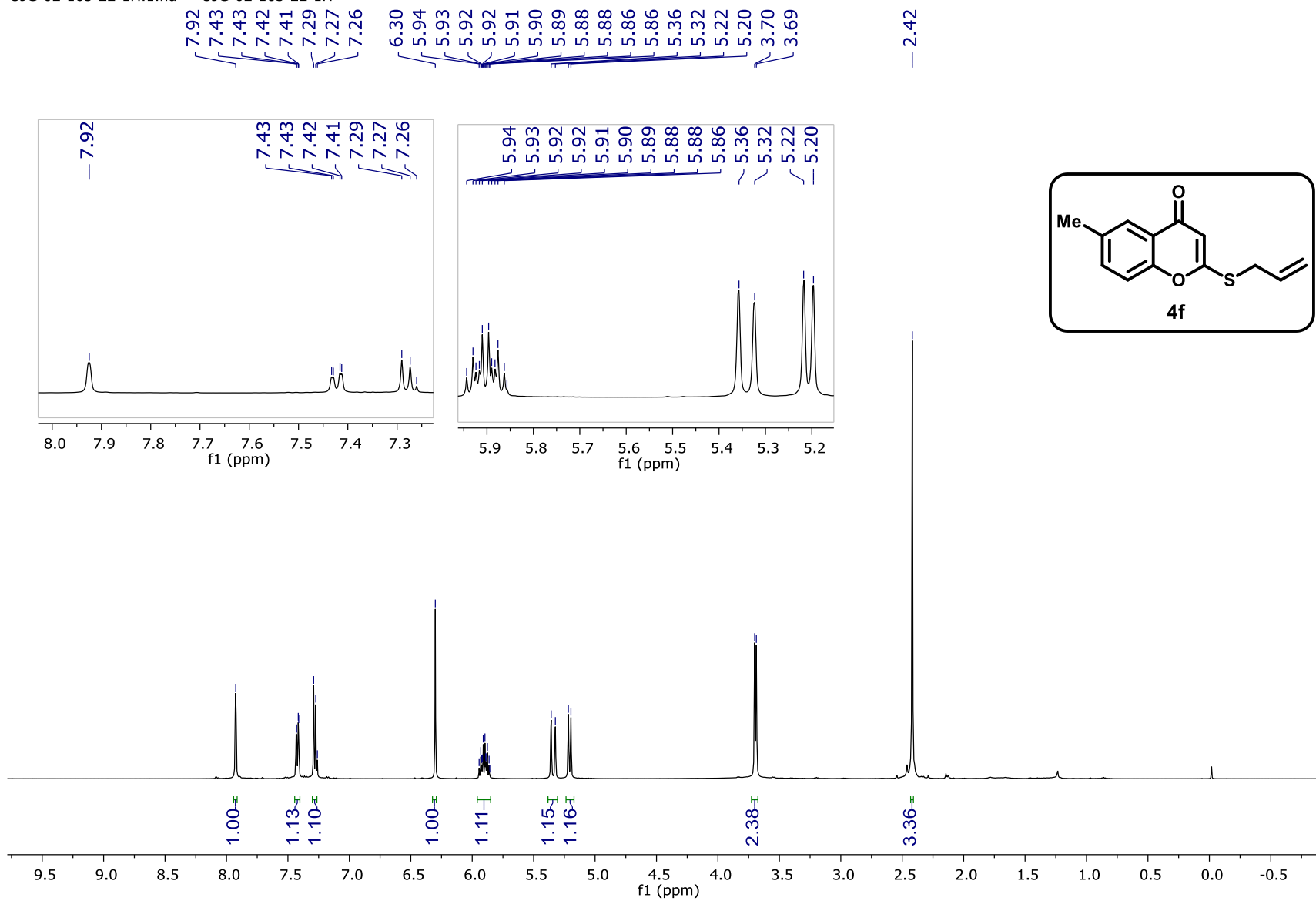


HRMS Spectrum of Compound 4e



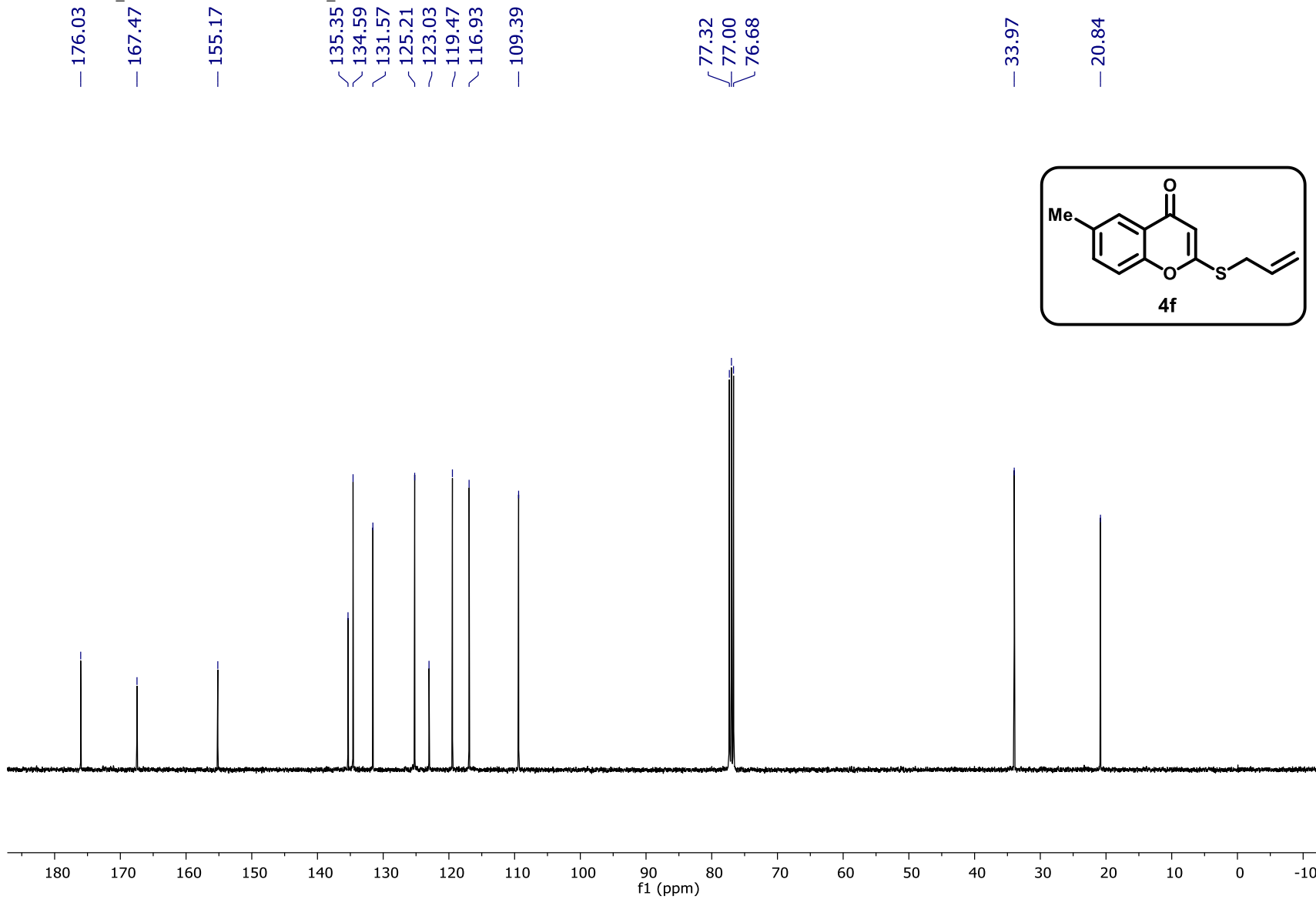
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4f

UJG-02-163-22-1H.1.fid — UJG-02-163-22-1H

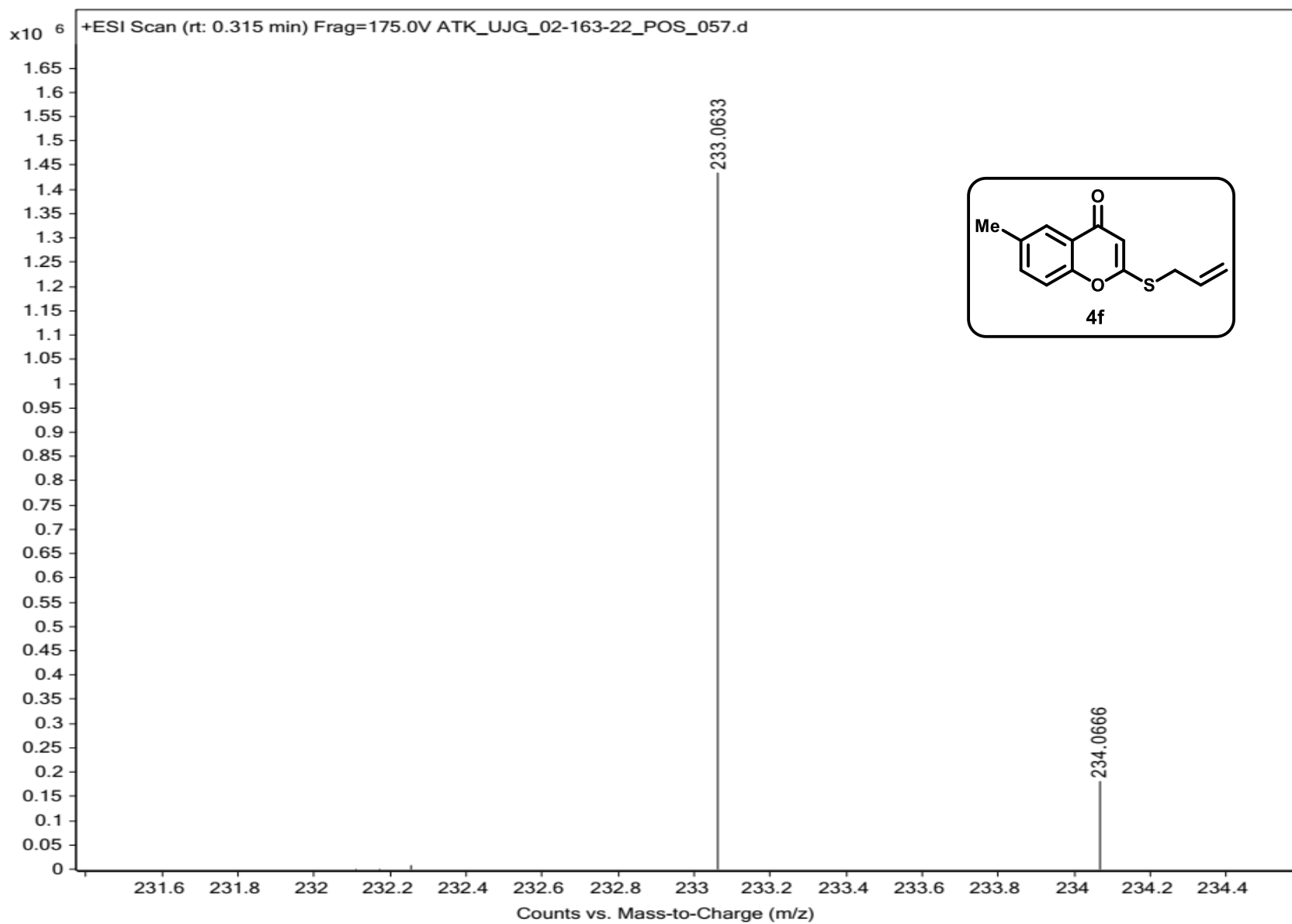


^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of Compound 4f

UJG-02-163-22_13C.10.fid — UJG-02-163-22_13C

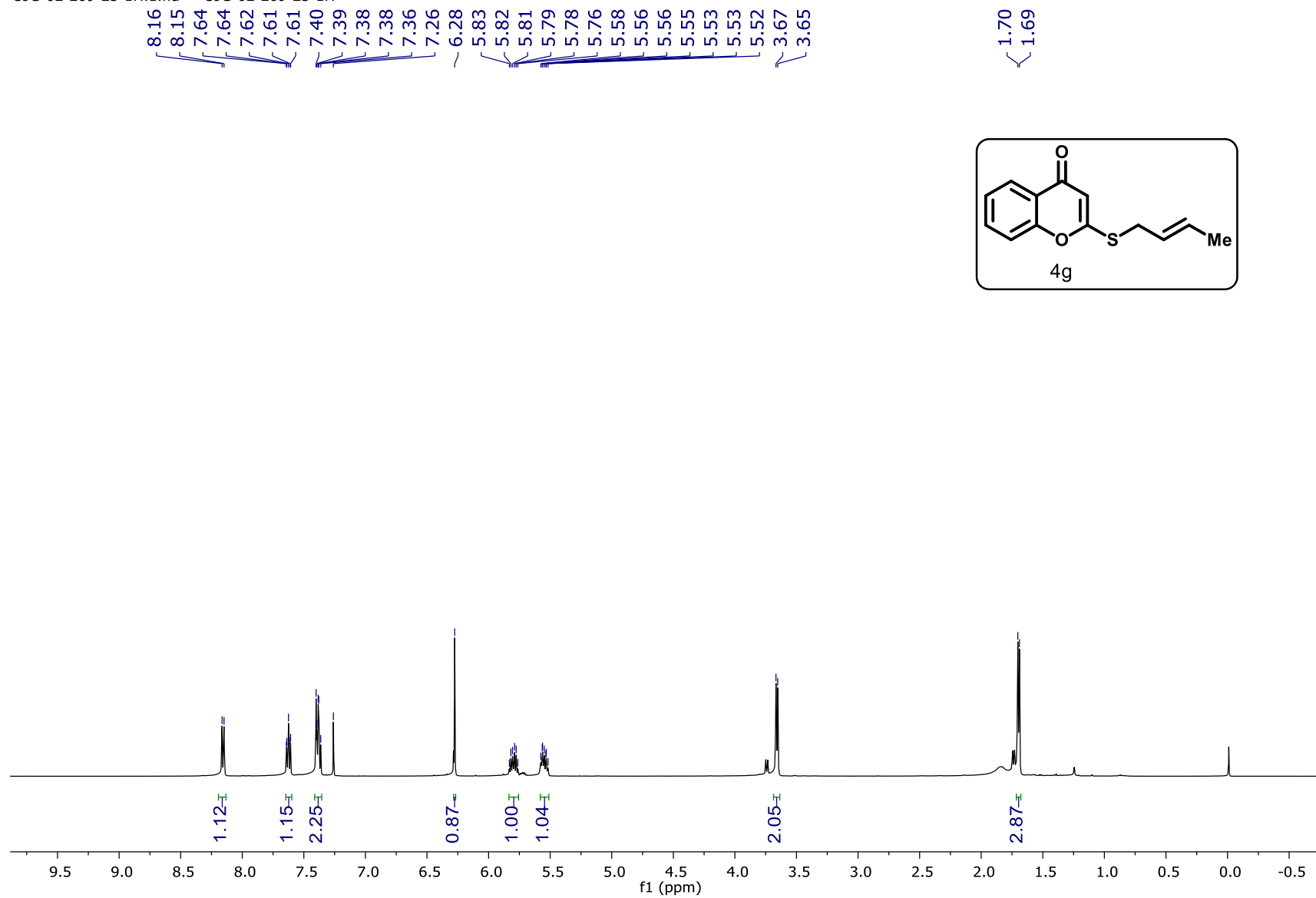


HRMS Spectrum of Compound 4f



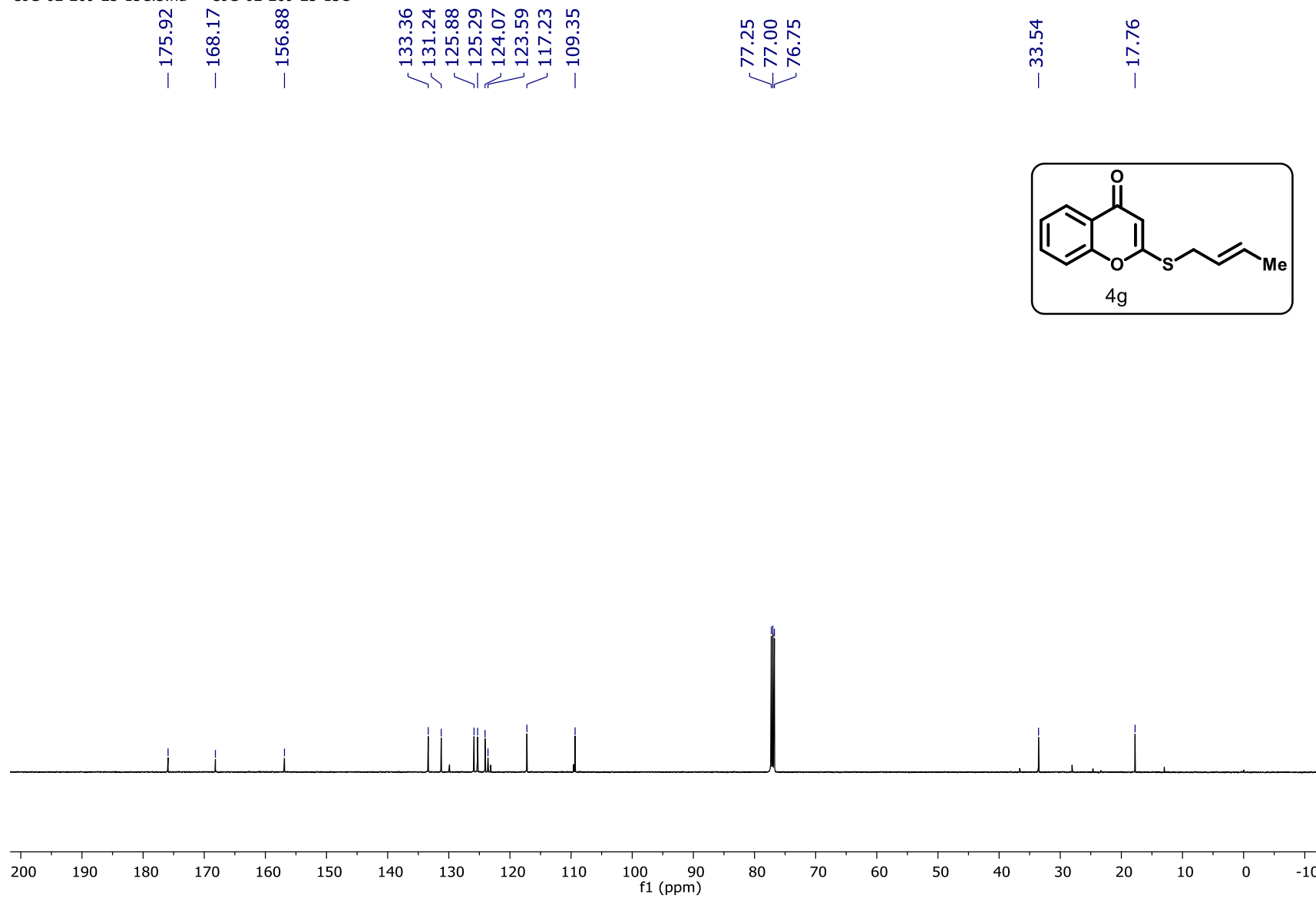
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4g

UJG-02-209-23-1H.1.fid — UJG-02-209-23-1H

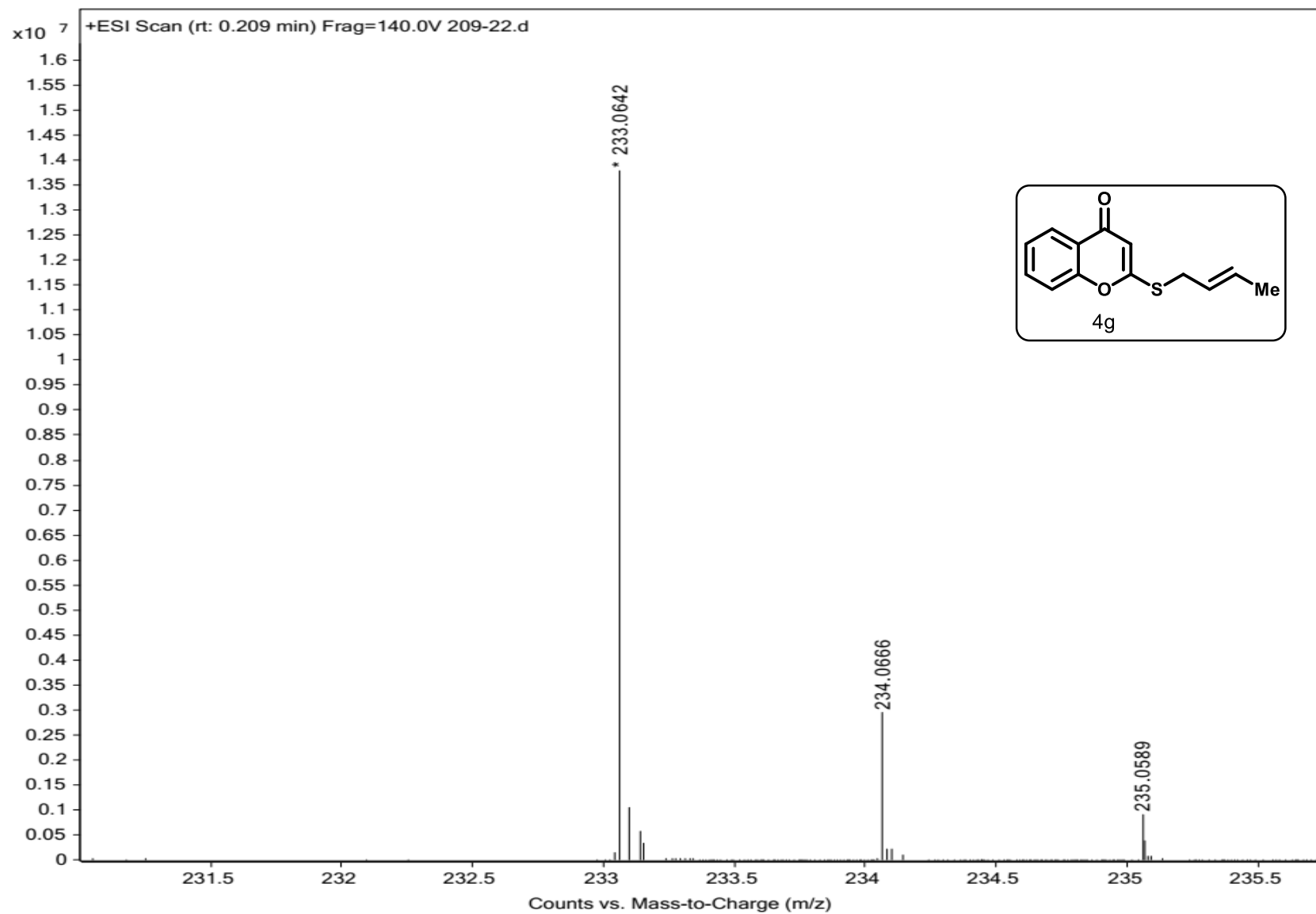


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4g

UJG-02-209-23-13C.3.fid — UJG-02-209-23-13C

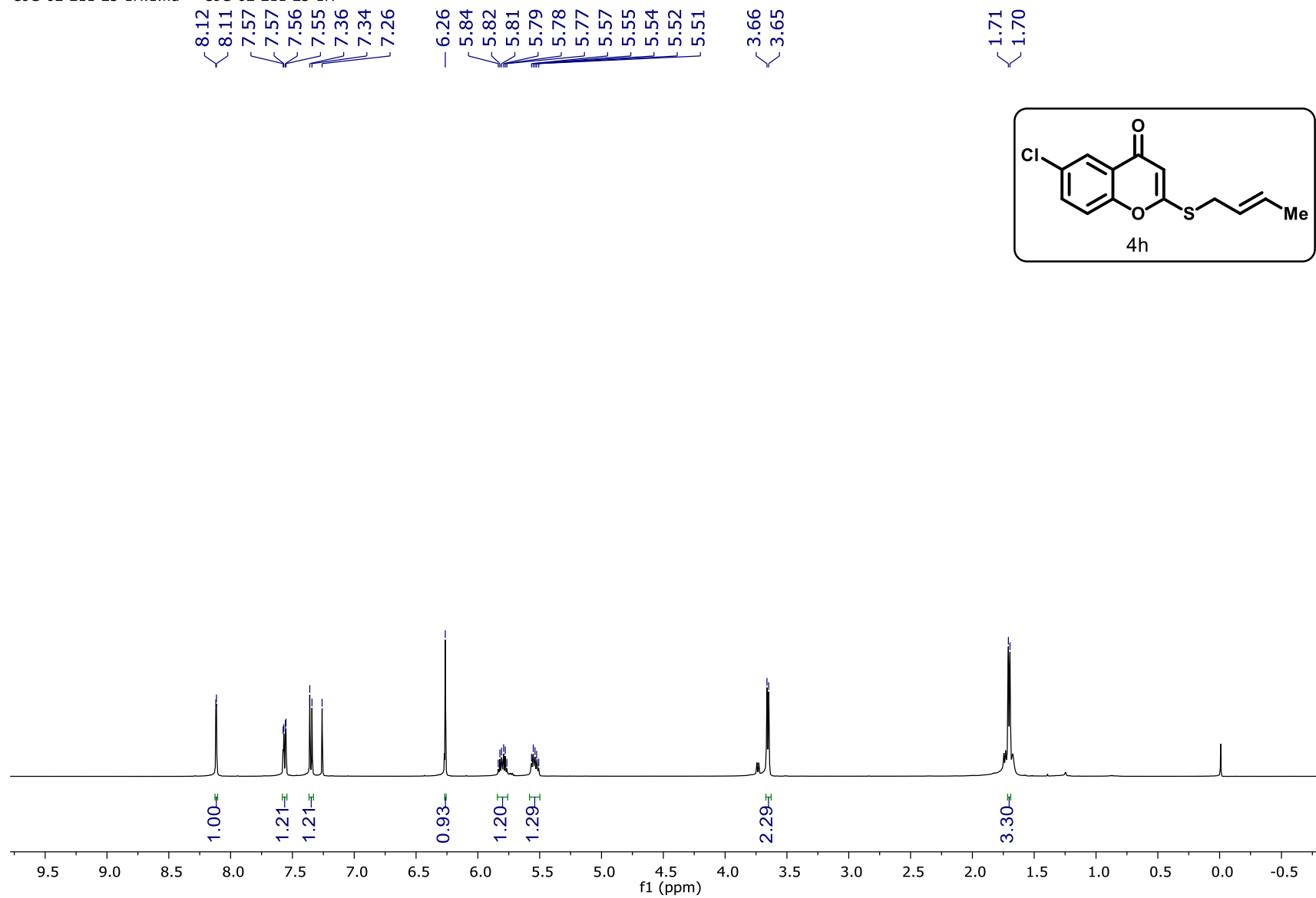


HRMS Spectrum of Compound 4g



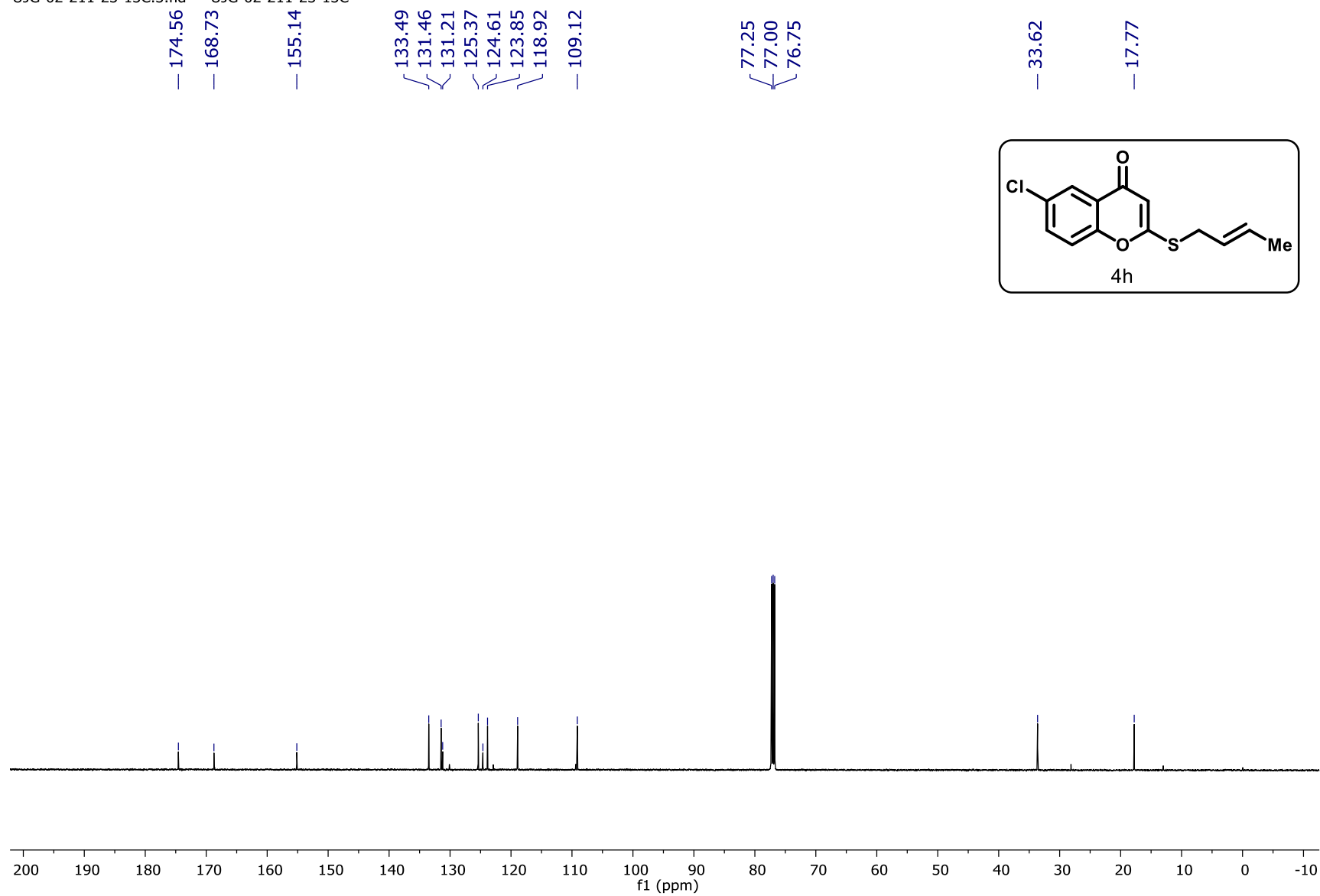
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4h

UJG-02-211-23-1H.1.fid — UJG-02-211-23-1H

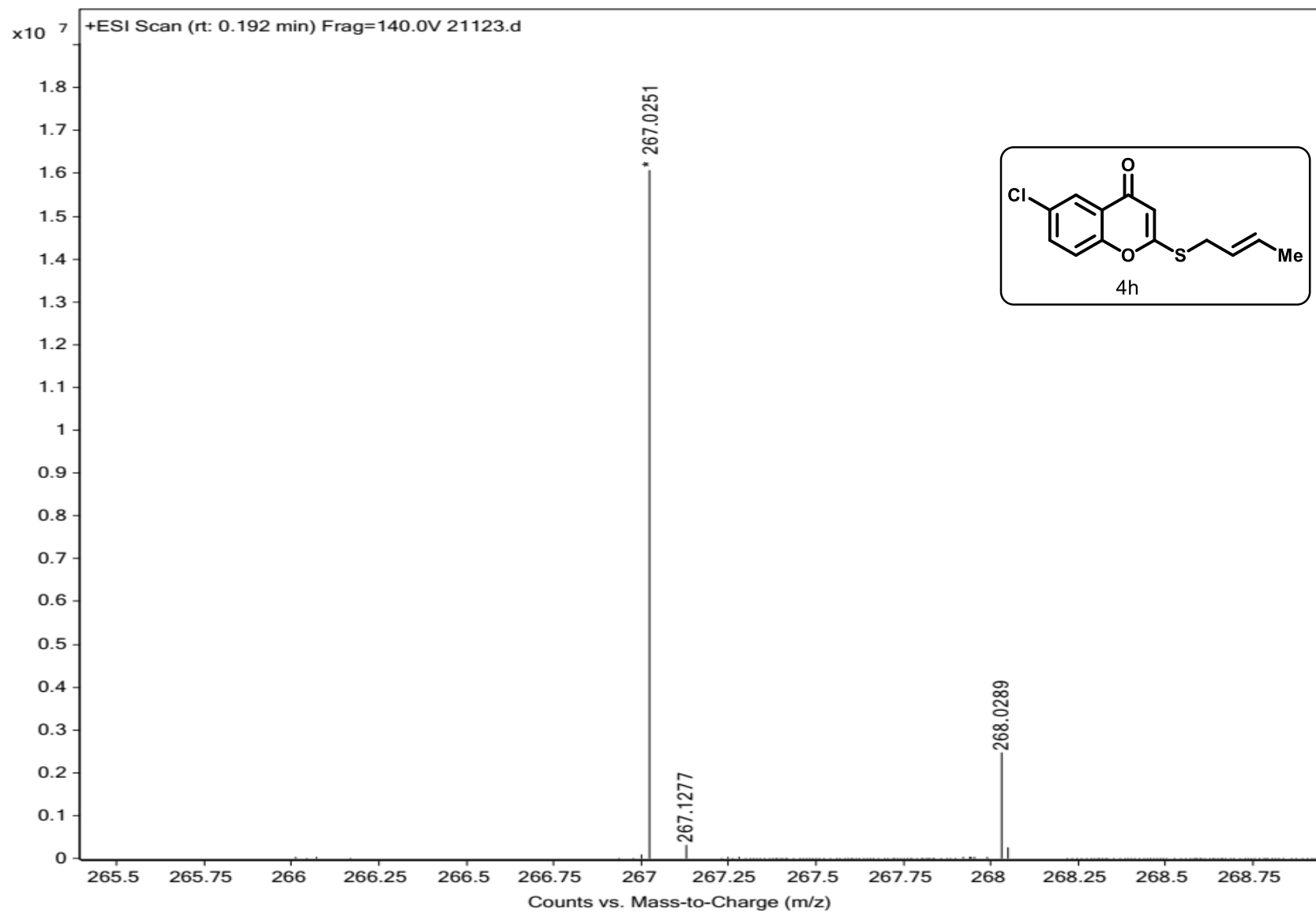


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4h

UJG-02-211-23-13C.3.fid — UJG-02-211-23-13C

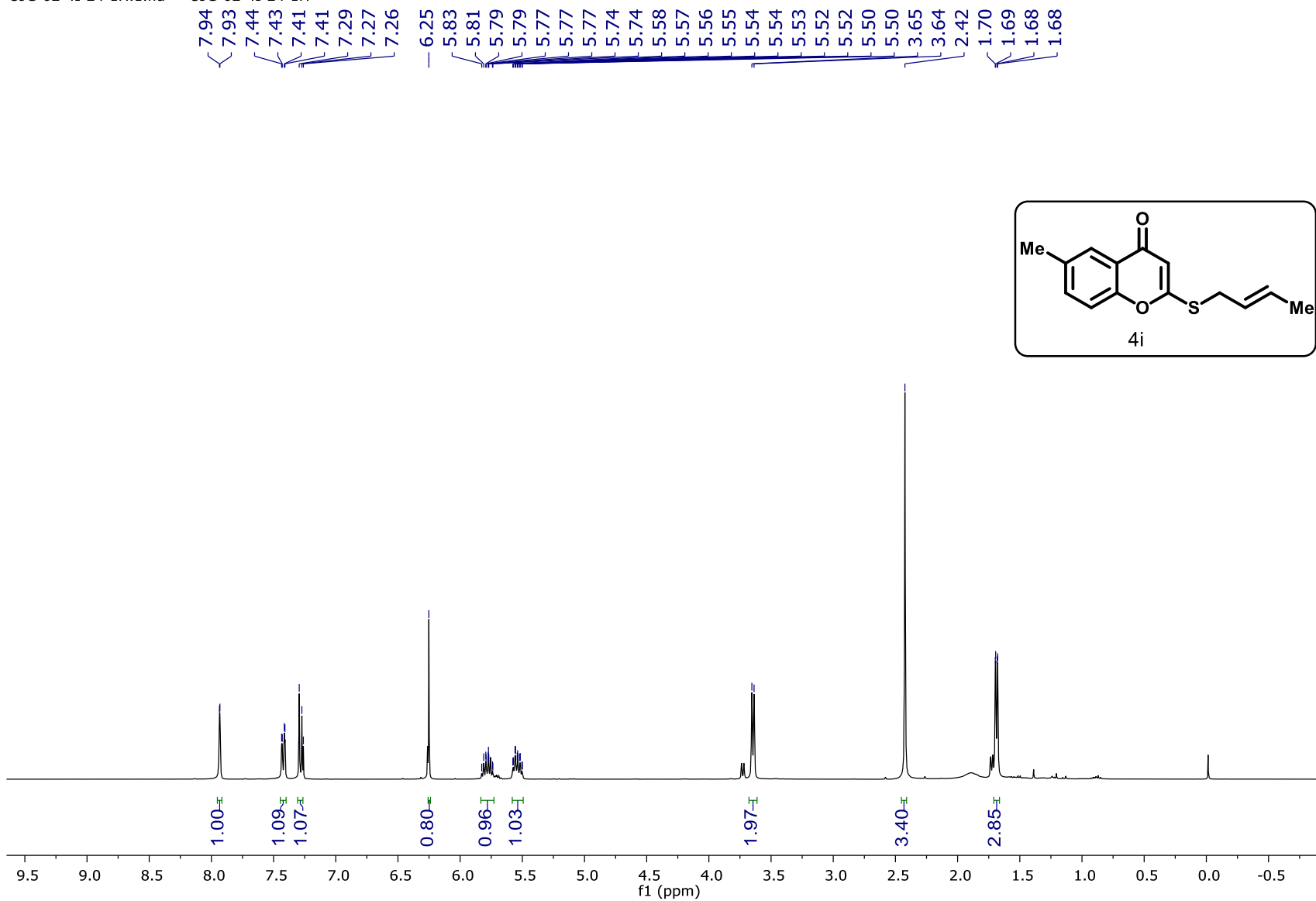


HRMS Spectrum of Compound 4h



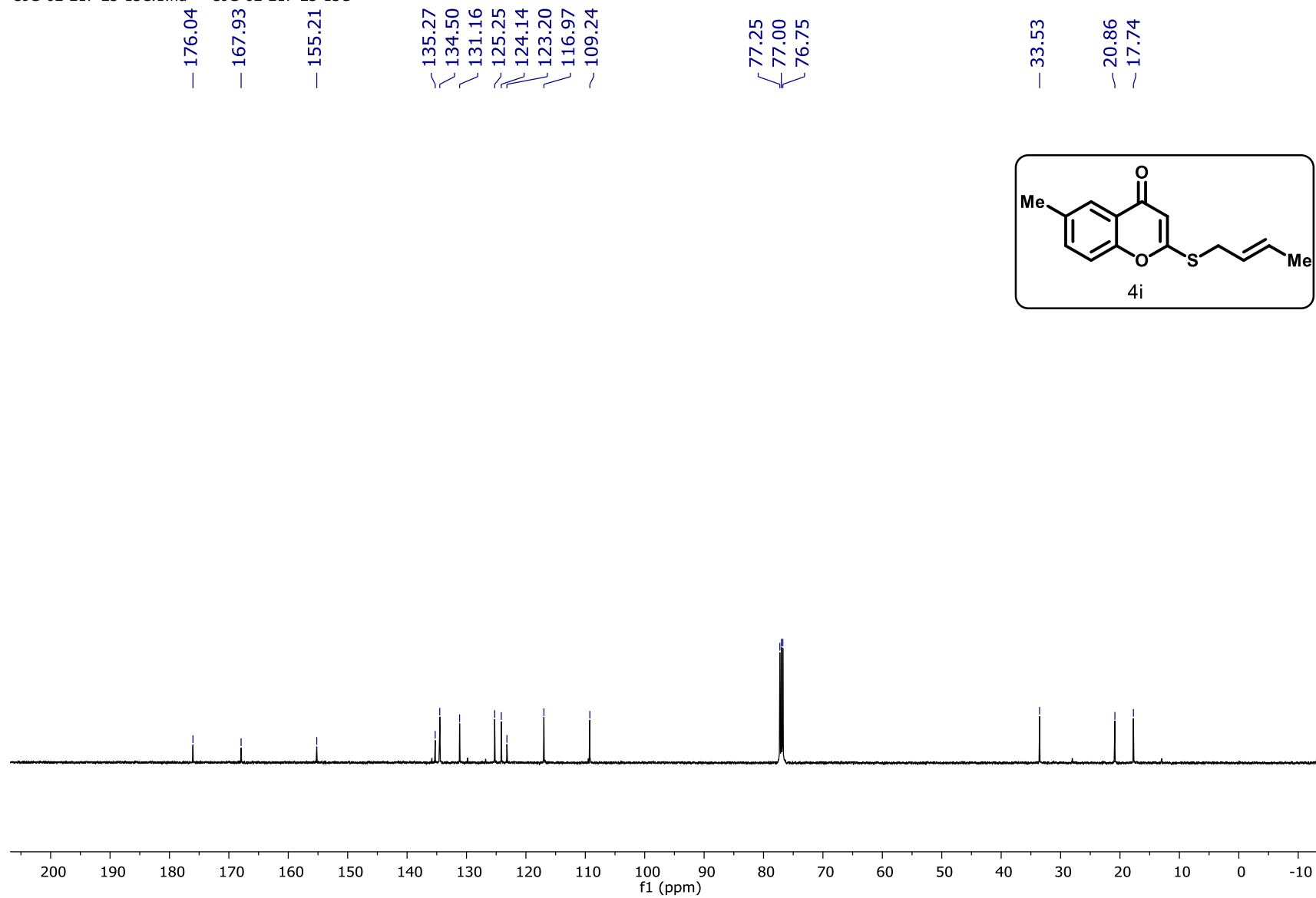
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 4i

UJG-02-4I-24-1H.1.fid — UJG-02-4I-24-1H

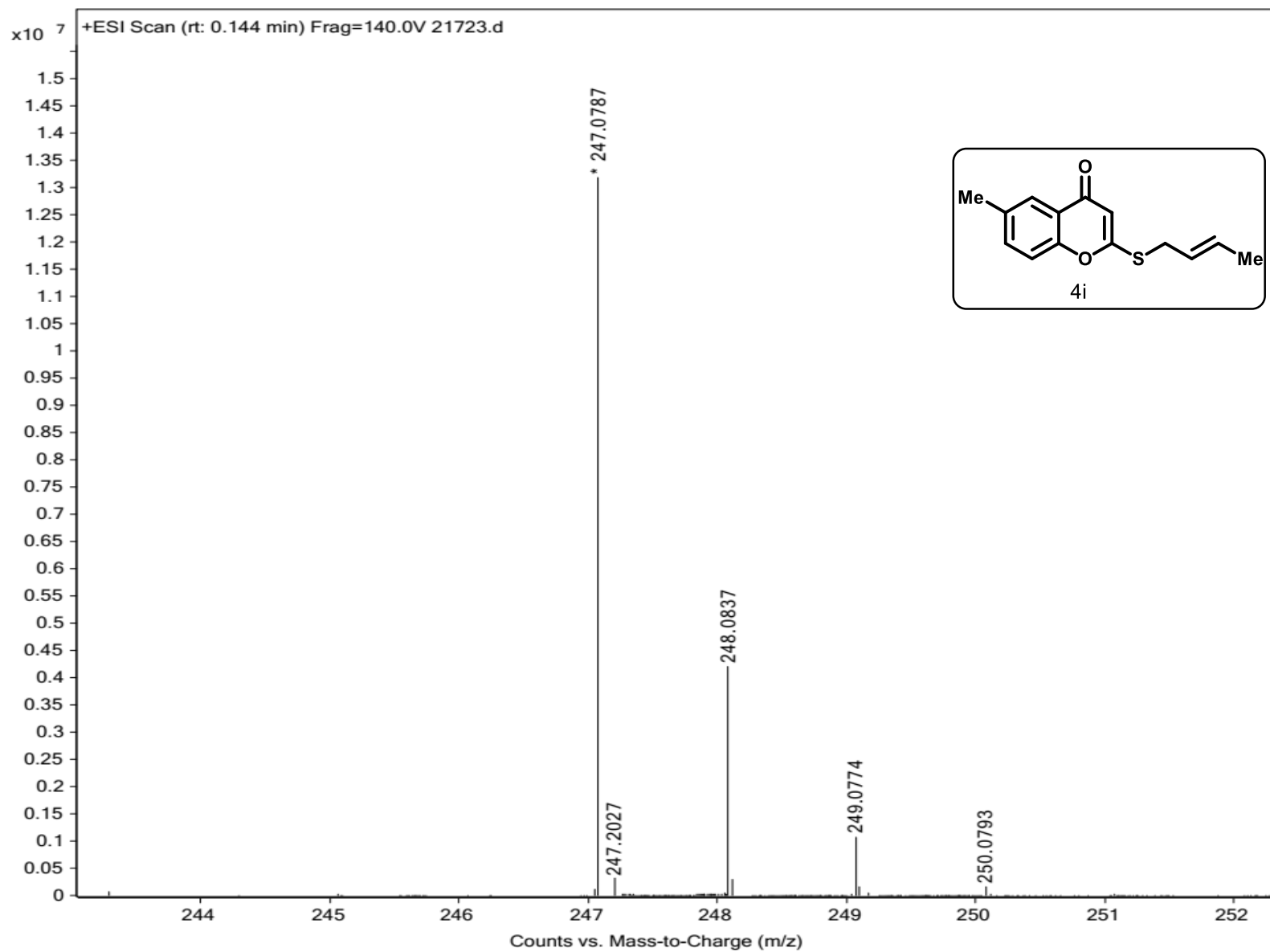


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4i

UJG-02-217-23-13C.1.fid — UJG-02-217-23-13C

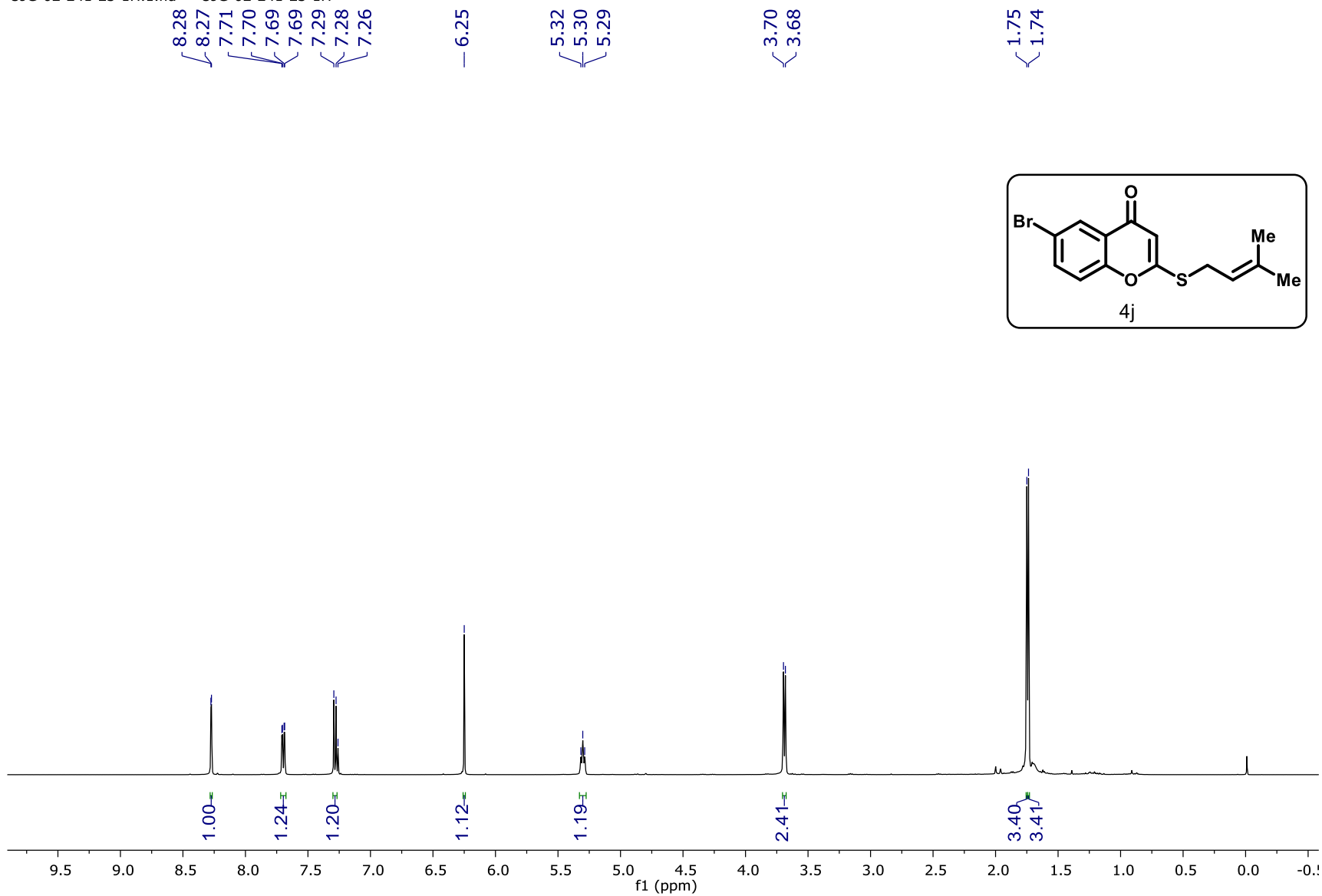


HRMS Spectrum of Compound 4i



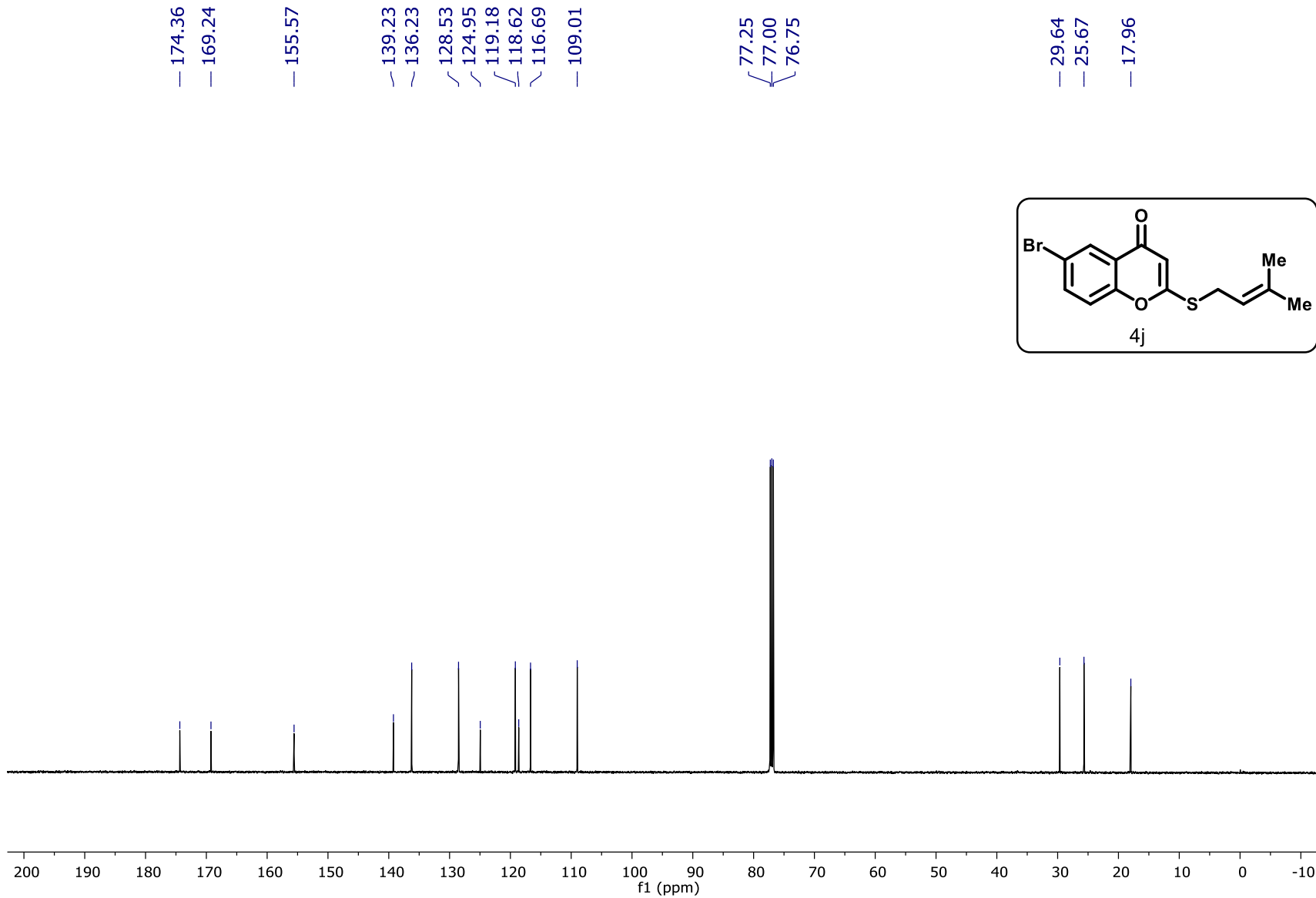
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4j

UJG-02-241-23-1H.1.fid — UJG-02-241-23-1H

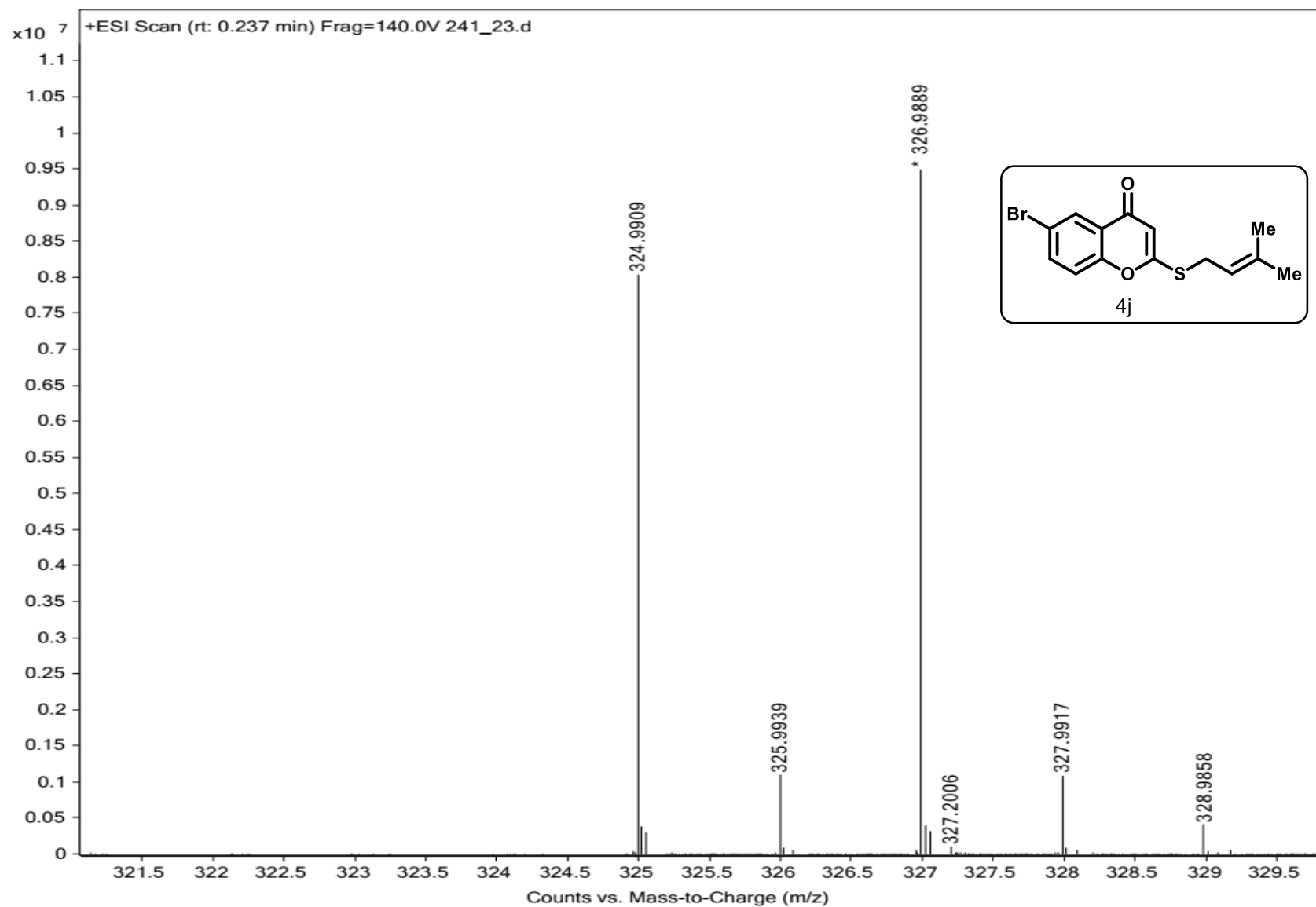


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4j

UJG-02-241-23-13C.3.fid — UJG-02-241-23-13C

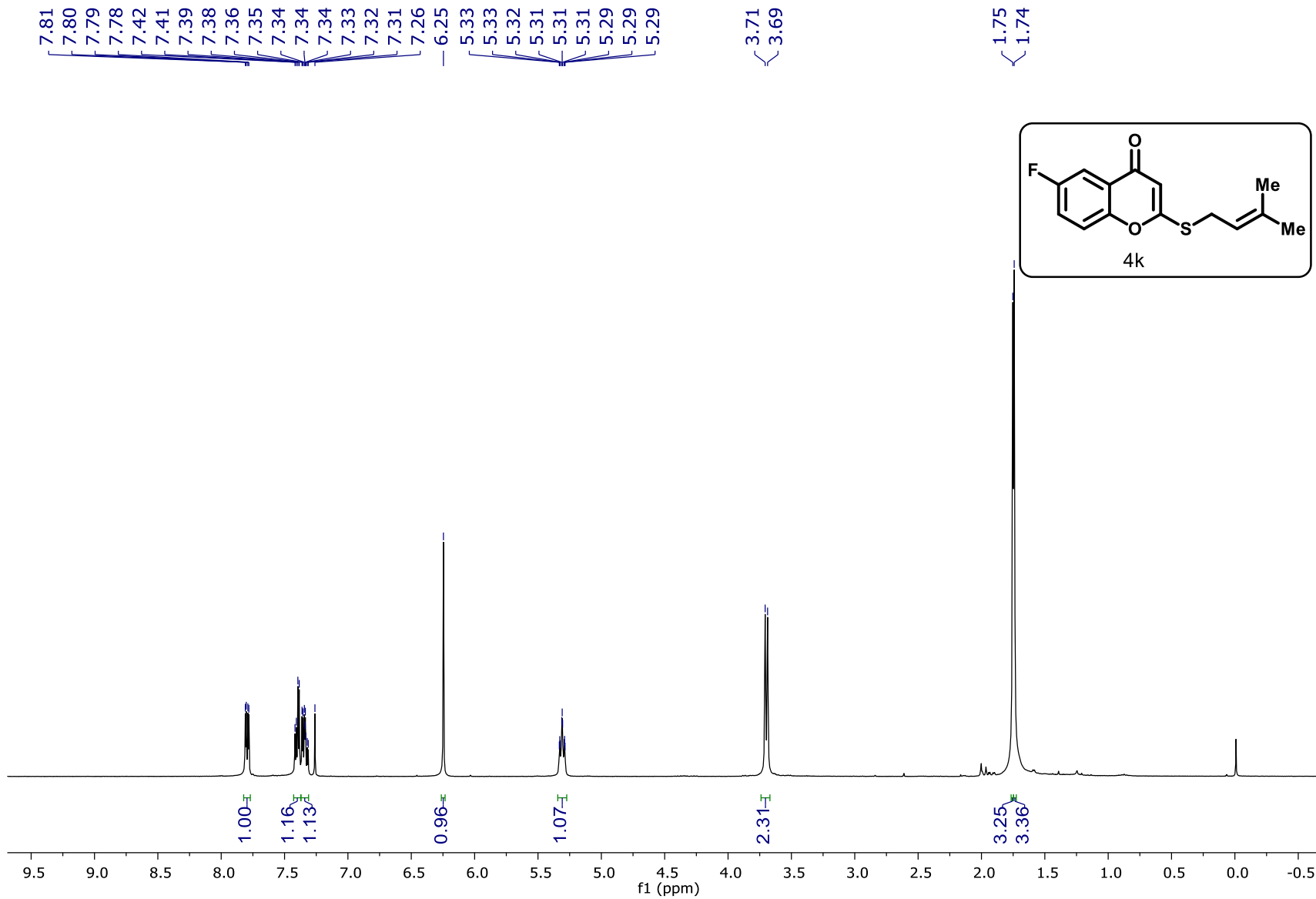


HRMS Spectrum of Compound 4j



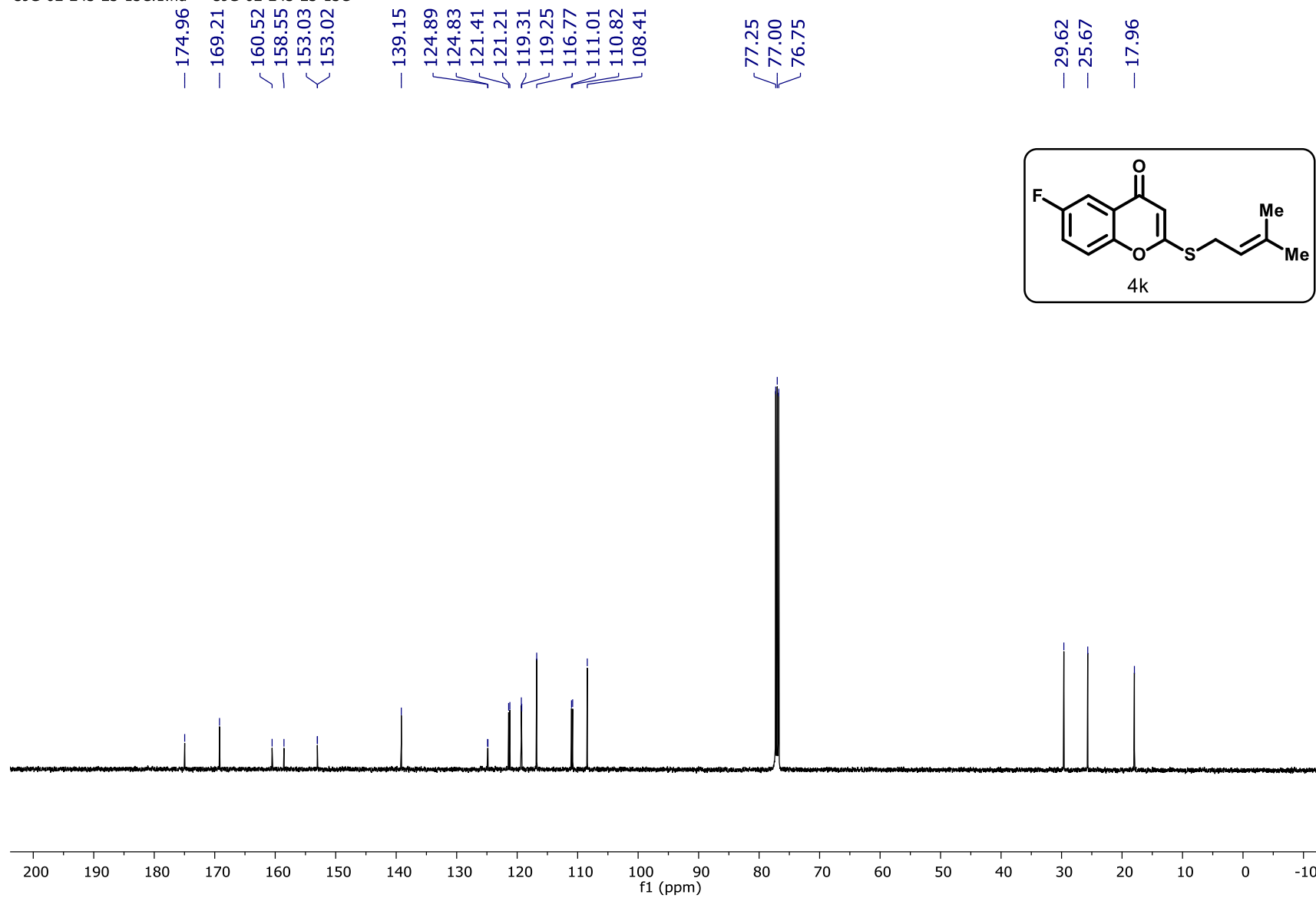
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 4k

UJG-02-243-23-1H.1.fid — UJG-02-243-23-1H



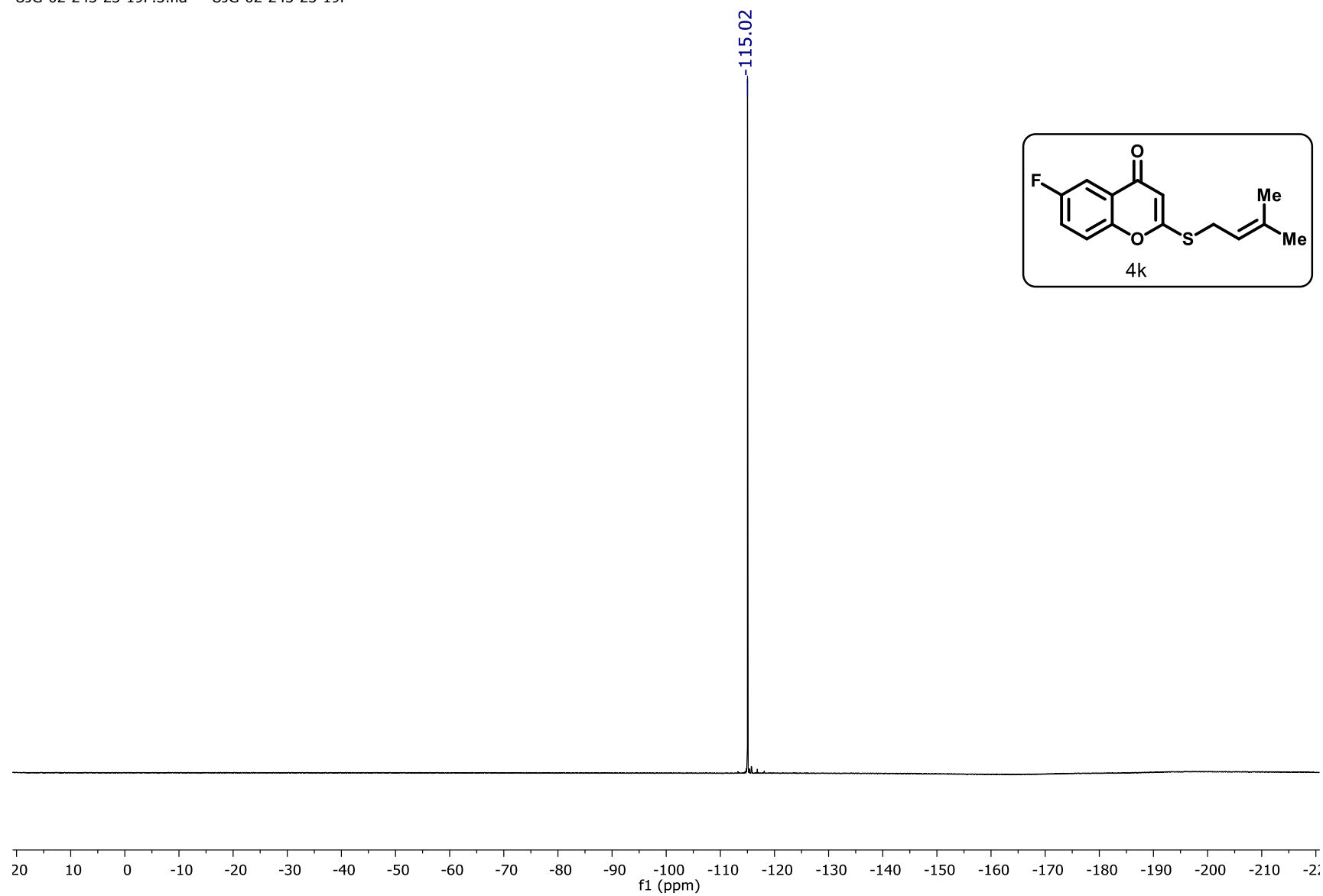
^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 4k

UJG-02-243-23-13C.1.fid — UJG-02-243-23-13C

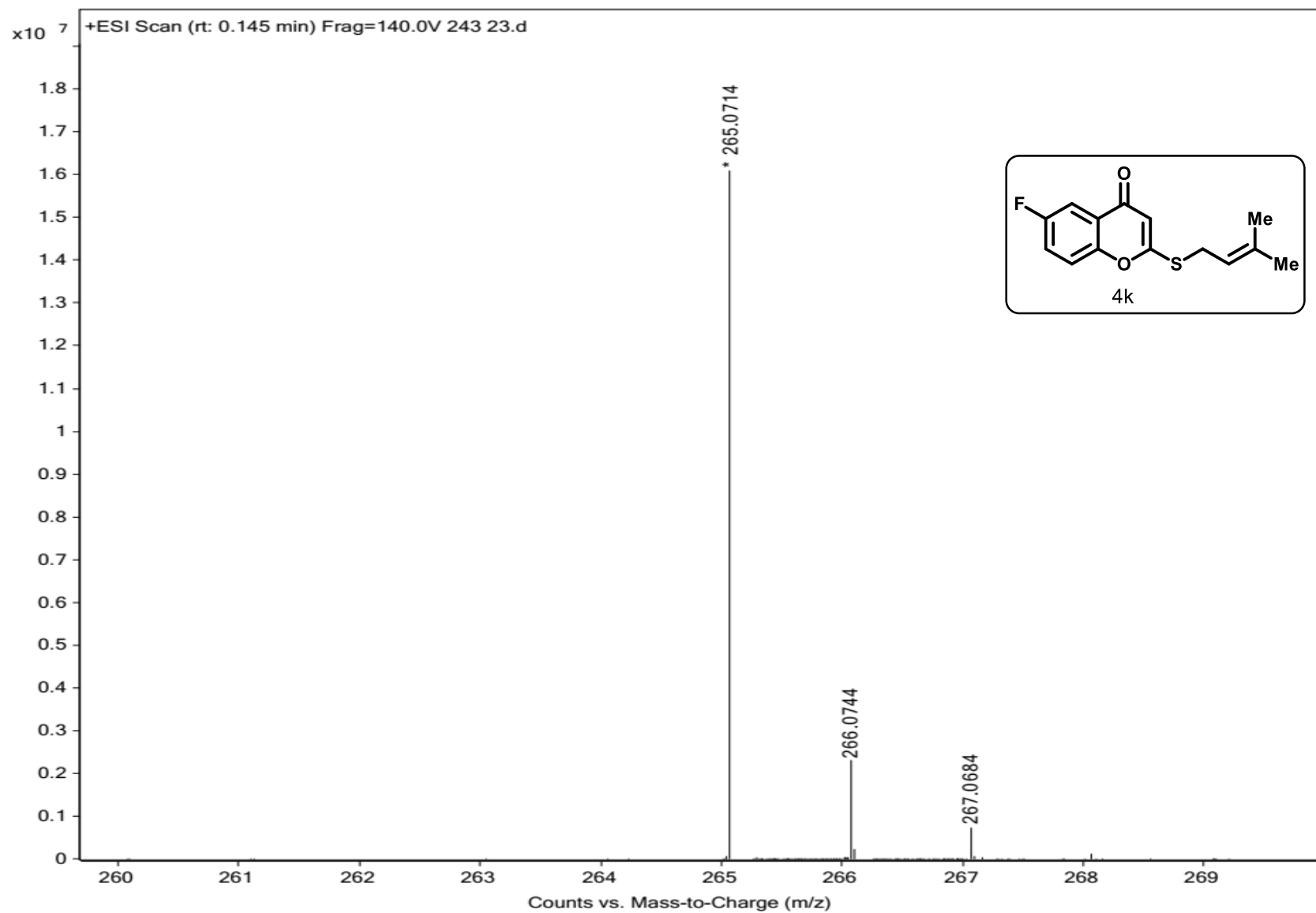


^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 4k

UJG-02-243-23-19F.3.fid — UJG-02-243-23-19F

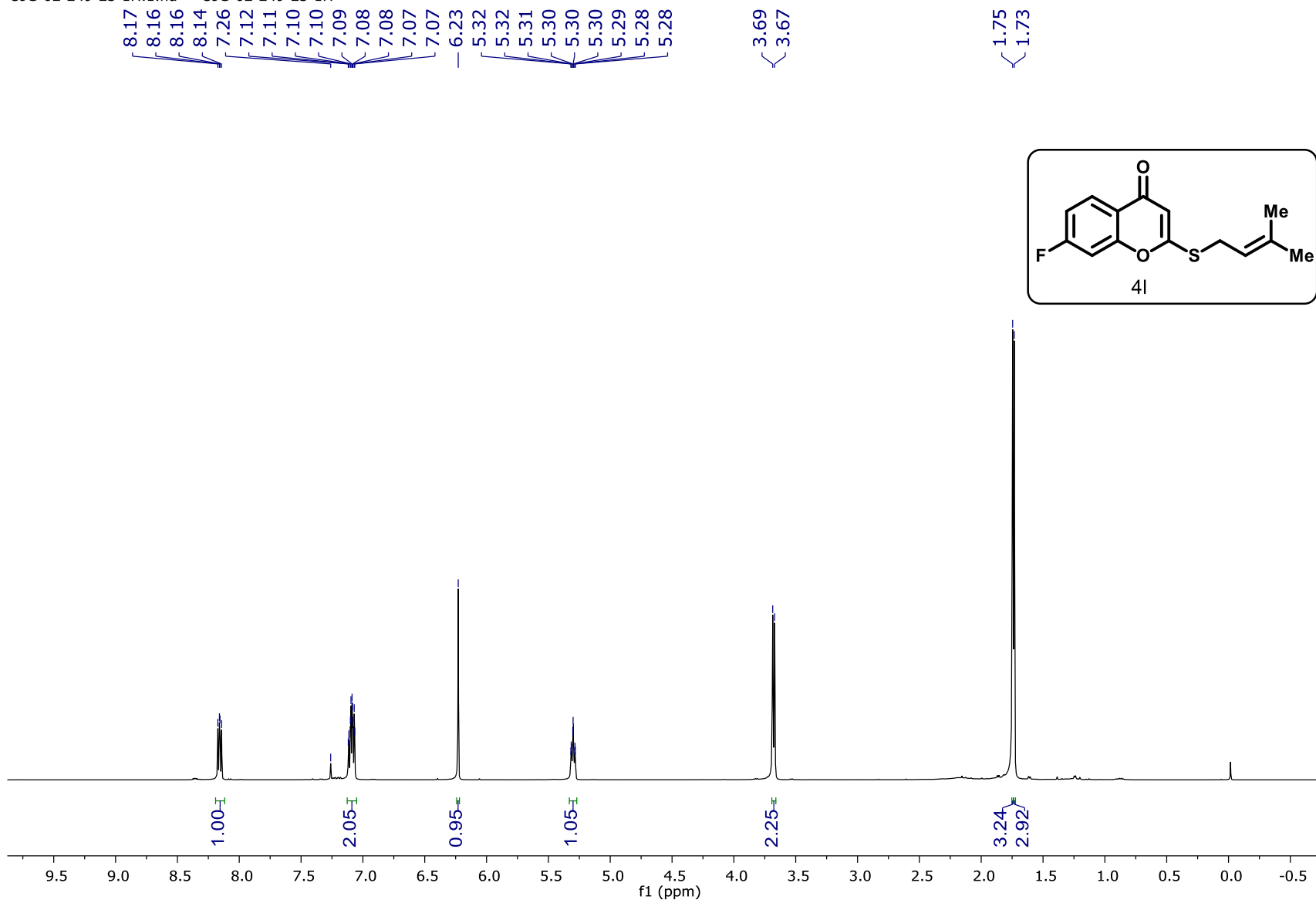


HRMS Spectrum of Compound 4k



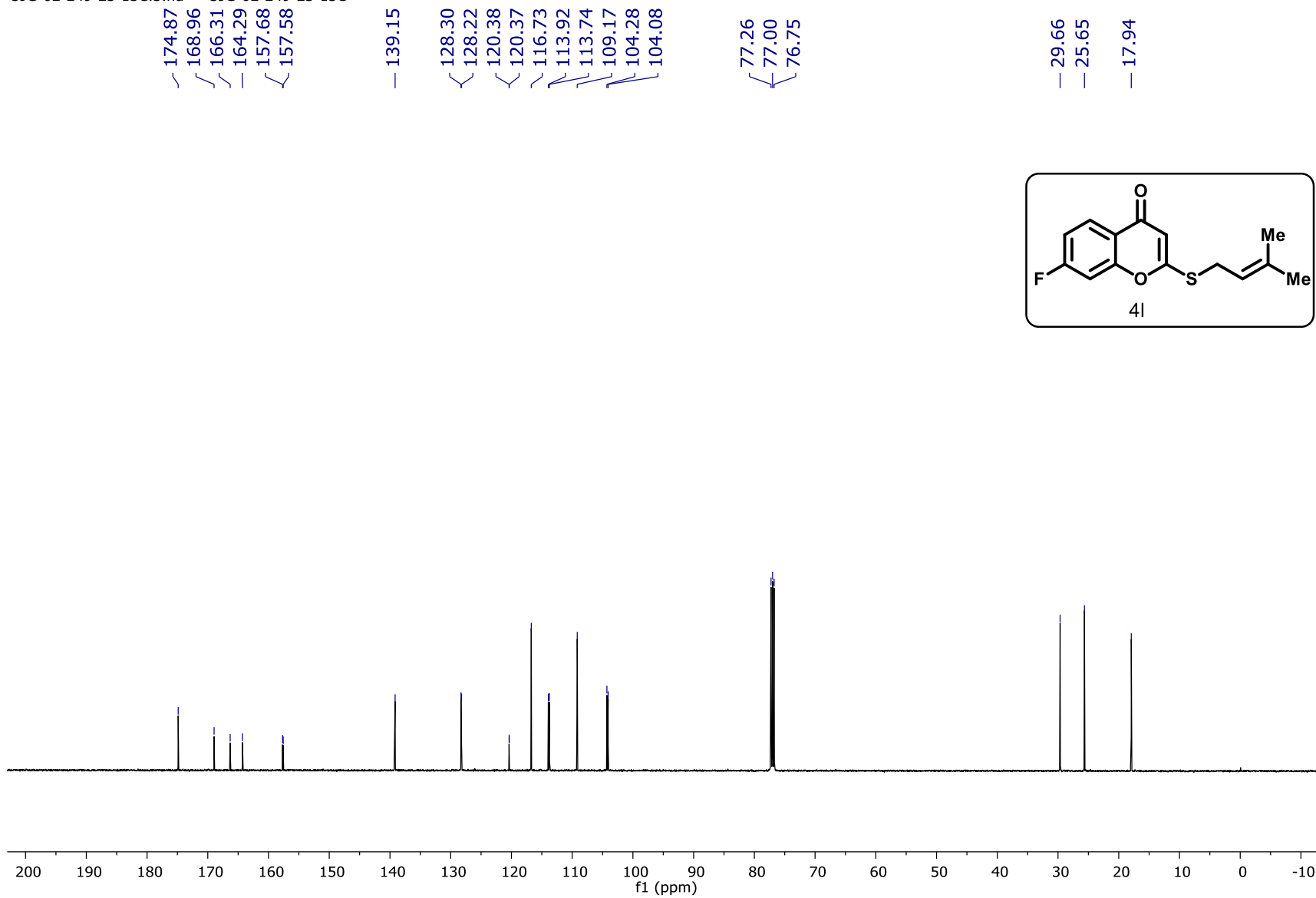
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 4l

UJG-02-249-23-1H.1.fid — UJG-02-249-23-1H



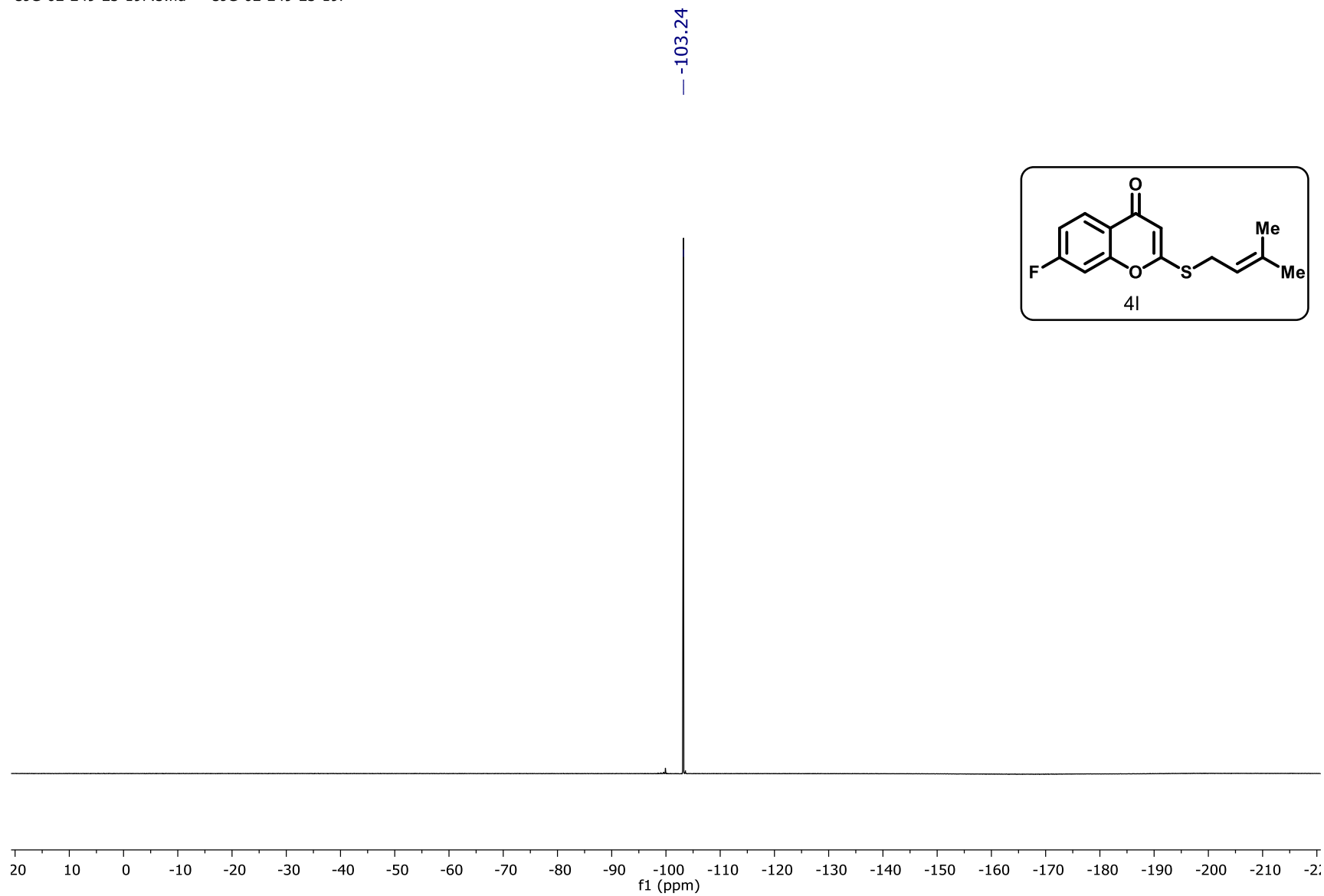
^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 4l

UJG-02-249-23-13C.3.fid — UJG-02-249-23-13C

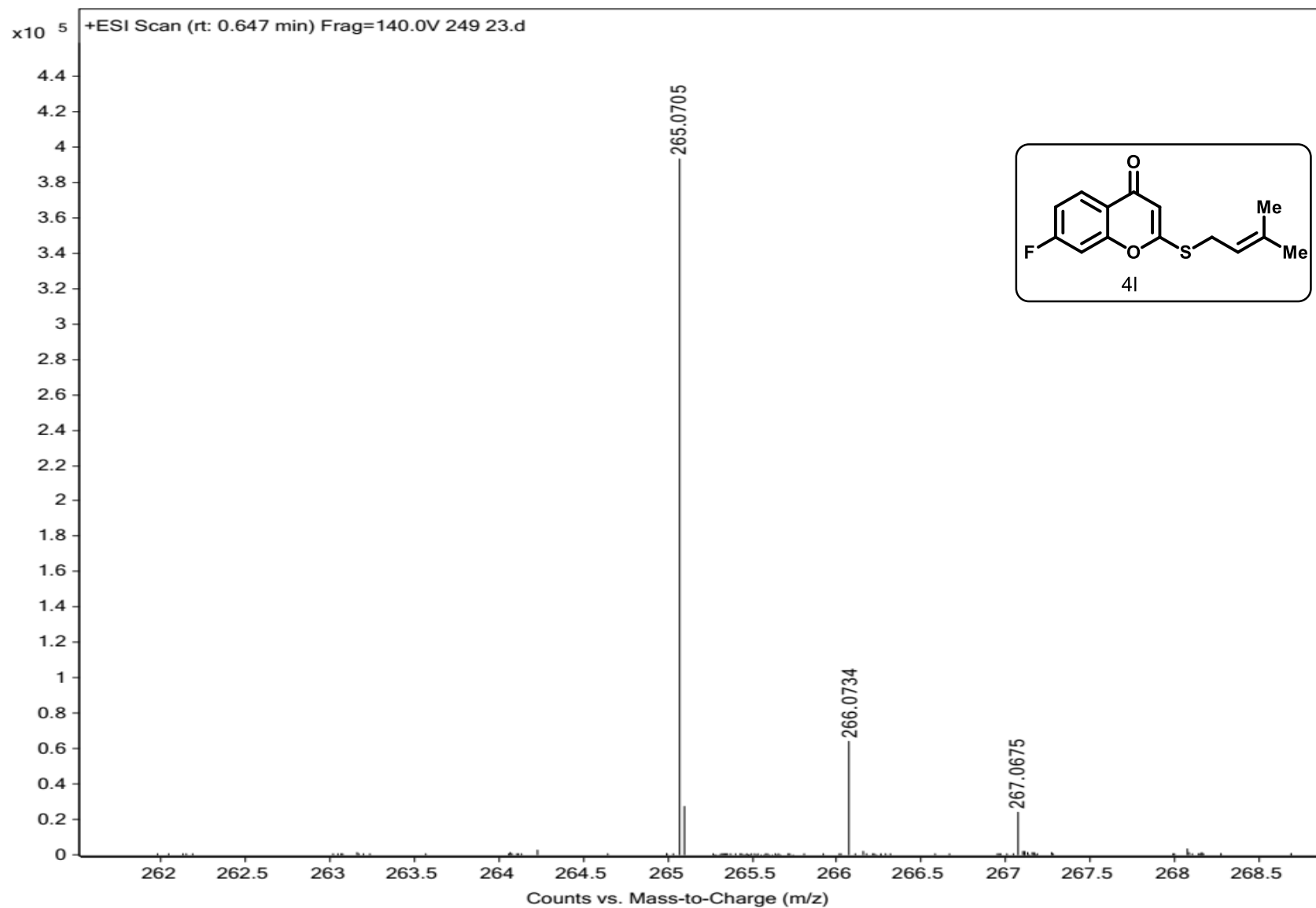


^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 4l

UJG-02-249-23-19F.5.fid — UJG-02-249-23-19F



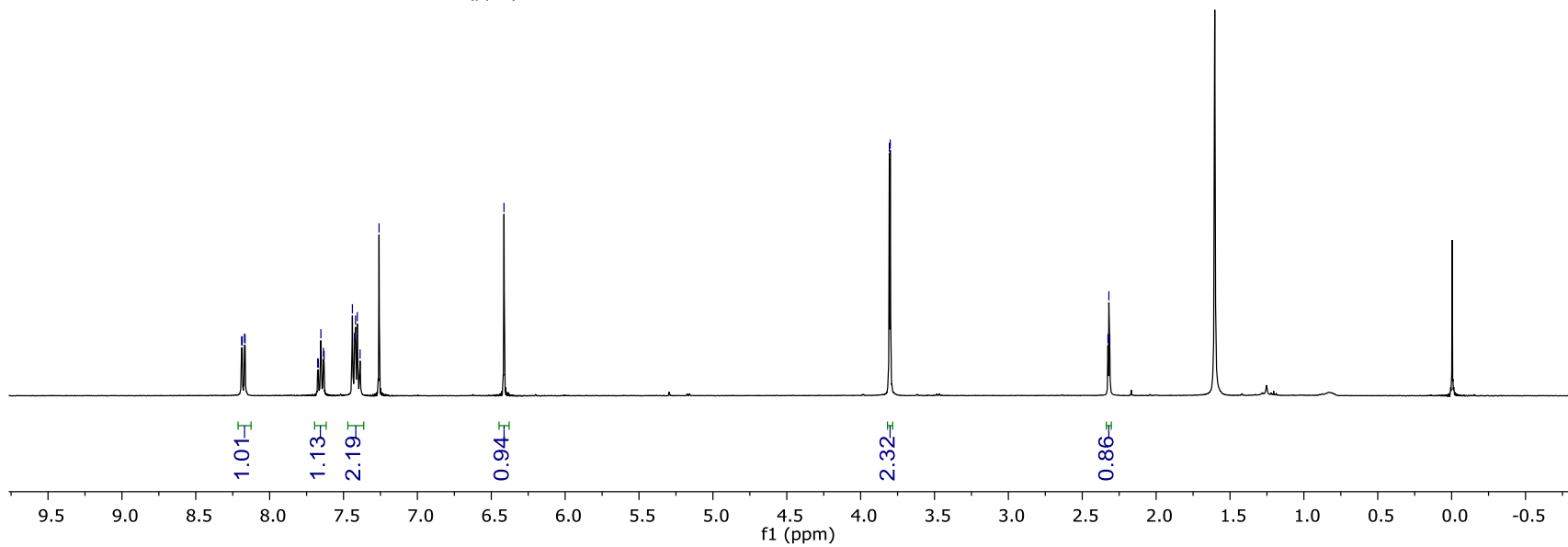
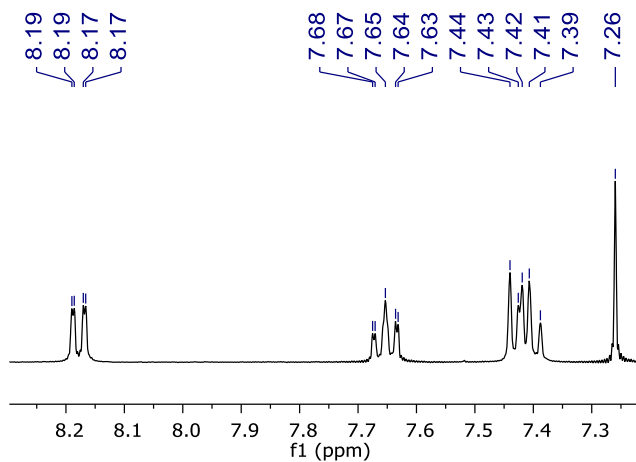
HRMS Spectrum of Compound 4l



¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5a

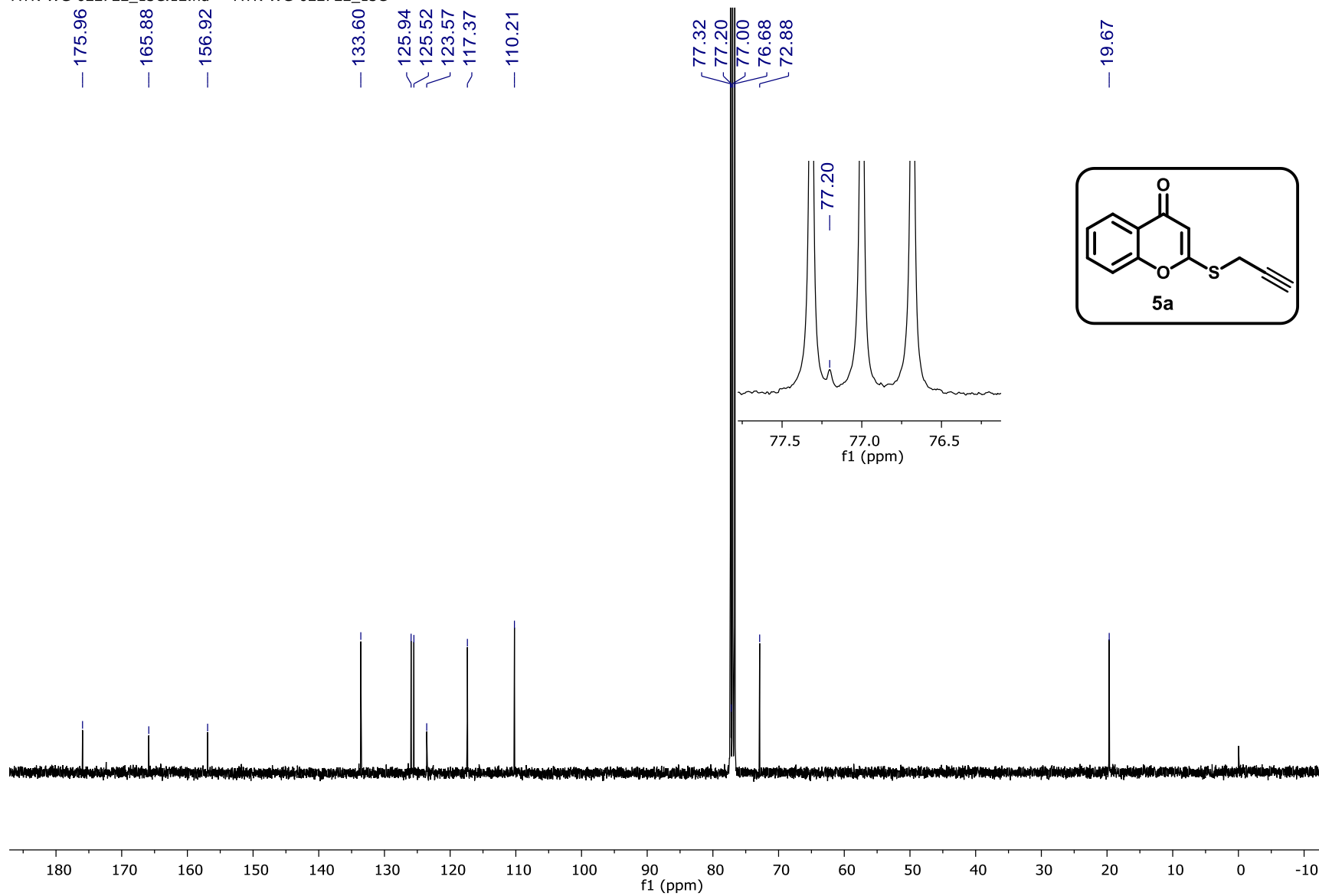
ATK-UJG-02-07-22-1111
ATK-UJG-02-07-22-1111

8.19, 8.19, 8.17, 8.17, 7.68, 7.67, 7.65, 7.64, 7.63, 7.44, 7.43, 7.42, 7.41, 7.39, 7.26, 6.41, 3.81, 3.80, 2.33, 2.32, 2.31

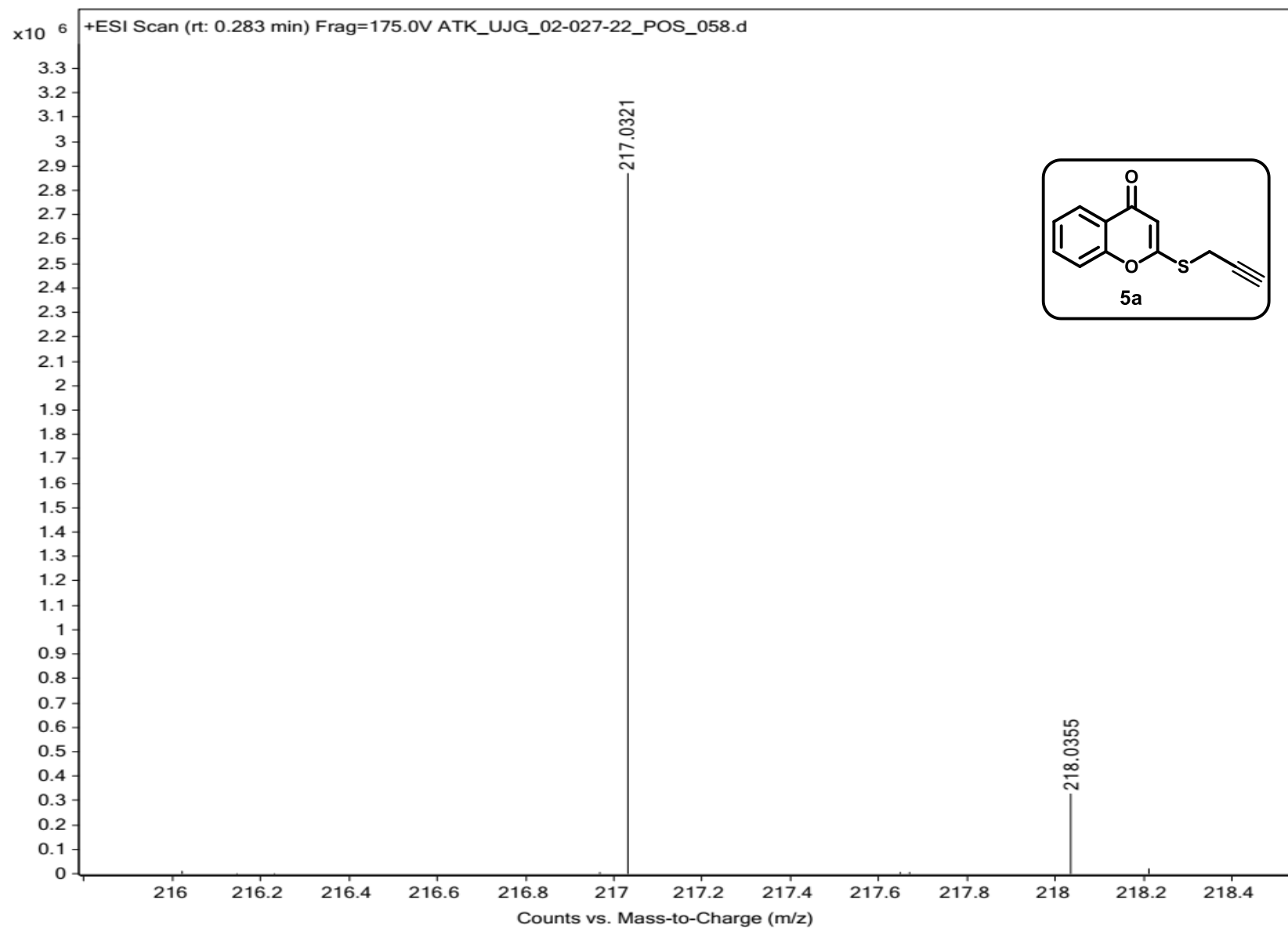


^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of Compound 5a

ATK-WG-022722_13C.12.fid — ATK-WG-022722_13C

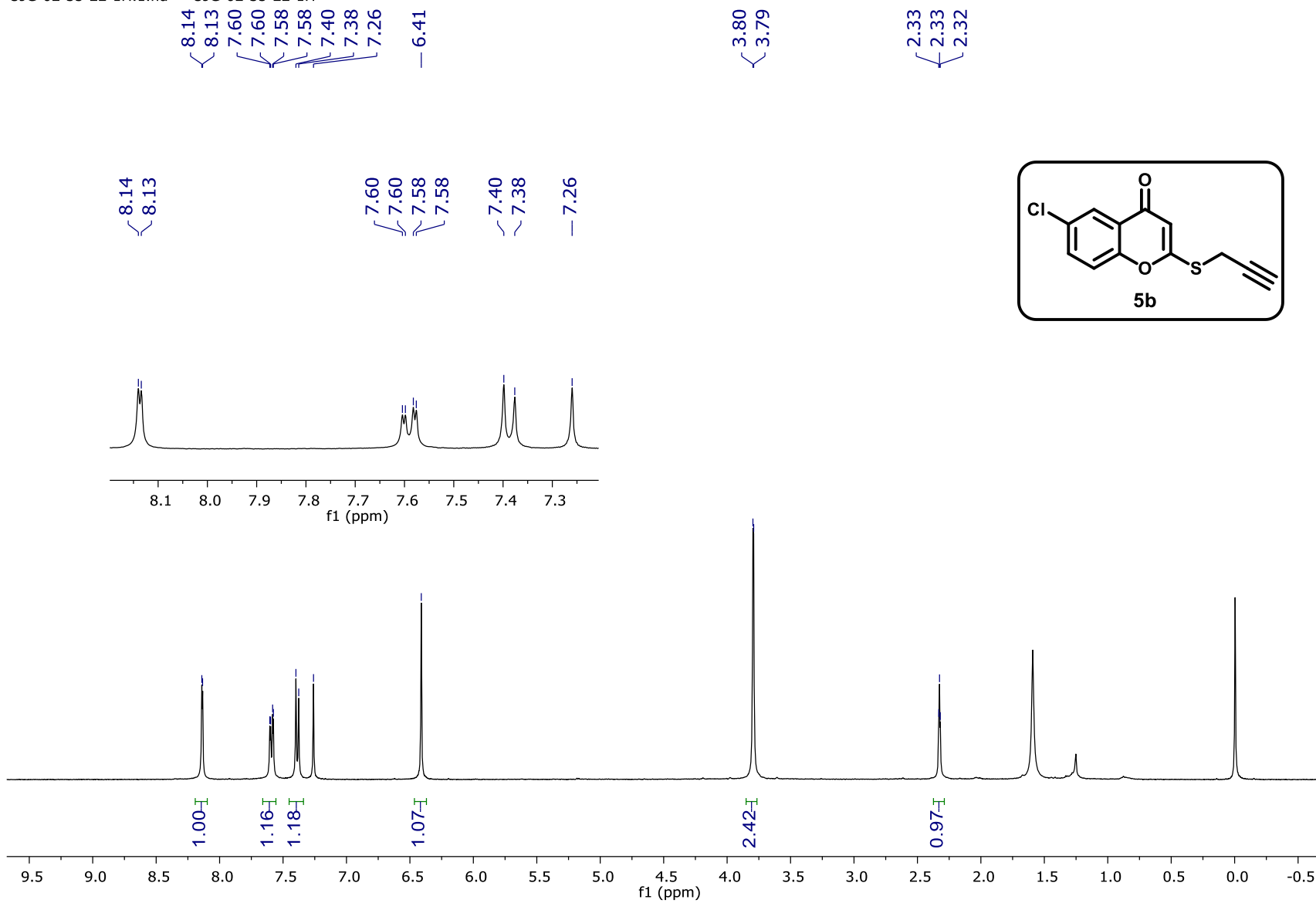


HRMS Spectrum of Compound 5a



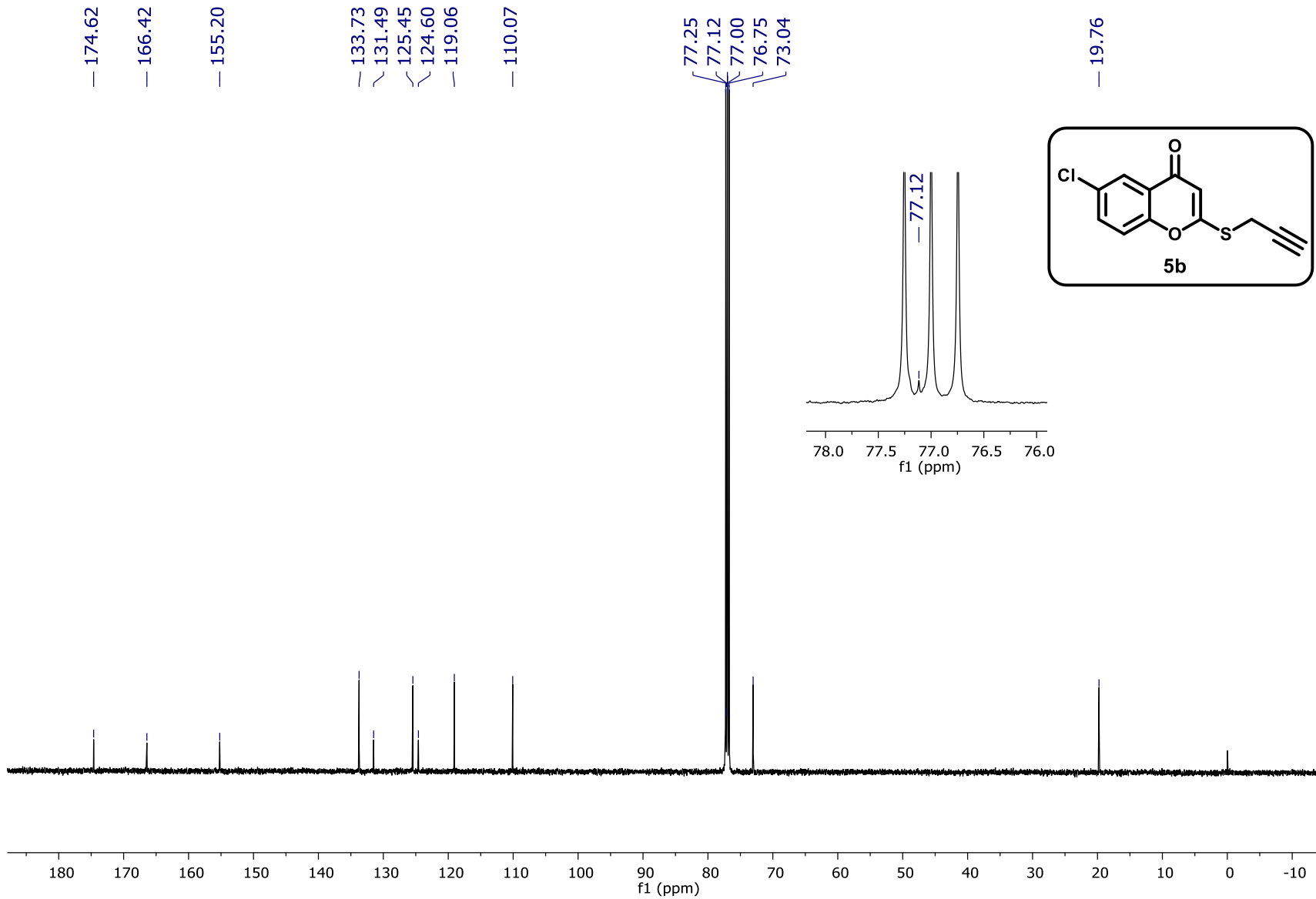
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5b

