

*Supporting Information*

**Iminophosphorane-mediated regioselective umpolung alkylation reaction of  $\alpha$ -iminoesters**

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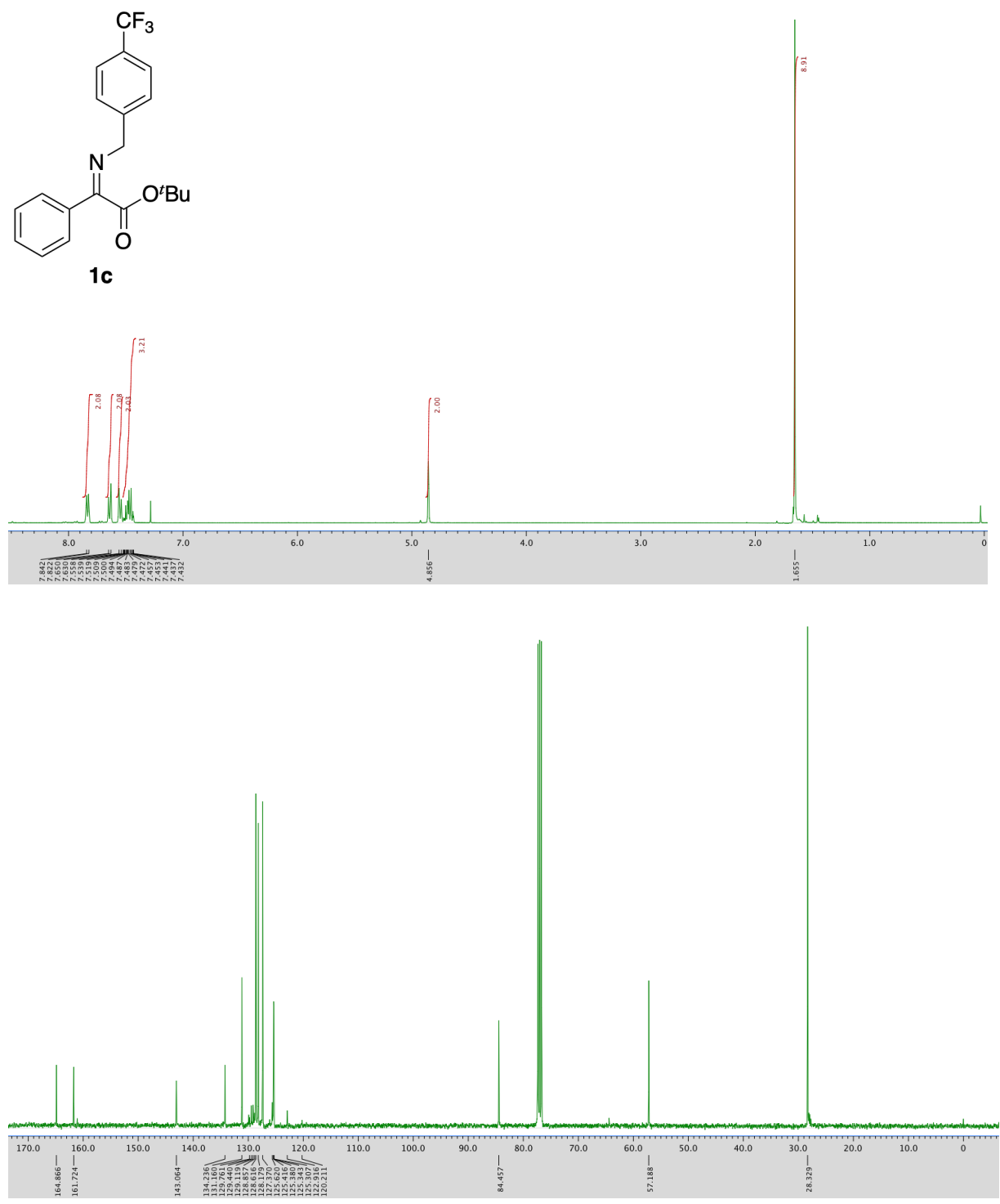