UJG-02-35-22-1H.1.fid — UJG-02-35-22-1H

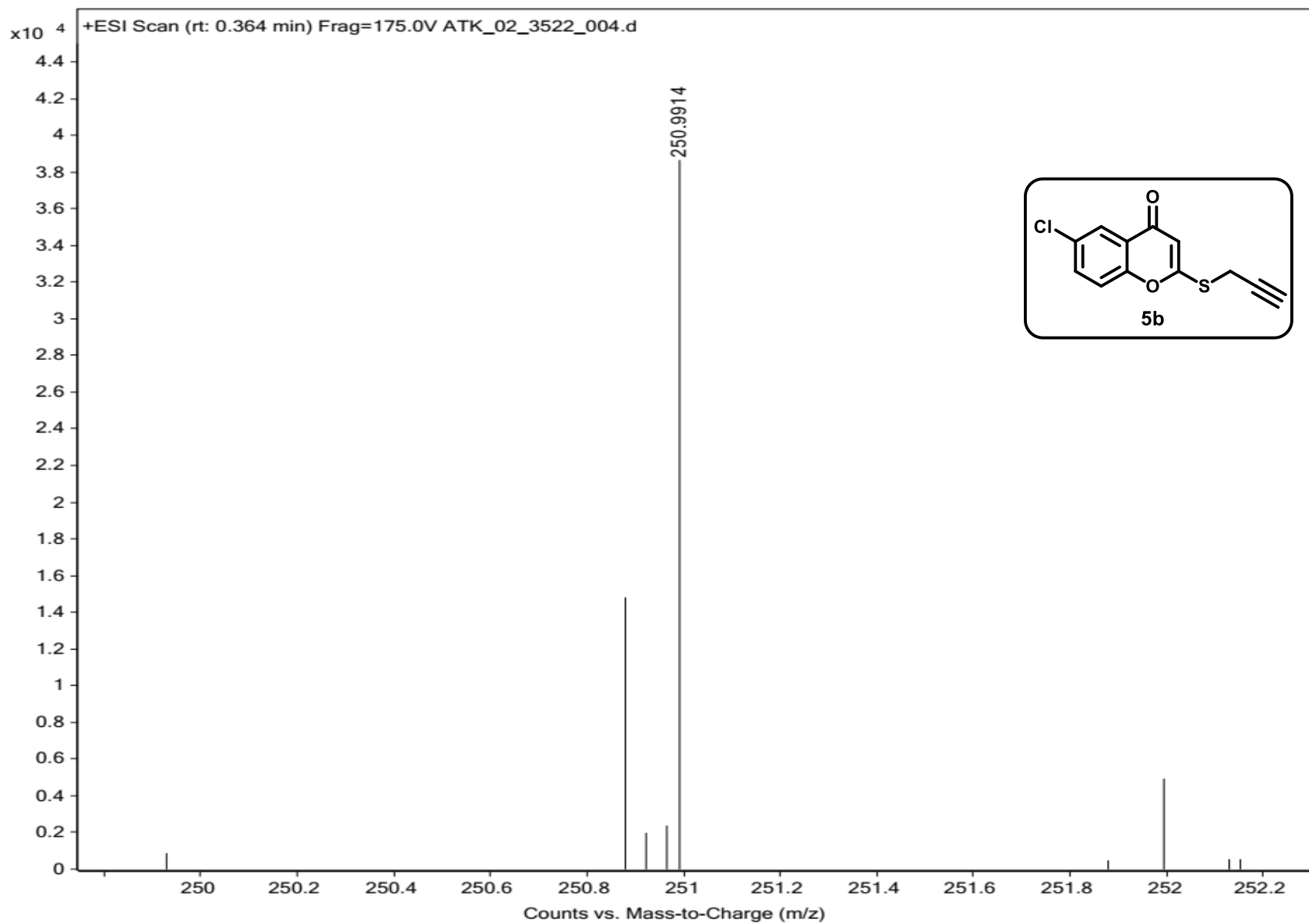


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5b

UJG-02-35-22-13C.1.fid — UJG-02-35-22-13C

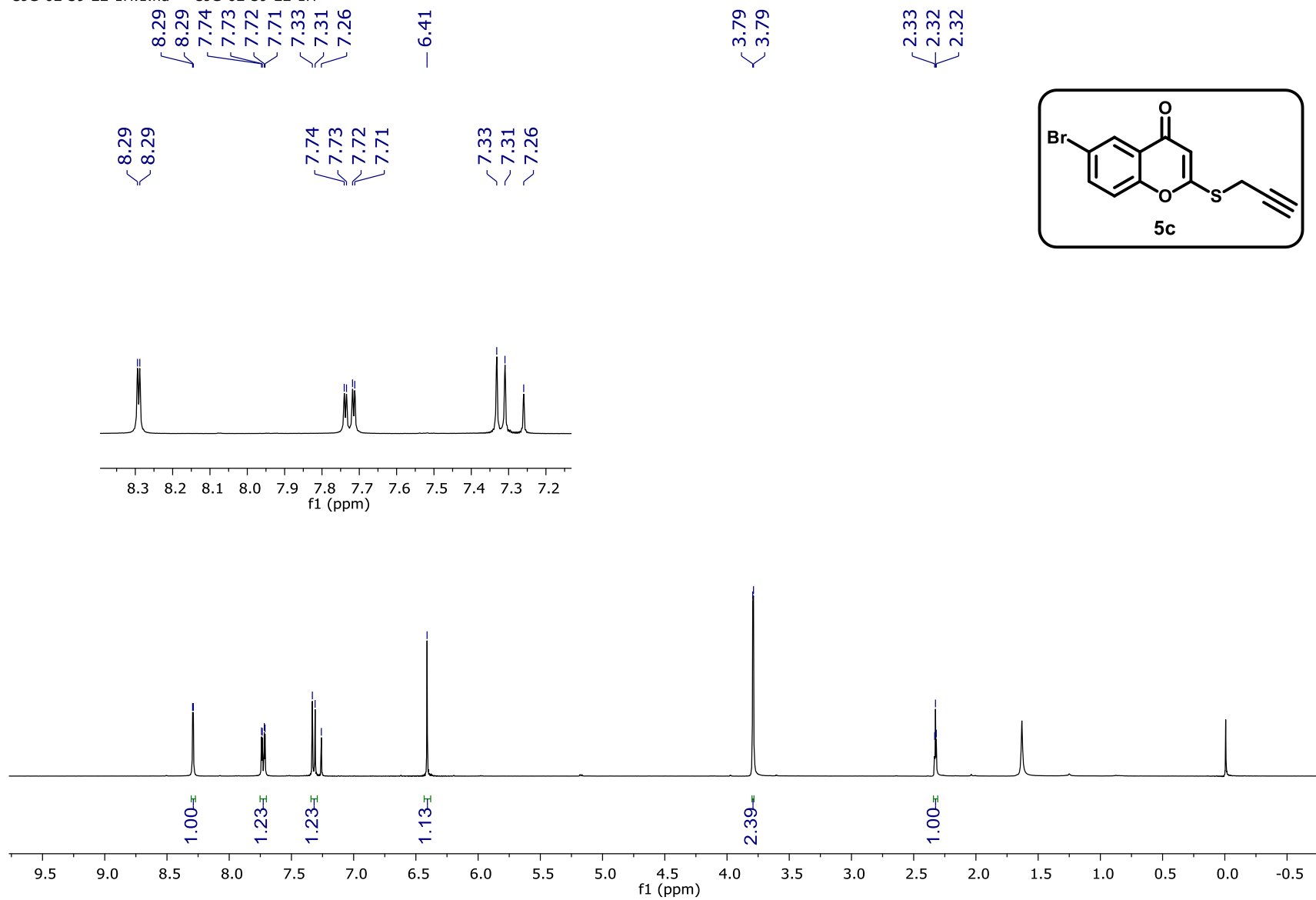


HRMS Spectrum of Compound 5b



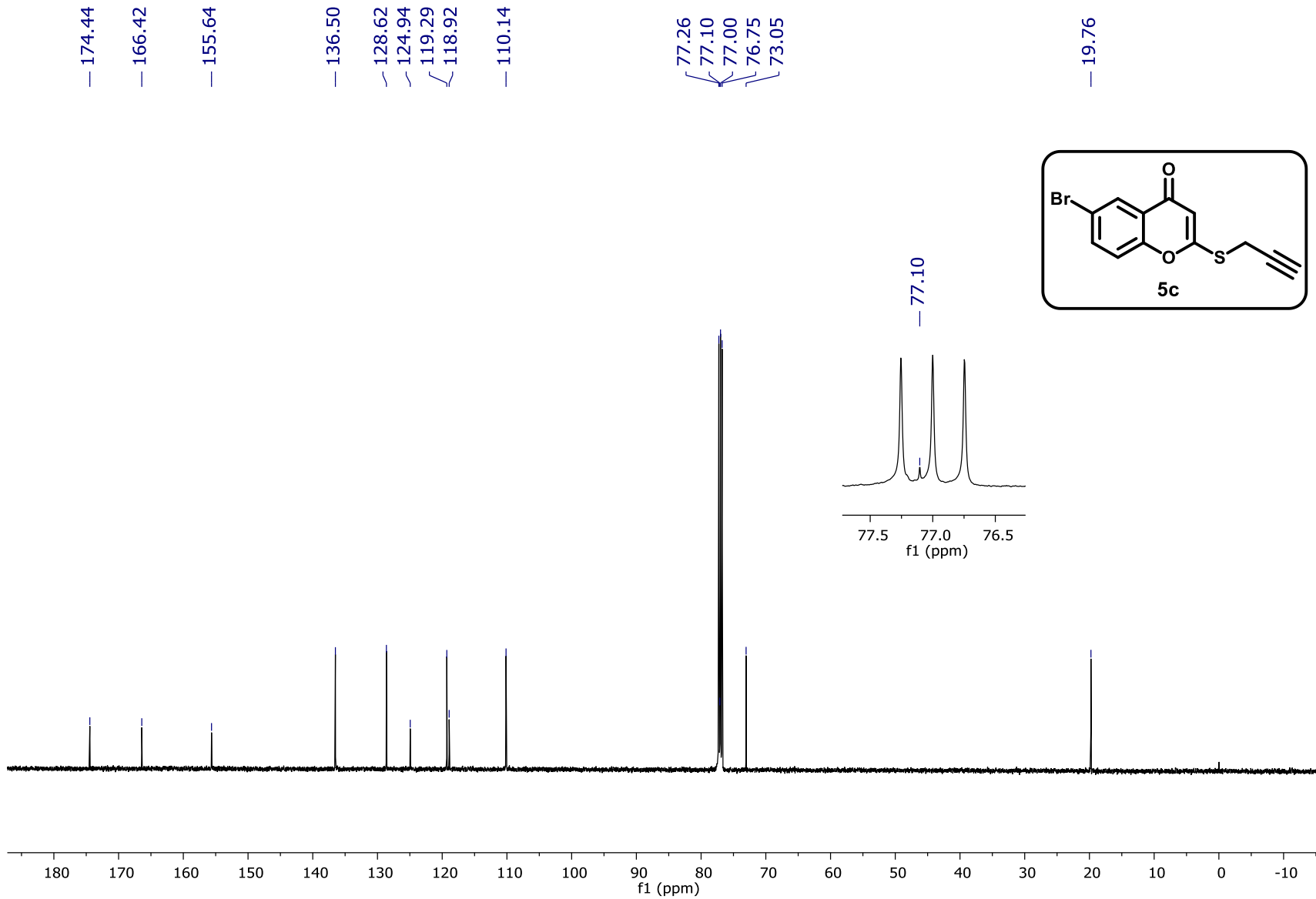
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5c

UJG-02-39-22-1H.1.fid — UJG-02-39-22-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5c

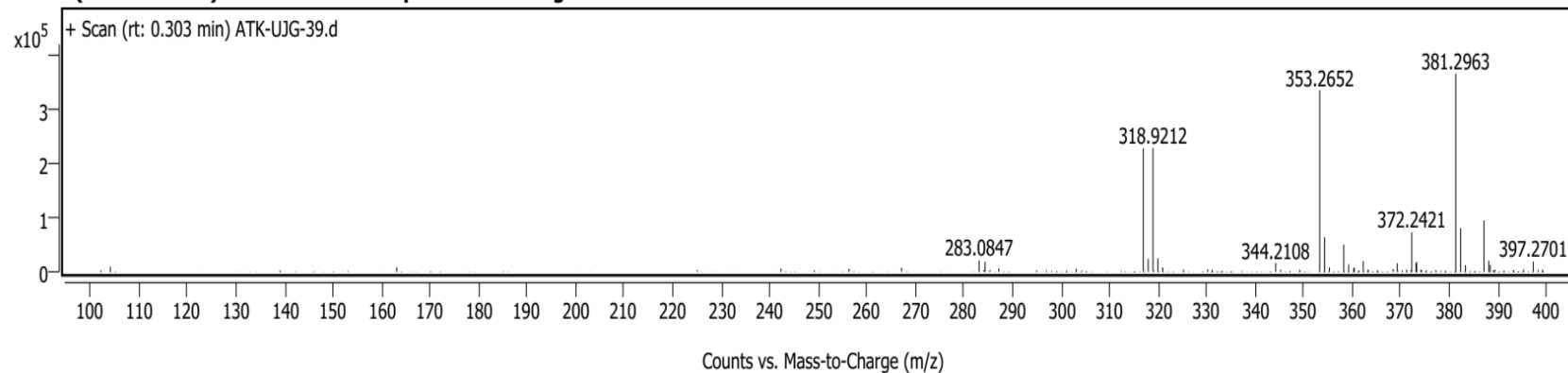
UJG-02-39-22-13C.1.fid — UJG-02-39-22-13C



HRMS Spectrum of Compound 5c

+ Scan (rt: 0.303 min)

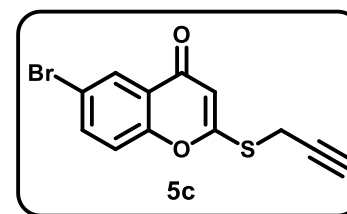
SpectrumIdString



SpectrumIdString

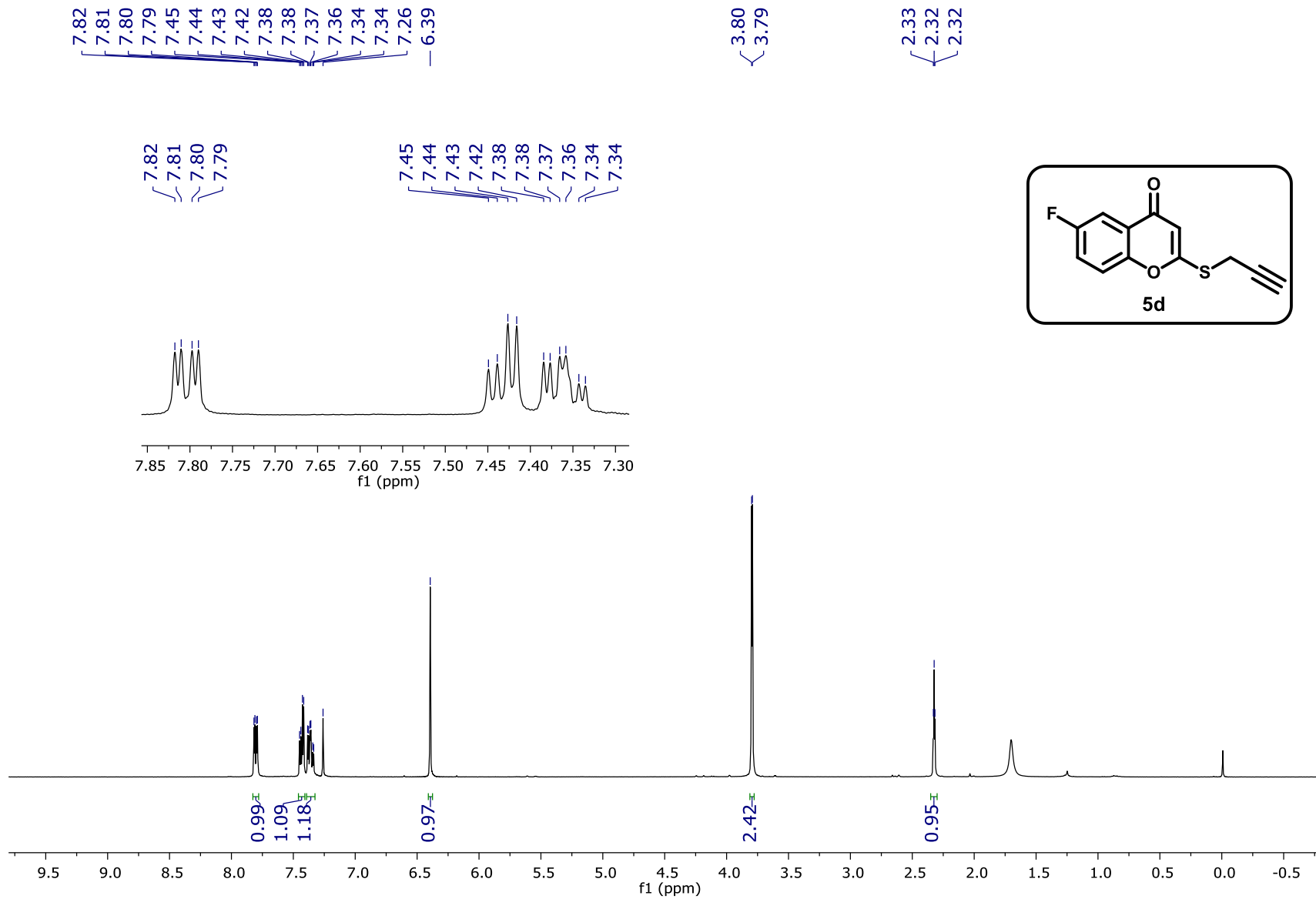
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284.3302		18524	5.06				
316.9232	1	228612	62.39				
317.9262	1	24015	6.55				
318.9212	1	228968	62.49				
319.9245	1	24685	6.74				
344.2108		16167	4.41				
353.2652	1	335909	91.68				
354.2686	1	63955	17.46				
358.2267		50403	13.76				
362.2399		19682	5.37				
369.2388		15727	4.29				
372.2421	1	73075	19.94				
373.0948		15699	4.28				
373.2456	1	18353	5.01				
381.2963	1	366396	100.00				
382.2996	1	80726	22.03				
387.1107	1	95007	25.93				
388.1142	1	20298	5.54				
397.2701		18824	5.14				

Ion Type



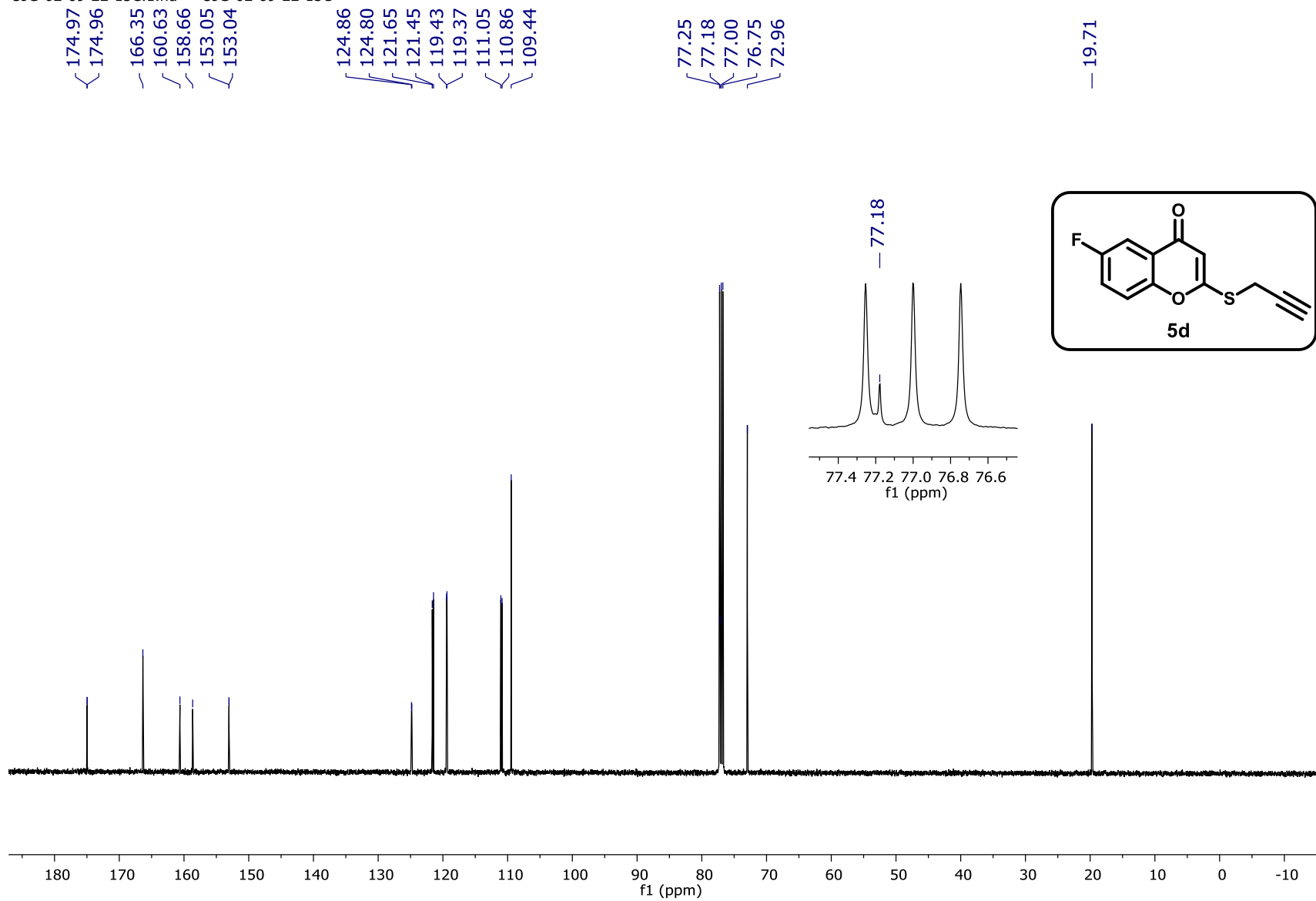
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5d

UJG-02-69-22-1H.1.fid — UJG-02-69-22-1H



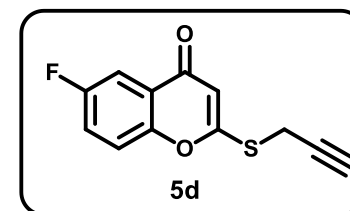
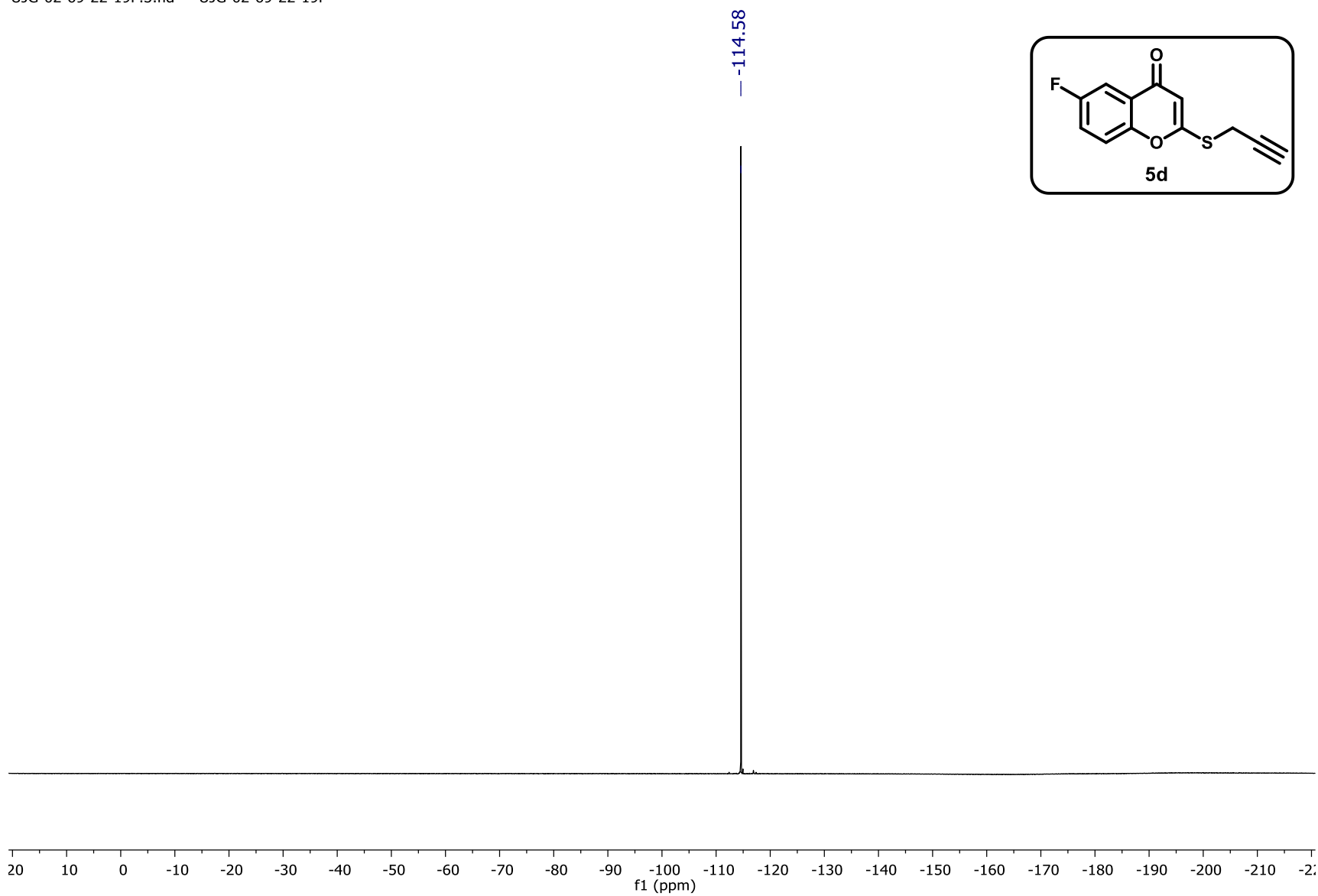
^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5d

UJG-02-69-22-13C.1.fid — UJG-02-69-22-13C

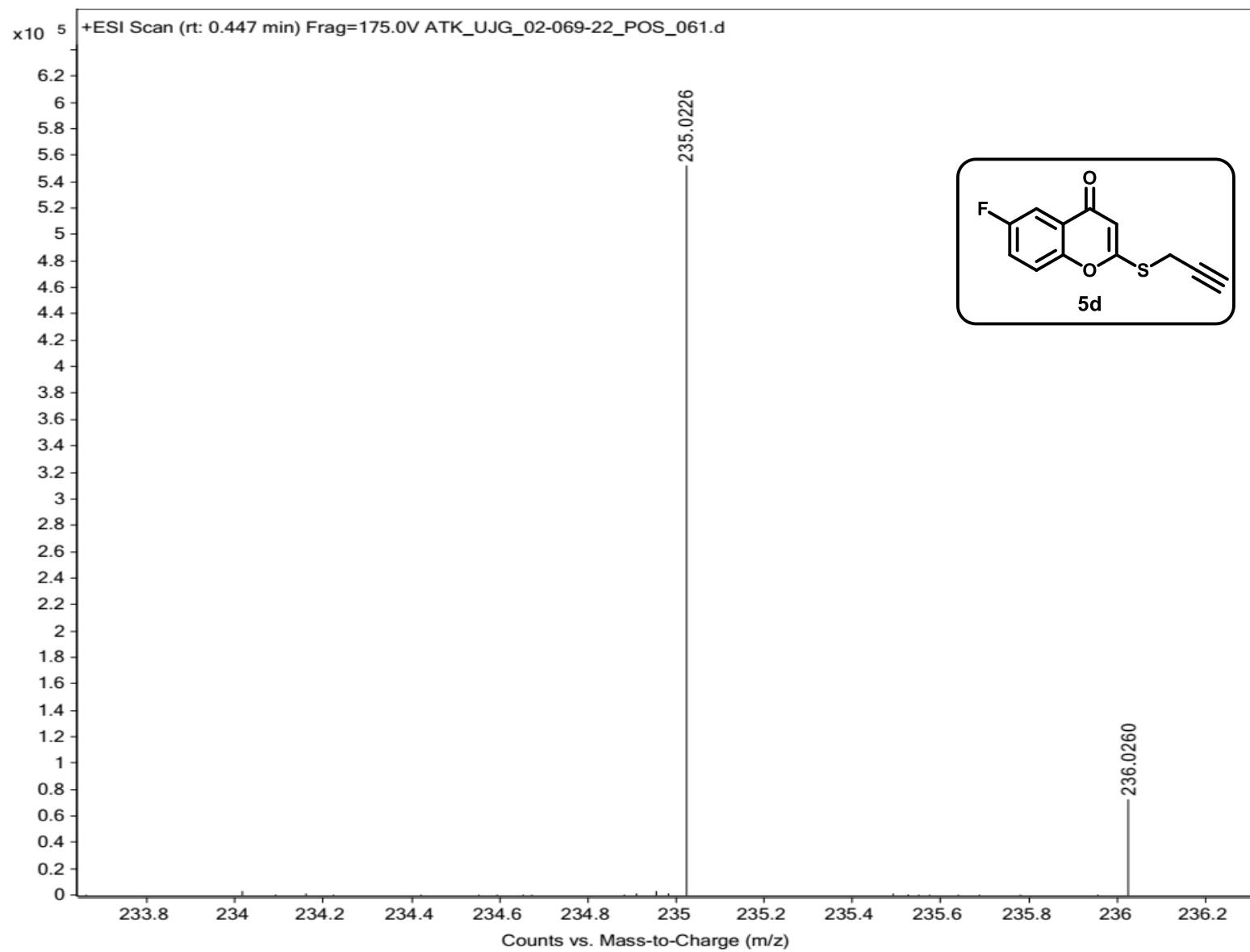


^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 5d

UJG-02-69-22-19F.3.fid — UJG-02-69-22-19F

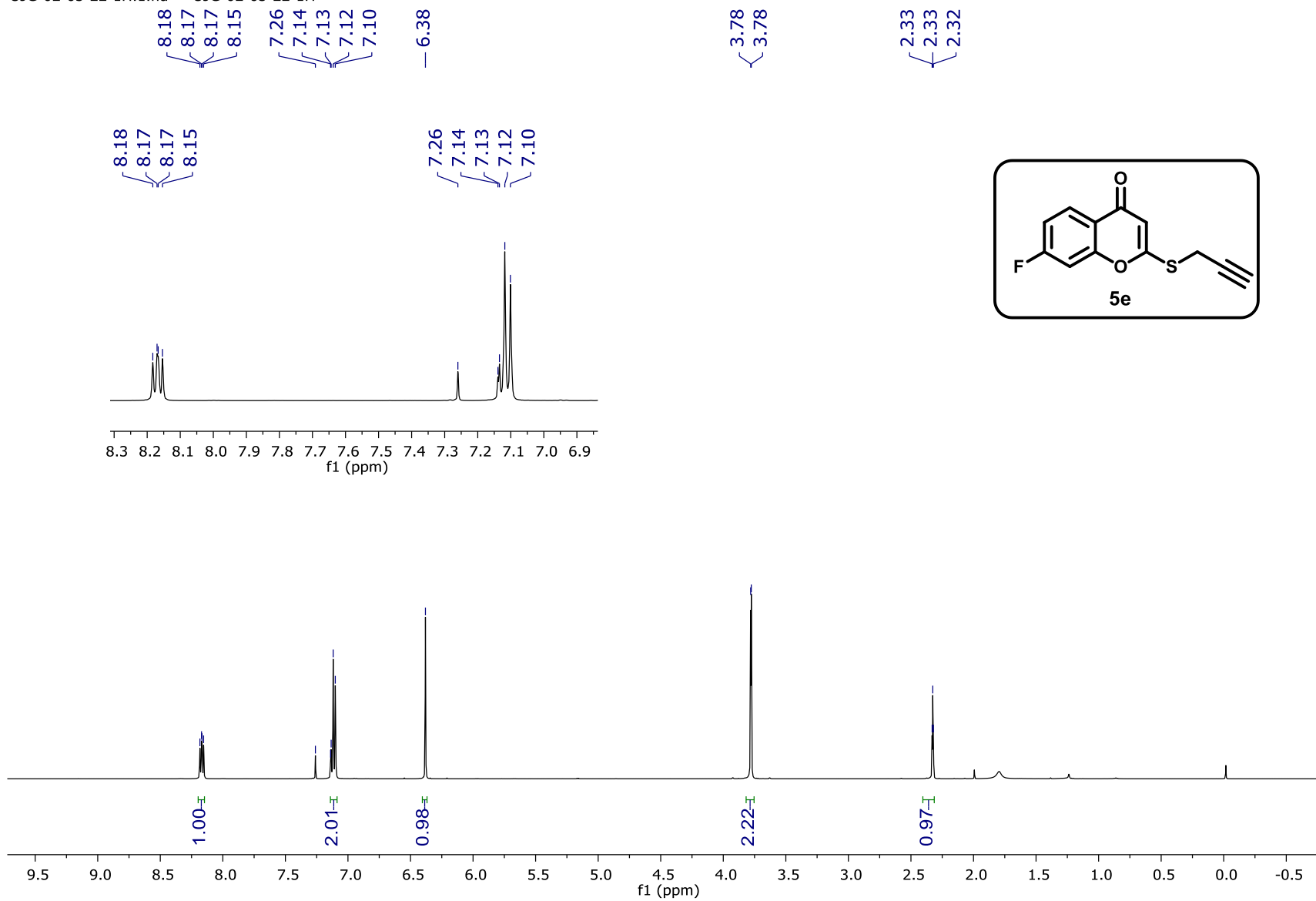


HRMS Spectrum of Compound 5d



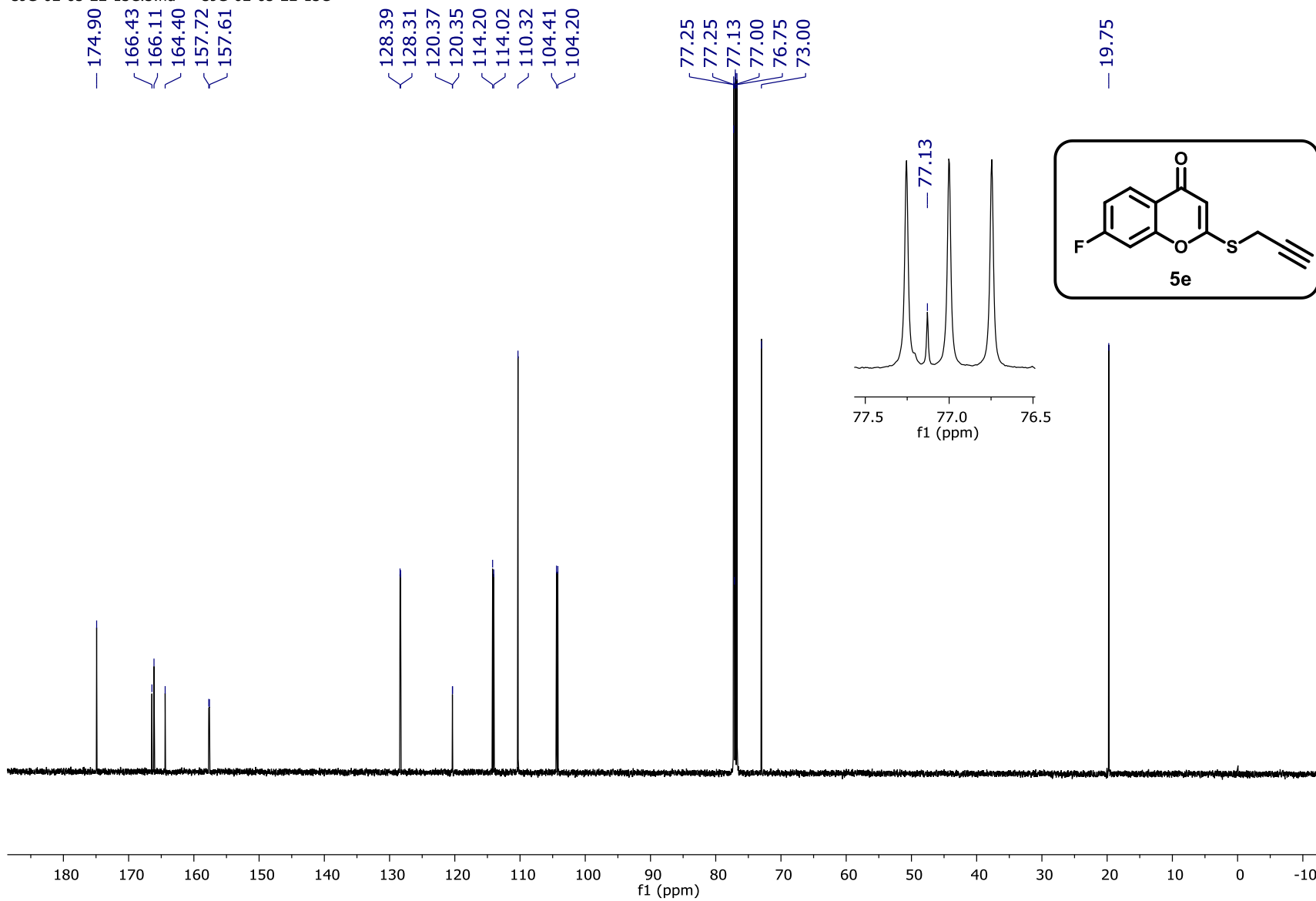
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 5e

UJG-02-65-22-1H.1.fid — UJG-02-65-22-1H



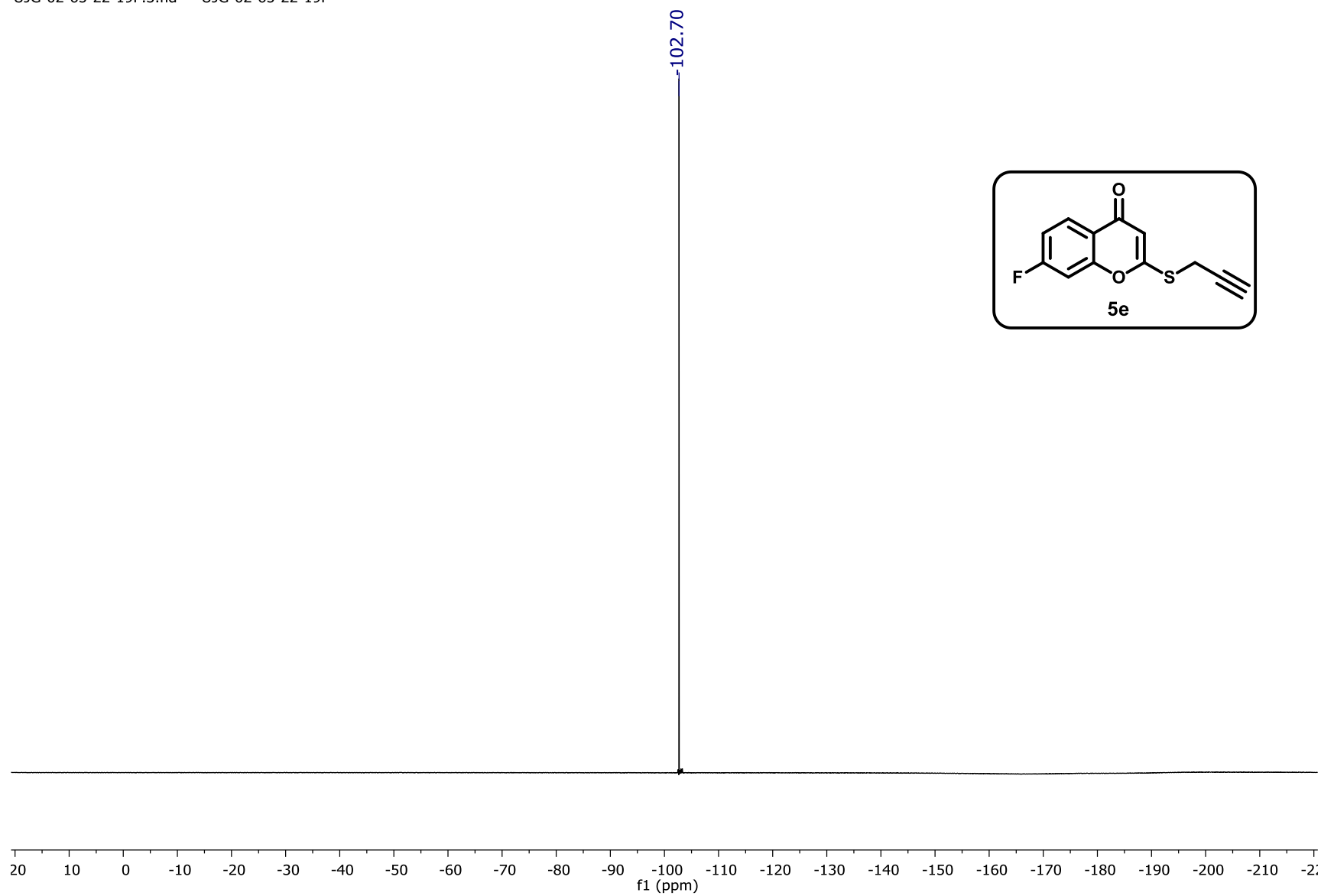
^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 5e

UJG-02-65-22-13C.3.fid — UJG-02-65-22-13C

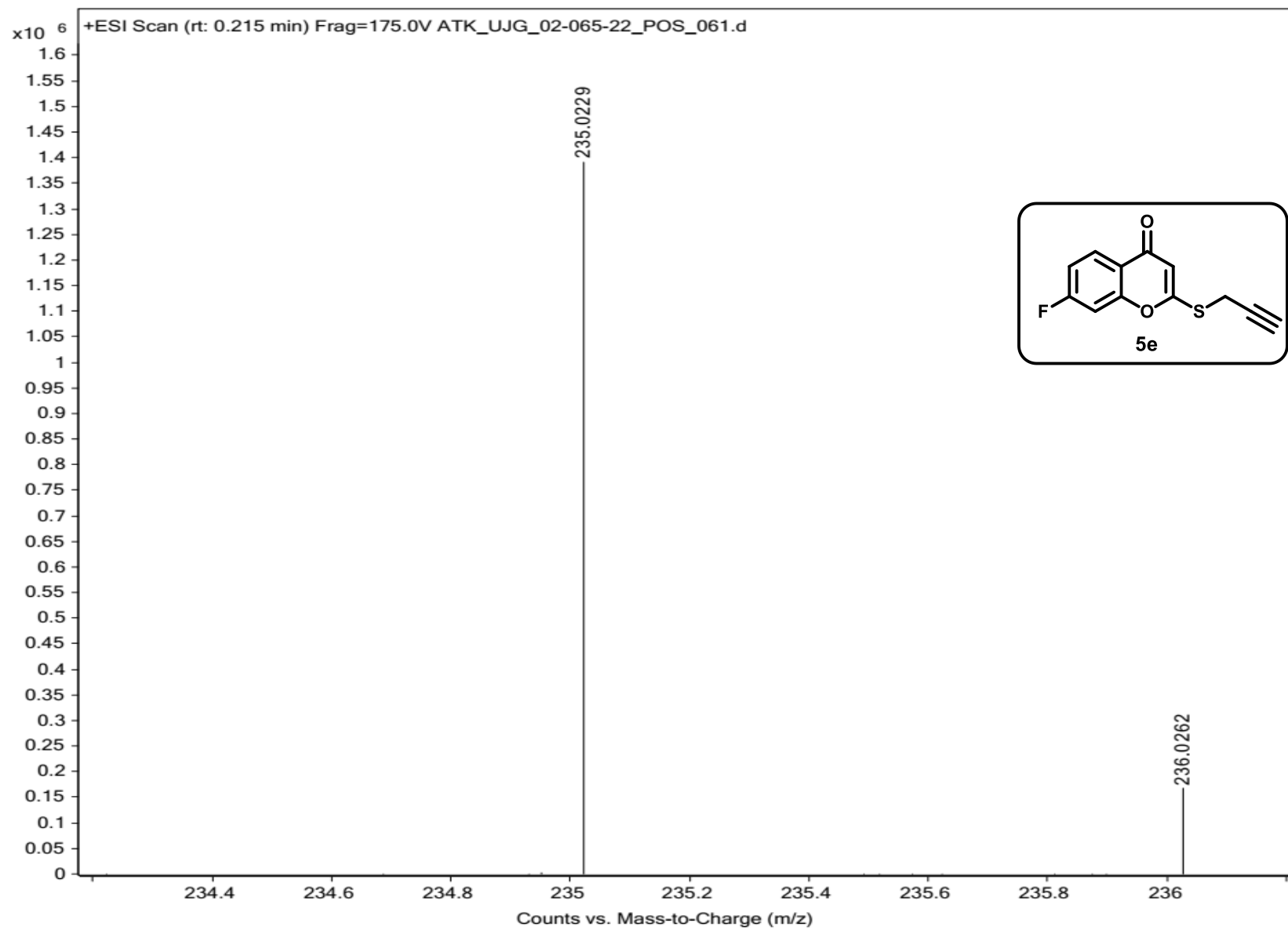


^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 5e

UJG-02-65-22-19F.3.fid — UJG-02-65-22-19F

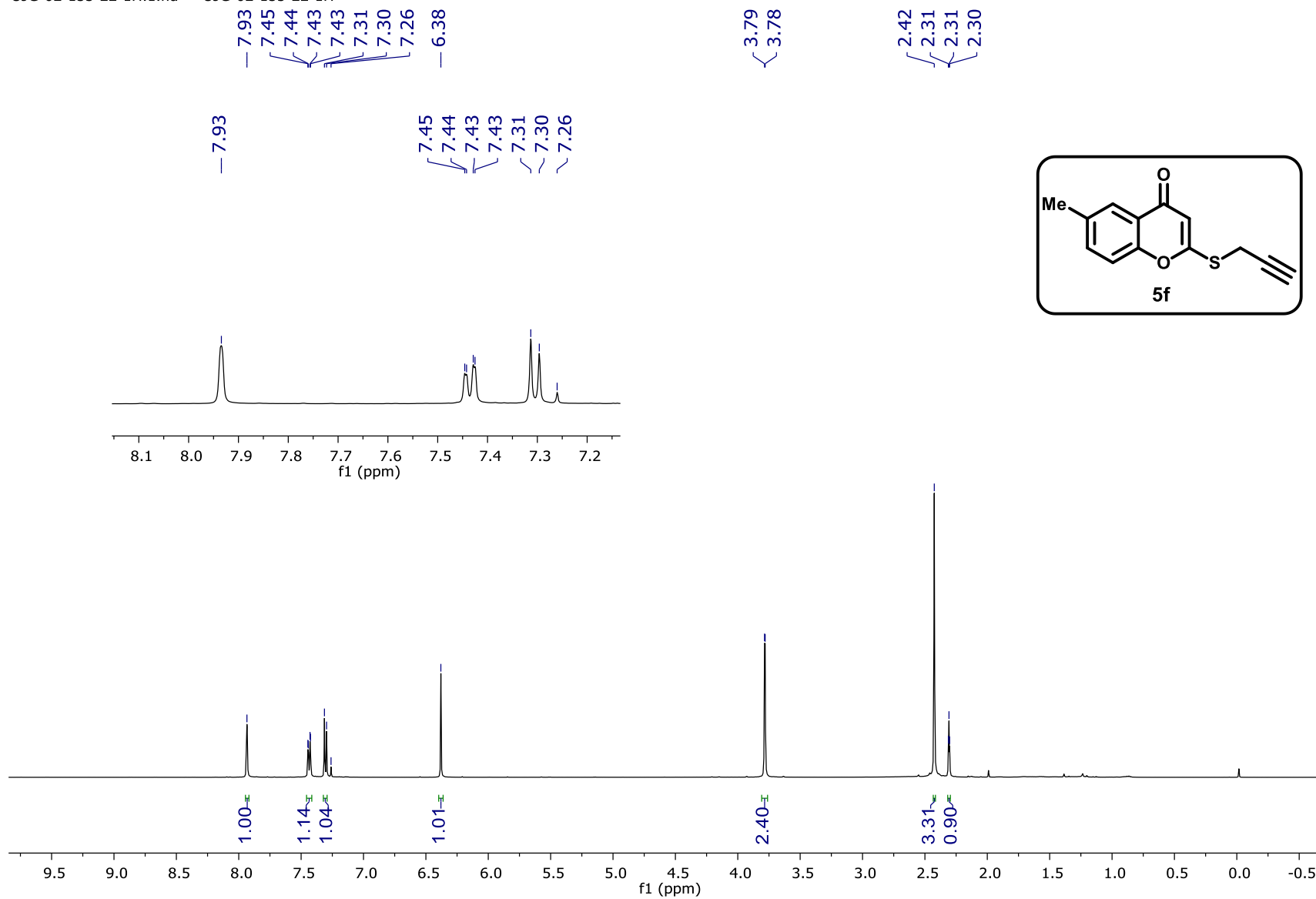


HRMS Spectrum of Compound 5e



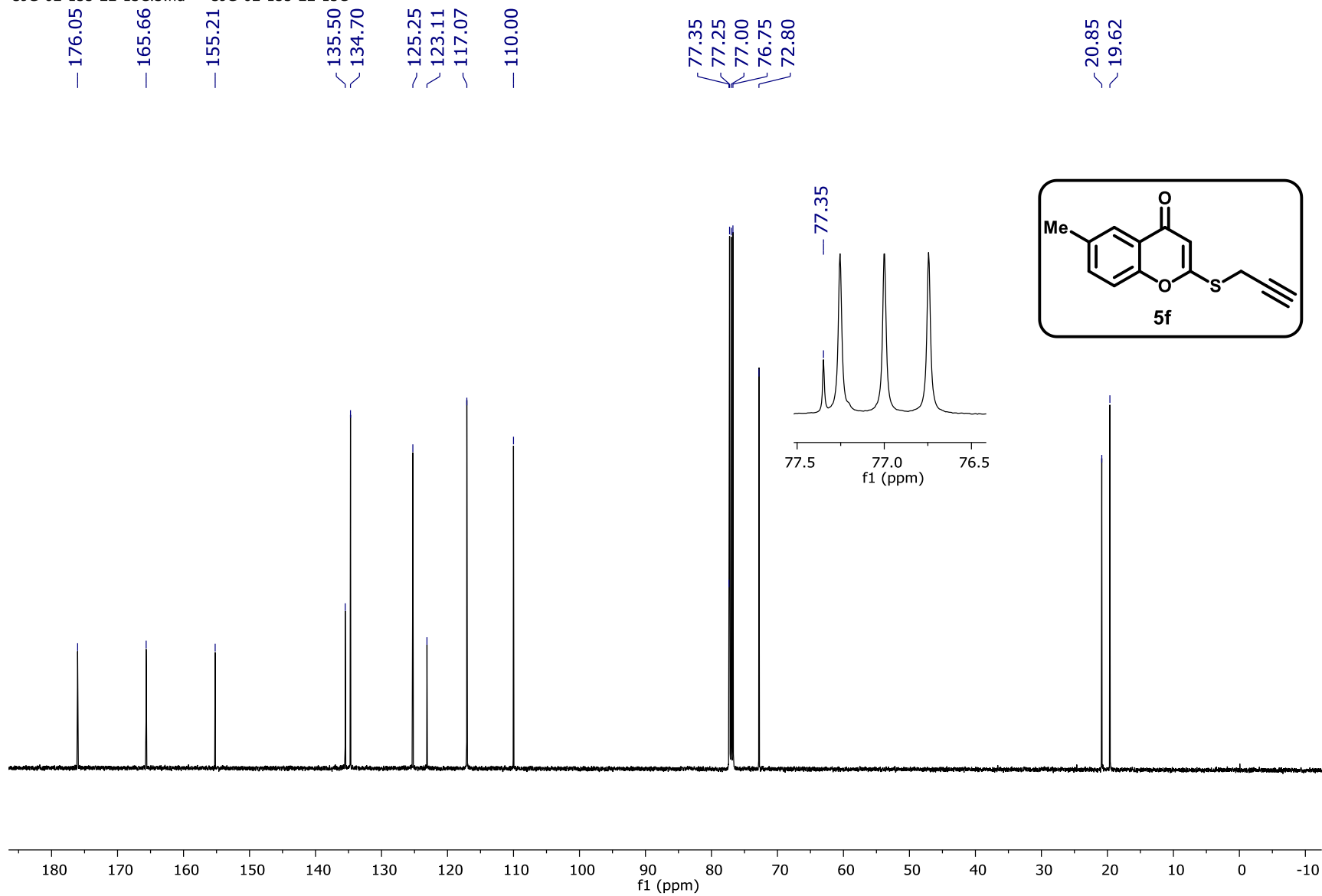
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 5f

UJG-02-155-22-1H.1.fid — UJG-02-155-22-1H

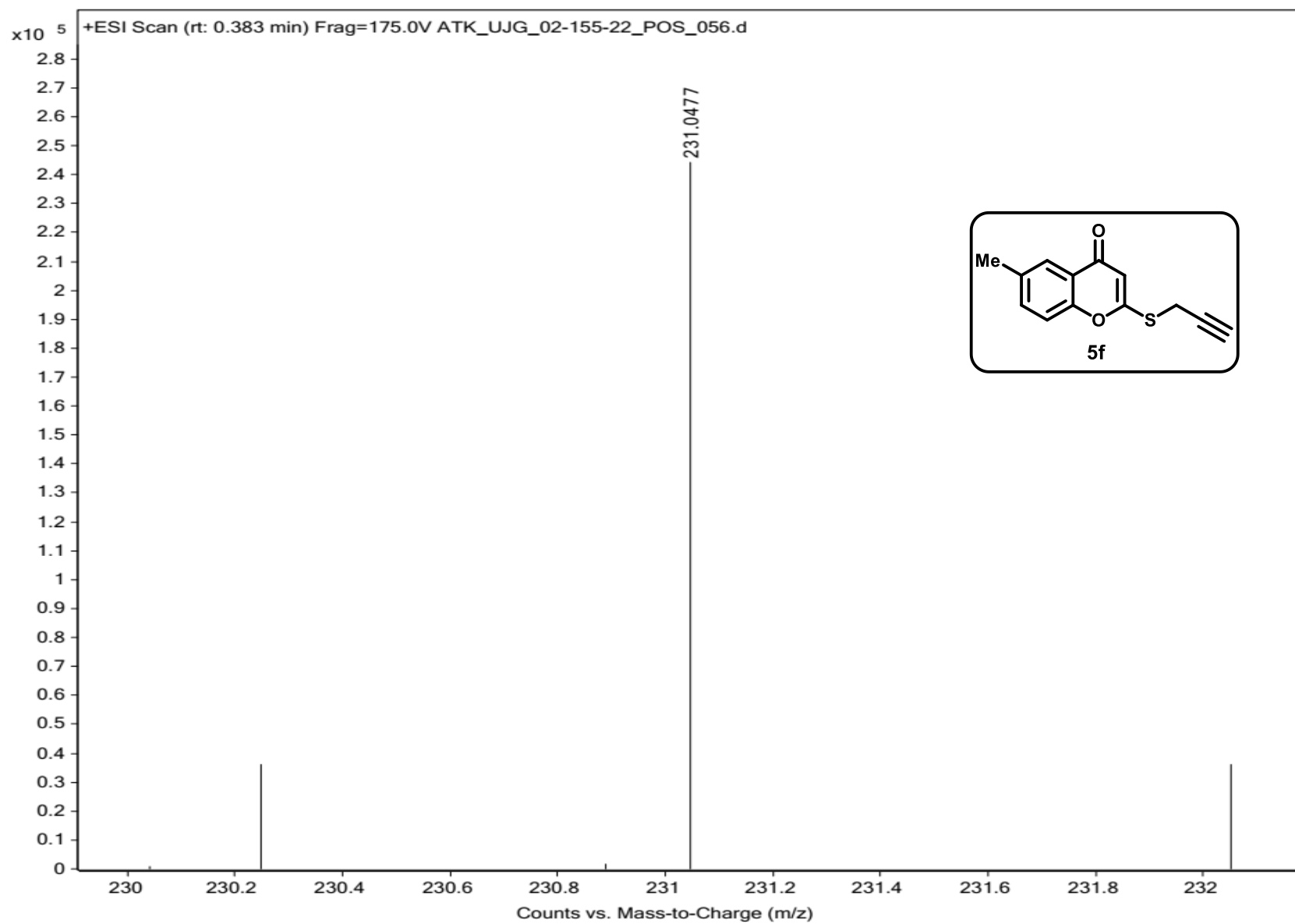


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 5f

UJG-02-155-22-13C.3.fid — UJG-02-155-22-13C

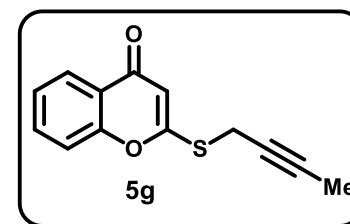
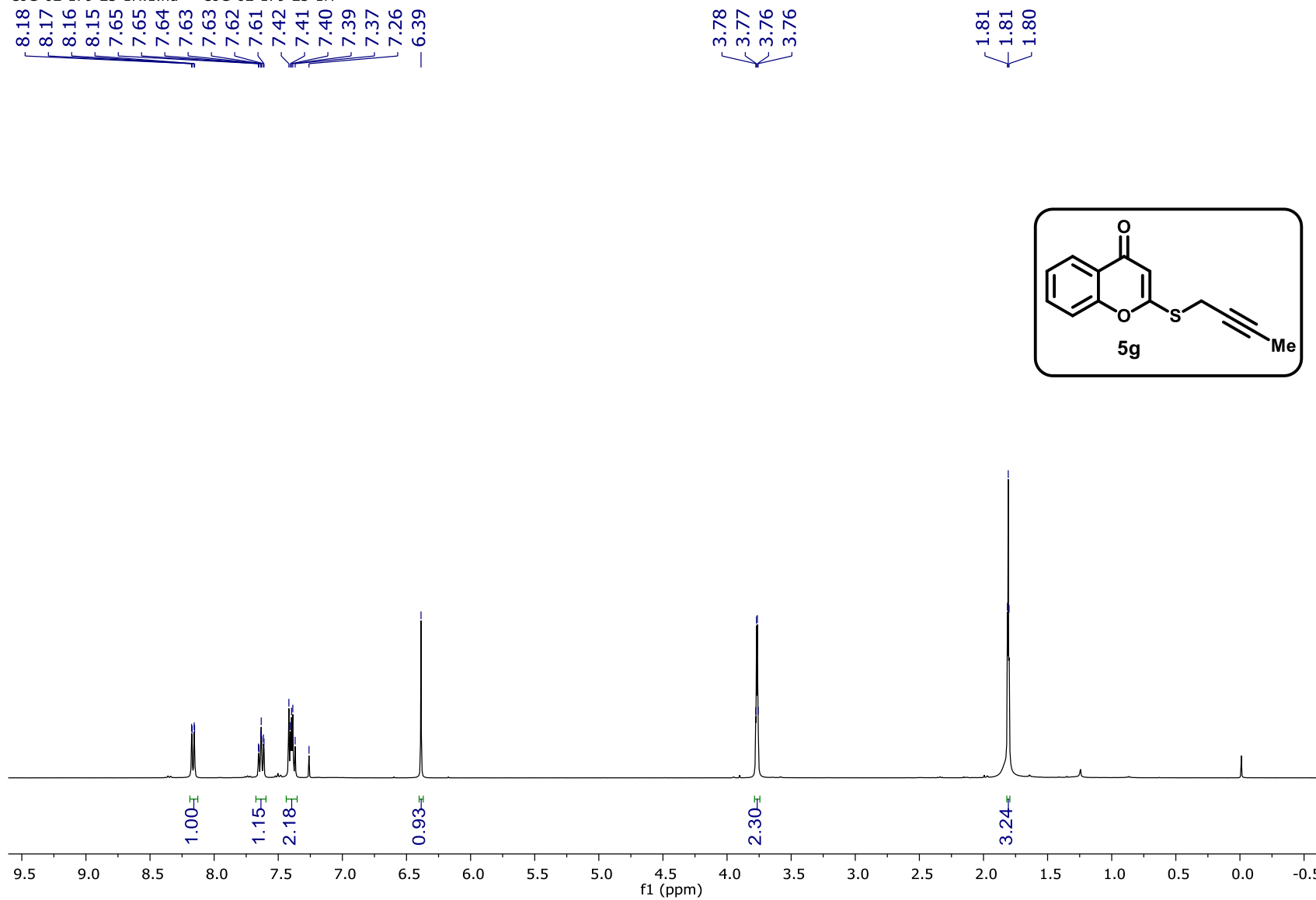


HRMS Spectrum of Compound 5f



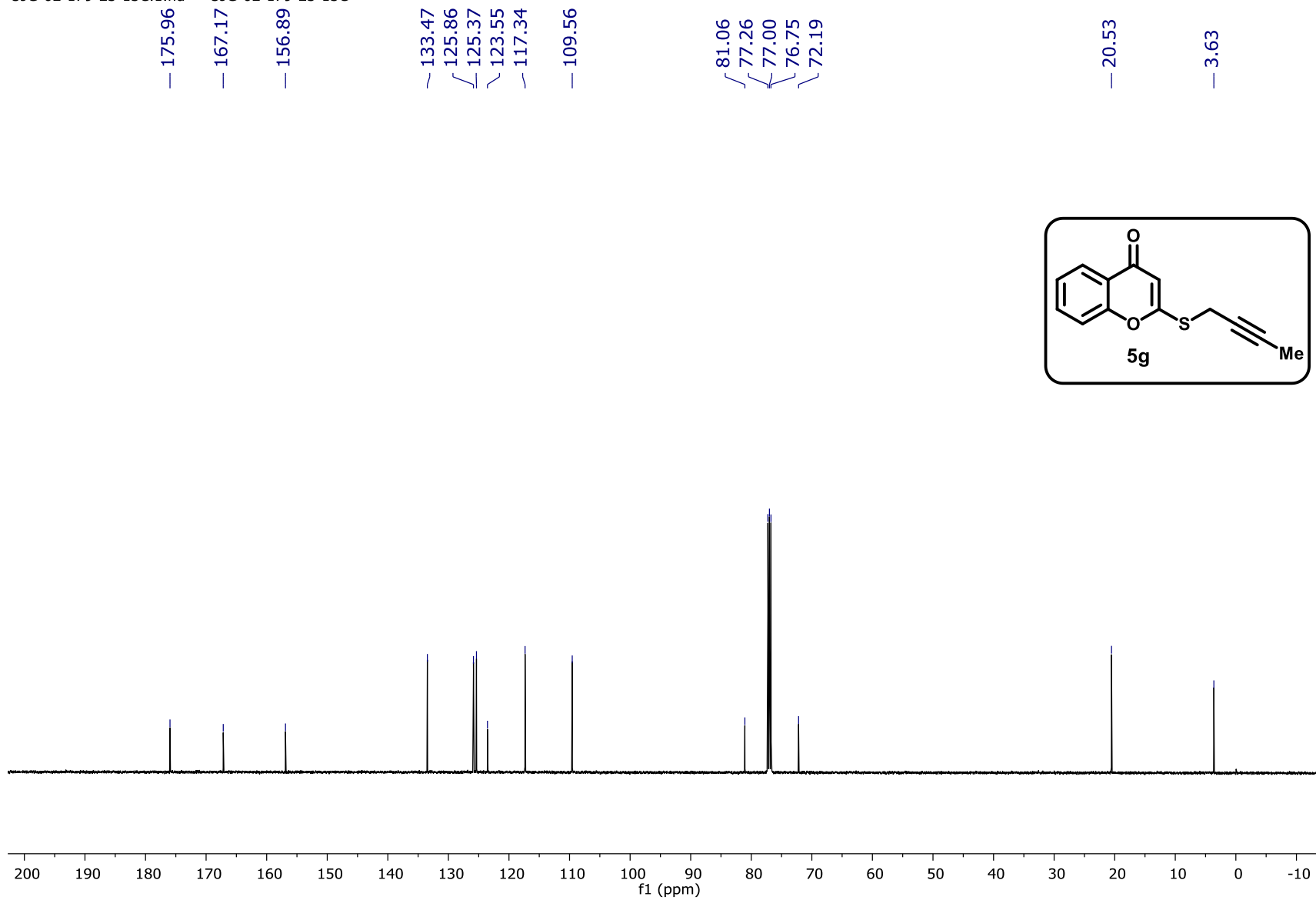
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5g

UJG-02-179-23-1H.1.fid — UJG-02-179-23-1H

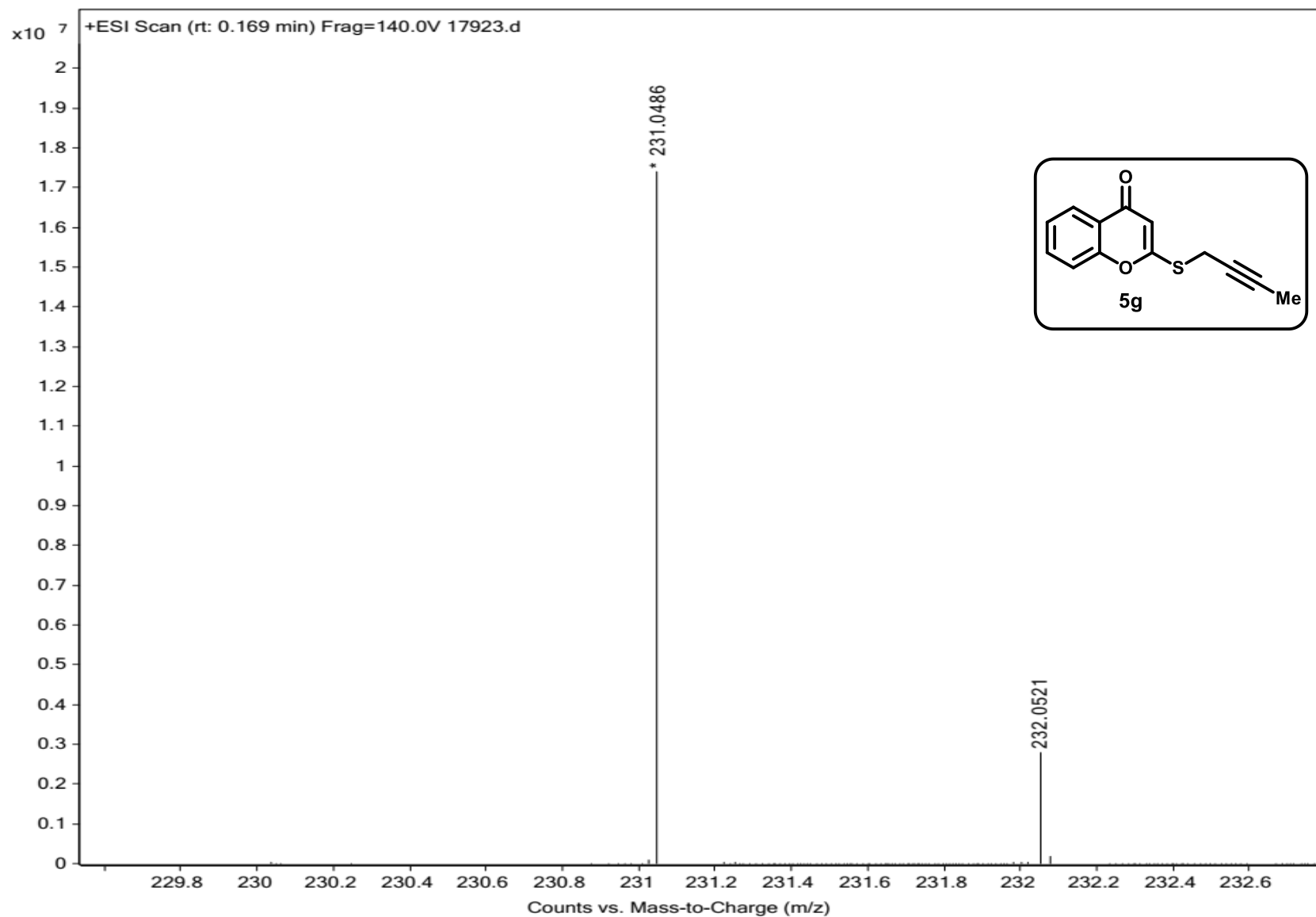


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5g

UJG-02-179-23-13C.1.fid — UJG-02-179-23-13C

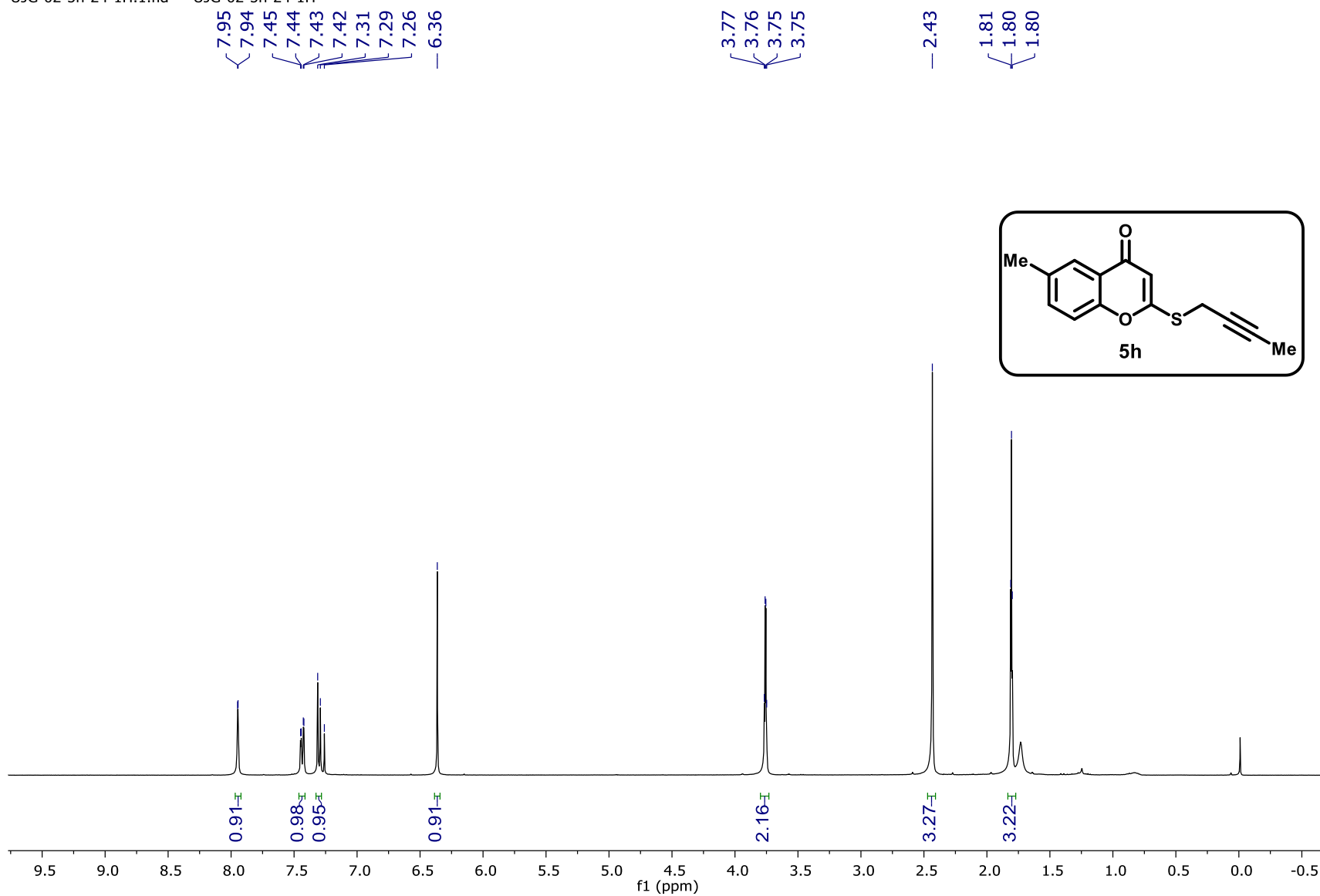


HRMS Spectrum of Compound 5g



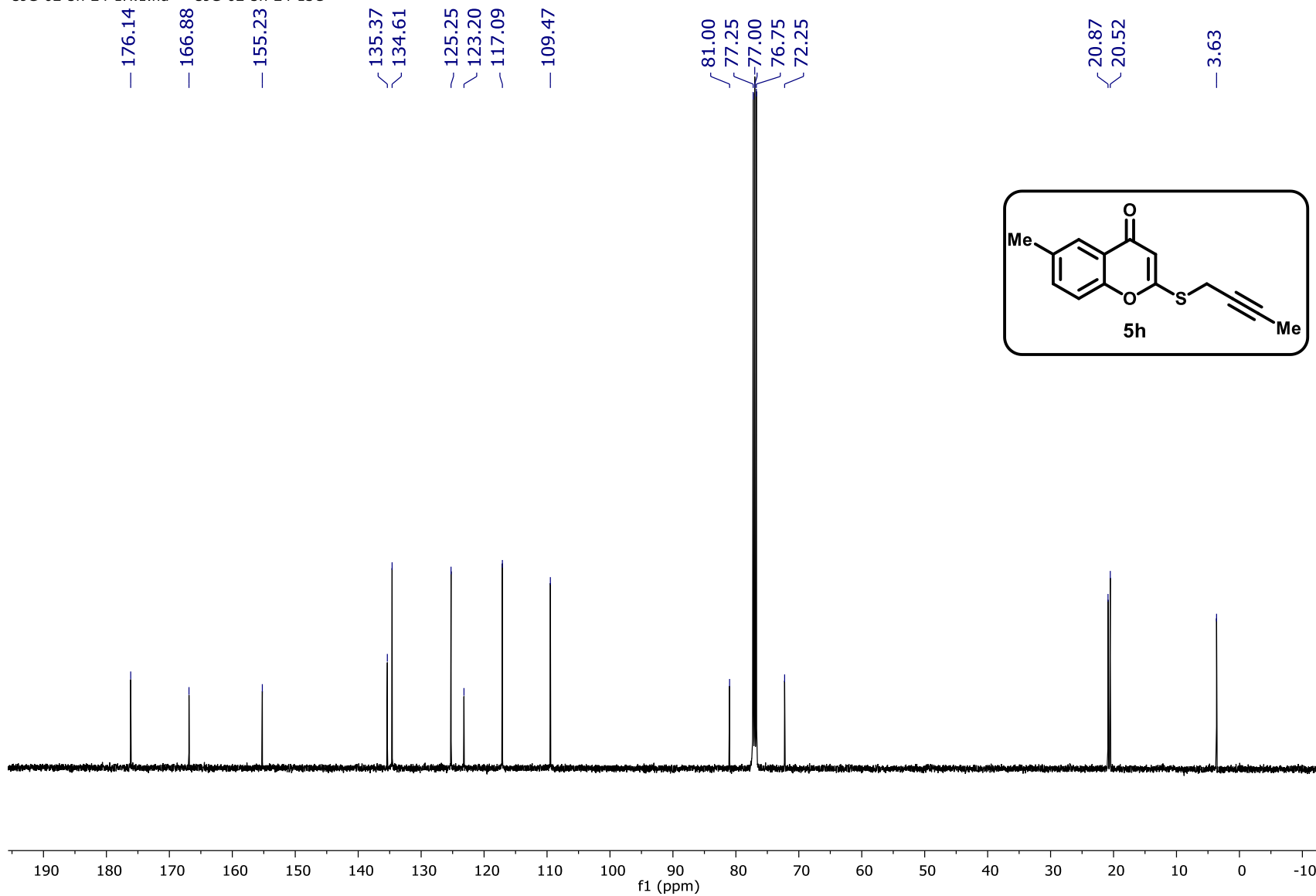
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 5h

UJG-02-5h-24-1H.1.fid — UJG-02-5h-24-1H

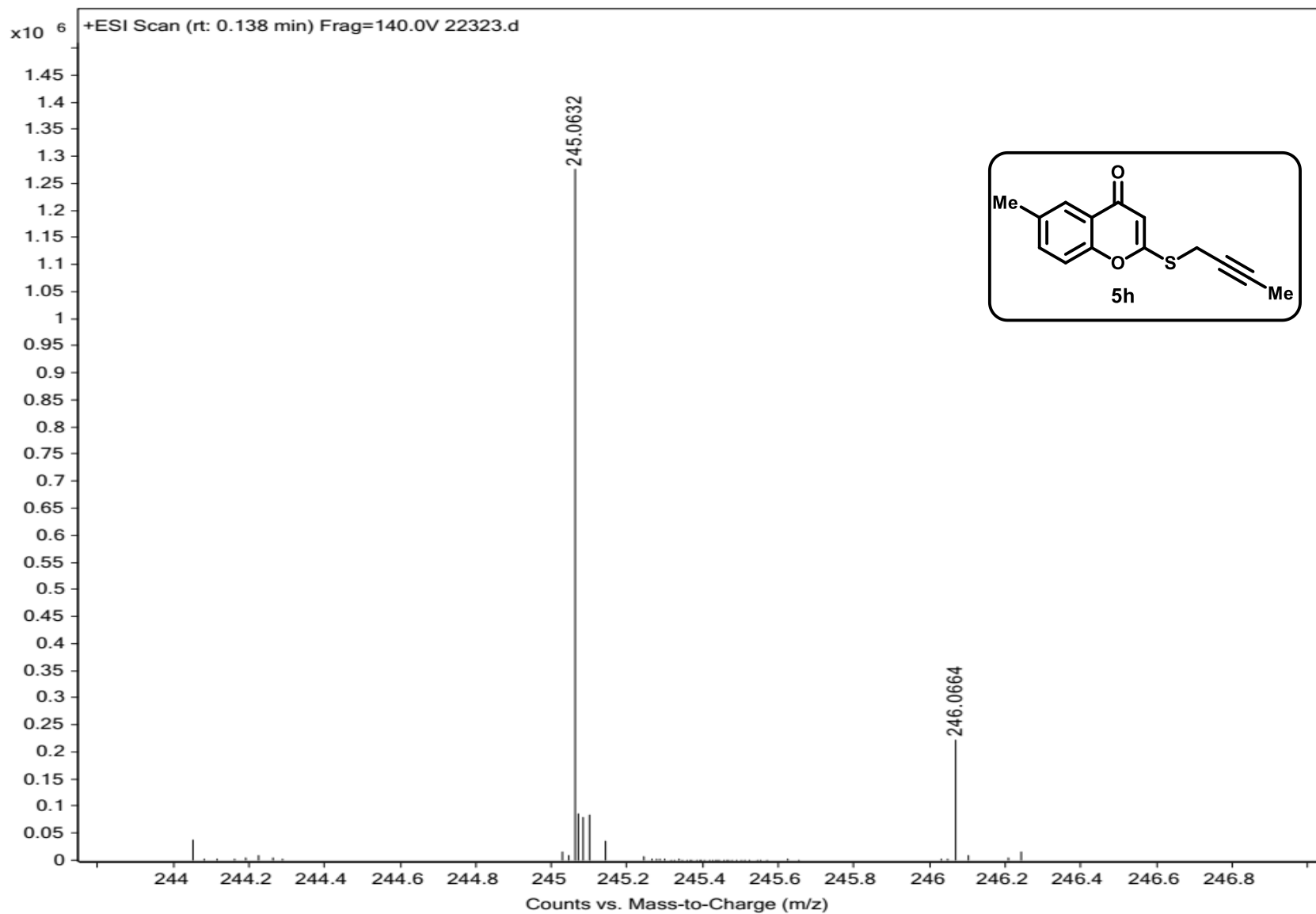


¹³C {¹H} NMR (125 MHz, CDCl₃) Spectrum of Compound 5h

UJG-02-5h-24-1H.1.fid — UJG-02-5h-24-13C

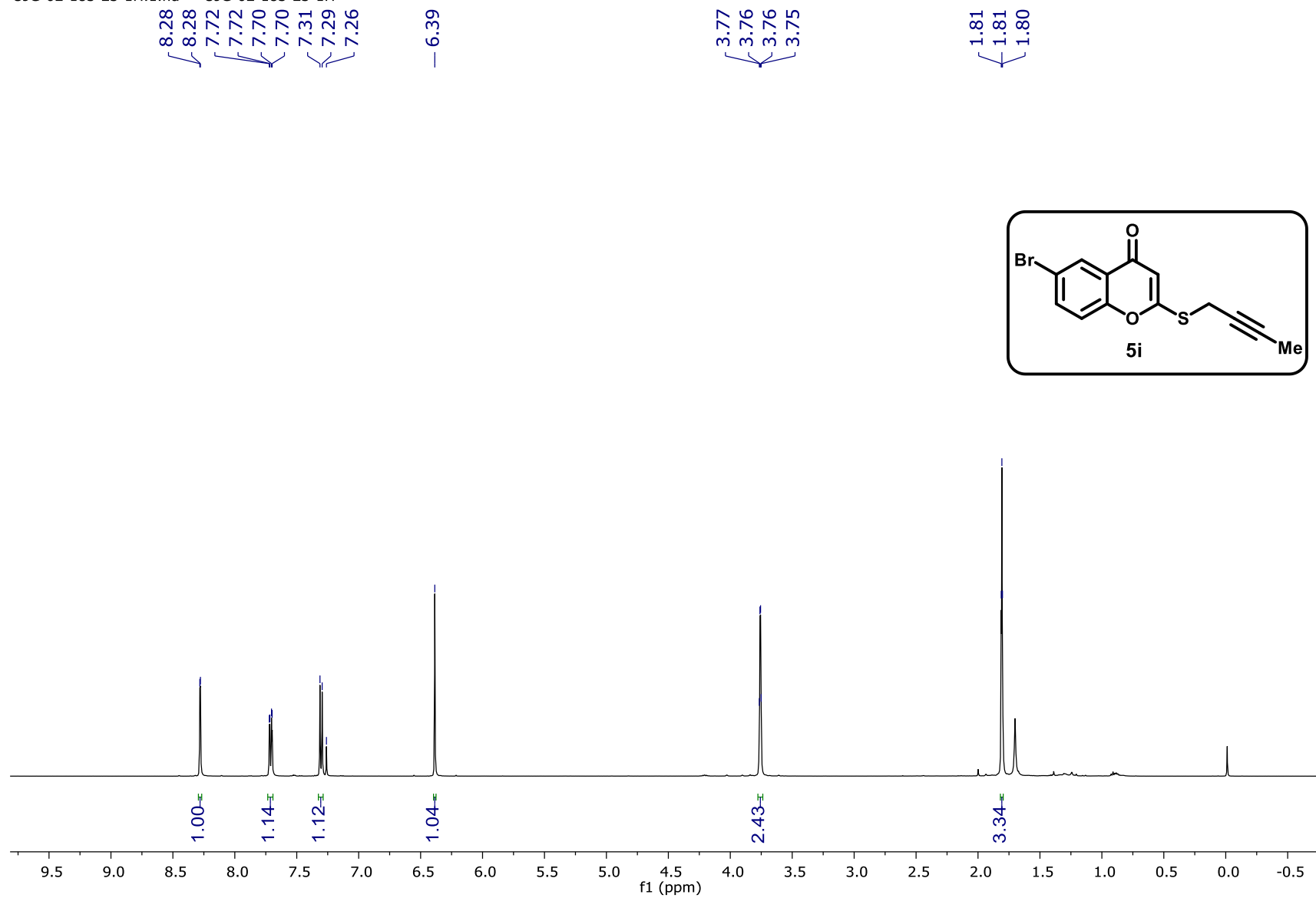


HRMS Spectrum of Compound 5h



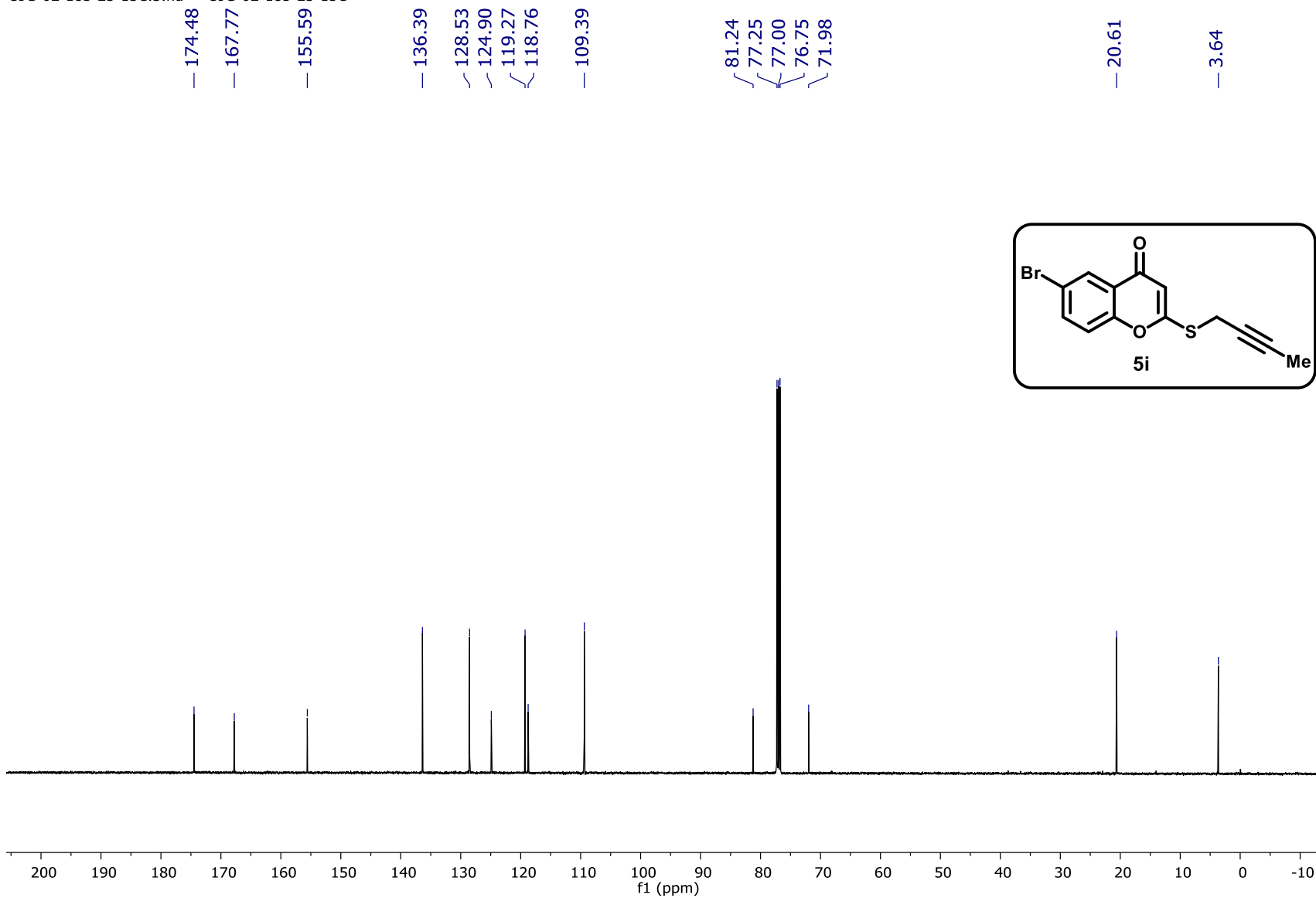
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 5i

UJG-02-183-23-1H.1.fid — UJG-02-183-23-1H

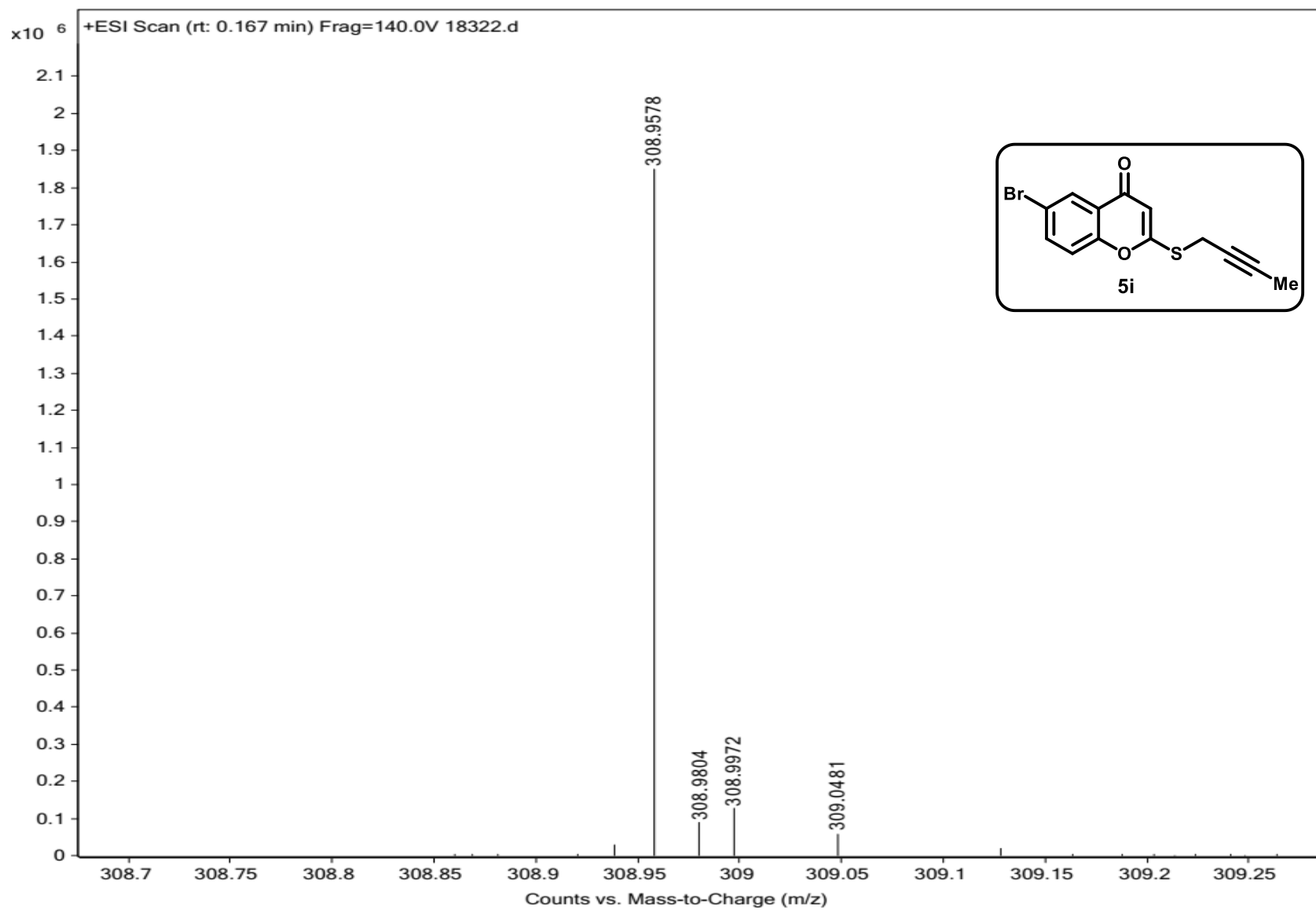


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5i

UJG-02-183-23-13C.3.fid — UJG-02-183-23-13C

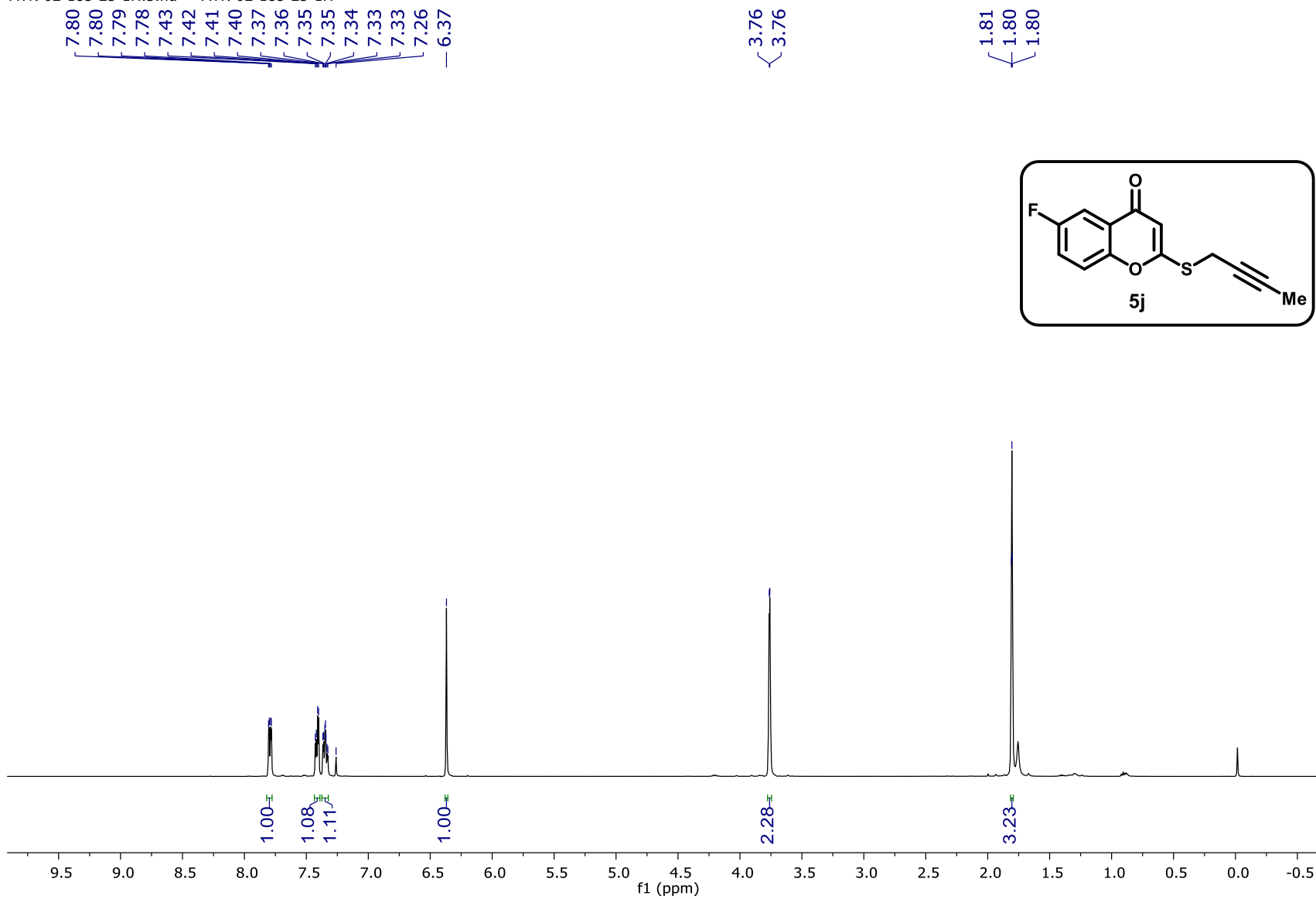


HRMS Spectrum of Compound 5i



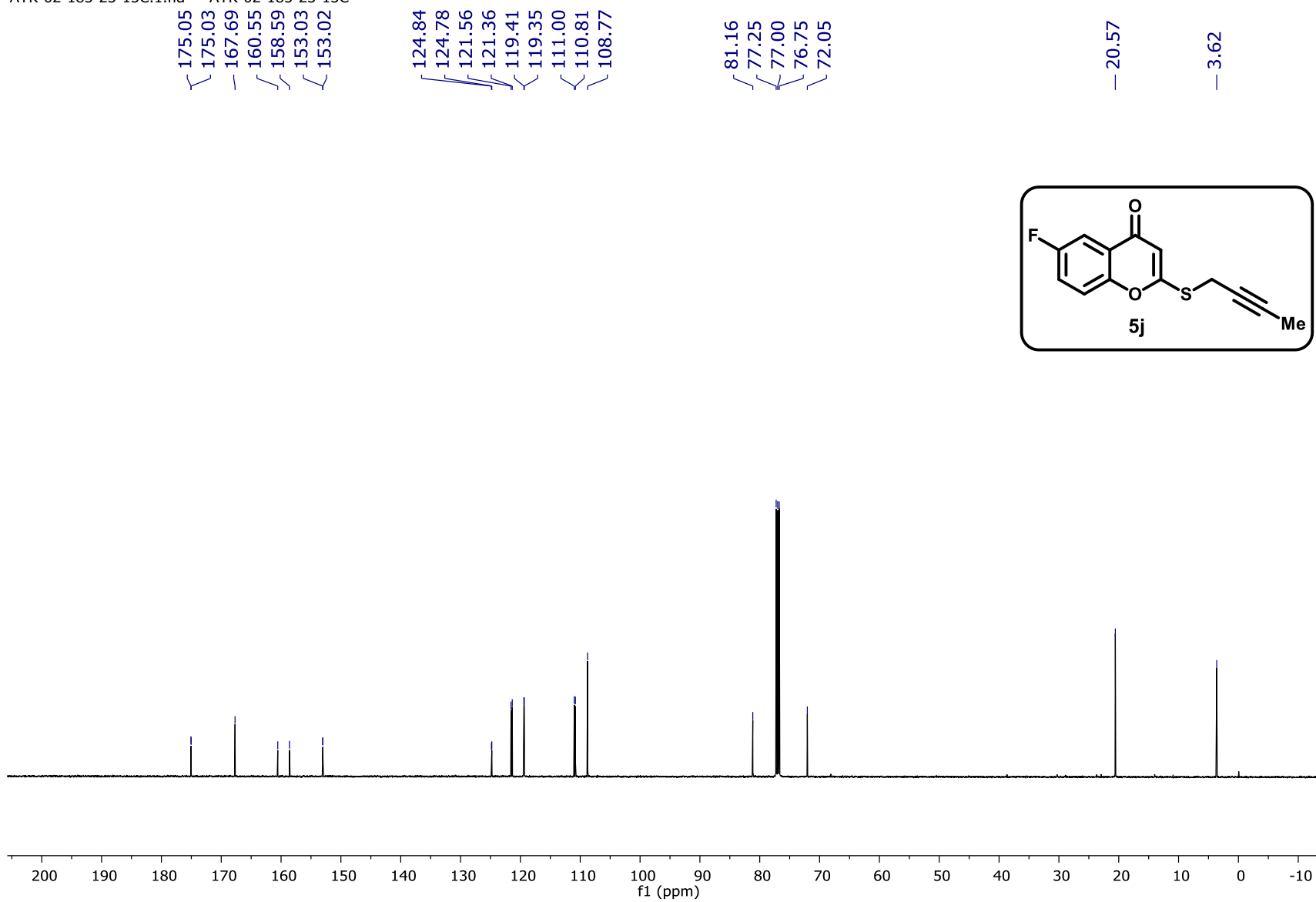
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 5j

ATK-02-185-23-1H.3.fid — ATK-02-185-23-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5j

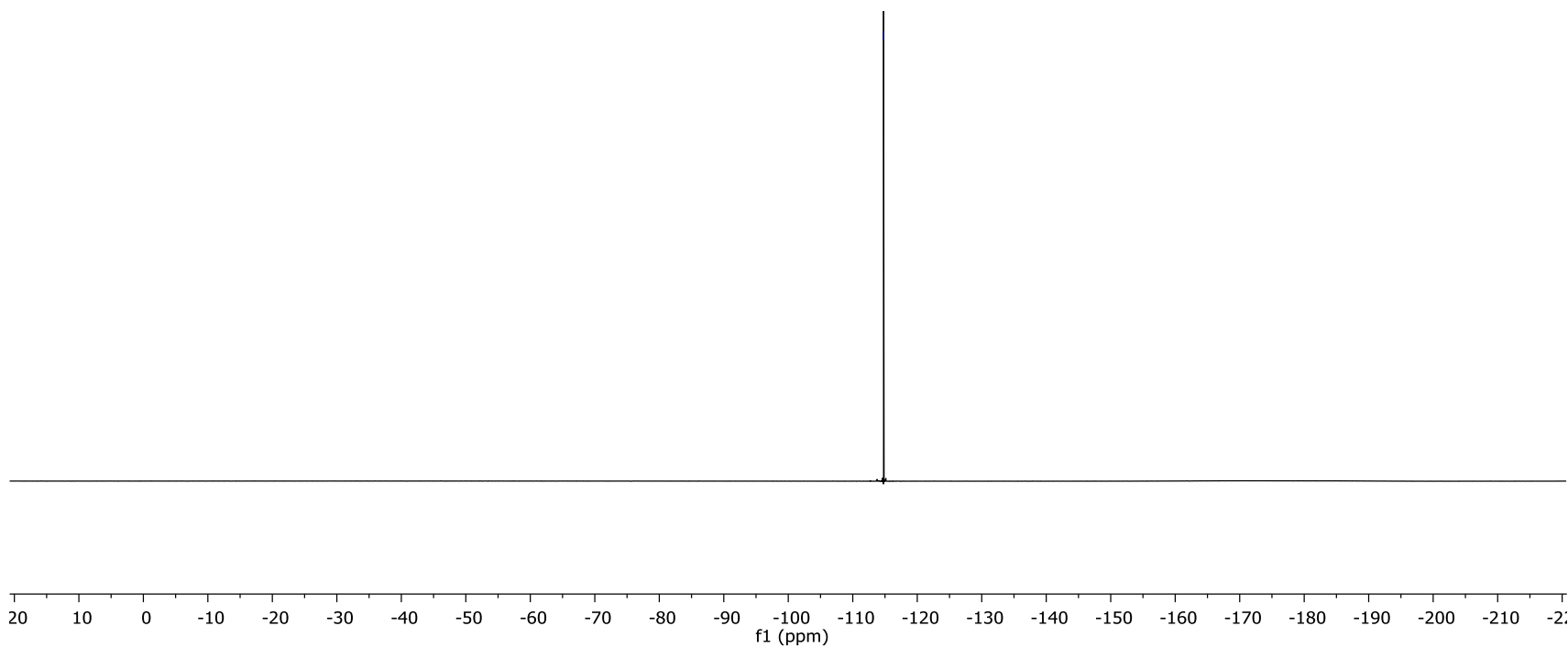
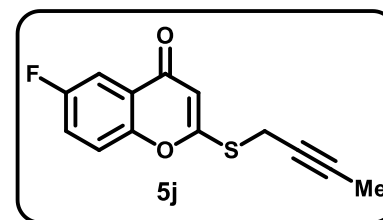
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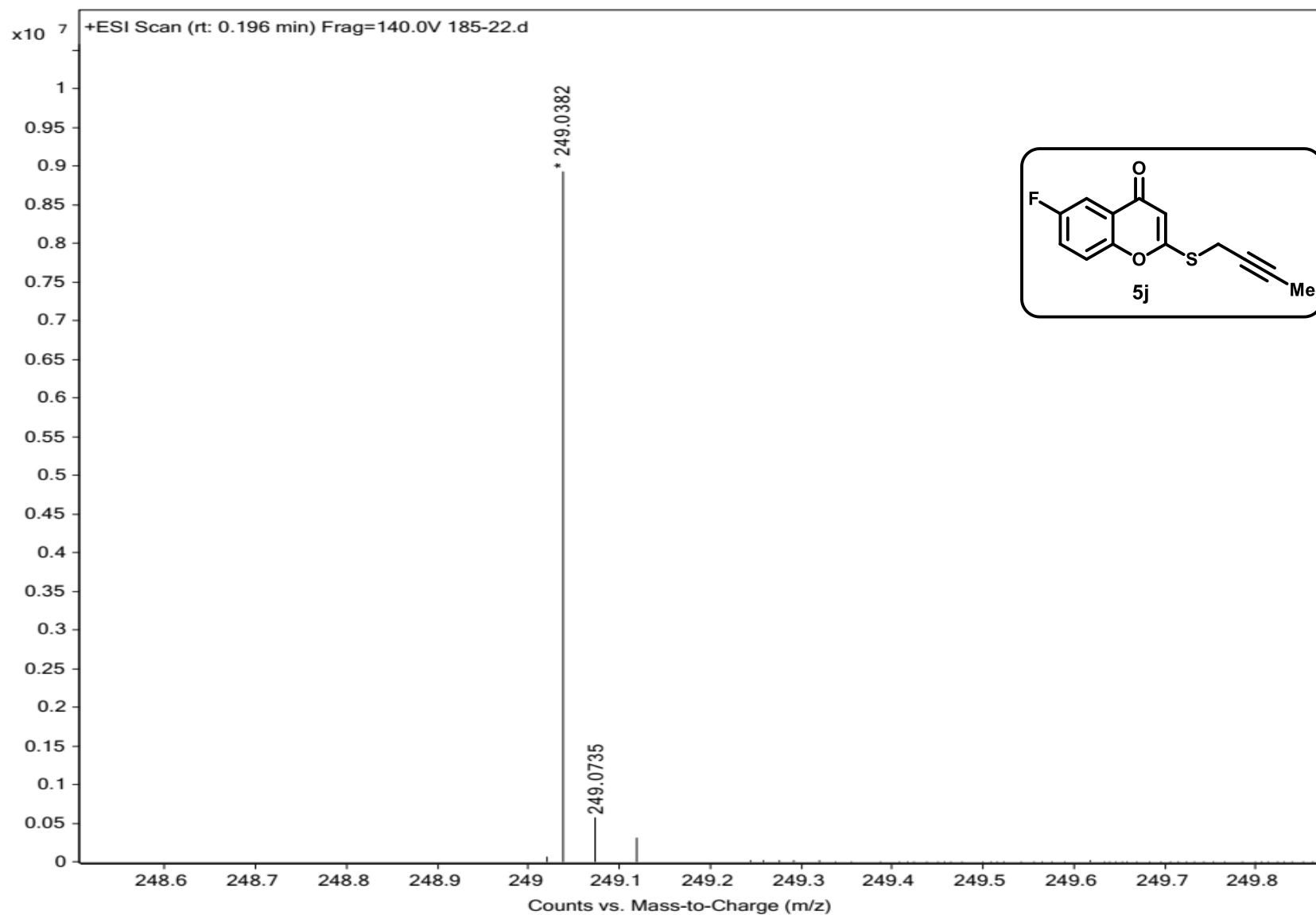
¹⁹F NMR (471 MHz, CDCl₃) Spectrum of Compound 5j

ATK-02-185-23-19F.5.fid — ATK-02-185-23-19F

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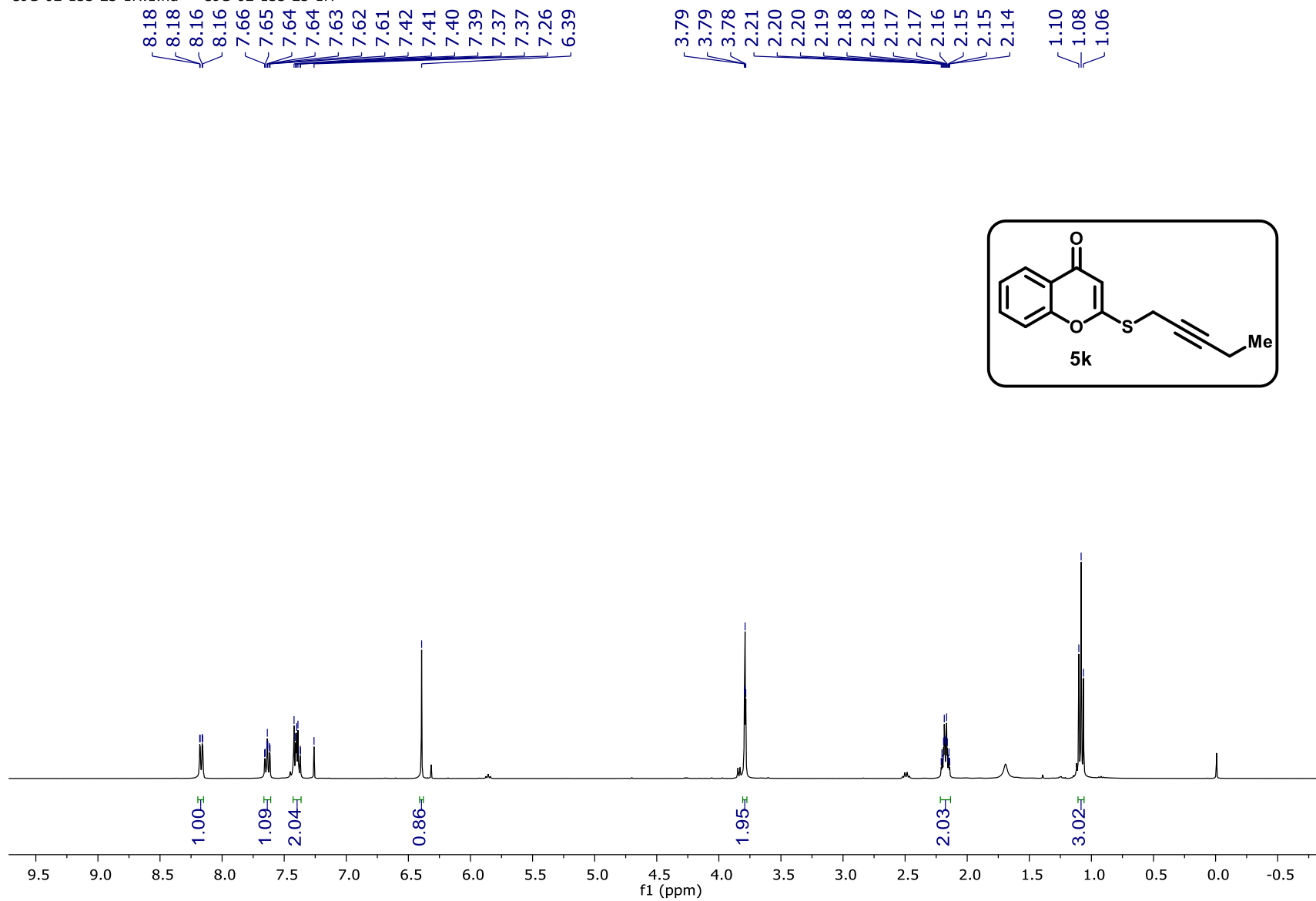


HRMS Spectrum of Compound 5j



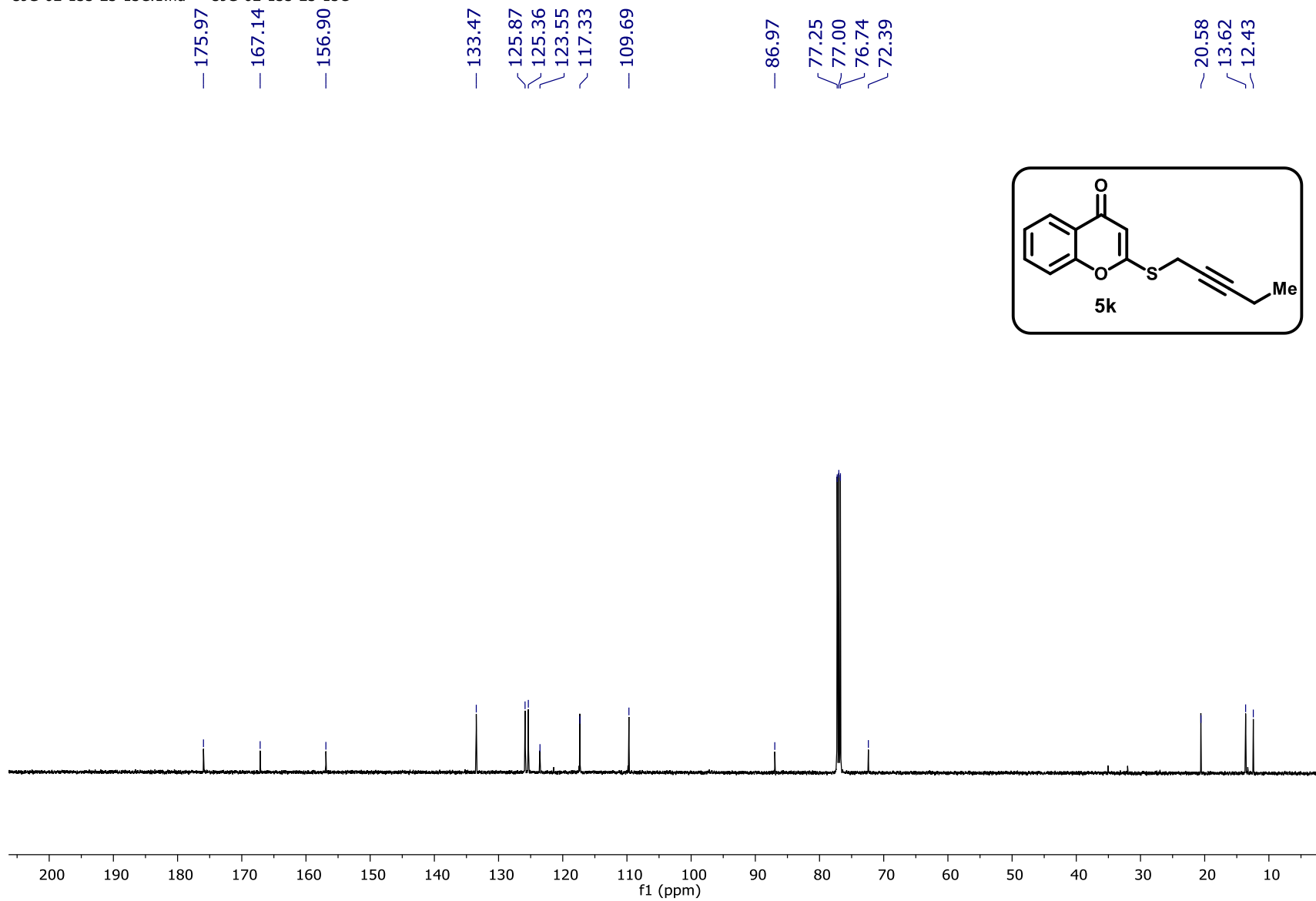
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5k

UJG-02-133-23-1H.1.fid — UJG-02-133-23-1H

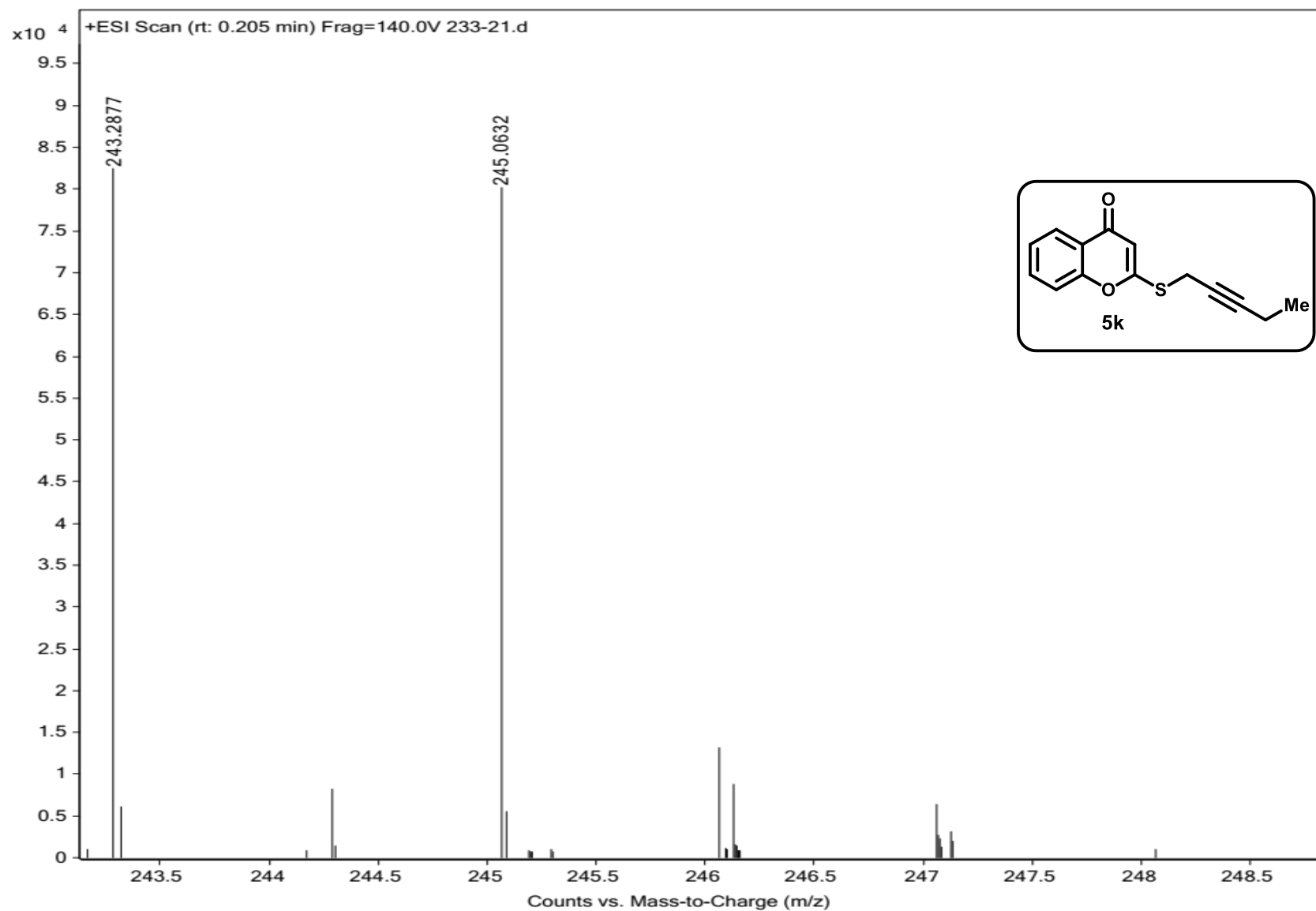


¹³C {¹H} NMR (125 MHz, CDCl₃) Spectrum of Compound 5k

UJG-02-133-23-13C.1.fid — UJG-02-133-23-13C

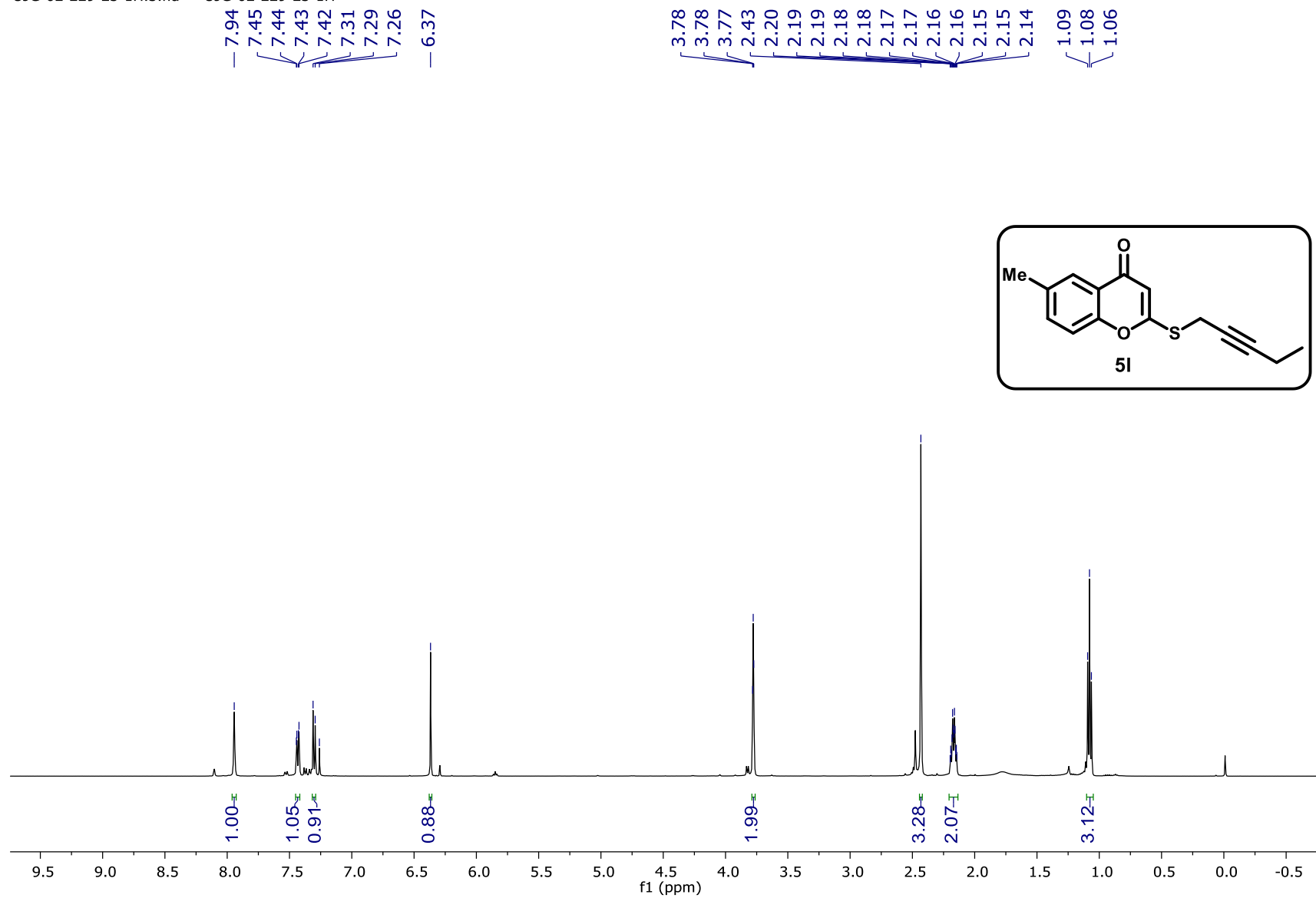


HRMS Spectrum of Compound 5k



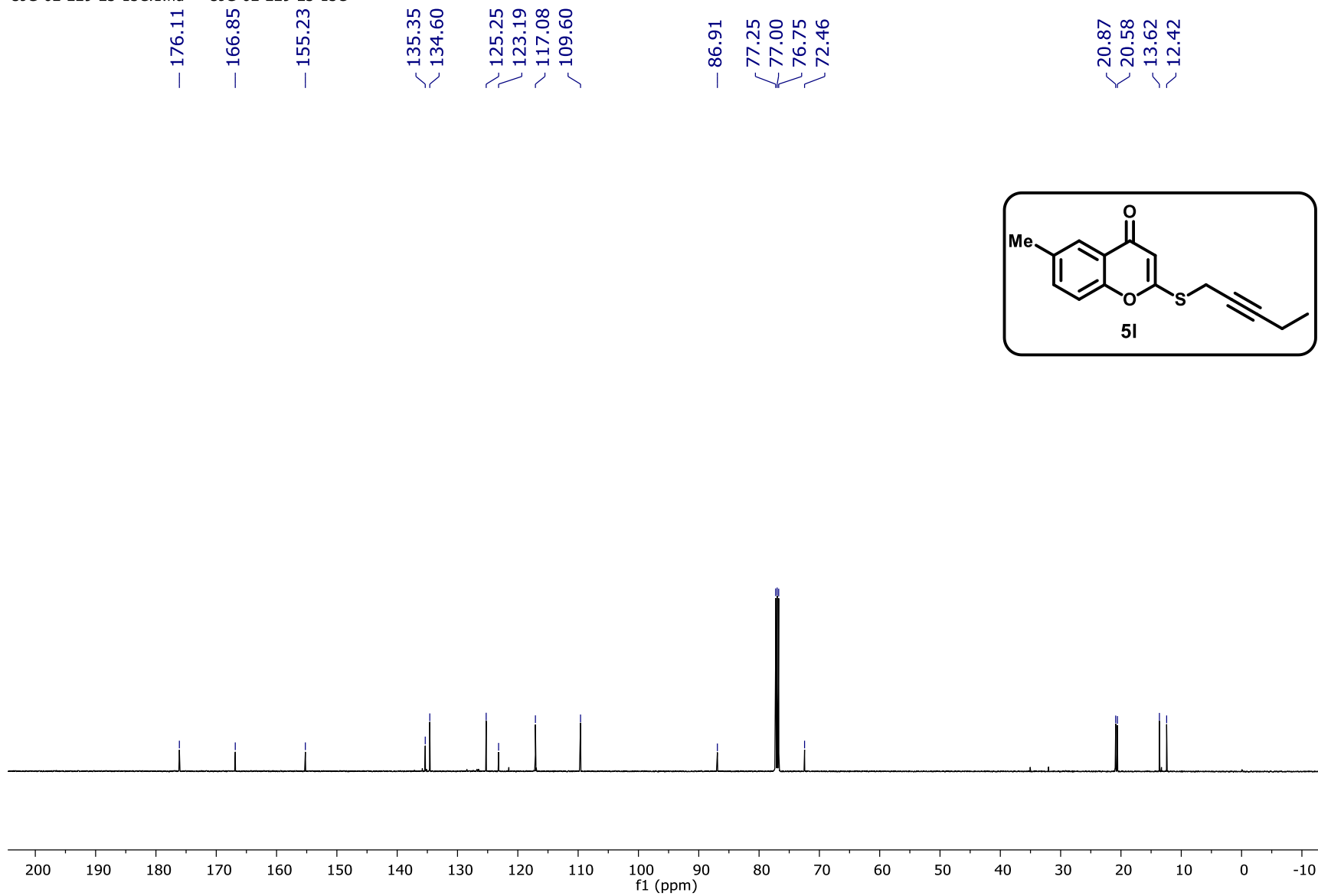
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 5I

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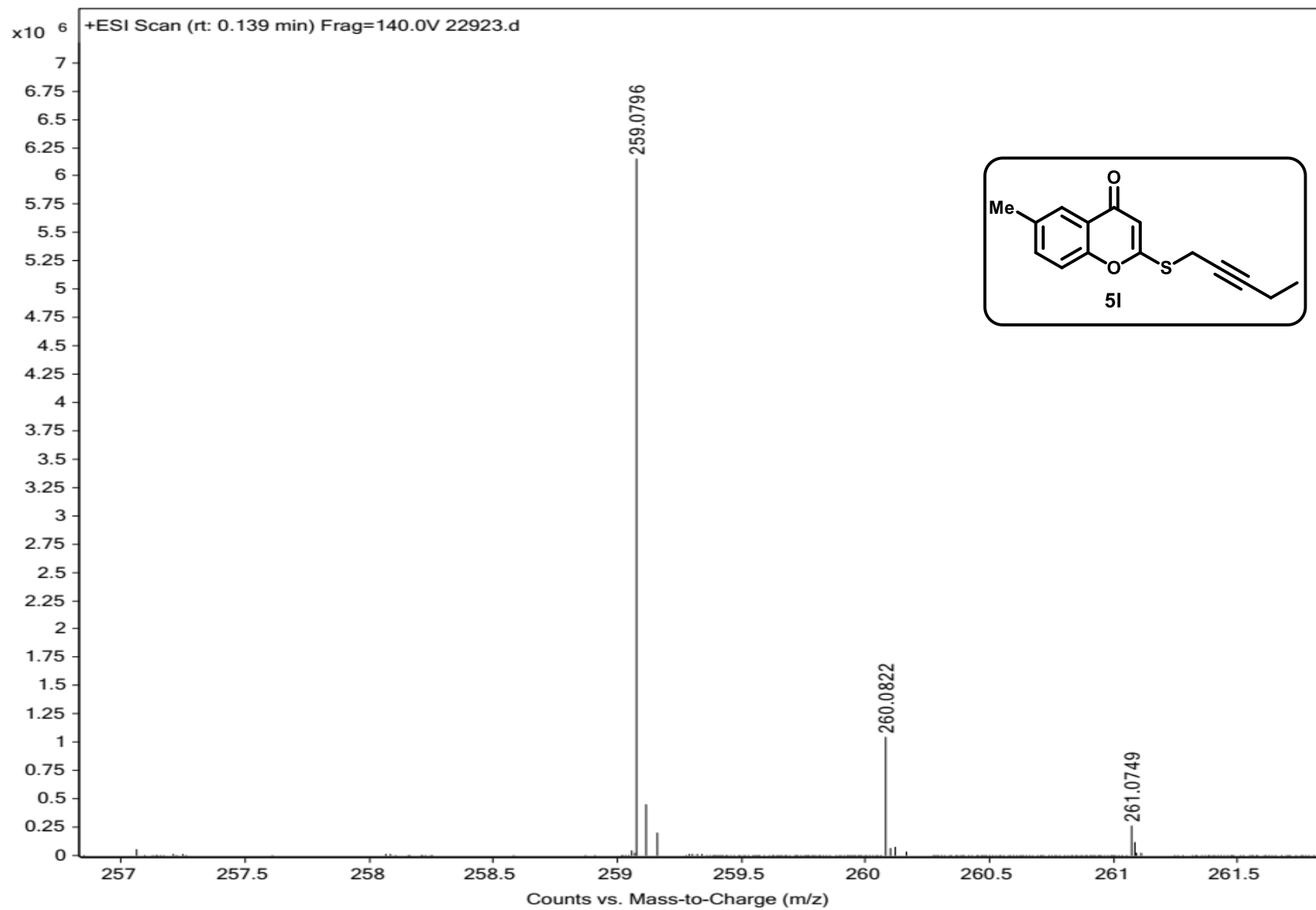


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 5l

UJG-02-229-23-13C.1.fid — UJG-02-229-23-13C

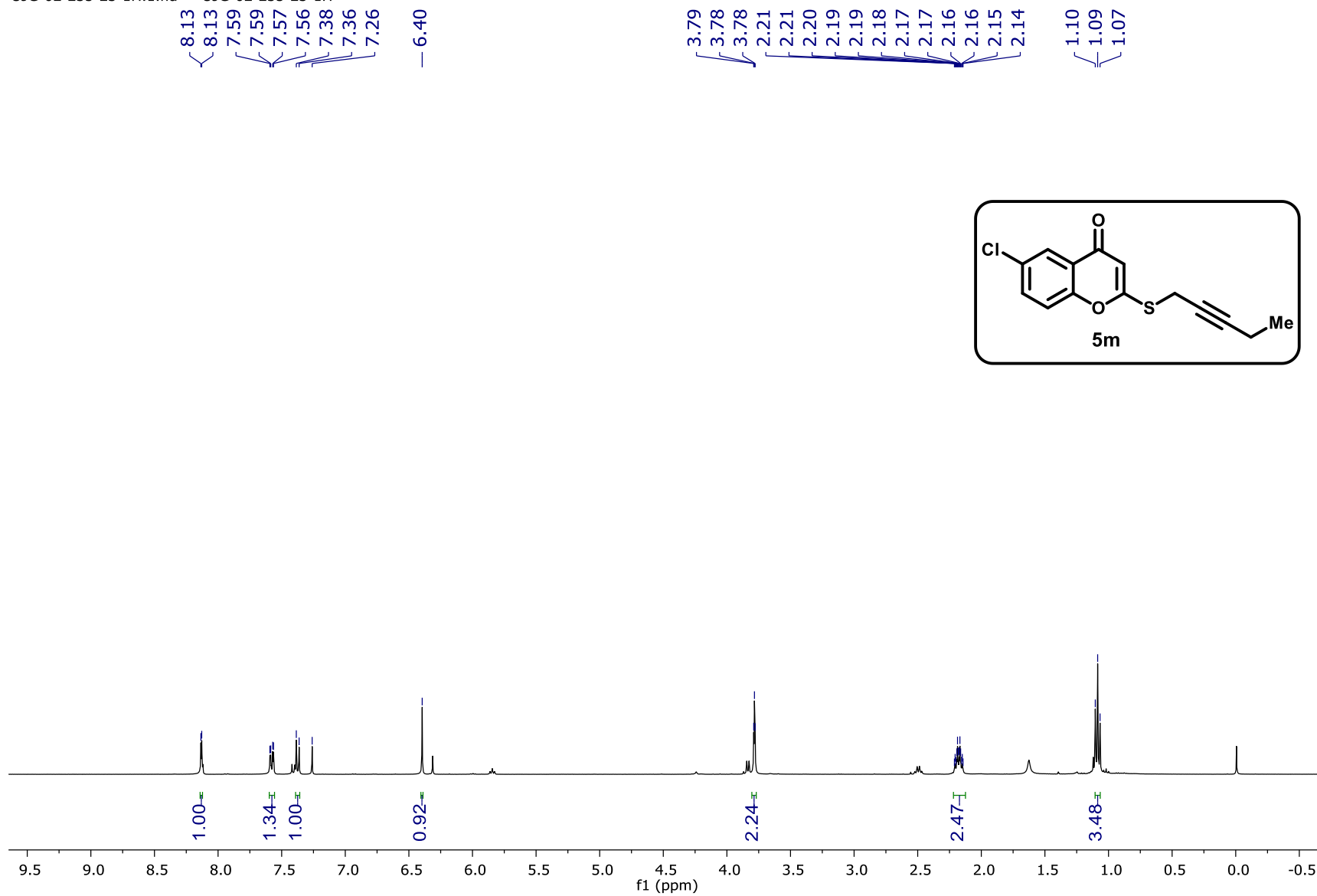


HRMS Spectrum of Compound 5l



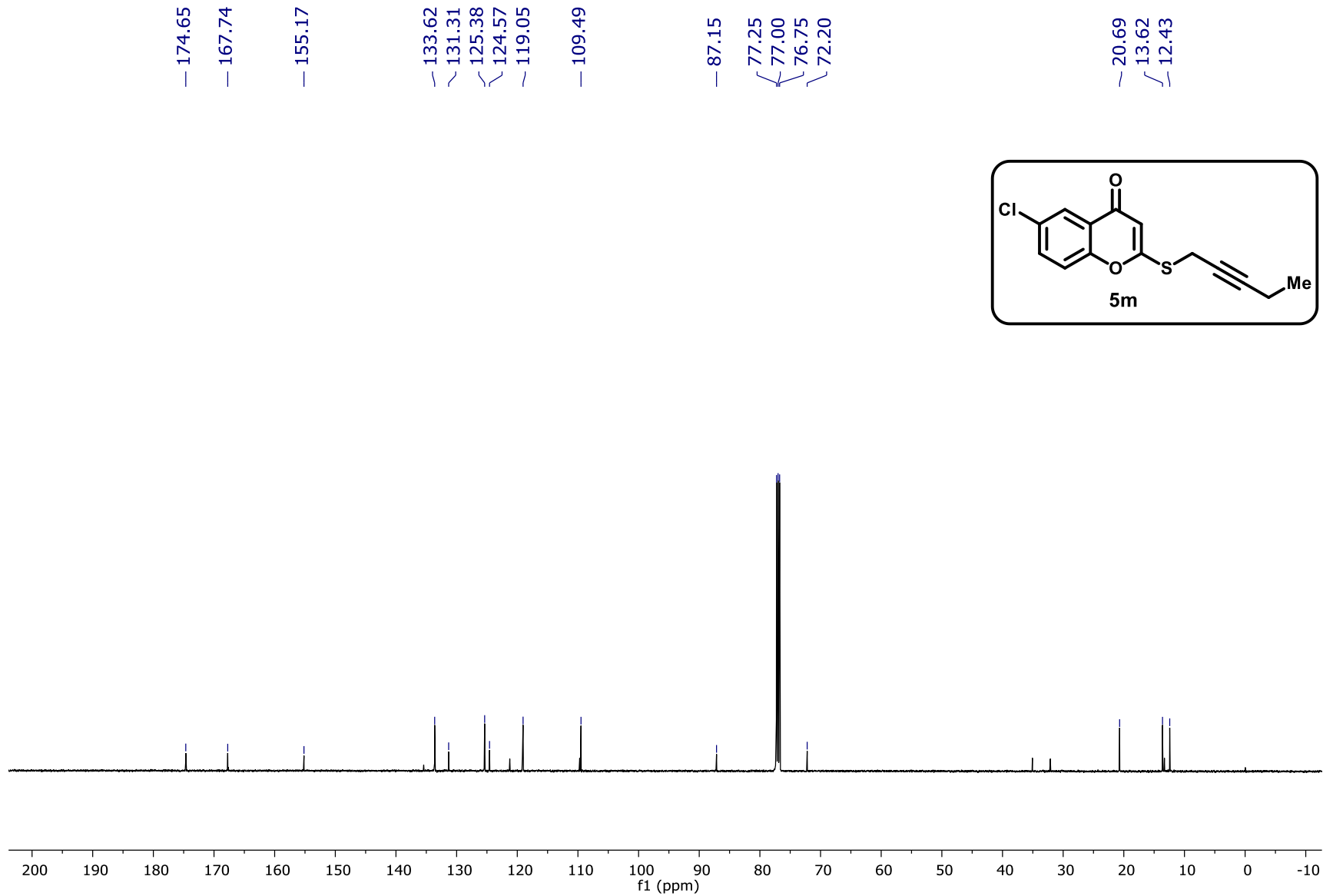
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5m

UJG-02-235-23-1H.1.fid — UJG-02-235-23-1H

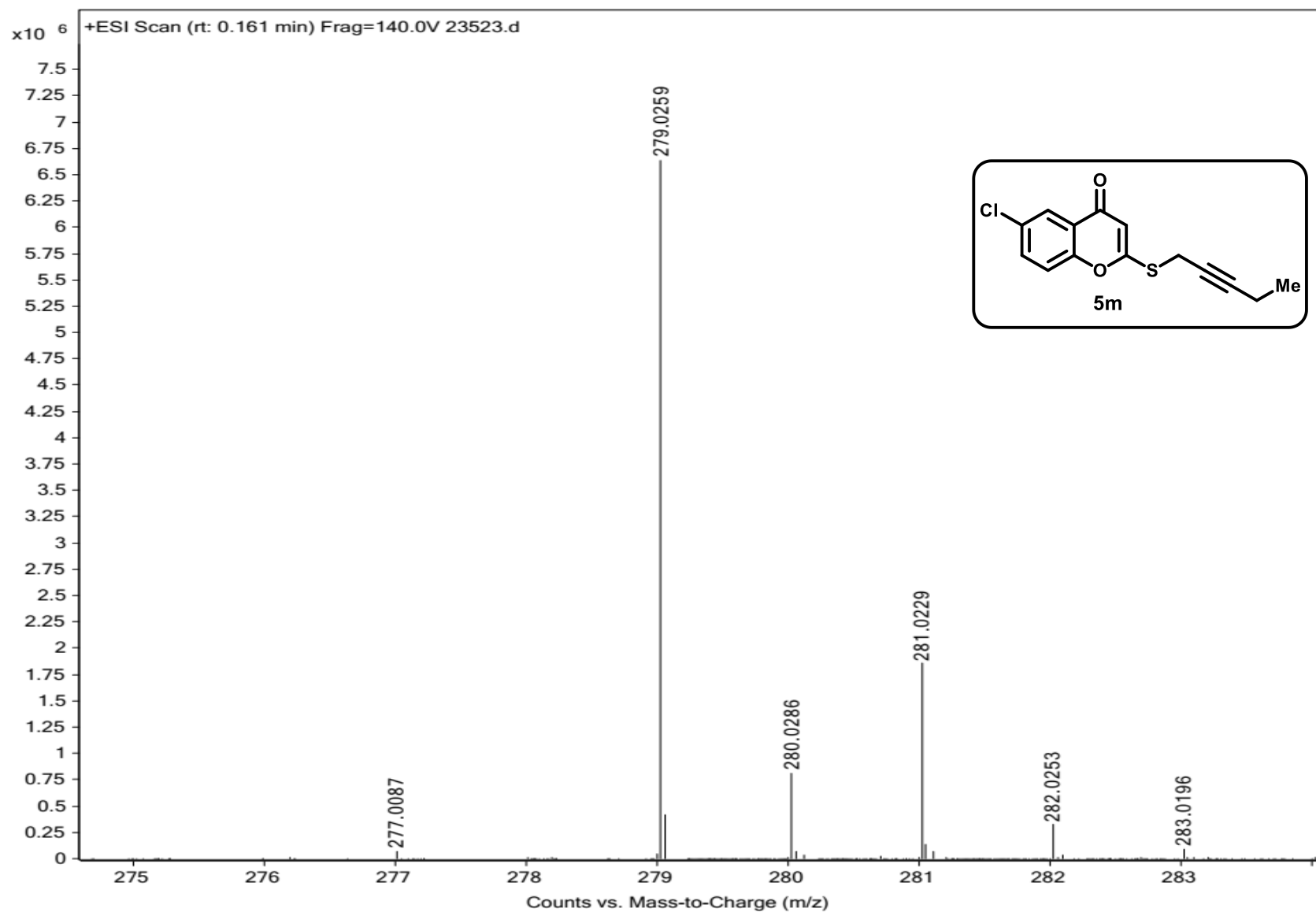


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5m

UJG-02-235-23-13C.1.fid — UJG-02-235-23-13C

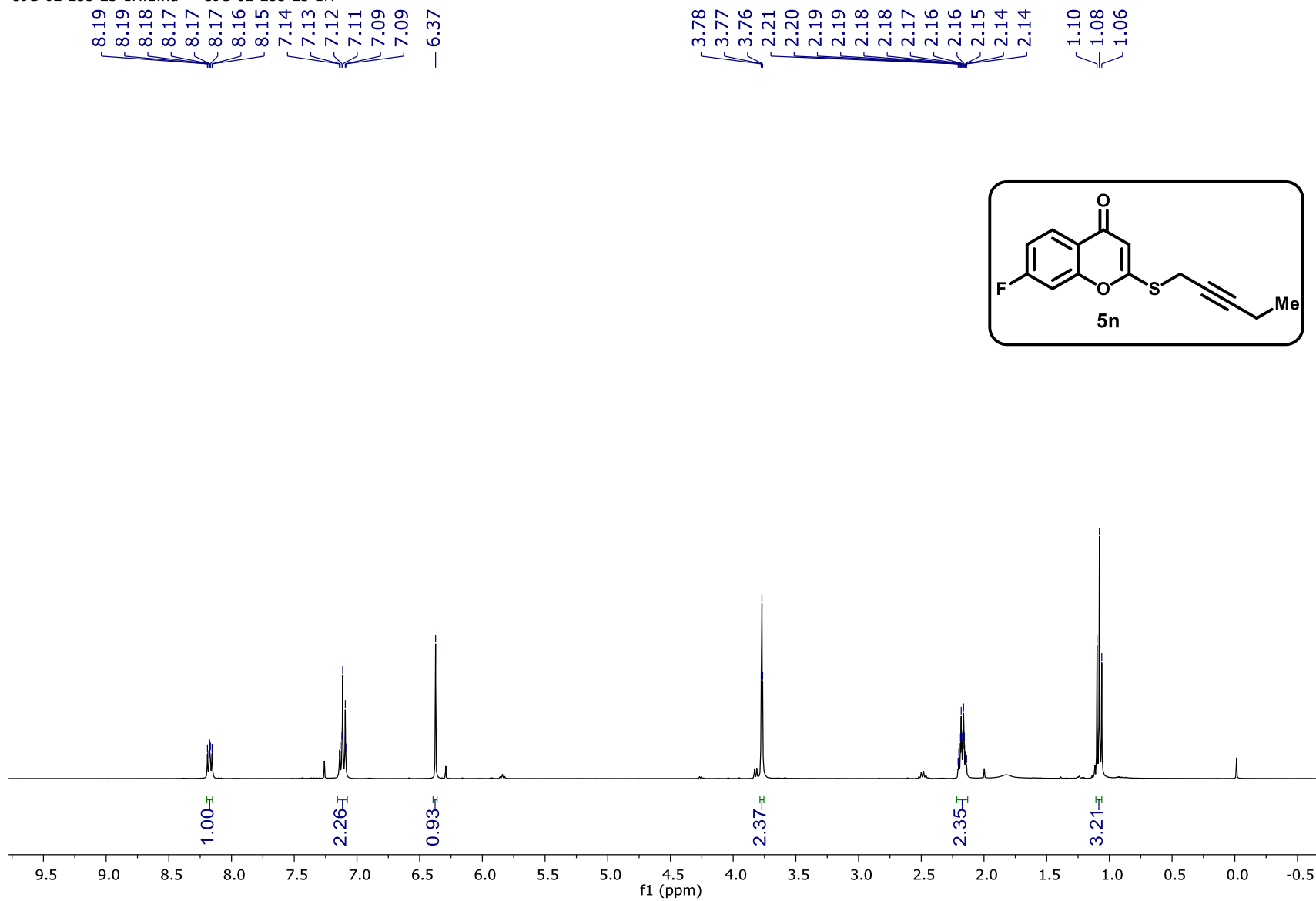


HRMS Spectrum of Compound 5m



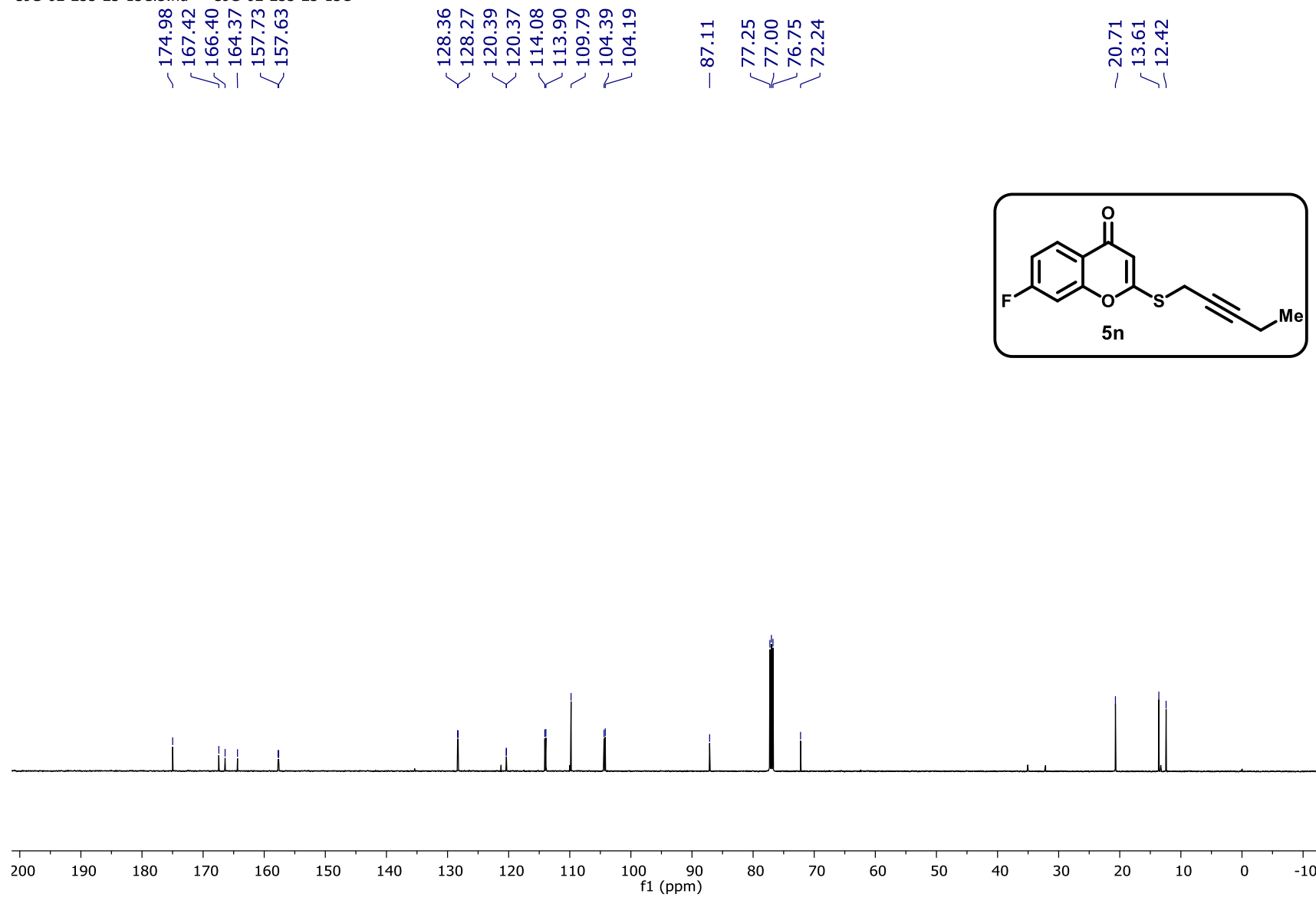
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 5n

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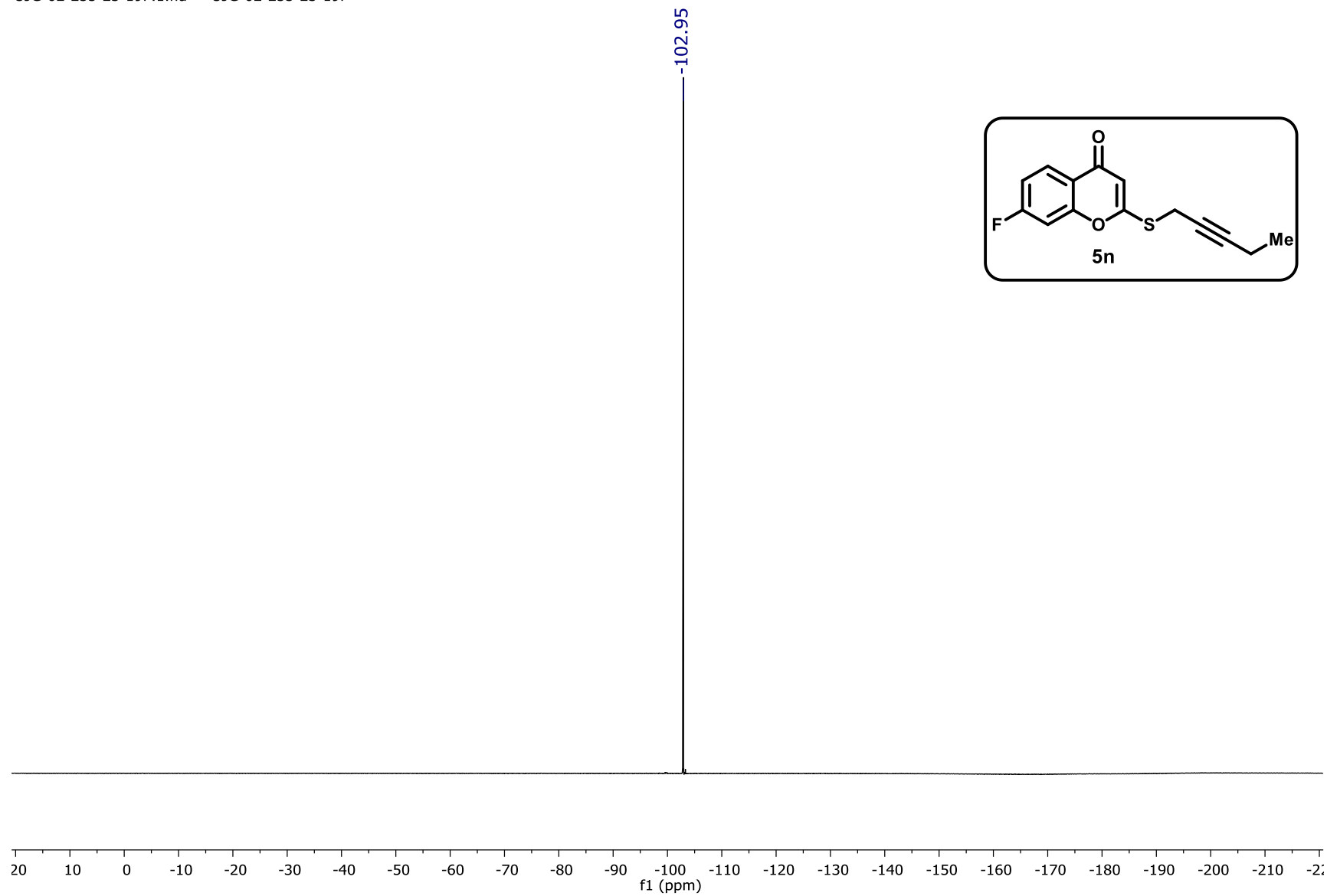
^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 5n

UJG-02-255-23-13C.3.fid — UJG-02-255-23-13C



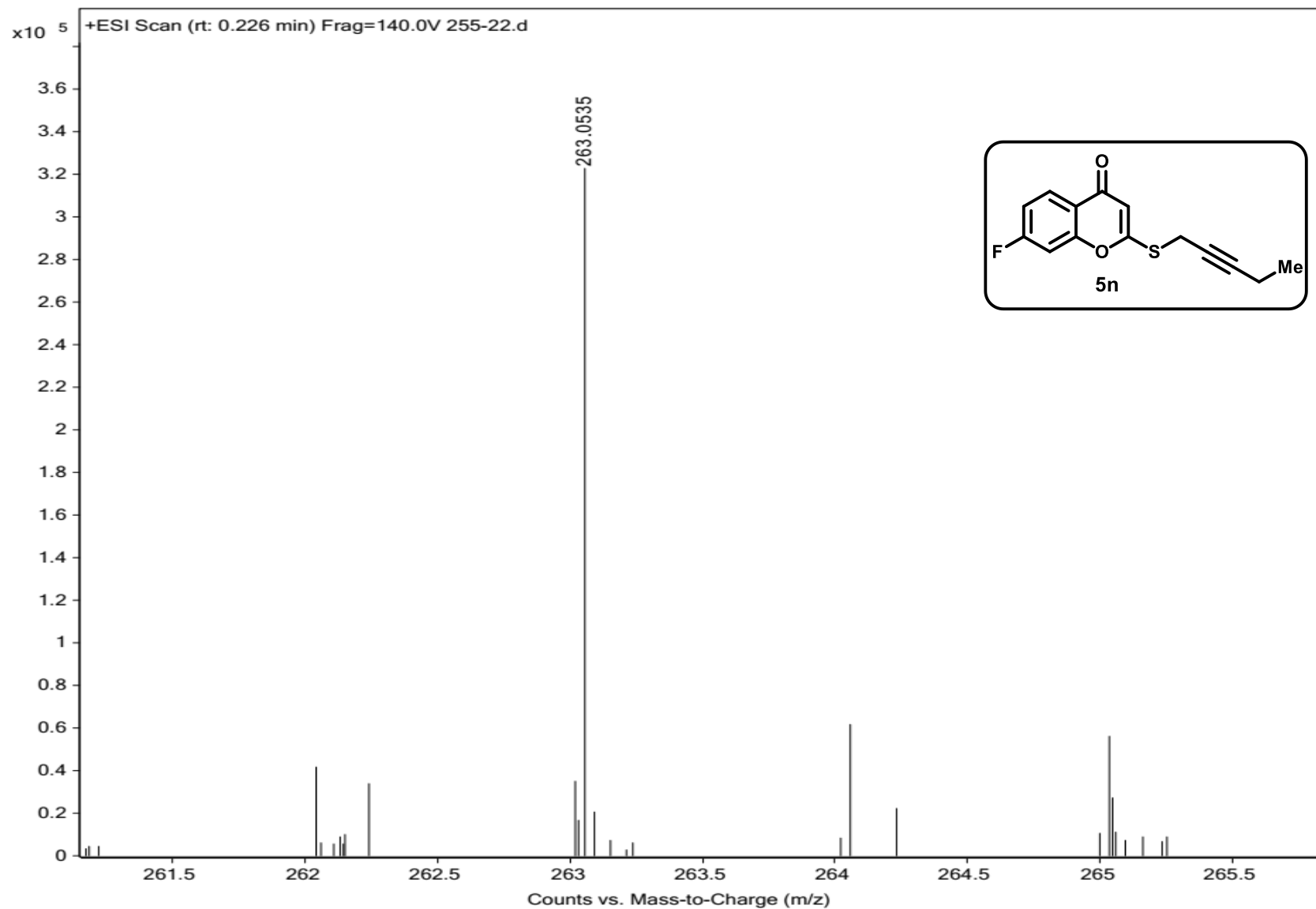
^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 5n

UJG-02-255-23-19F.1.fid — UJG-02-255-23-19F



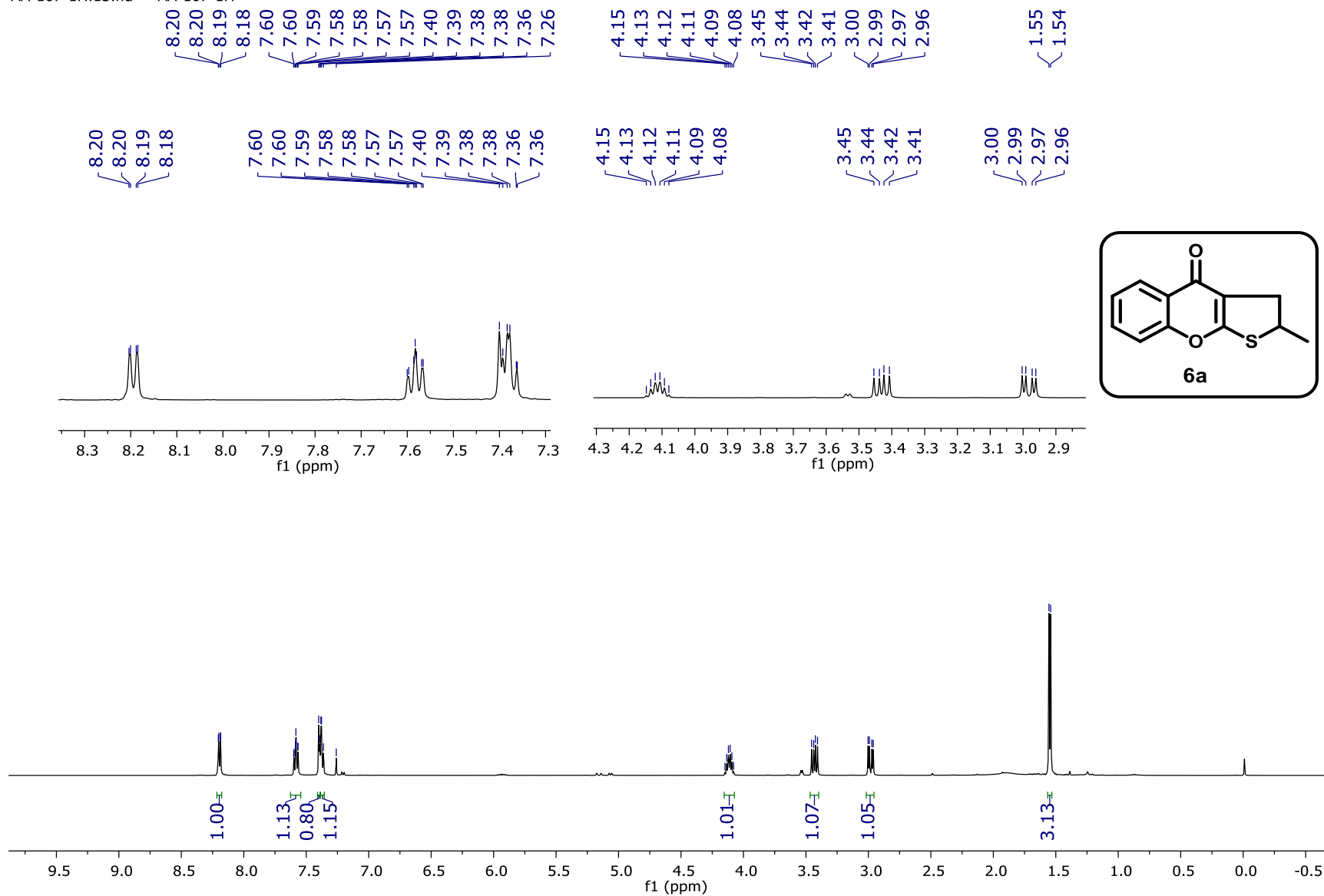
S103

HRMS Spectrum of Compound 5n



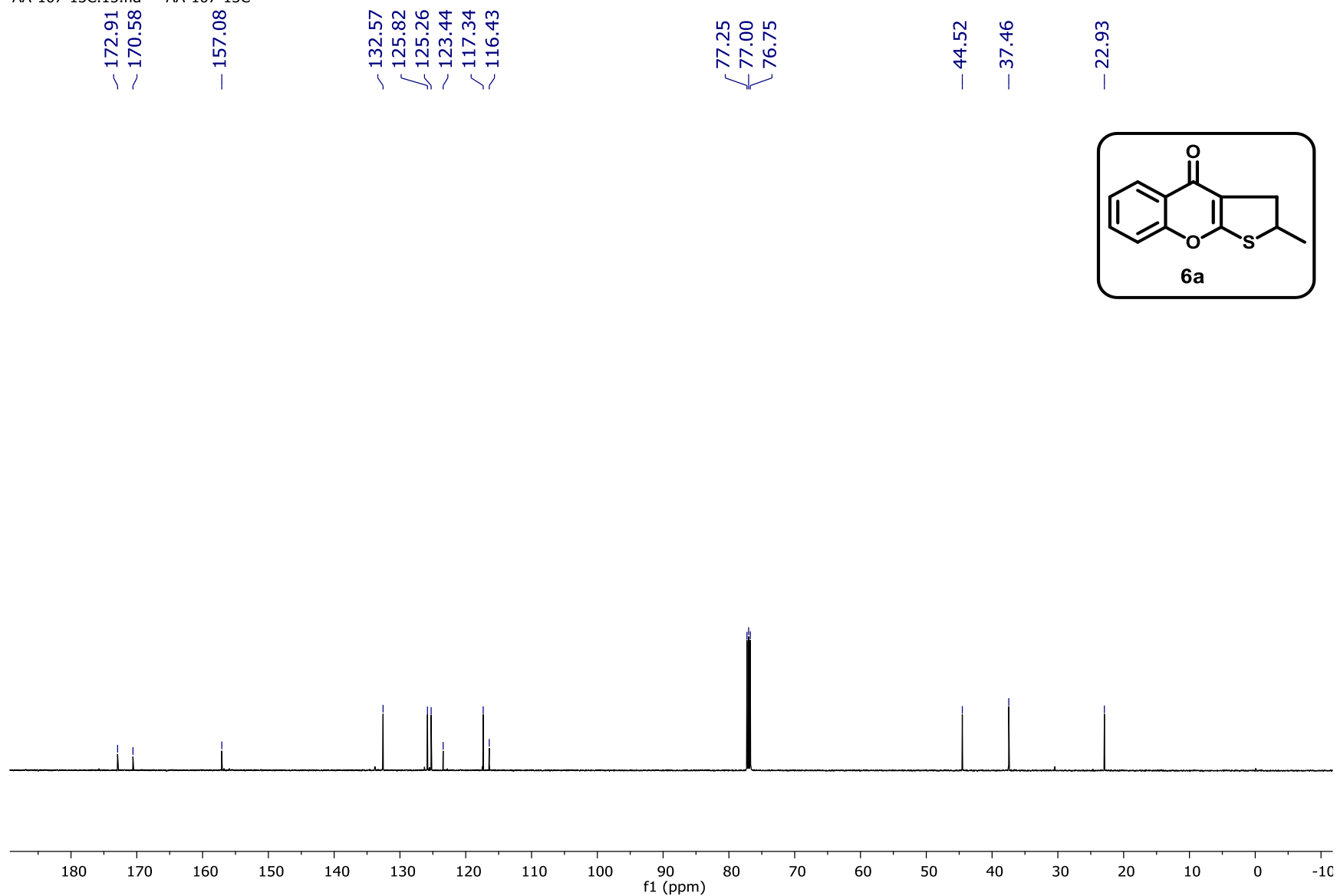
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 6a

AA-107-1H.13.fid — AA-107-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6a

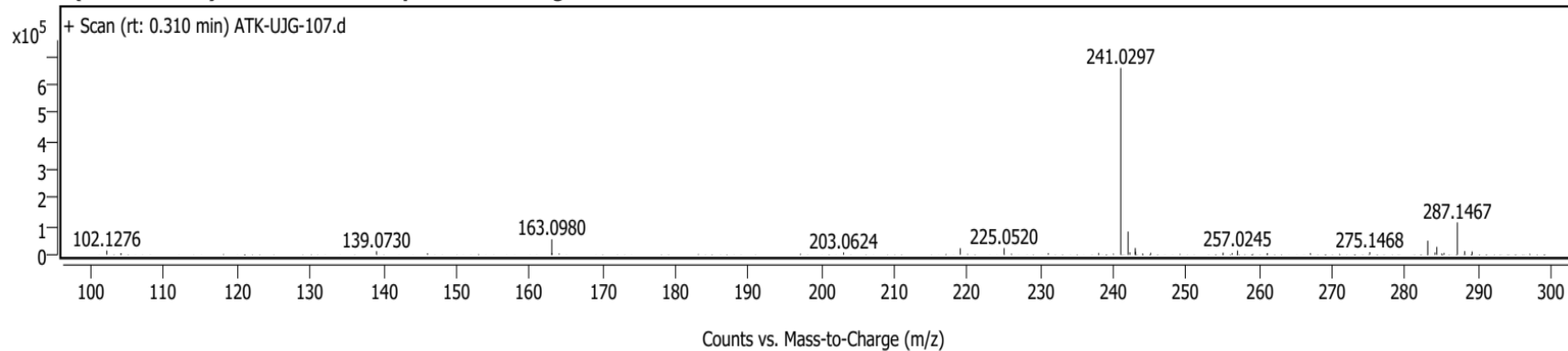
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HRMS Spectrum of Compound 6a

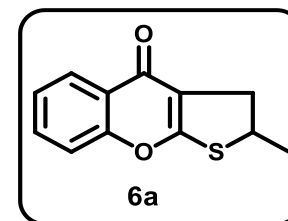
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SpectrumIdString



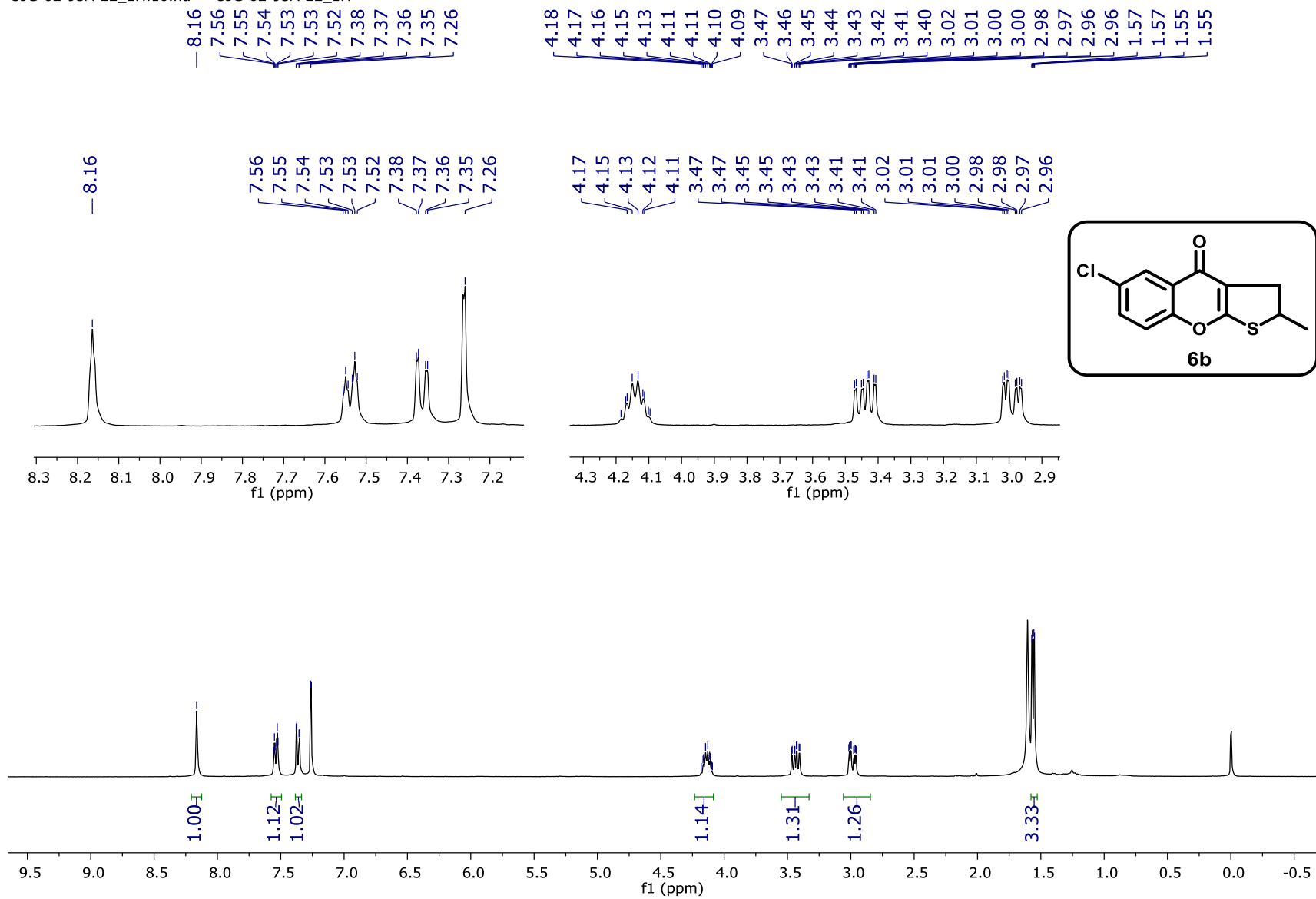
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219.0478		23084	3.50					
225.0520		23583	3.57					
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243.0260		23727	3.60					
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257.0245		14963	2.27					
275.1468		9199	1.39					
283.0859	1	49494	7.50					
284.0892	1	7616	1.15					
284.3314		27725	4.20					
287.1467	1	114242	17.31					
288.1501	1	12669	1.92					
289.1618		11292	1.71					



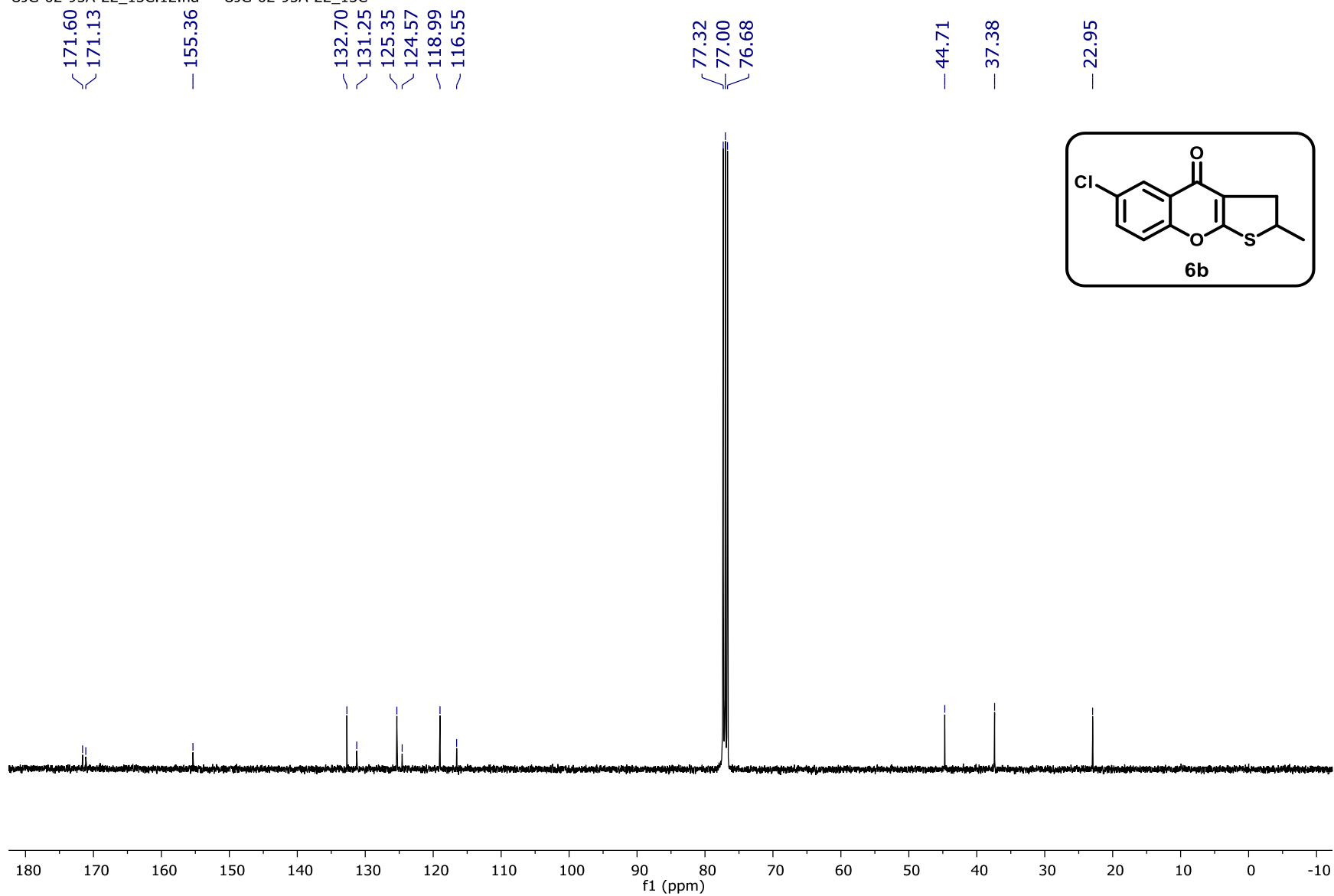
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 6b

UJG-02-95A-22_1H.10.fid — UJG-02-95A-22_1H

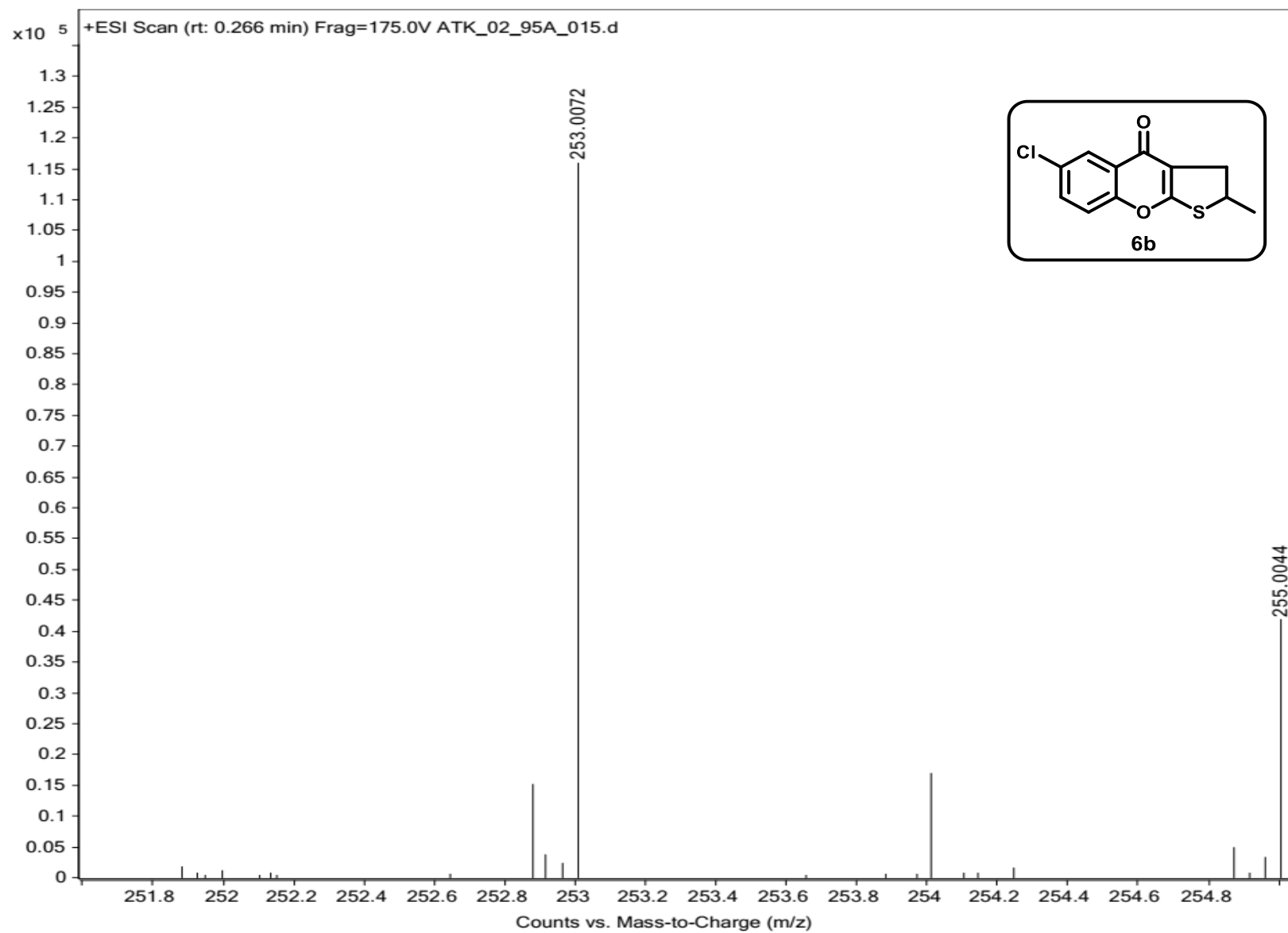


¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of Compound 6b

UJG-02-95A-22_13C.12.fid — UJG-02-95A-22_13C

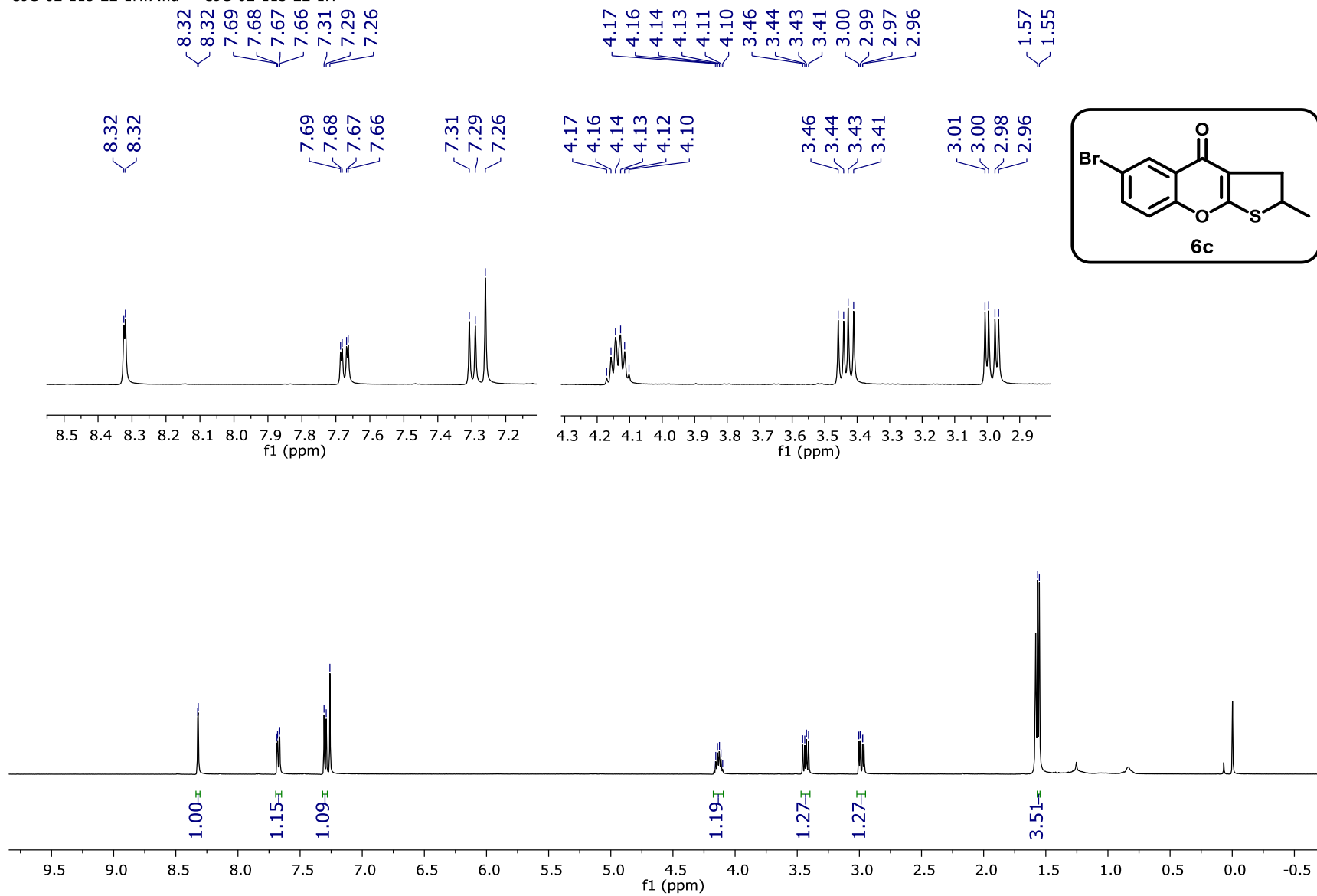


HRMS Spectrum of Compound 6b



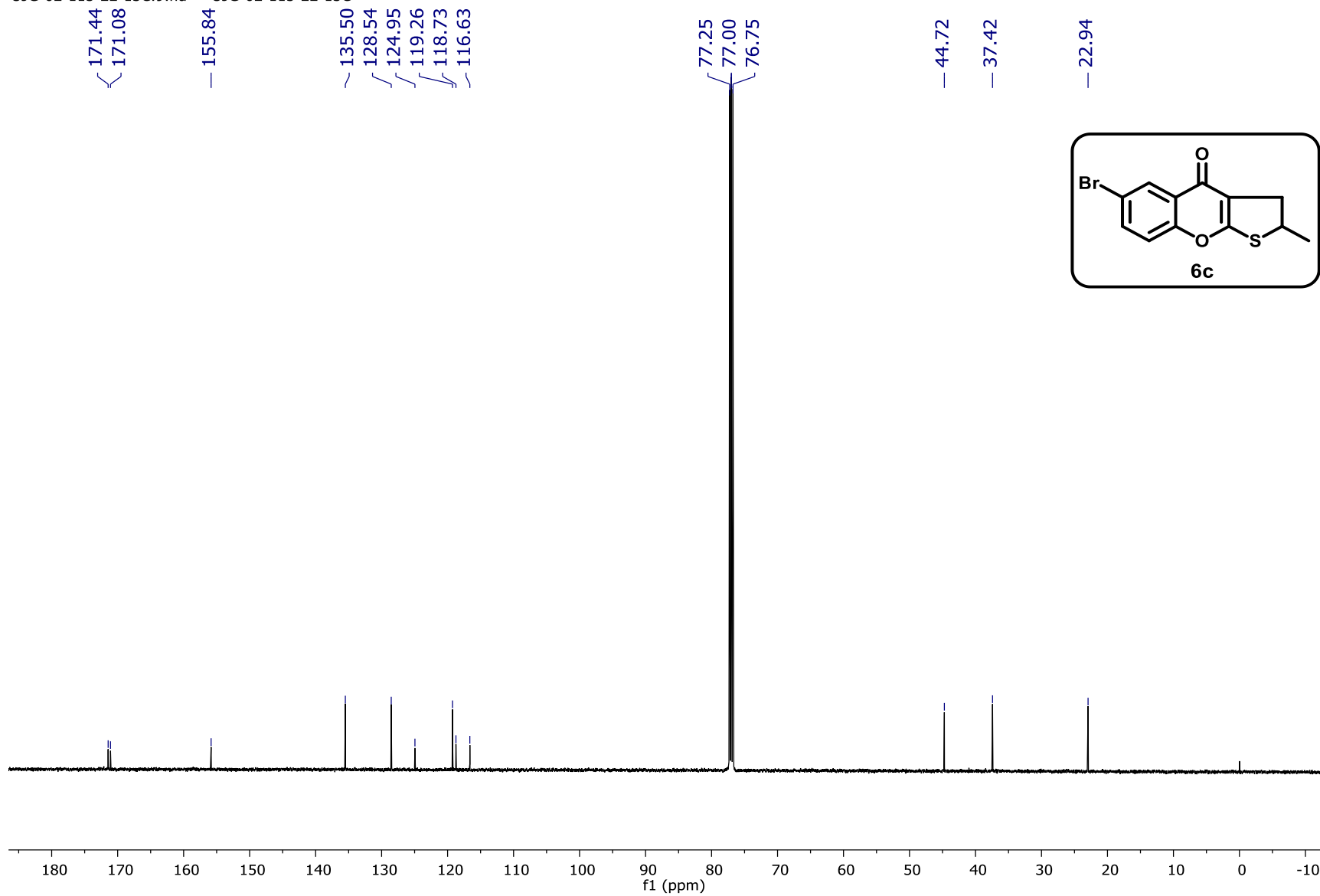
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 6c

UJG-02-115-22-1H.7.fid — UJG-02-115-22-1H

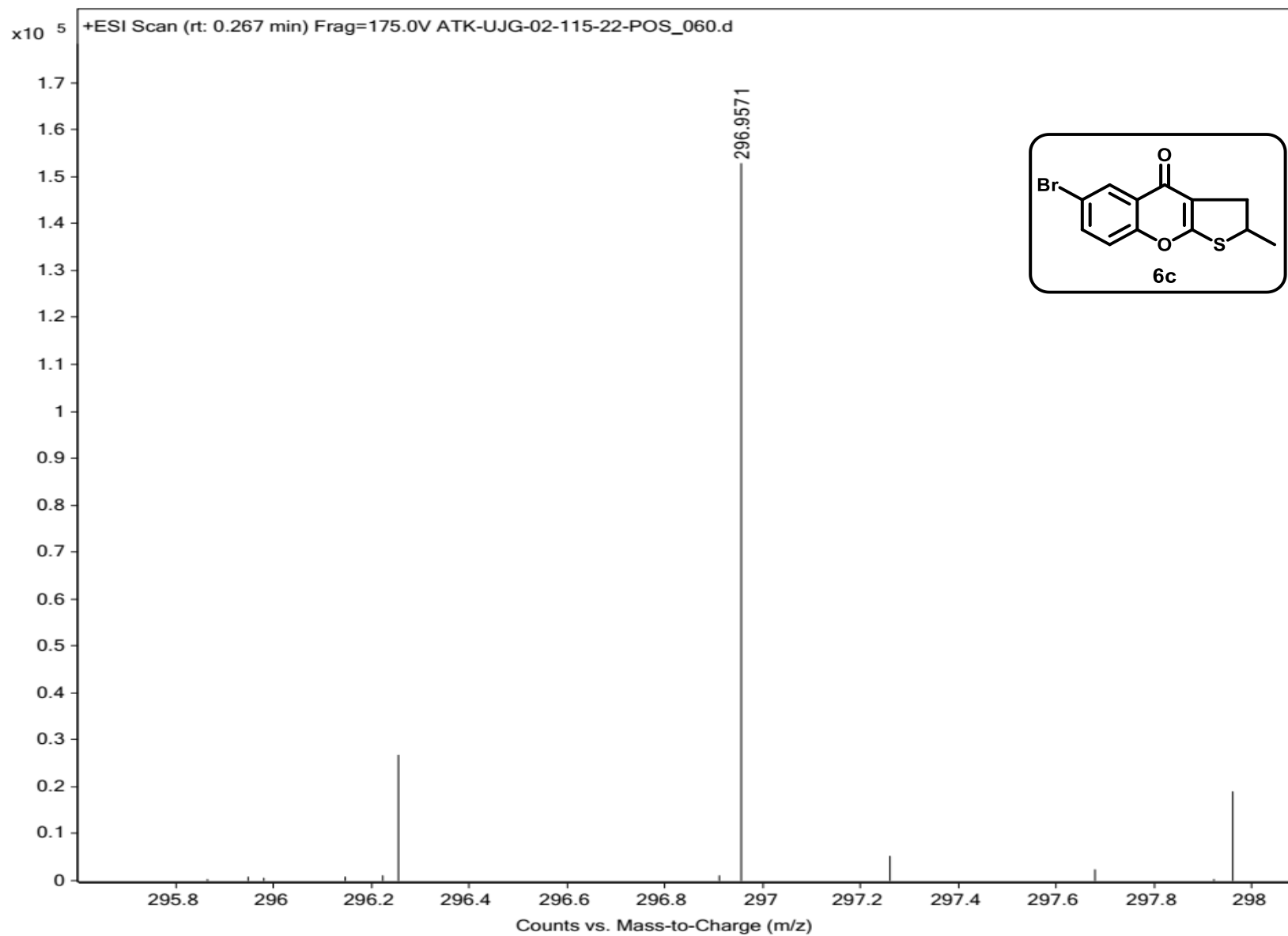


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6c

UJG-02-115-22-13C.9.fid — UJG-02-115-22-13C

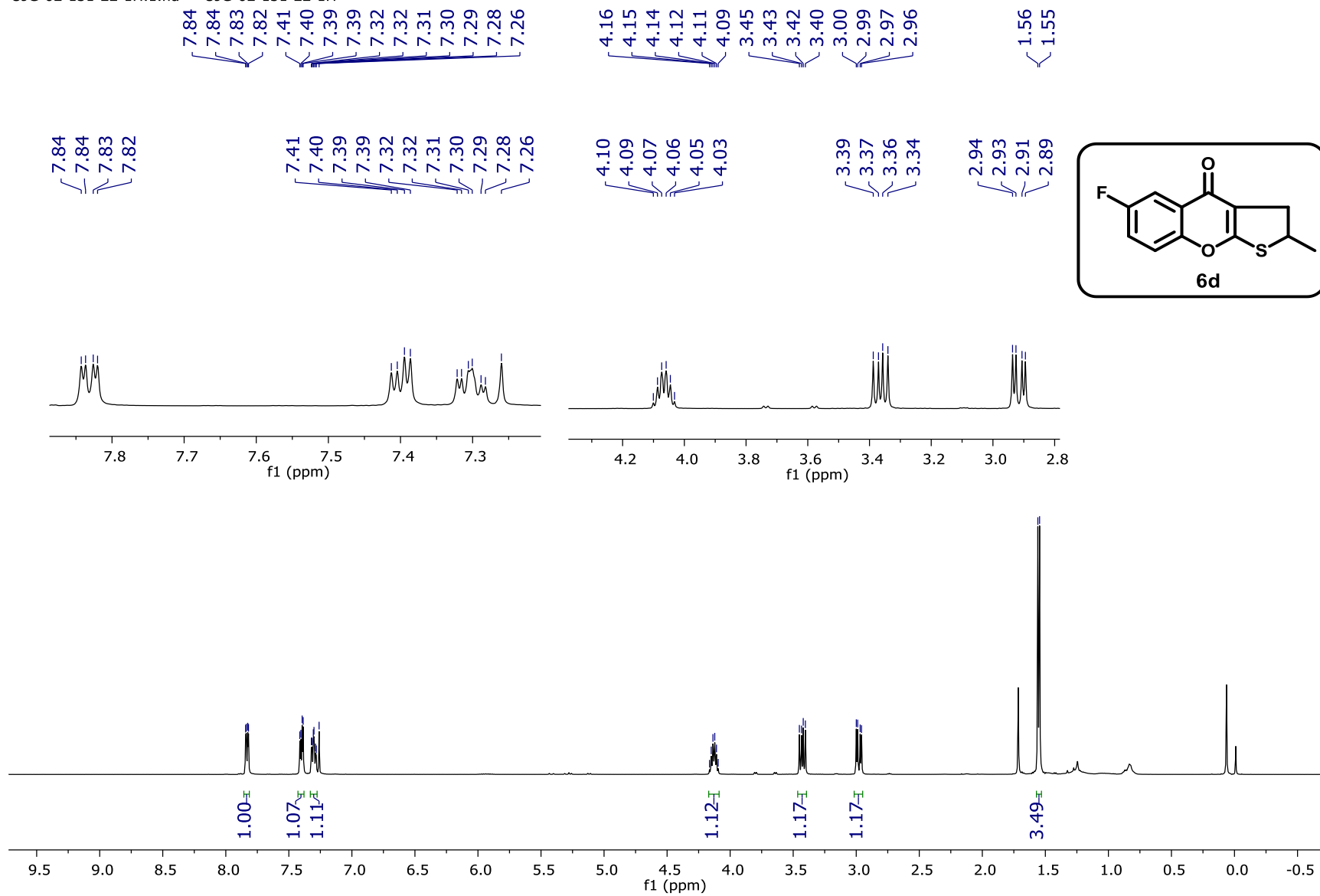


HRMS Spectrum of Compound 6c

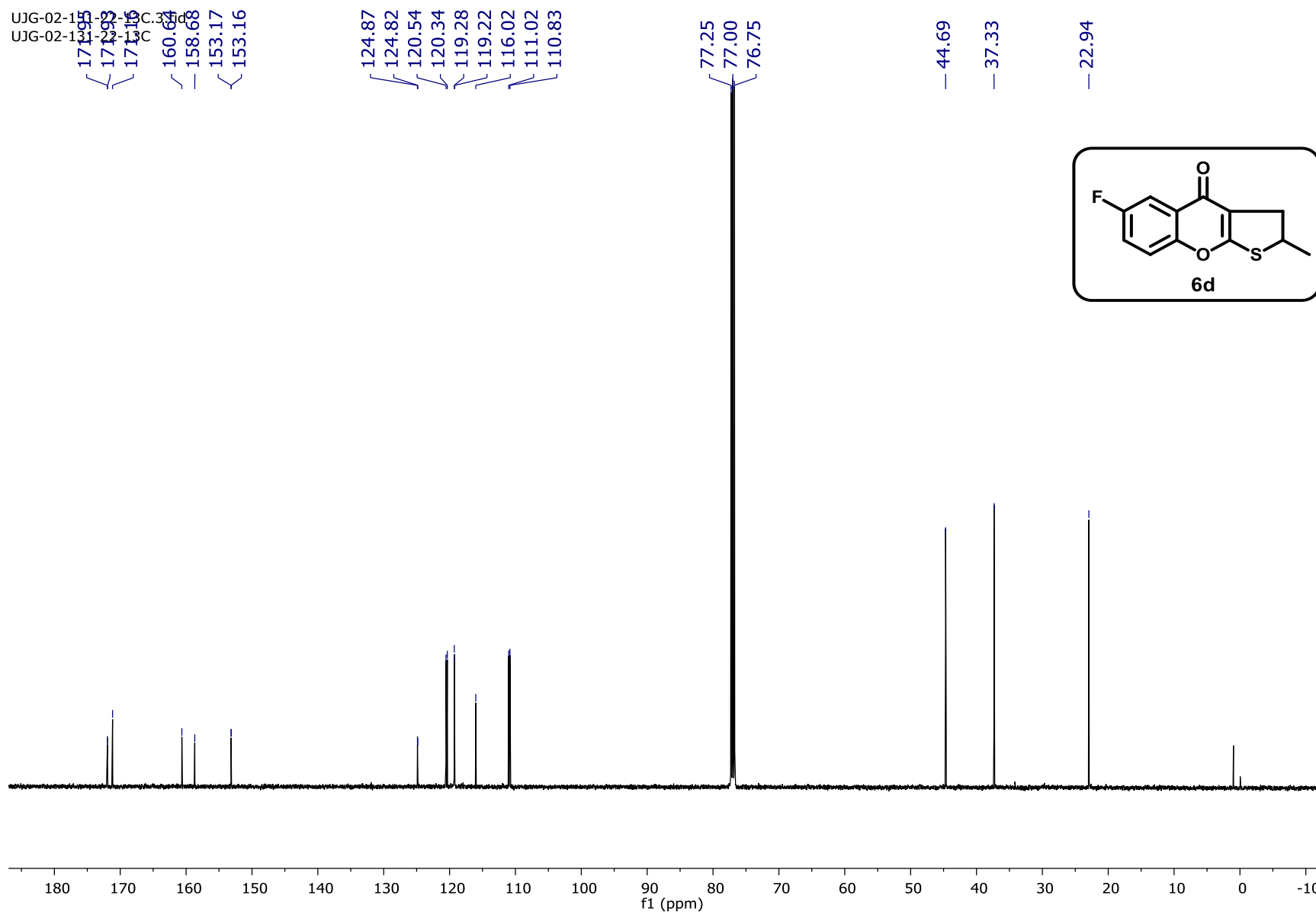


¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 6d

UJG-02-131-22-1H.1.fid — UJG-02-131-22-1H

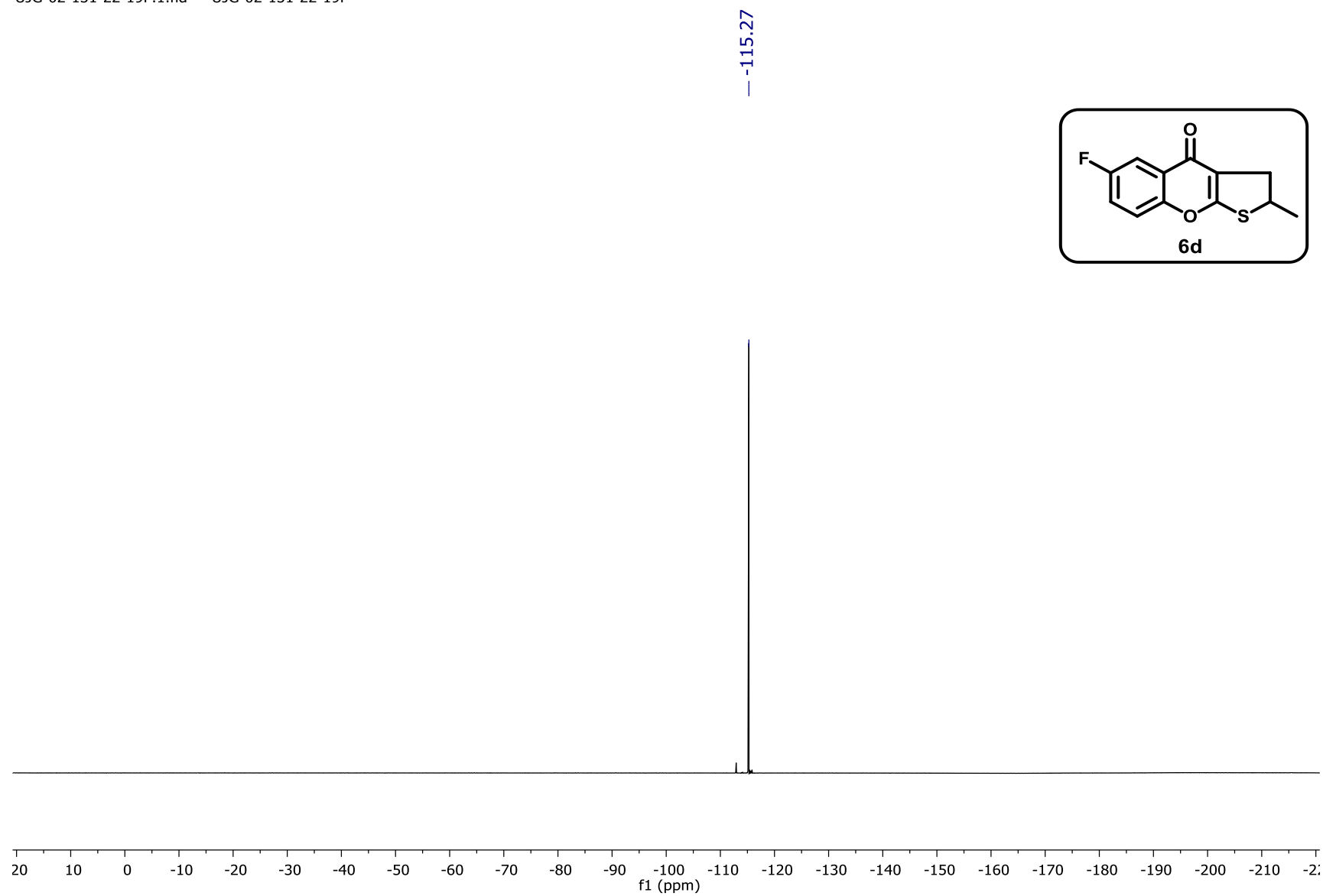


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6d



^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 6d

UJG-02-131-22-19F.1.fid — UJG-02-131-22-19F

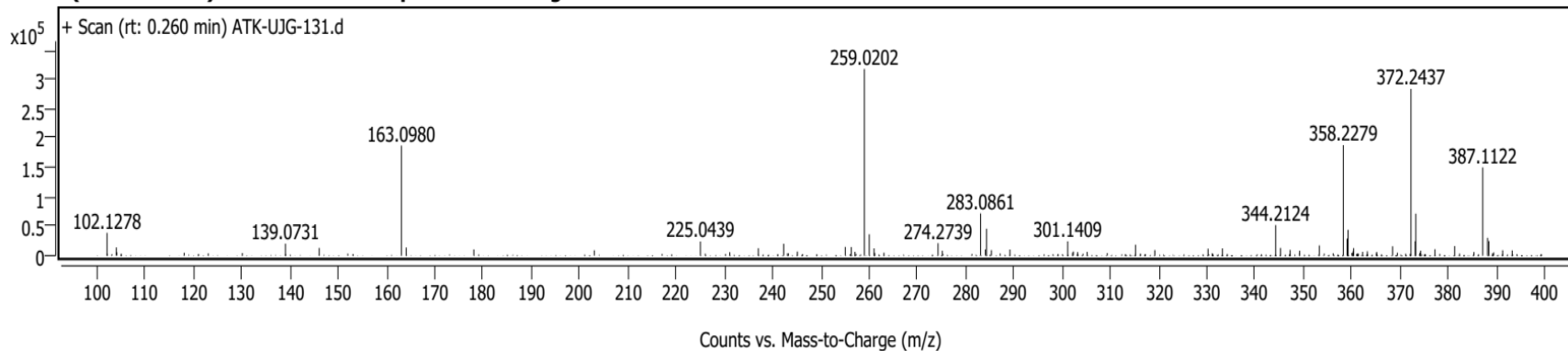


S116

HRMS Spectrum of Compound 6d

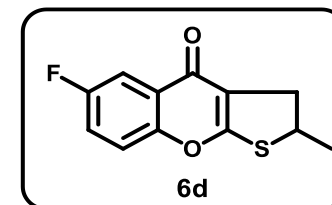
+ Scan (rt: 0.260 min)

SpectrumIdString



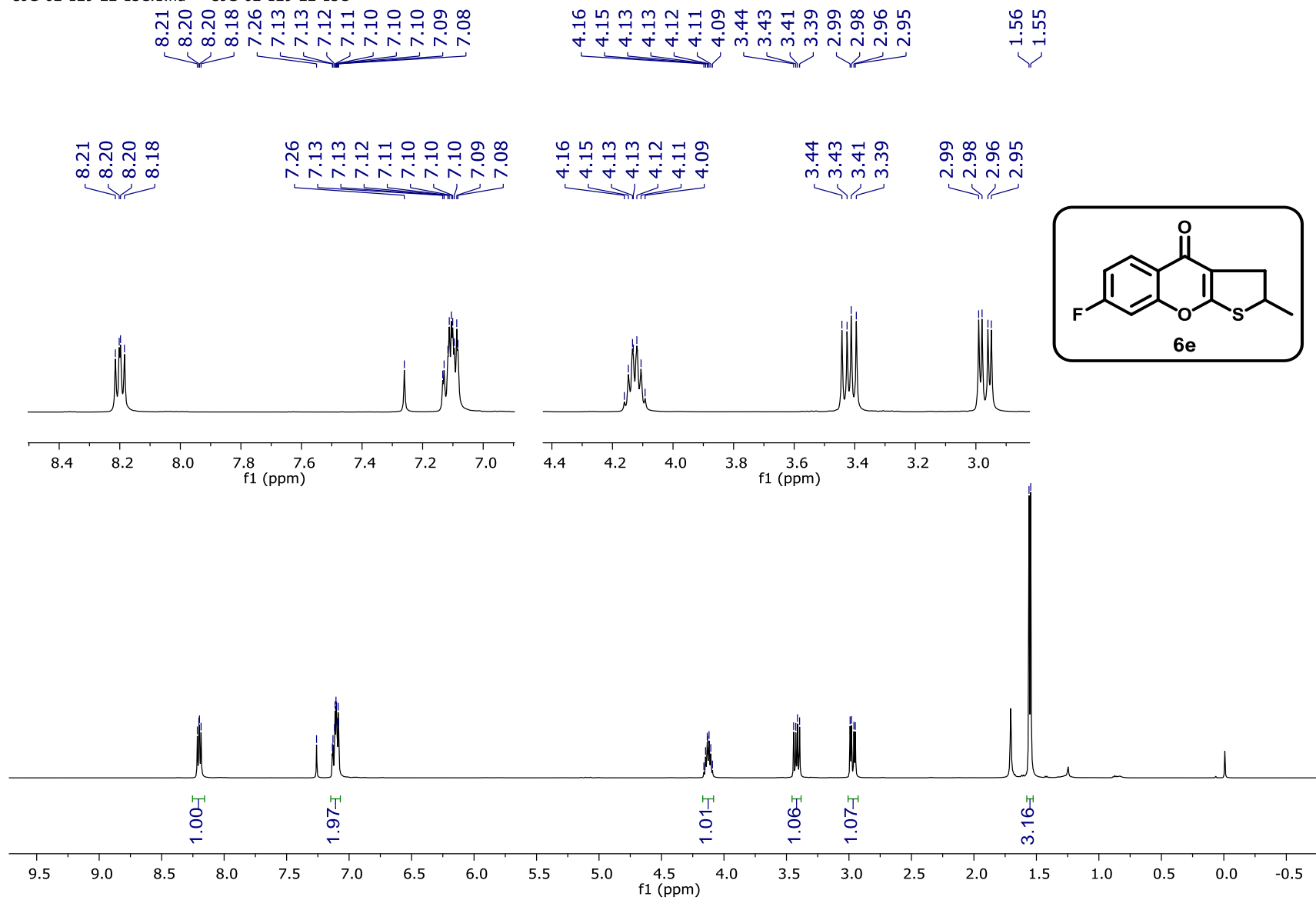
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139.0731		20424	6.43				
163.0980		187074	58.92				
225.0439		23915	7.53				
259.0202	1	317481	100.00				
260.0232	1	36337	11.45				
274.2739		21247	6.69				
283.0861		71713	22.59				
284.3312		45855	14.44				
301.1409		24259	7.64				
344.2124		52031	16.39				
358.2279	1	187856	59.17				
359.0185		28960	9.12				
359.2313	1	43936	13.84				
372.2437	1	283463	89.28				
373.0966		24408	7.69				
373.2469	1	71276	22.45				
387.1122	1	149933	47.23				
388.1156	1	30350	9.56				
388.3939		24809	7.81				