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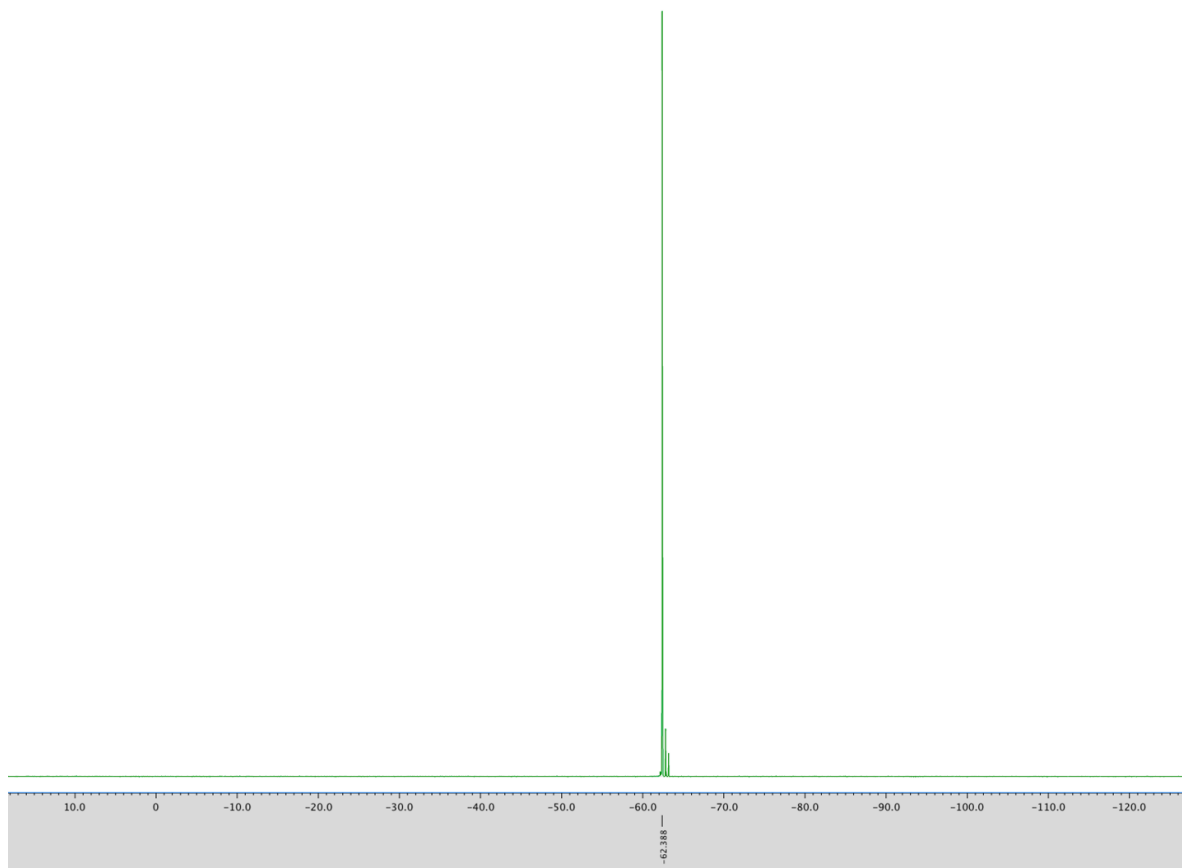
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