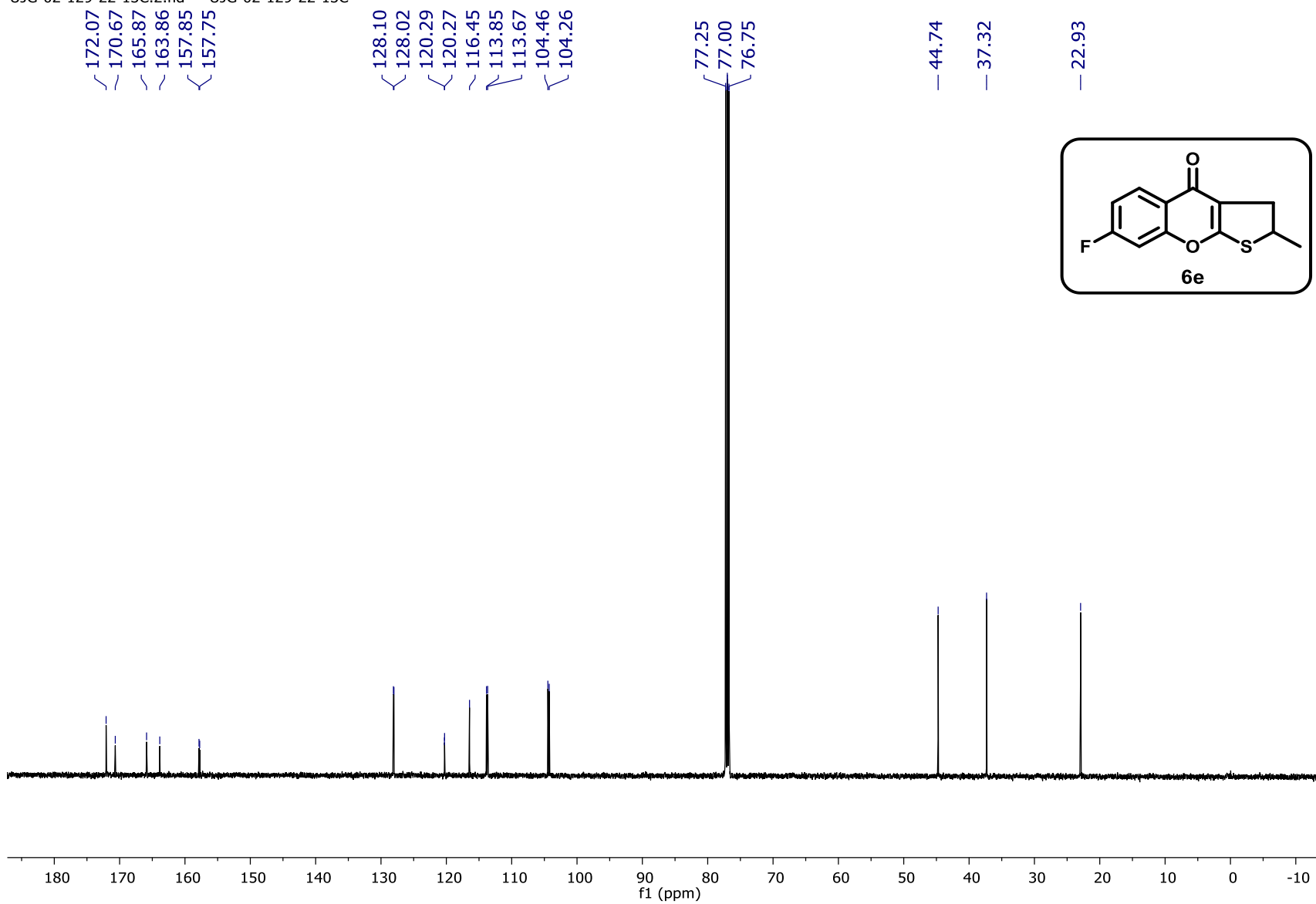
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 6e

UJG-02-129-22-13C.1.fid — UJG-02-129-22-13C



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6e

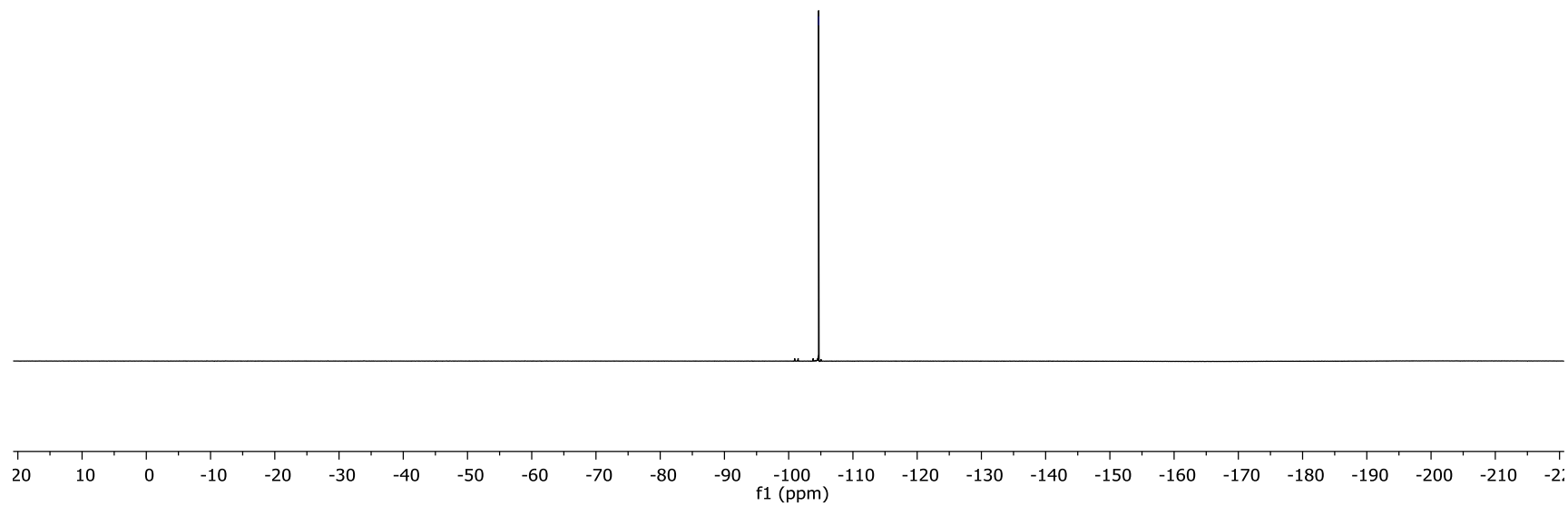
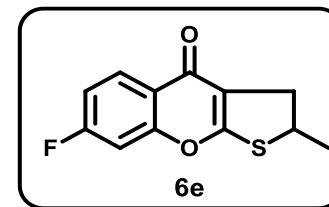
UJG-02-129-22-13C.2.fid — UJG-02-129-22-13C



^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 6e

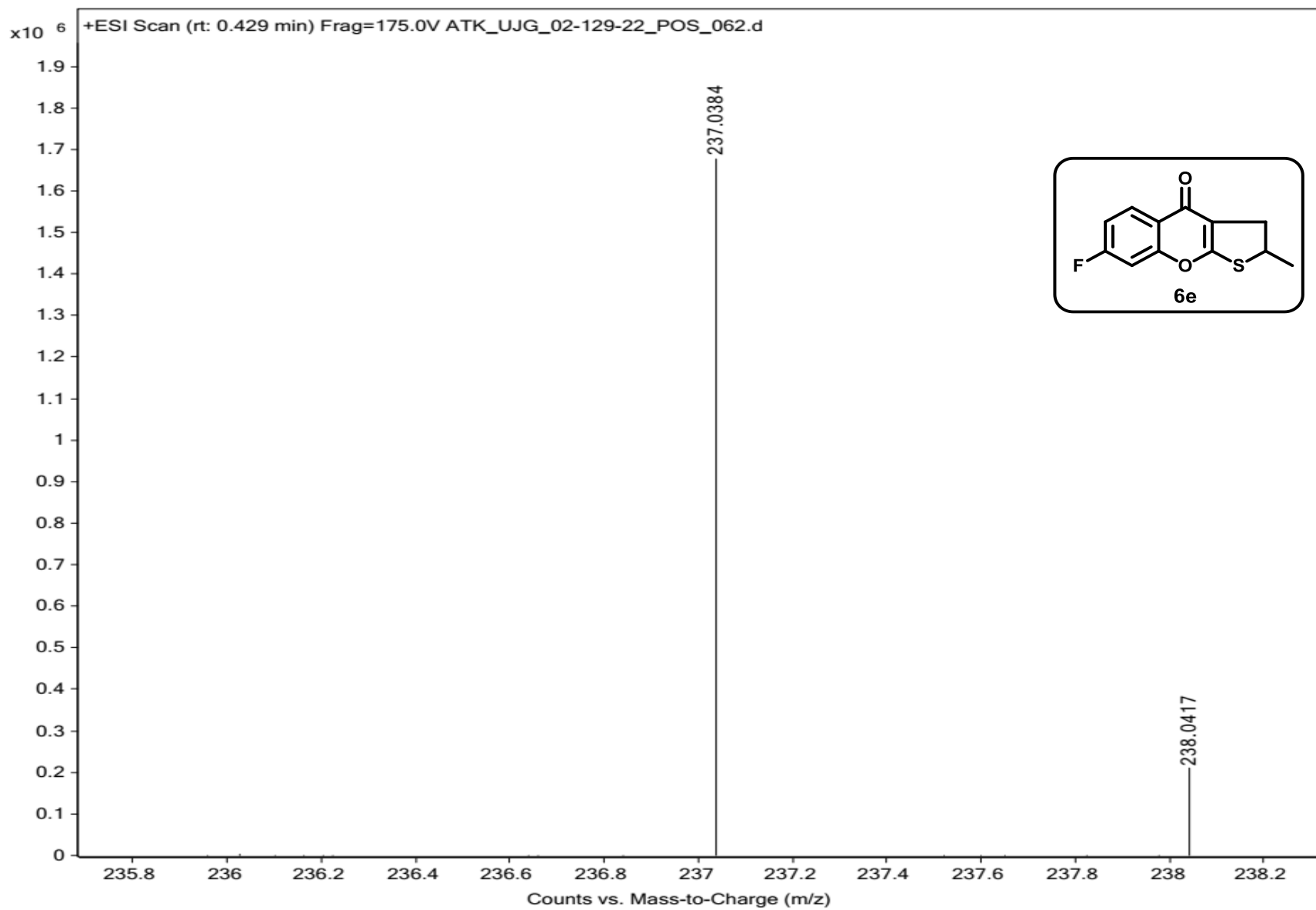
UJG-02-129-22-19F.1.fid — UJG-02-129-22-19F

— -104.66



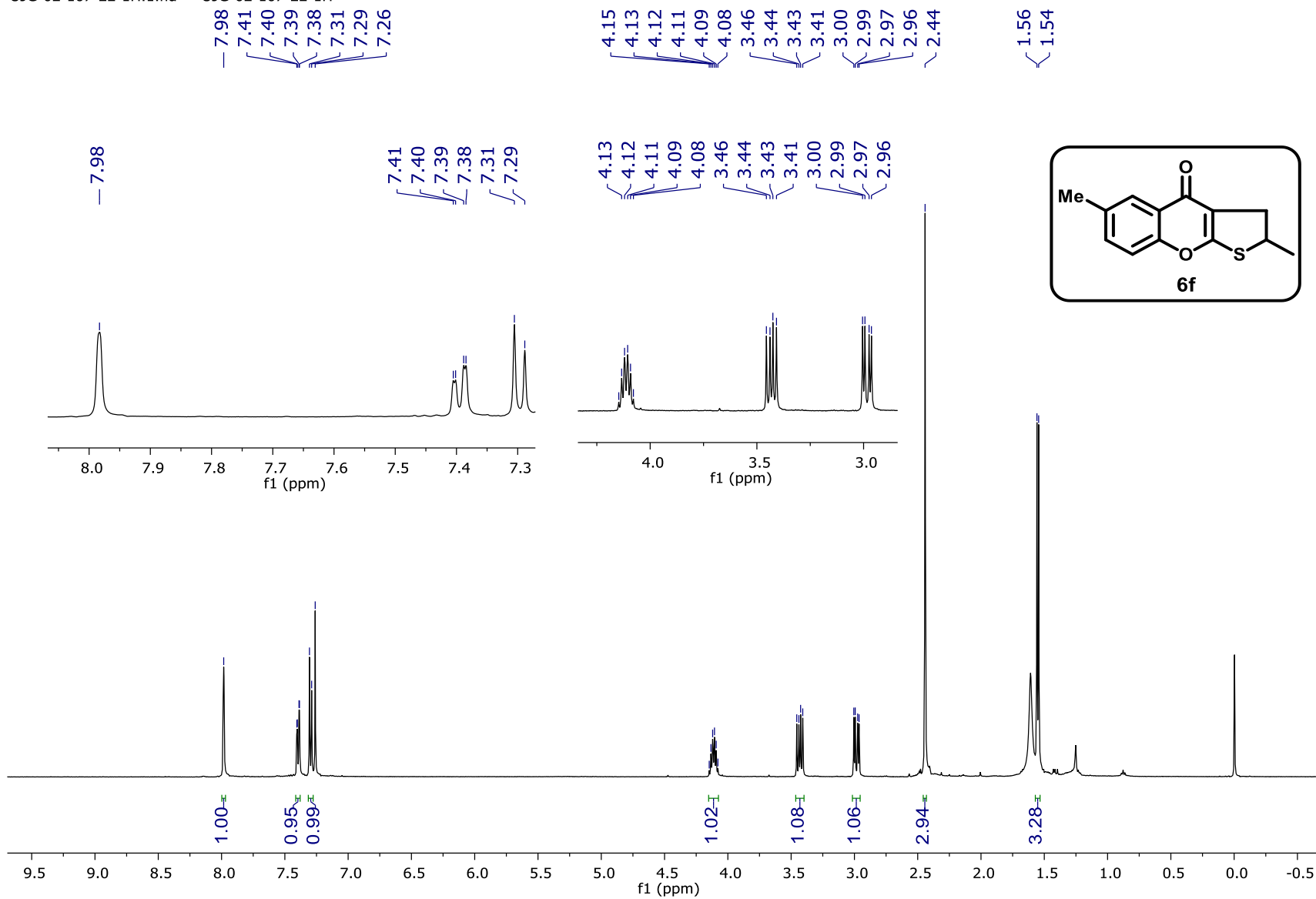
S120

HRMS Spectrum of Compound 6e



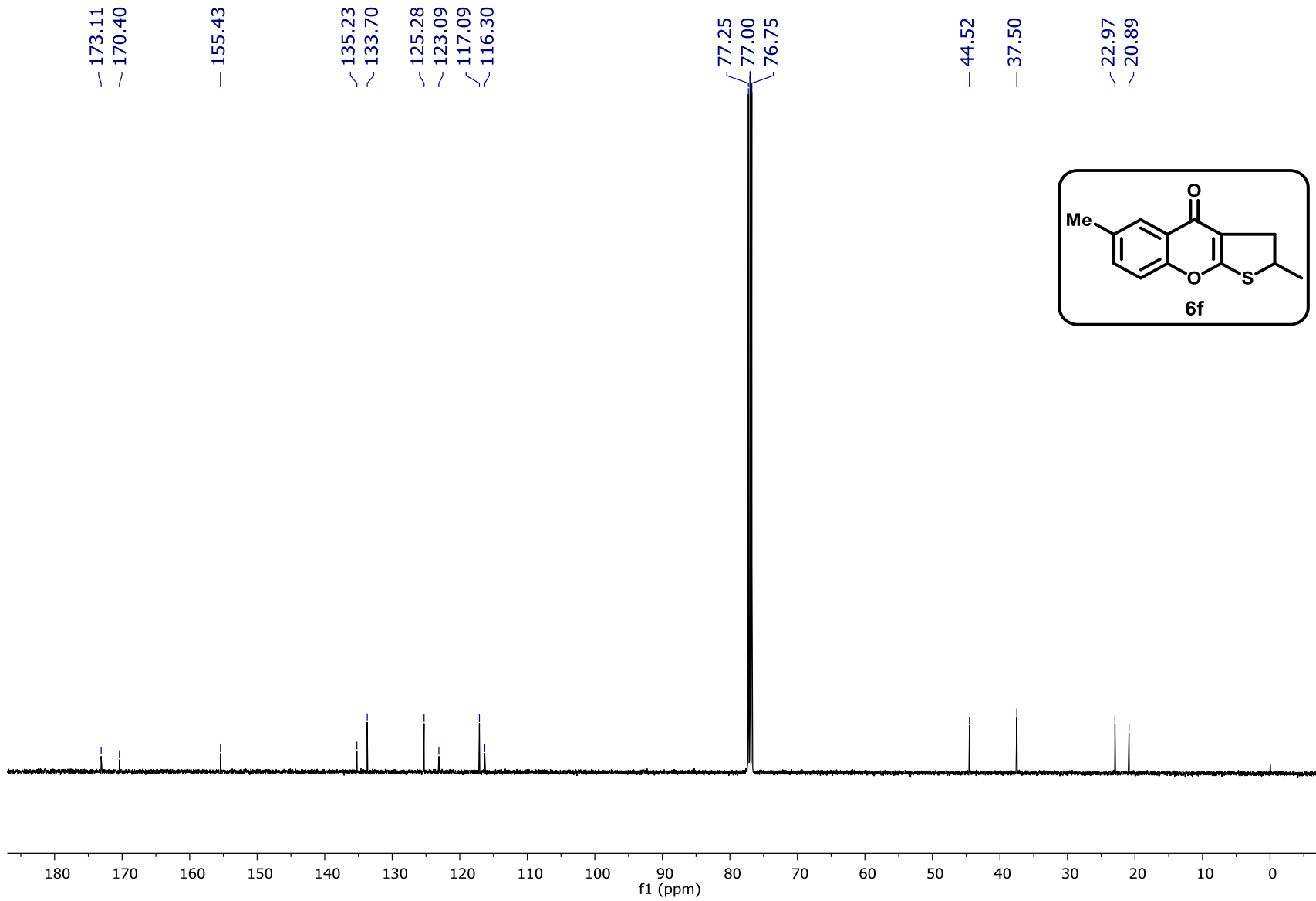
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 6f

UJG-02-167-22-1H.1.fid — UJG-02-167-22-1H

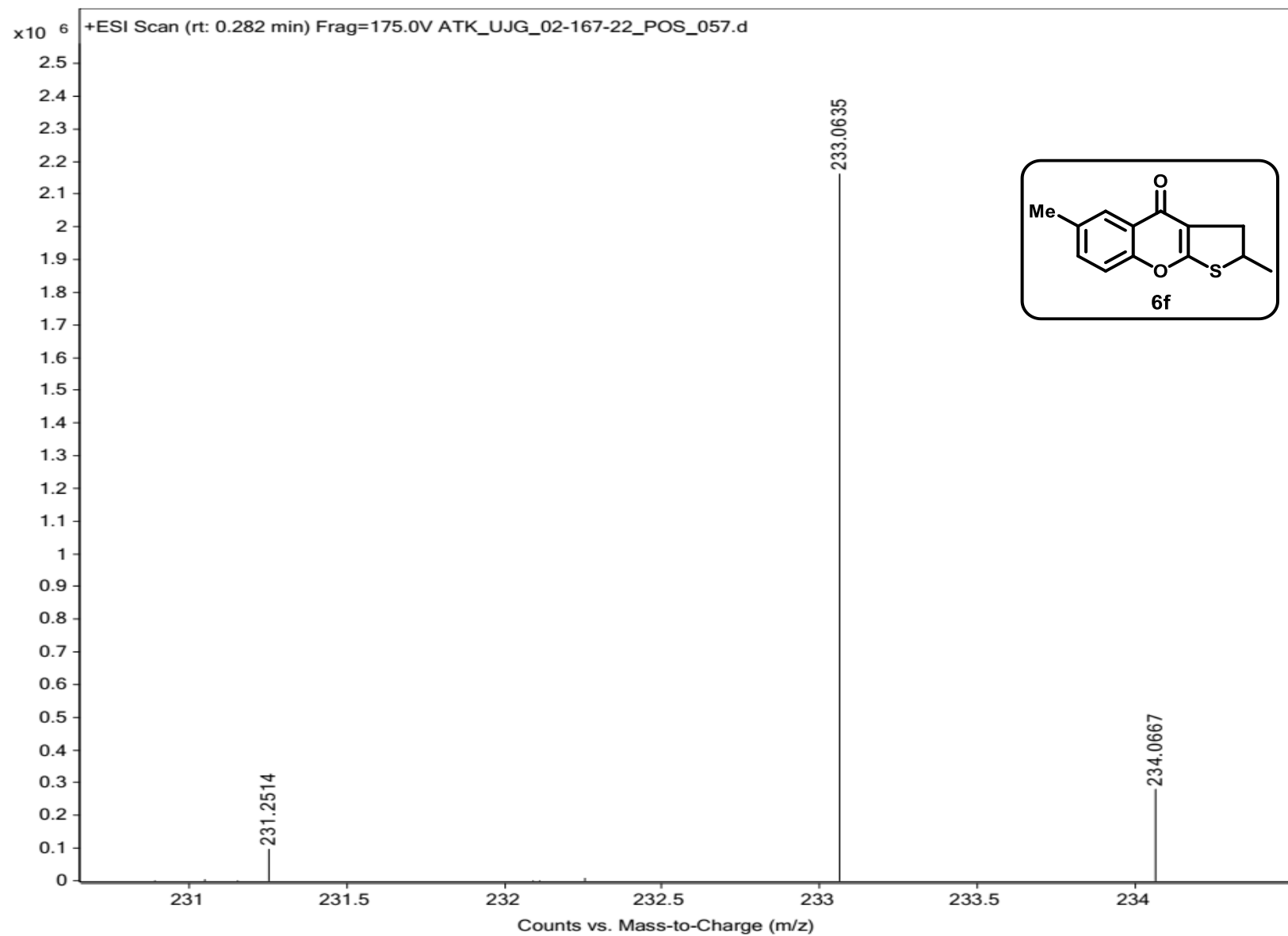


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 6f

UJG-02-167-22-13C.3.fid — UJG-02-167-22-13C

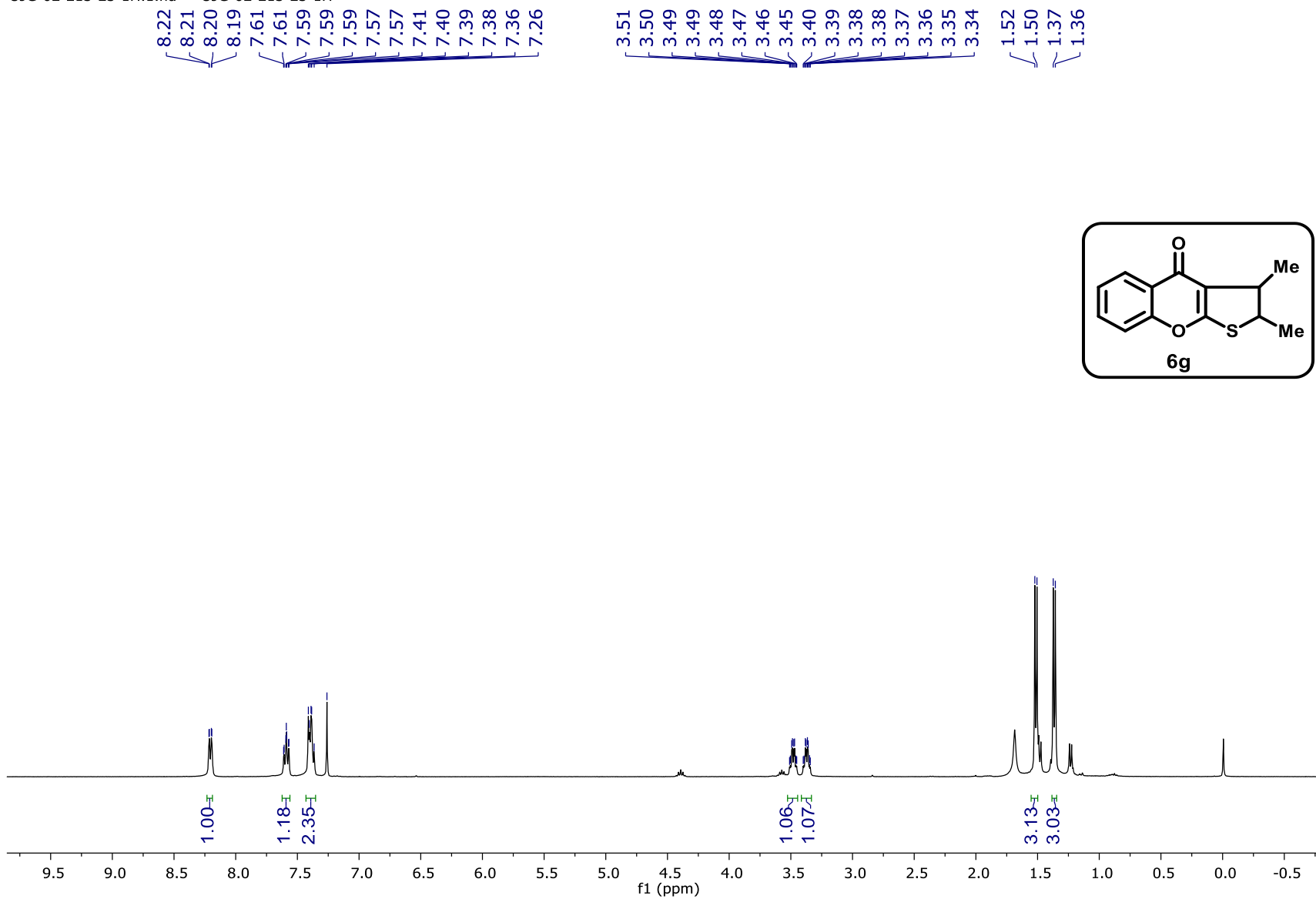


HRMS Spectrum of Compound 6f



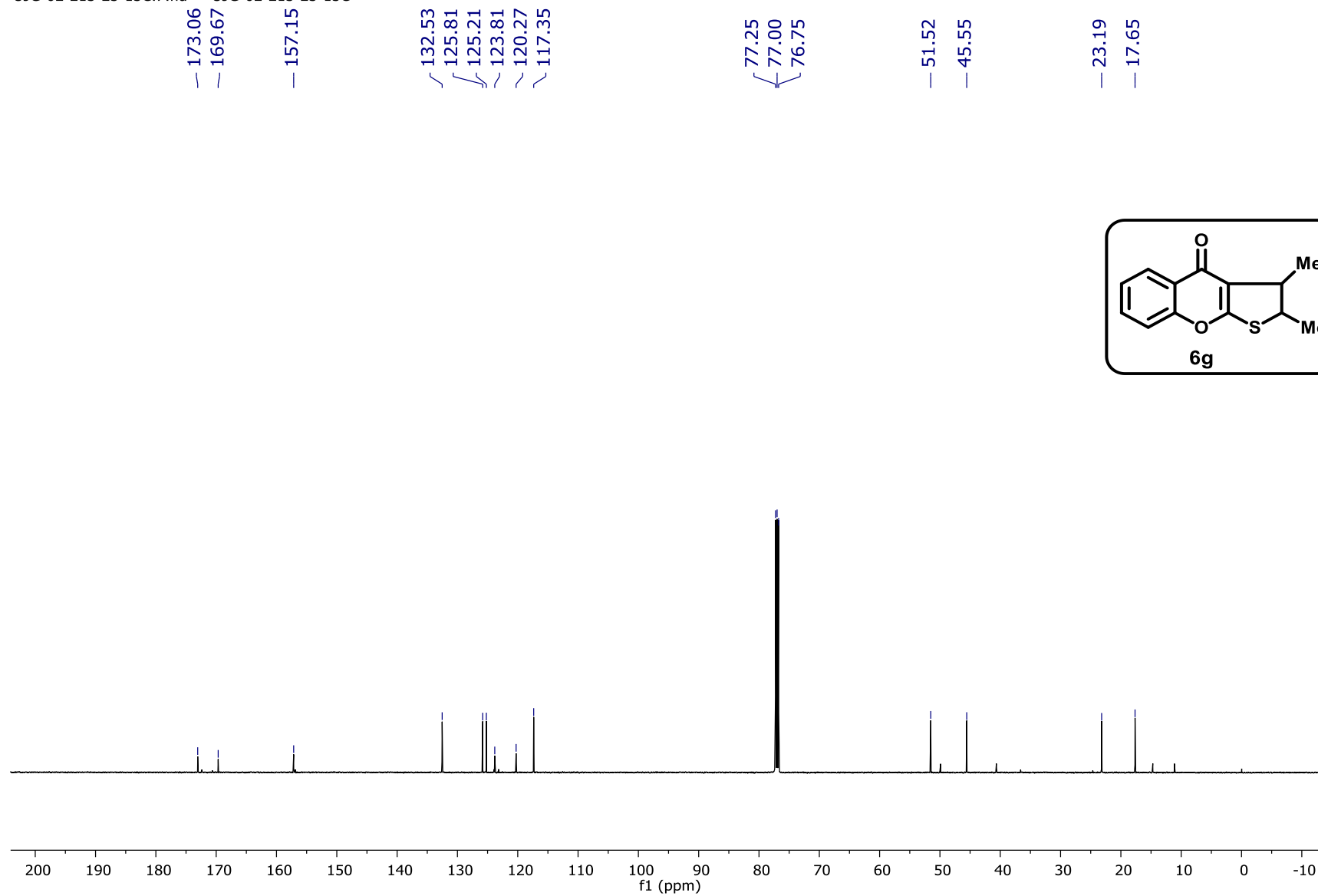
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 6g

UJG-02-213-23-1H.1.fid — UJG-02-213-23-1H

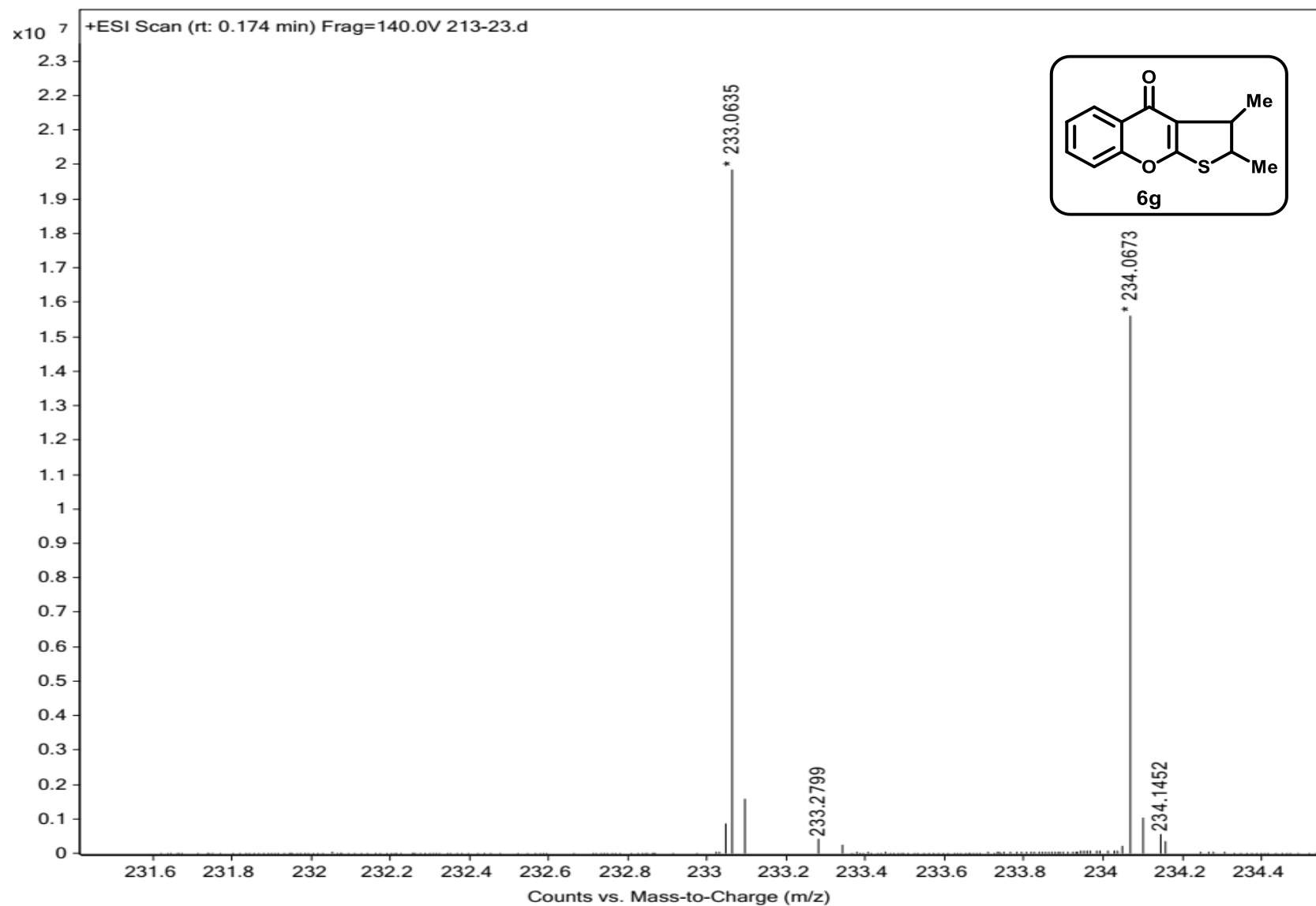


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6g

UJG-02-213-23-13C.7.fid — UJG-02-213-23-13C

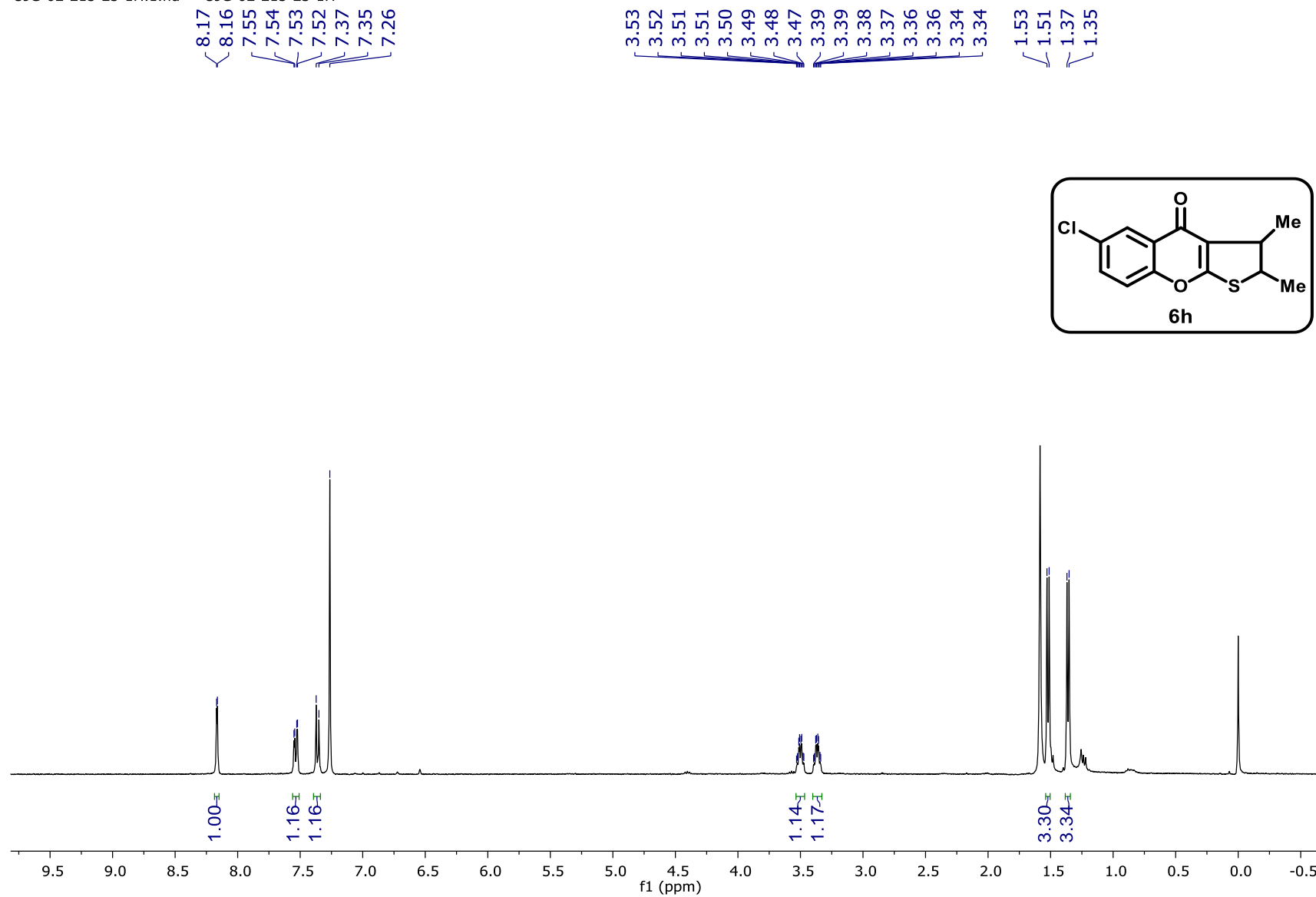


HRMS Spectrum of Compound 6g



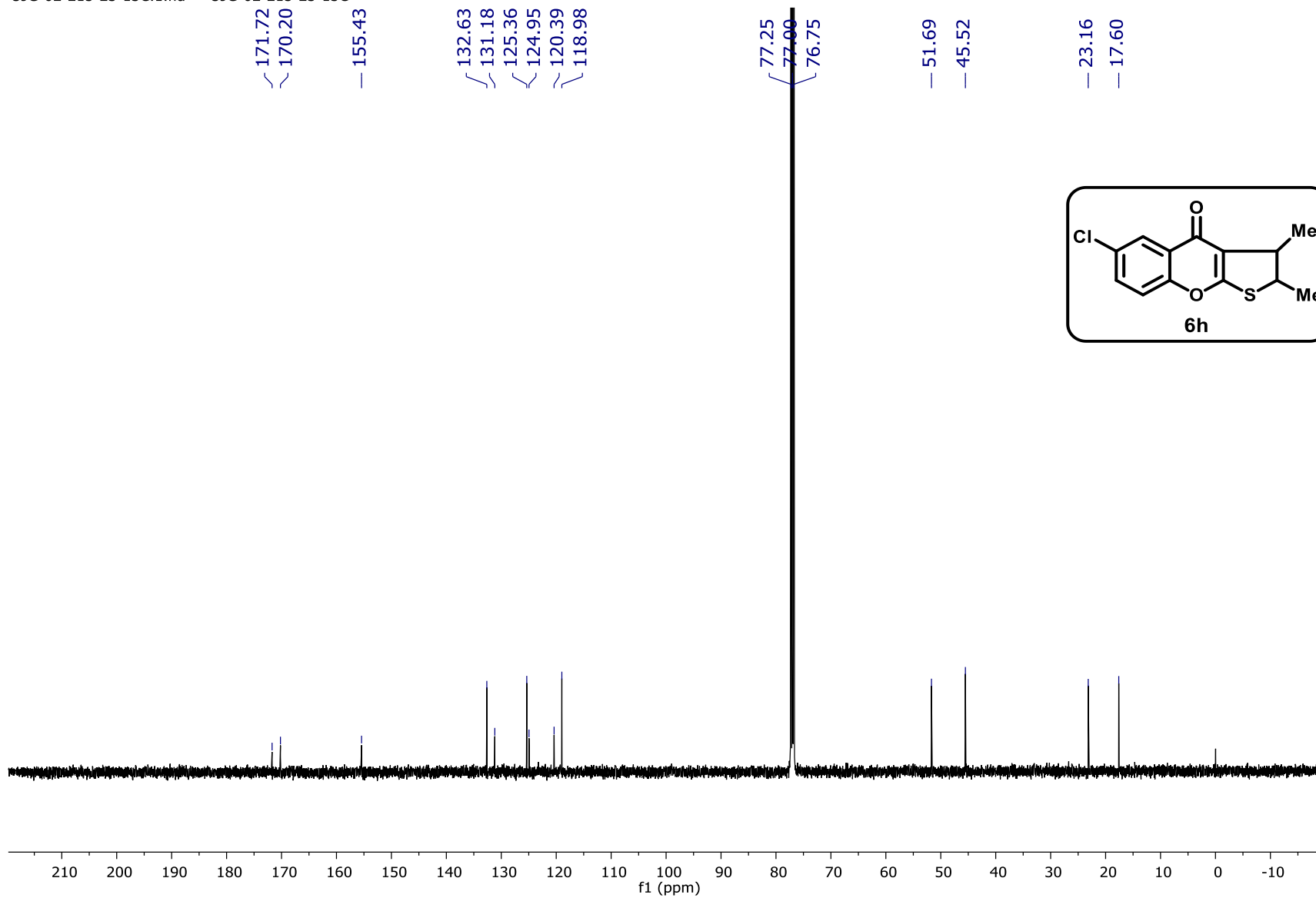
^1H NMR (400 MHz, CDCl_3) Spectrum of Compound 6h

UJG-02-215-23-1H.1.fid — UJG-02-215-23-1H

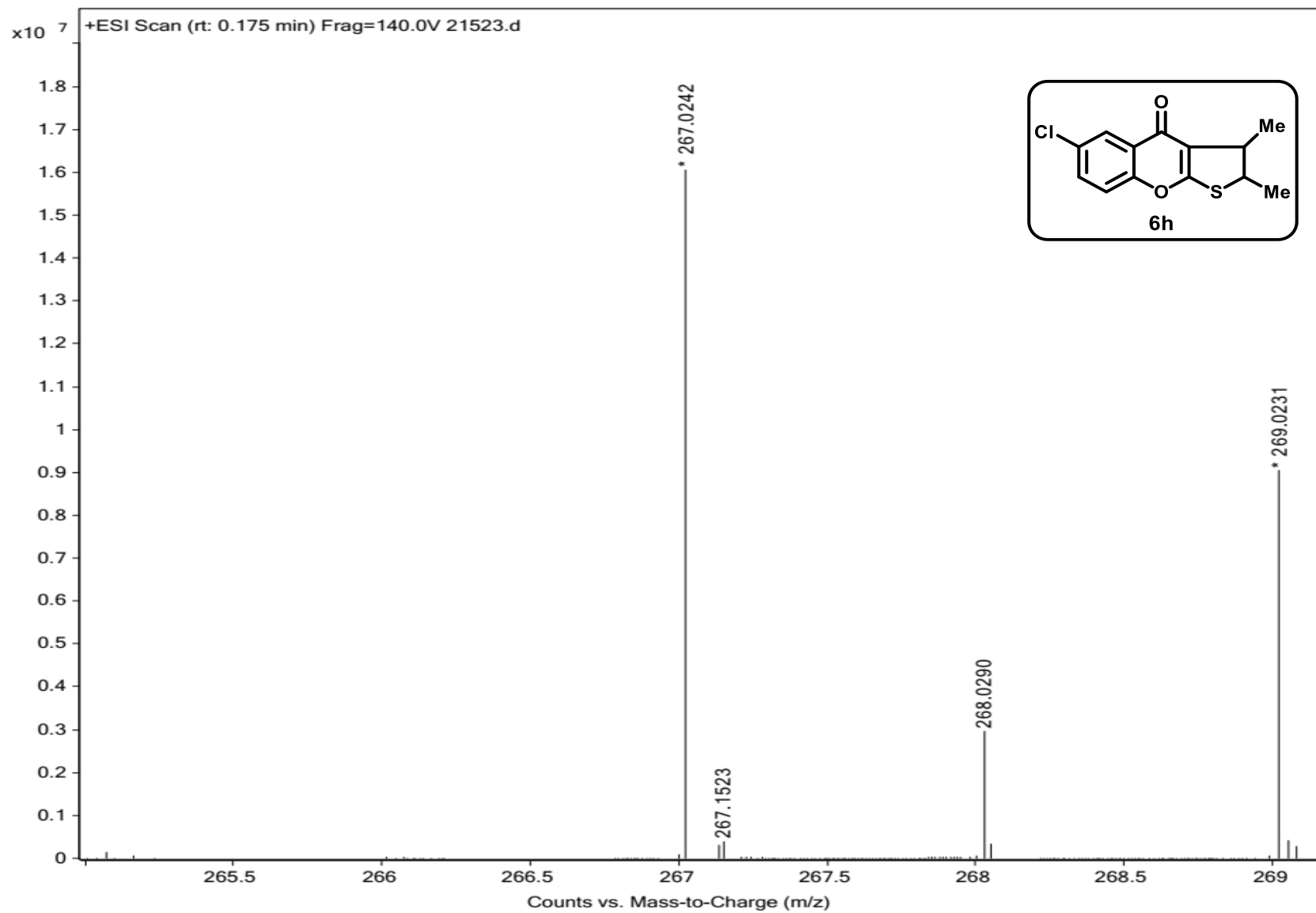


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6h

UJG-02-215-23-13C.1.fid — UJG-02-215-23-13C

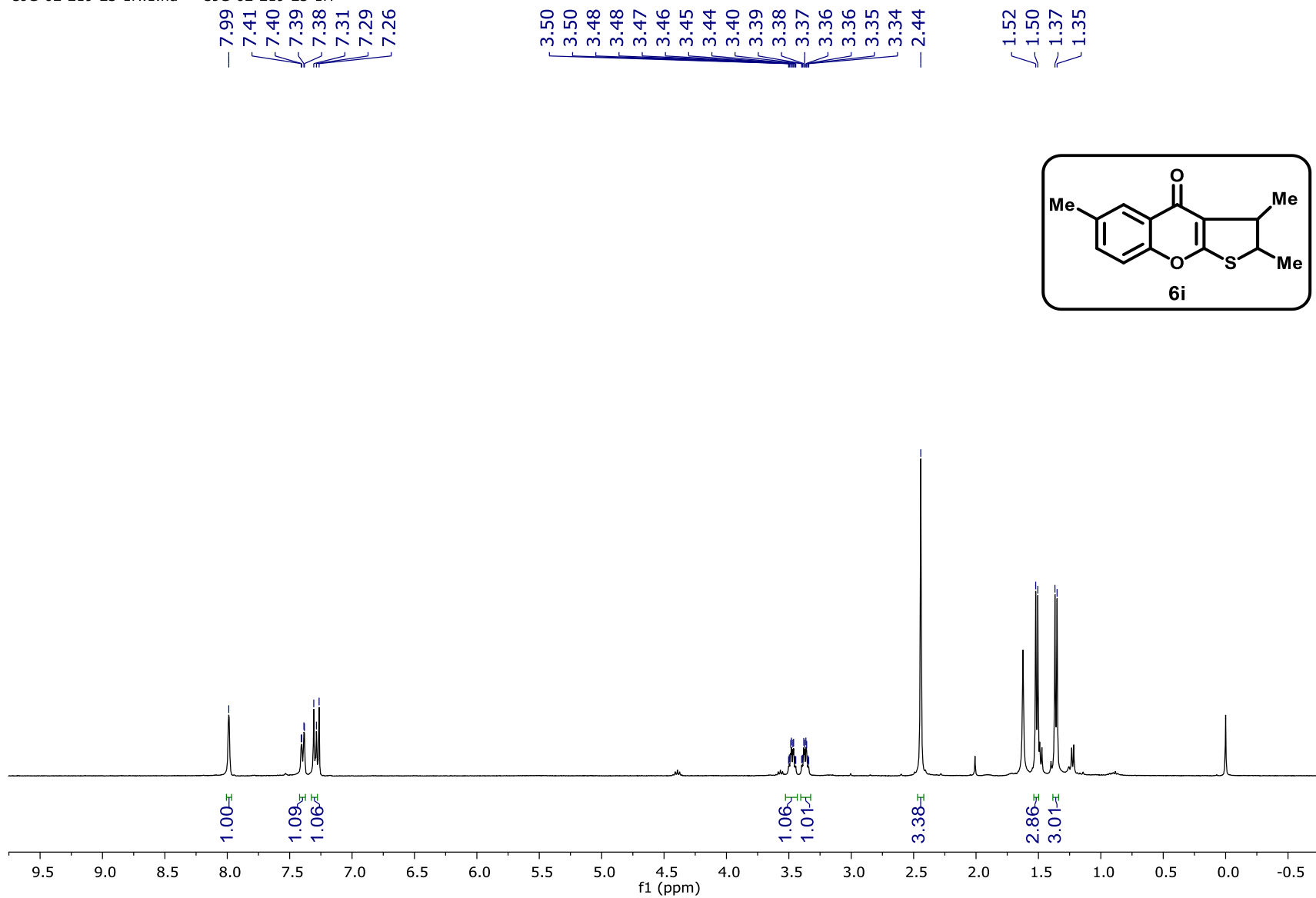


HRMS Spectrum of Compound 6h



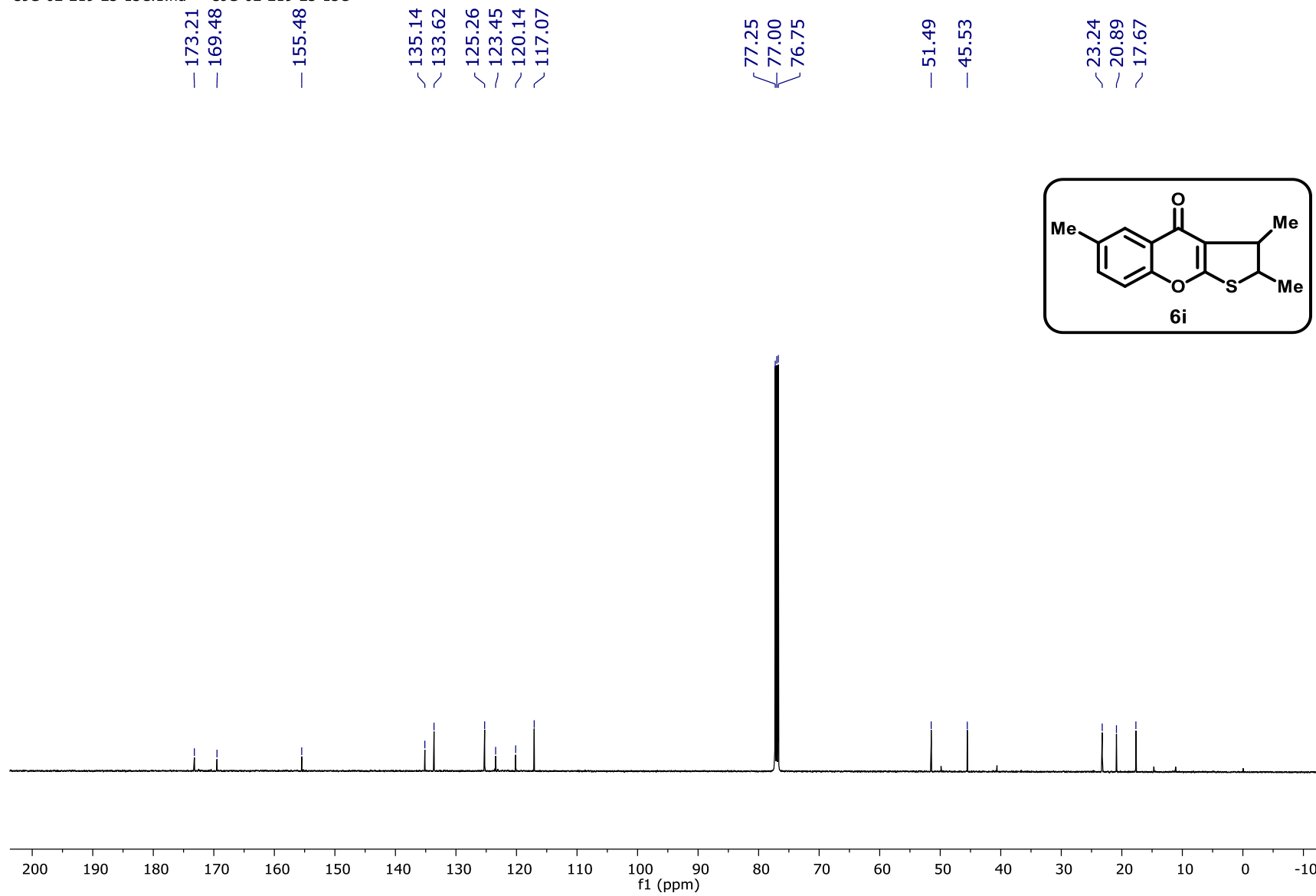
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 6i

UJG-02-219-23-1H.1.fid — UJG-02-219-23-1H

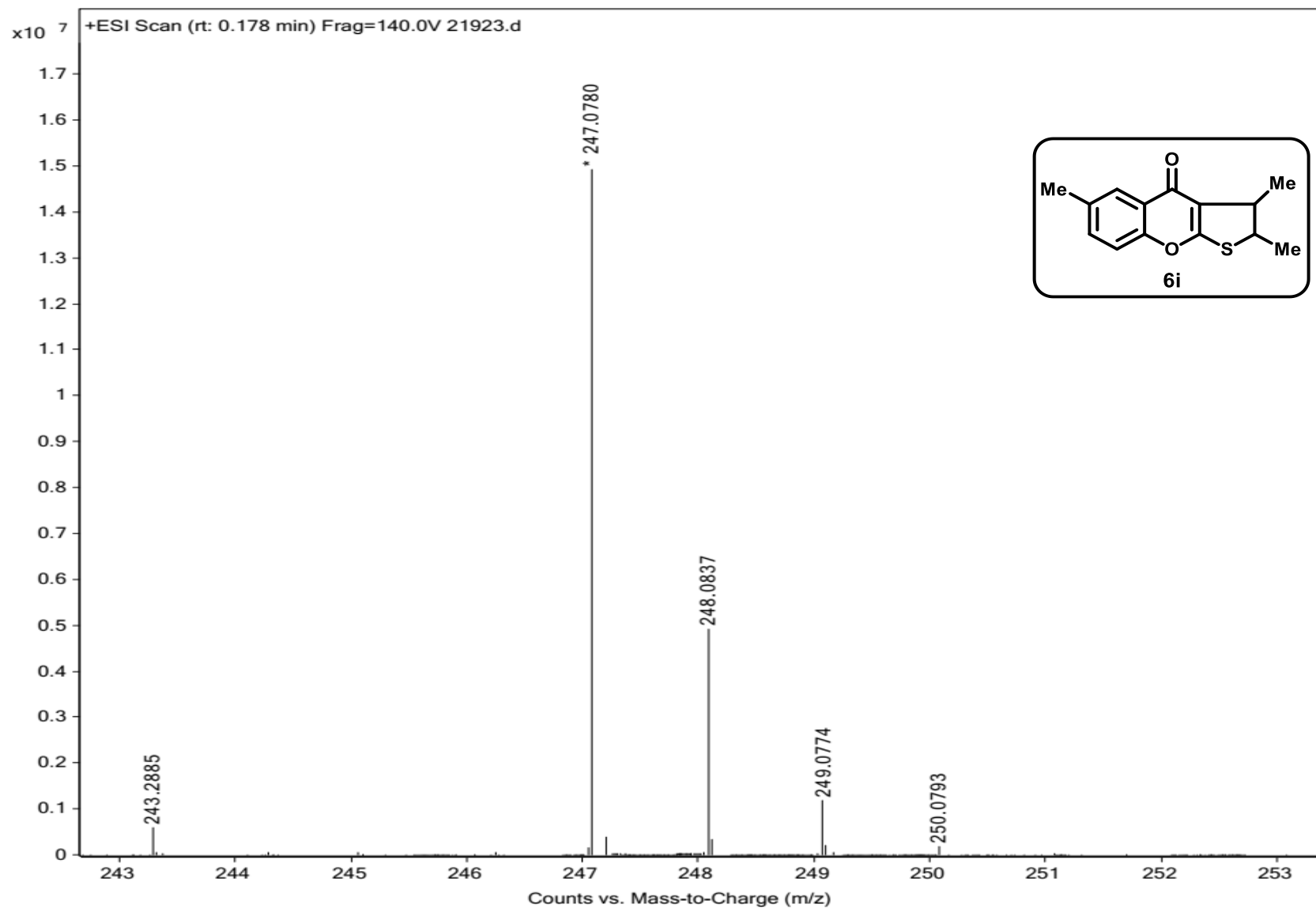


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6i

UJG-02-219-23-13C.1.fid — UJG-02-219-23-13C



HRMS Spectrum of Compound 6i



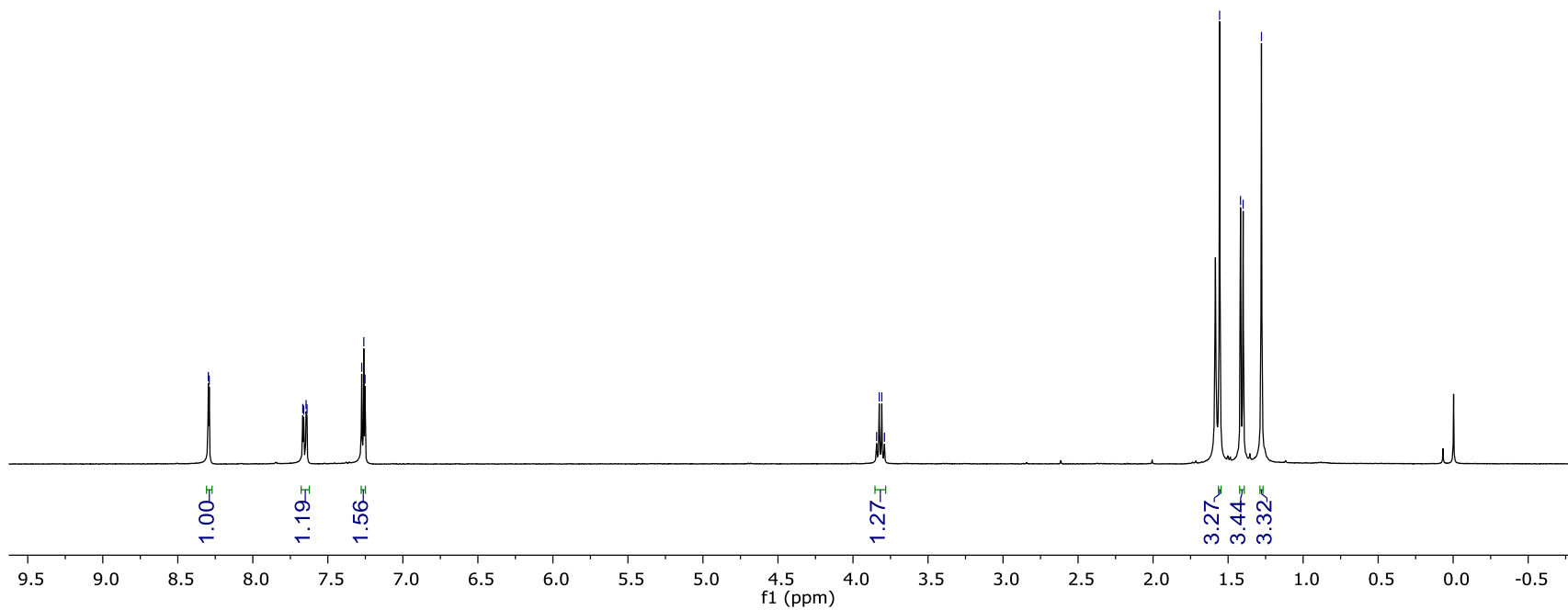
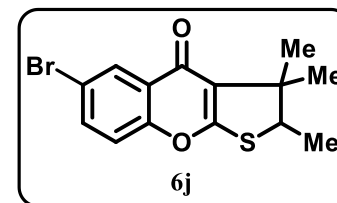
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 6j

UJG-02-245-23-1H.1.fid — UJG-02-245-23-1H

8.30
8.29
7.67
7.66
7.65
7.64
7.27
7.26
7.25

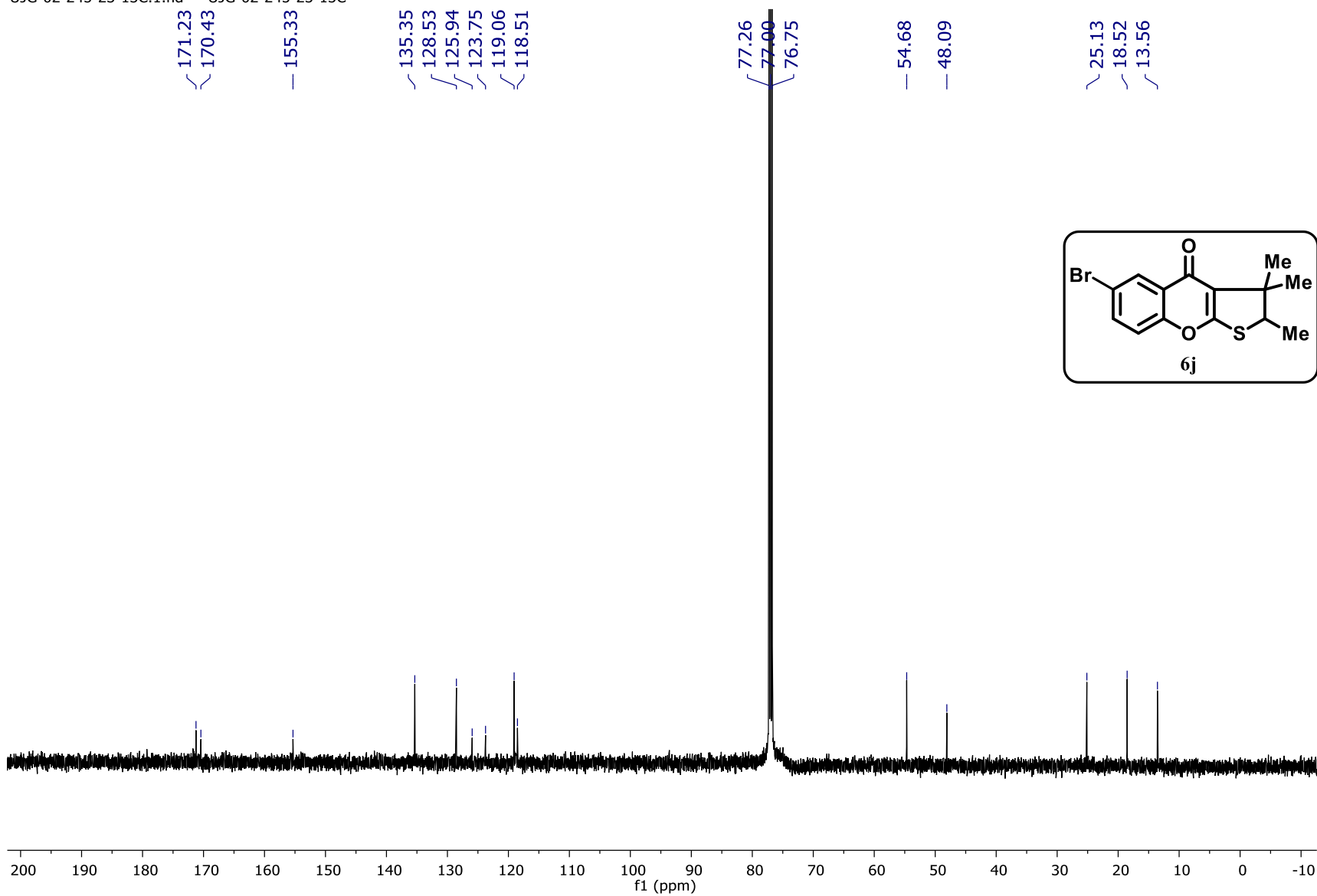
3.84
3.83
3.81
3.79

1.56
1.42
1.40
1.28

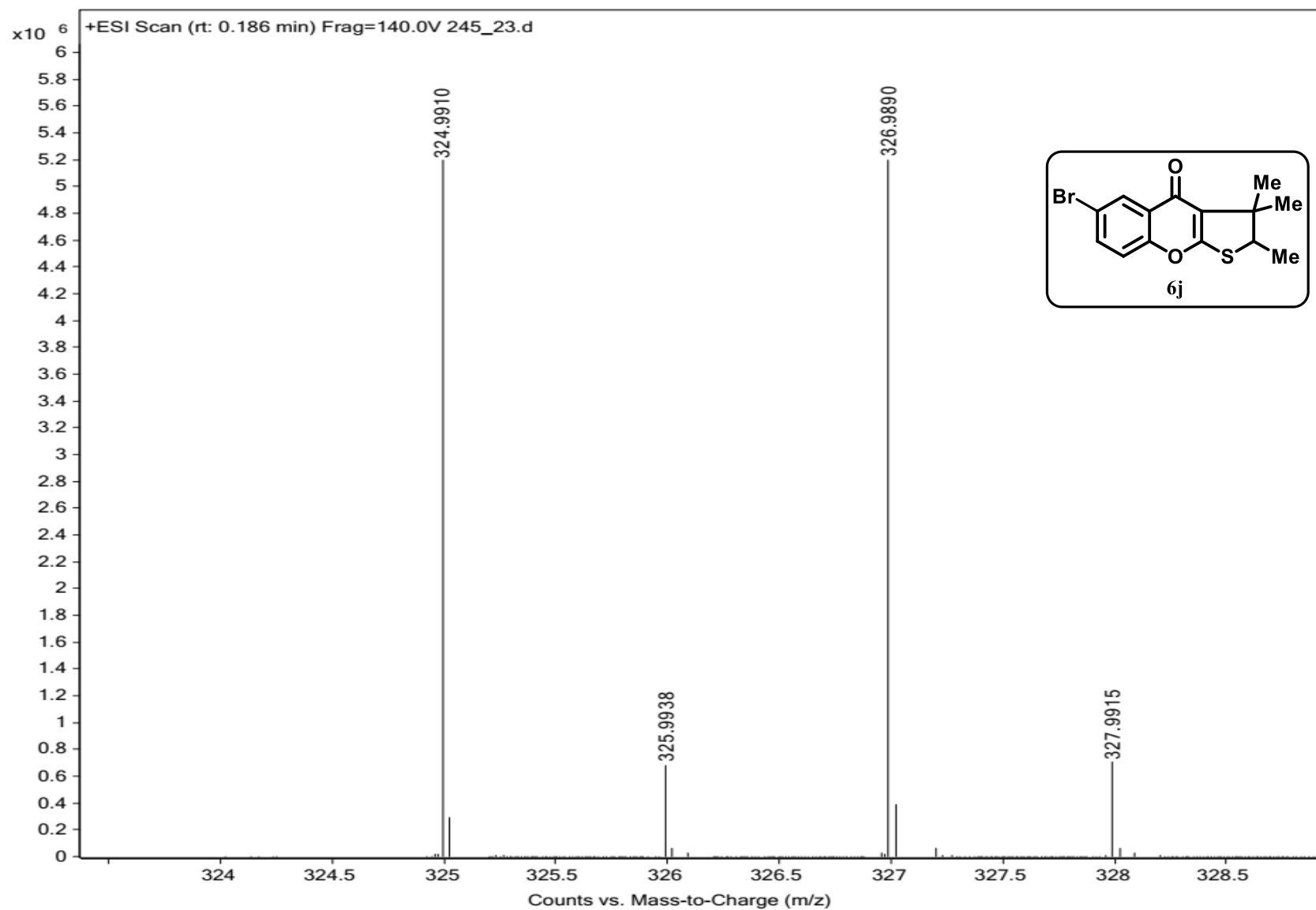


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6j

UJG-02-245-23-13C.1.fid — UJG-02-245-23-13C

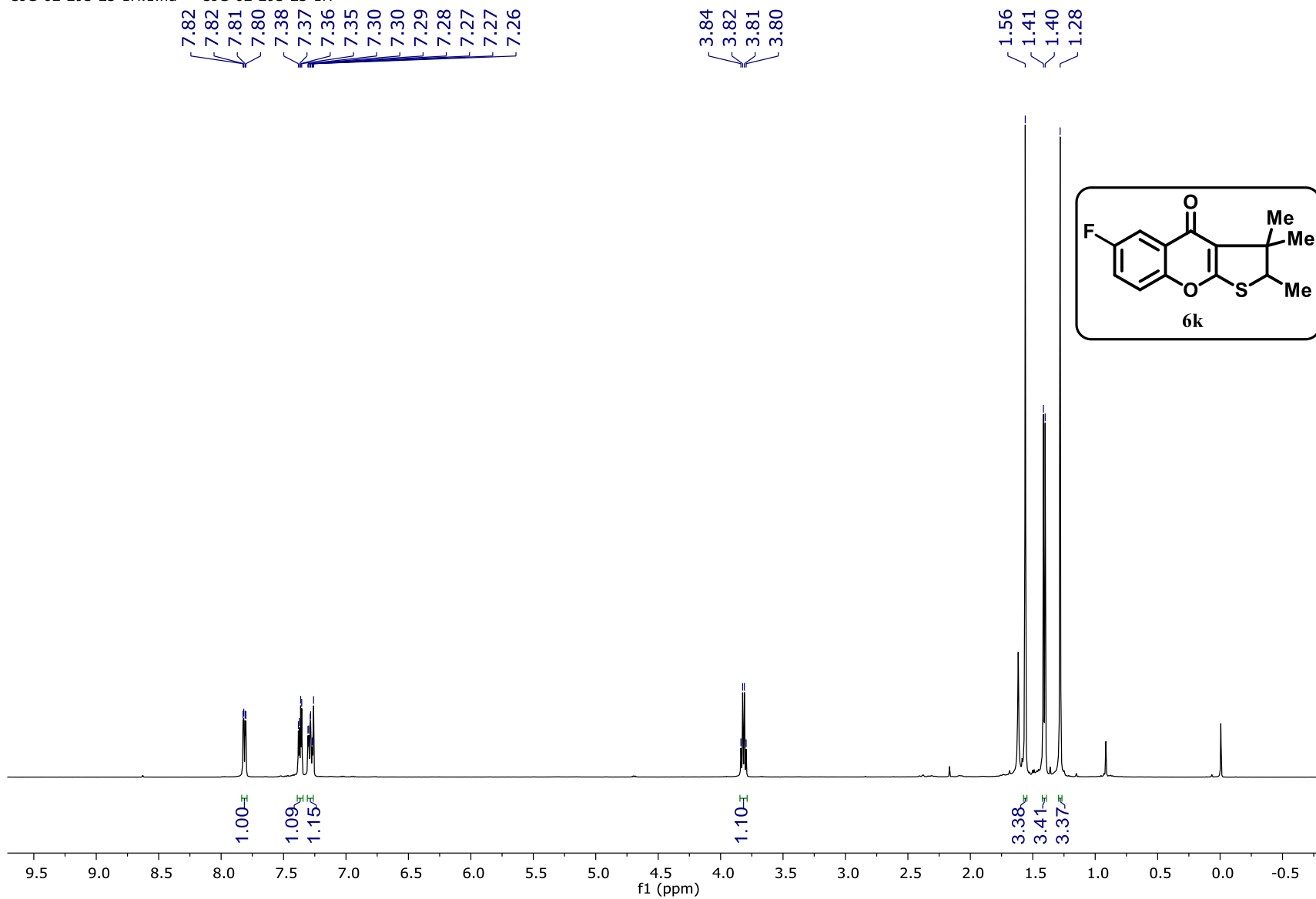


HRMS Spectrum of Compound 6j



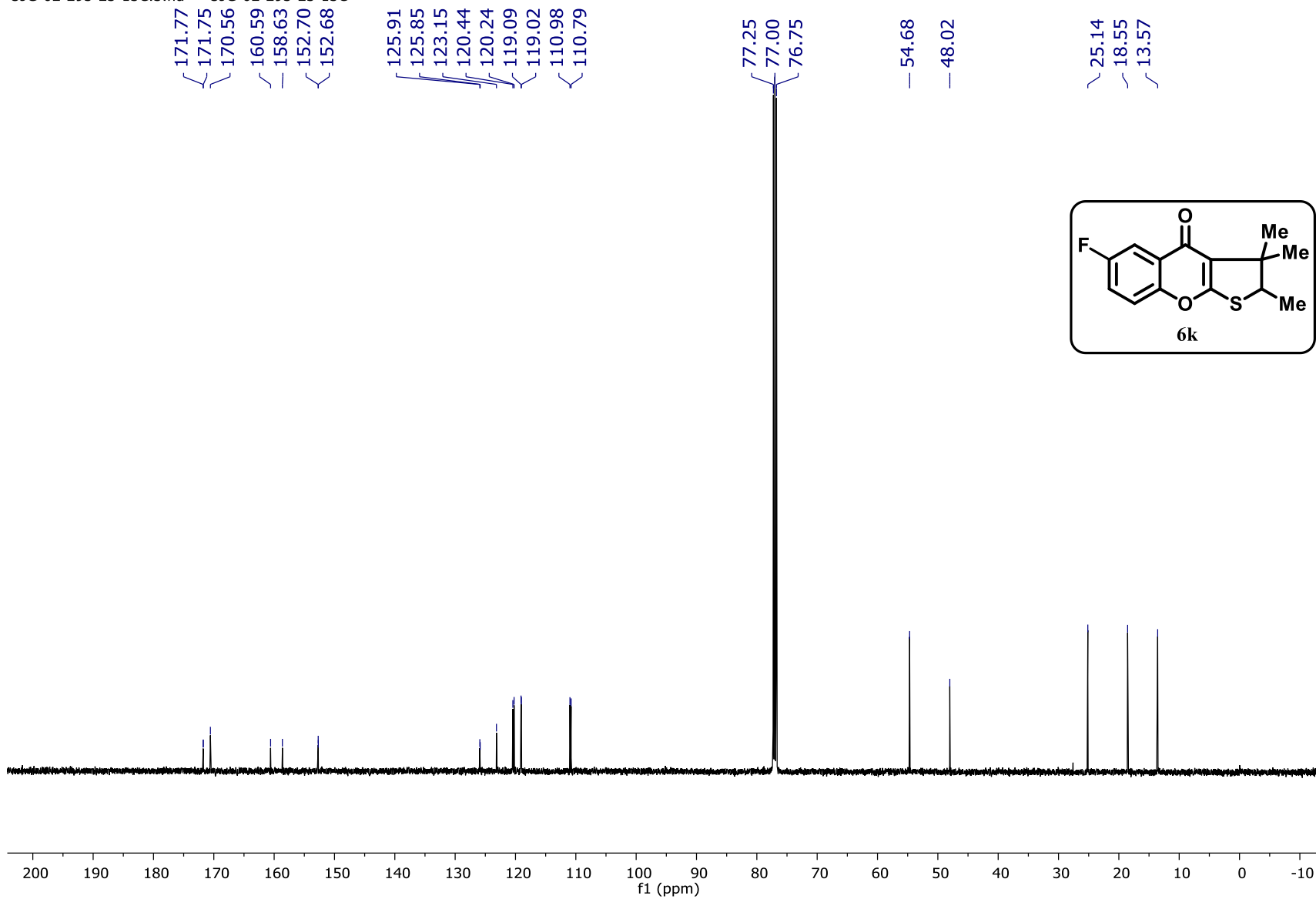
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 6k

UJG-02-293-23-1H.1.fid — UJG-02-293-23-1H



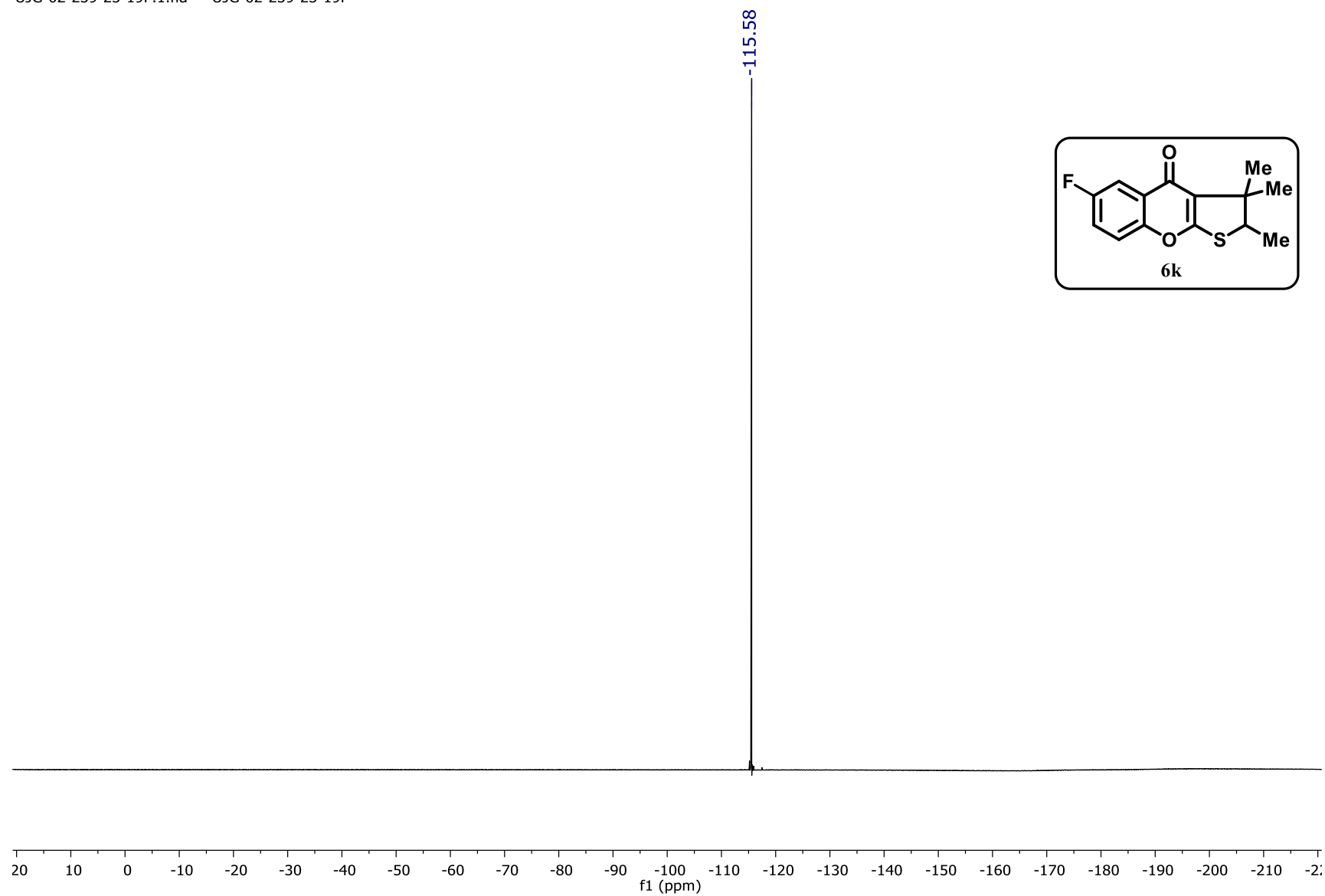
^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 6k

UJG-02-293-23-13C.3.fid — UJG-02-293-23-13C

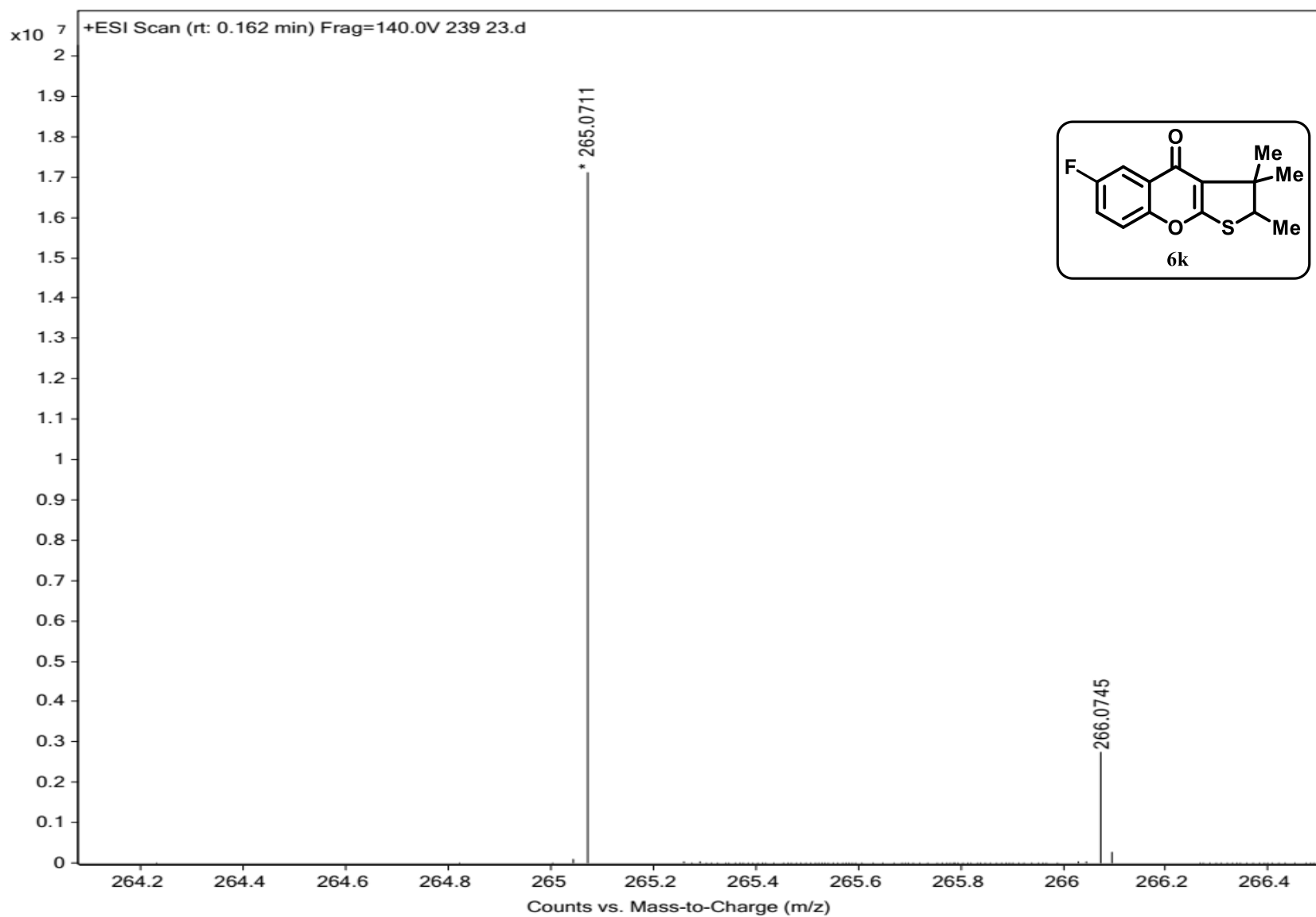


^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 6k

UJG-02-239-23-19F.1.fid — UJG-02-239-23-19F

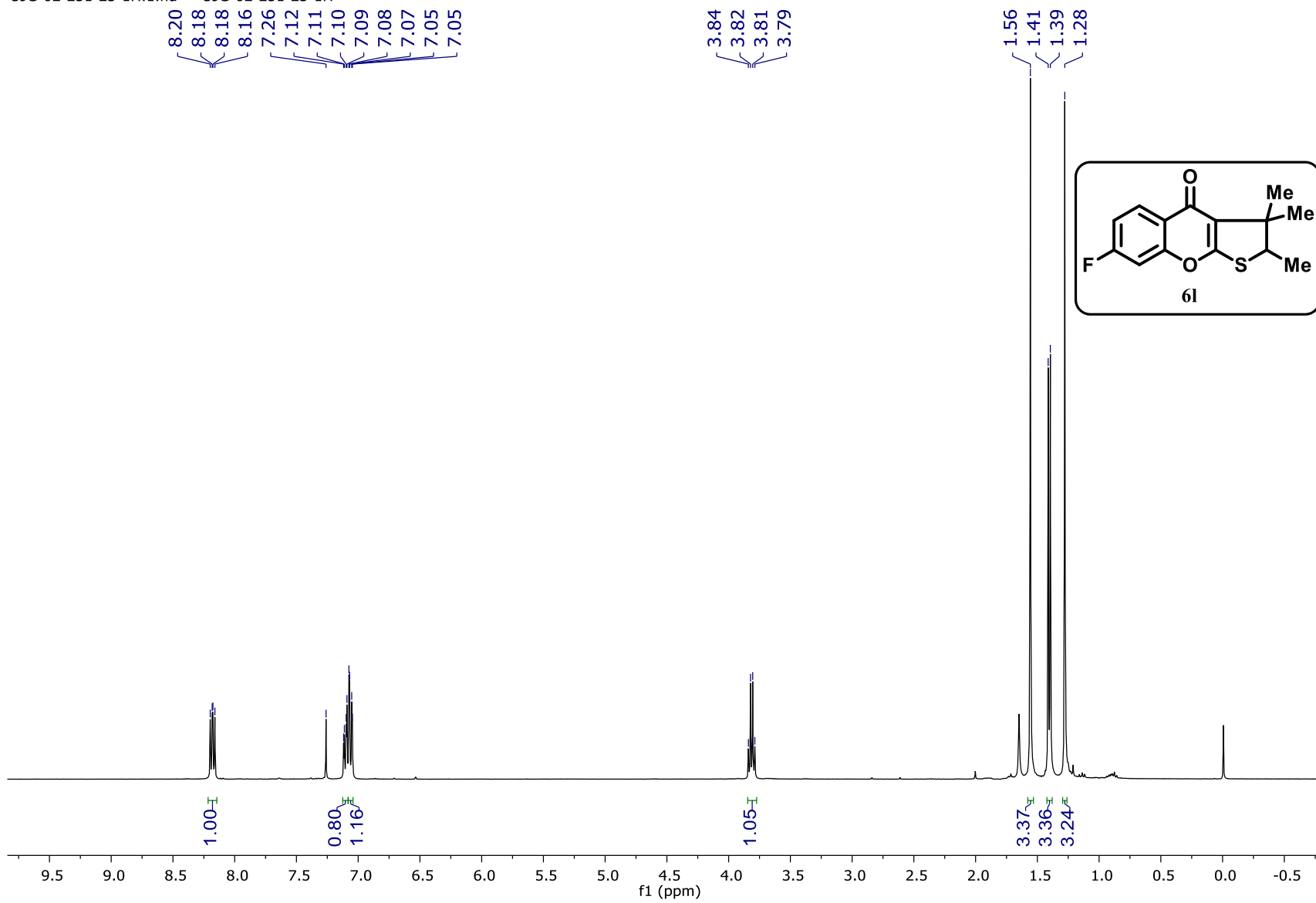


HRMS Spectrum of Compound 6k



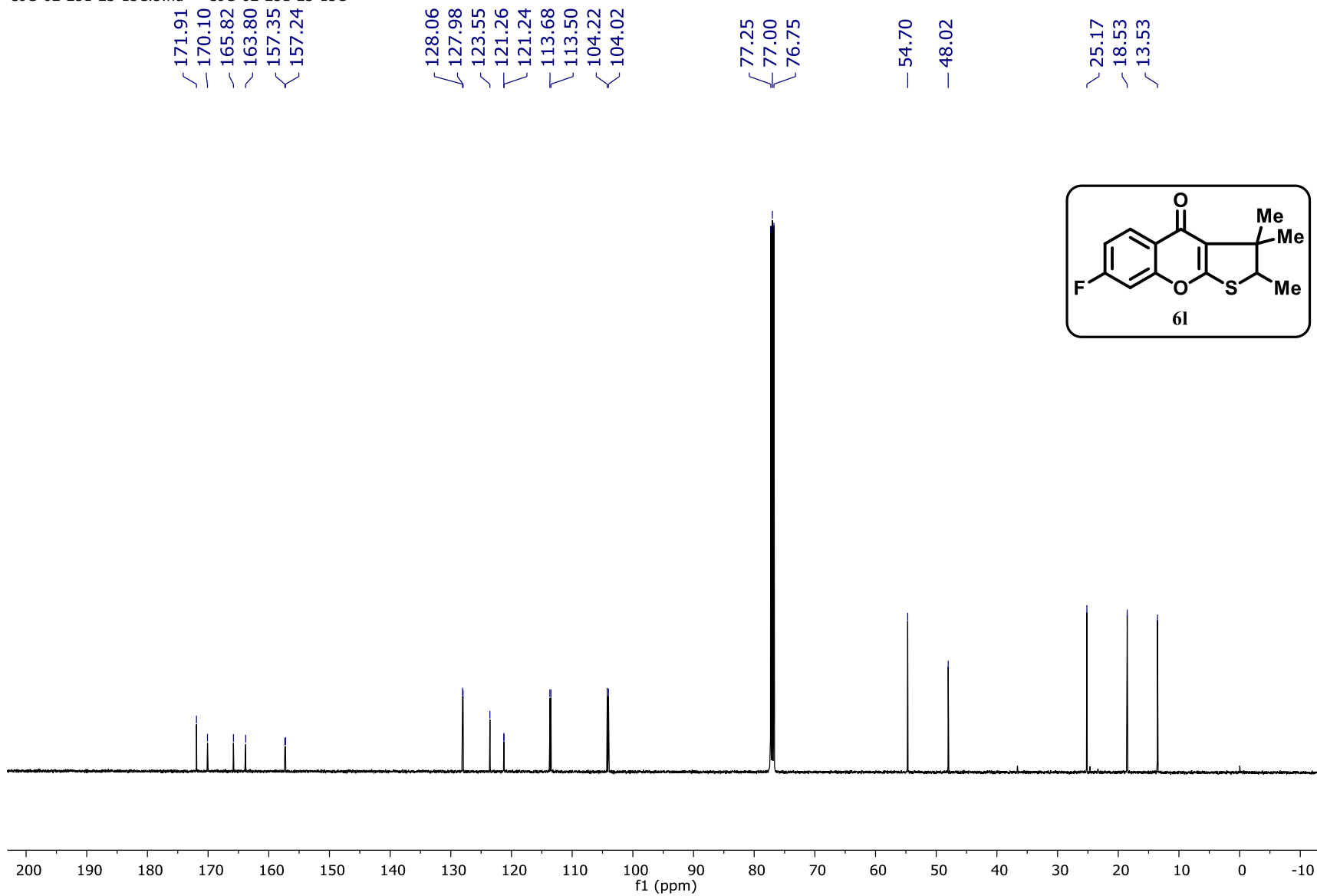
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 6l

UJG-02-251-23-1H.1.fid — UJG-02-251-23-1H



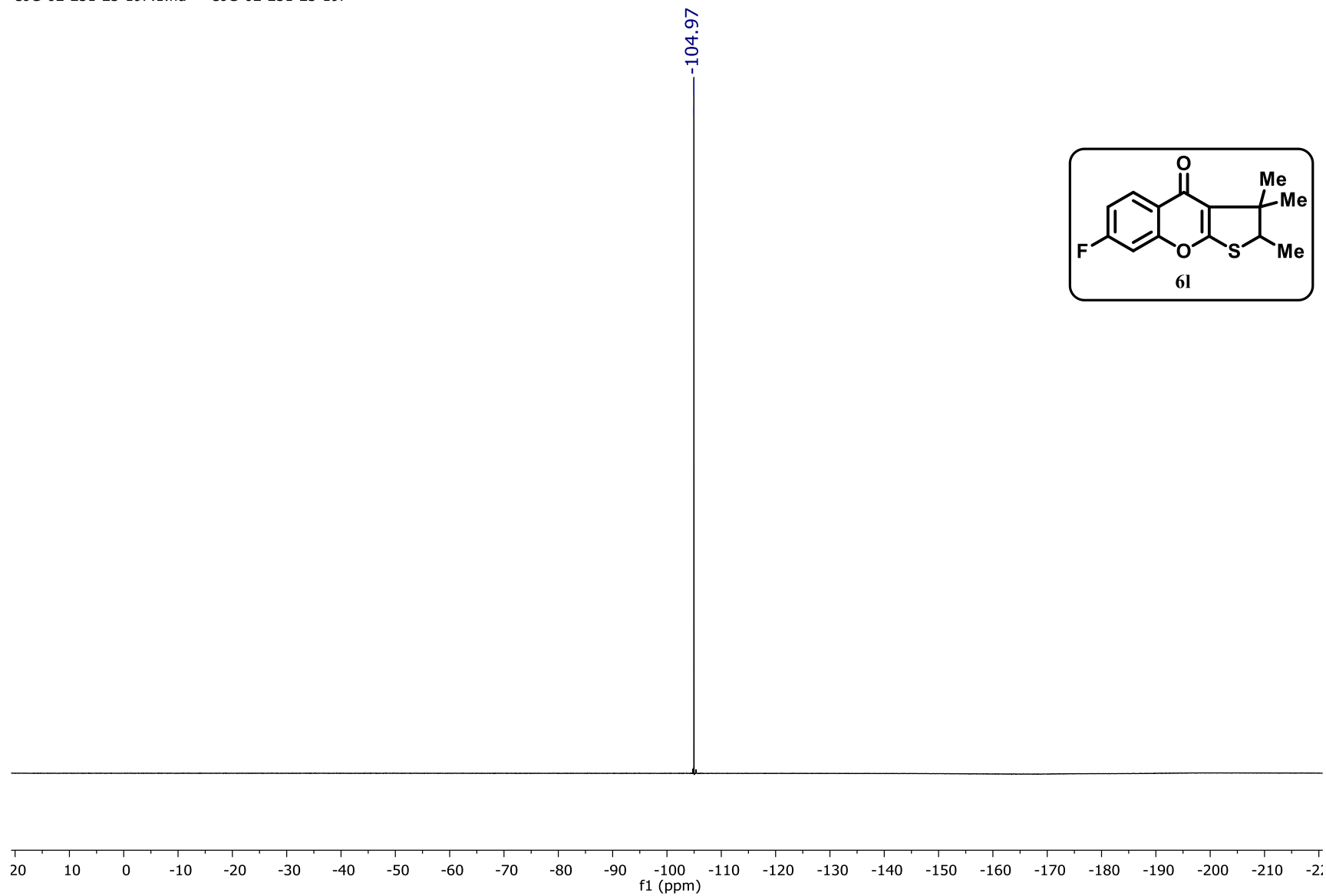
^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 6l

UJG-02-251-23-13C.5.fid — UJG-02-251-23-13C



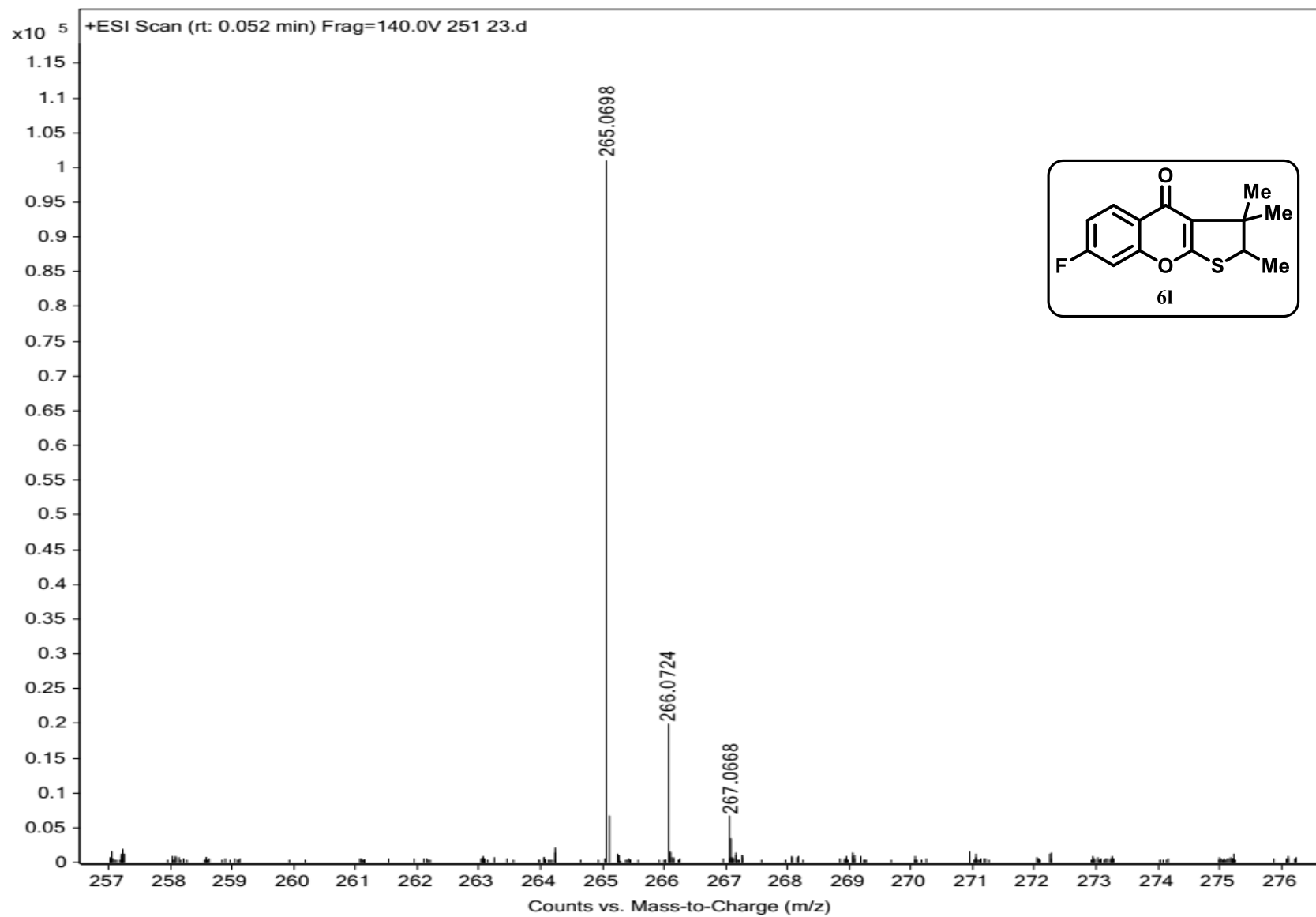
^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 6l

UJG-02-251-23-19F.1.fid — UJG-02-251-23-19F



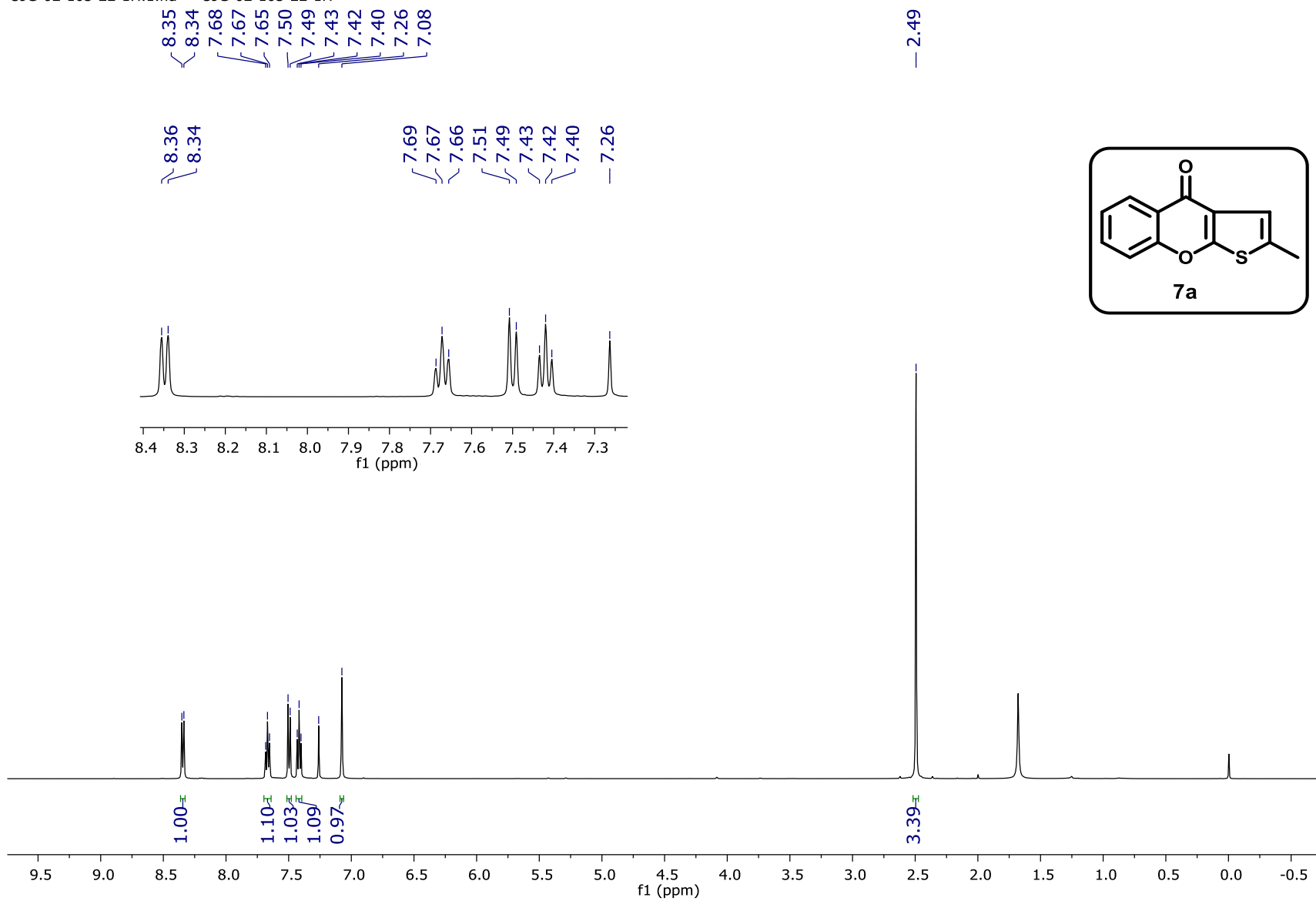
S143

HRMS Spectrum of Compound 6l



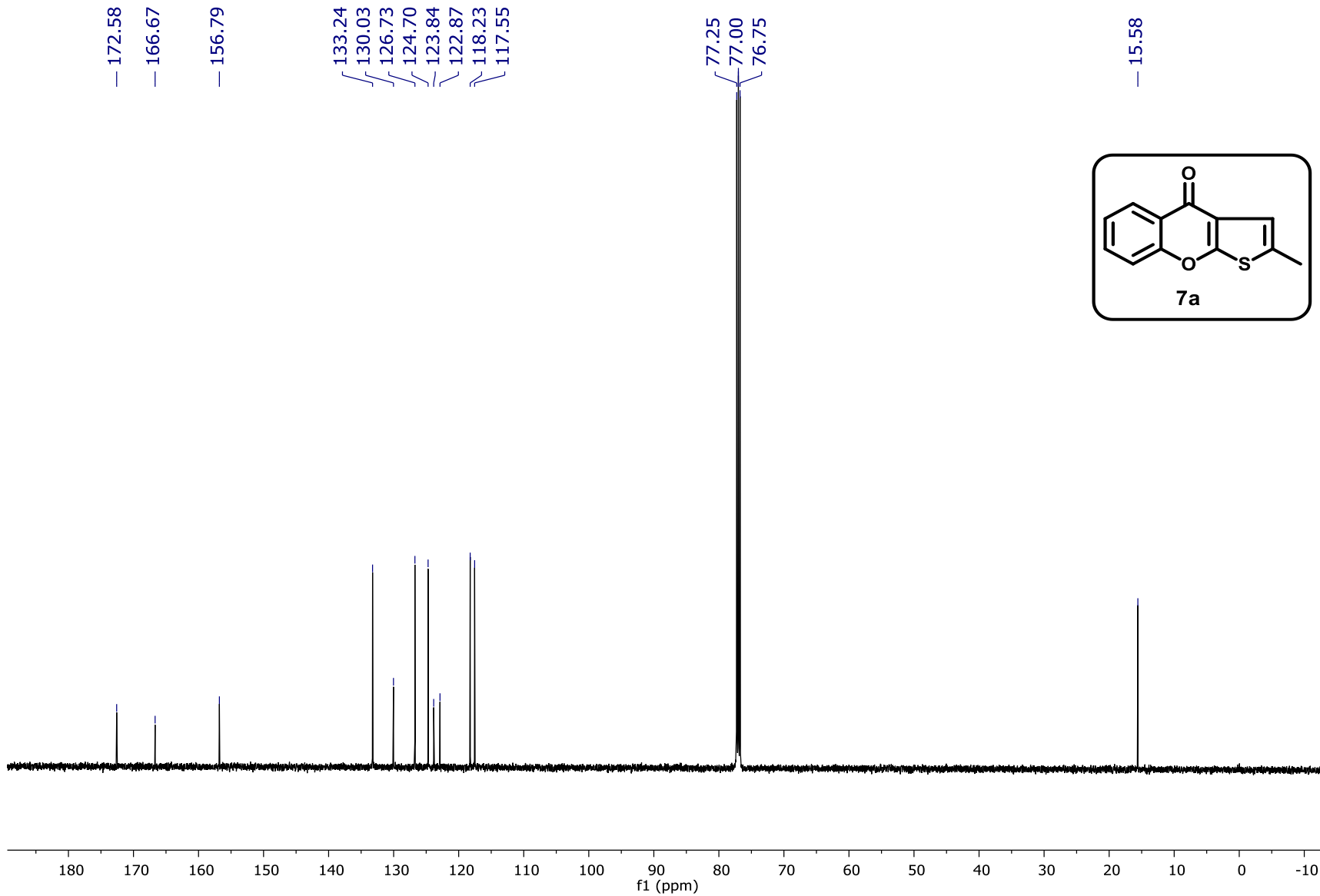
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7a