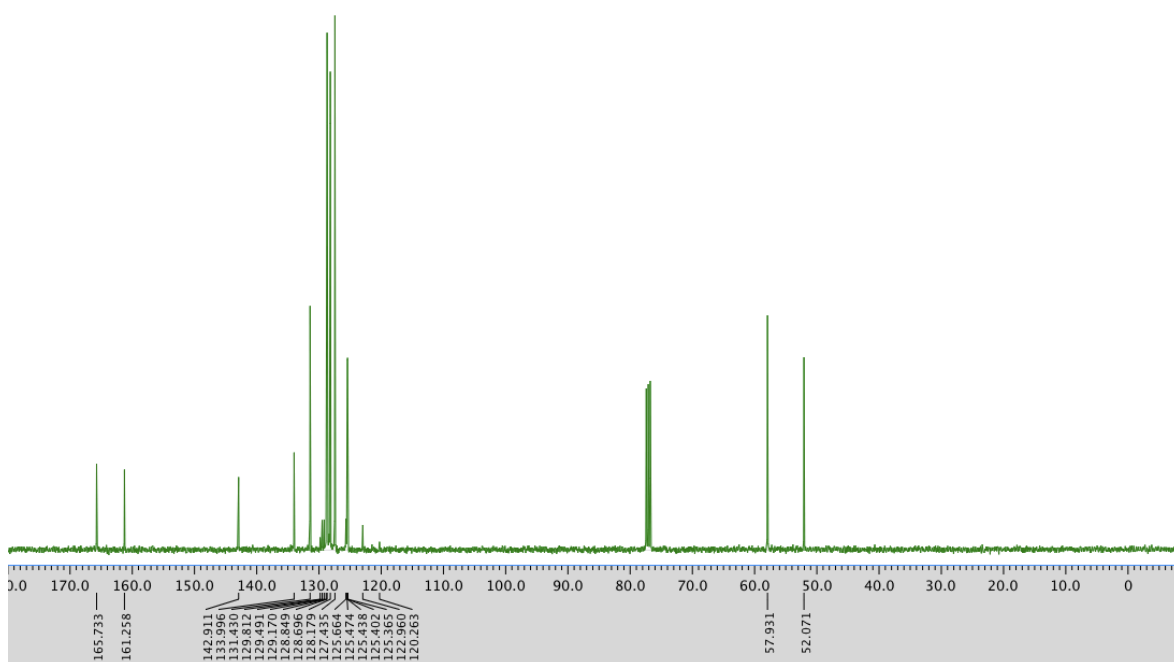
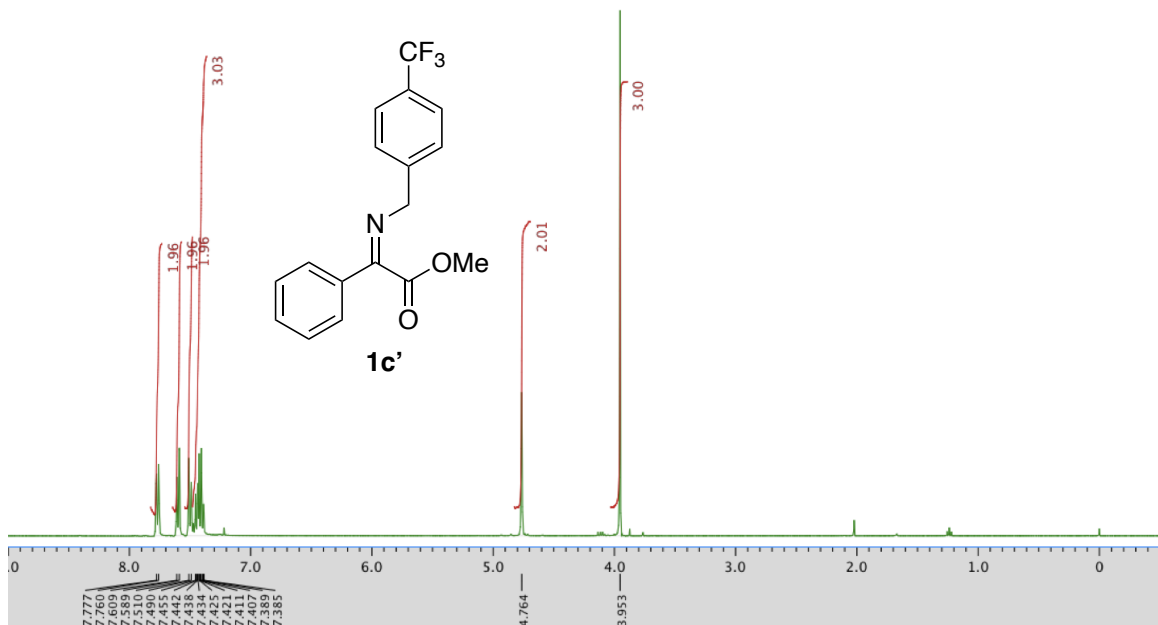
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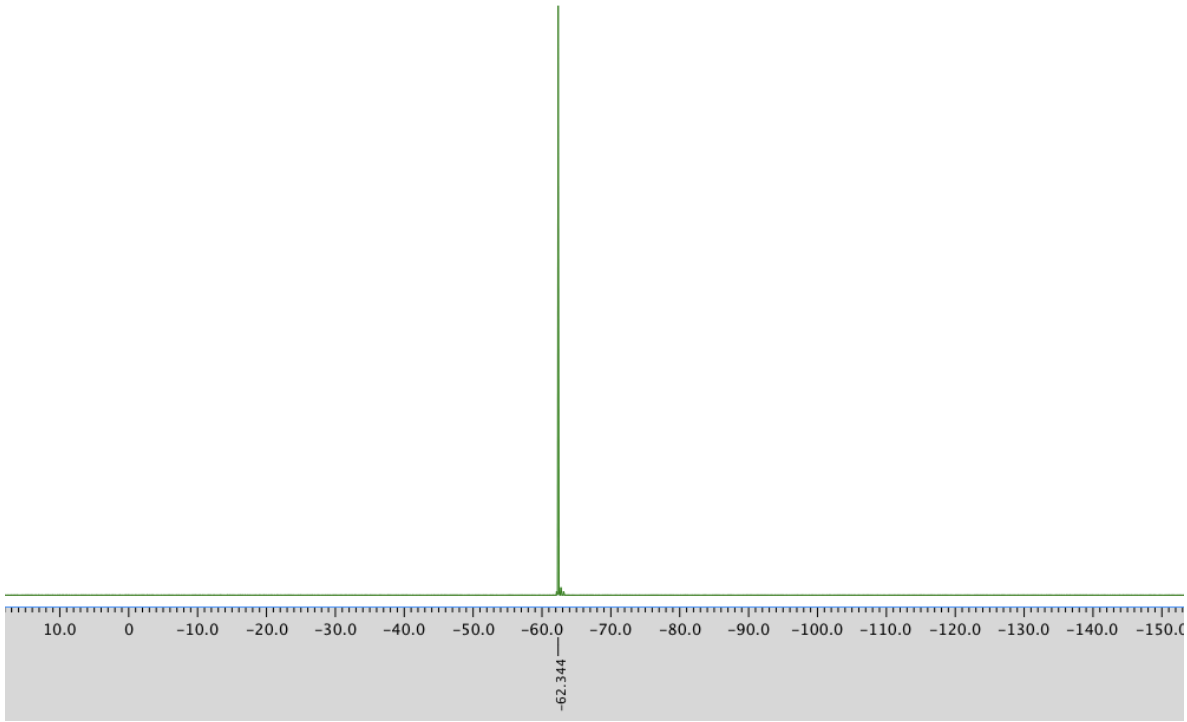
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