UJG-02-105-22-1H.1.fid — UJG-02-105-22-1H

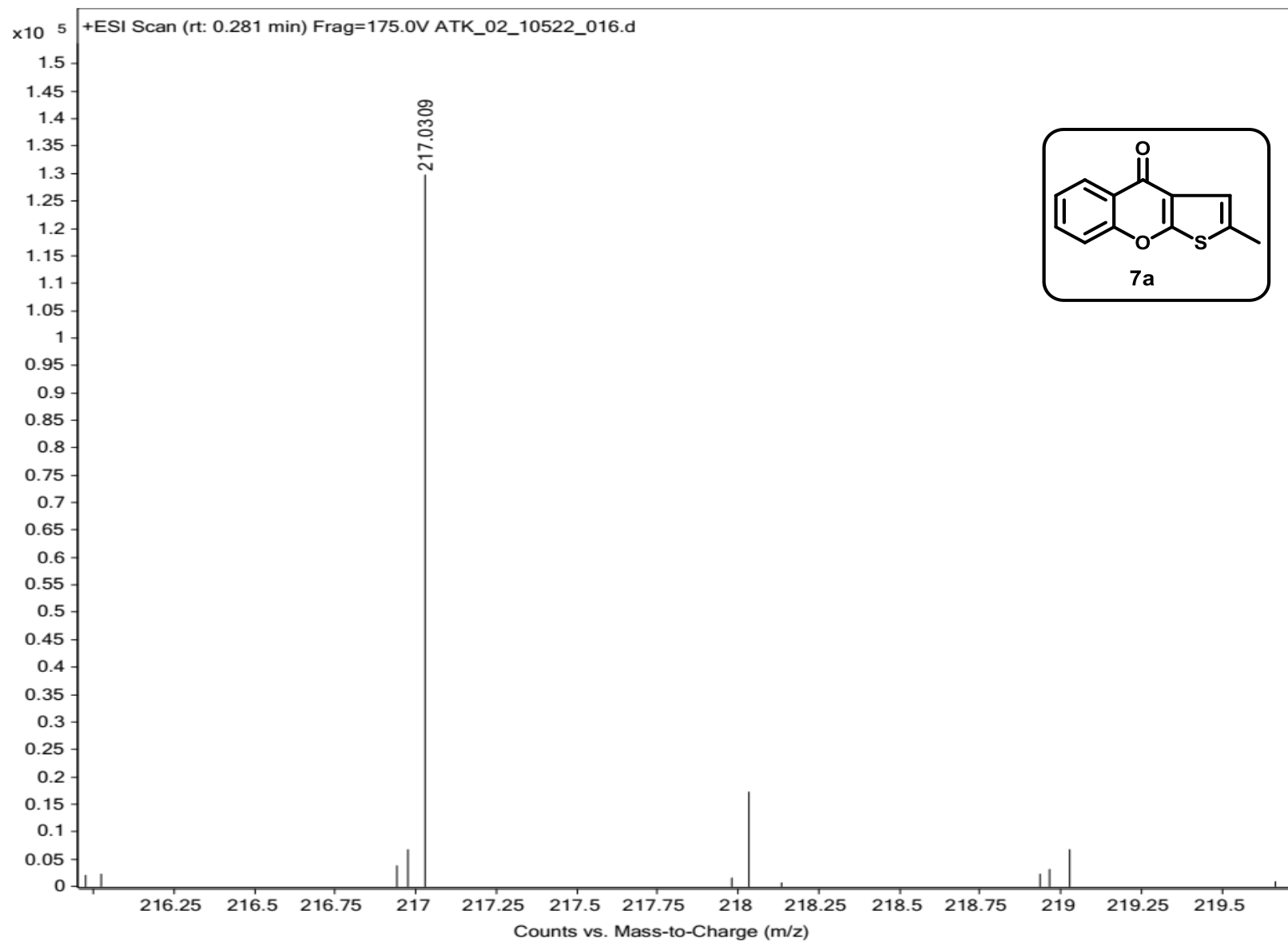


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7a

UJG-02-103-22-13C.7.fid — UJG-02-103-22-13C

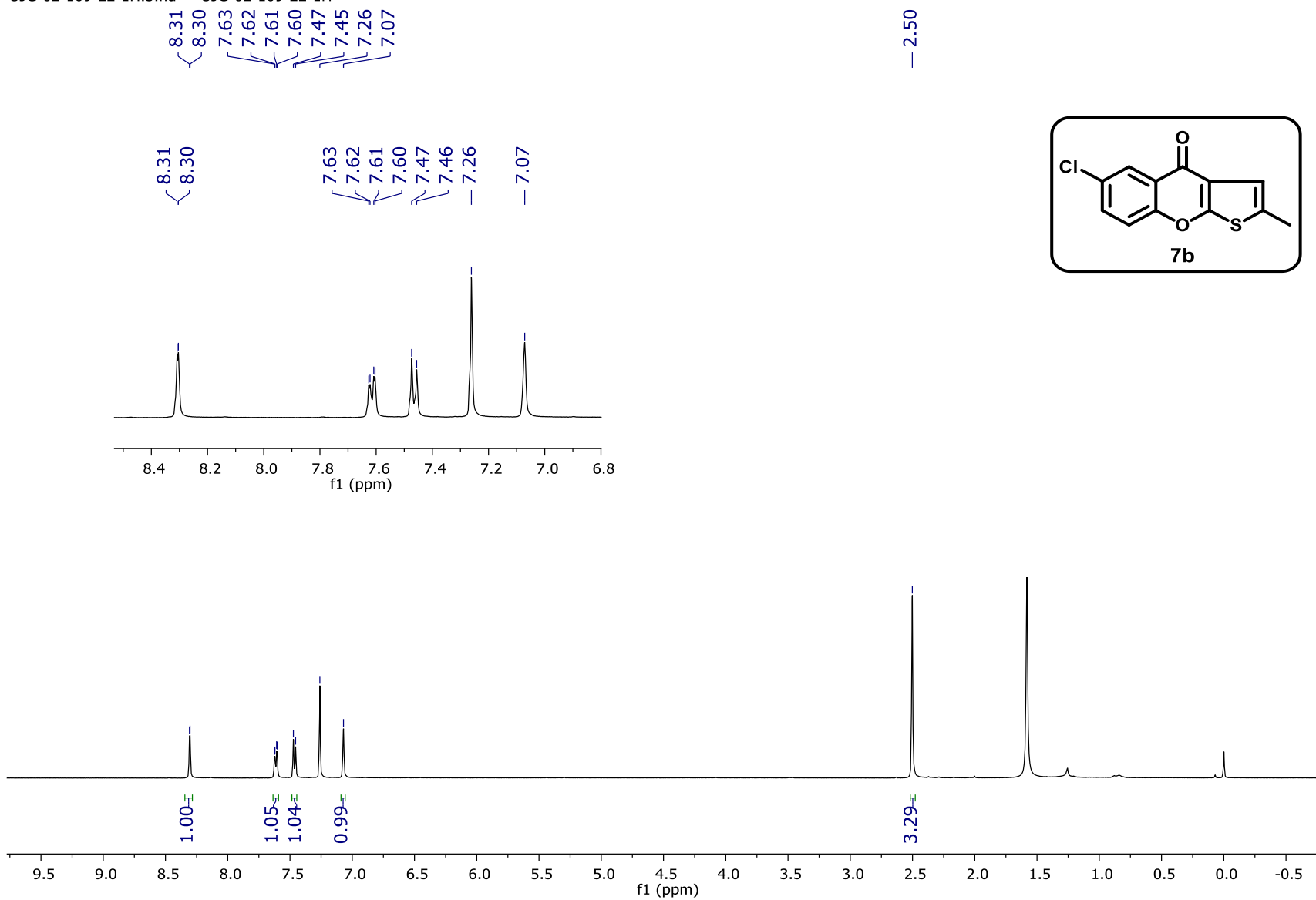


HRMS Spectrum of Compound 7a



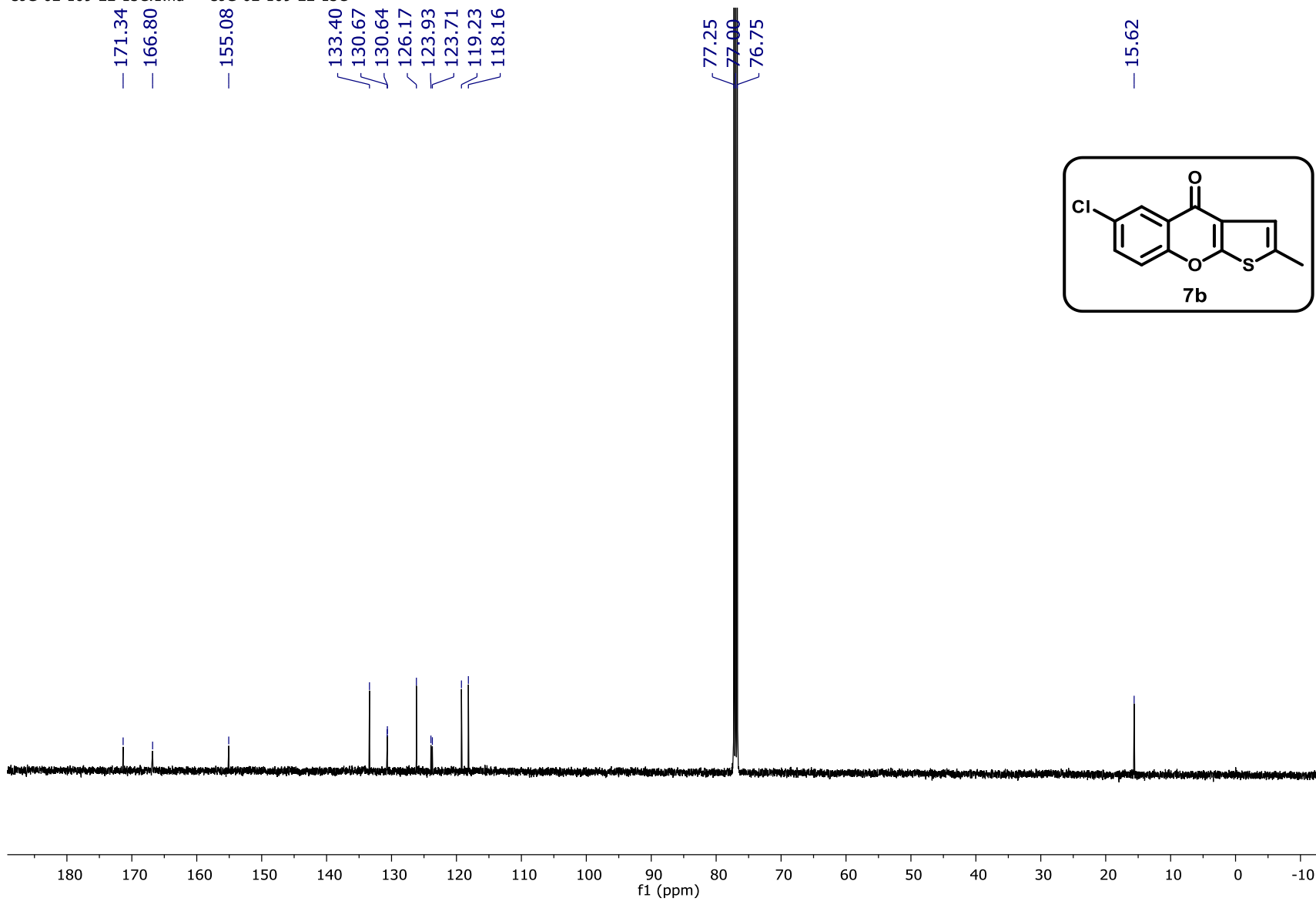
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7b

UJG-02-109-22-1H.3.fid — UJG-02-109-22-1H

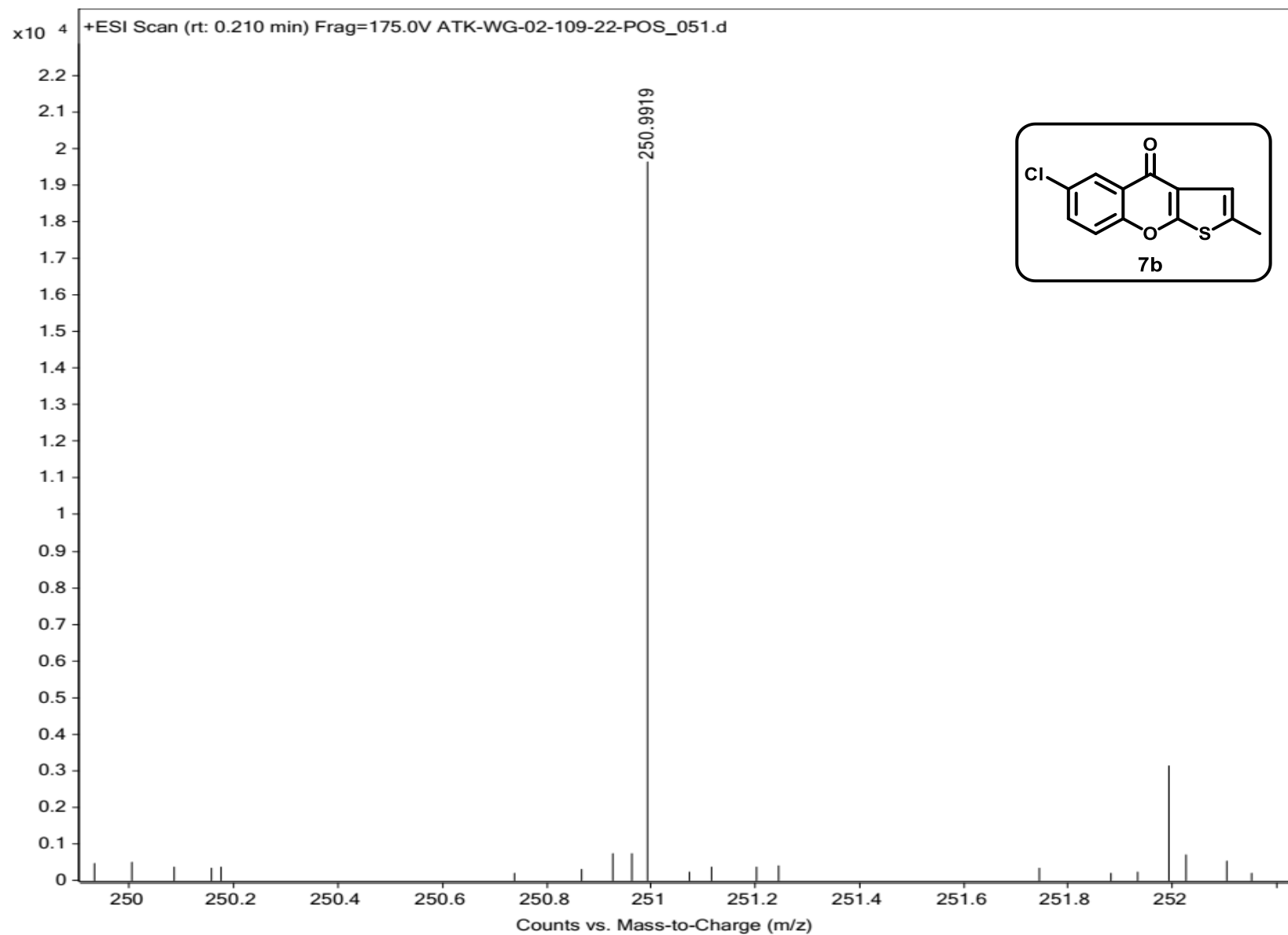


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7b

UJG-02-109-22-13C.1.fid — UJG-02-109-22-13C



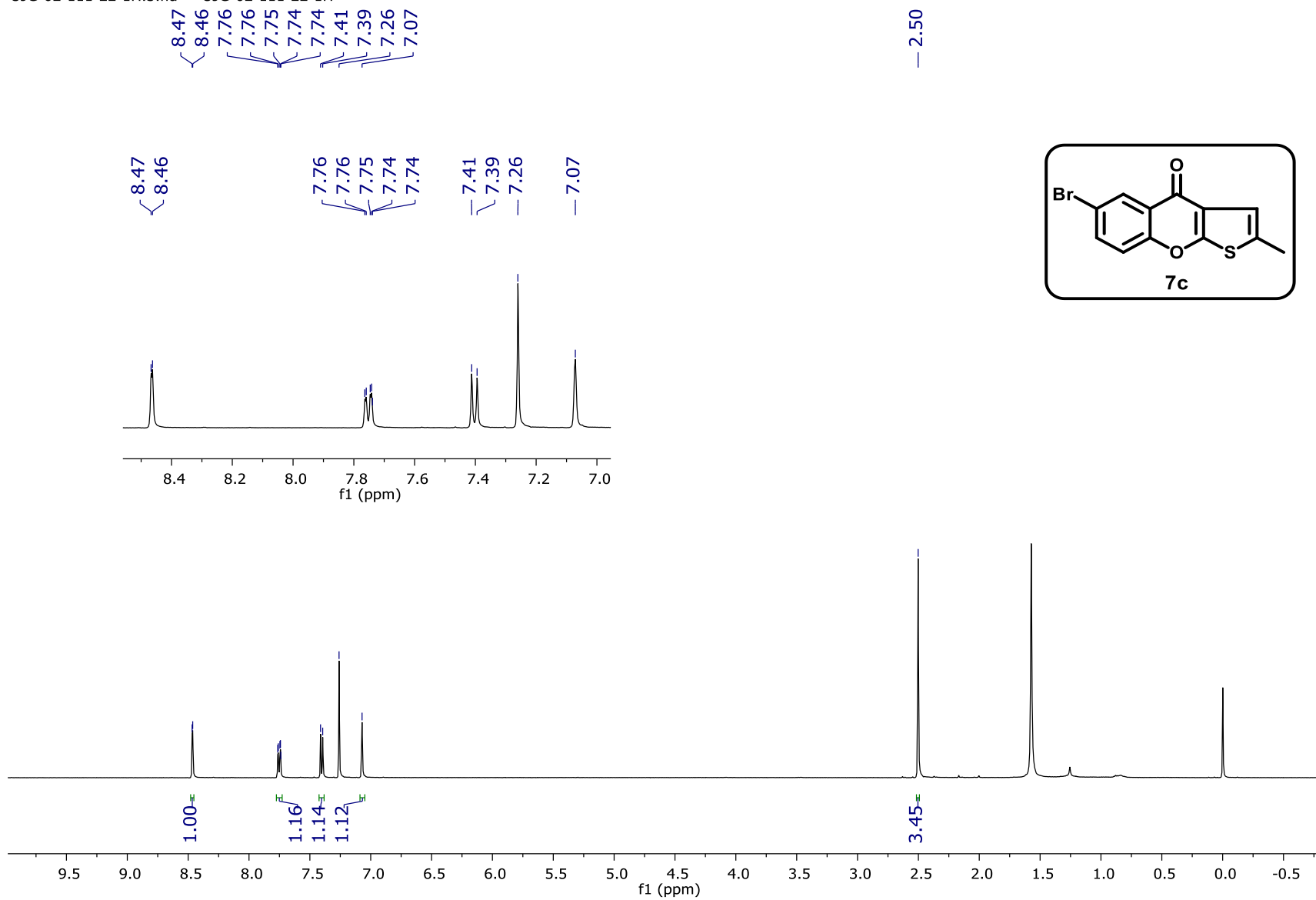
HRMS Spectrum of Compound 7b



S150

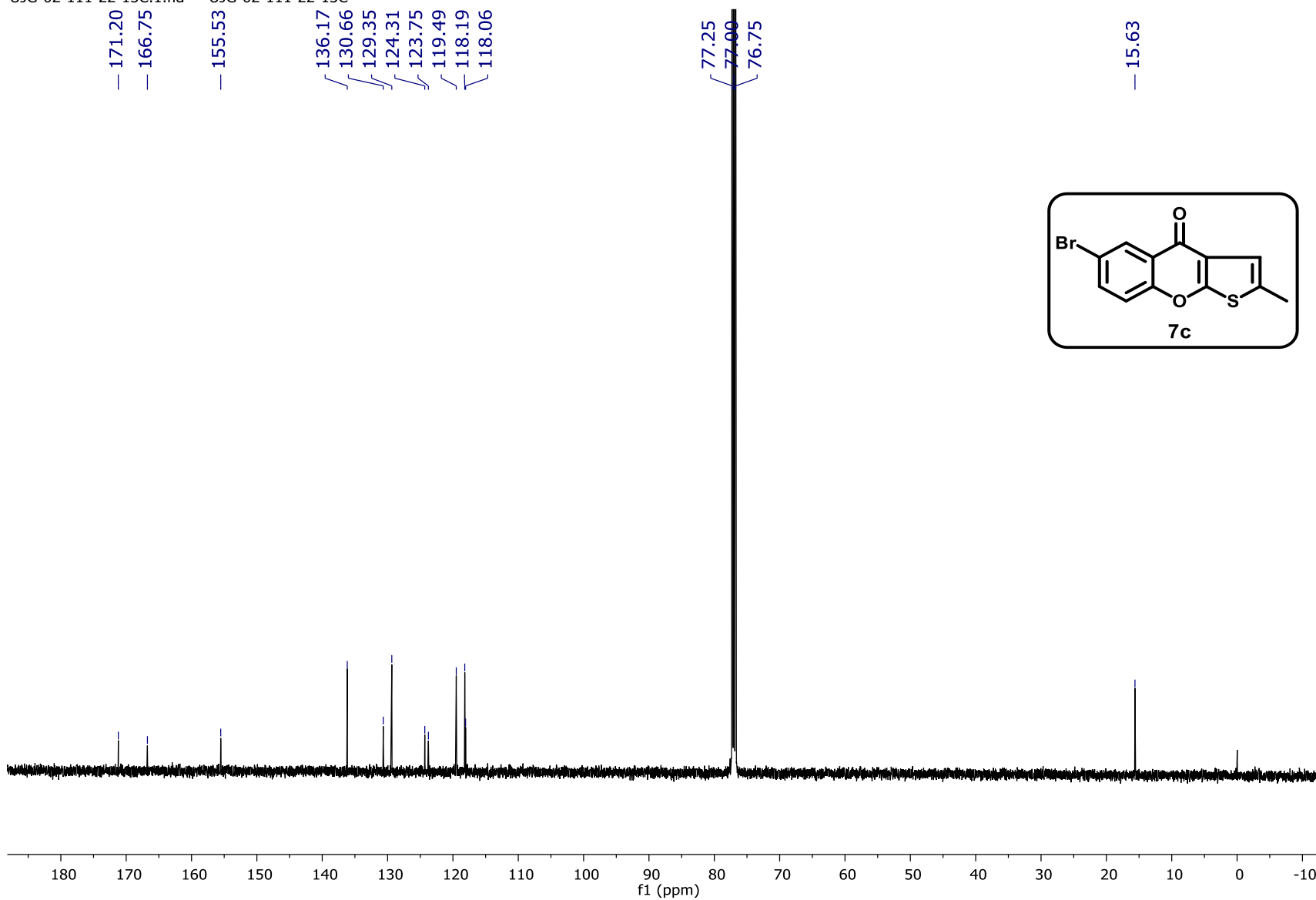
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7c

UJG-02-111-22-1H.3.fid — UJG-02-111-22-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7c

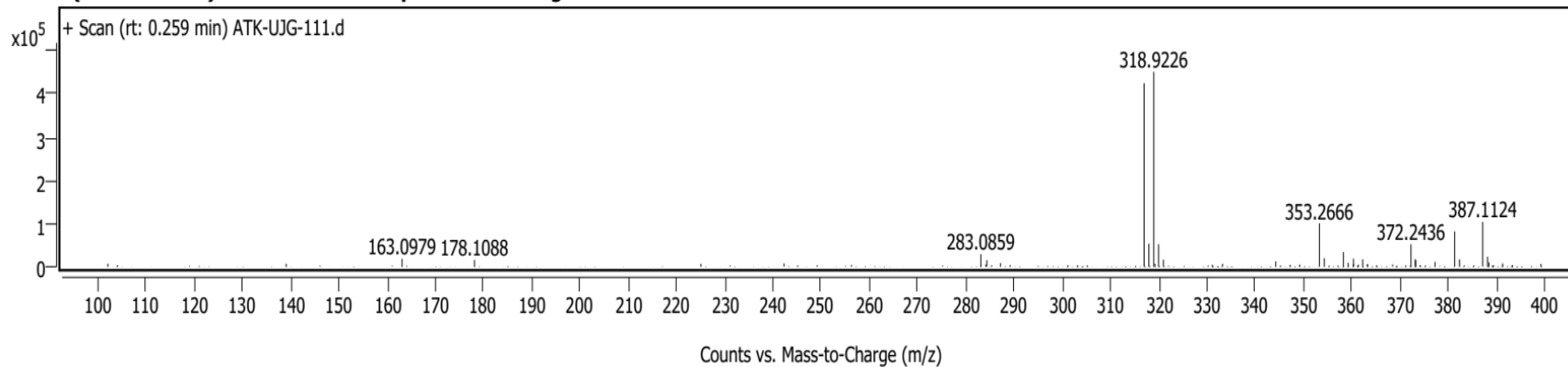
UJG-02-111-22-13C.1.fid — UJG-02-111-22-13C



HRMS Spectrum of Compound 7c

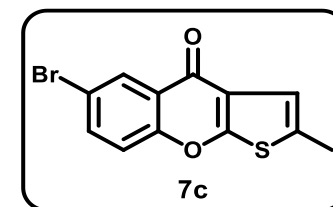
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SpectrumIdString



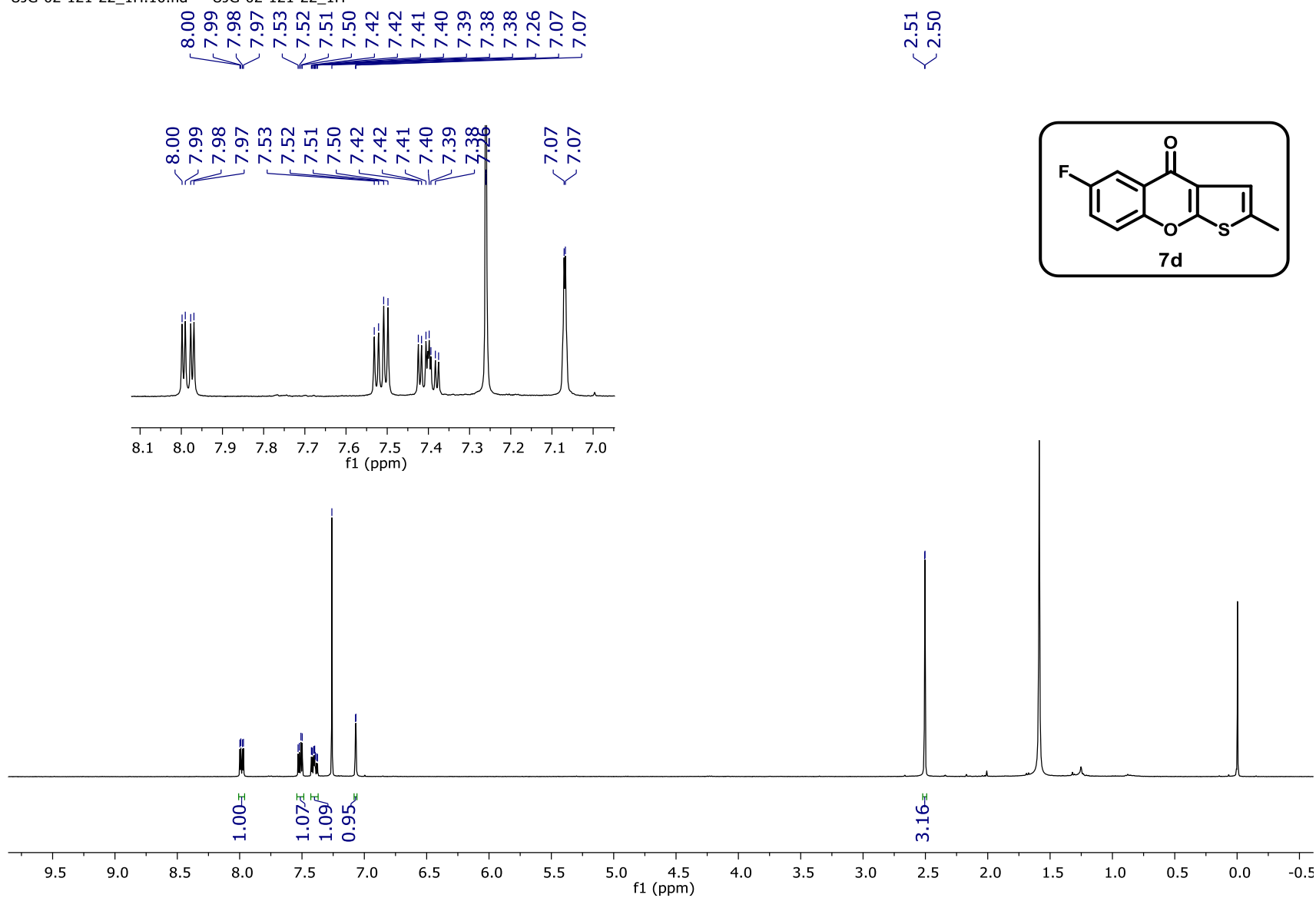
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m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula
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178.1088		15695	3.48				
283.0859		28922	6.41				
316.9246	1	424439	94.11				
317.9279	1	52886	11.73				
318.9226	1	451020	100.00				
319.9255	1	52205	11.57				
320.9196	1	16173	3.59				
353.2666	1	100400	22.26				
354.2695	1	19674	4.36				
358.2278		33894	7.51				
360.3237		18477	4.10				
362.2420		17027	3.78				
372.2436	1	51937	11.52				
373.0968		16950	3.76				
373.2470	1	15366	3.41				
381.2978	1	81728	18.12				
382.3014	1	16774	3.72				
387.1124	1	103734	23.00				
388.1152	1	23275	5.16				



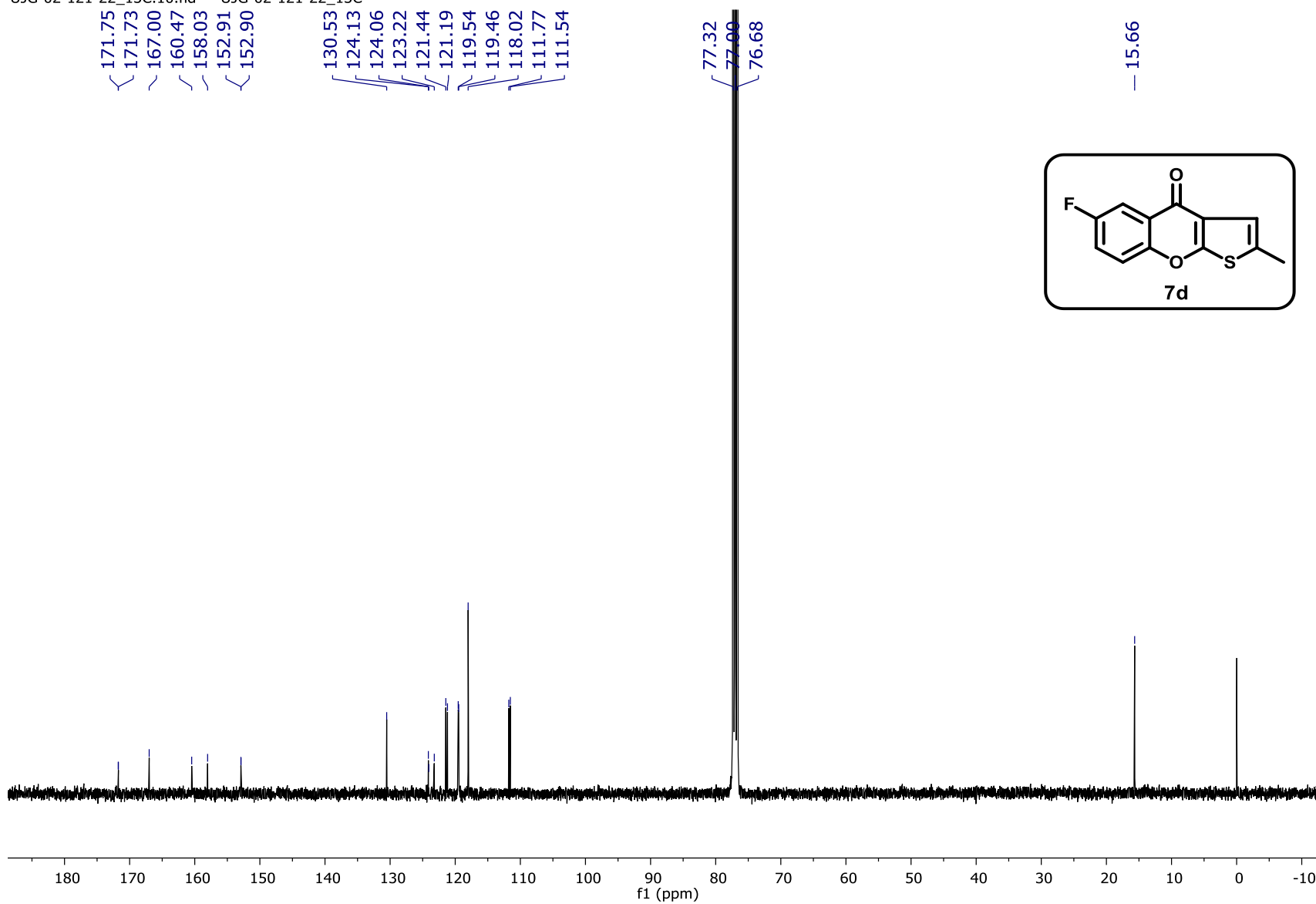
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 7d

UJG-02-121-22_1H.10.fid — UJG-02-121-22_1H



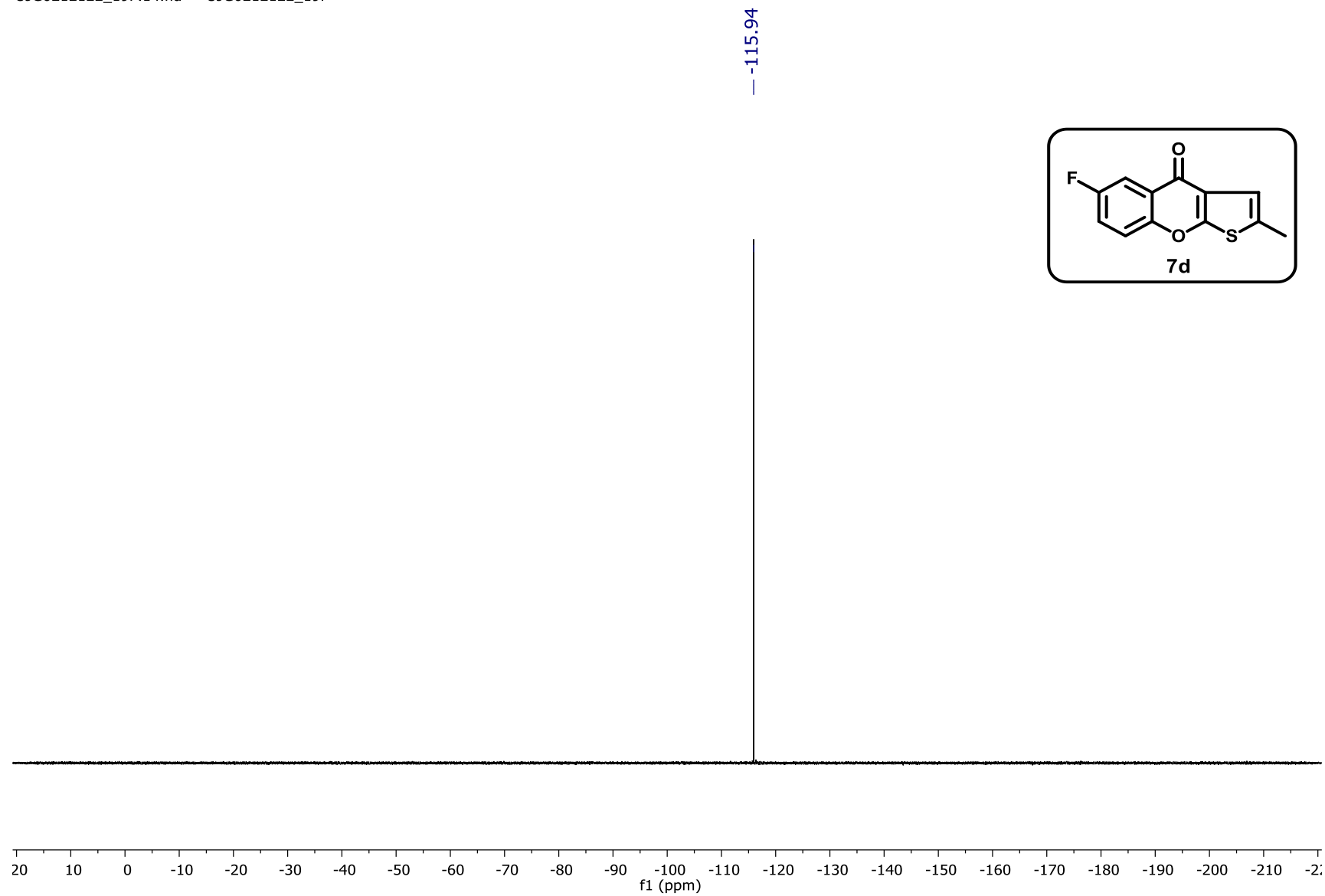
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of Compound 7d

UJG-02-121-22_13C.10.fid — UJG-02-121-22_13C

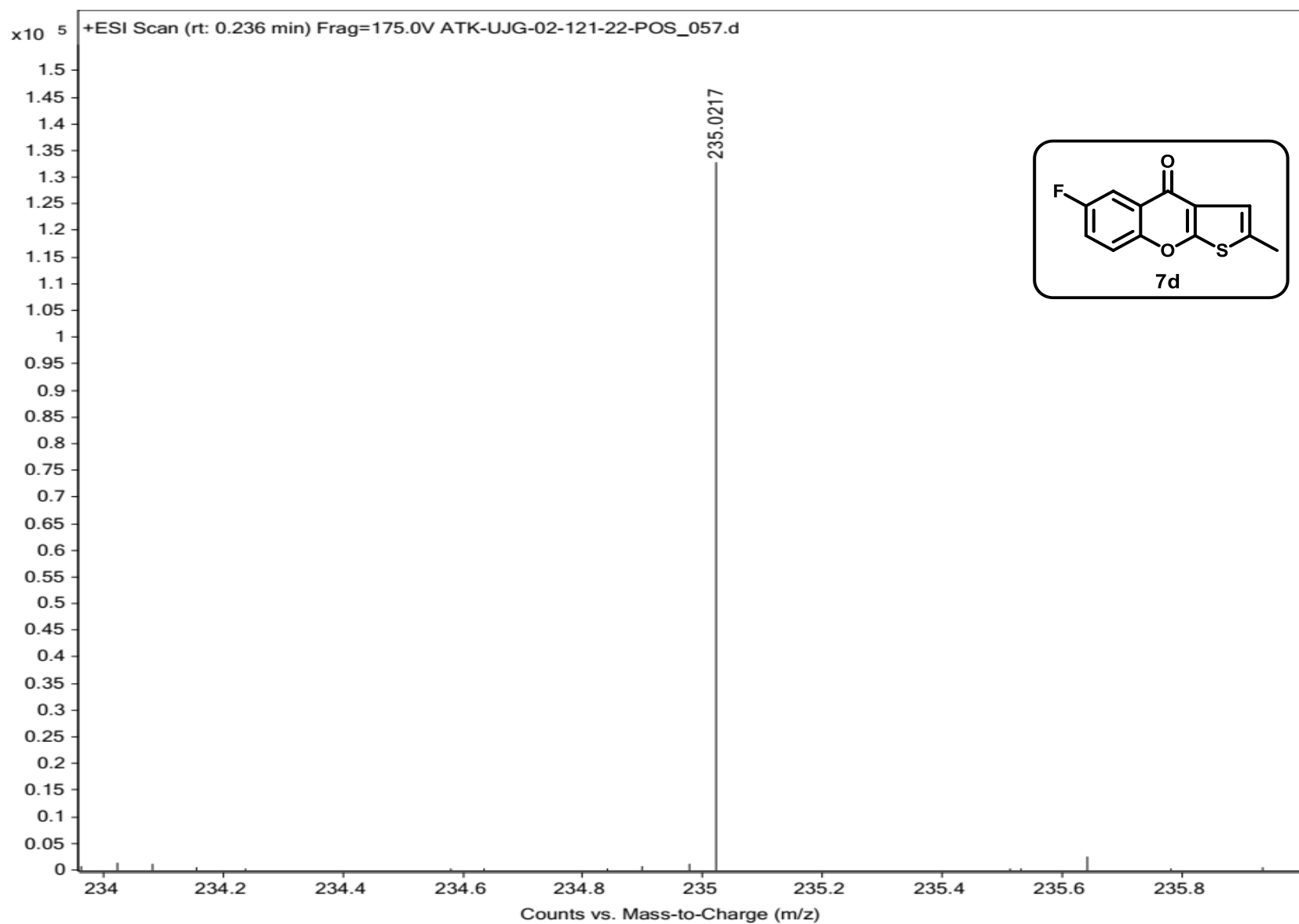


^{19}F NMR (376 MHz, CDCl_3) Spectrum of Compound 7d

UJG0212122_19F.14.fid — UJG0212122_19F

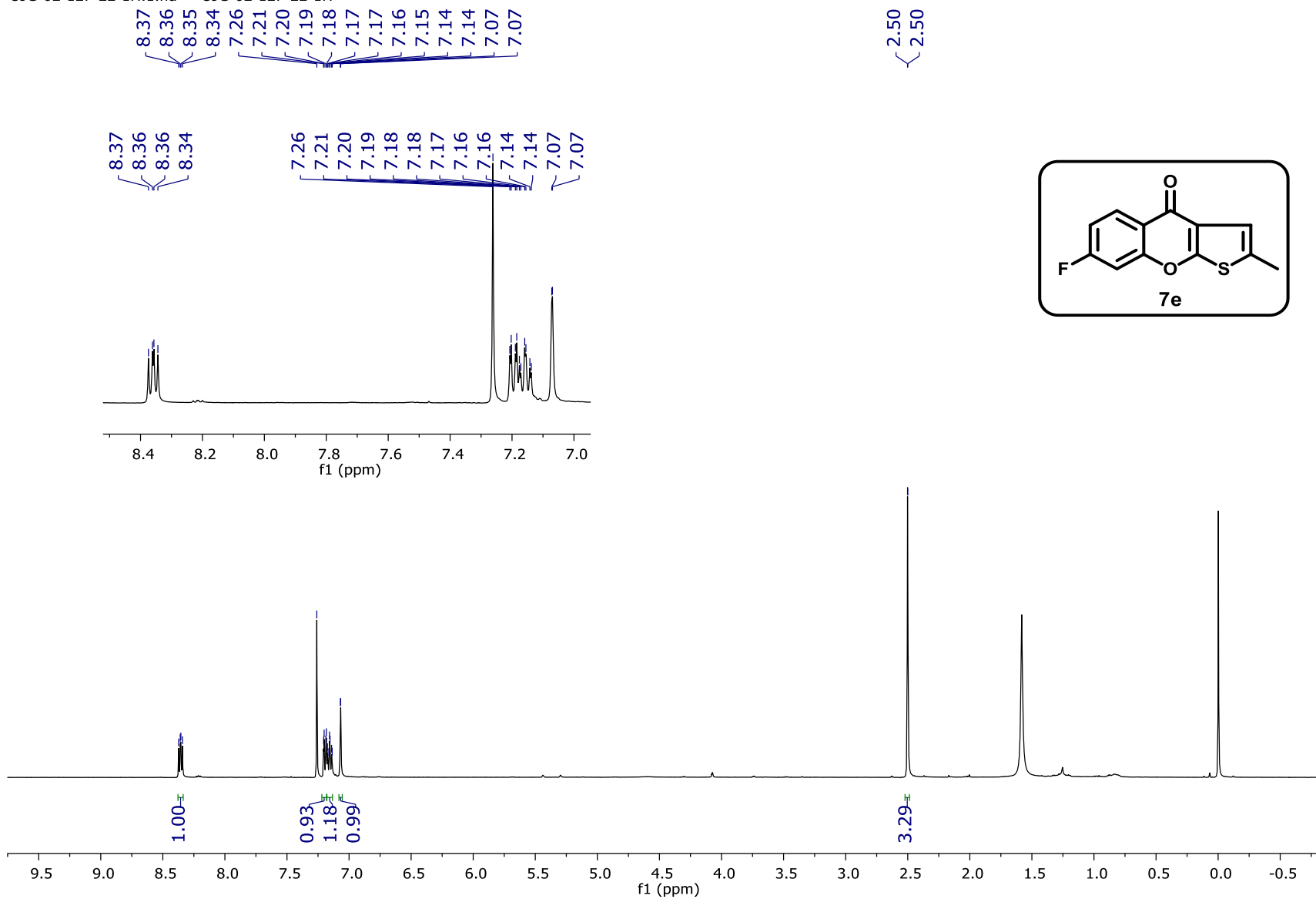


HRMS Spectrum of Compound 7d



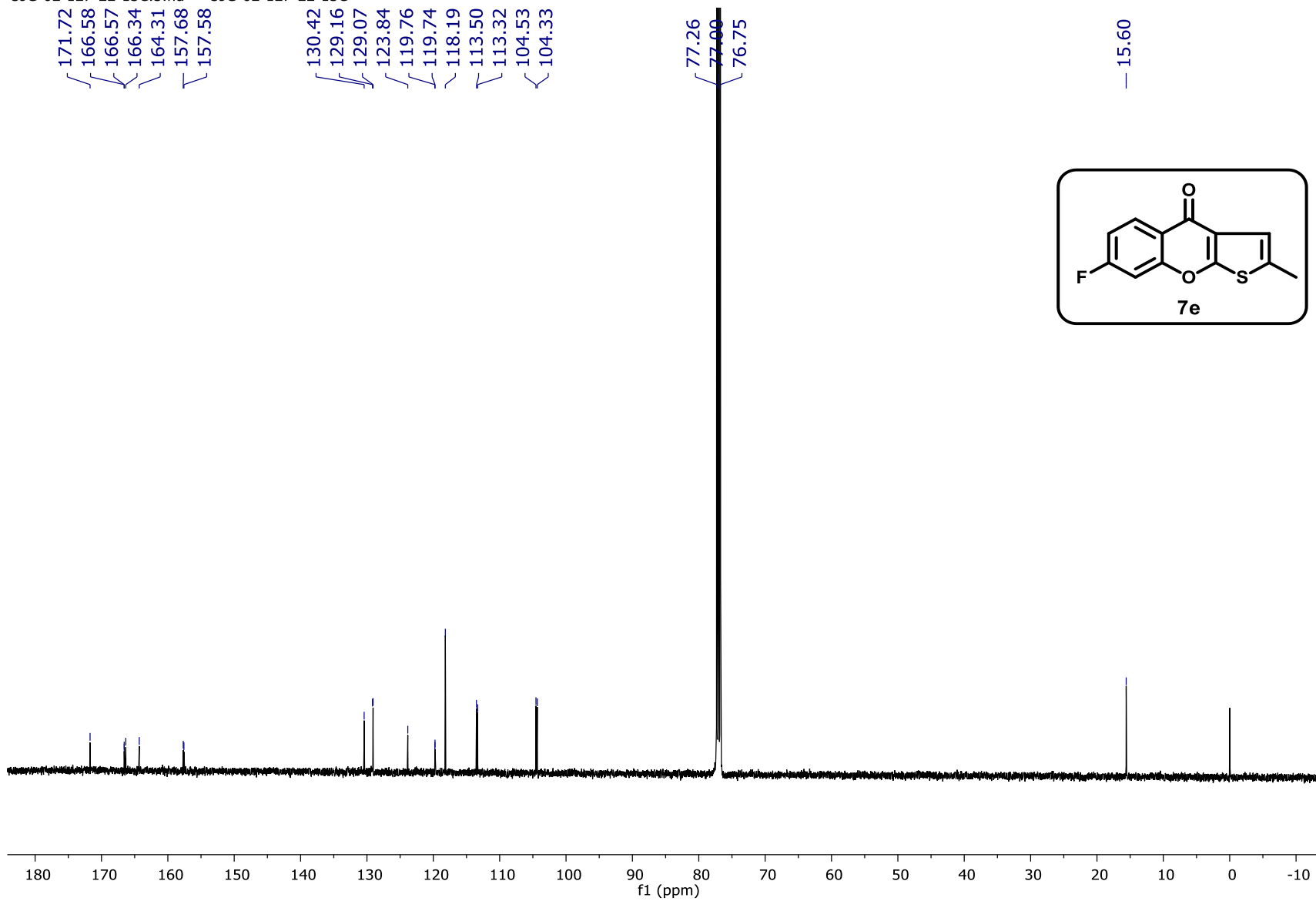
^1H NMR (500 MHz, CDCl_3) Spectrum of Compound 7e

UJG-02-127-22-1H.1.fid — UJG-02-127-22-1H



^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 7e

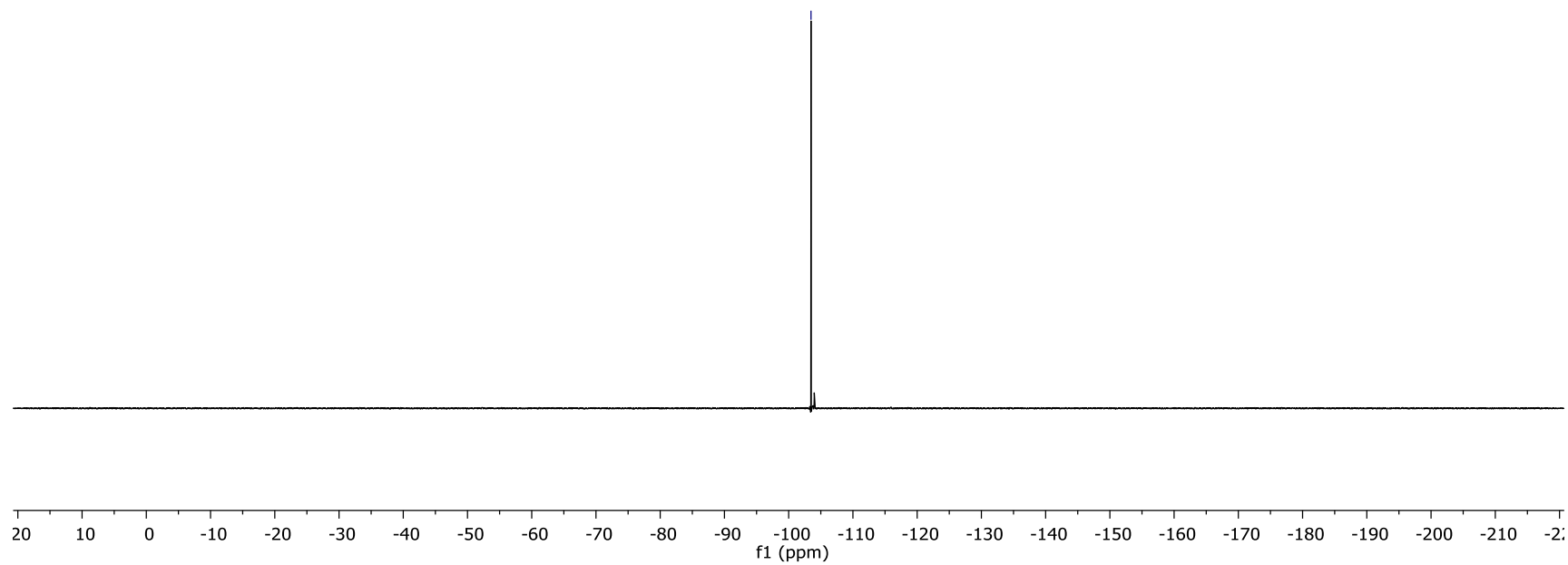
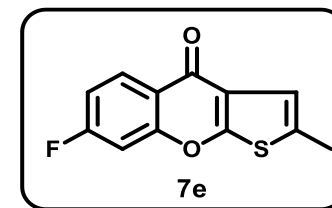
UJG-02-127-22-13C.5.fid — UJG-02-127-22-13C



^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 7e

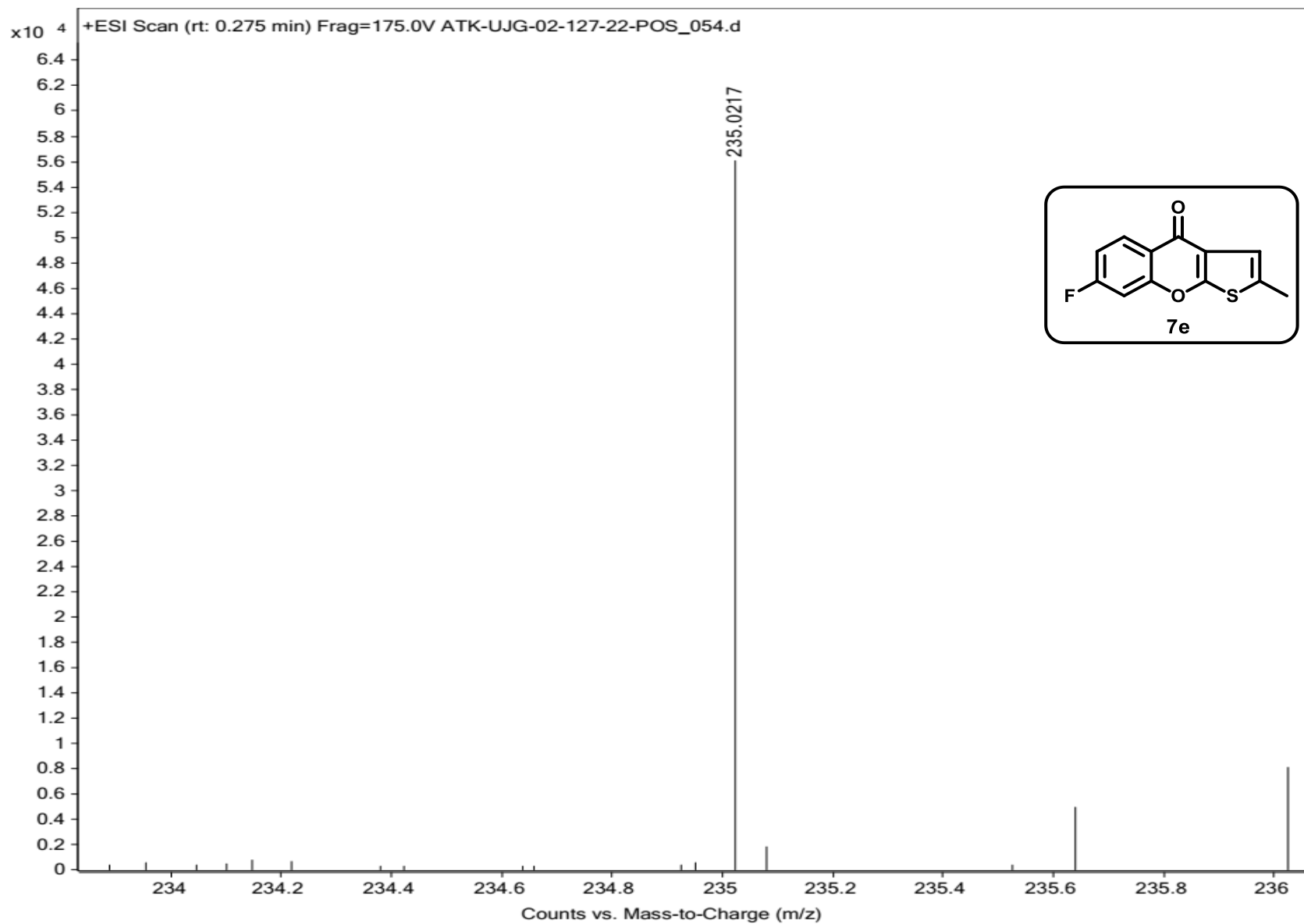
UJG-02-127-22-19F.3.fid — UJG-02-127-22-19F

— -103.48



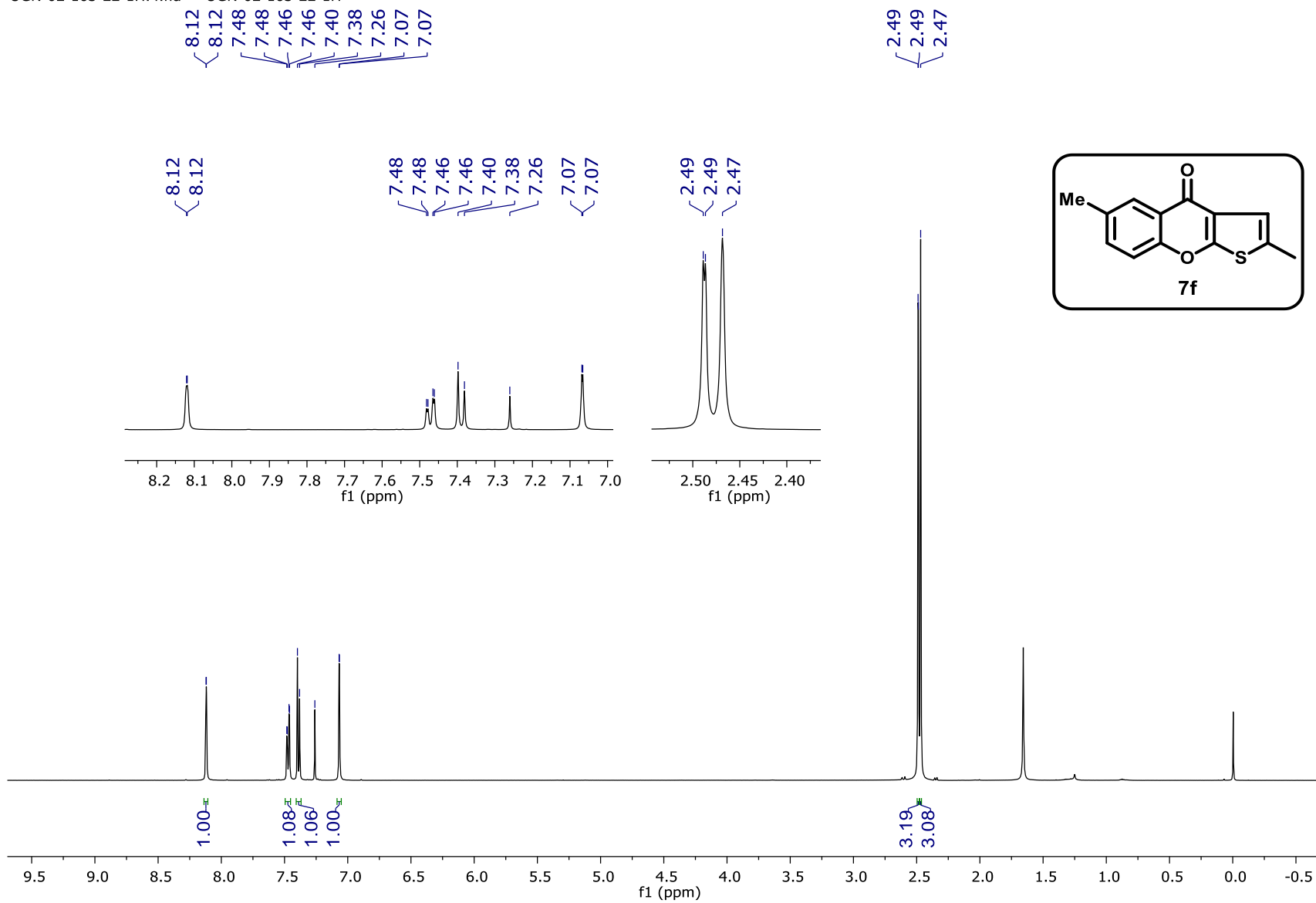
S160

HRMS Spectrum of Compound 7e



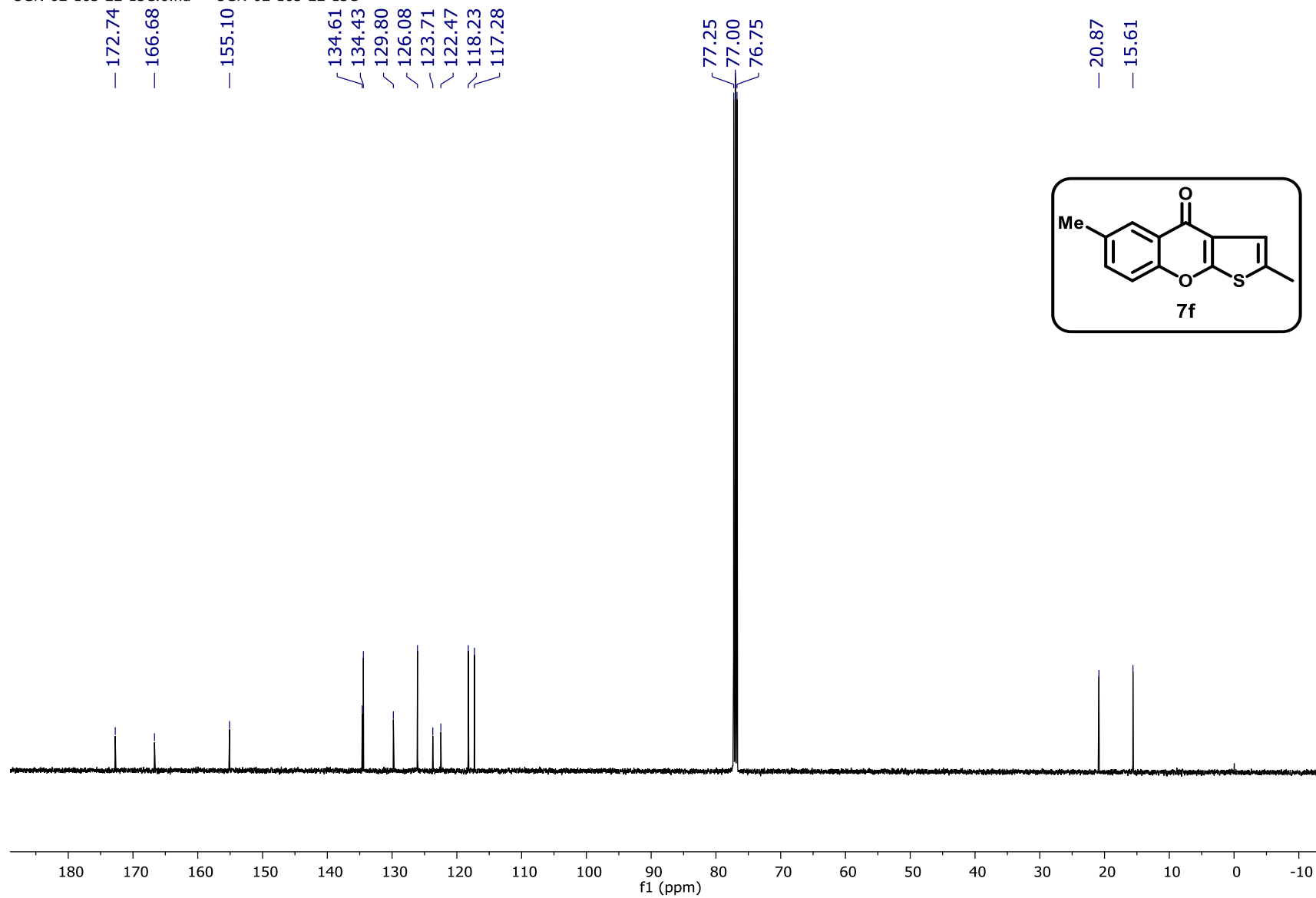
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7f

UGN-02-163-22-1H.4.fid — UGN-02-163-22-1H

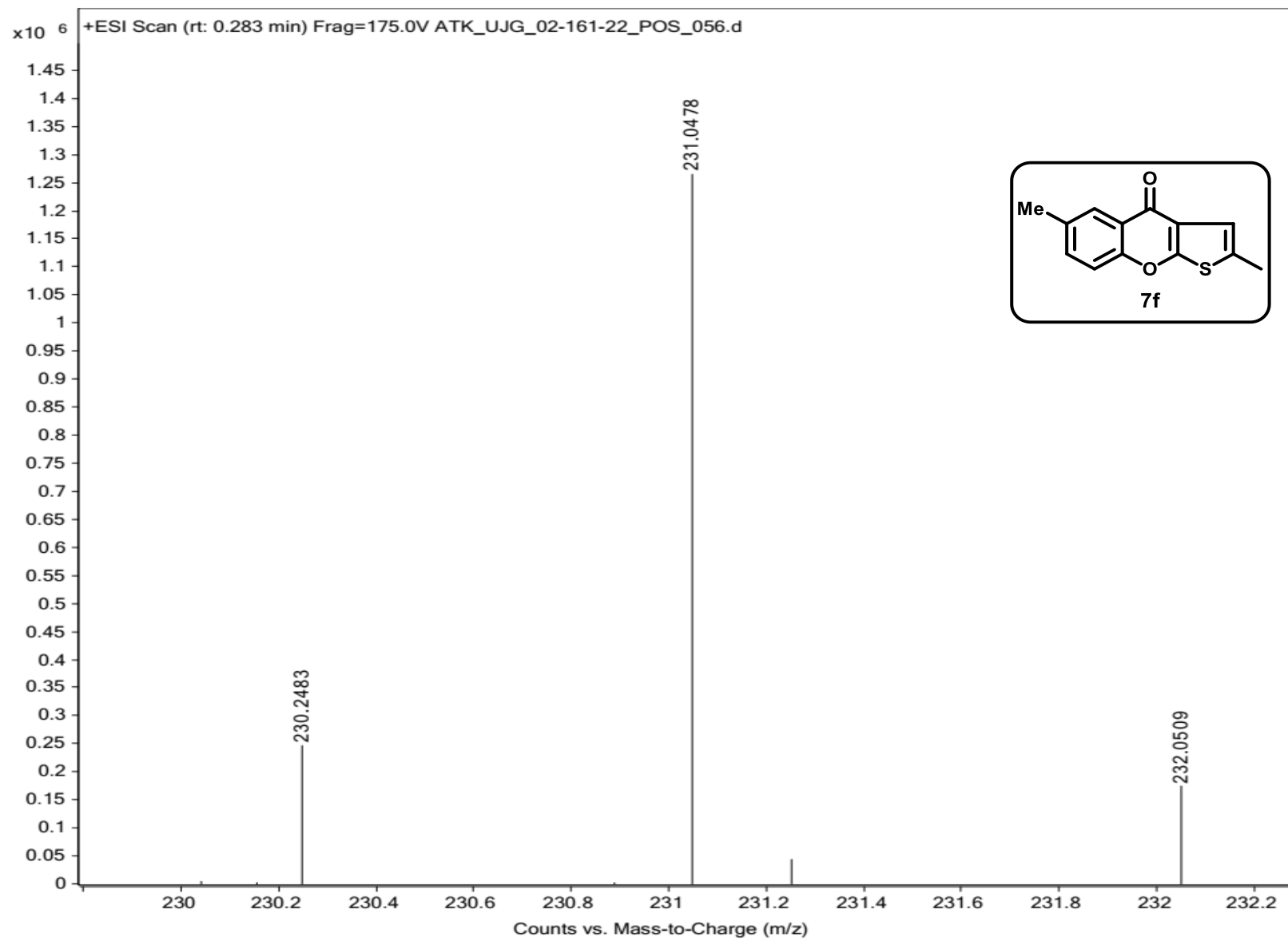


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 7f

UGN-02-163-22-13C.6.fid — UGN-02-163-22-13C

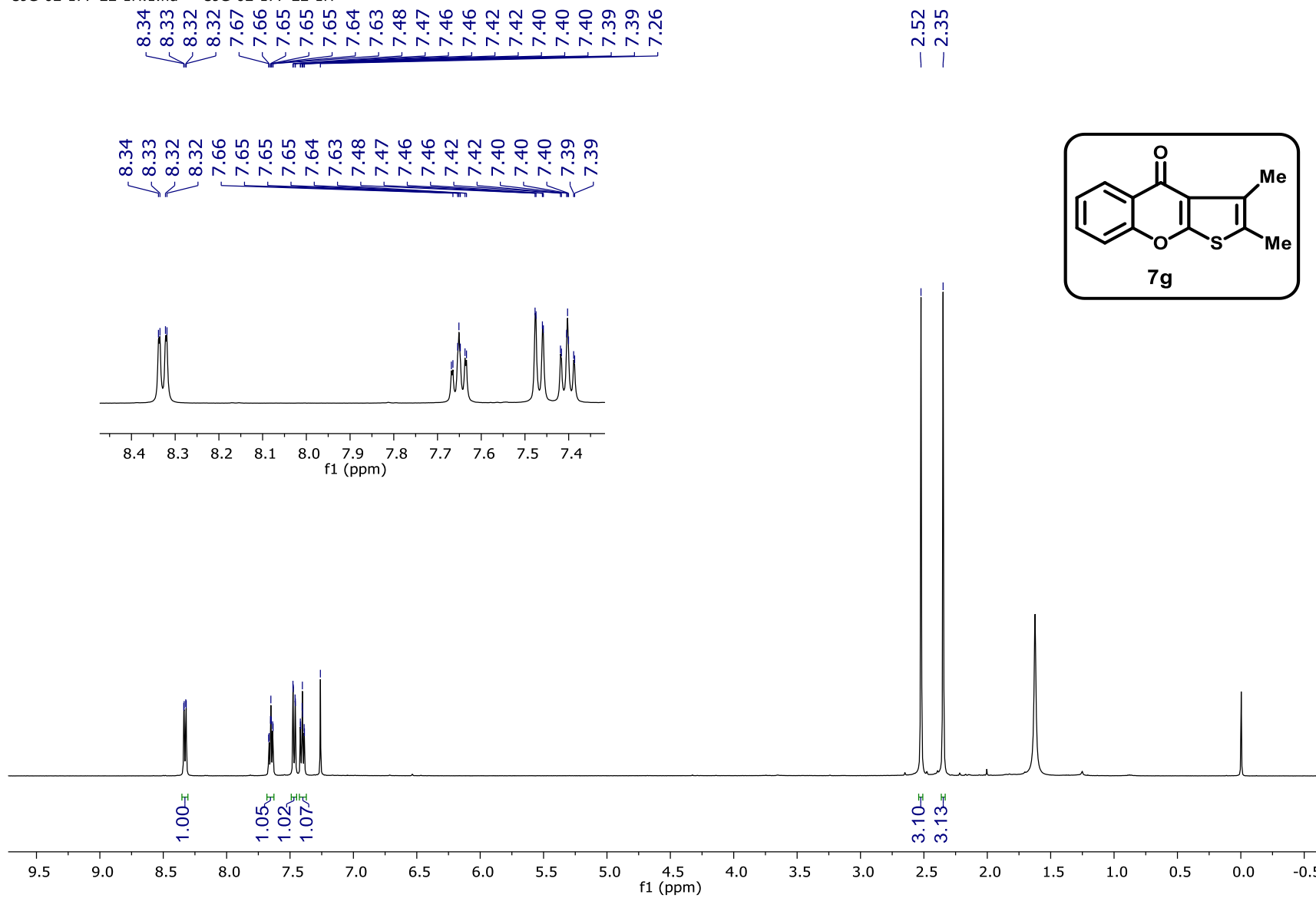


HRMS Spectrum of Compound 7f



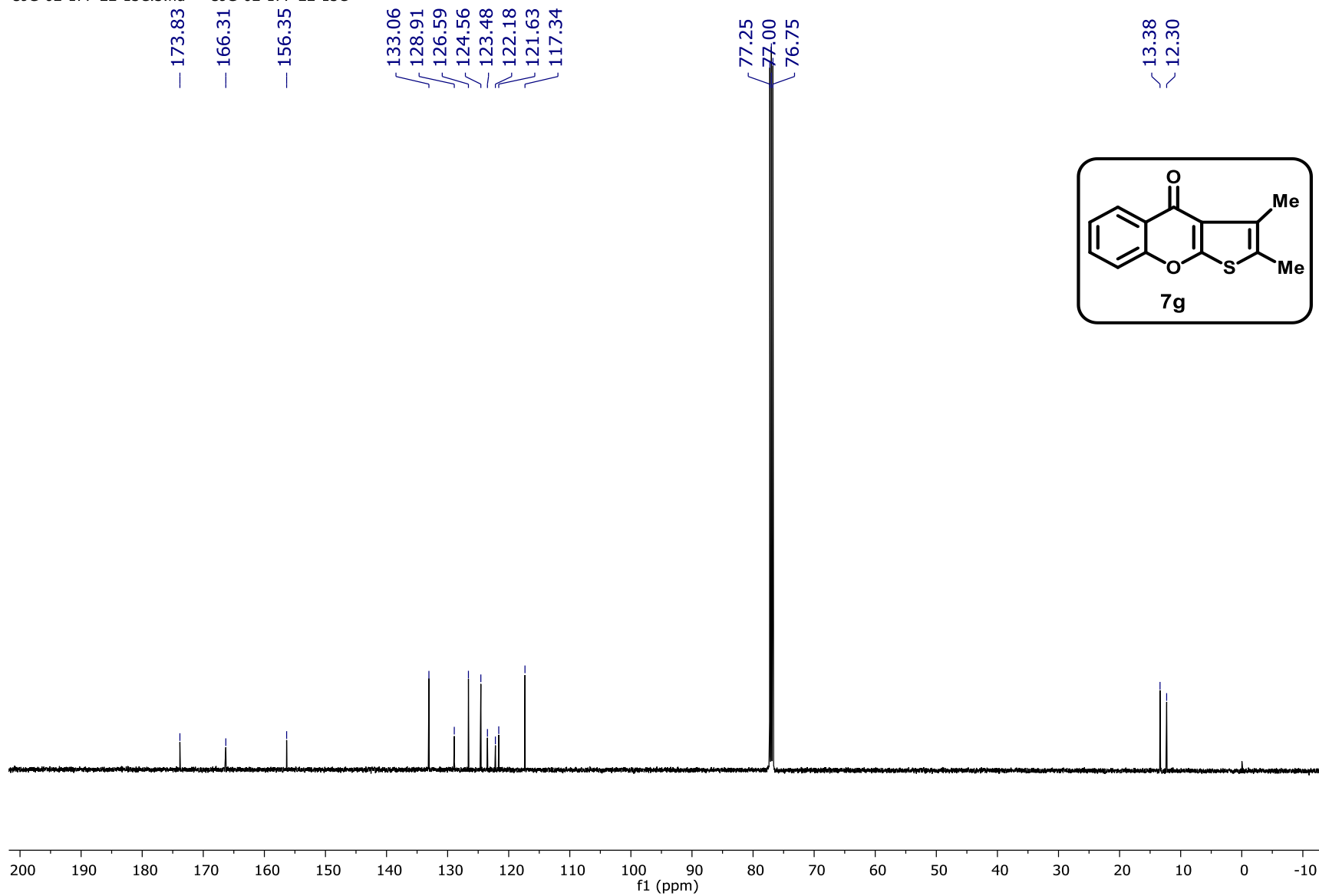
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7g

UJG-02-177-22-1H.1.fid — UJG-02-177-22-1H

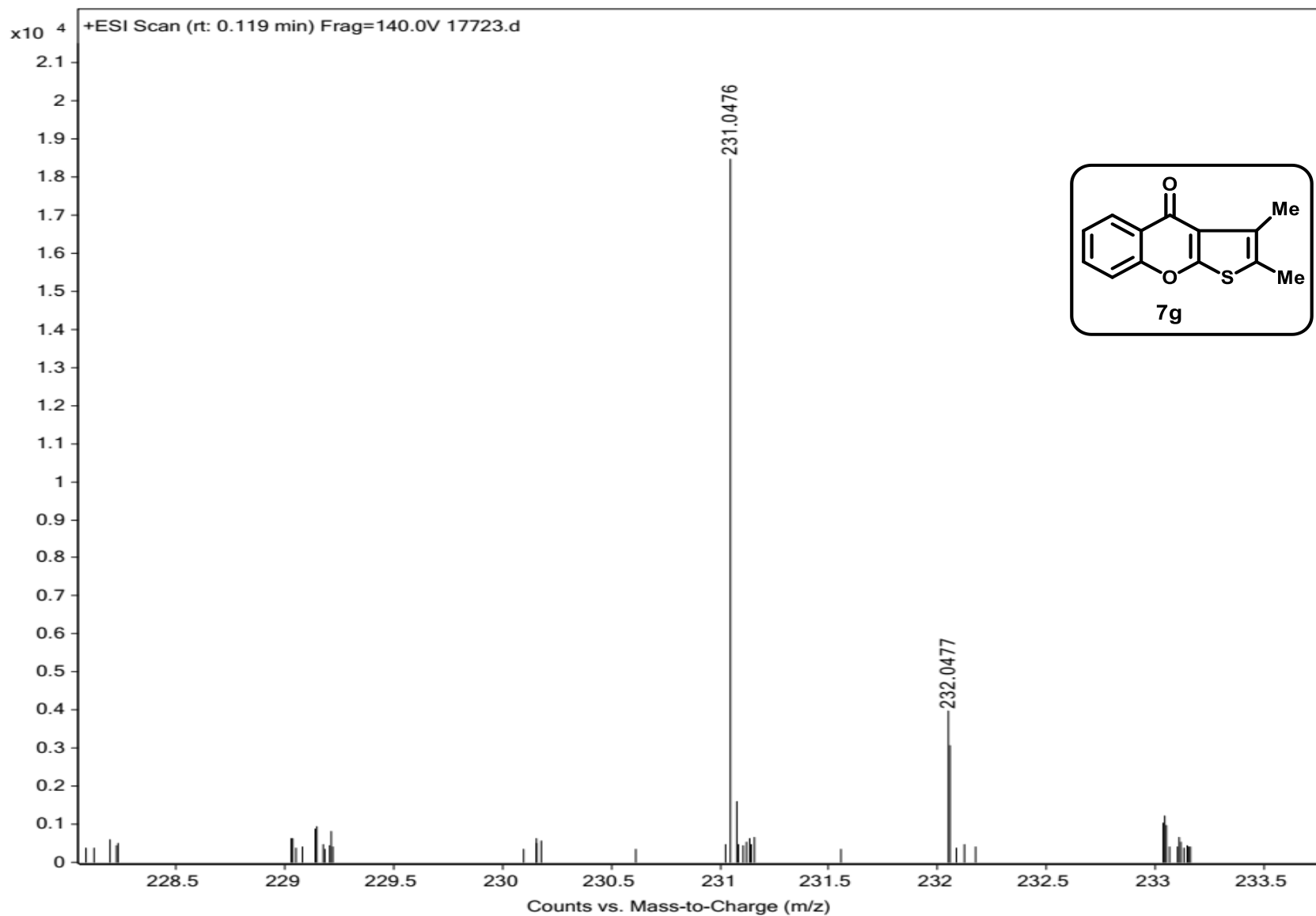


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7g

UJG-02-177-22-13C.3.fid — UJG-02-177-22-13C

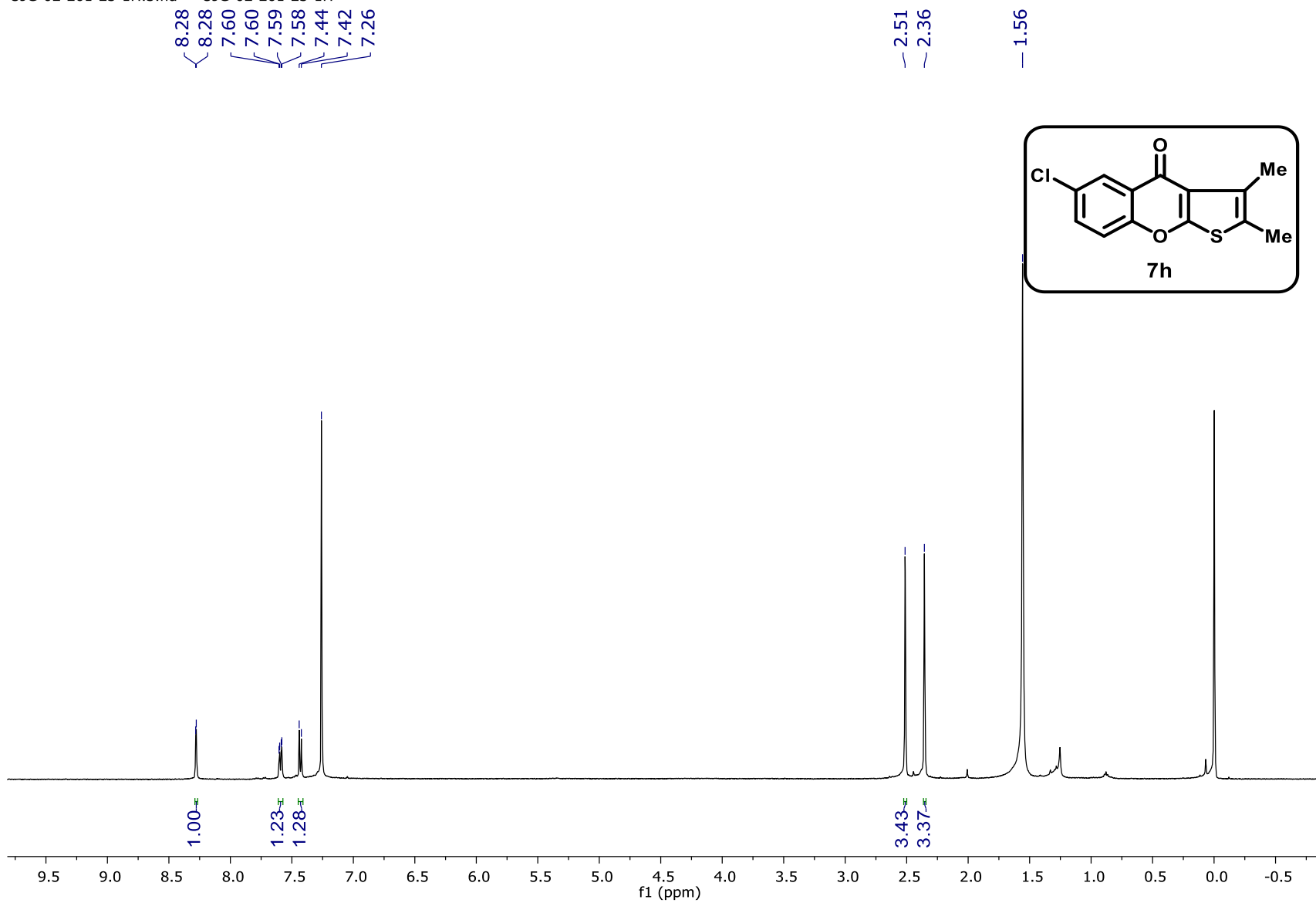


HRMS Spectrum of Compound 7g



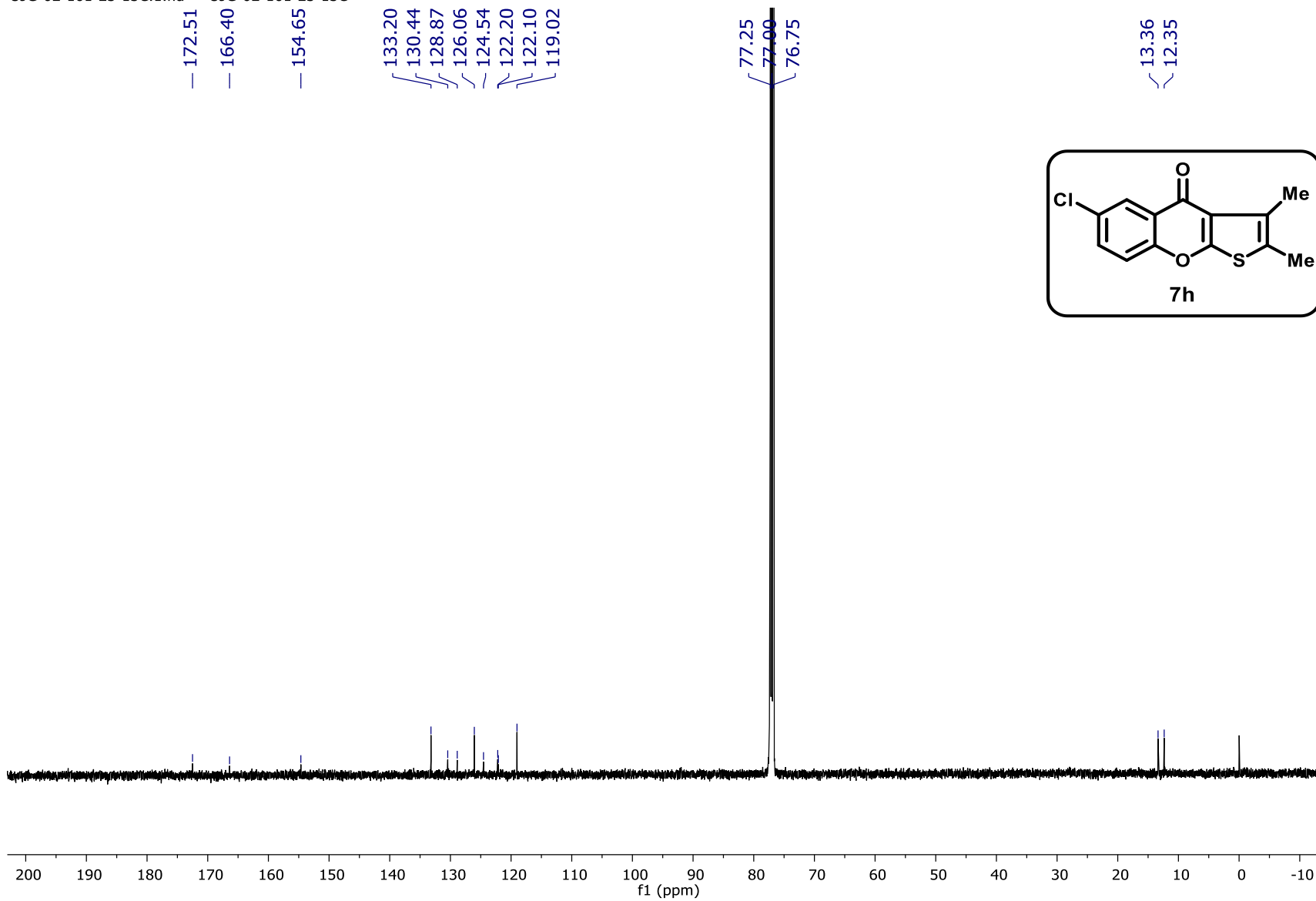
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7h

UJG-02-261-23-1H.3.fid — UJG-02-261-23-1H



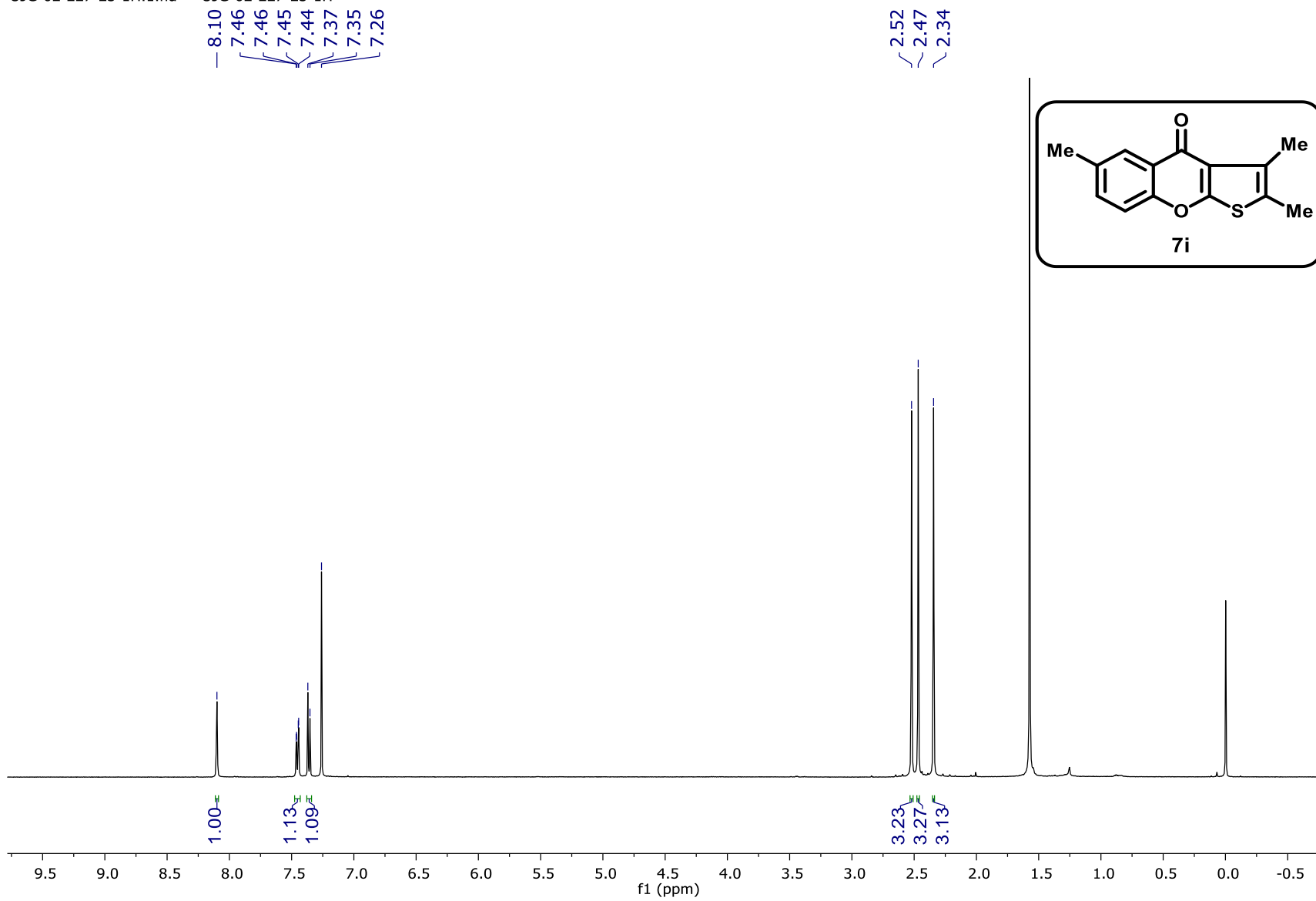
¹³C {¹H} NMR (125 MHz, CDCl₃) Spectrum of Compound 7h

UJG-02-161-23-13C.1.fid — UJG-02-161-23-13C



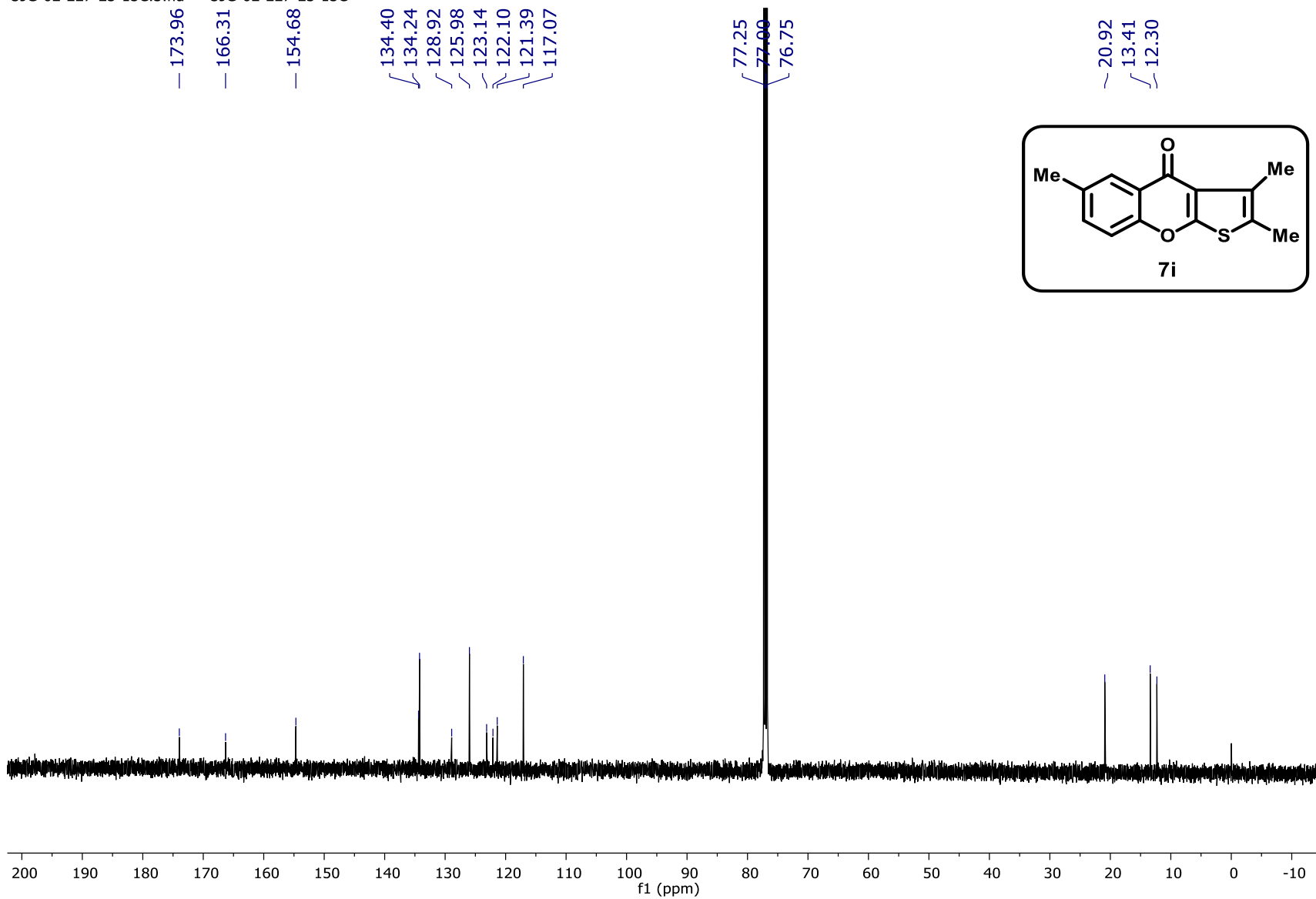
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7i

UJG-02-227-23-1H.1.fid — UJG-02-227-23-1H

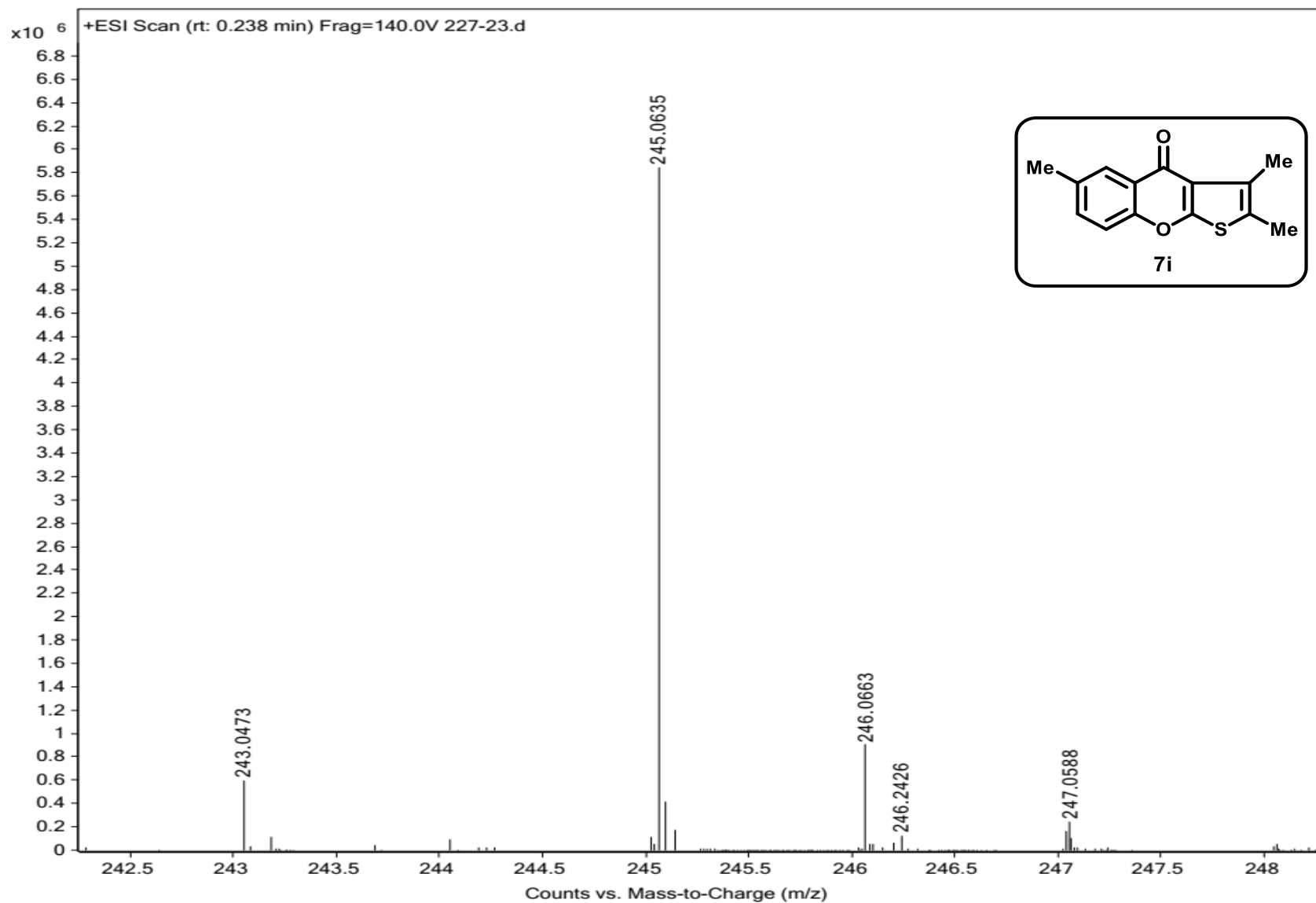


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7i

UJG-02-227-23-13C.3.fid — UJG-02-227-23-13C



HRMS Spectrum of Compound 7i

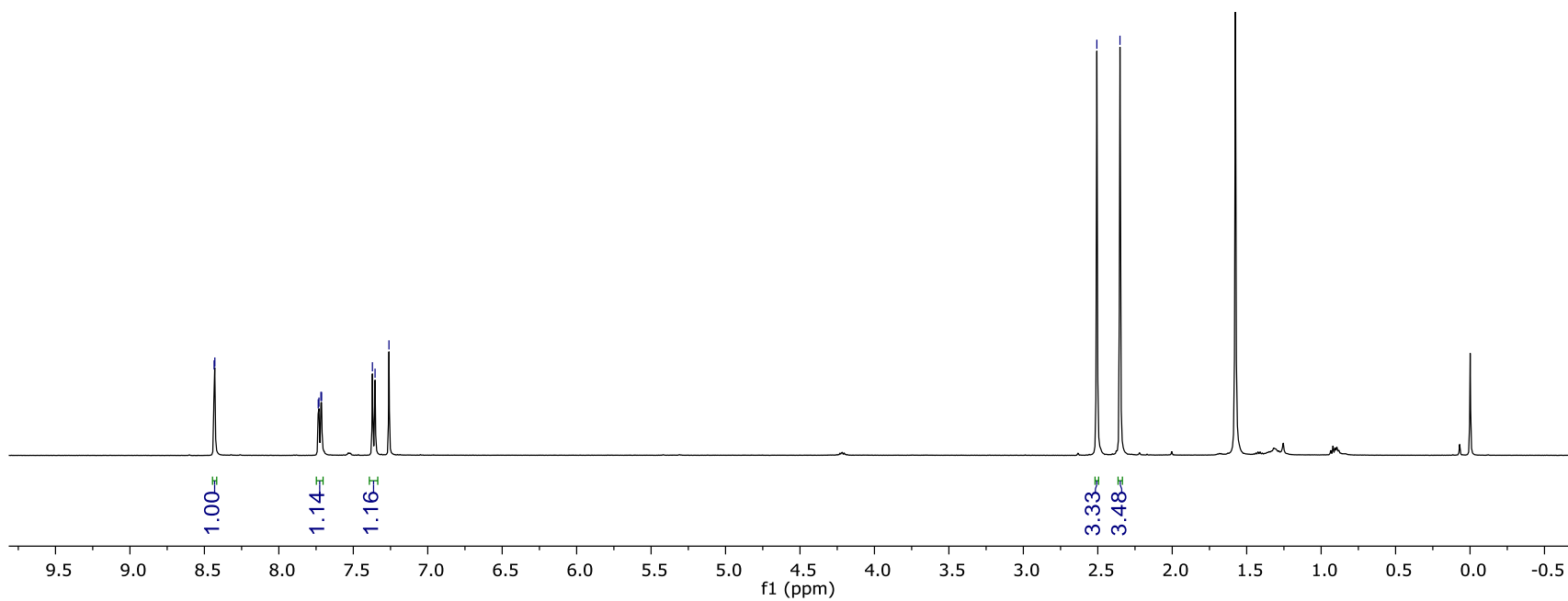
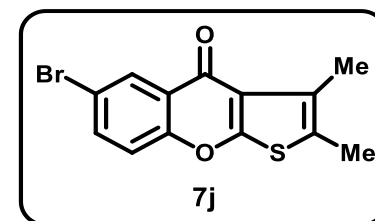


¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7j

UJG-02-191-23-1H.1.fid — UJG-02-191-23-1H

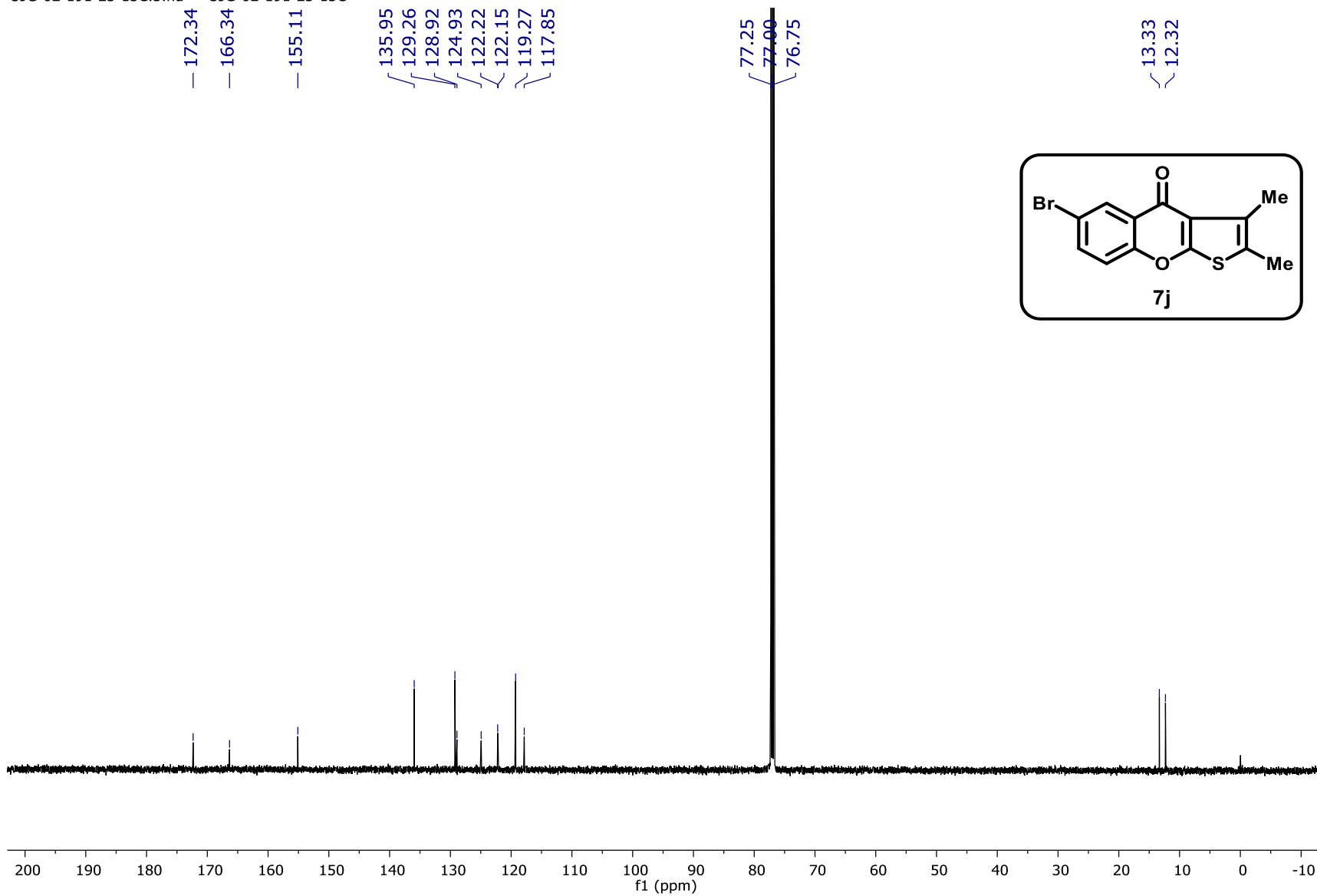
8.43
8.43
7.74
7.73
7.72
7.71
7.37
7.35
7.26

2.51
2.35

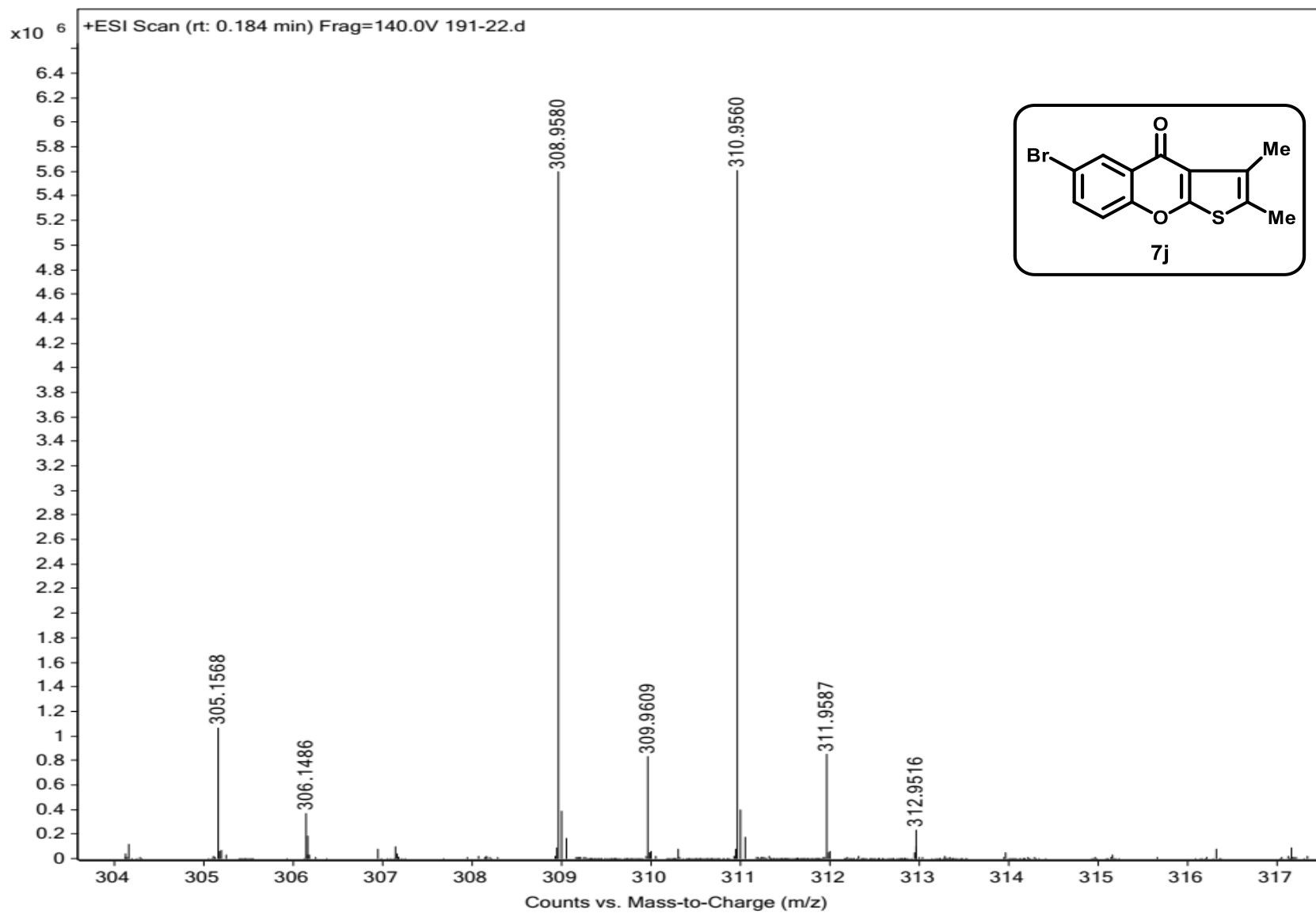


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7j

UJG-02-191-23-13C.3.fid — UJG-02-191-23-13C

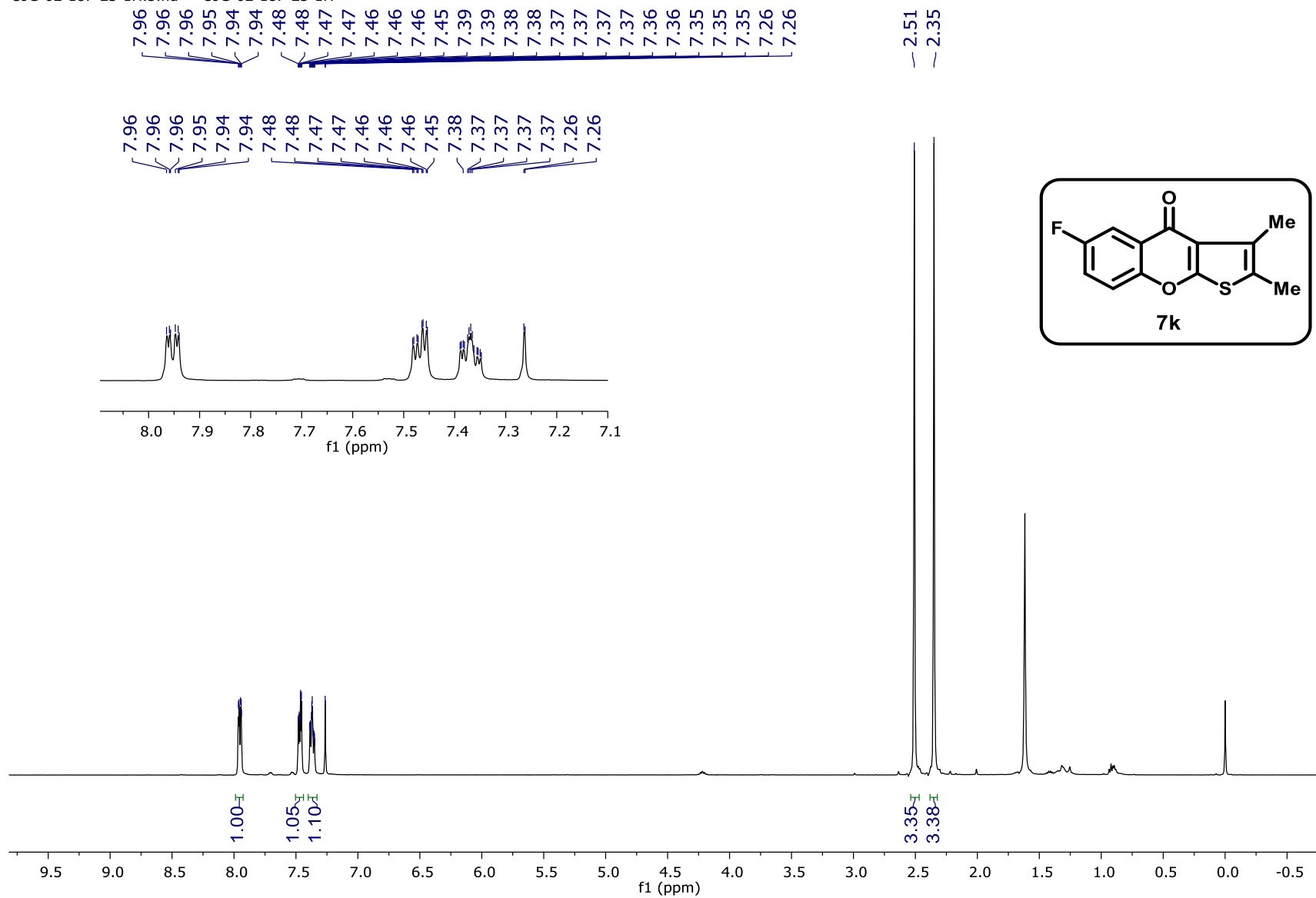


HRMS Spectrum of Compound 7j



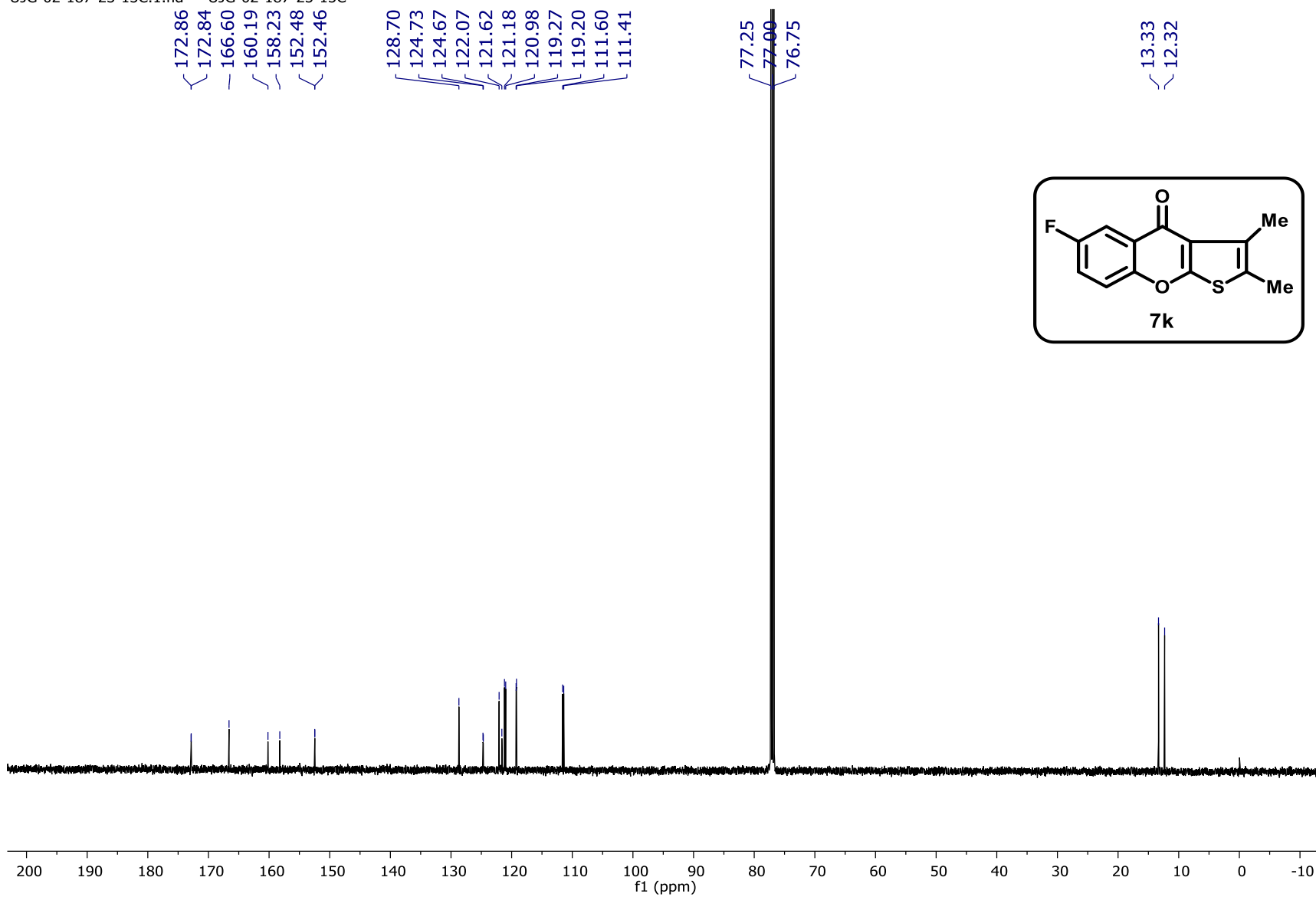
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7k

UJG-02-187-23-1H.5.fid — UJG-02-187-23-1H



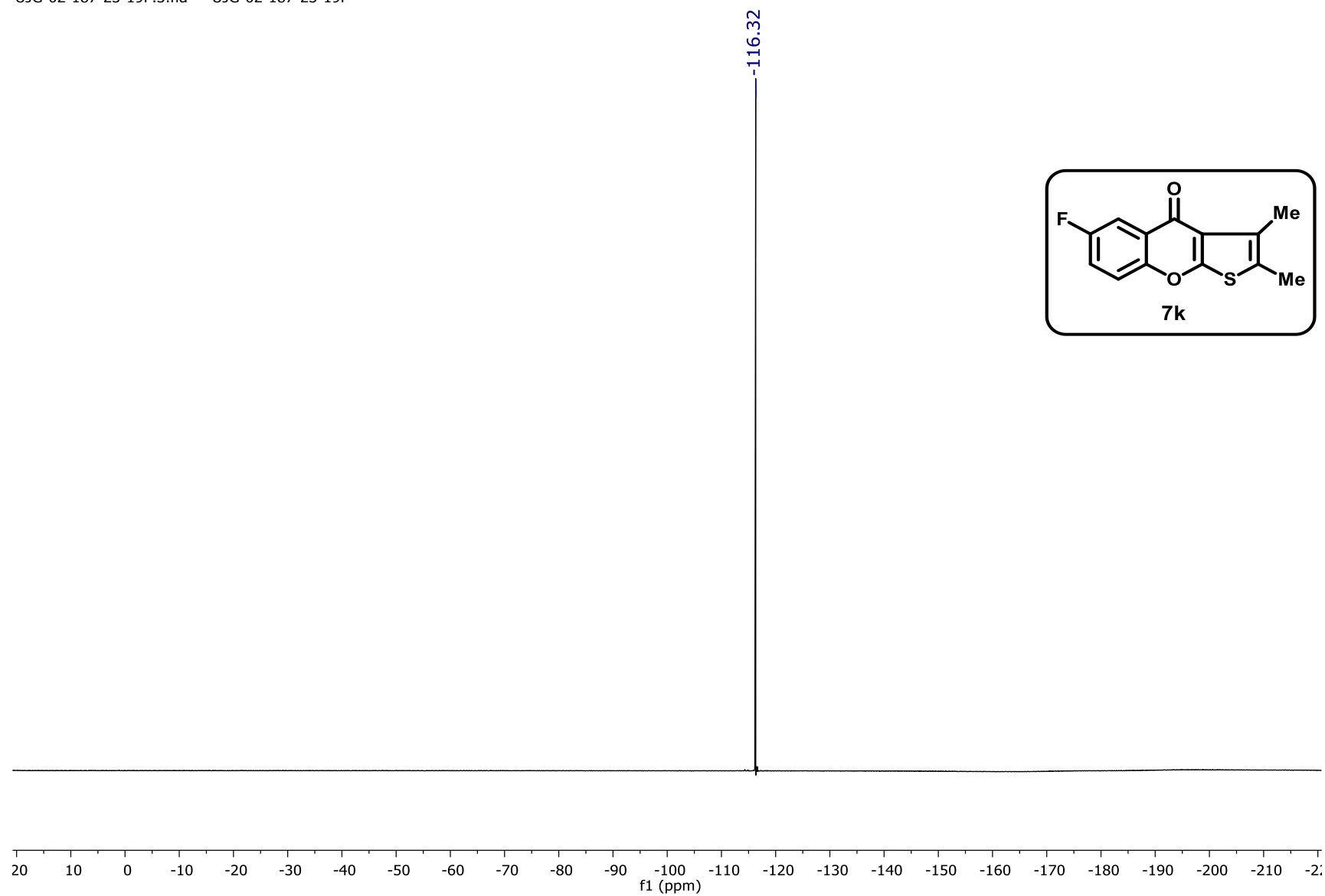
^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 7k

UJG-02-187-23-13C.1.fid — UJG-02-187-23-13C



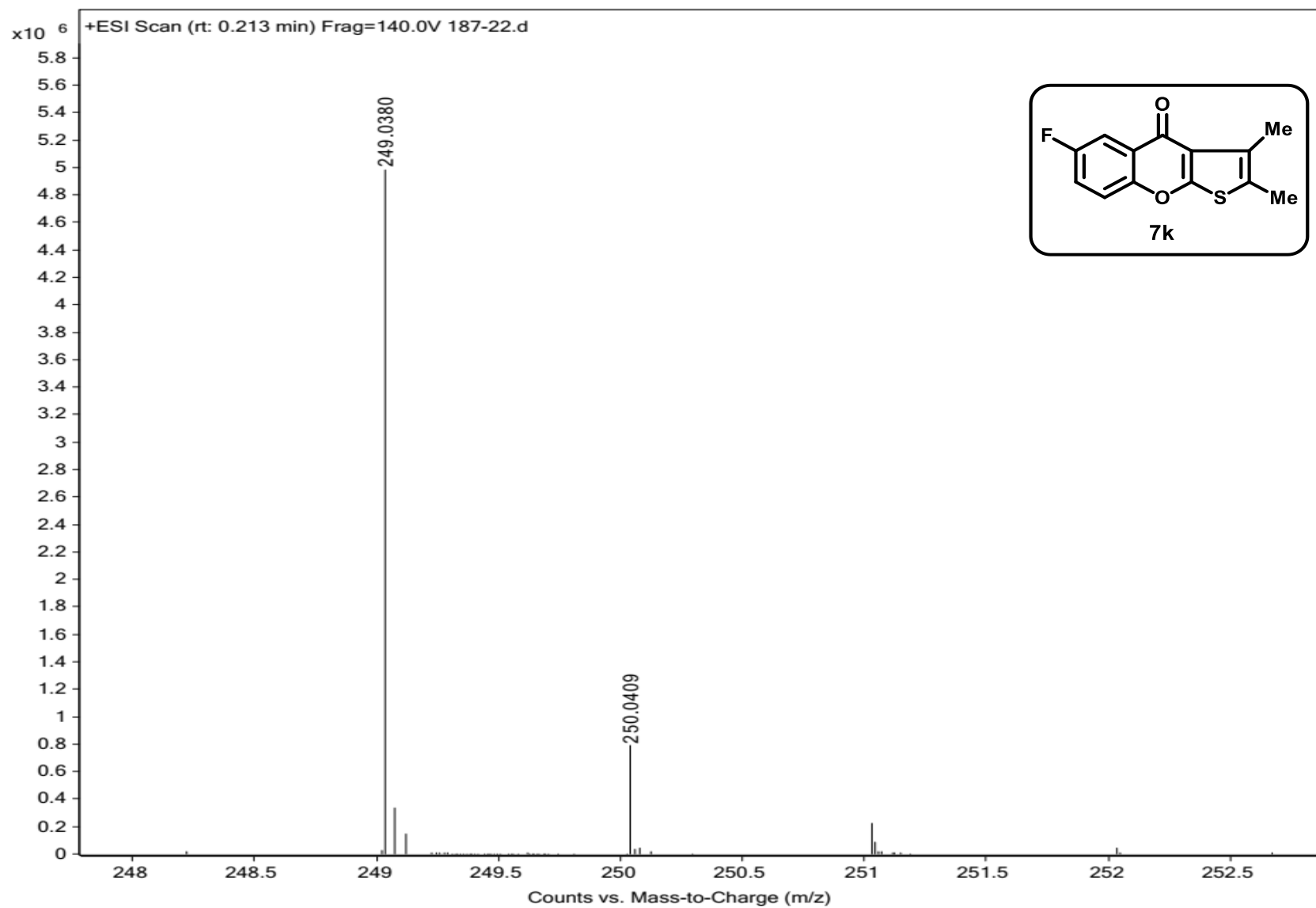
^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 7k

UJG-02-187-23-19F.3.fid — UJG-02-187-23-19F



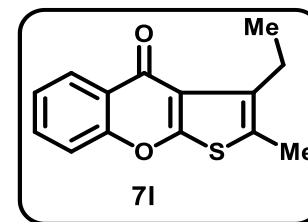
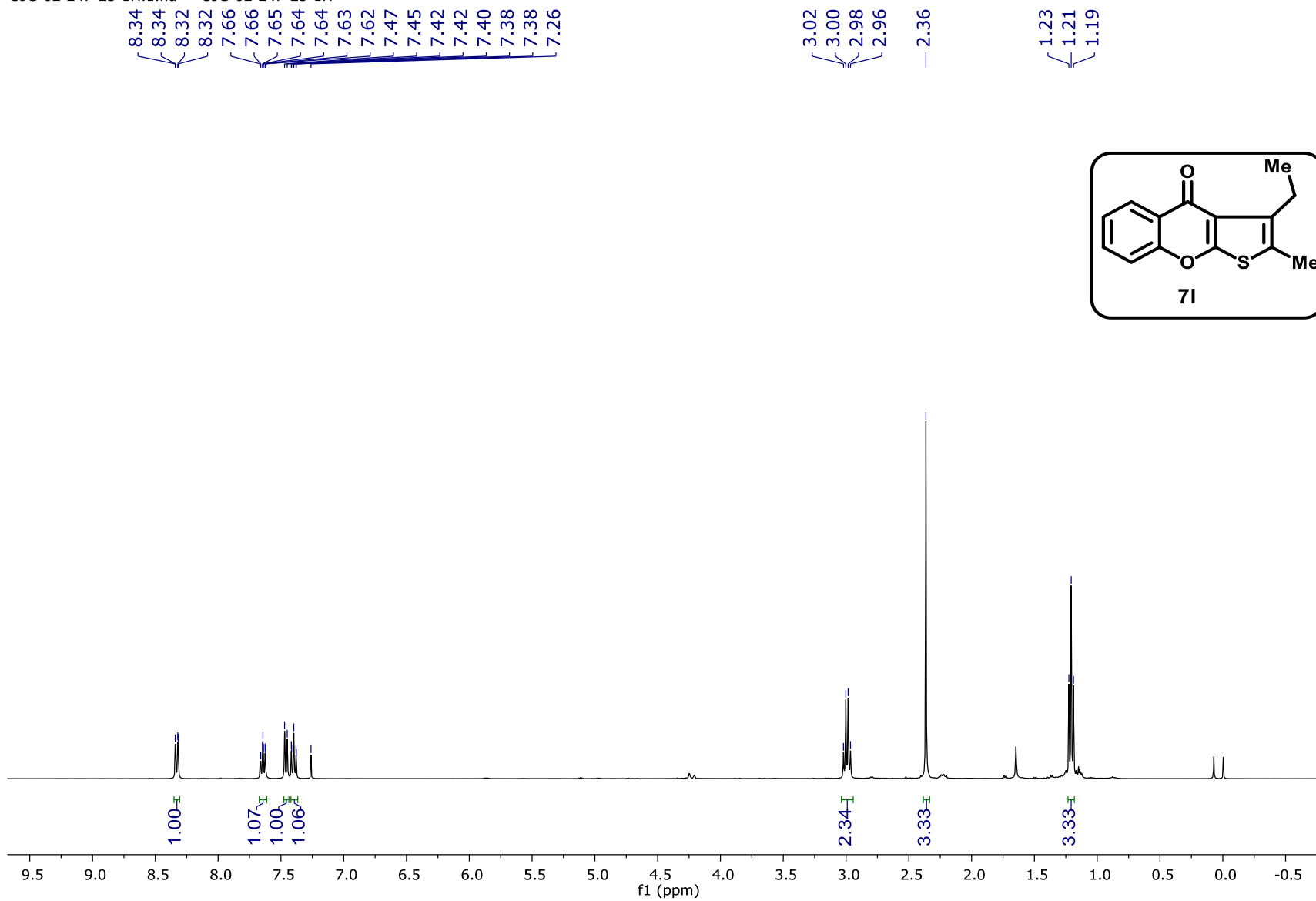
S178

HRMS Spectrum of Compound 7k



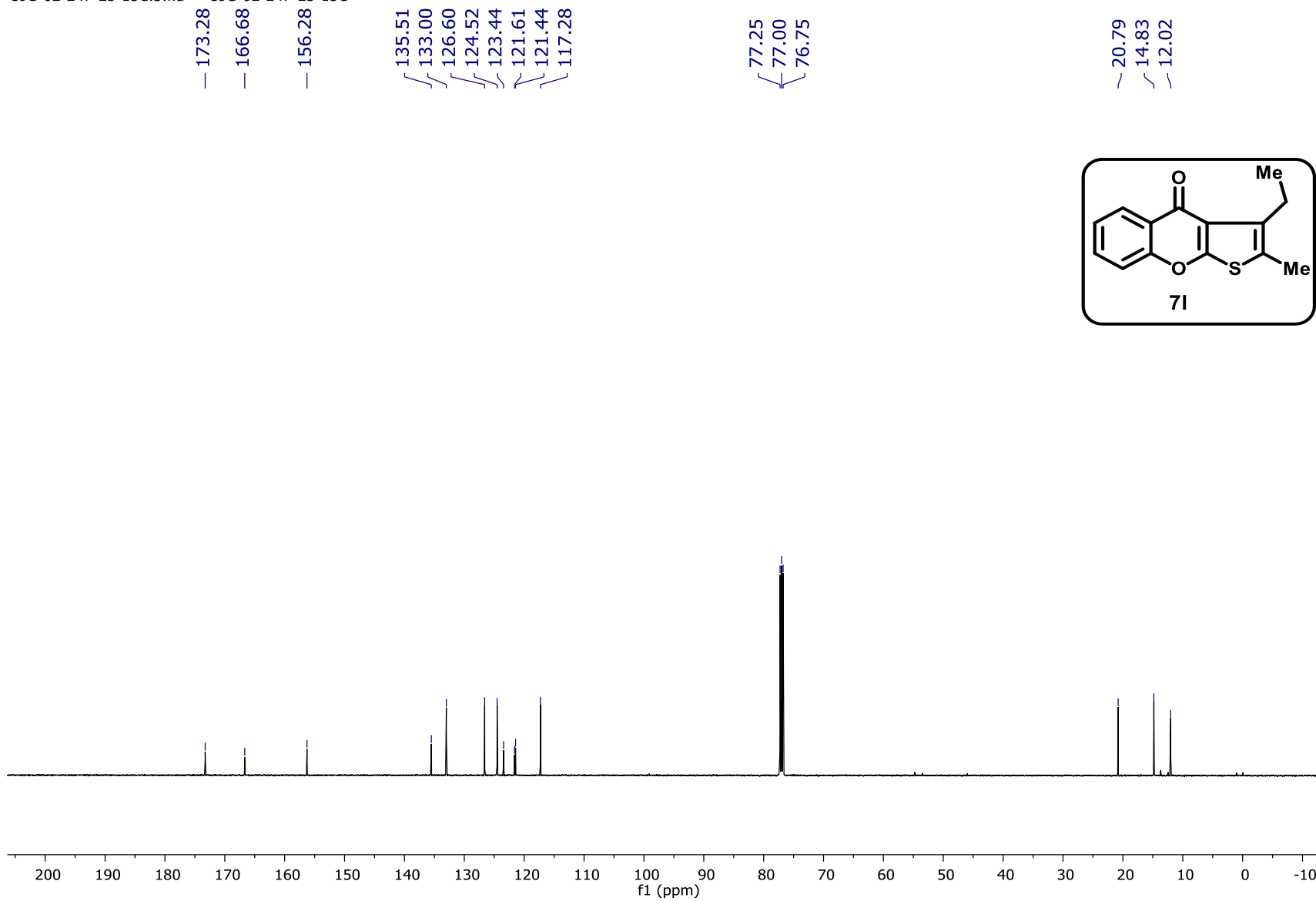
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 7l

UJG-02-247-23-1H.1.fid — UJG-02-247-23-1H

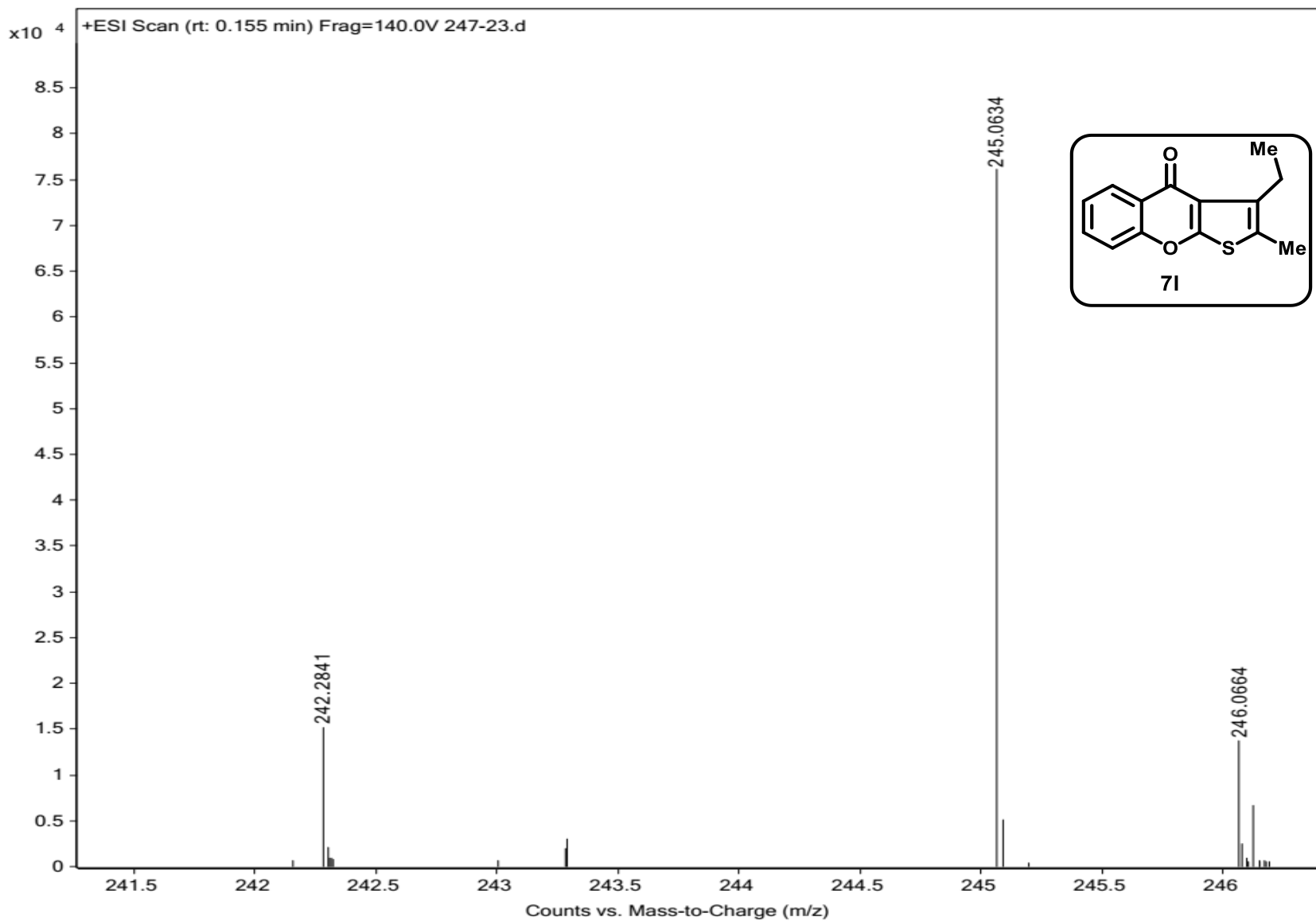


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7l

UJG-02-247-23-13C.3.fid — UJG-02-247-23-13C



HRMS Spectrum of Compound 71



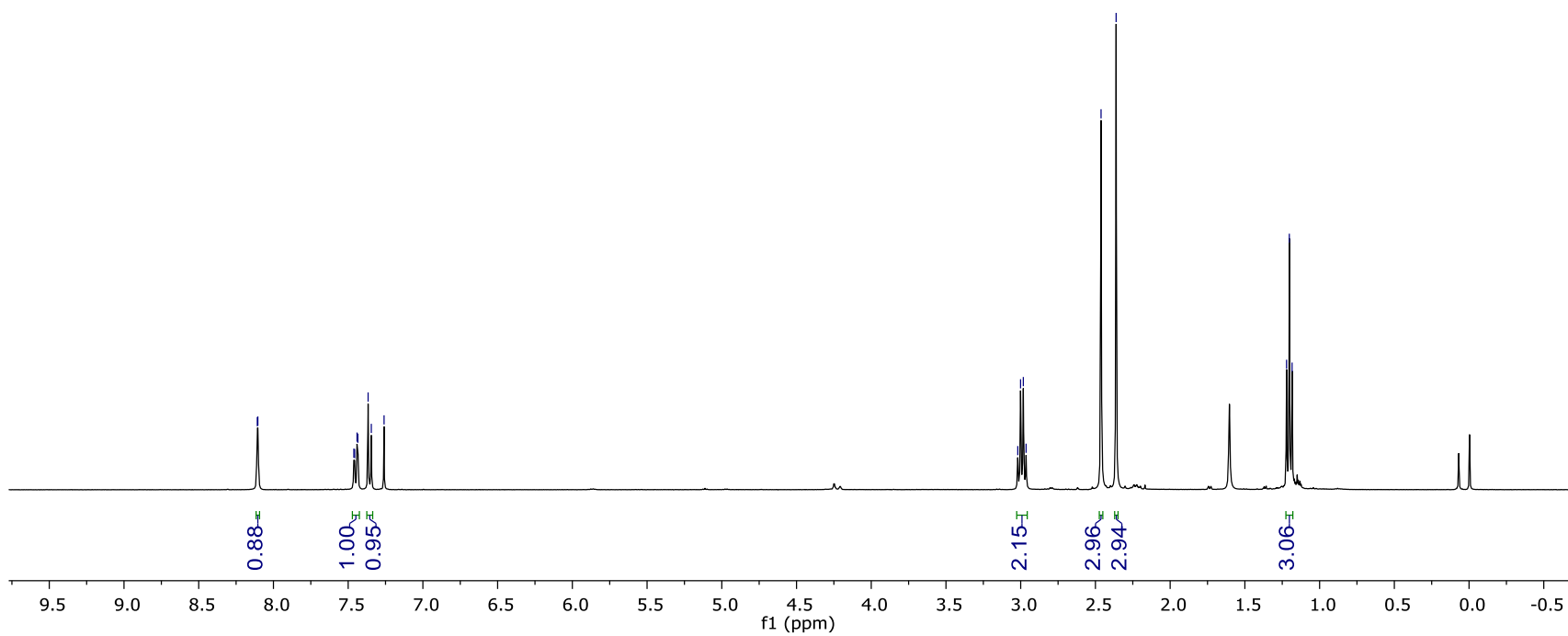
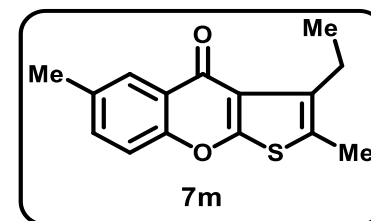
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 7m

UJG-02-237-23-1H.1.fid — UJG-02-237-23-1H

8.11
8.10
7.46
7.46
7.44
7.44
7.37
7.35
7.26

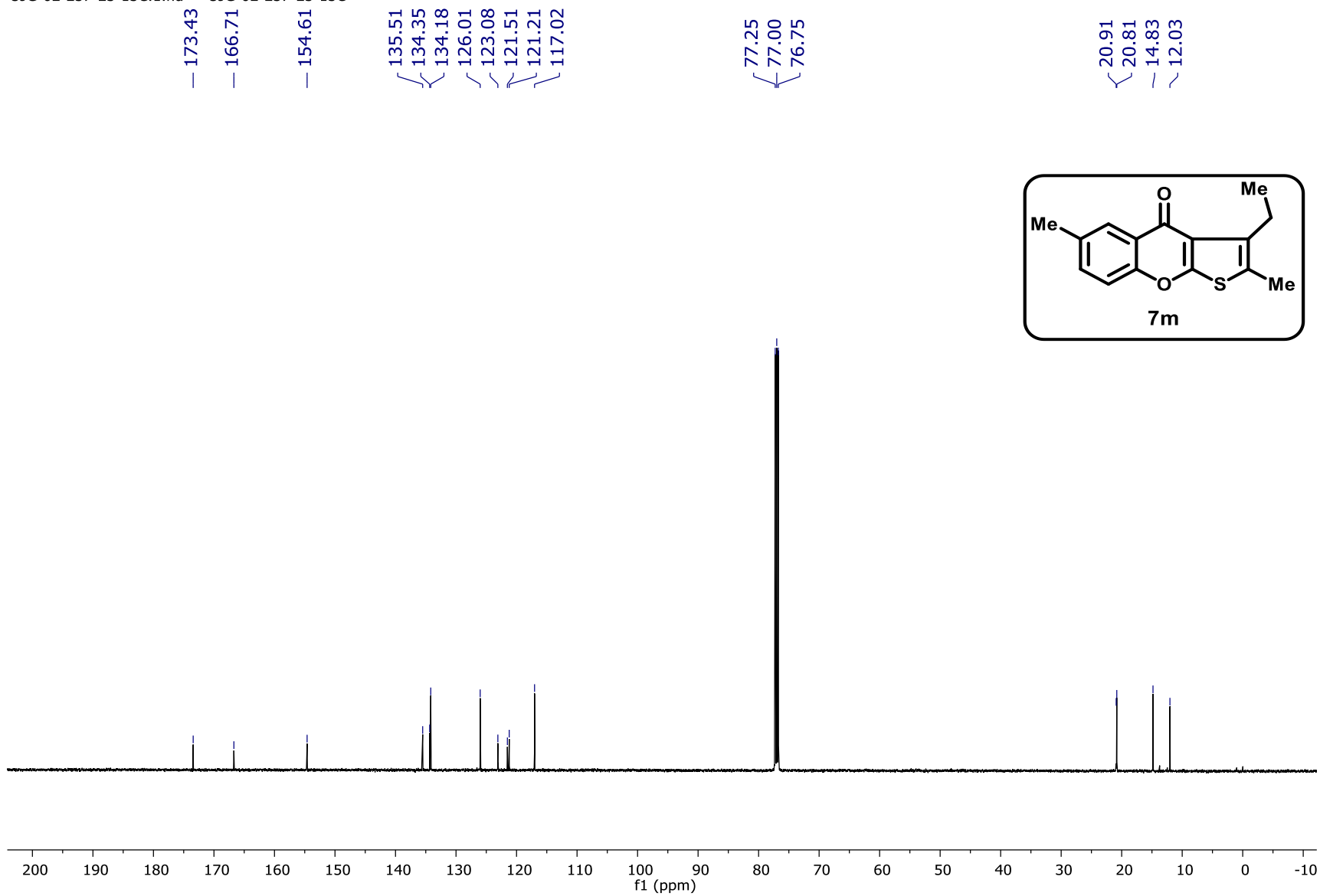
3.02
3.00
2.98
2.96
2.46
2.36

1.22
1.20
1.18

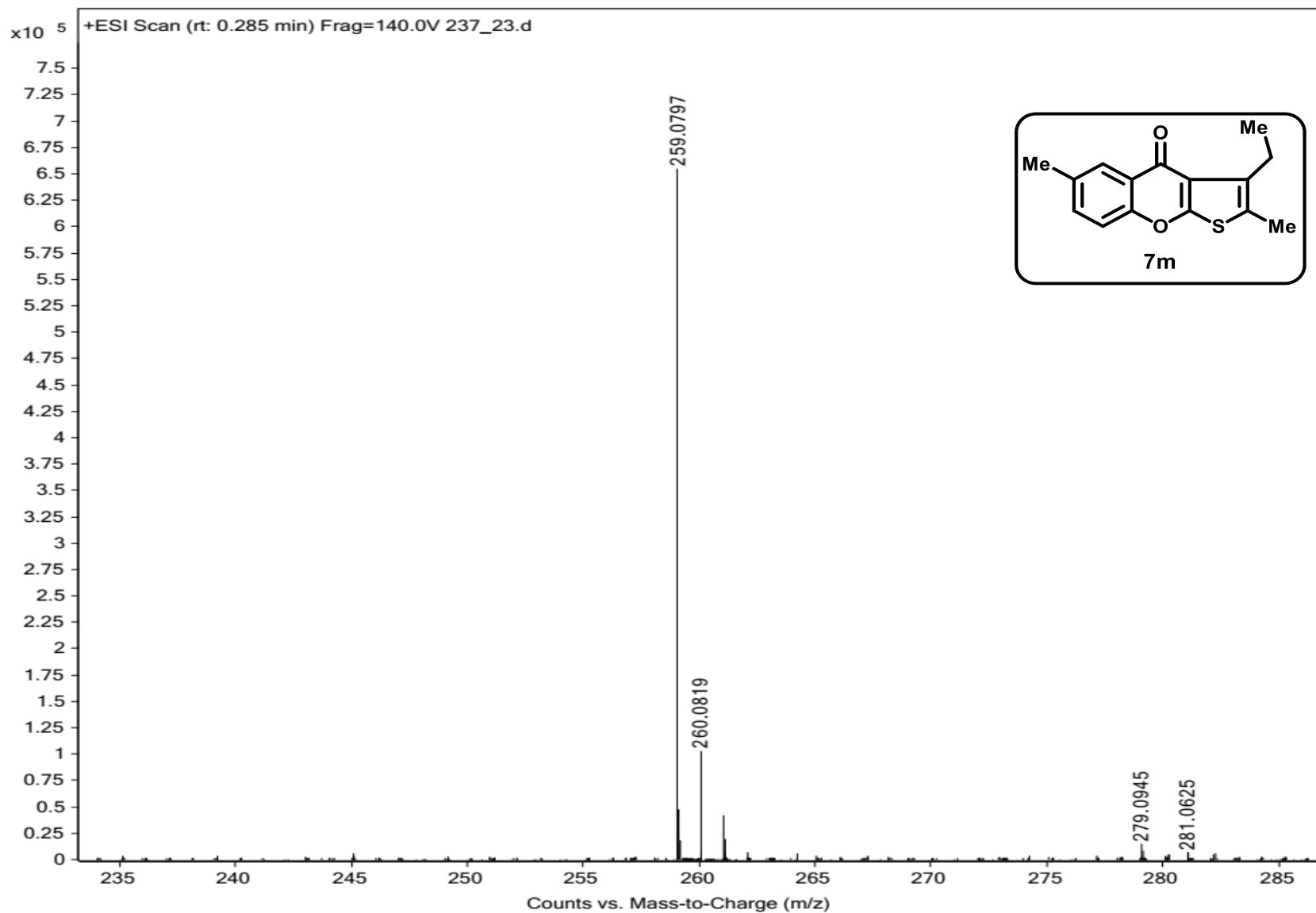


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7m

UJG-02-237-23-13C.1.fid — UJG-02-237-23-13C

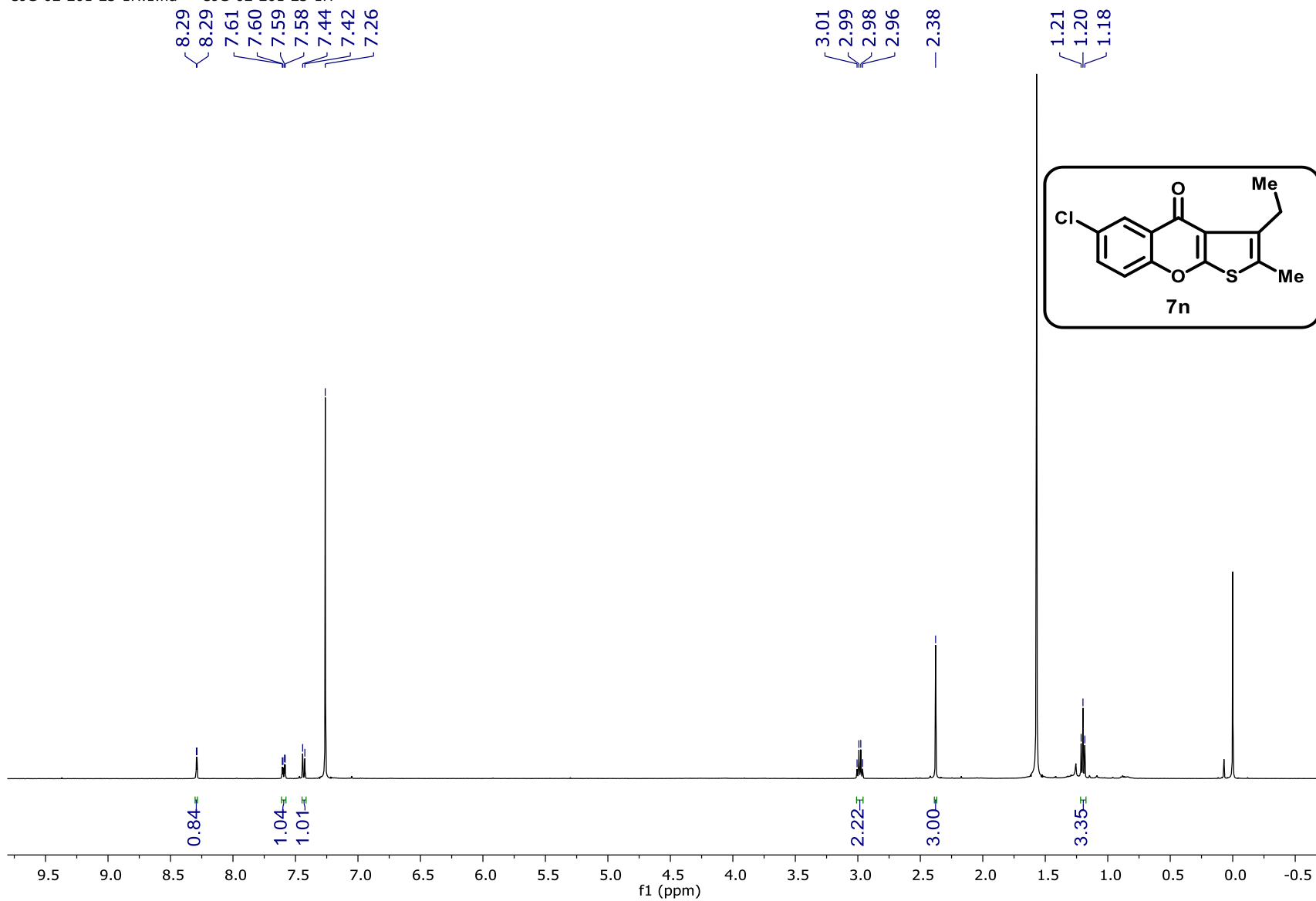


HRMS Spectrum of Compound 7m



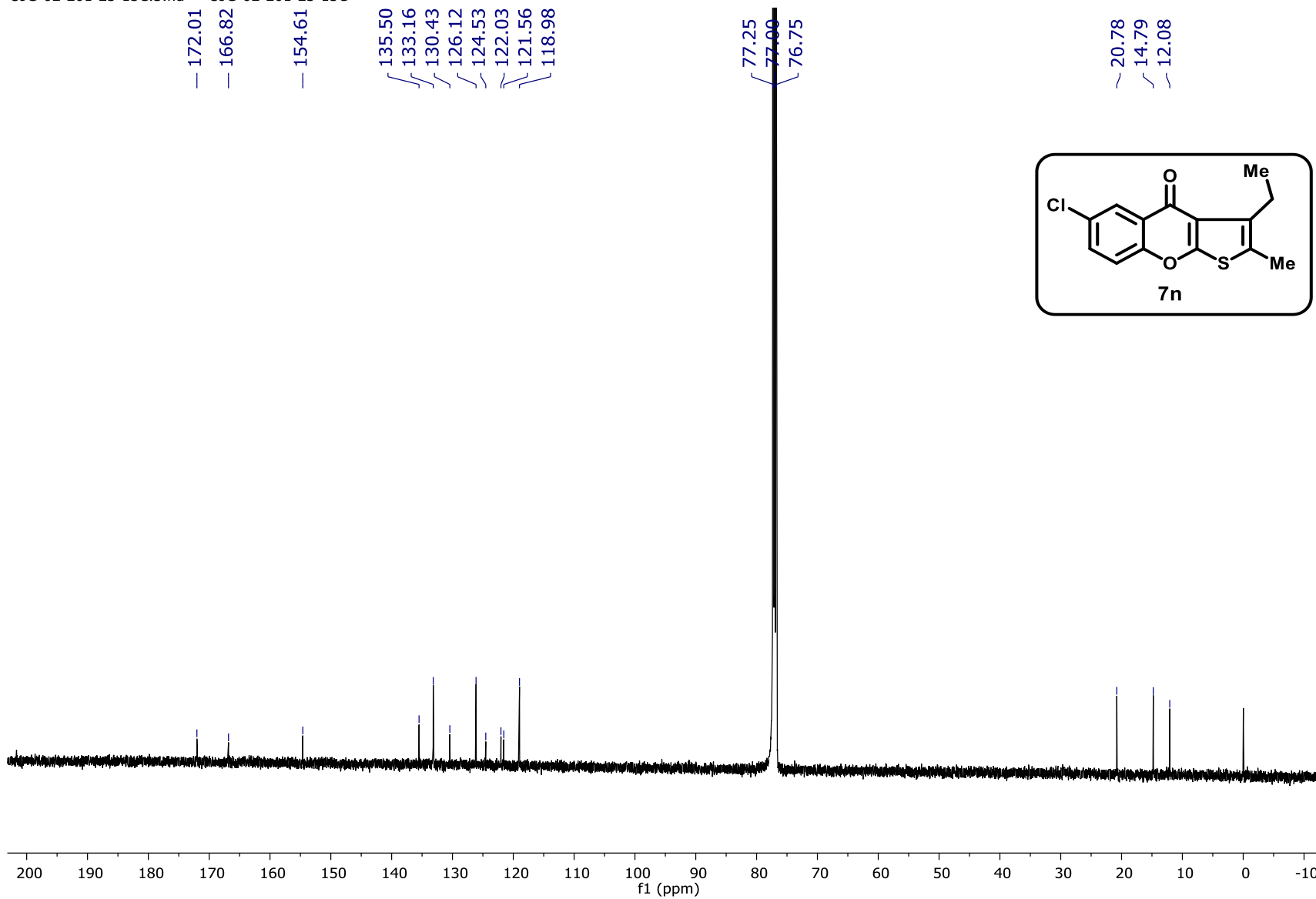
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7n

UJG-02-201-23-1H.1.fid — UJG-02-201-23-1H

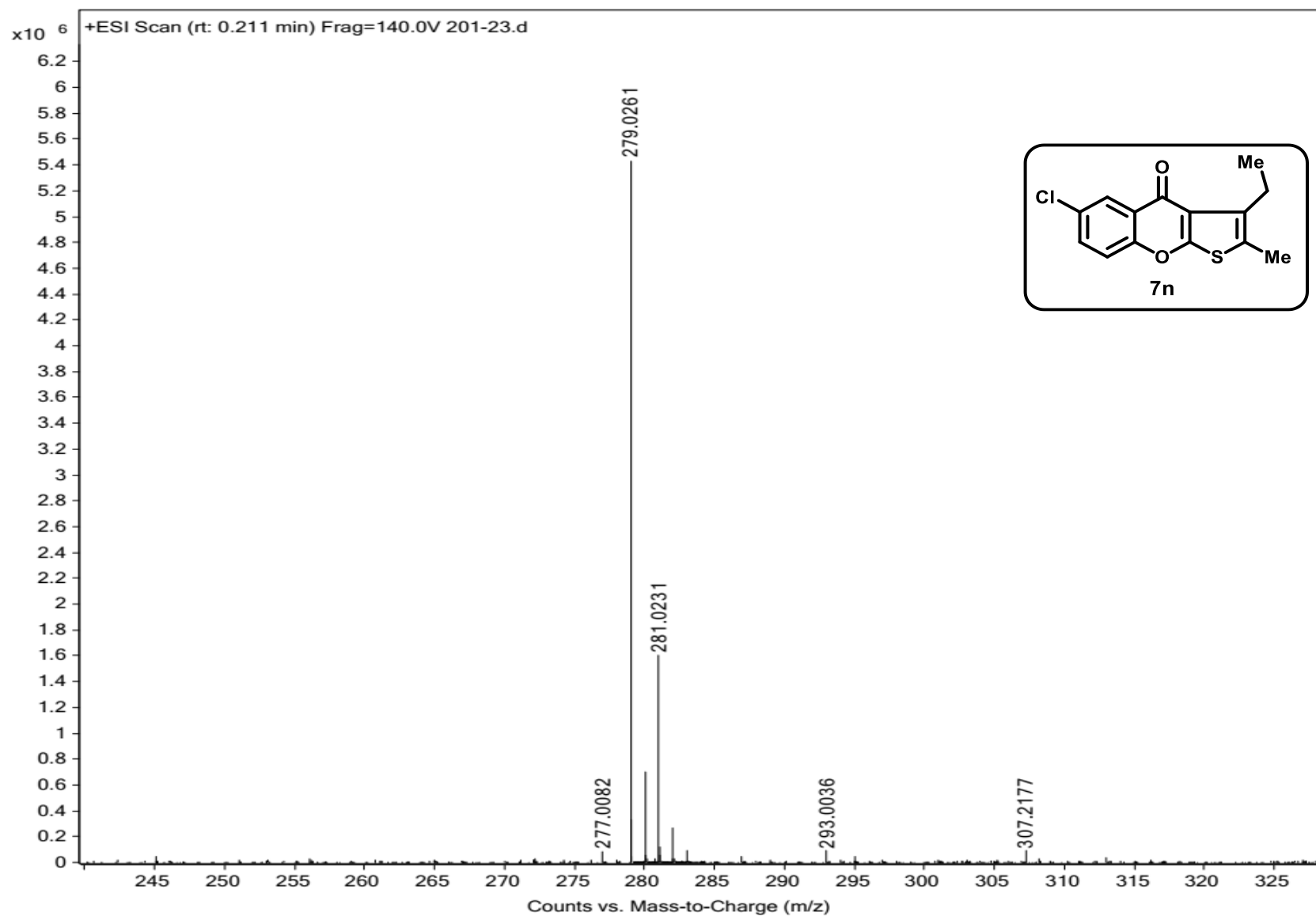


¹³C {¹H} NMR (125 MHz, CDCl₃) Spectrum of Compound 7n

UJG-02-201-23-13C.3.fid — UJG-02-201-23-13C

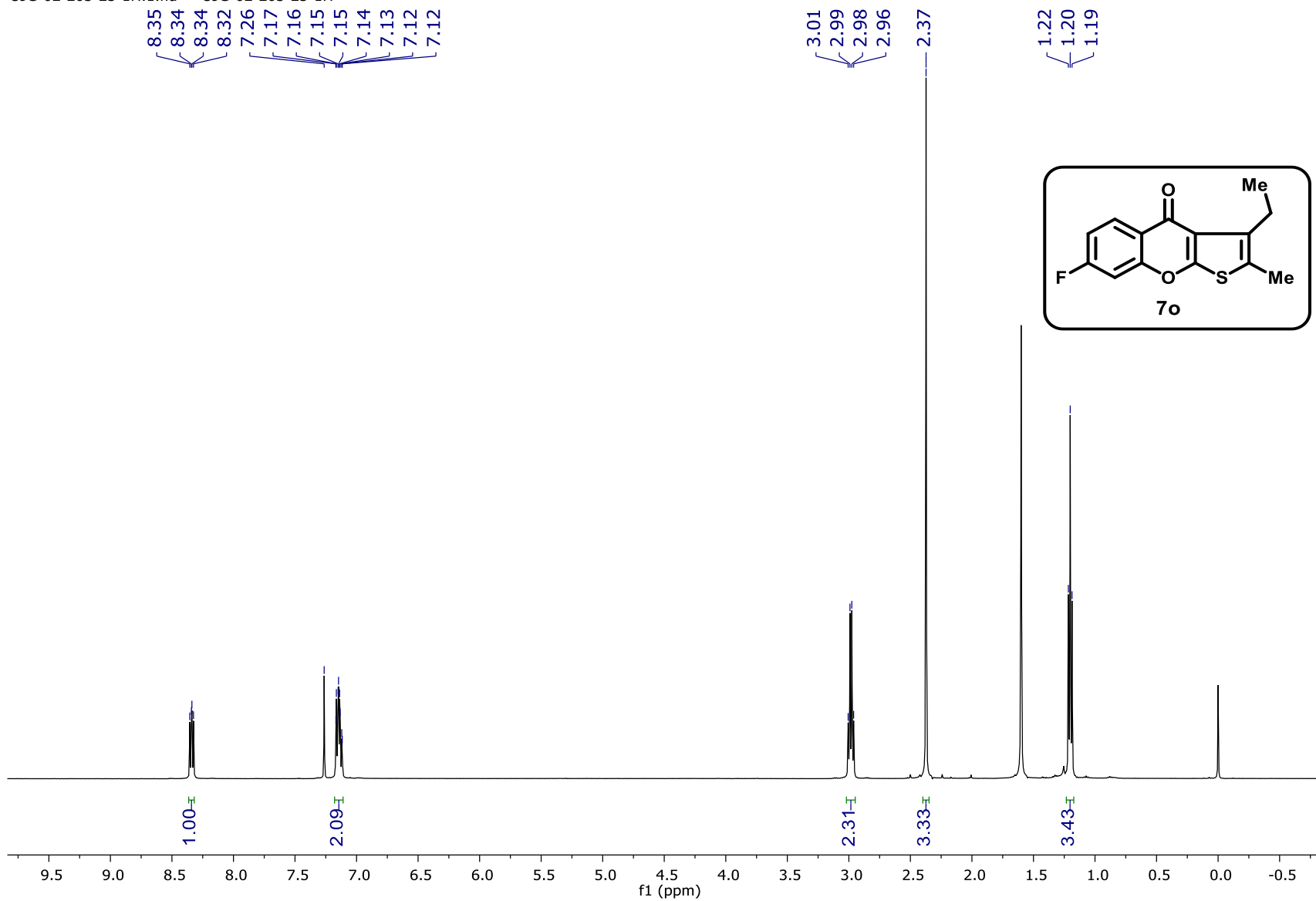


HRMS Spectrum of Compound 7n



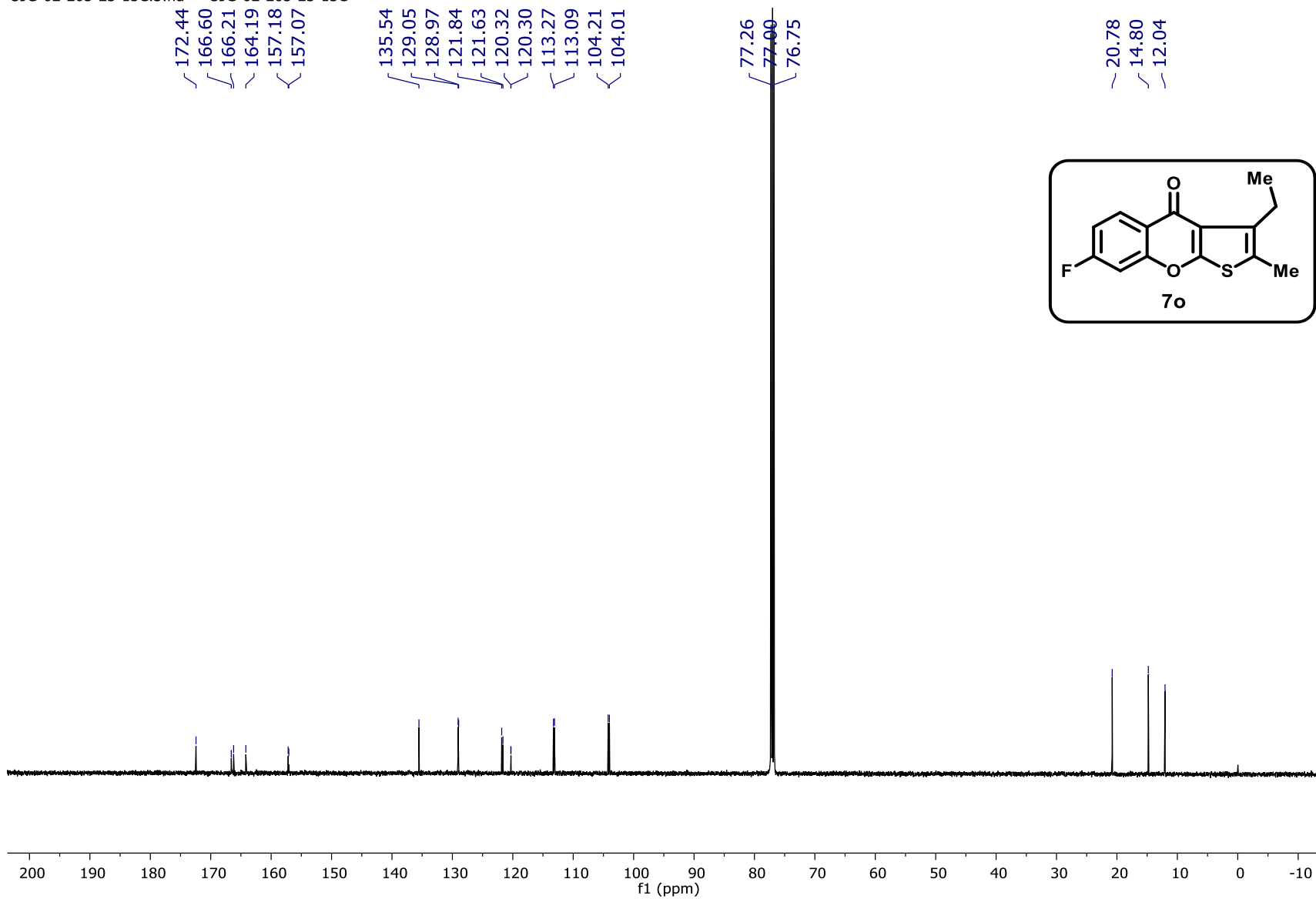
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 7o

UJG-02-203-23-1H.1.fid — UJG-02-203-23-1H



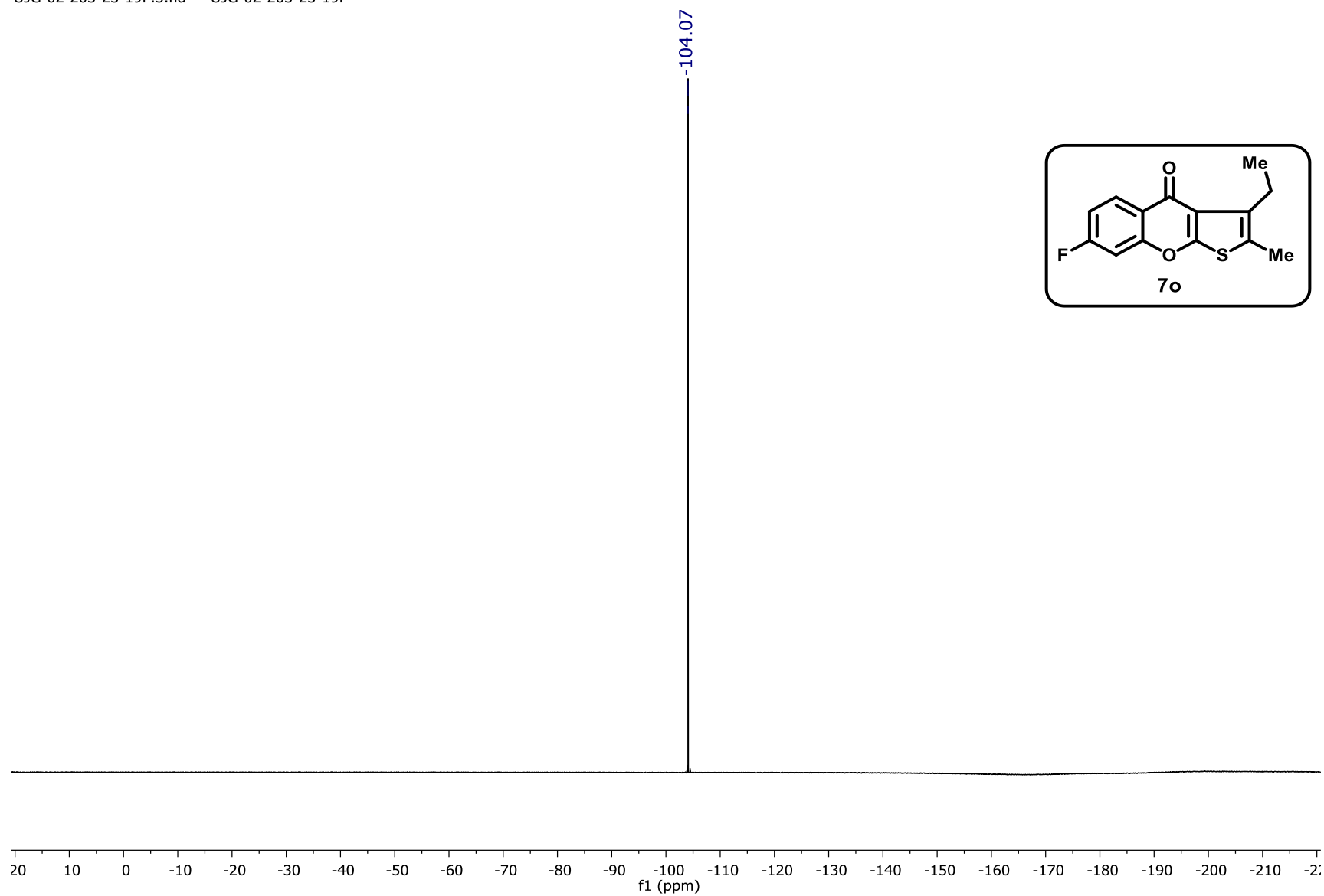
^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 7o

UJG-02-203-23-13C.3.fid — UJG-02-203-23-13C

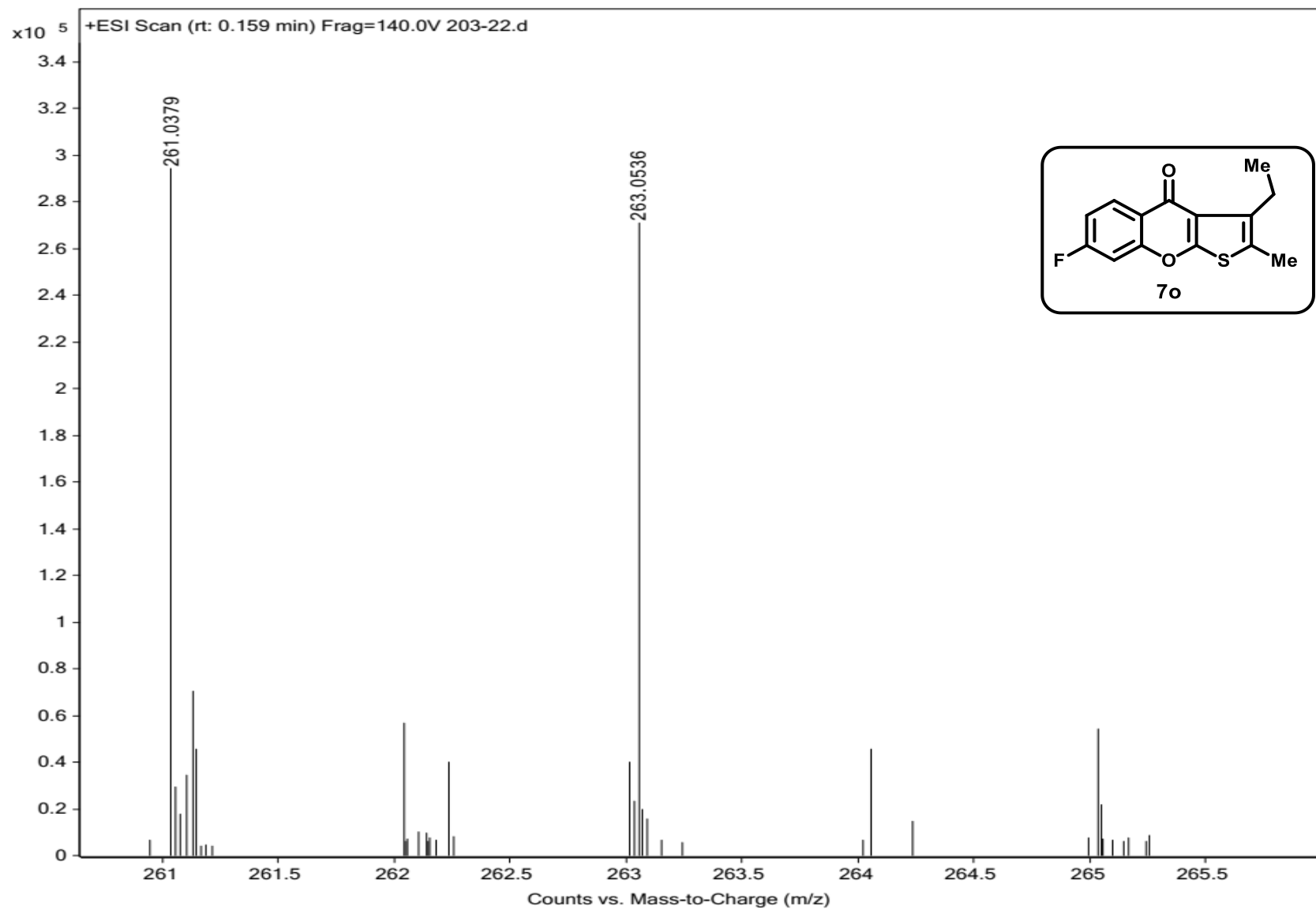


^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 7o

UJG-02-203-23-19F.5.fid — UJG-02-203-23-19F



HRMS Spectrum of Compound 7o



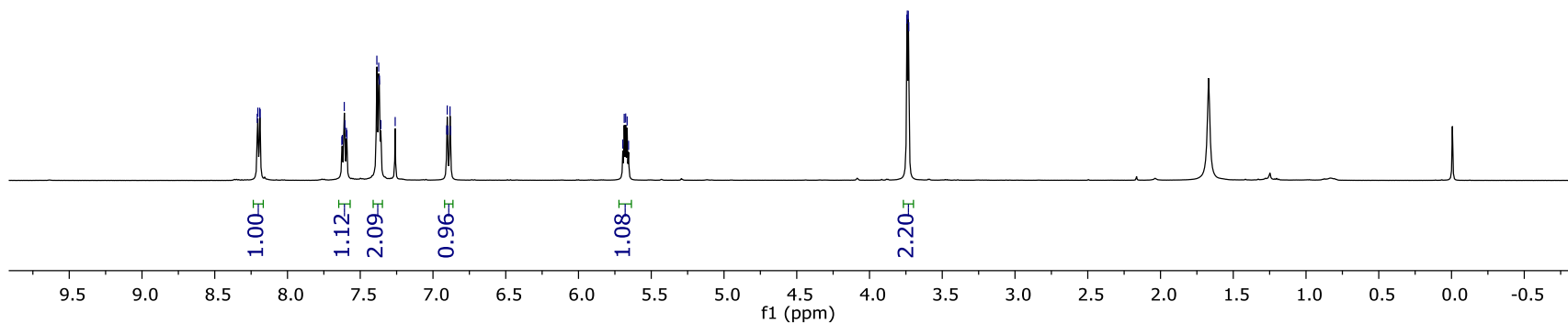
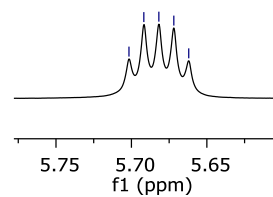
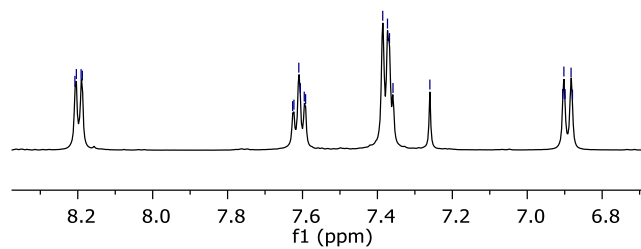
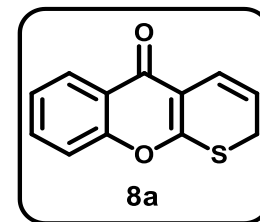
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8a

UJG-02-033-22-1H.1.fid — UJG-02-033-22-1H

8.21
8.20
8.19
8.19
7.63
7.62
7.61
7.61
7.60
7.59
7.39
7.37
7.37
7.36
7.26
7.26
6.91
6.90
6.90
6.88
6.88
5.70
5.69
5.68
5.67
5.66
3.74
3.74
3.73
3.73

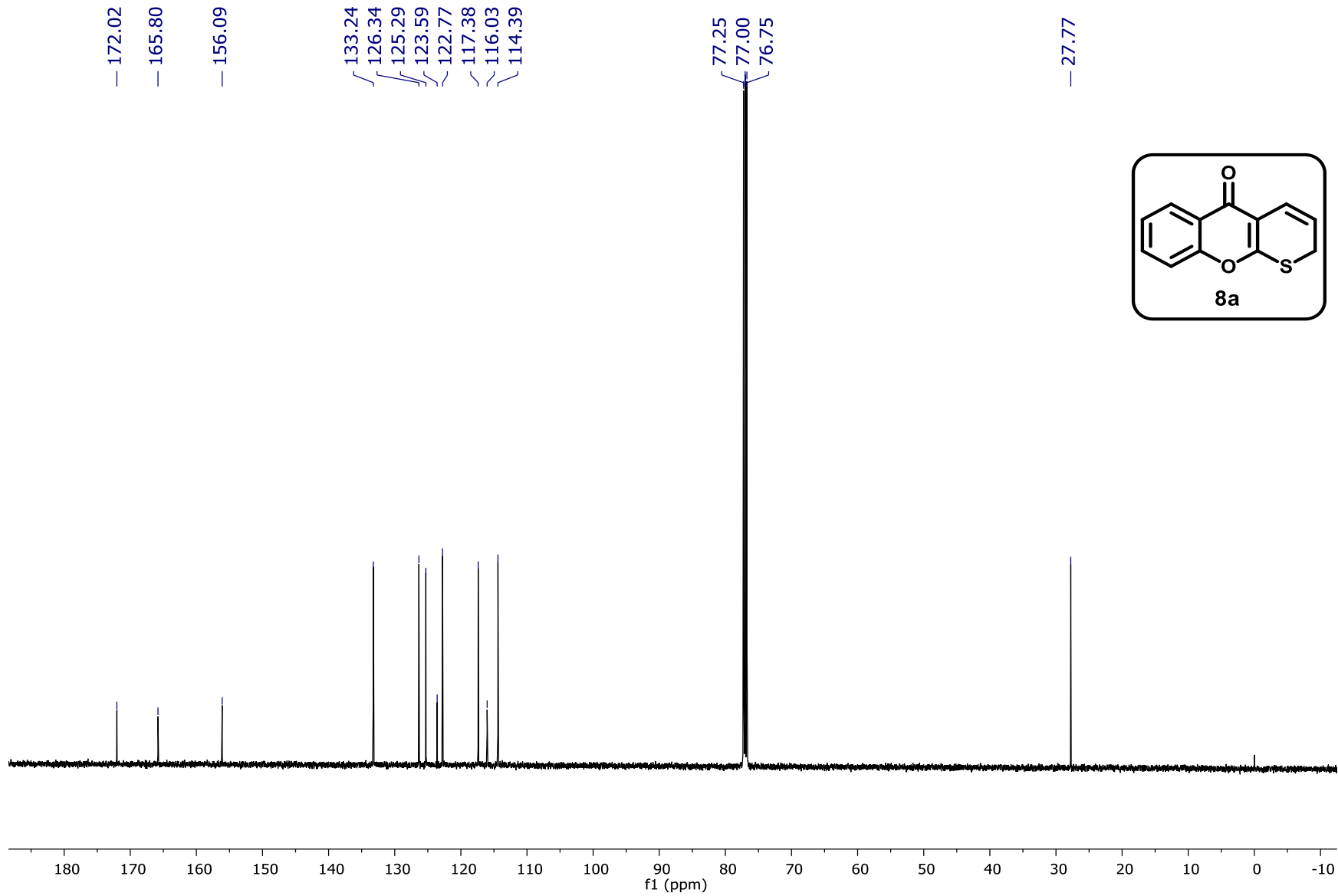
8.21
8.20
8.19
8.19
7.63
7.62
7.61
7.61
7.60
7.59
7.39
7.37
7.37
7.36
7.26
6.91
6.90
6.90
6.88

5.70
5.69
5.68
5.67
5.66

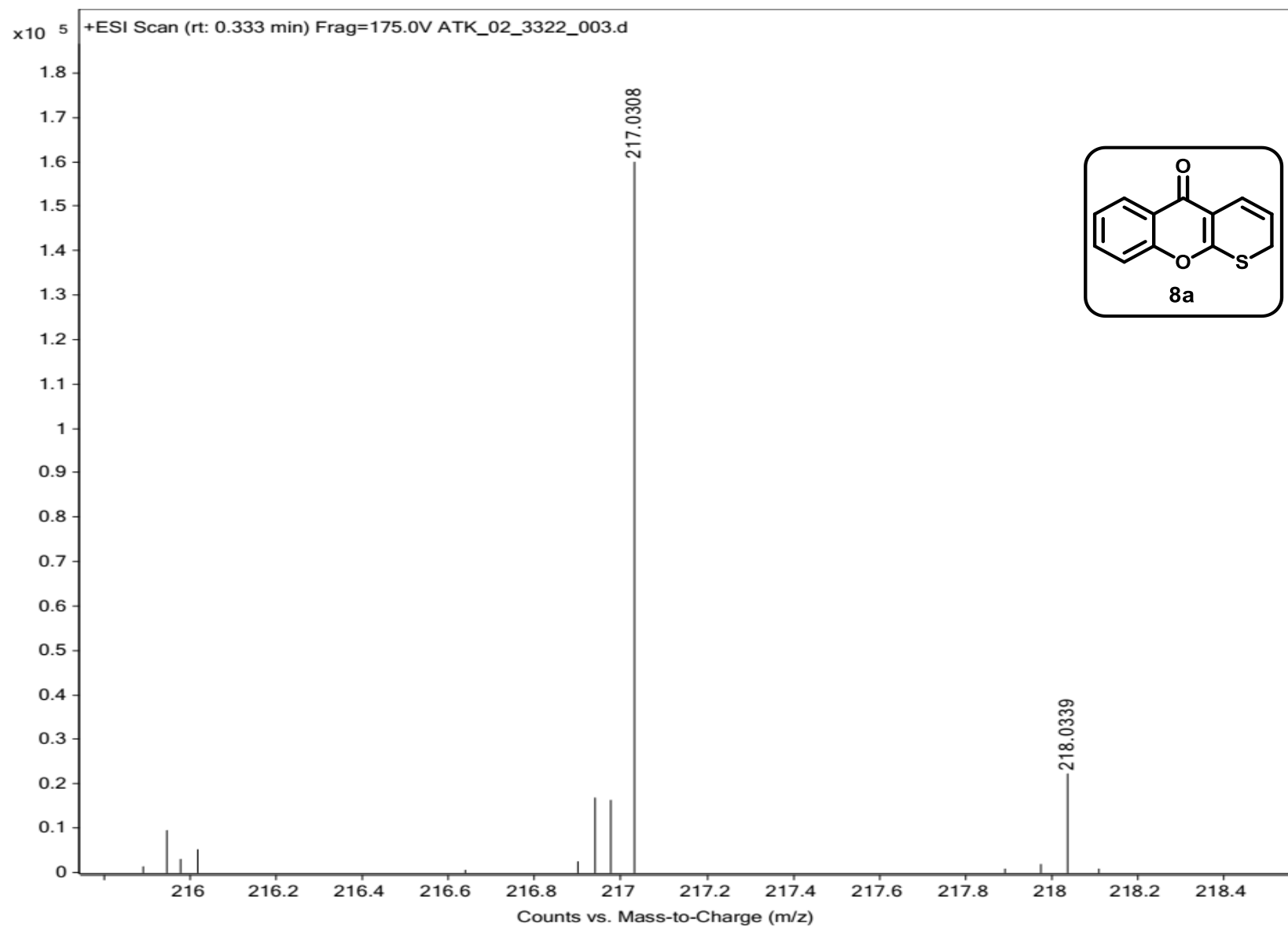


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8a

UJG-02-033-22-13C.3.fid — UJG-02-033-22-13C

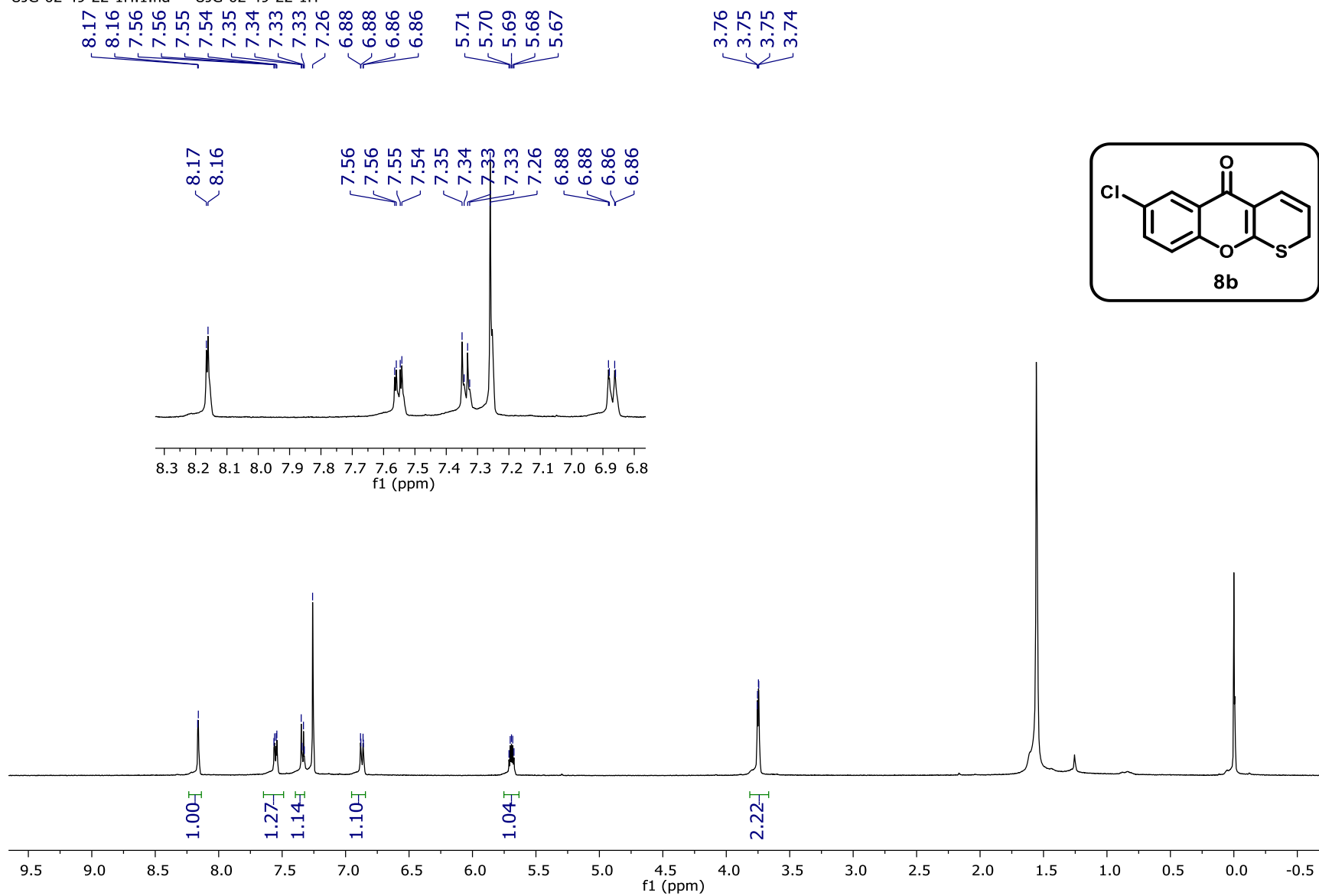


HRMS Spectrum of Compound 8a



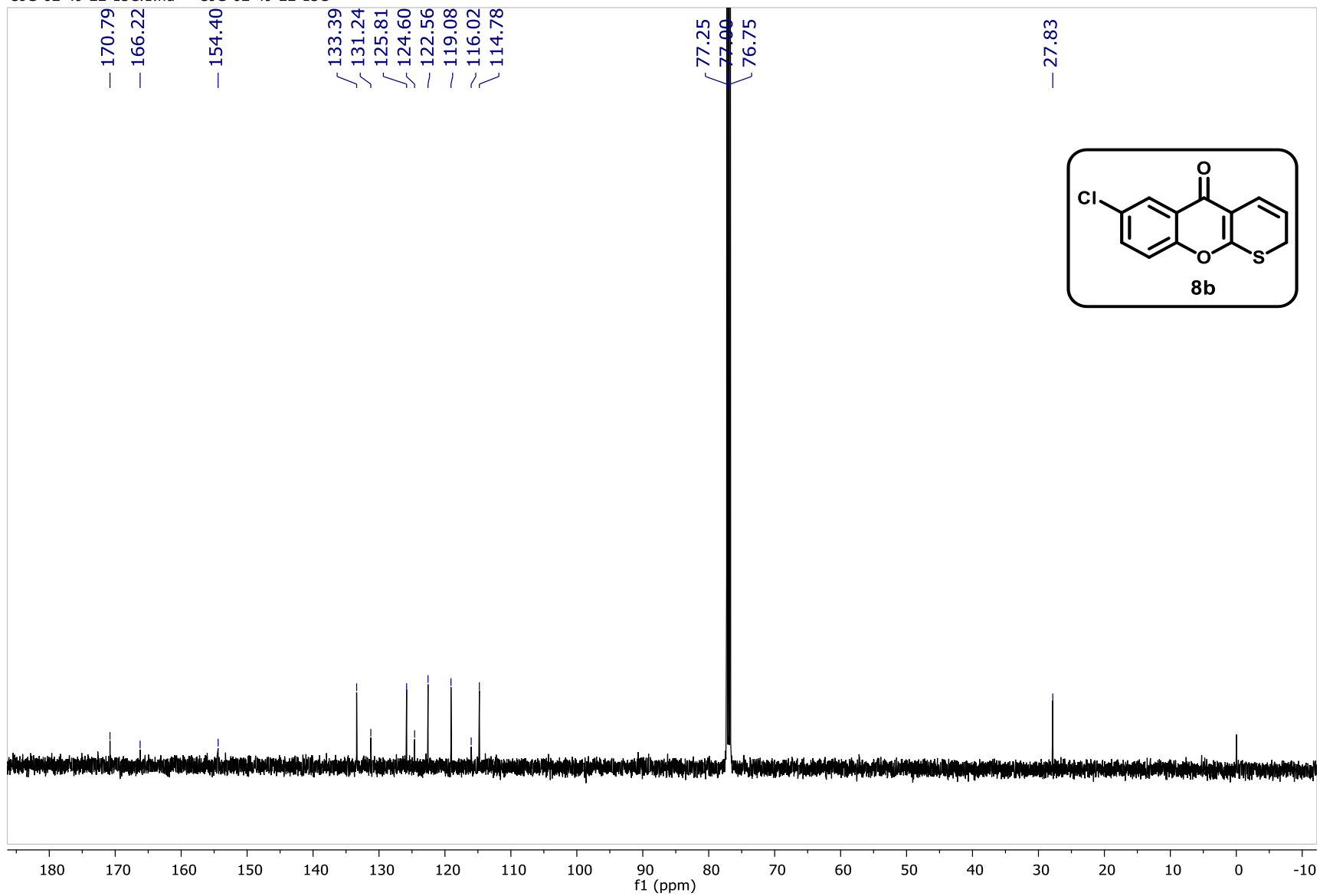
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8b

UJG-02-49-22-1H.1.fid — UJG-02-49-22-1H

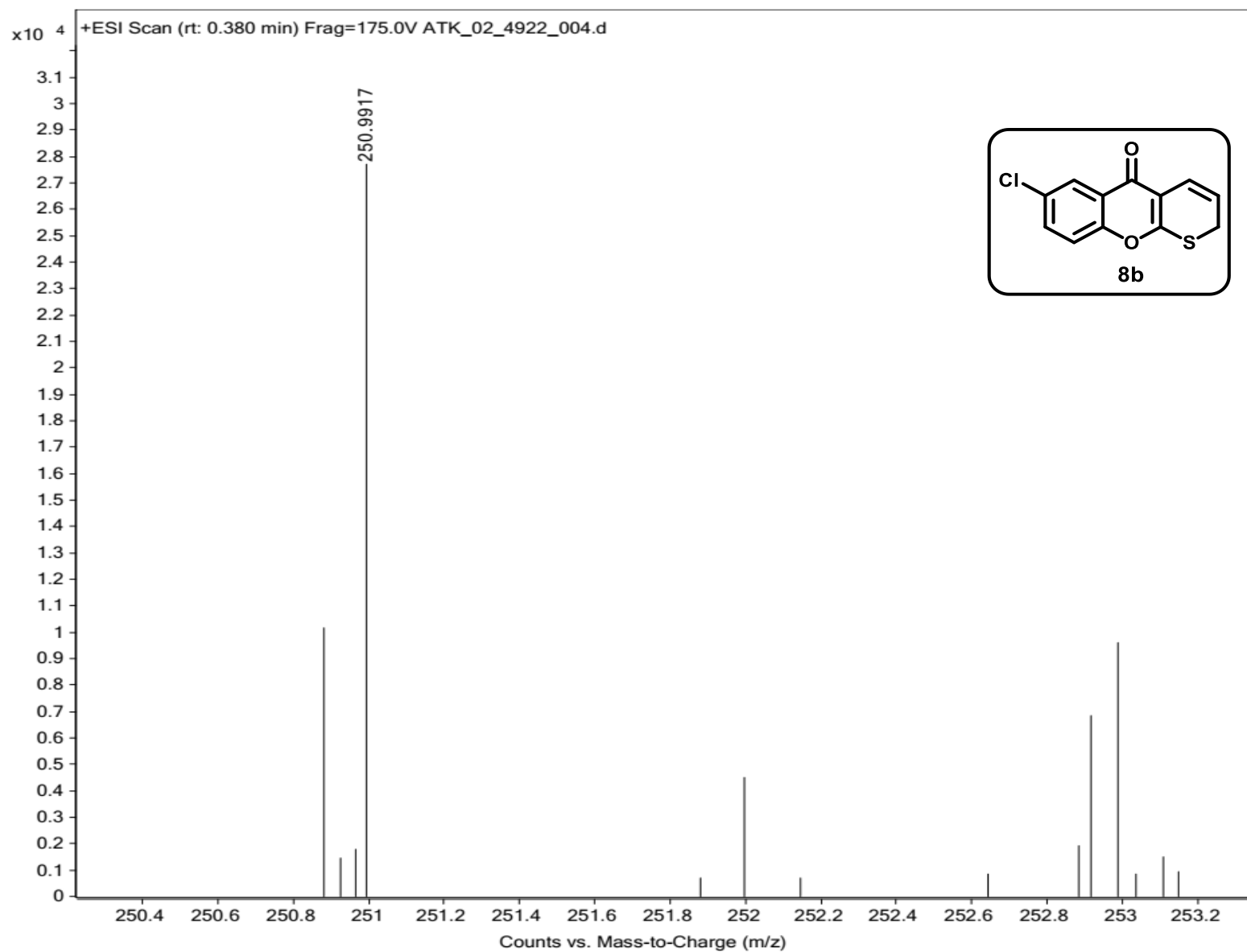


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8b

UJG-02-49-22-13C.1.fid — UJG-02-49-22-13C

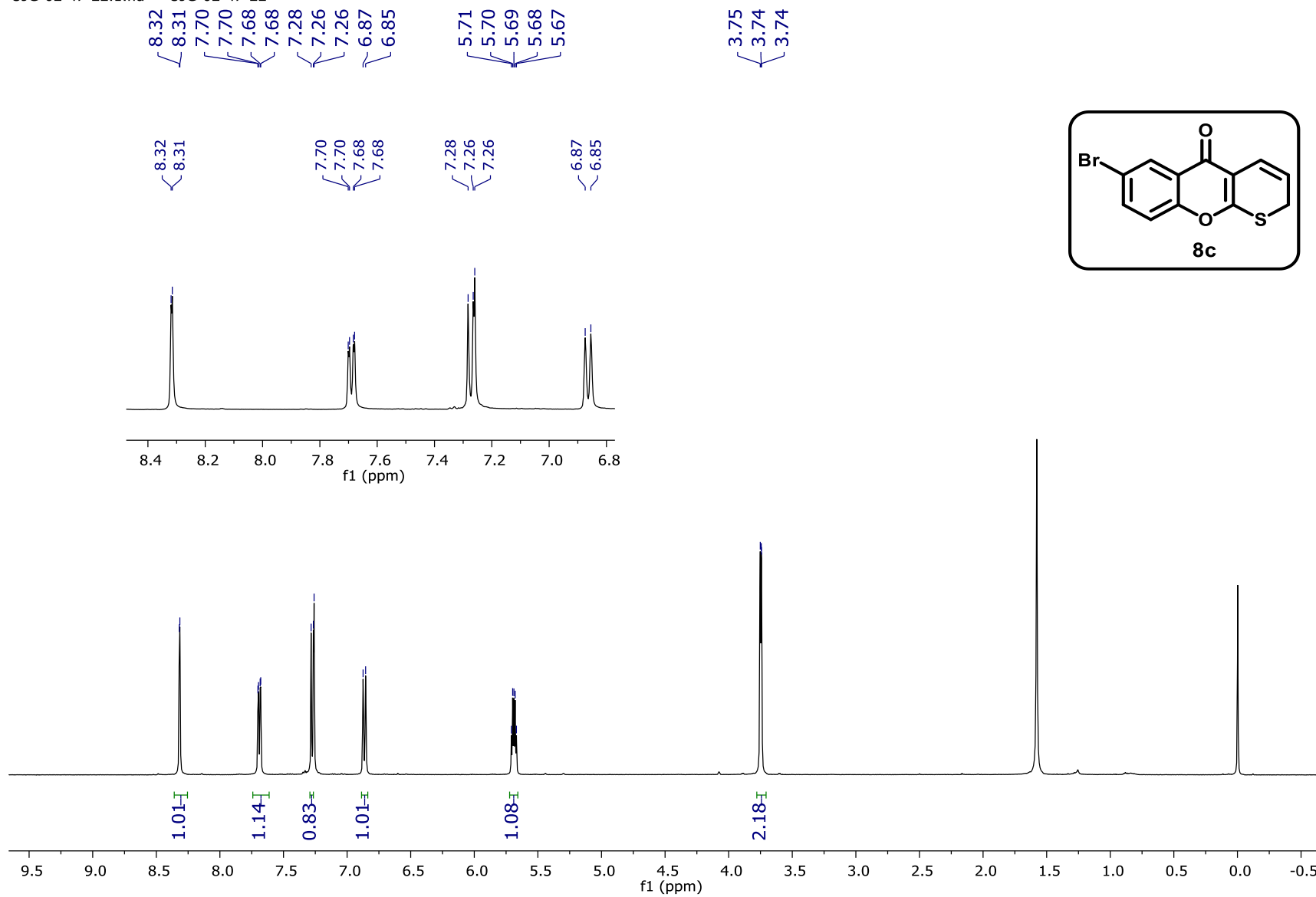


HRMS Spectrum of Compound 8b



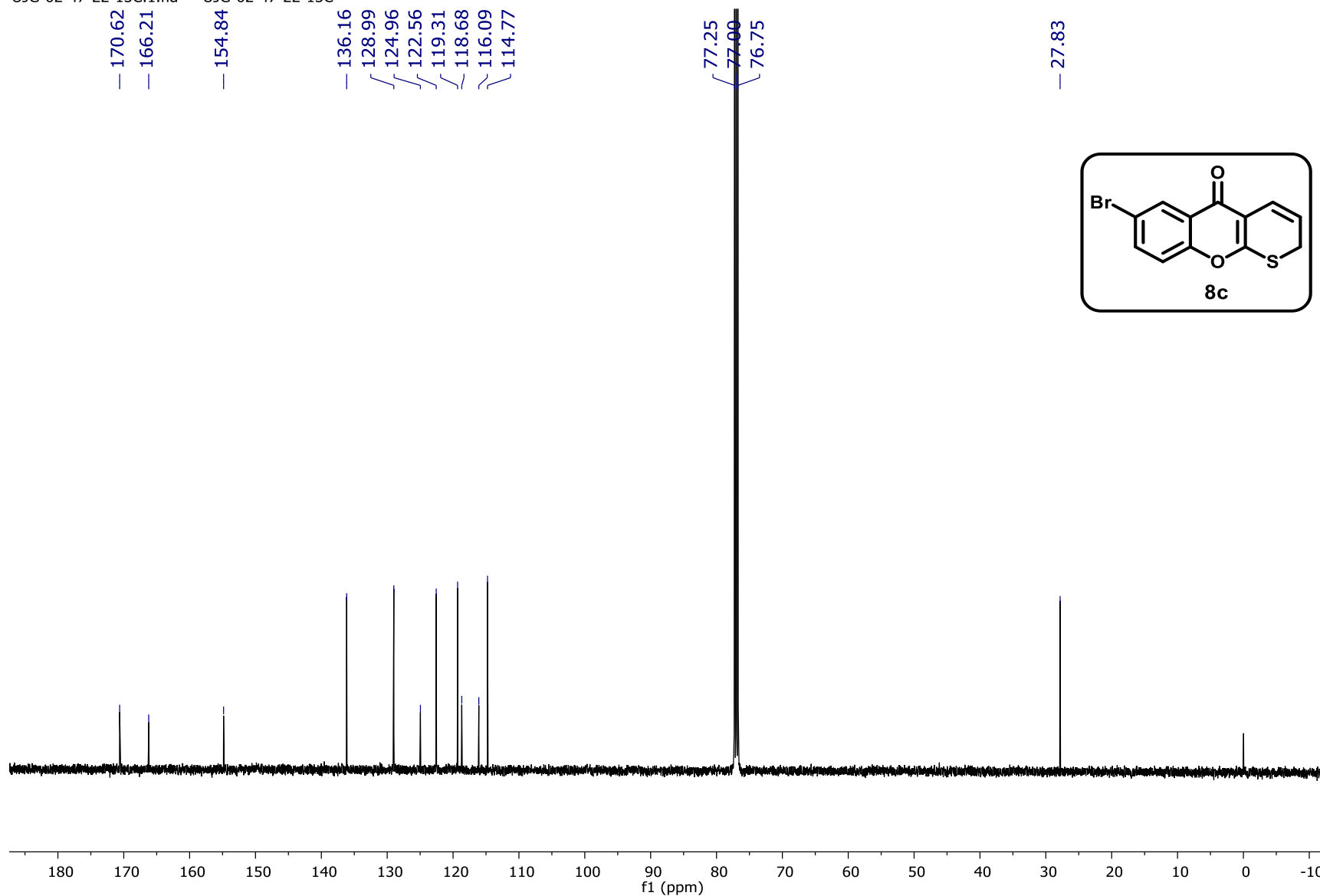
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8c

UJG-02-47-22.1.fid — UJG-02-47-22



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8c

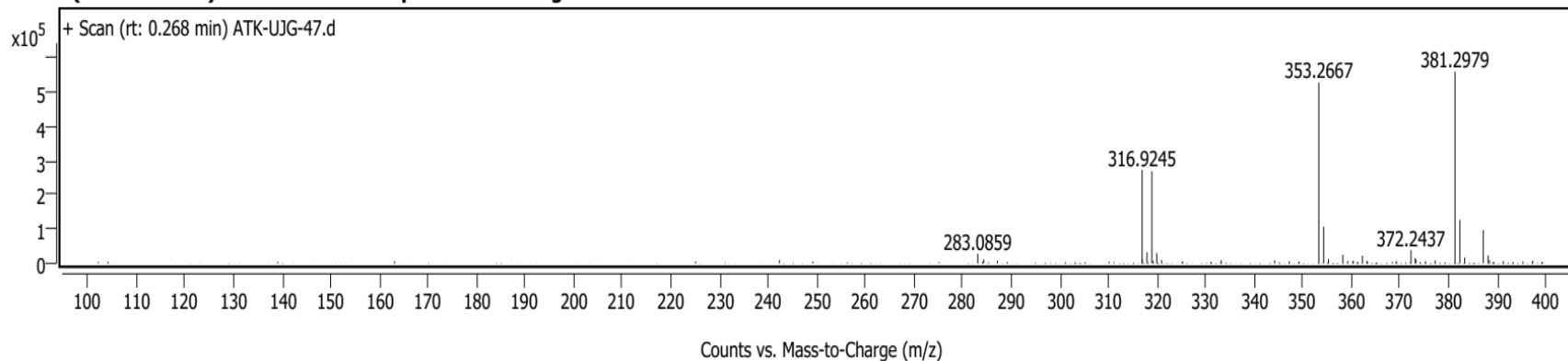
UJG-02-47-22-13C.1.fid — UJG-02-47-22-13C



HRMS Spectrum of Compound 8c

+ Scan (rt: 0.268 min)

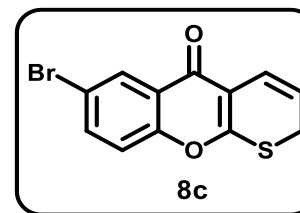
SpectrumIdString



SpectrumIdString

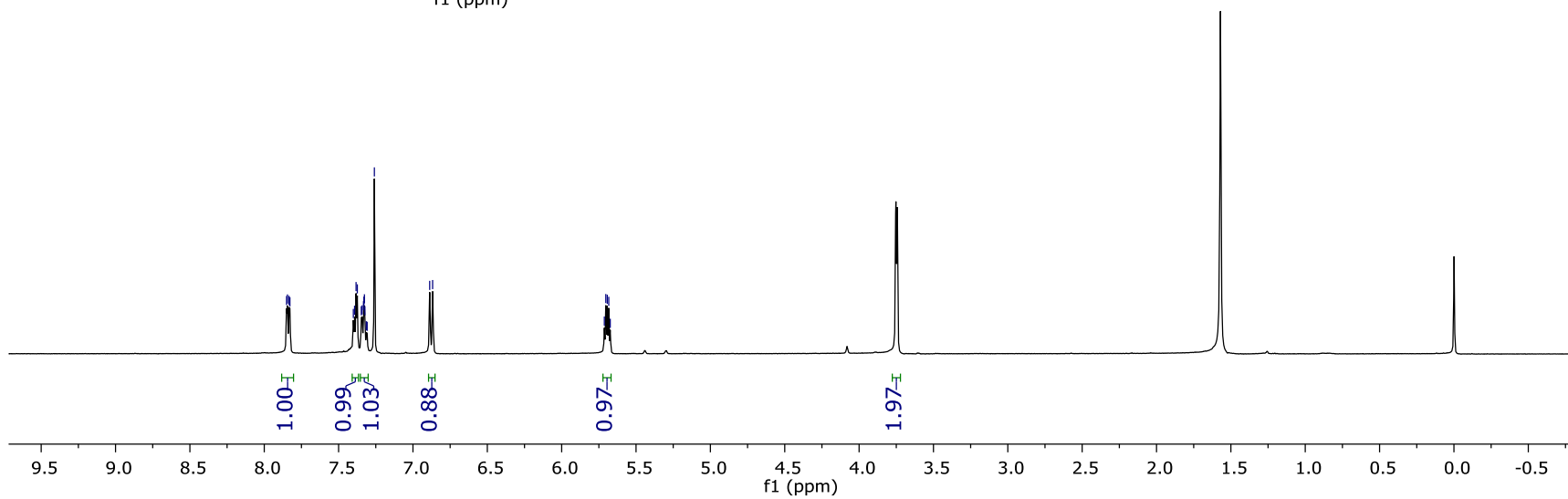
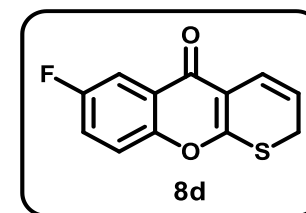
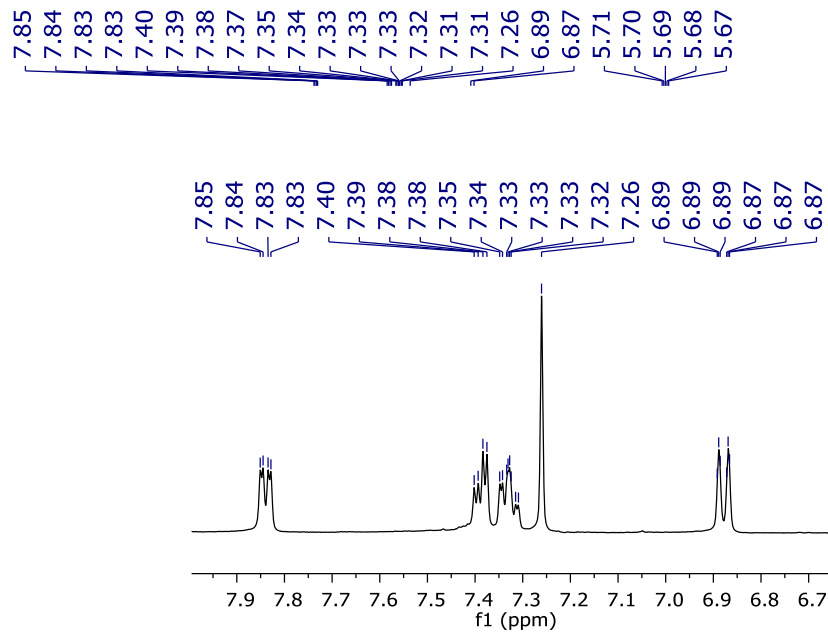
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula
283.0859		27801	4.97				
284.3315		11477	2.05				
316.9245	1	272636	48.70				
316.9350		13254	2.37				
317.9277	1	32429	5.79				
318.9225	1	269032	48.05				
319.9255	1	29957	5.35				
353.2667	1	527755	94.26				
354.2700	1	106931	19.10				
355.2727	1	12592	2.25				
358.2278		25035	4.47				
362.2413		22249	3.97				
372.2437	1	38293	6.84				
373.0965		15841	2.83				
373.2467	1	11208	2.00				
381.2979	1	559879	100.00				
382.3011	1	126708	22.63				
383.3039	1	16985	3.03				
387.1123	1	97276	17.37				
388.1155	1	22720	4.06				

Ion Type



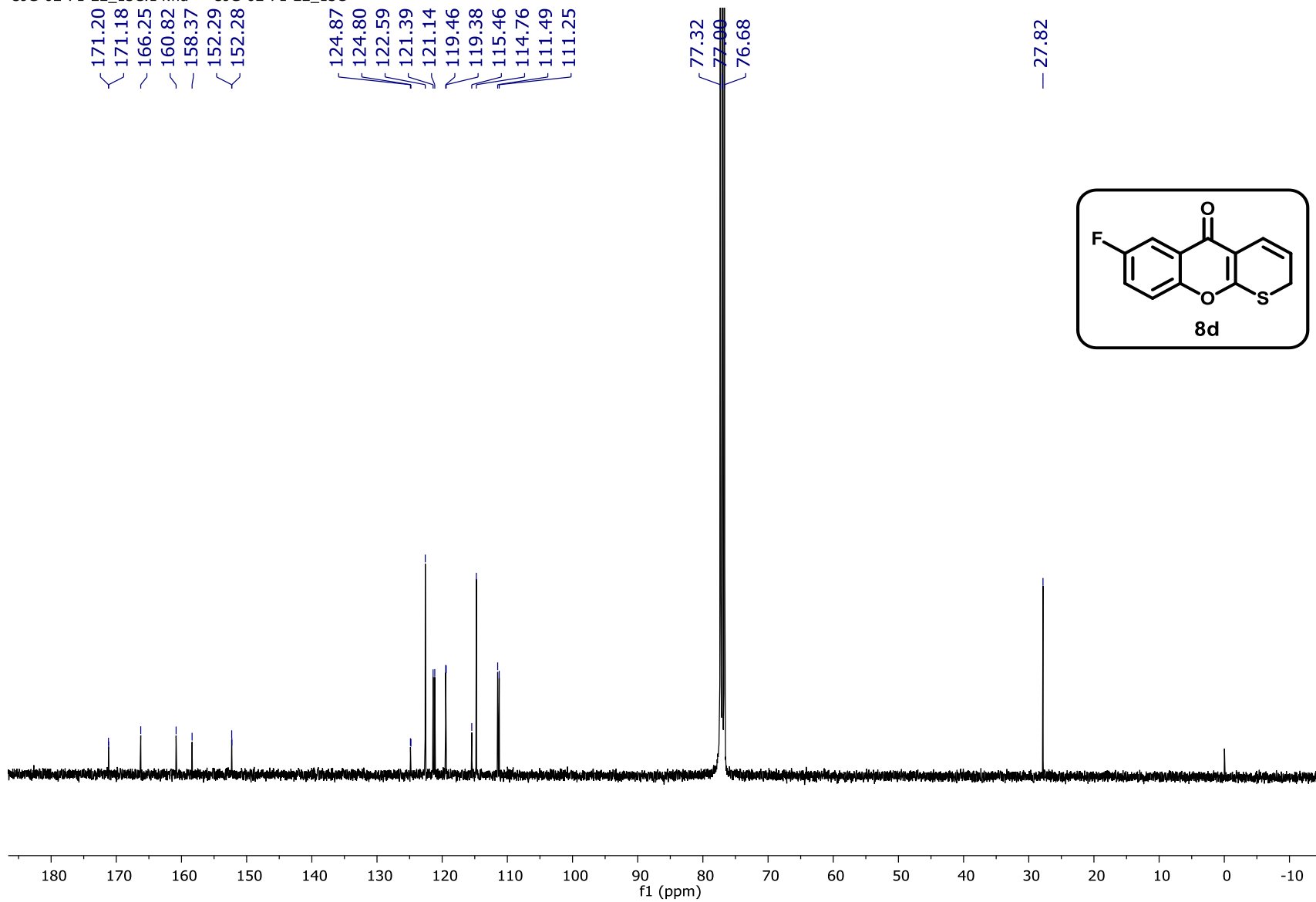
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8d

UJG-02-71-22I-1H.5.fid — UJG-02-71-22I-1H



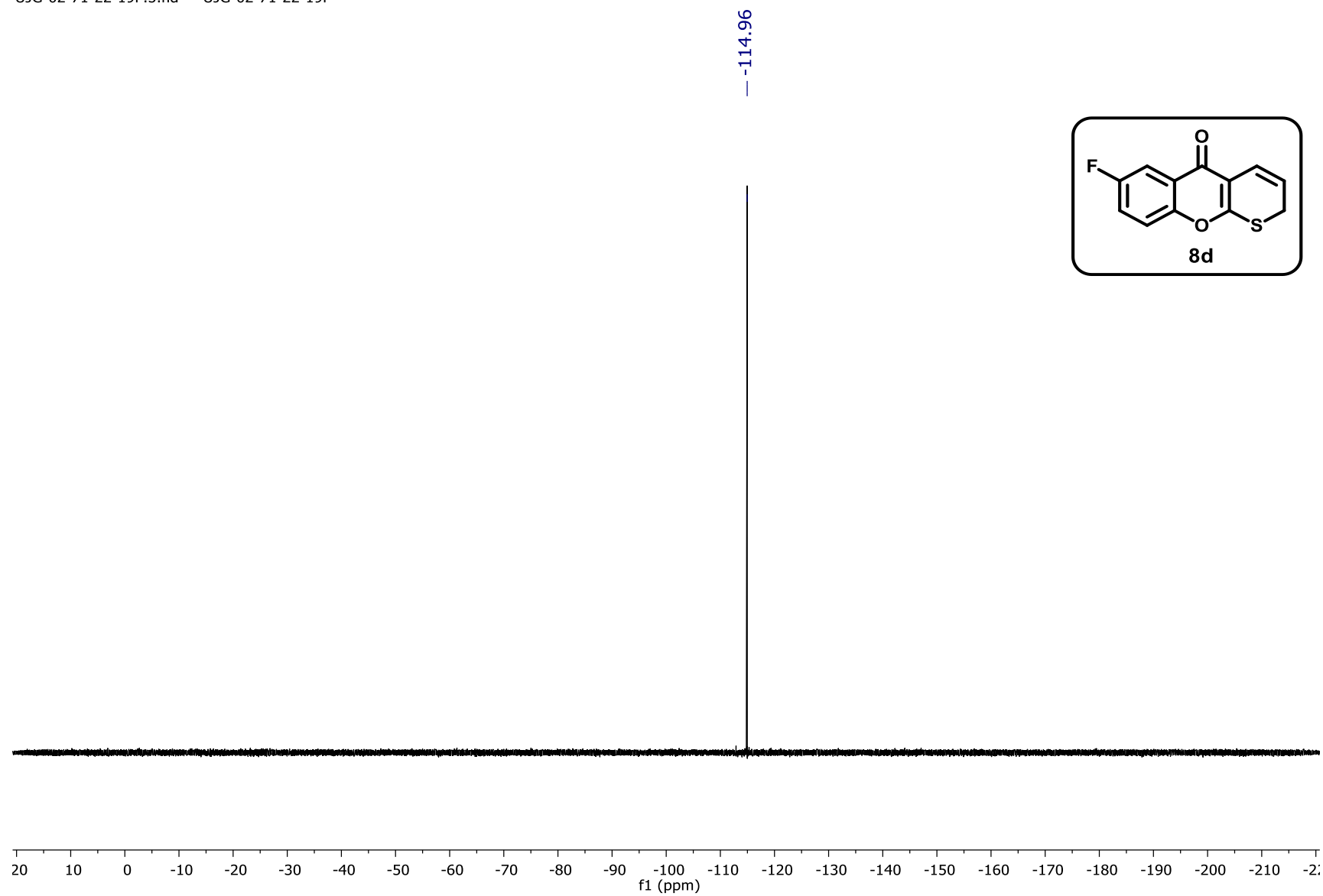
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of Compound 8d

UJG-02-71-22_13C.14.fid — UJG-02-71-22_13C



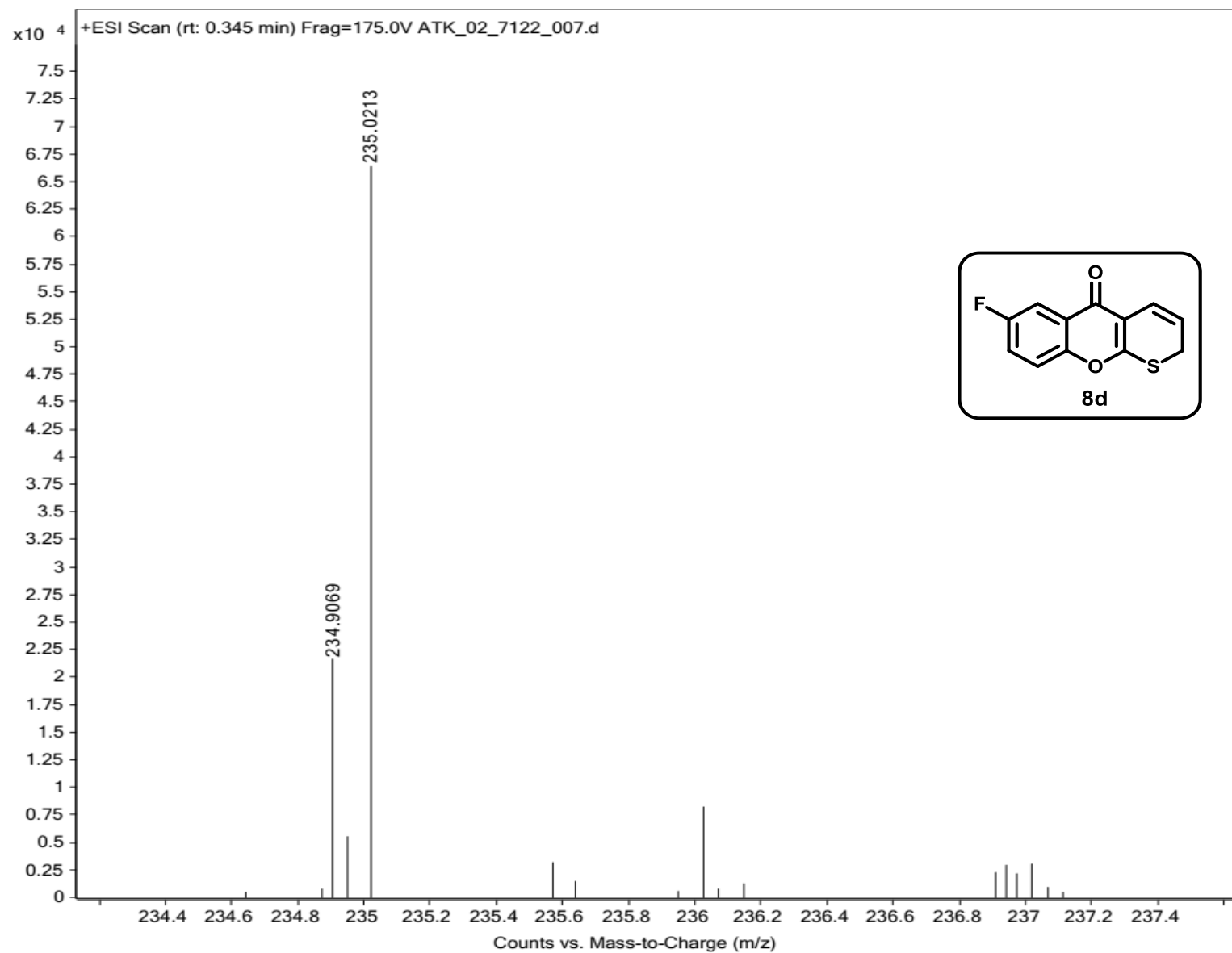
^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 8d

UJG-02-71-22-19F.5.fid — UJG-02-71-22-19F



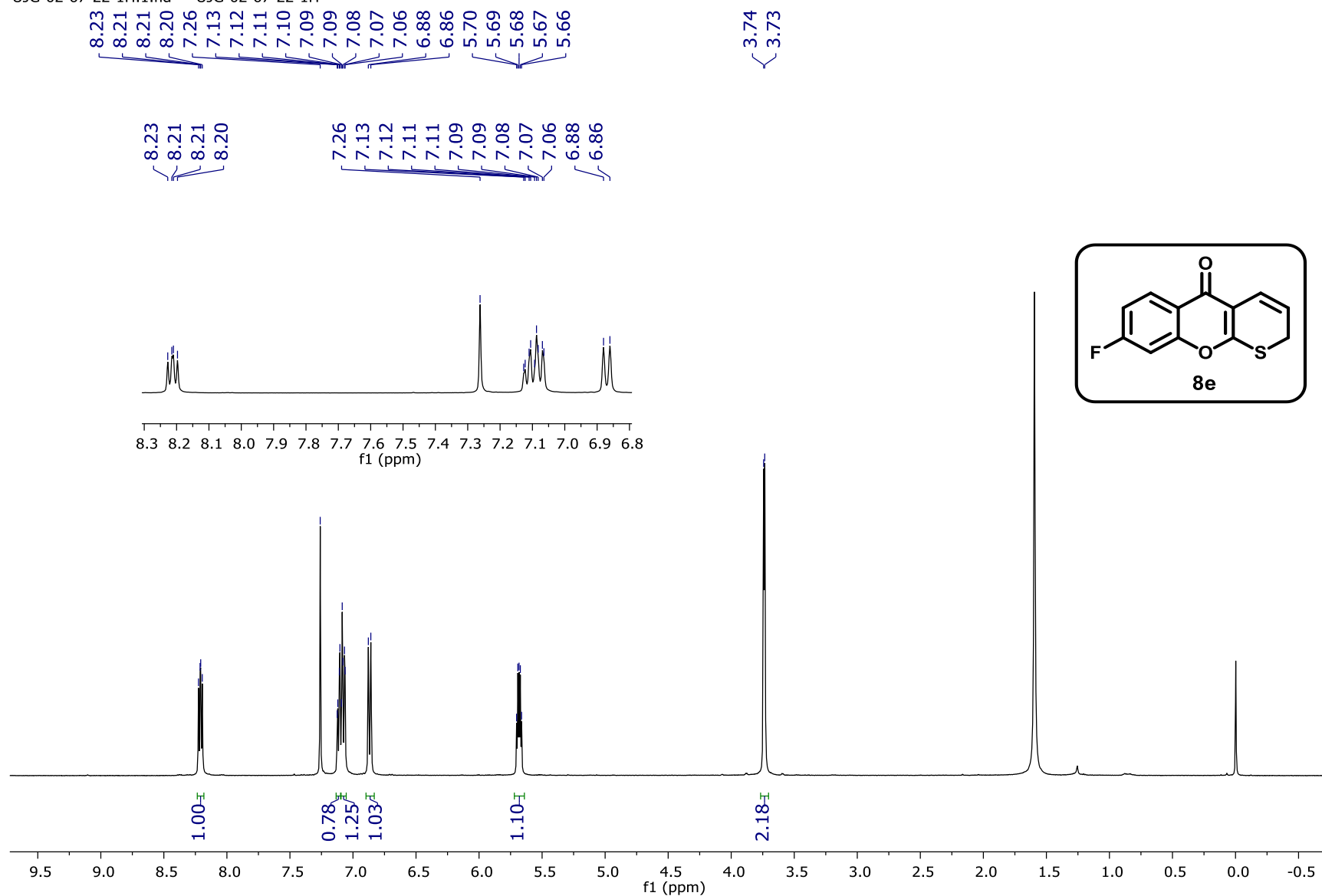
S204

HRMS Spectrum of Compound 8d



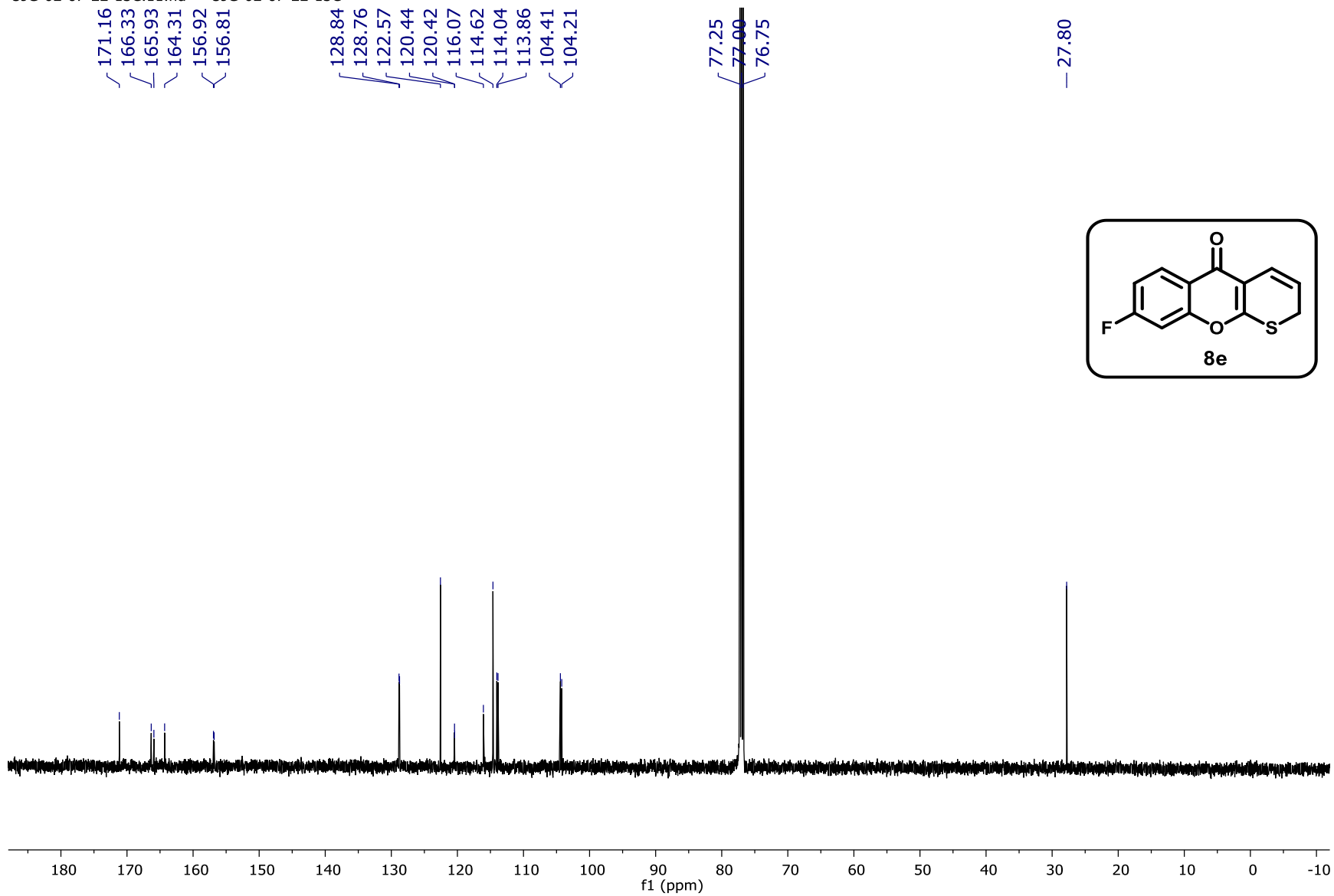
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8e

UJG-02-67-22-1H.1.fid — UJG-02-67-22-1H



^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 8e

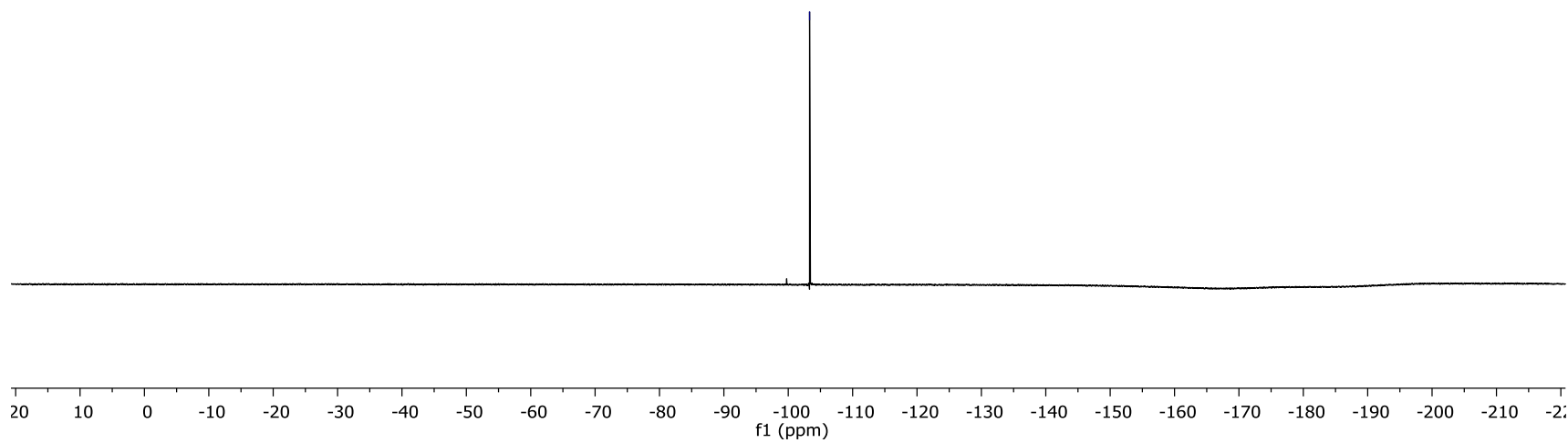
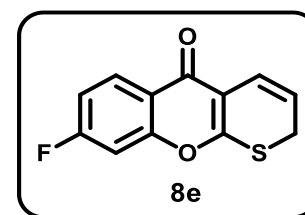
UJG-02-67-22-13C.11.fid — UJG-02-67-22-13C



^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 8e

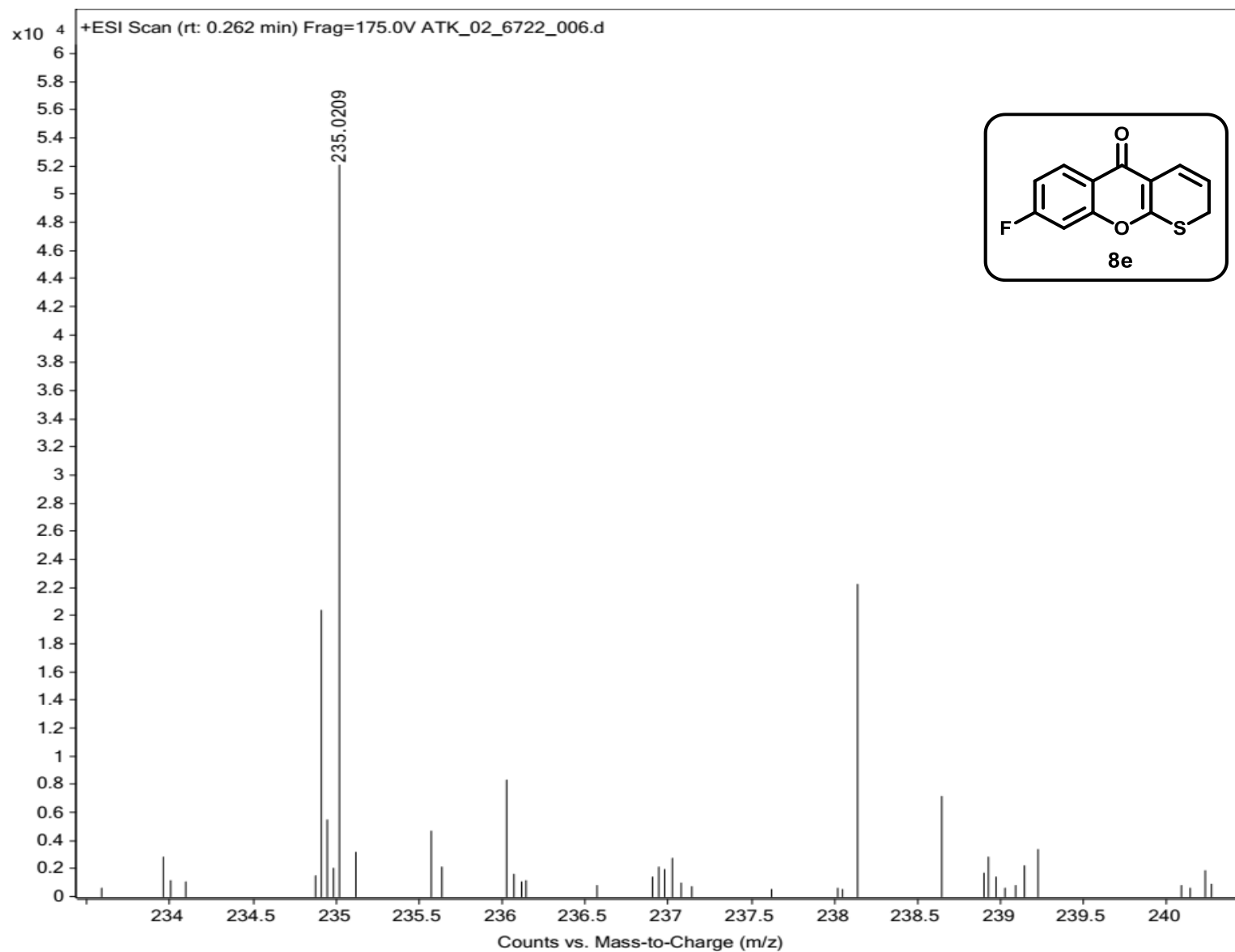
UJG-02-67-22-19F.5.fid — UJG-02-67-22-19F

— -103.31



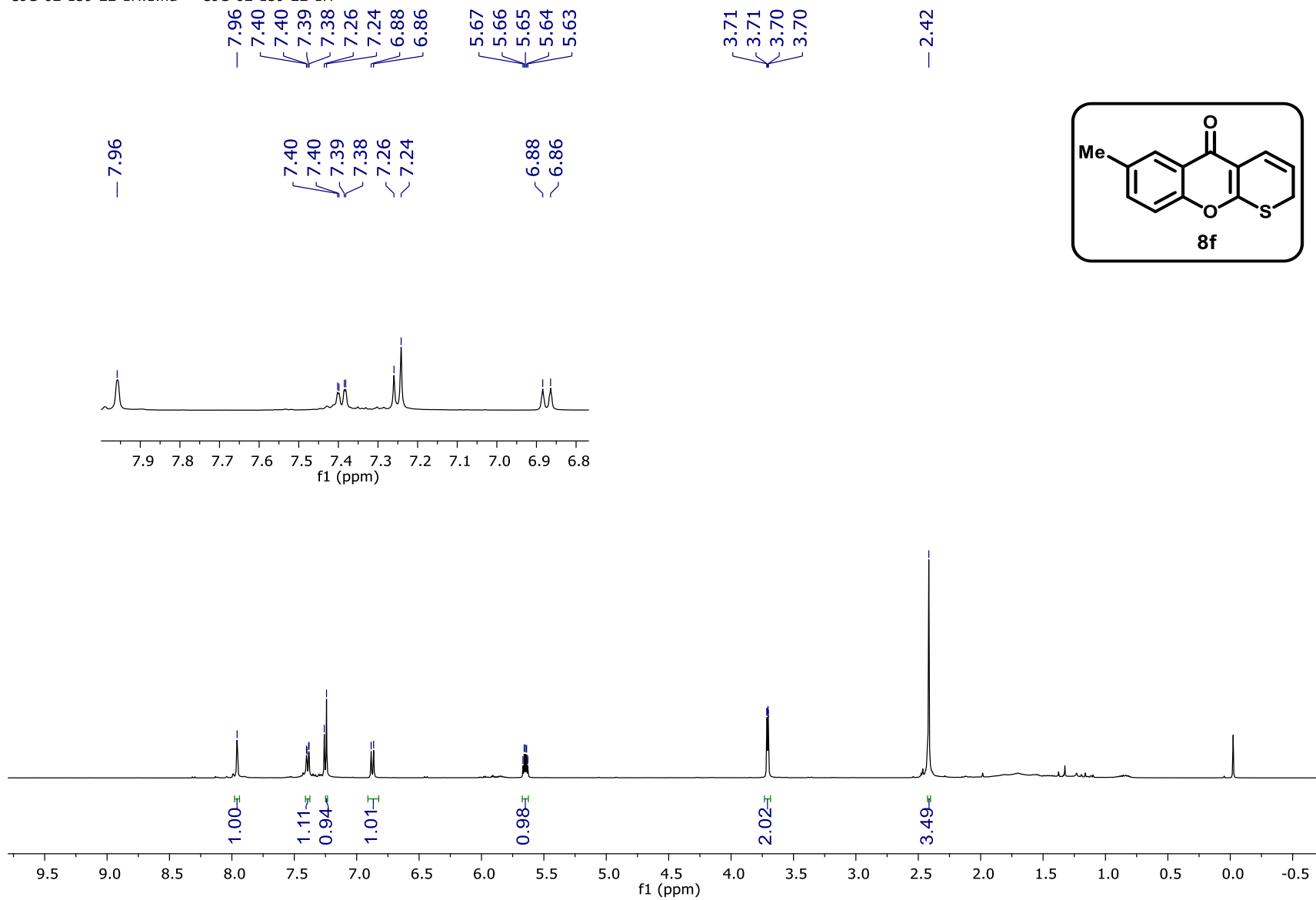
S208

HRMS Spectrum of Compound 8e



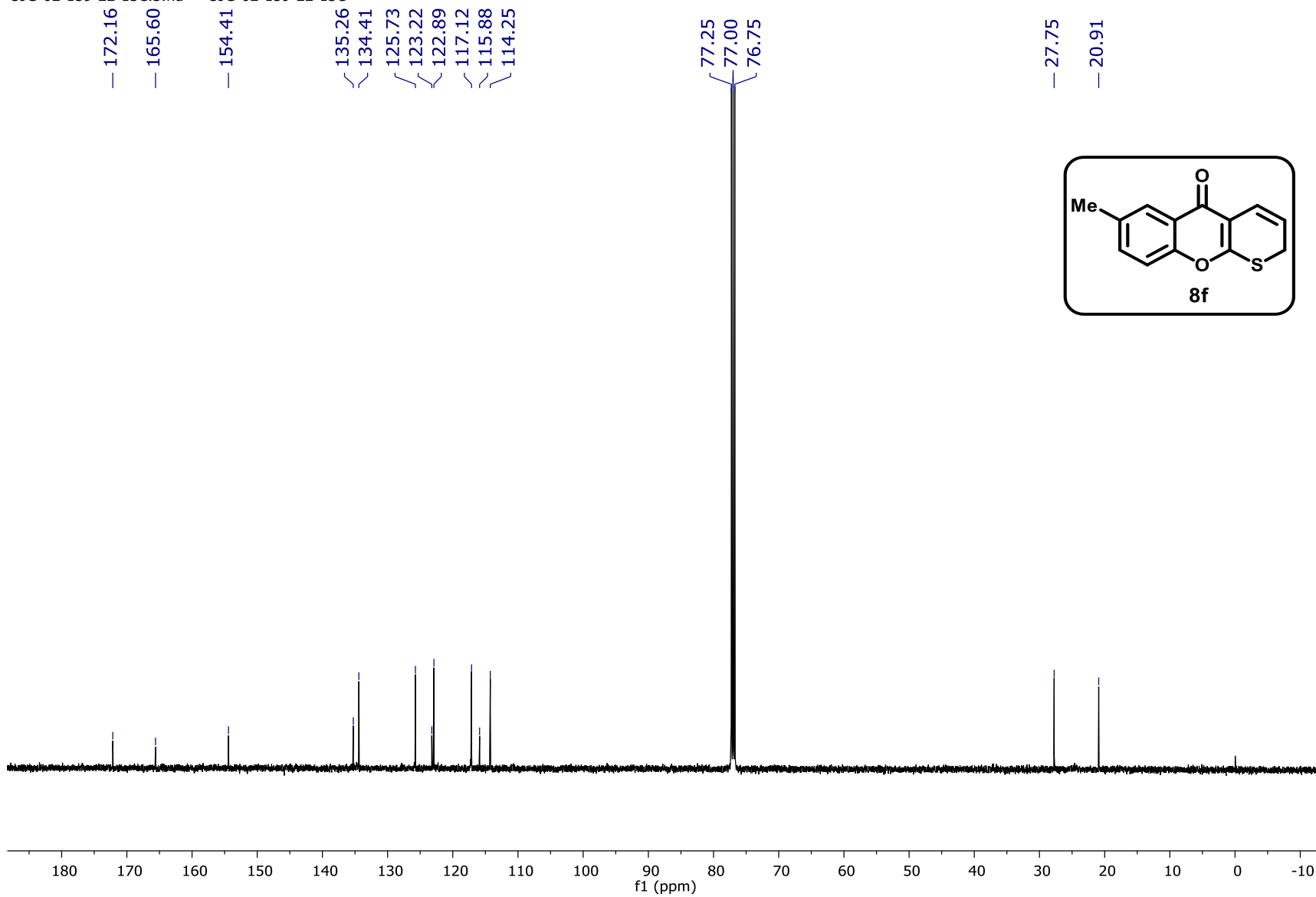
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8f

UJG-02-159-22-1H.1.fid — UJG-02-159-22-1H

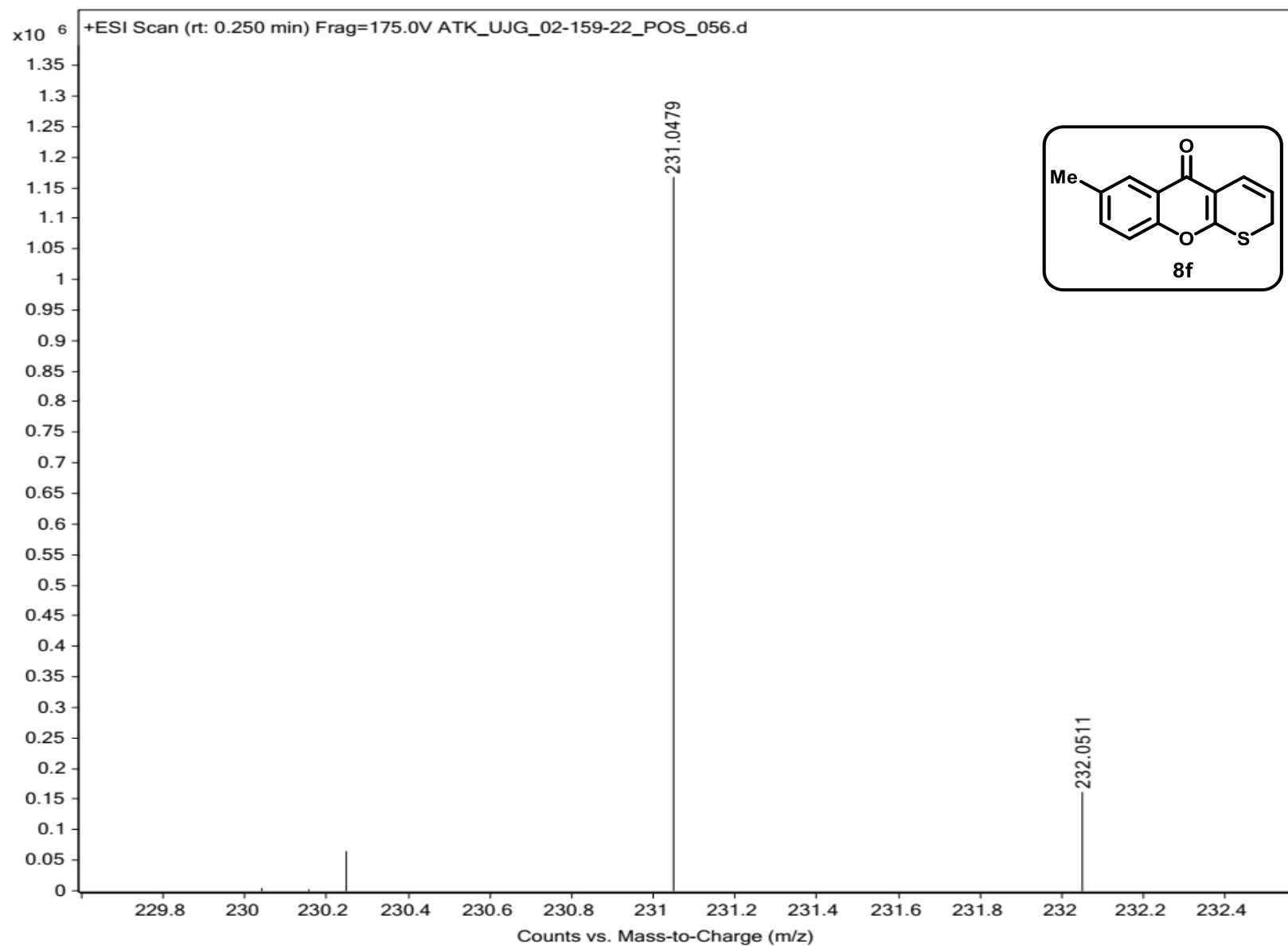


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8f

UJG-02-159-22-13C.3.fid — UJG-02-159-22-13C

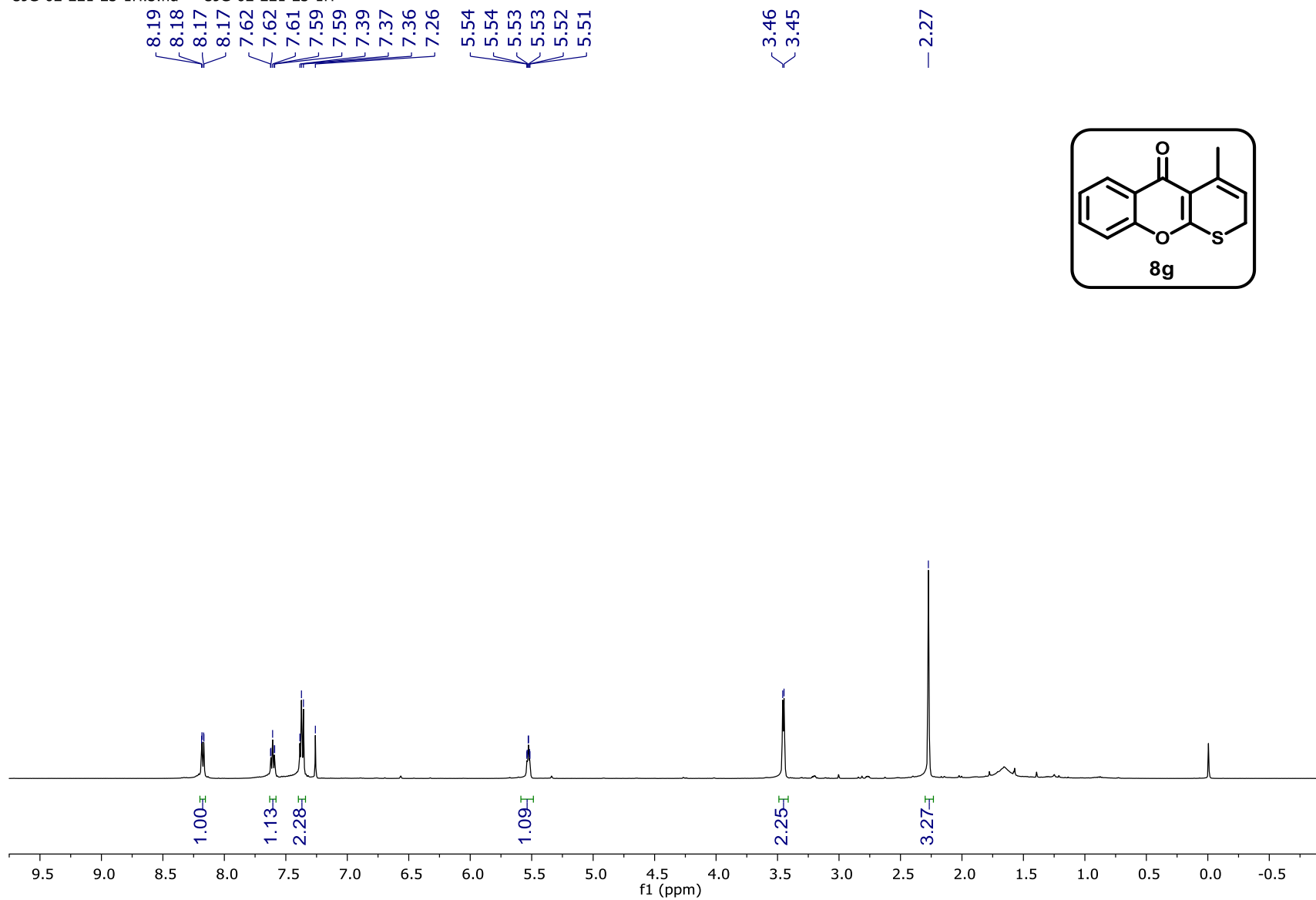


HRMS Spectrum of Compound 8f



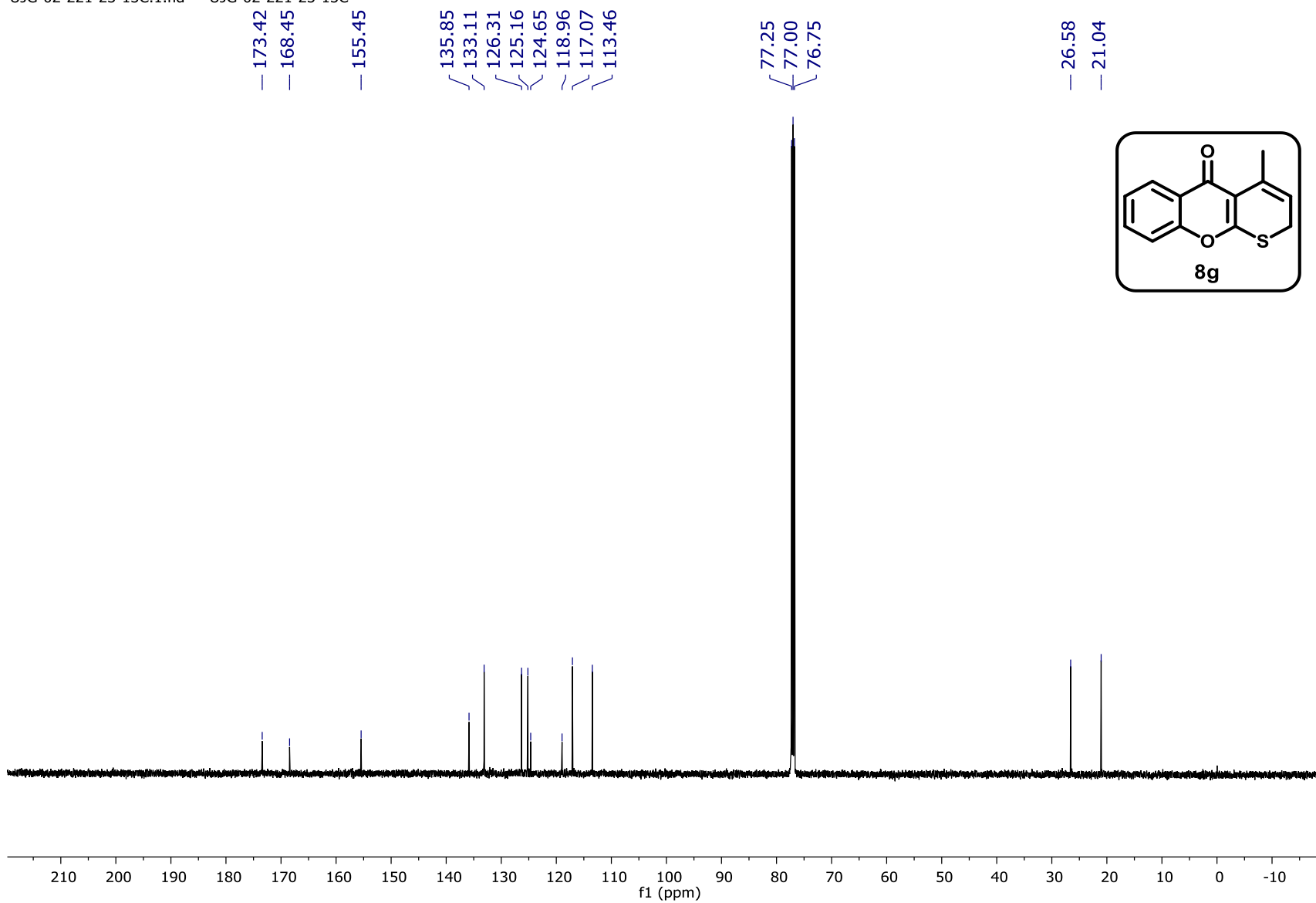
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8g

UJG-02-221-23-1H.3.fid — UJG-02-221-23-1H

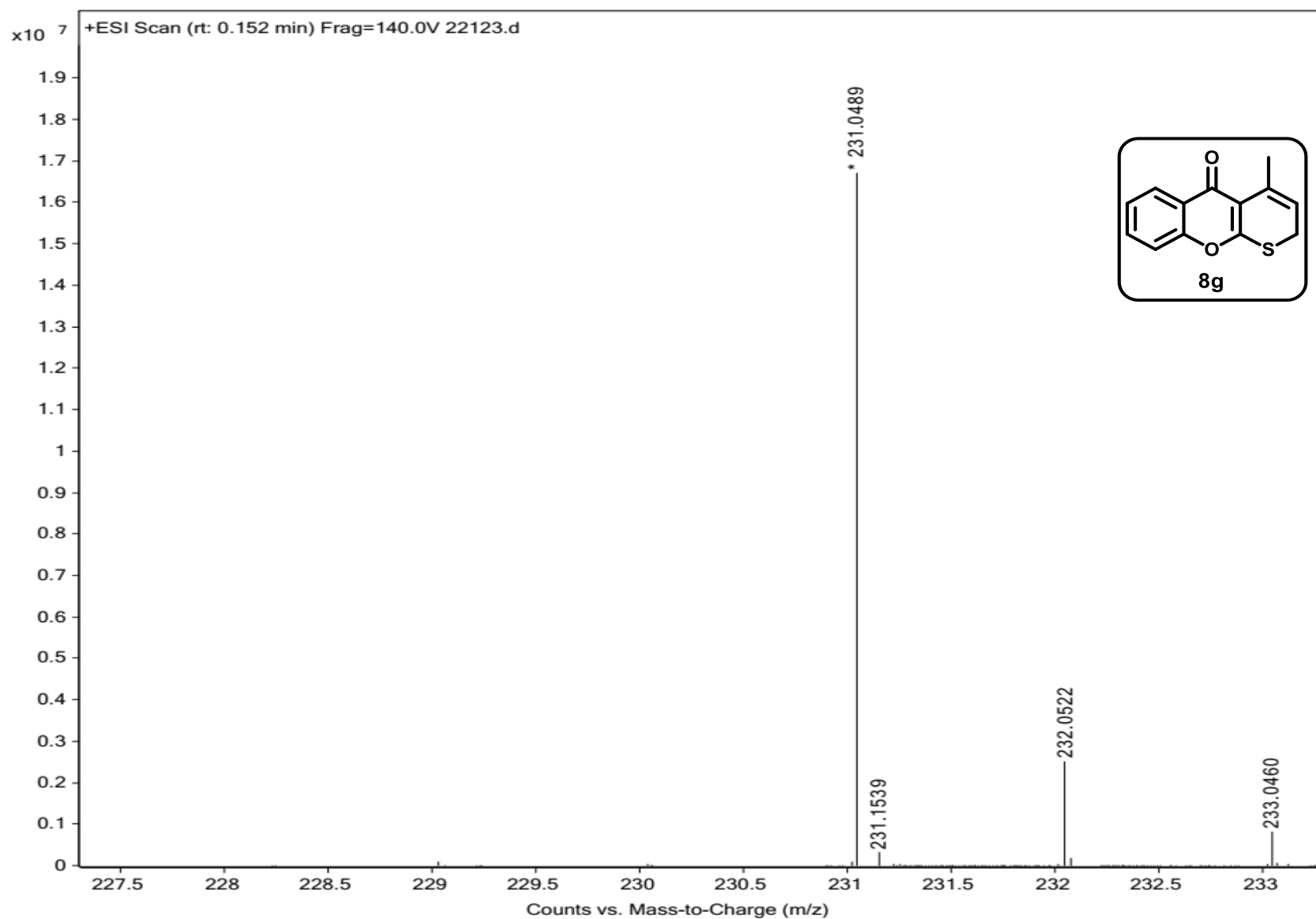


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8g

UJG-02-221-23-13C.1.fid — UJG-02-221-23-13C

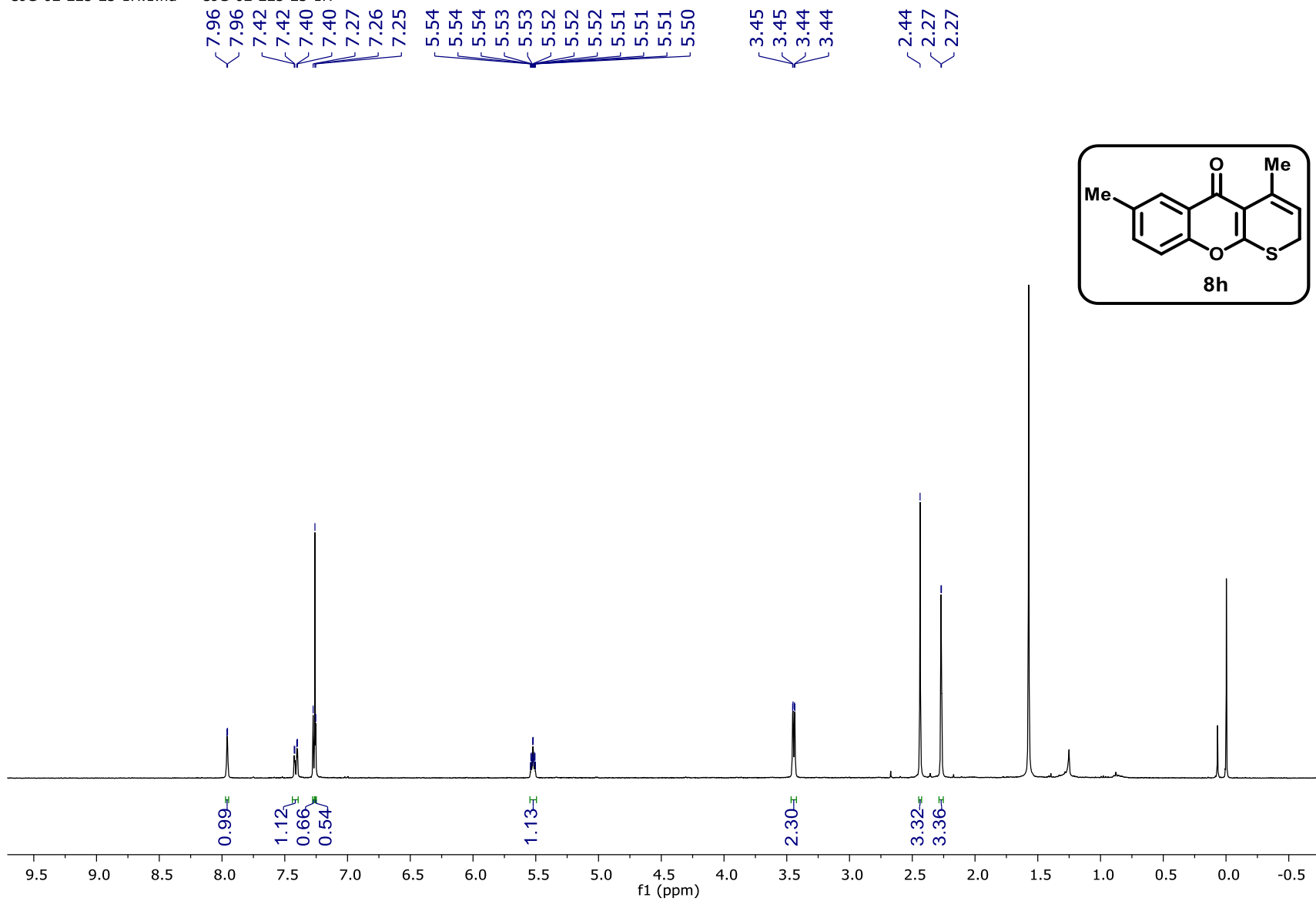


HRMS Spectrum of Compound 8g



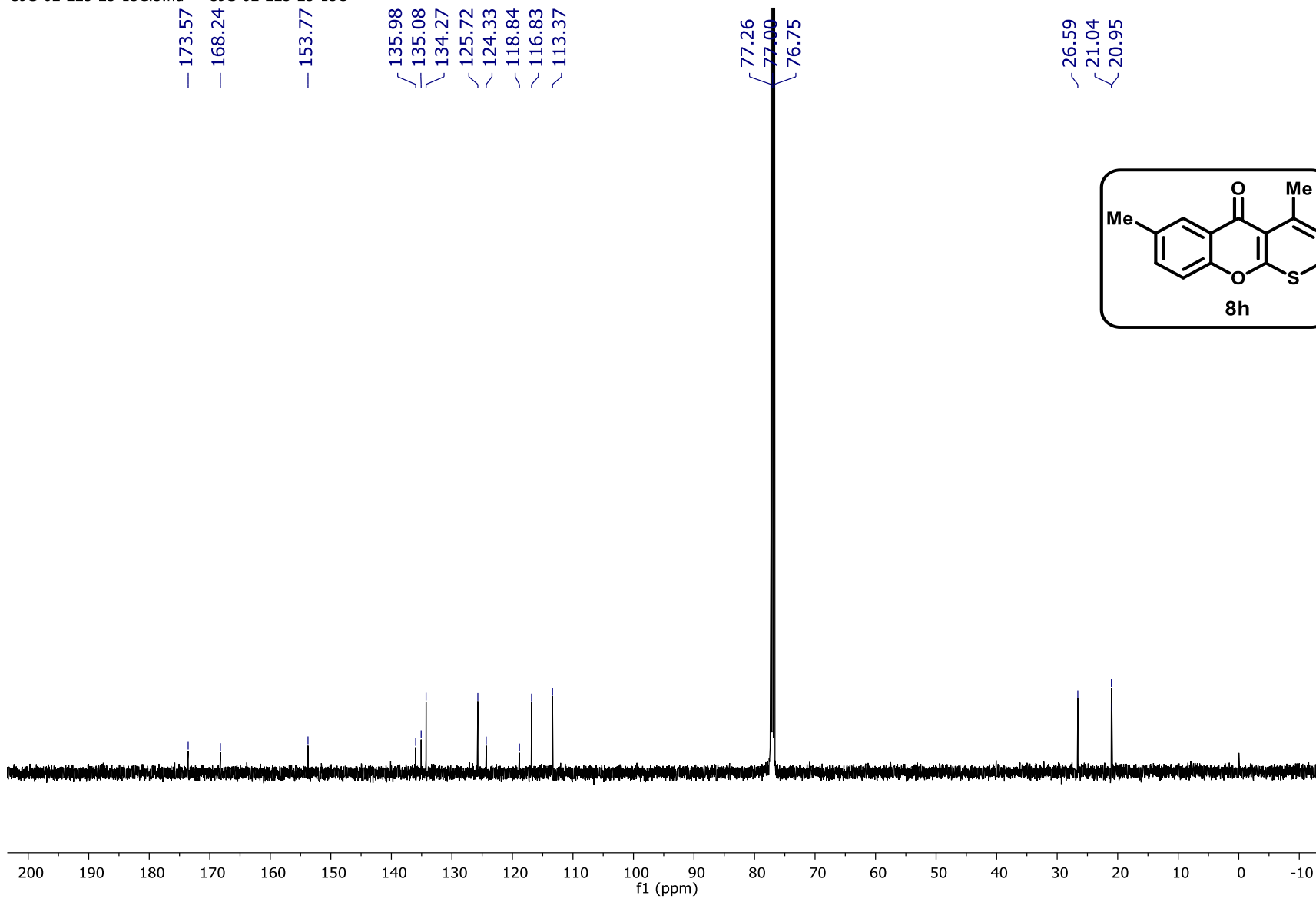
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 8h

UJG-02-225-23-1H.1.fid — UJG-02-225-23-1H

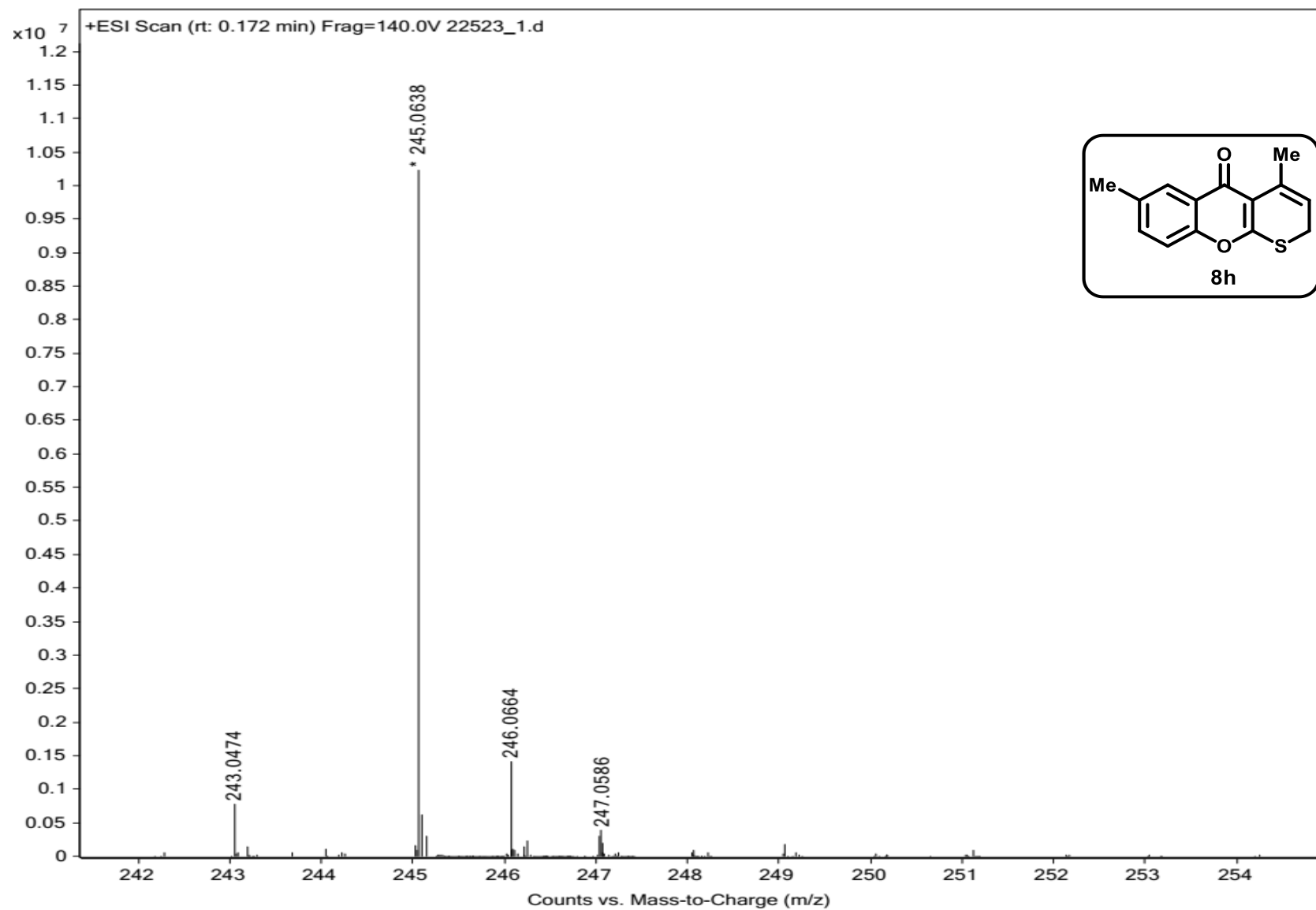


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8h

UJG-02-225-23-13C.3.fid — UJG-02-225-23-13C

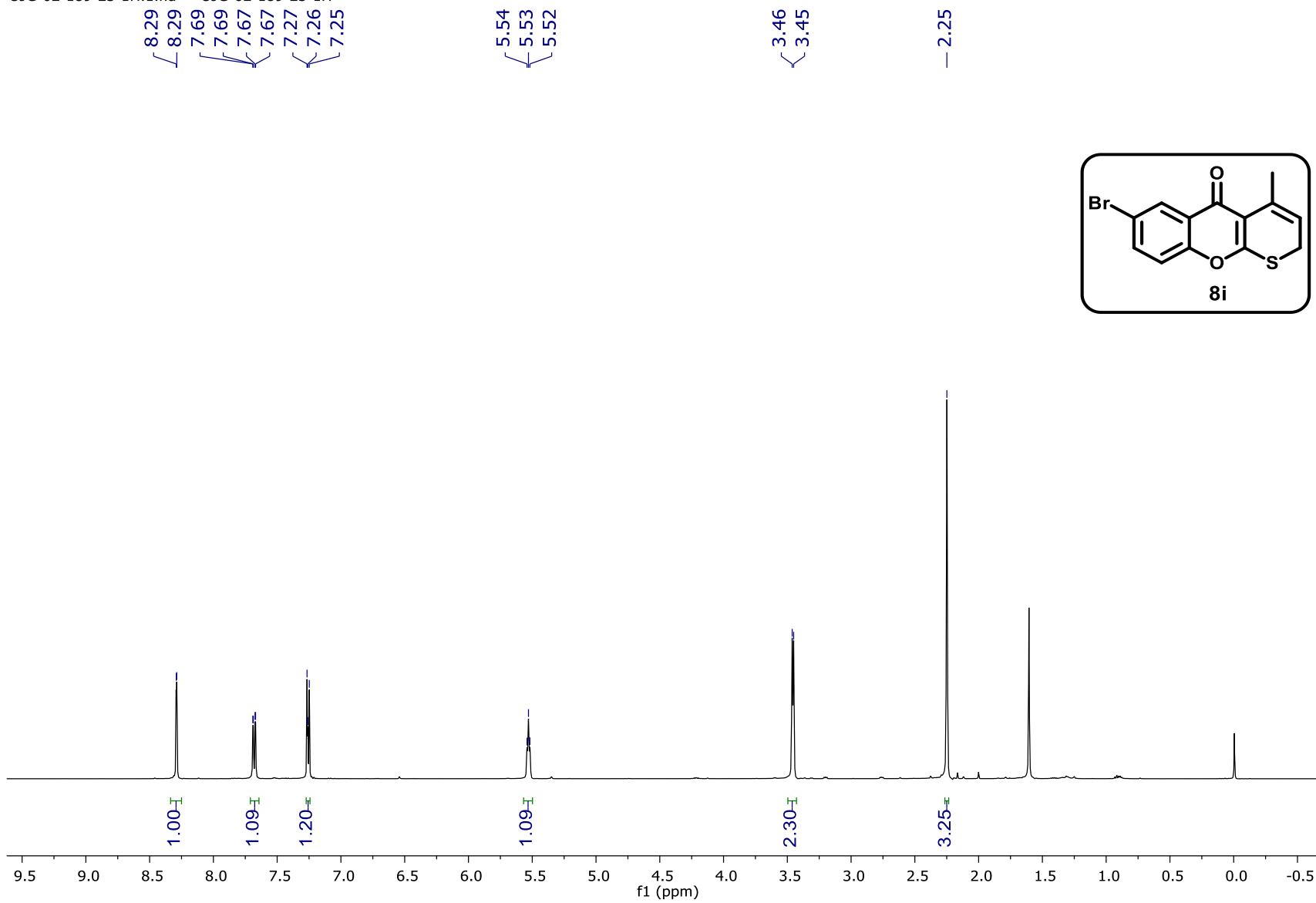


HRMS Spectrum of Compound 8h



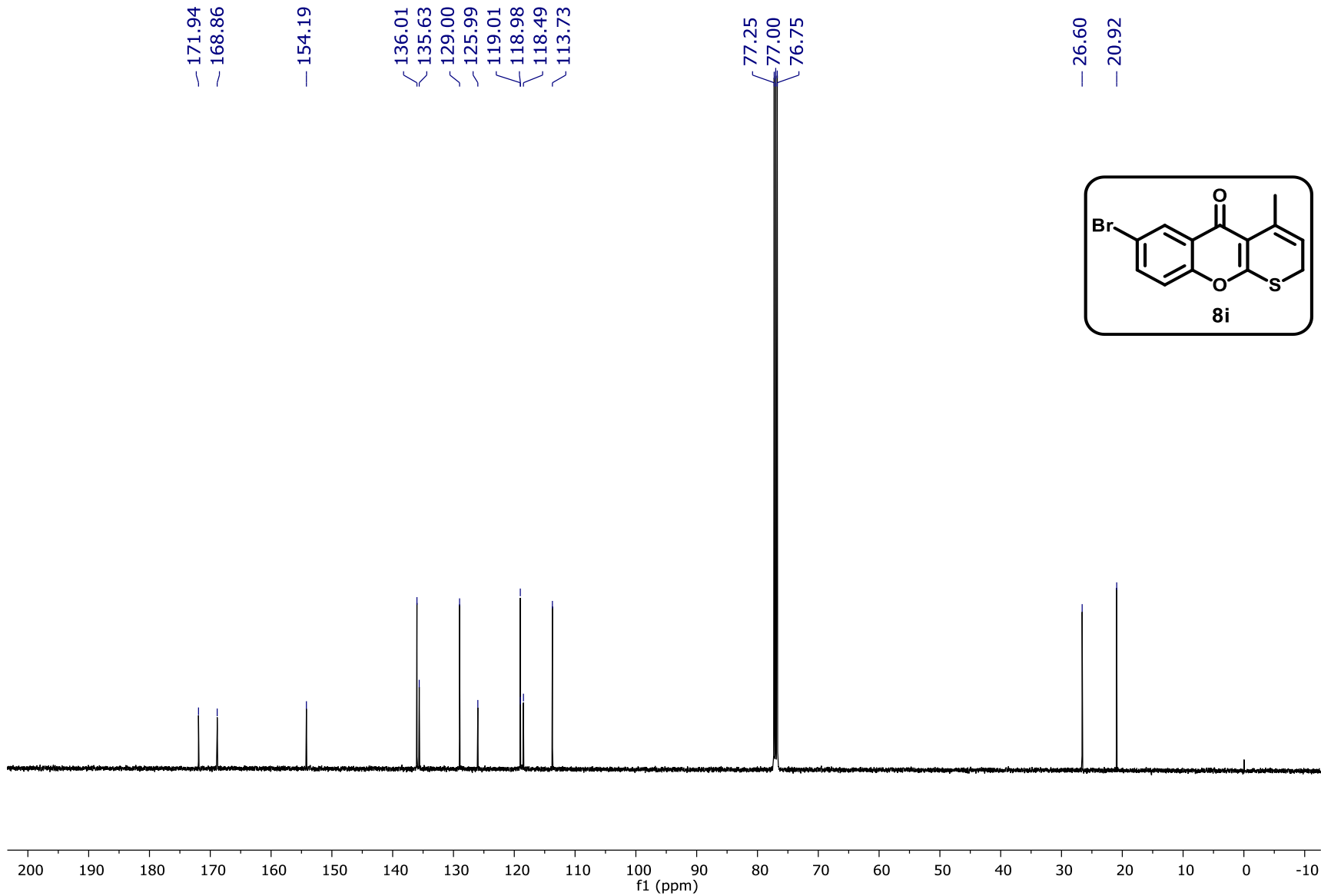
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8i

UJG-02-189-23-1H.1.fid — UJG-02-189-23-1H

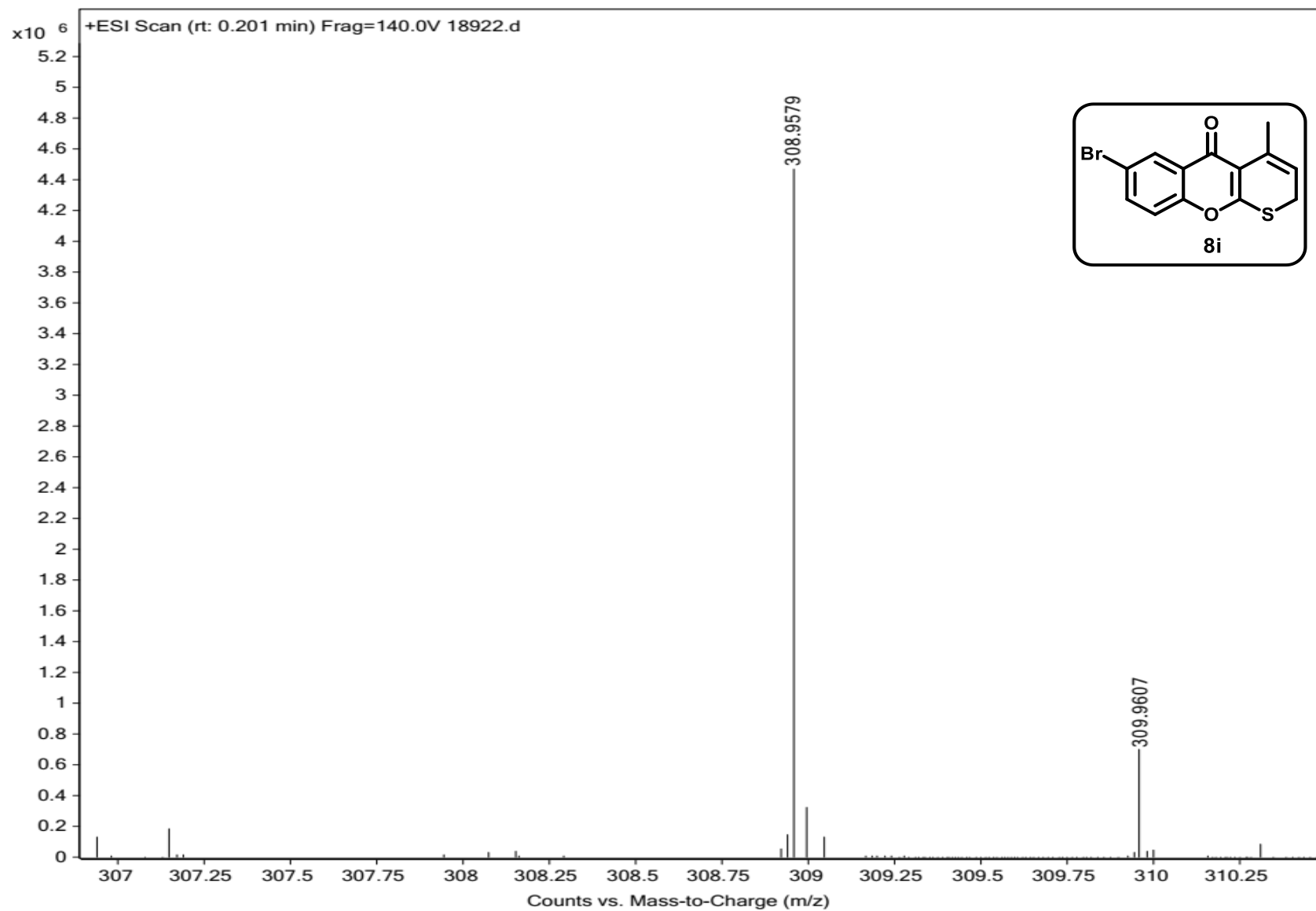


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8i

UJG-02-189-23-13C.3.fid — UJG-02-189-23-13C

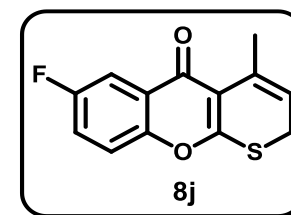
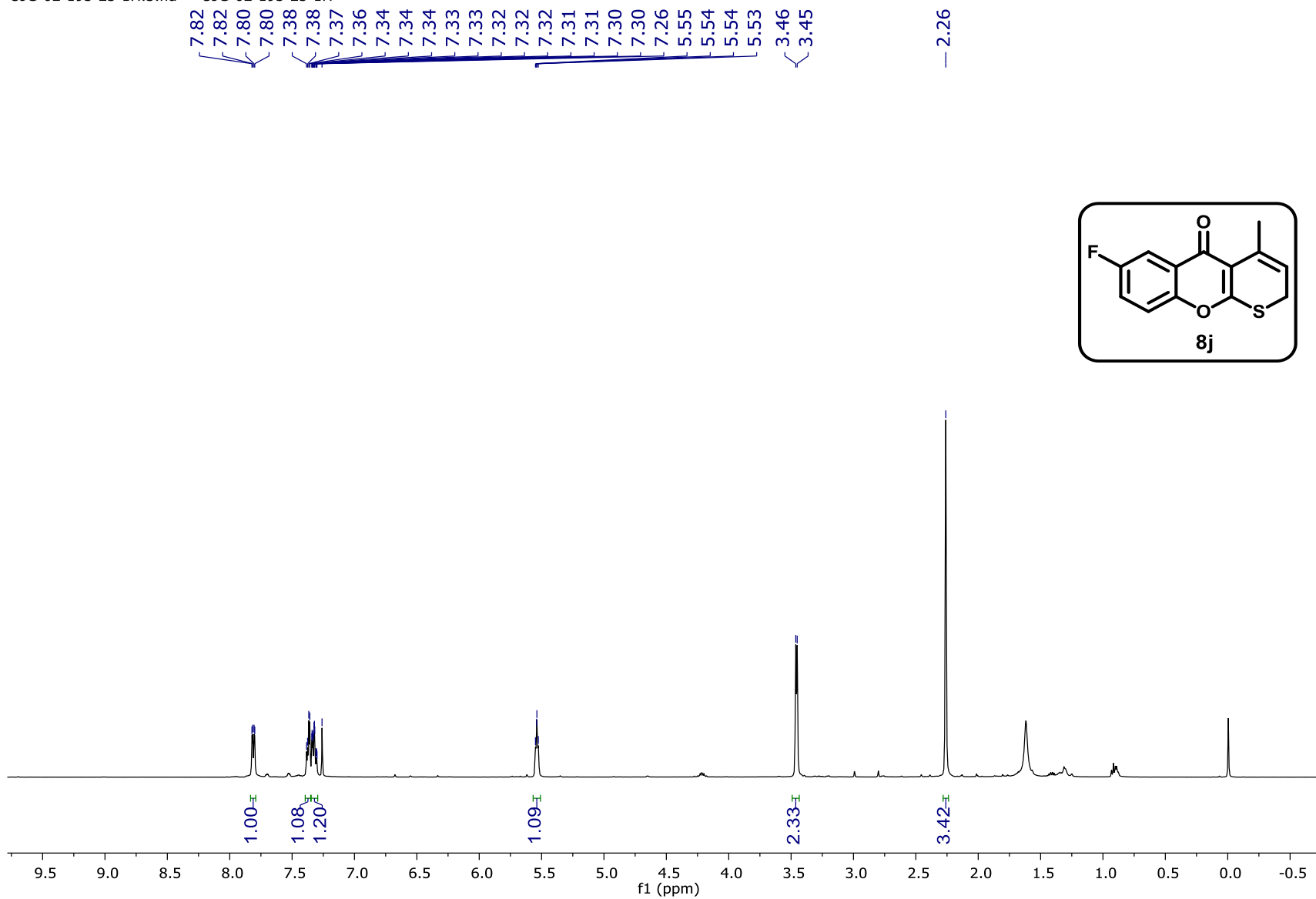


HRMS Spectrum of Compound 8i



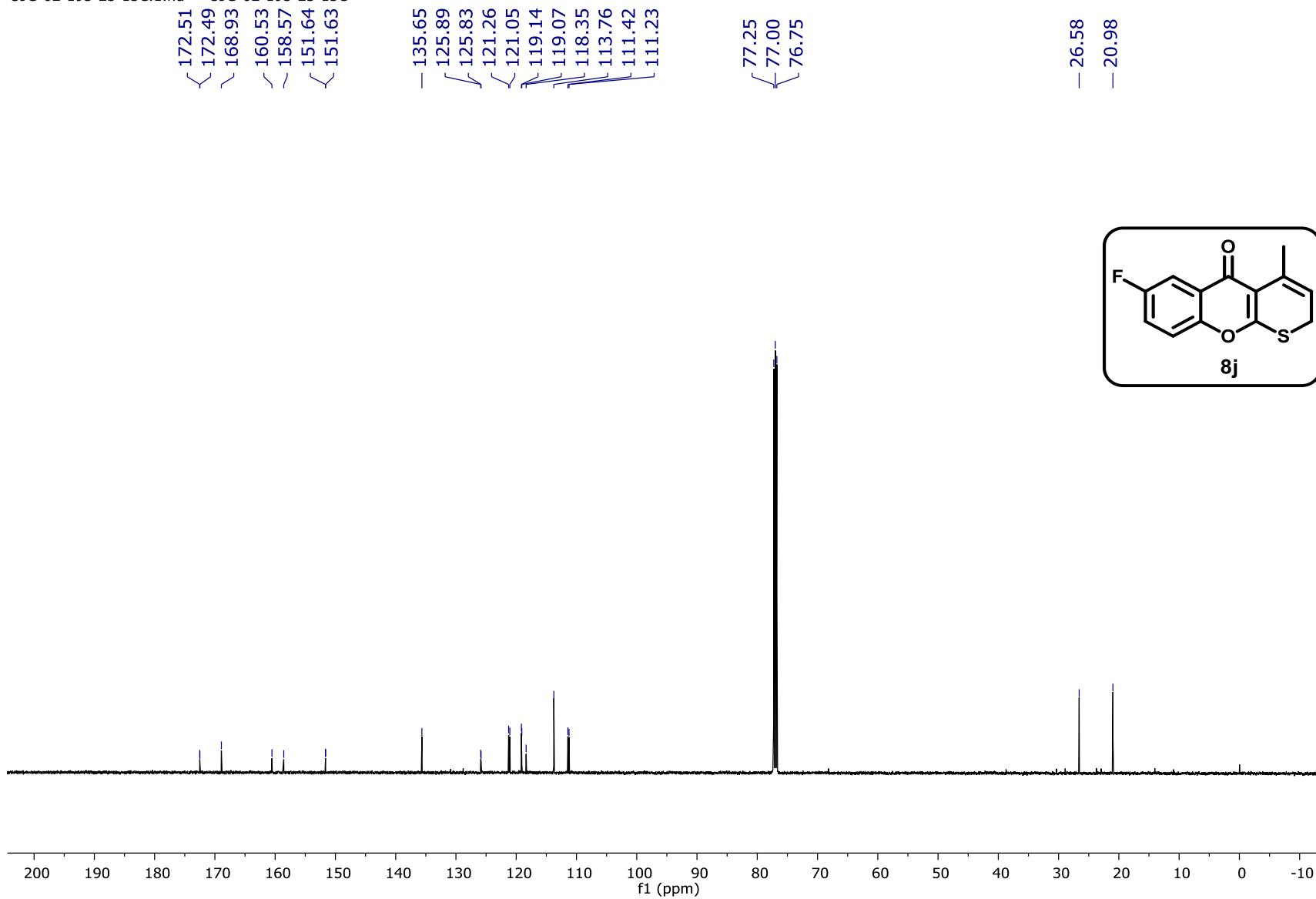
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8j

UJG-02-193-23-1H.3.fid — UJG-02-193-23-1H

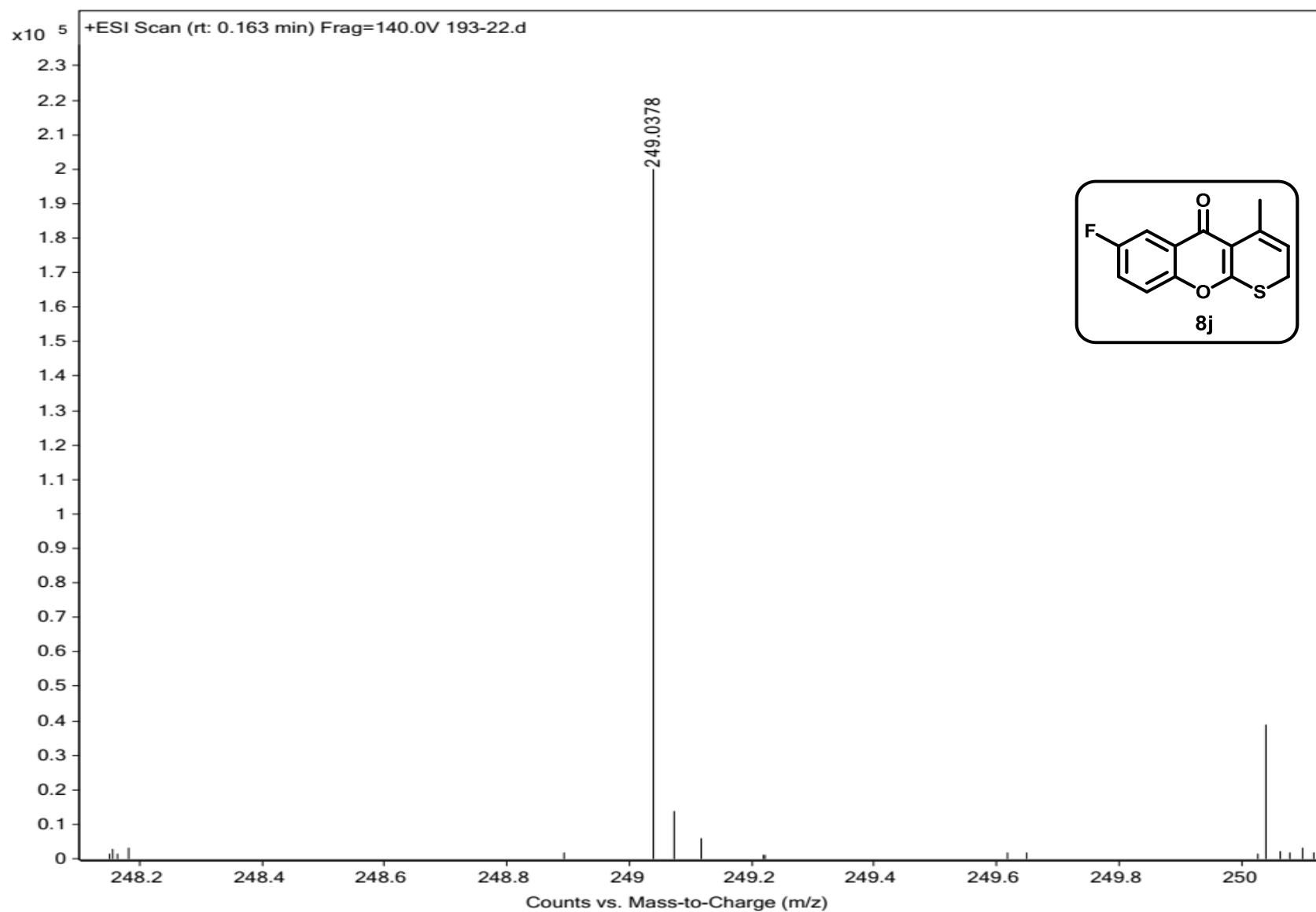


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 8j

UJG-02-193-23-13C.1.fid — UJG-02-193-23-13C

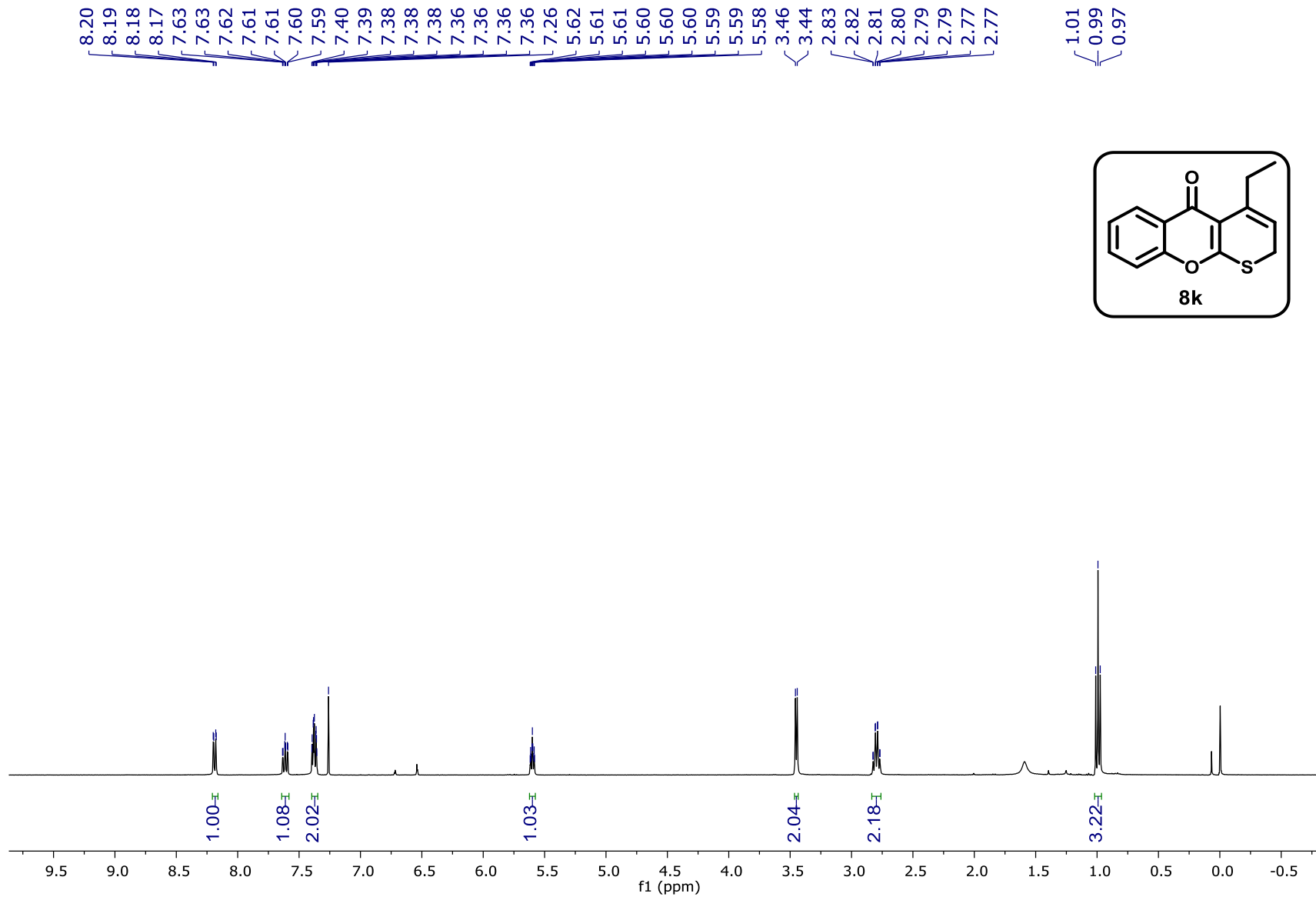


HRMS Spectrum of Compound 8j



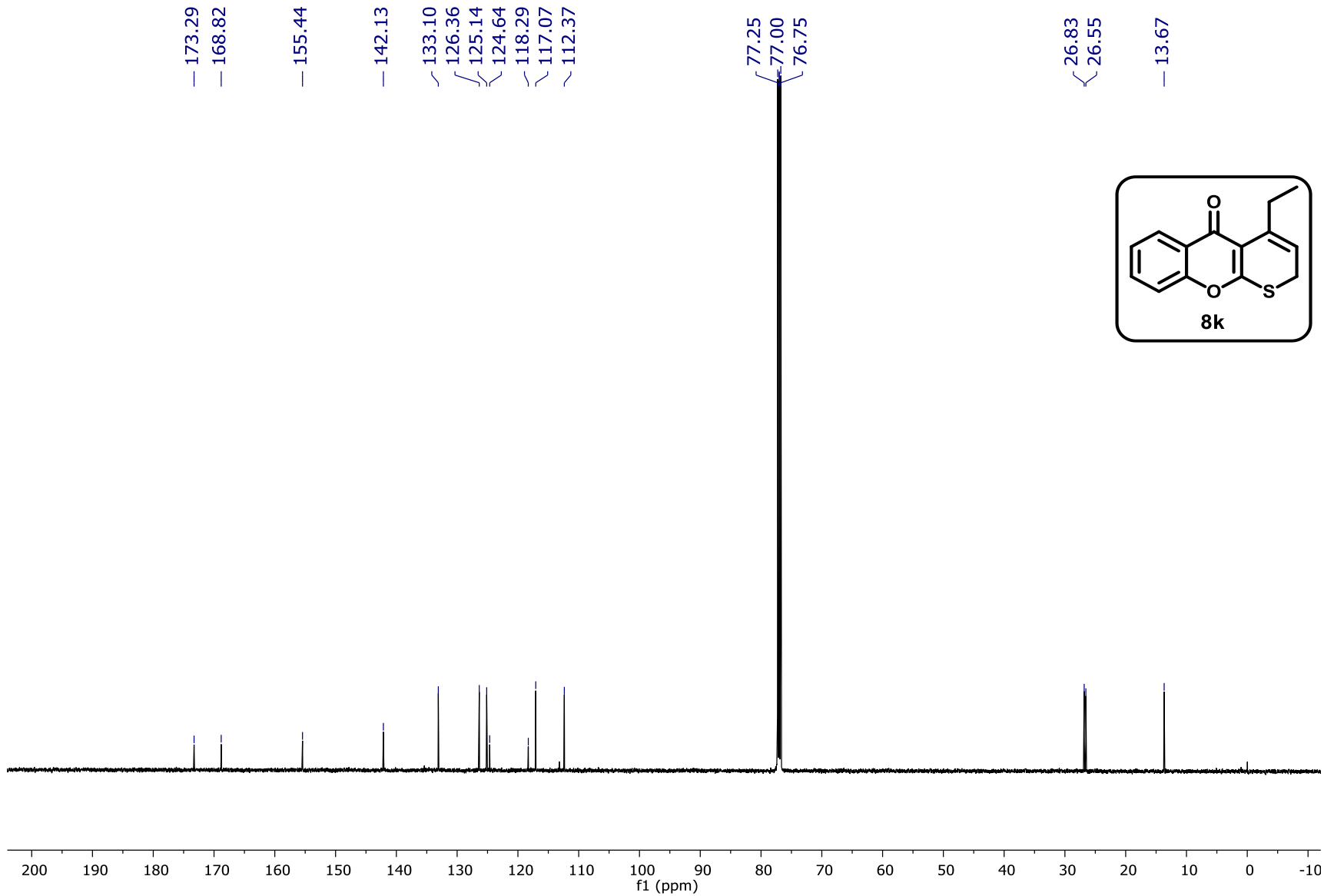
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 8k

UJG-02-231-23-1H.1.fid — UJG-02-231-23-1H

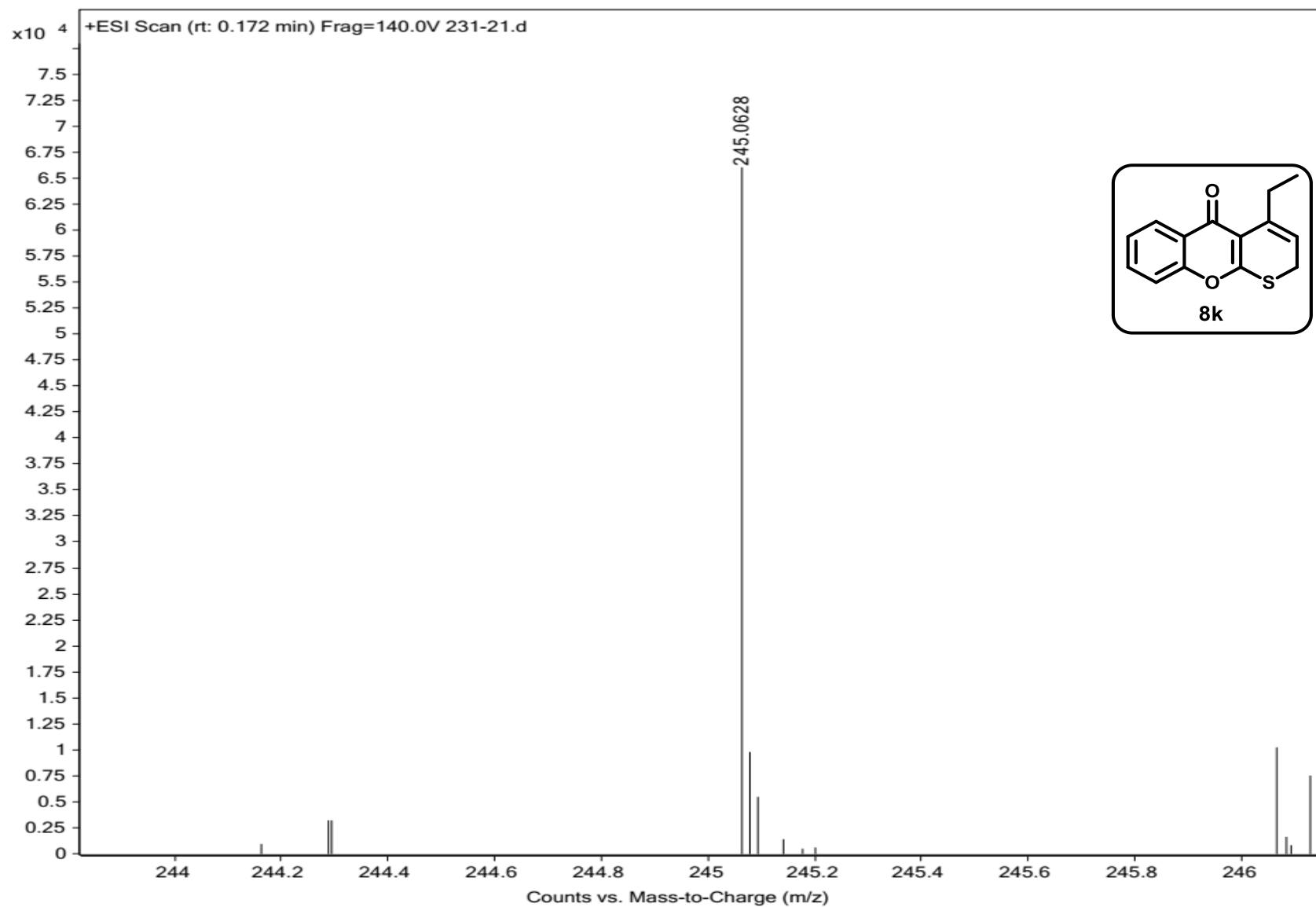


¹³C {¹H} NMR (125 MHz, CDCl₃) Spectrum of Compound 8k

UJG-02-231-23-13C.5.fid — UJG-02-231-23-13C

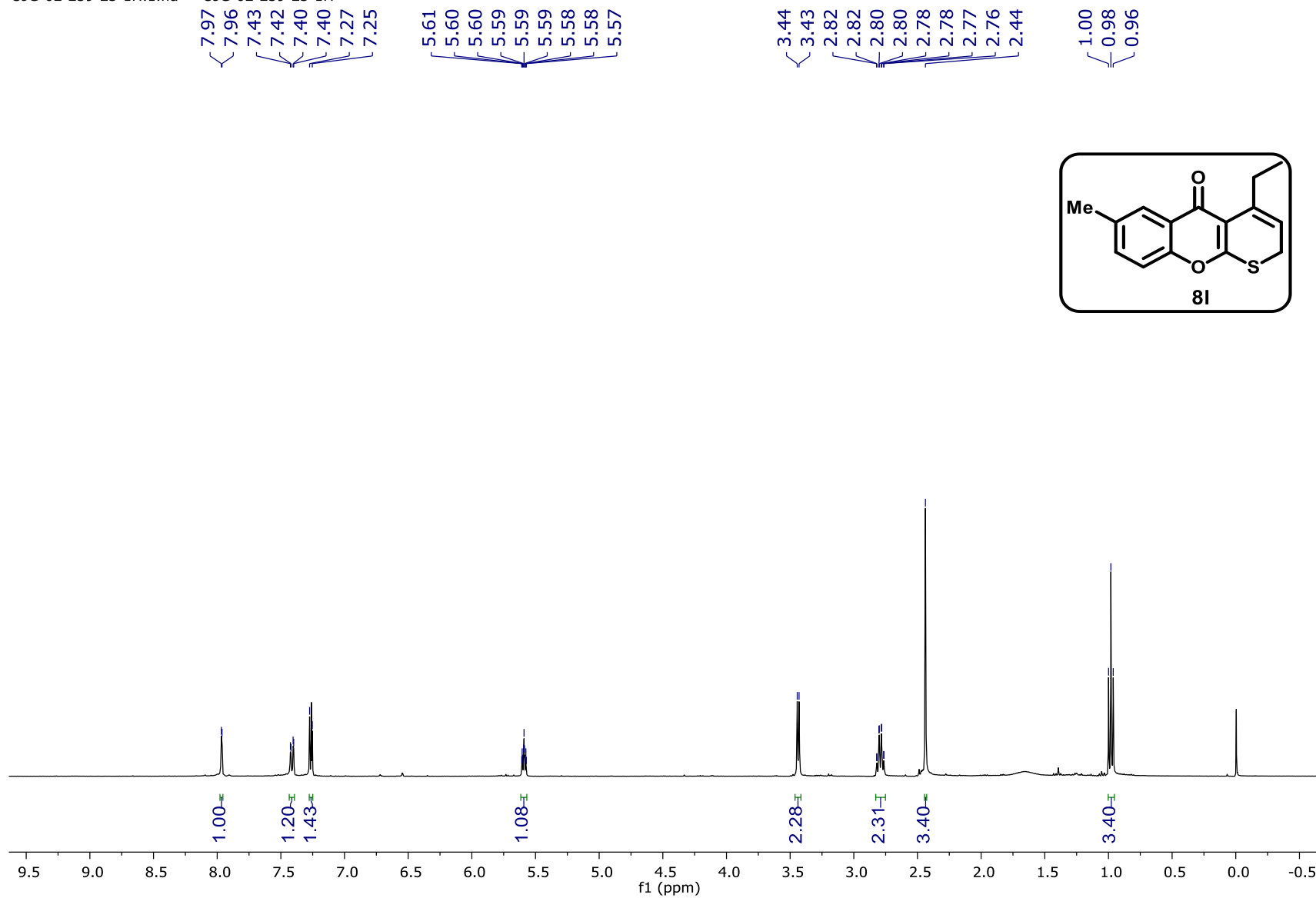


HRMS Spectrum of Compound 8k



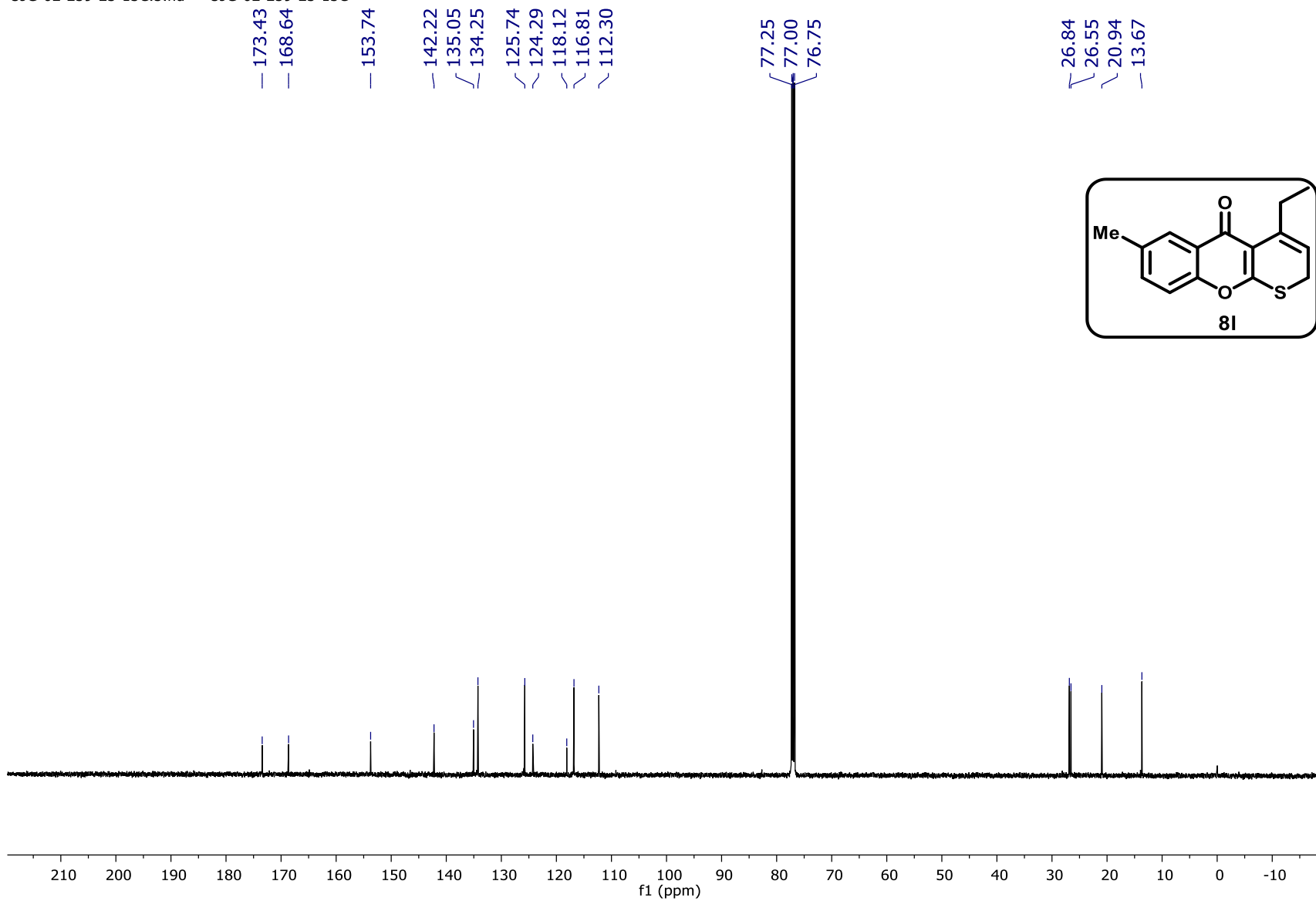
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 8l