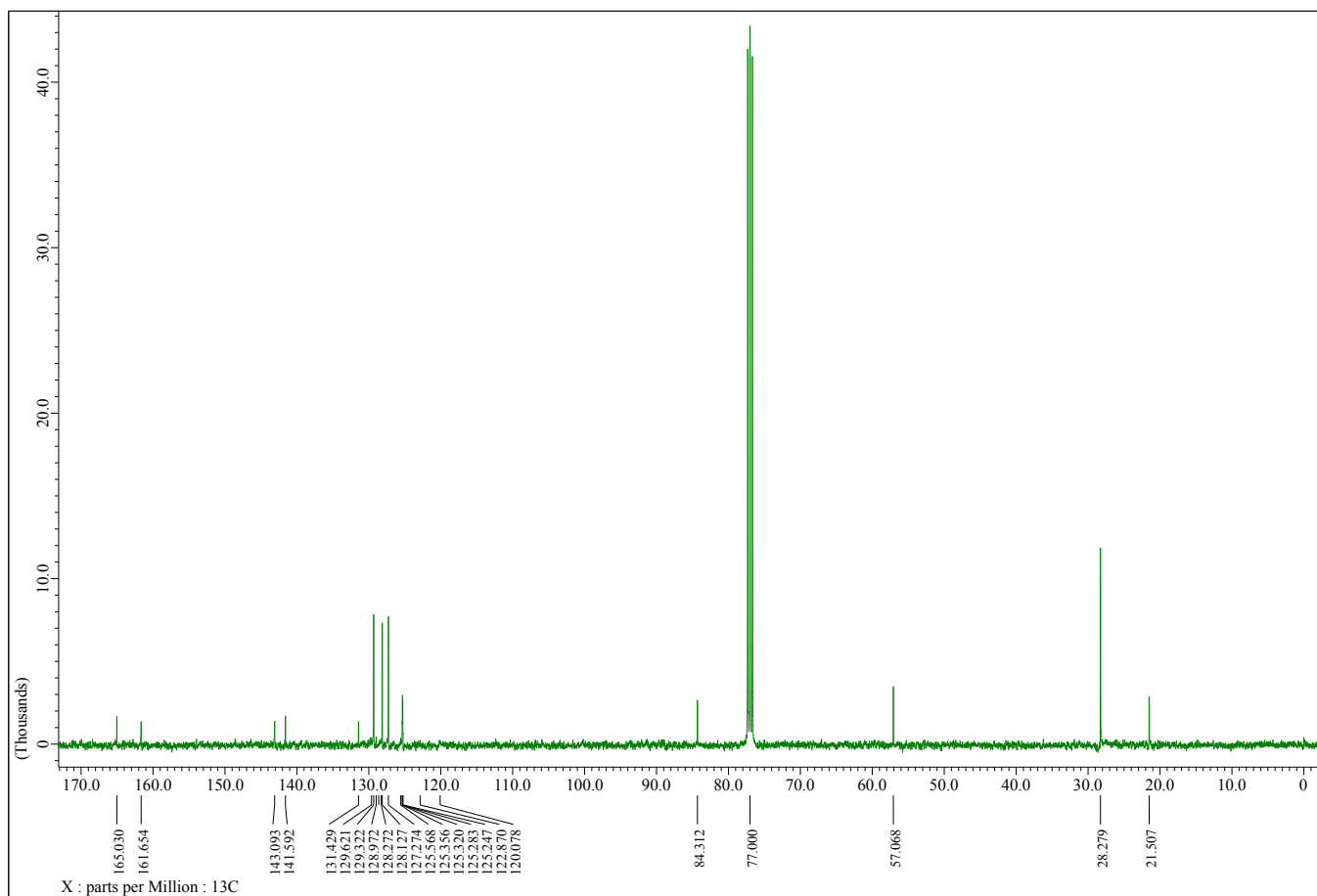
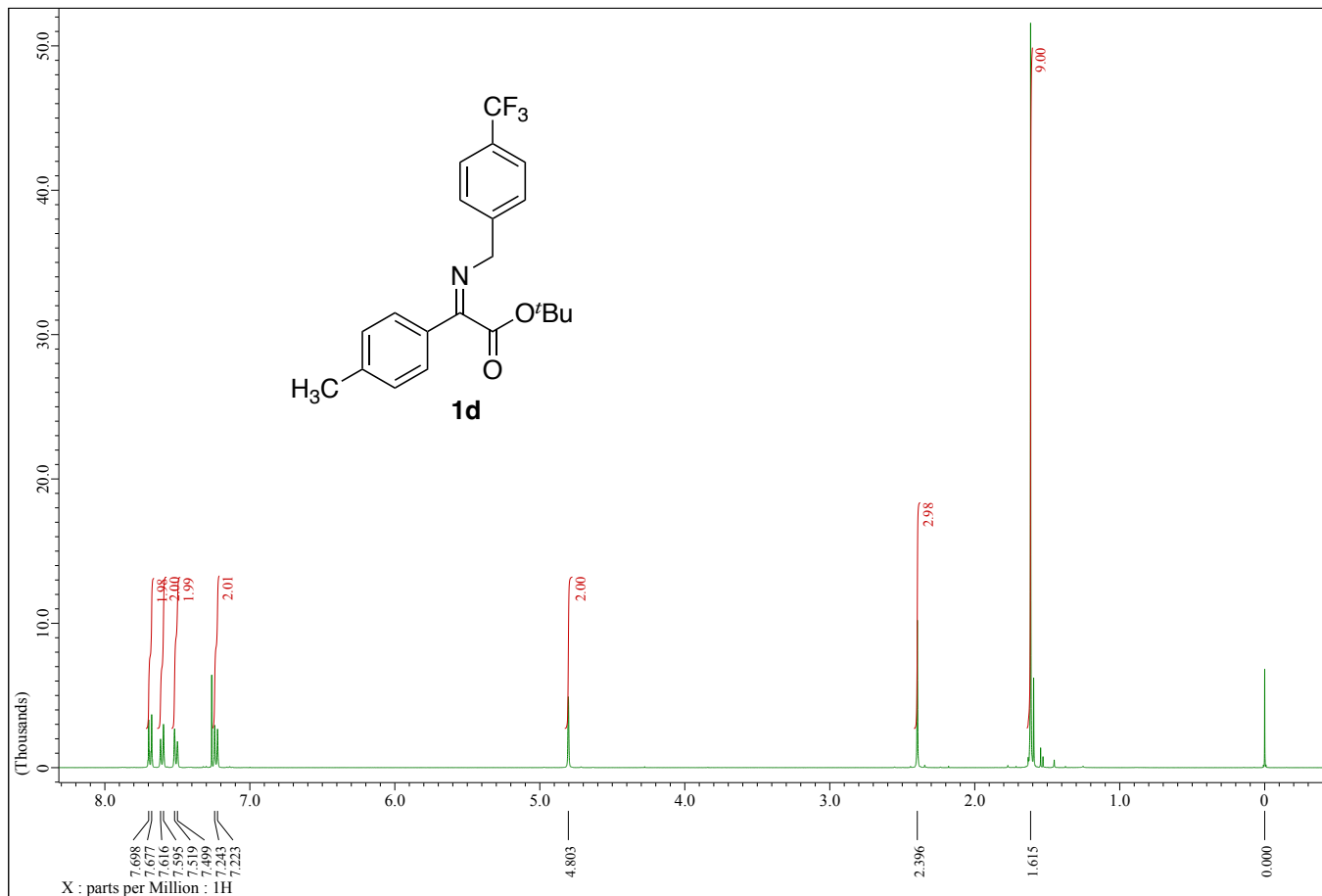
# 1. NMR and HPLC charts for new compounds

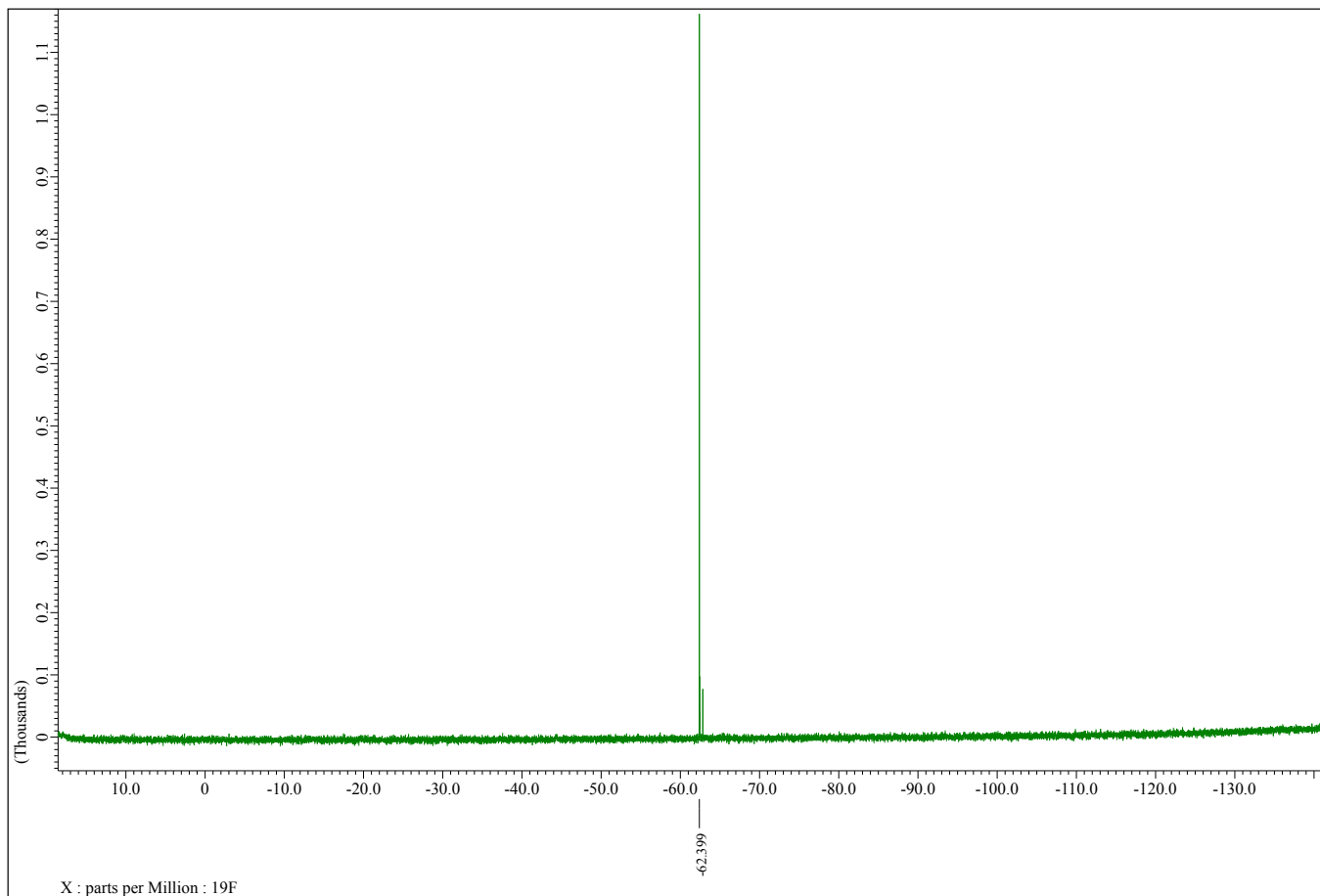


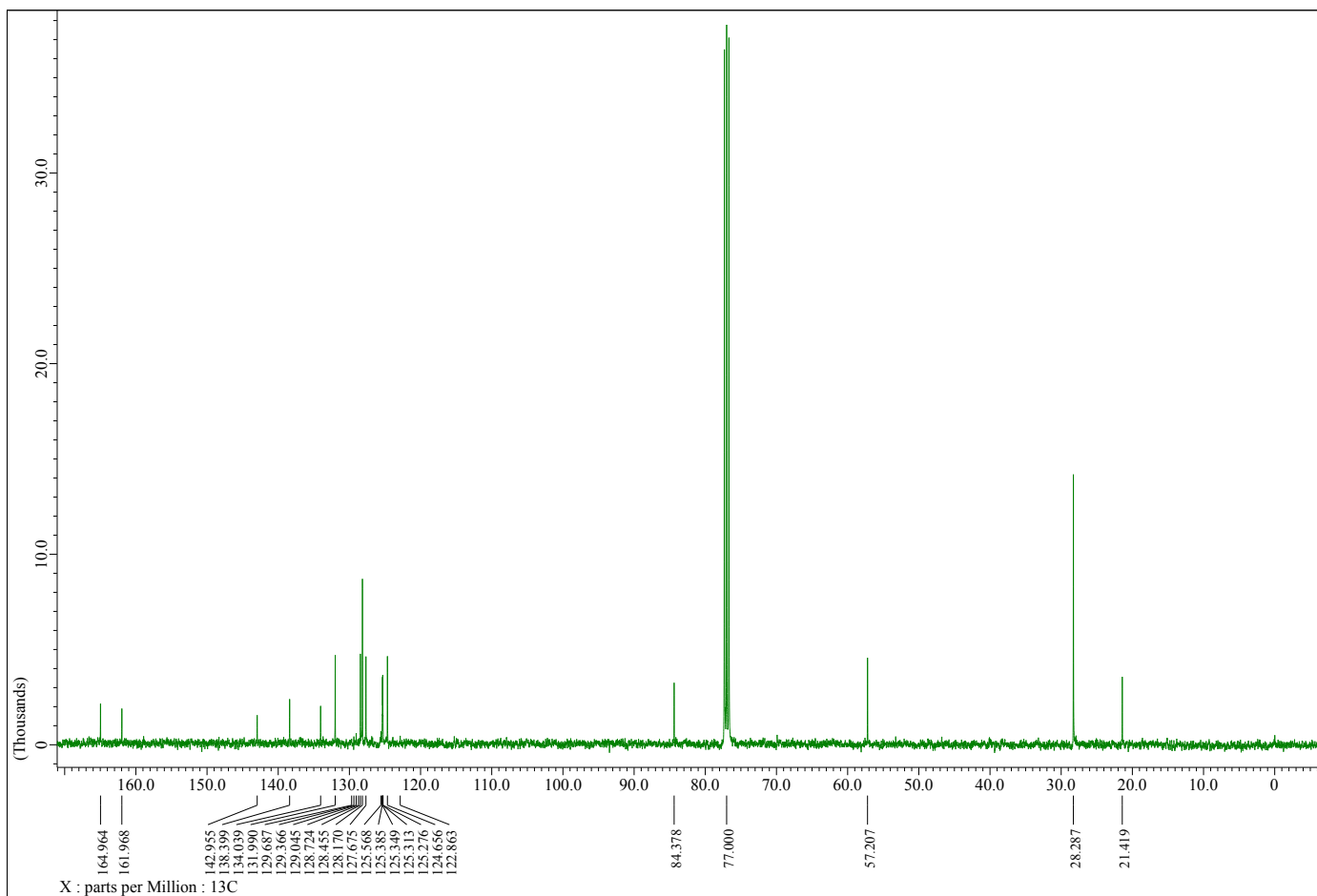
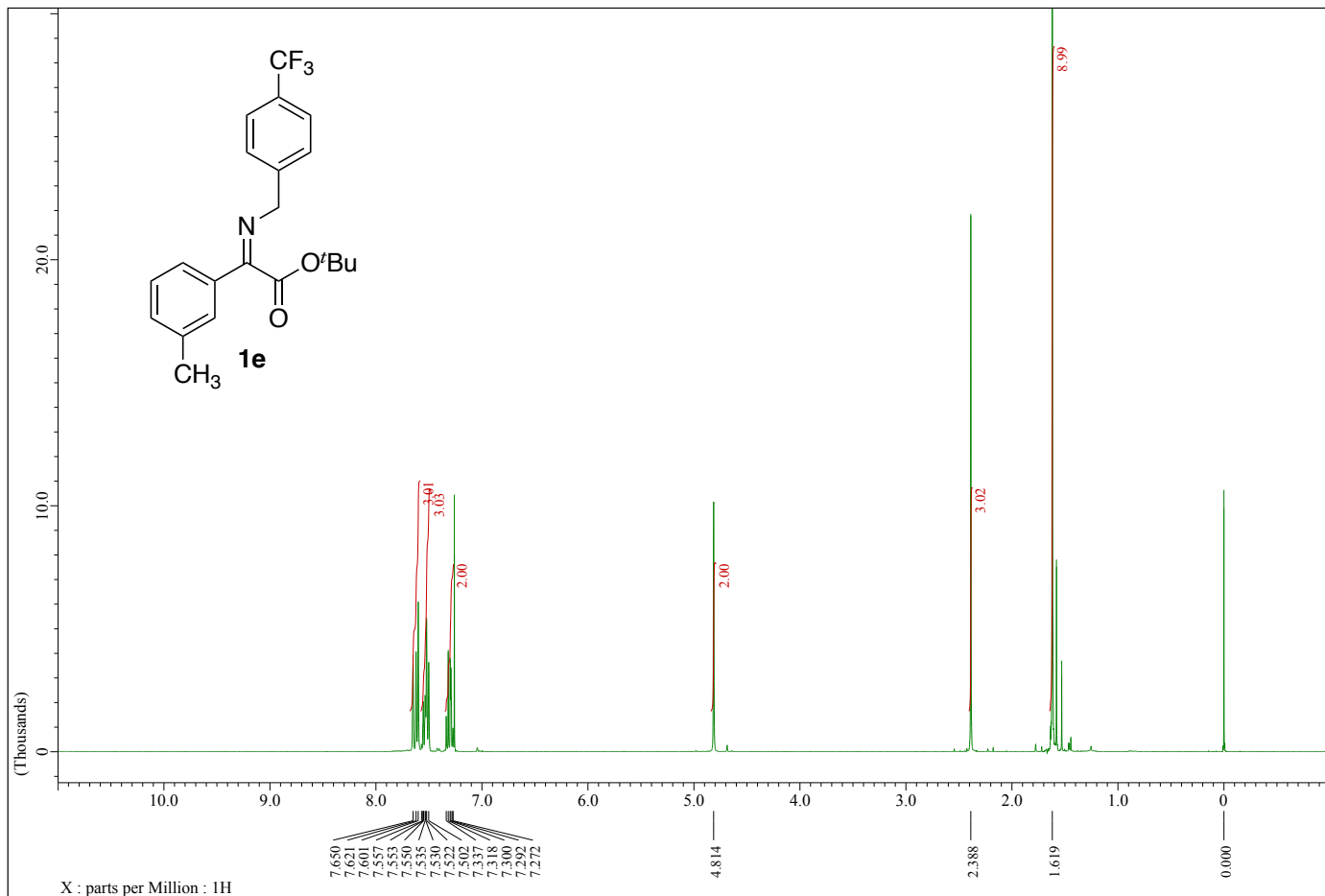