UJG-02-259-23-1H.1.fid — UJG-02-259-23-1H

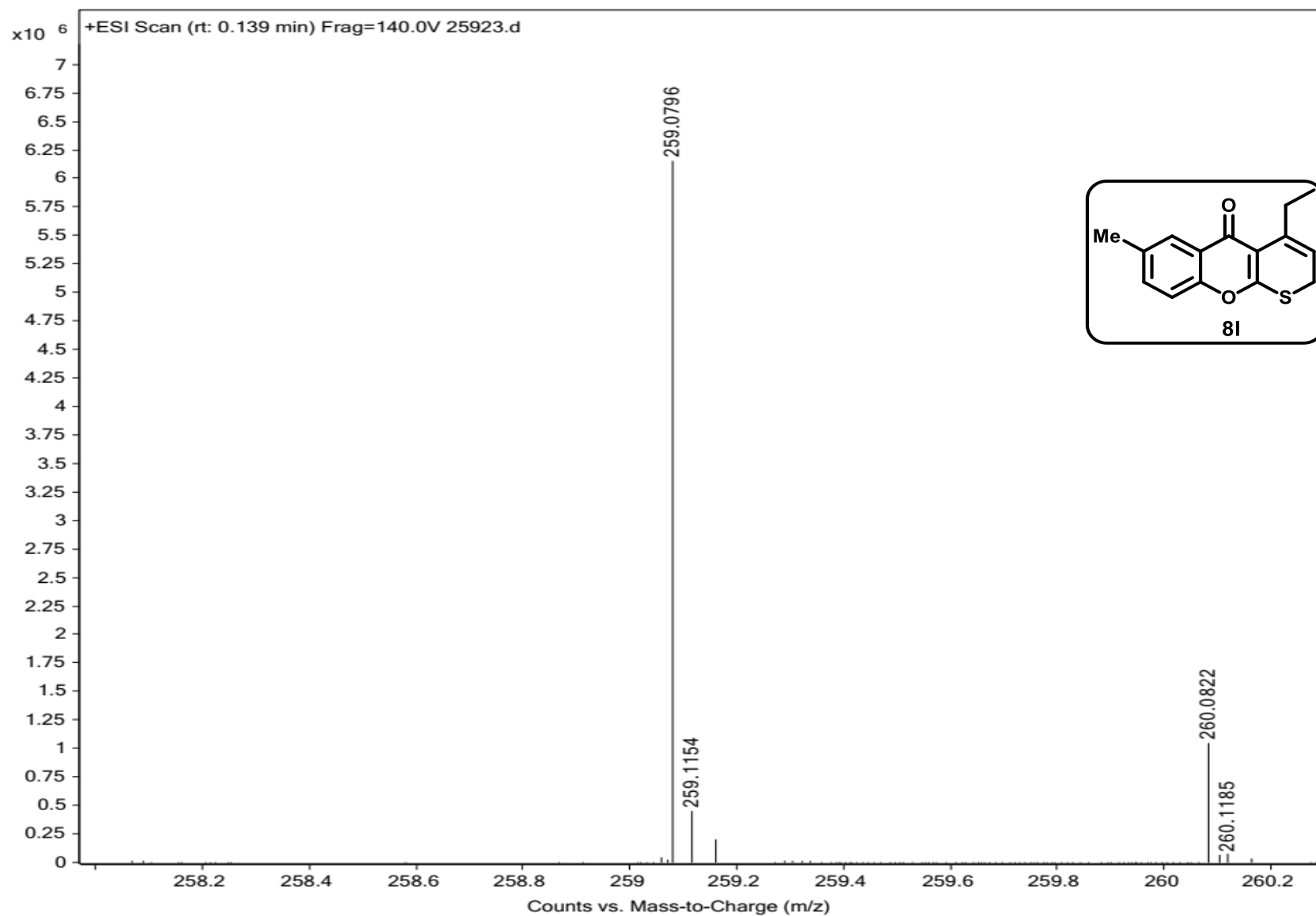


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 8l

UJG-02-259-23-13C.5.fid — UJG-02-259-23-13C

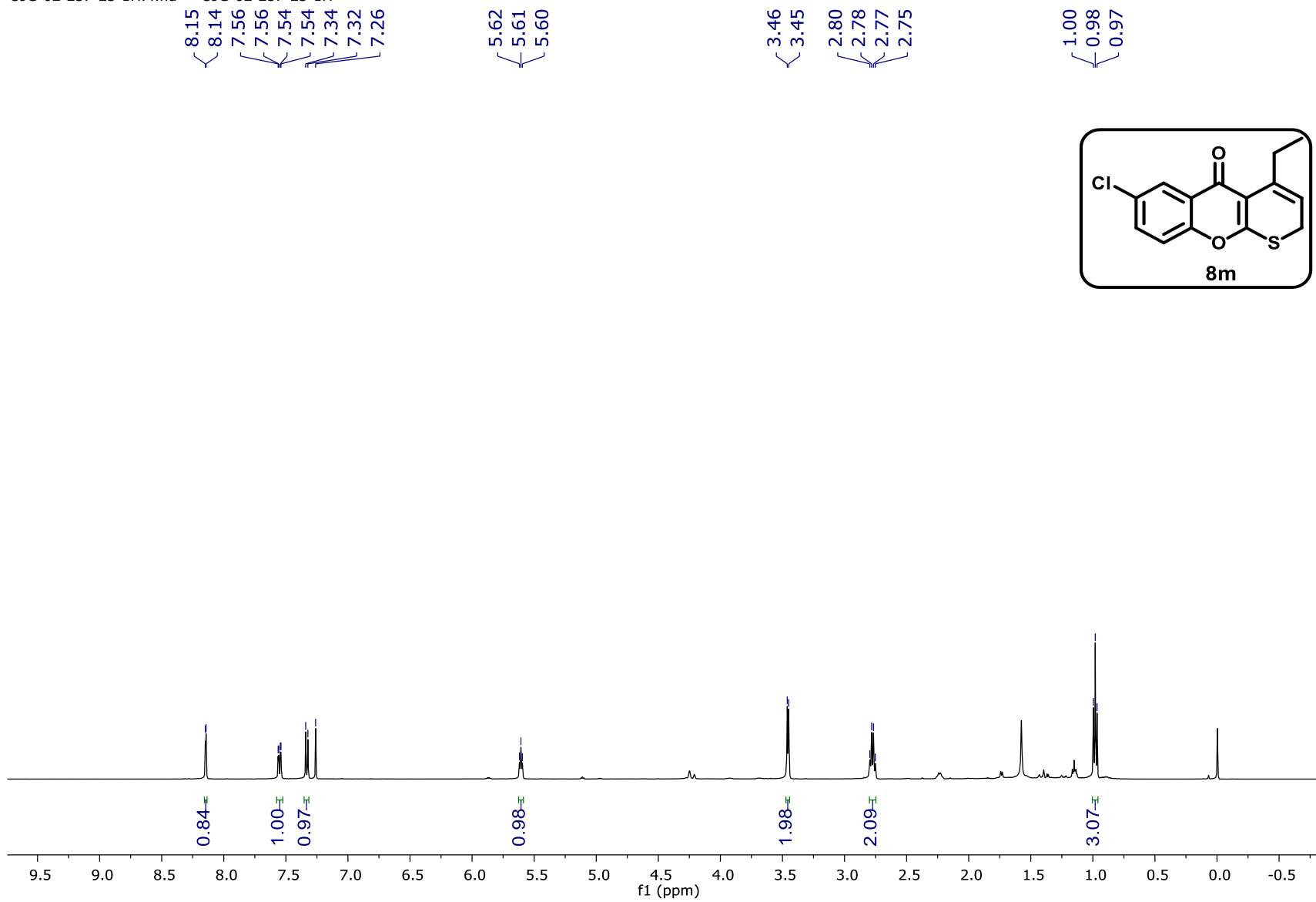


Spectrum of Compound 8l



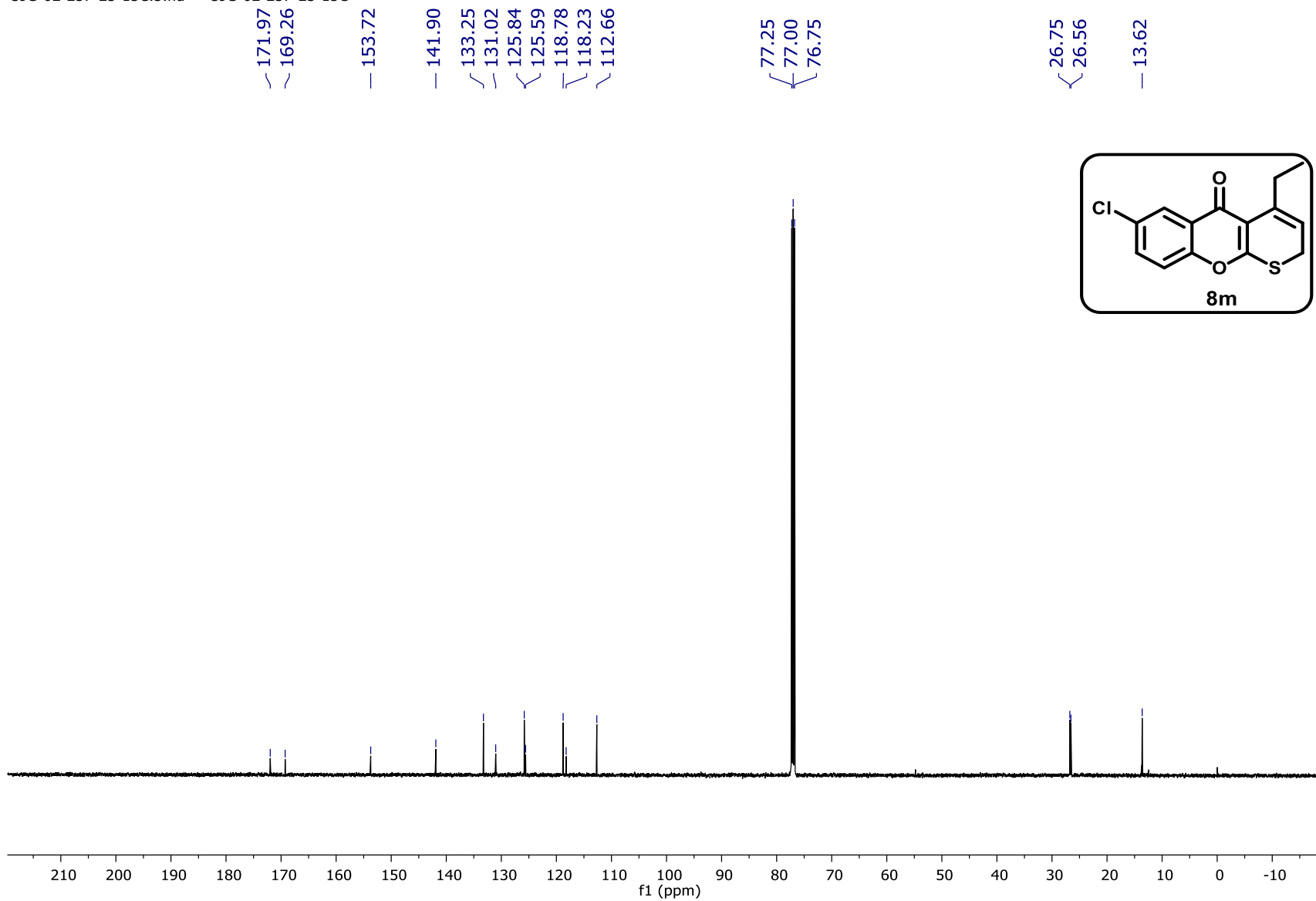
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 8m

UJG-02-257-23-1H.4.fid — UJG-02-257-23-1H

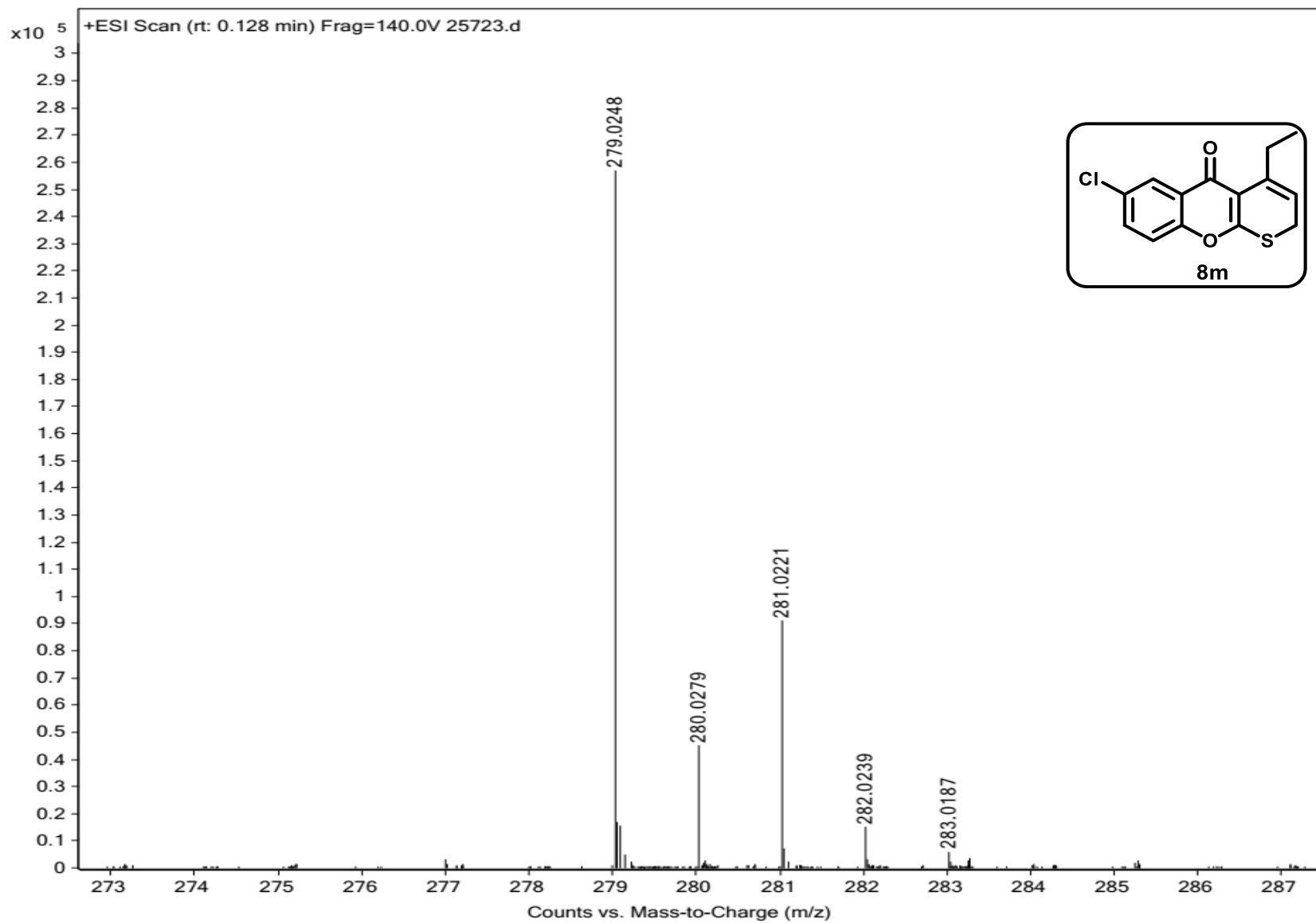


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 8m

UJG-02-257-23-13C.5.fid — UJG-02-257-23-13C

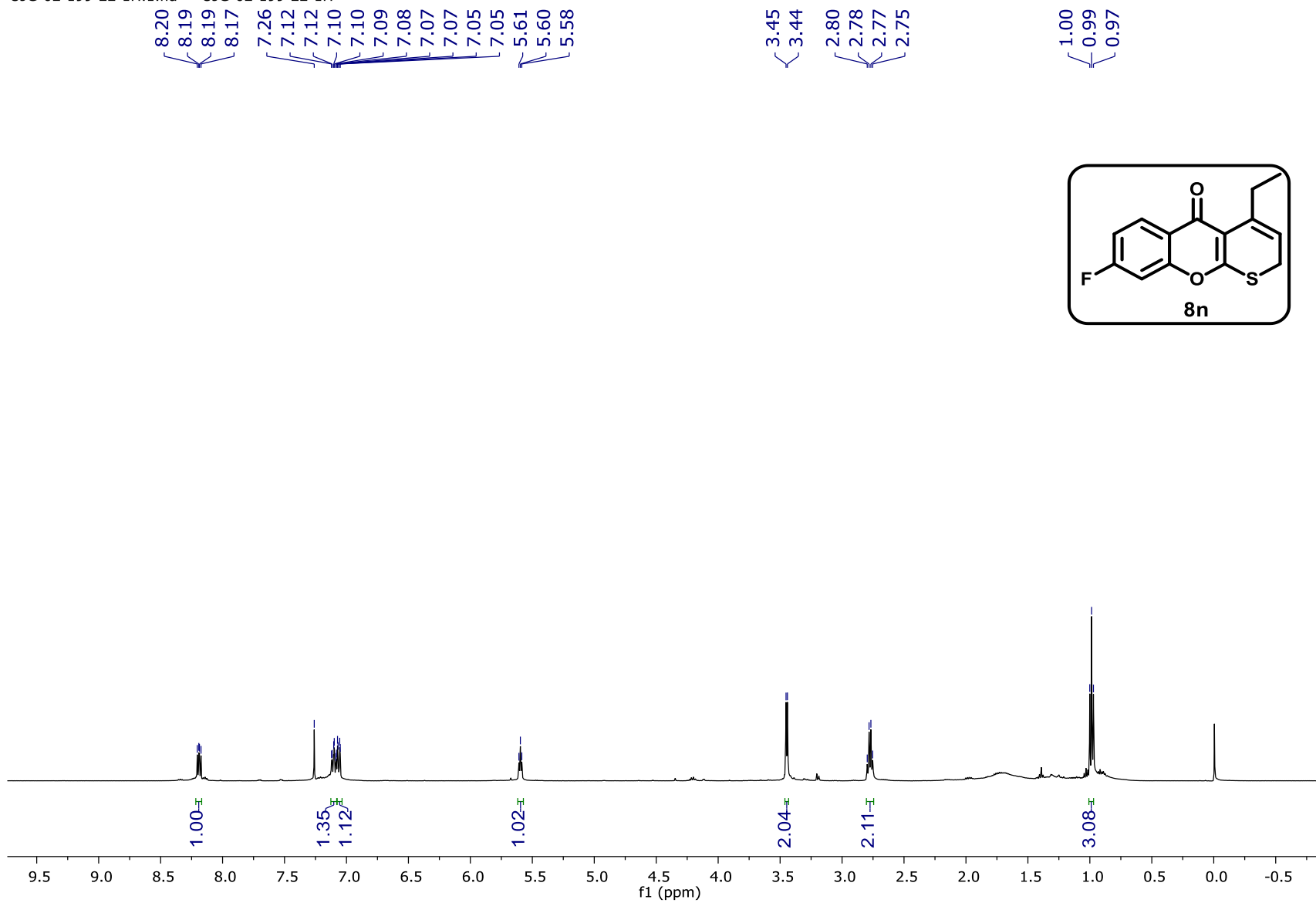


HRMS Spectrum of Compound 8m



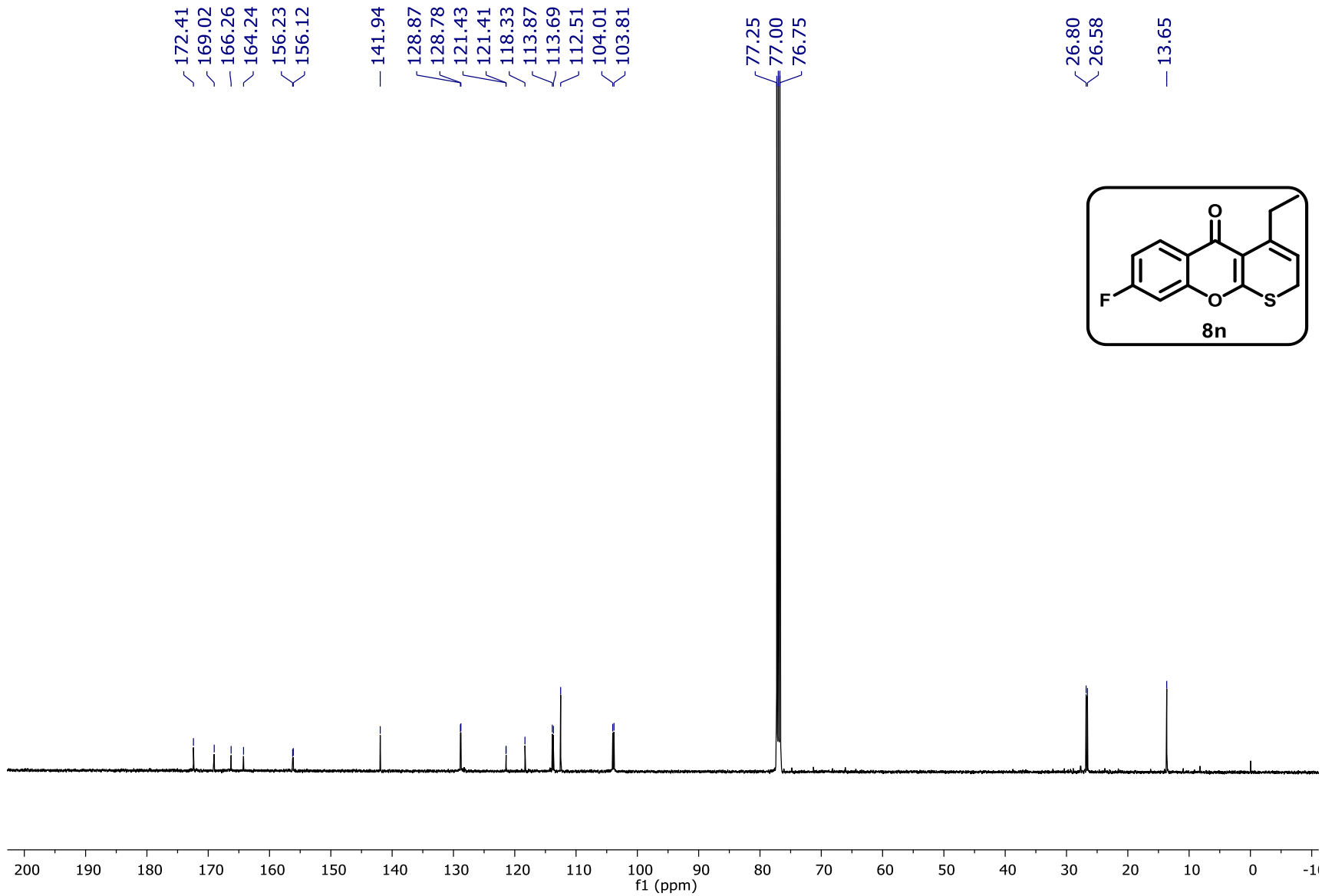
^1H NMR (500 MHz, CDCl_3) Spectrum of Compound 8n

UJG-02-199-22-1H.1.fid — UJG-02-199-22-1H



^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 8n

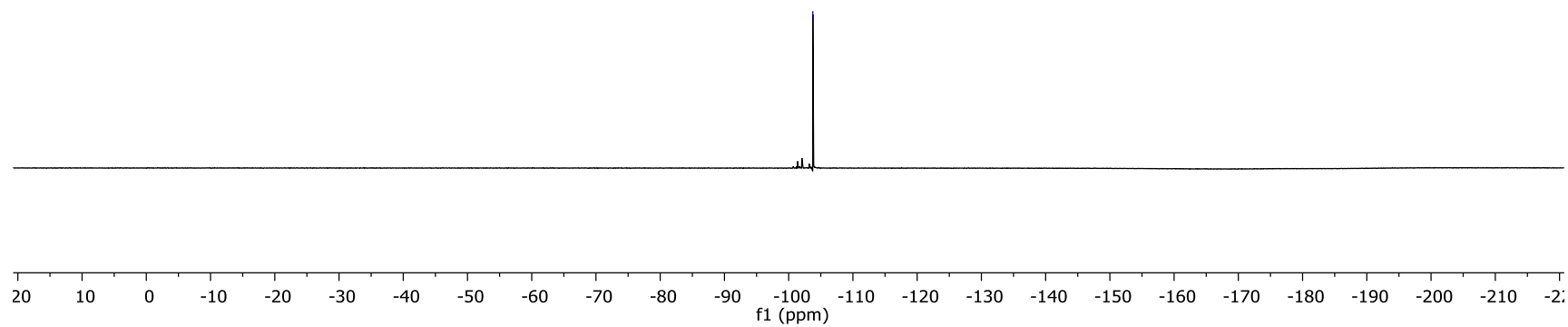
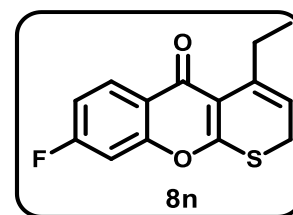
UJG-02-199-22-13C.3.fid — UJG-02-199-22-13C



^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 8n

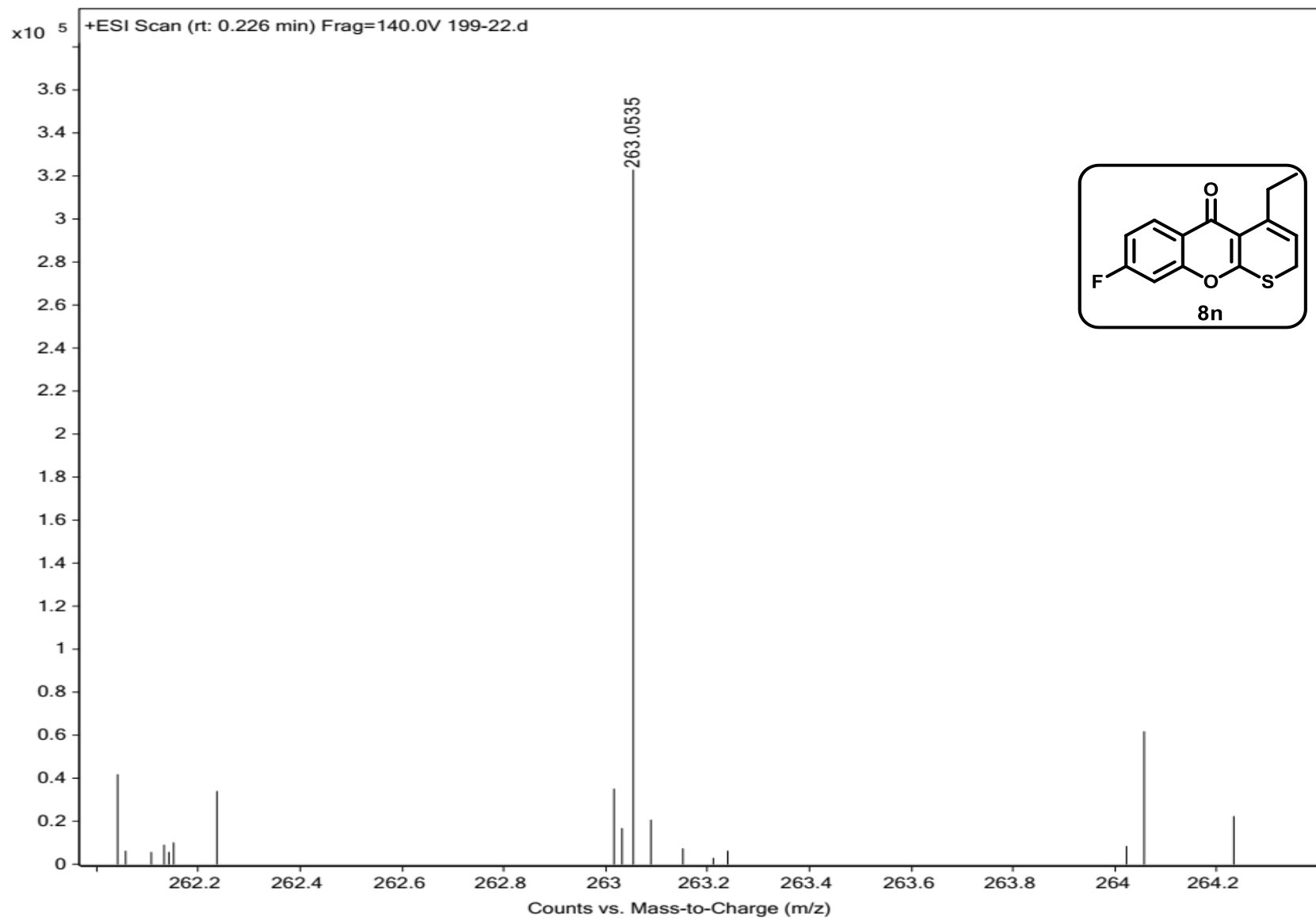
UJG-02-199-22-19F.5.fid — UJG-02-199-22-19F

— -103.76



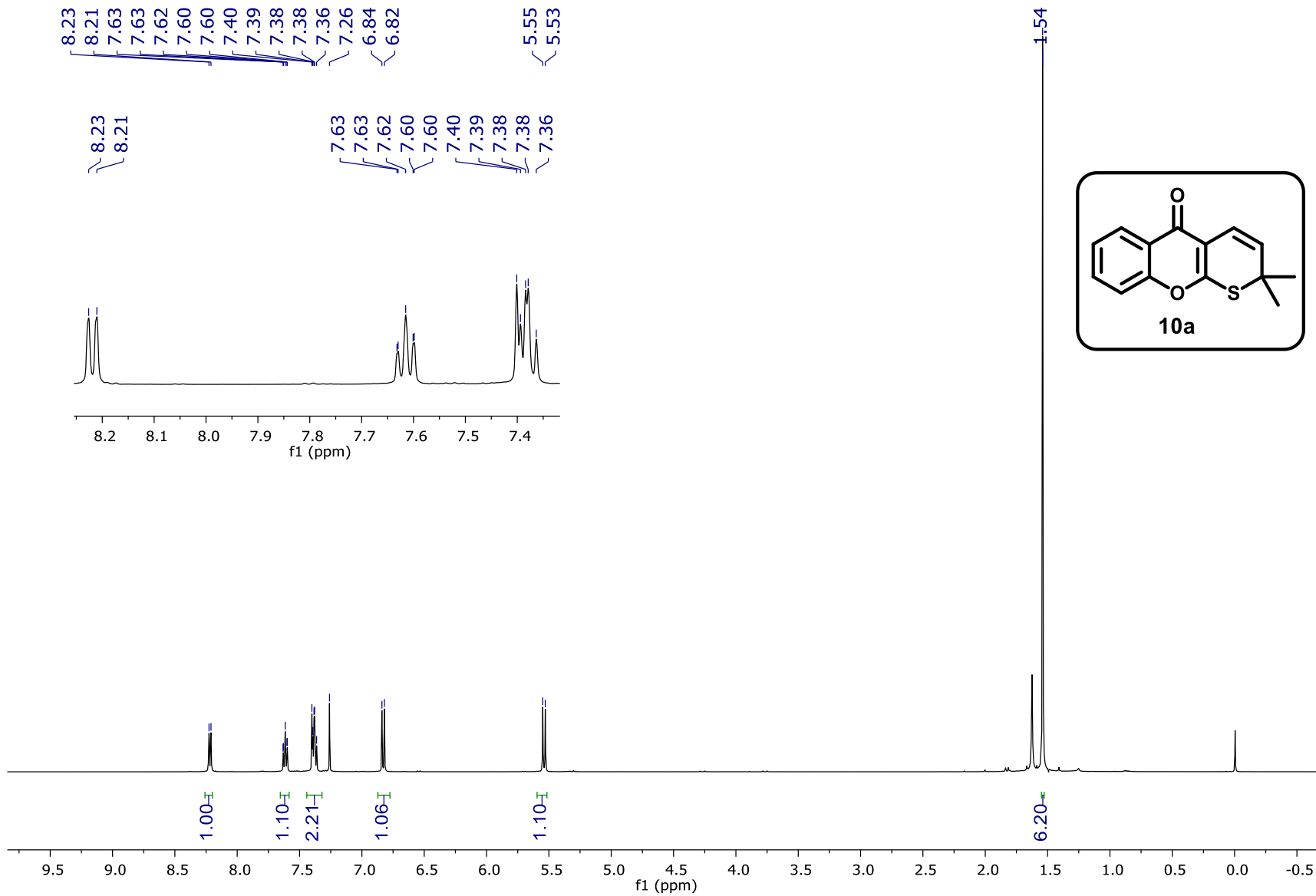
S236

Spectrum of Compound 8n



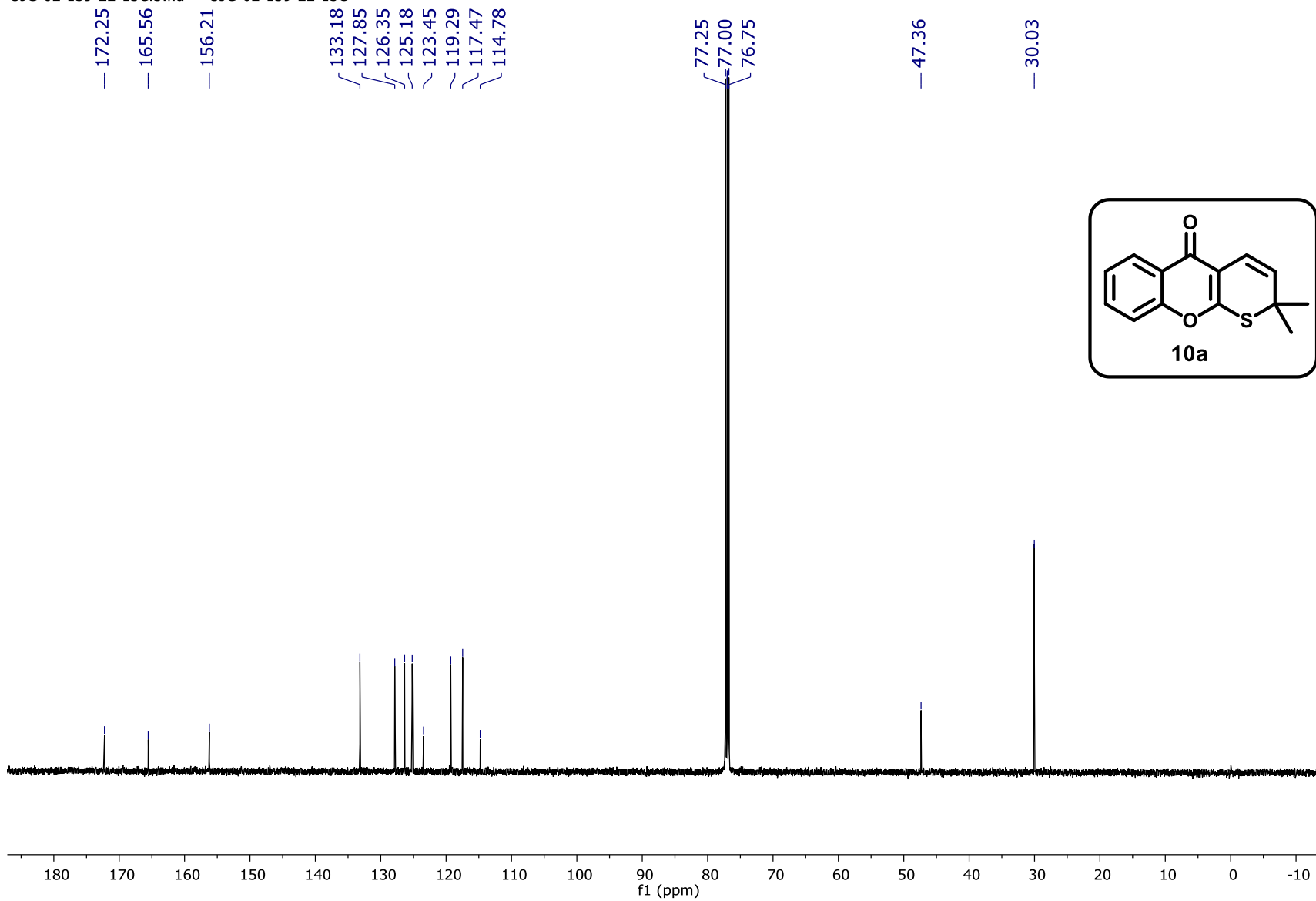
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 10a

UJG-02-139-22-1H.8.fid — UJG-02-139-22-1H



^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 10a

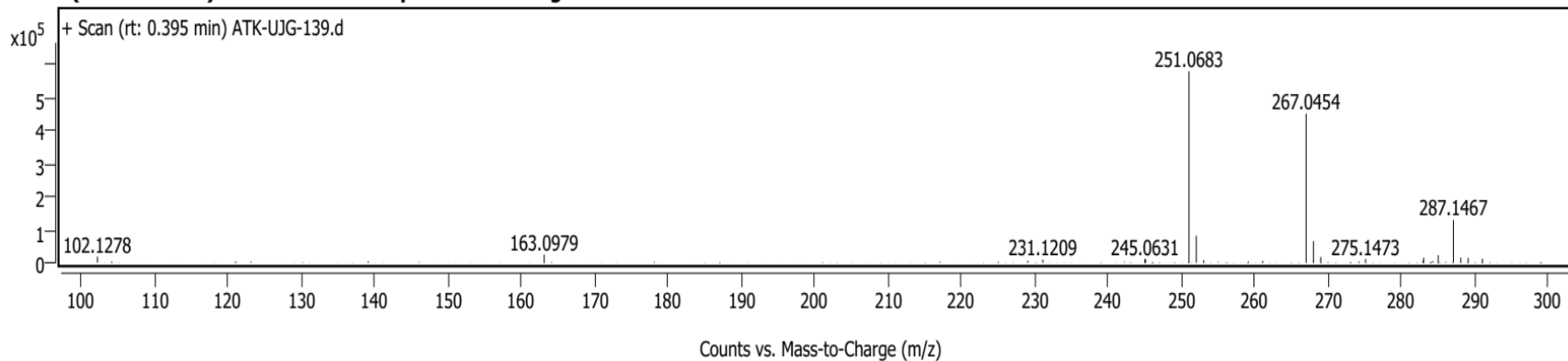
UJG-02-139-22-13C.3.fid — UJG-02-139-22-13C



HRMS Spectrum of Compound 10a

+ Scan (rt: 0.395 min)

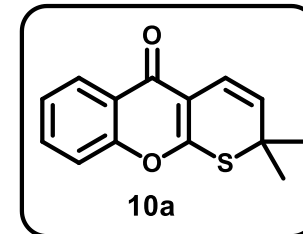
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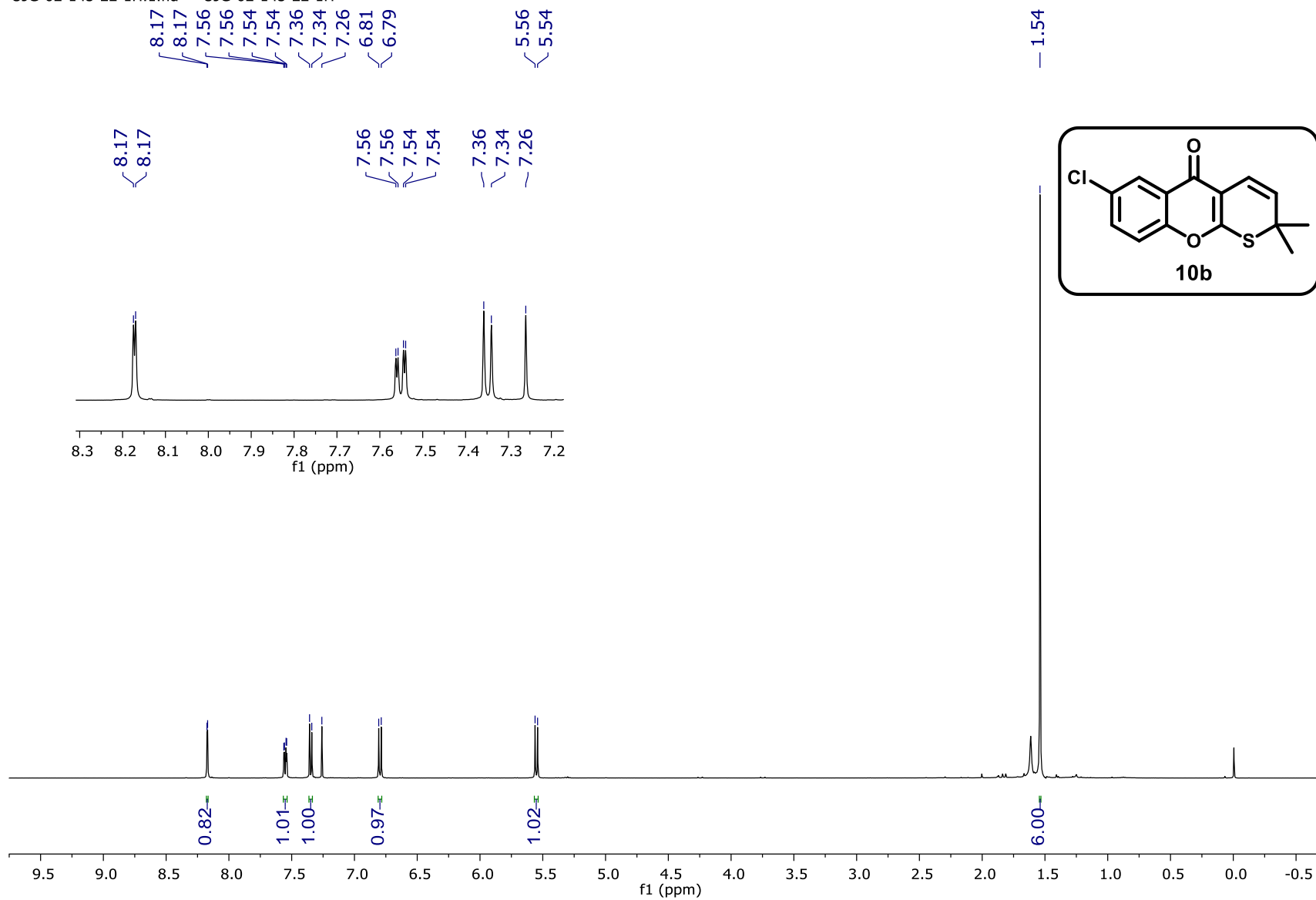
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula
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163.0979		24372	4.20				
229.0860		6284	1.08				
231.1209		9360	1.61				
245.0631		11200	1.93				
245.1366		10228	1.76				
251.0683	1	579849	100.00				
252.0717	1	81601	14.07				
253.0736	1	8049	1.39				
267.0454	1	450766	77.74				
268.0483	1	65115	11.23				
269.0422	1	17112	2.95				
275.1473		11244	1.94				
283.0573		8937	1.54				
283.0868		14913	2.57				
285.0737		22943	3.96				
287.1467	1	129308	22.30				
288.1500	1	15376	2.65				
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291.0999		12176	2.10				

Ion Type



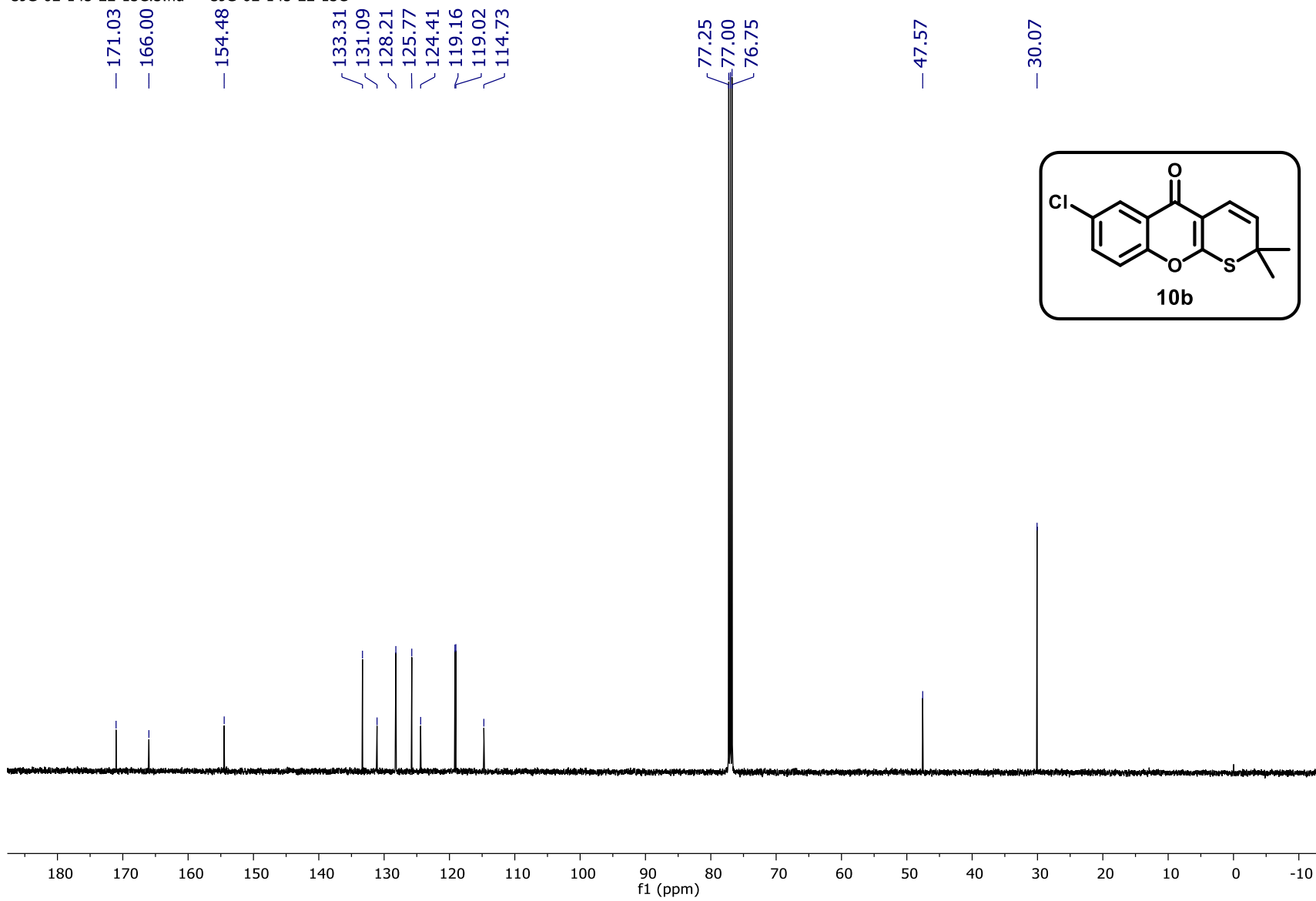
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 10b

UJG-02-145-22-1H.1.fid — UJG-02-145-22-1H

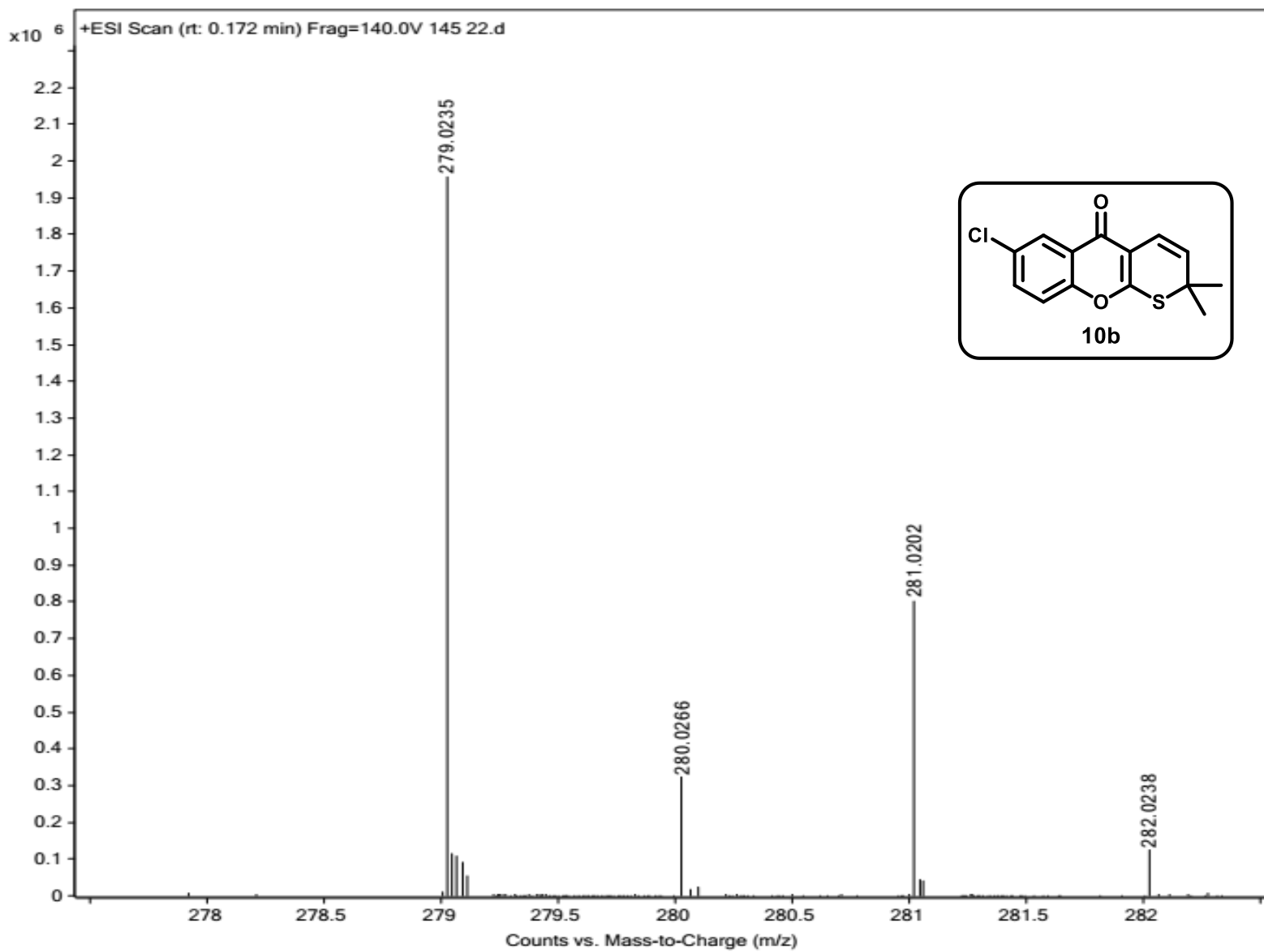


^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) Spectrum of Compound 10b

UJG-02-145-22-13C.3.fid — UJG-02-145-22-13C

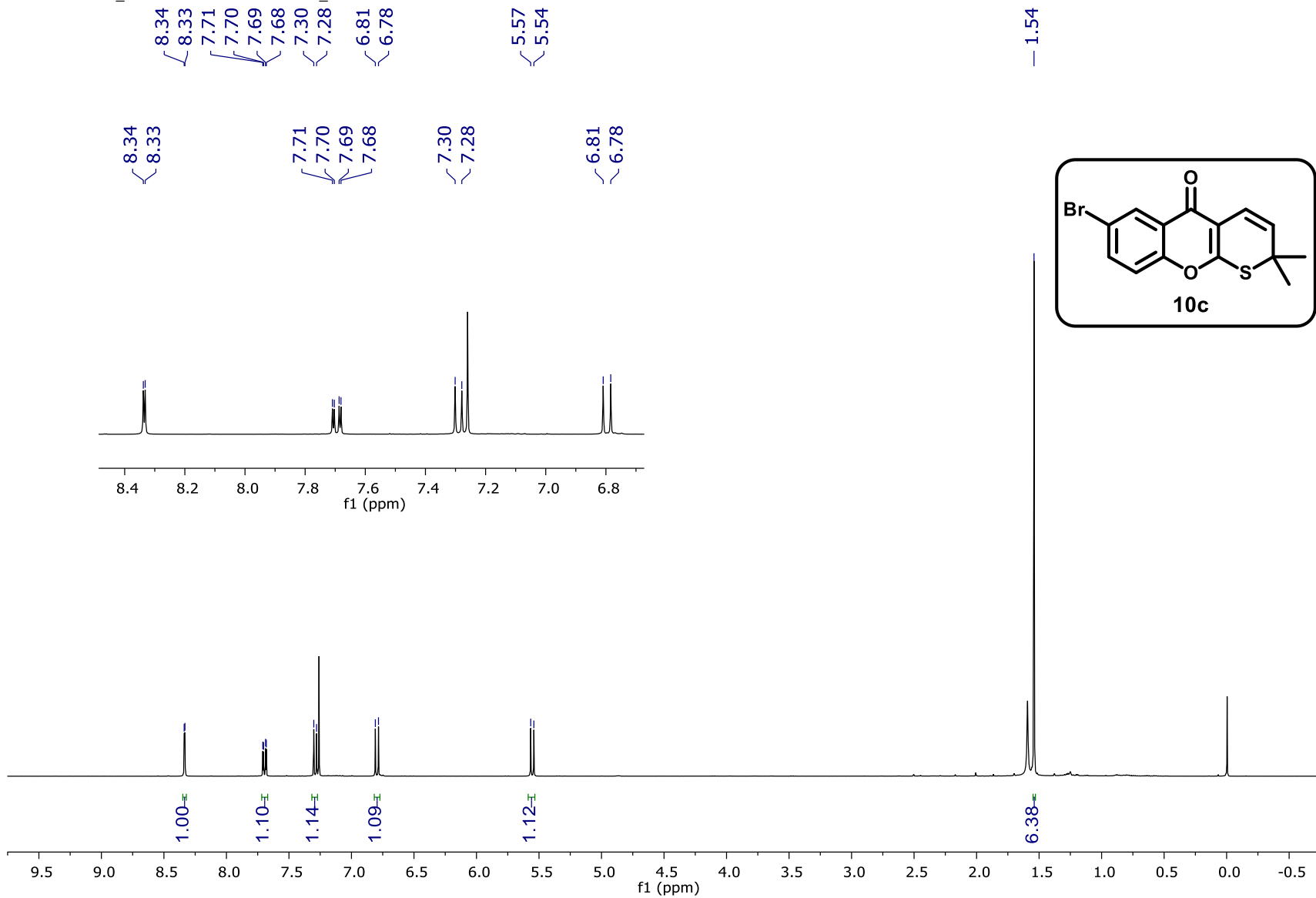


HRMS Spectrum of Compound 10b



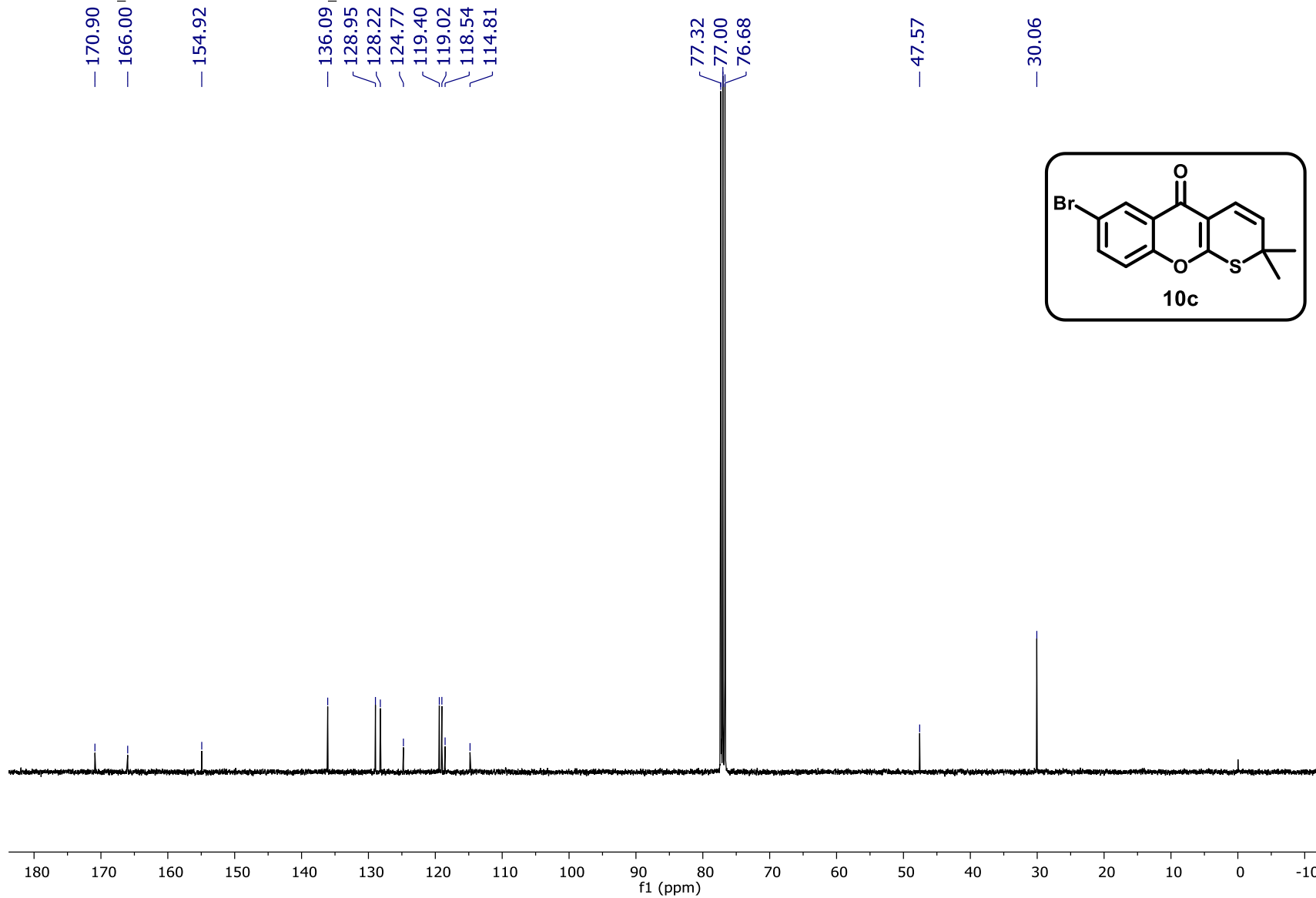
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 10c

UJG-02-145-22_1H.10.fid — UJG-02-145-22_1H



^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of Compound 10c

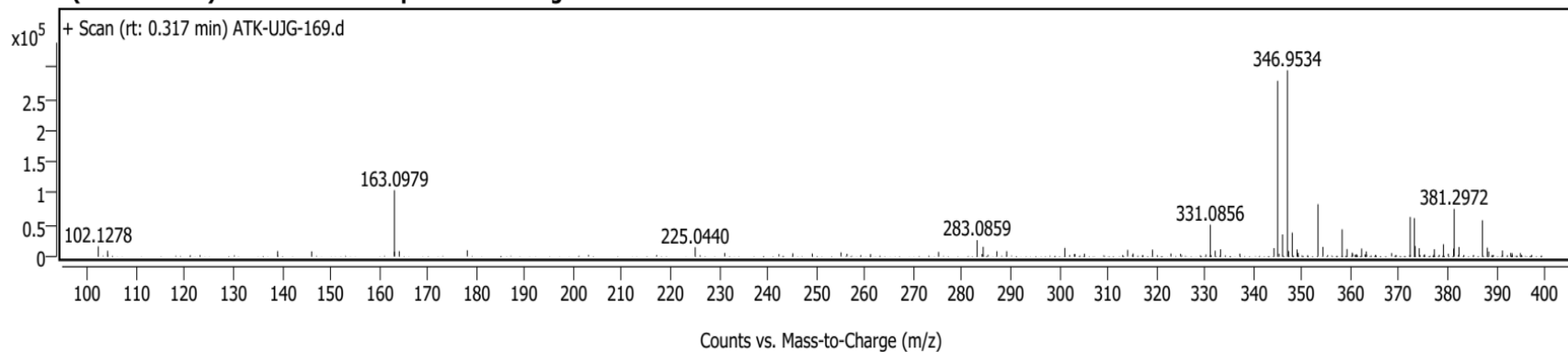
UJG-02-145-22_13C.12.fid — UJG-02-145-22_13C



HRMS Spectrum of Compound 10c

+ Scan (rt: 0.317 min)

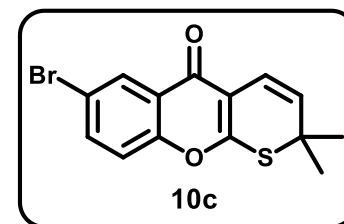
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SpectrumIdString

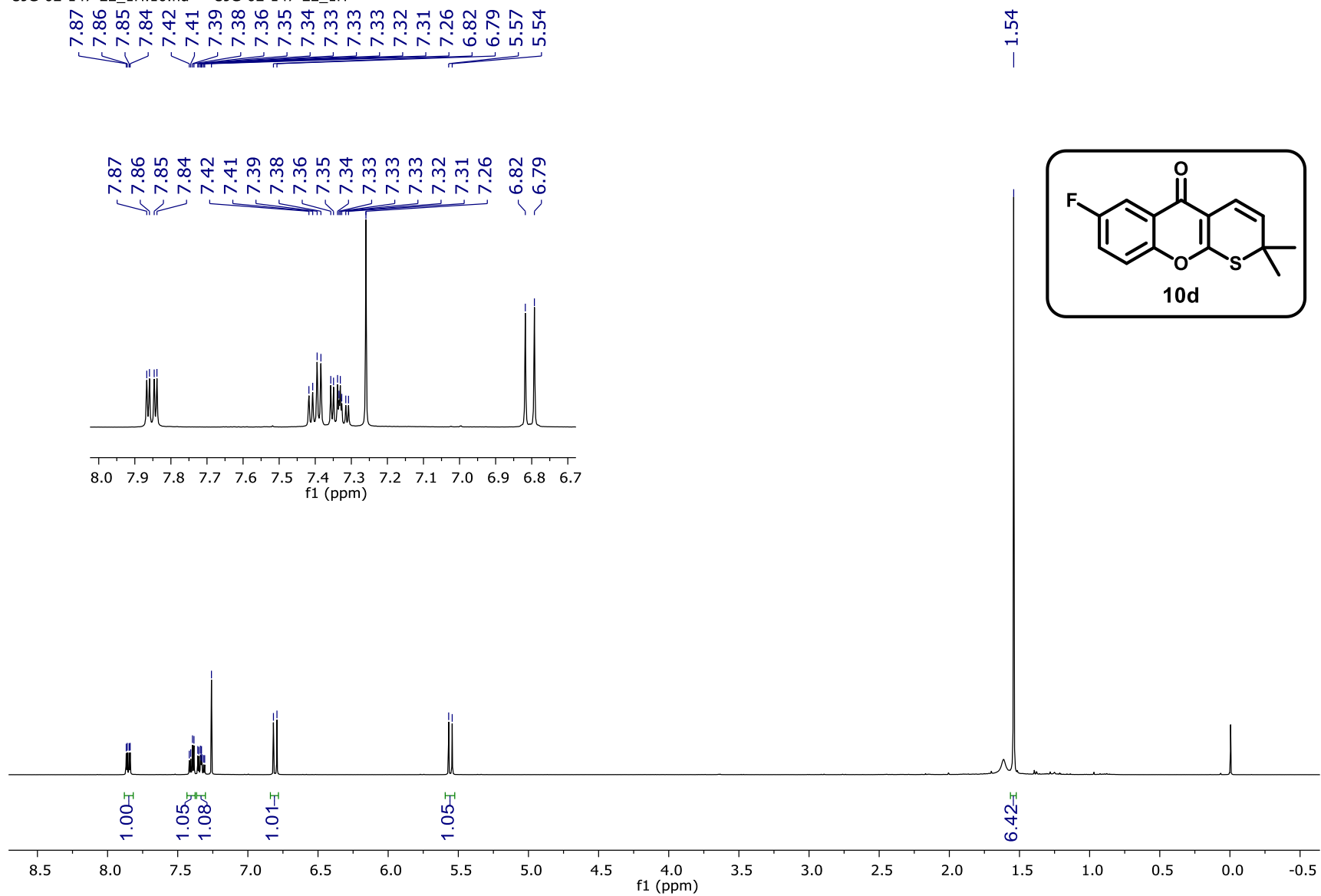
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225.0440		14641	4.96				
283.0859		25913	8.78				
284.3310		15411	5.22				
331.0856		50461	17.09				
344.9555	1	278577	94.36				
345.9587	1	34980	11.85				
346.9534	1	295217	100.00				
347.9564	1	37826	12.81				
353.2660	1	82913	28.09				
354.2696	1	15203	5.15				
358.2273		43118	14.61				
372.2430	1	62719	21.24				
373.0962		60888	20.62				
373.2467	1	16637	5.64				
379.0965		19499	6.61				
381.2972	1	75517	25.58				
382.3005	1	14956	5.07				
387.1117		57482	19.47				

Ion Type



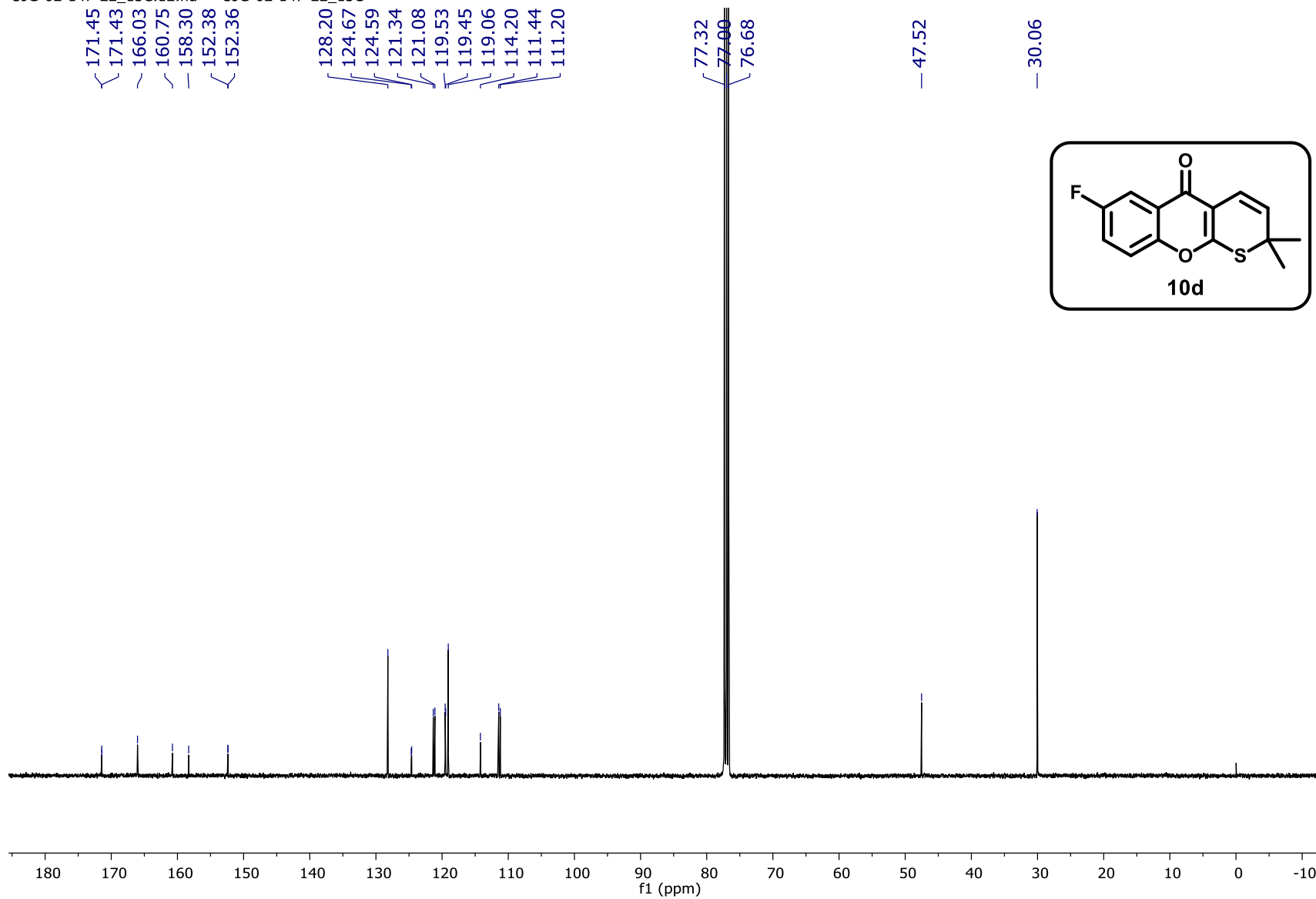
¹H NMR (400 MHz, CDCl₃) Spectrum of Compound 10d

UJG-02-147-22_1H.10.fid — UJG-02-147-22_1H



^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of Compound 10d

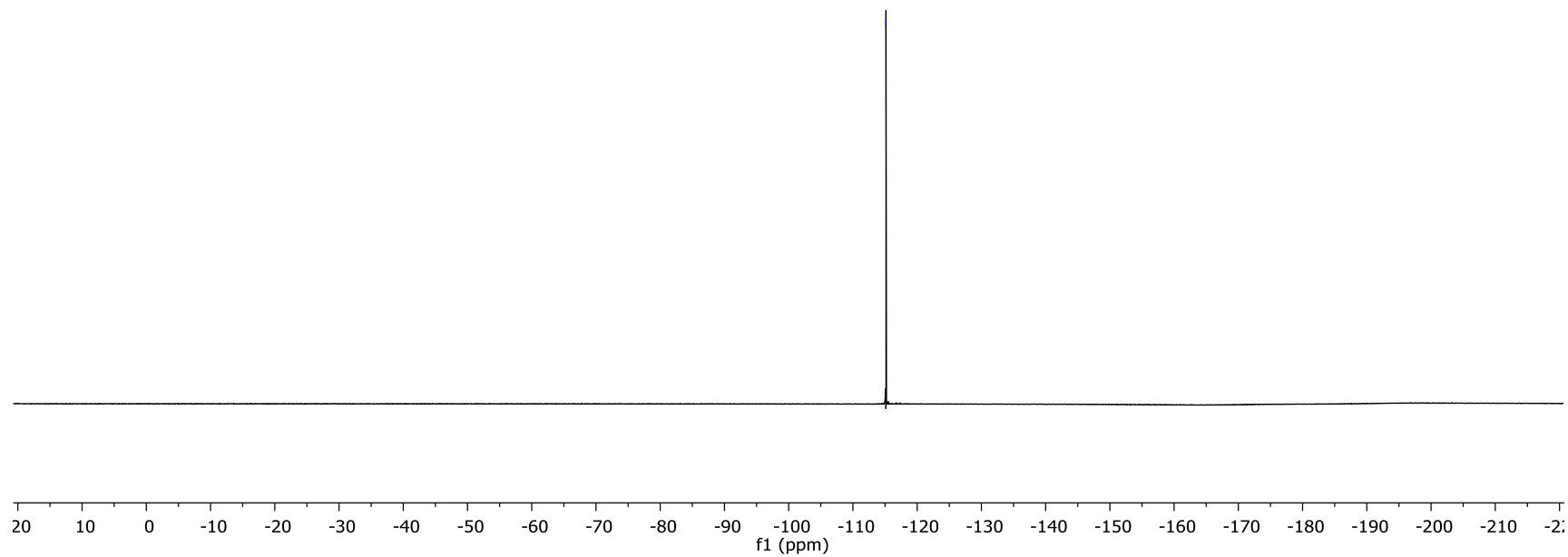
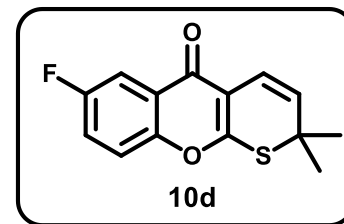
UJG-02-147-22_13C.12.fid — UJG-02-147-22_13C



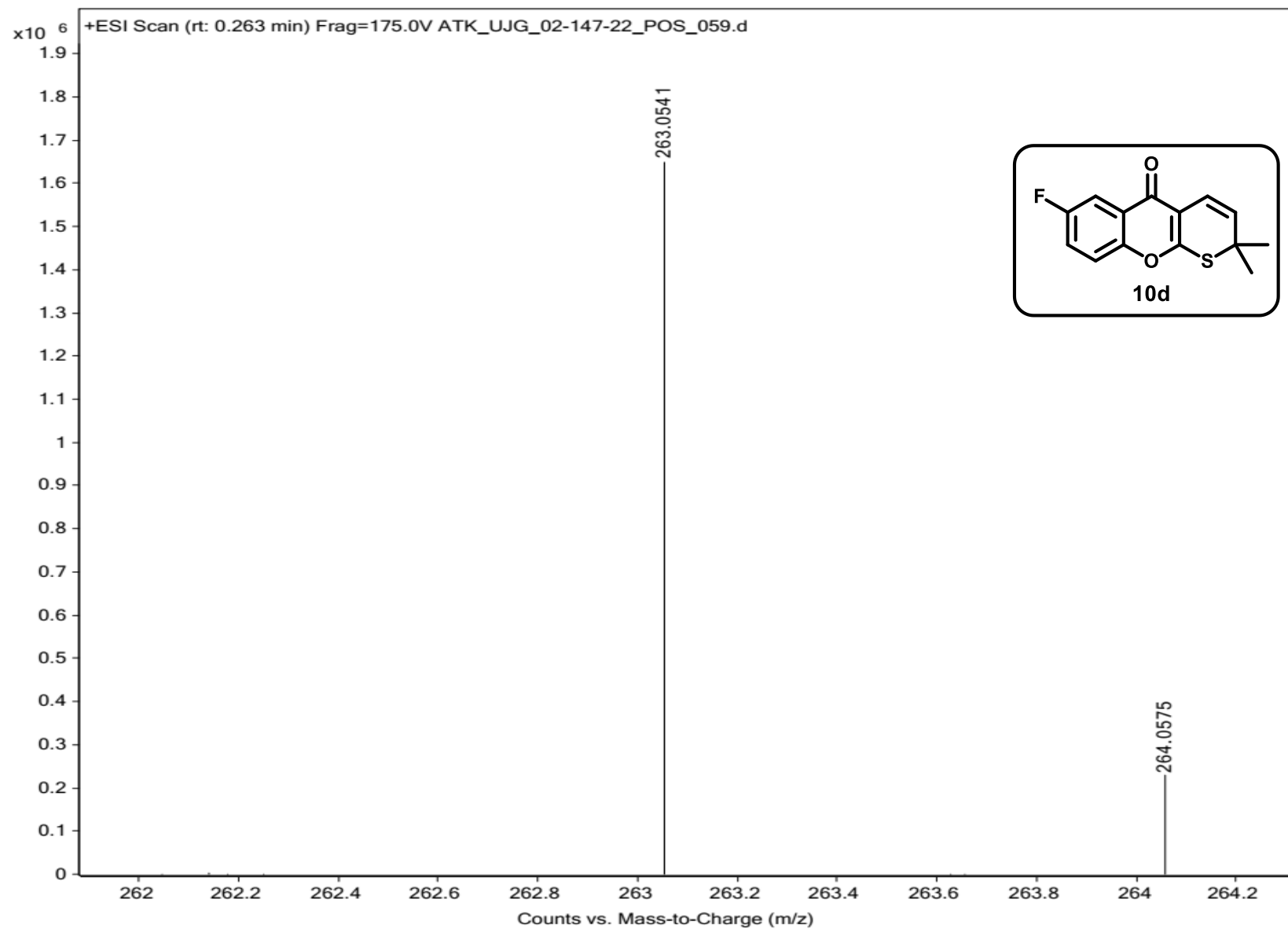
^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 10d

UJG-02-147-22-19F.1.fid — UJG-02-147-22-19F

— -115.15

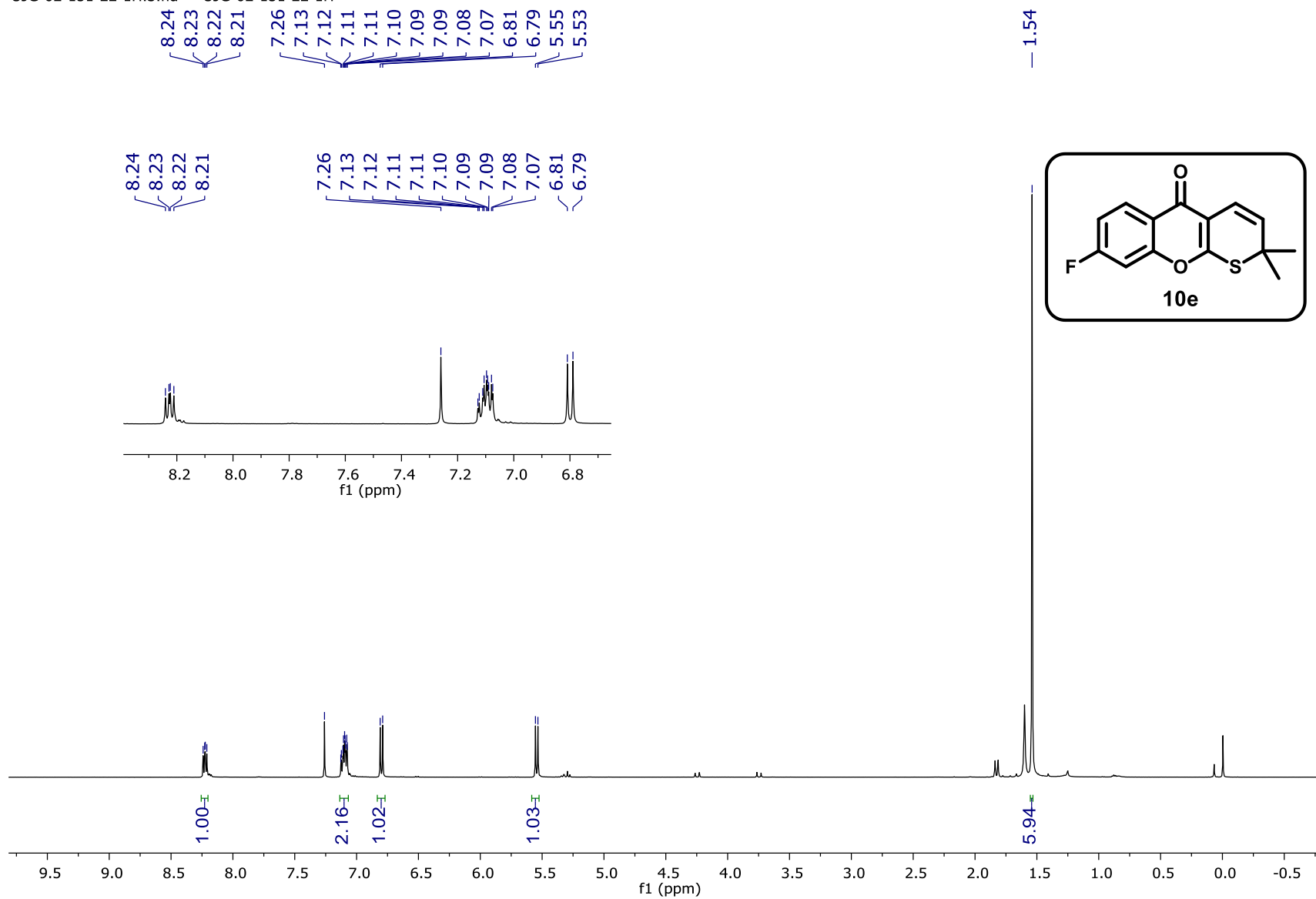


HRMS Spectrum of Compound 10d



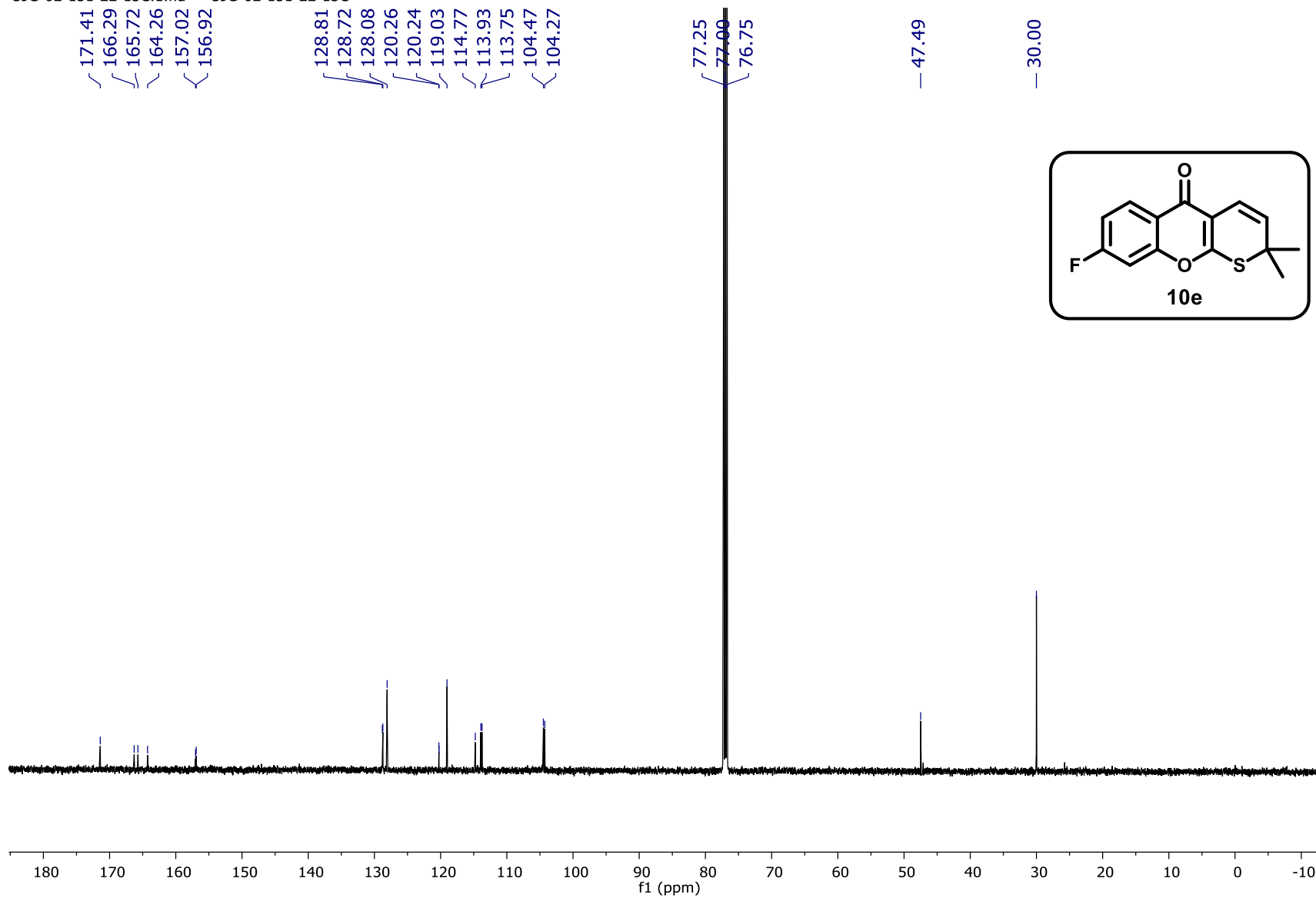
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 10e

UJG-02-151-22-1H.3.fid — UJG-02-151-22-1H



^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 10e

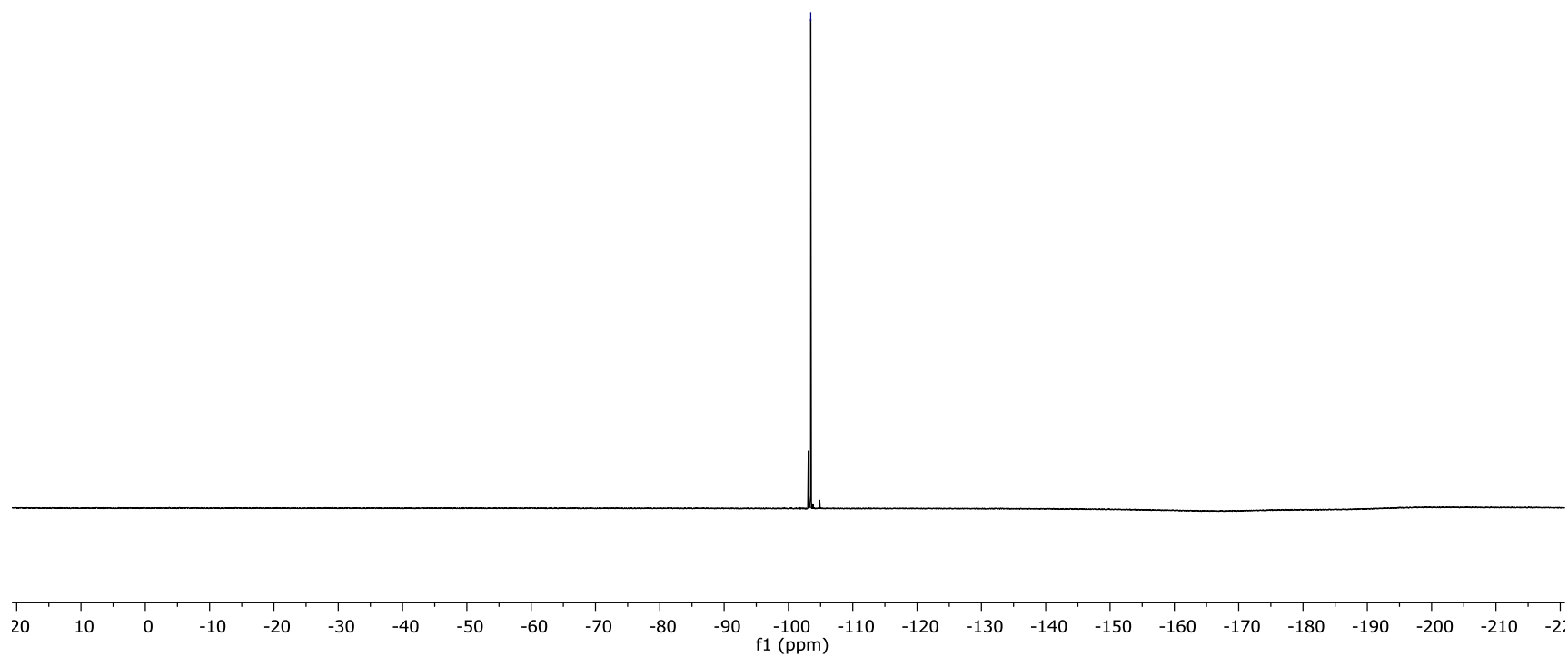
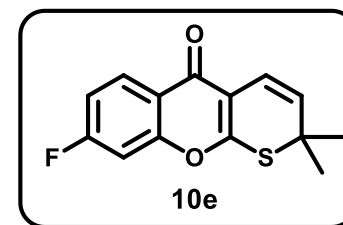
UJG-02-151-22-13C.1.fid — UJG-02-151-22-13C



^{19}F NMR (471 MHz, CDCl_3) Spectrum of Compound 10e

UJG-02-129-22-19F.2.fid — UJG-02-129-22-19F

— -103.47

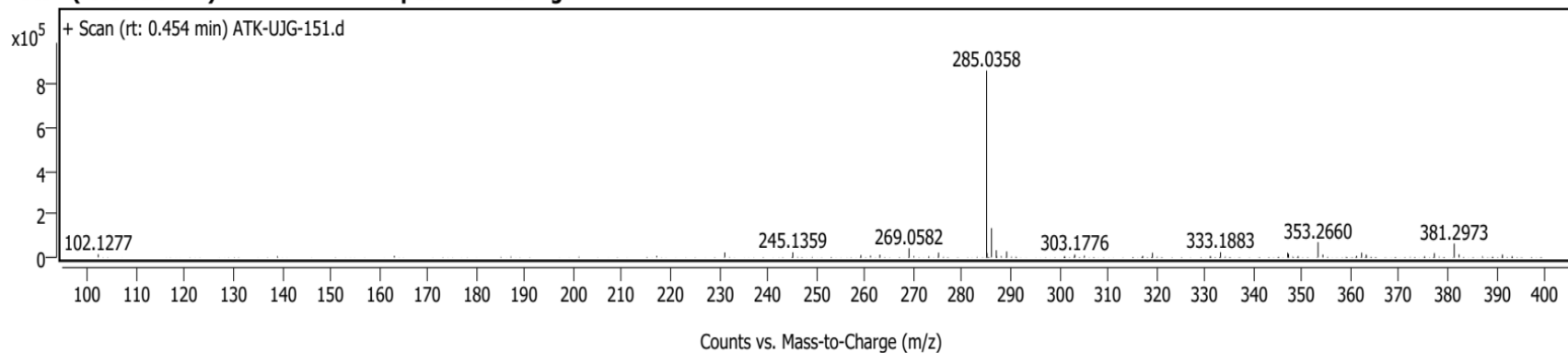


S253

HRMS Spectrum of Compound 10e

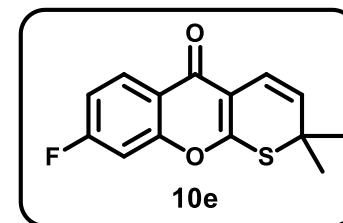
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SpectrumIdString



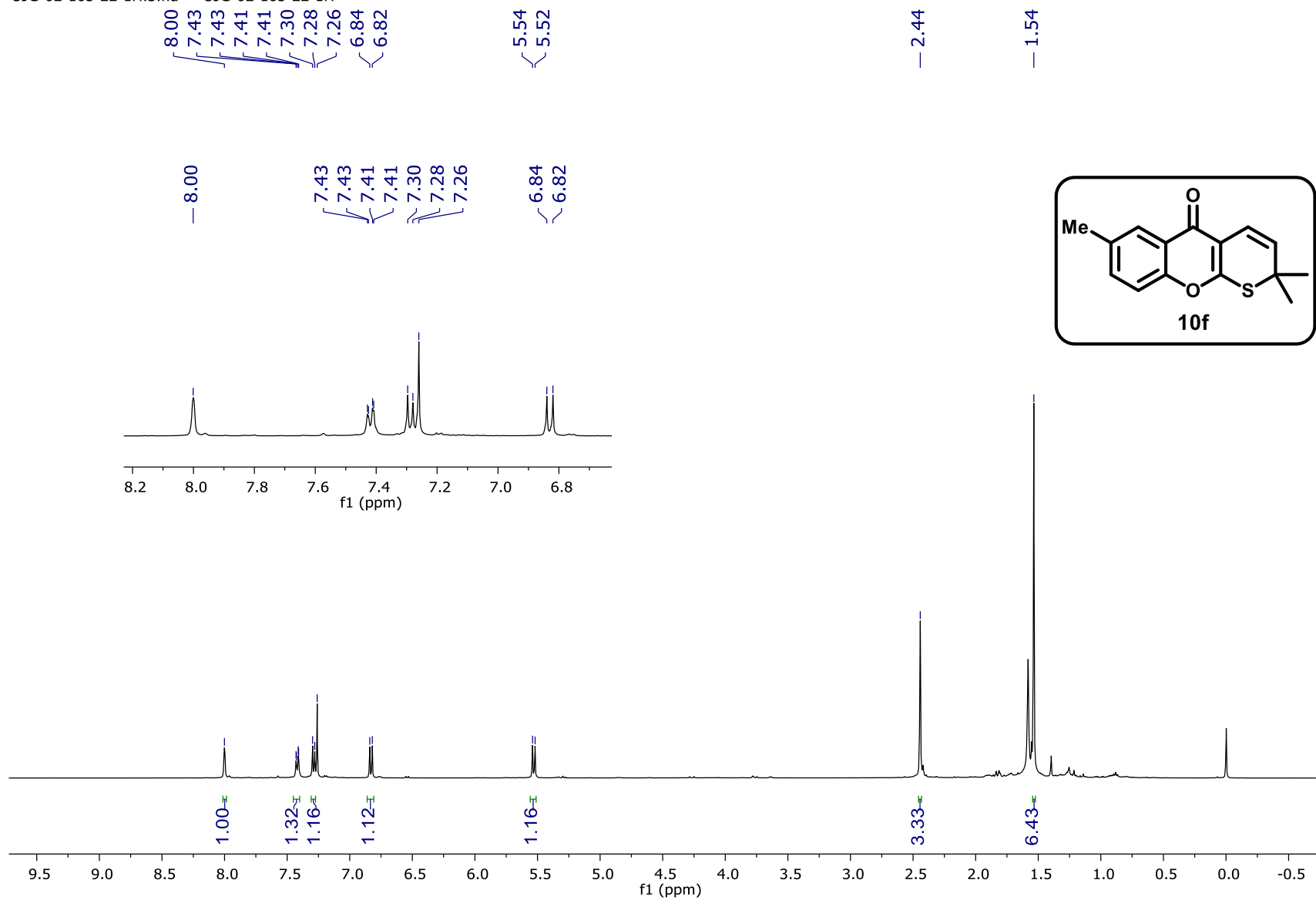
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m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula
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245.1359		23472	2.71				
269.0582		42391	4.89				
275.1465		21881	2.52				
285.0358	1	866670	100.00				
285.1235		20197	2.33				
286.0388	1	135832	15.67				
287.0329	1	33119	3.82				
289.1622		27257	3.14				
303.1776		13786	1.59				
319.1727		21368	2.47				
333.1883		24026	2.77				
347.0182		21409	2.47				
347.2039		16119	1.86				
353.2660		70426	8.13				
362.2412		21672	2.50				
377.2144		19971	2.30				
381.2973	1	64038	7.39				
382.3006	1	14270	1.65				



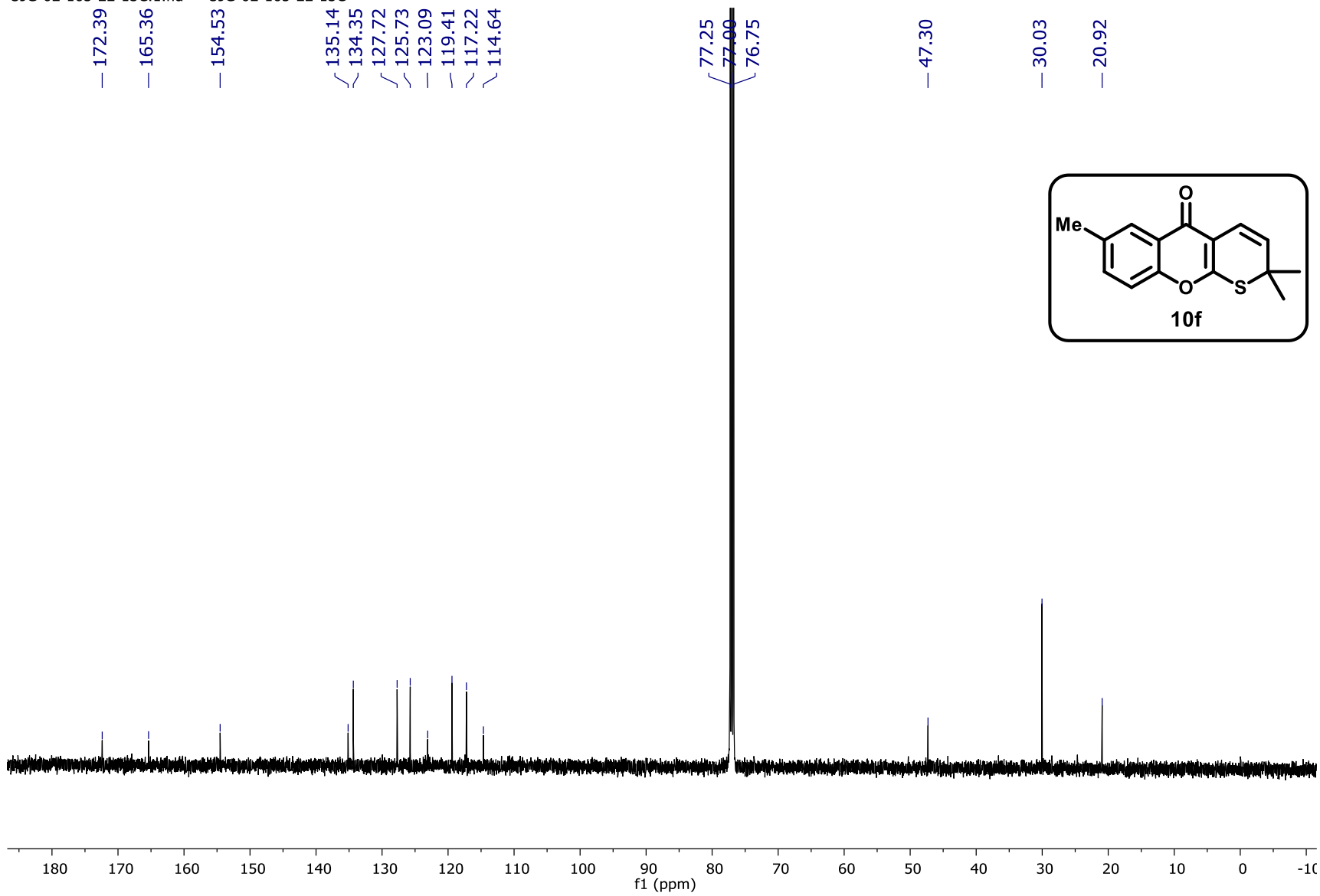
¹H NMR (500 MHz, CDCl₃) Spectrum of Compound 10f

UJG-02-165-22-1H.3.fid — UJG-02-165-22-1H

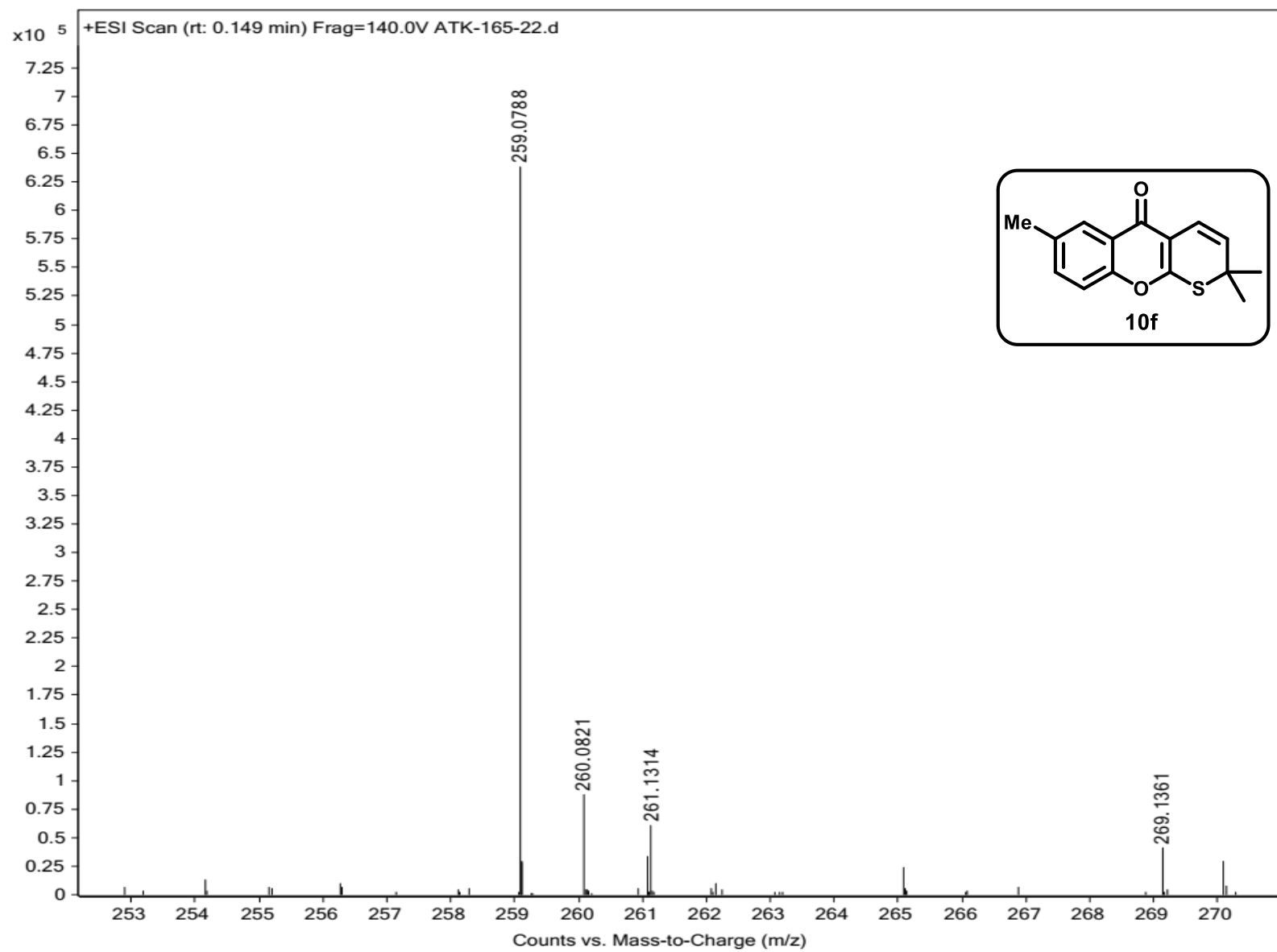


^{13}C { ^1H } NMR (125 MHz, CDCl_3) Spectrum of Compound 10f

UJG-02-165-22-13C.1.fid — UJG-02-165-22-13C



HRMS Spectrum of Compound 10f



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- S3. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, 113, 6378–6396.