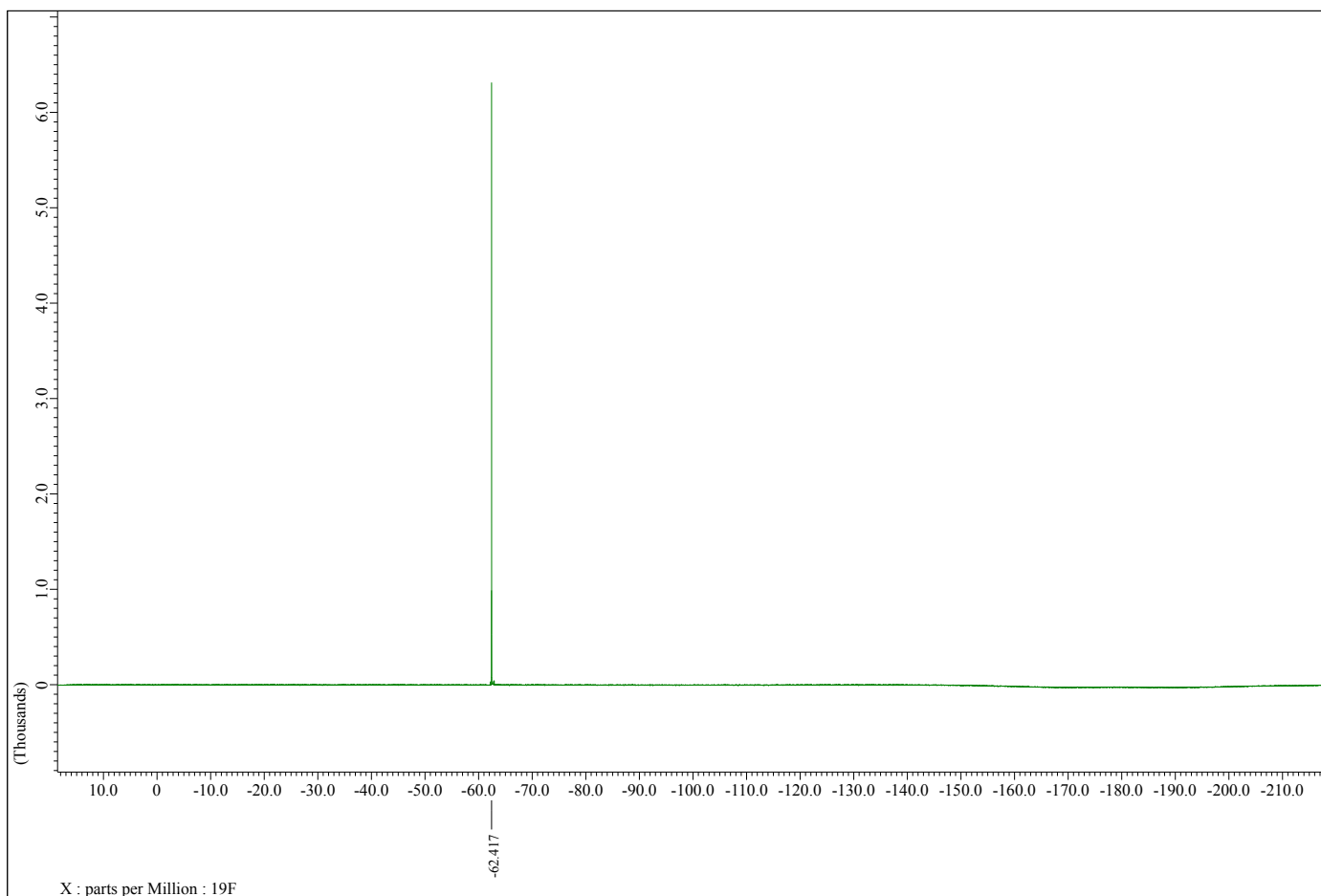


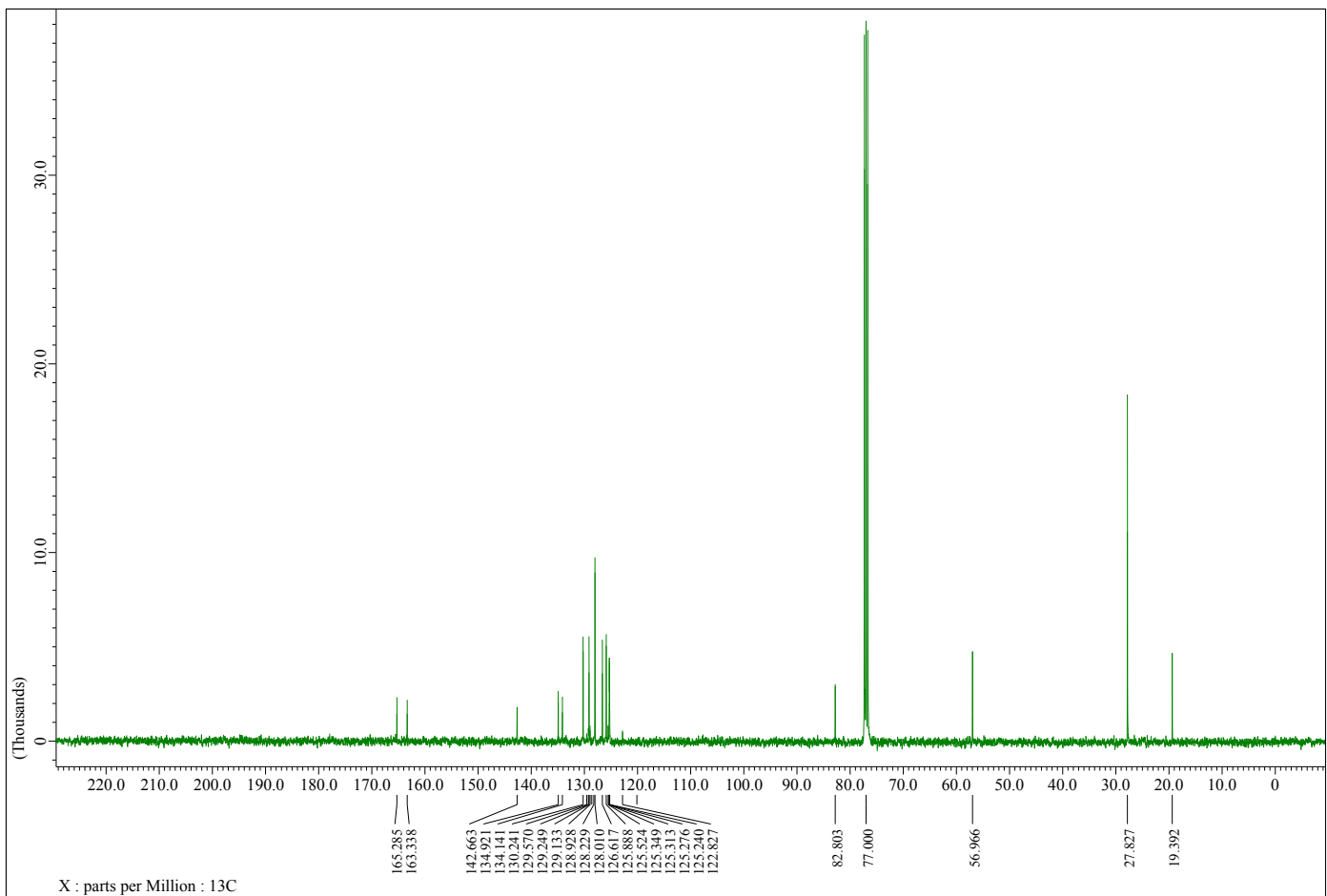
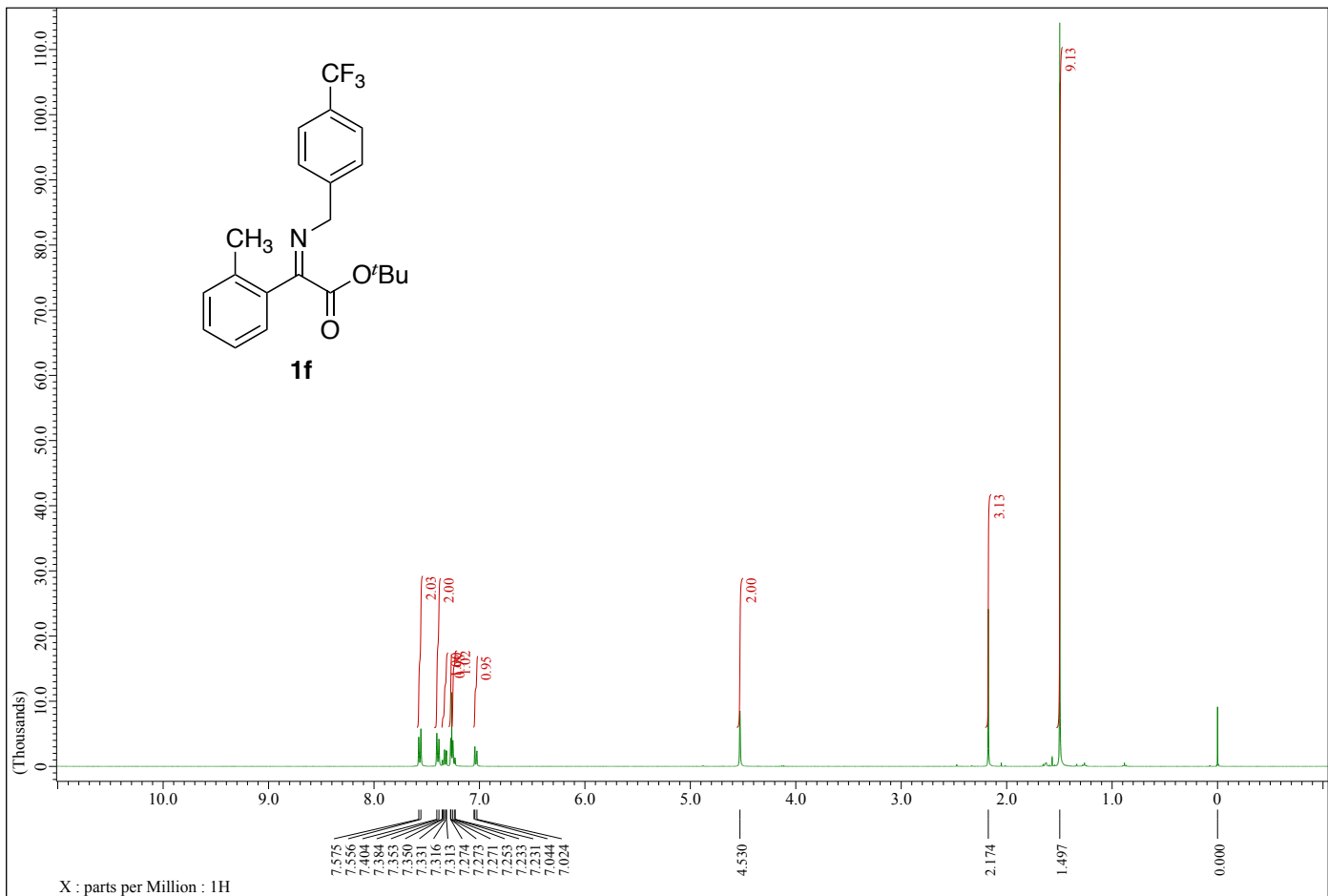


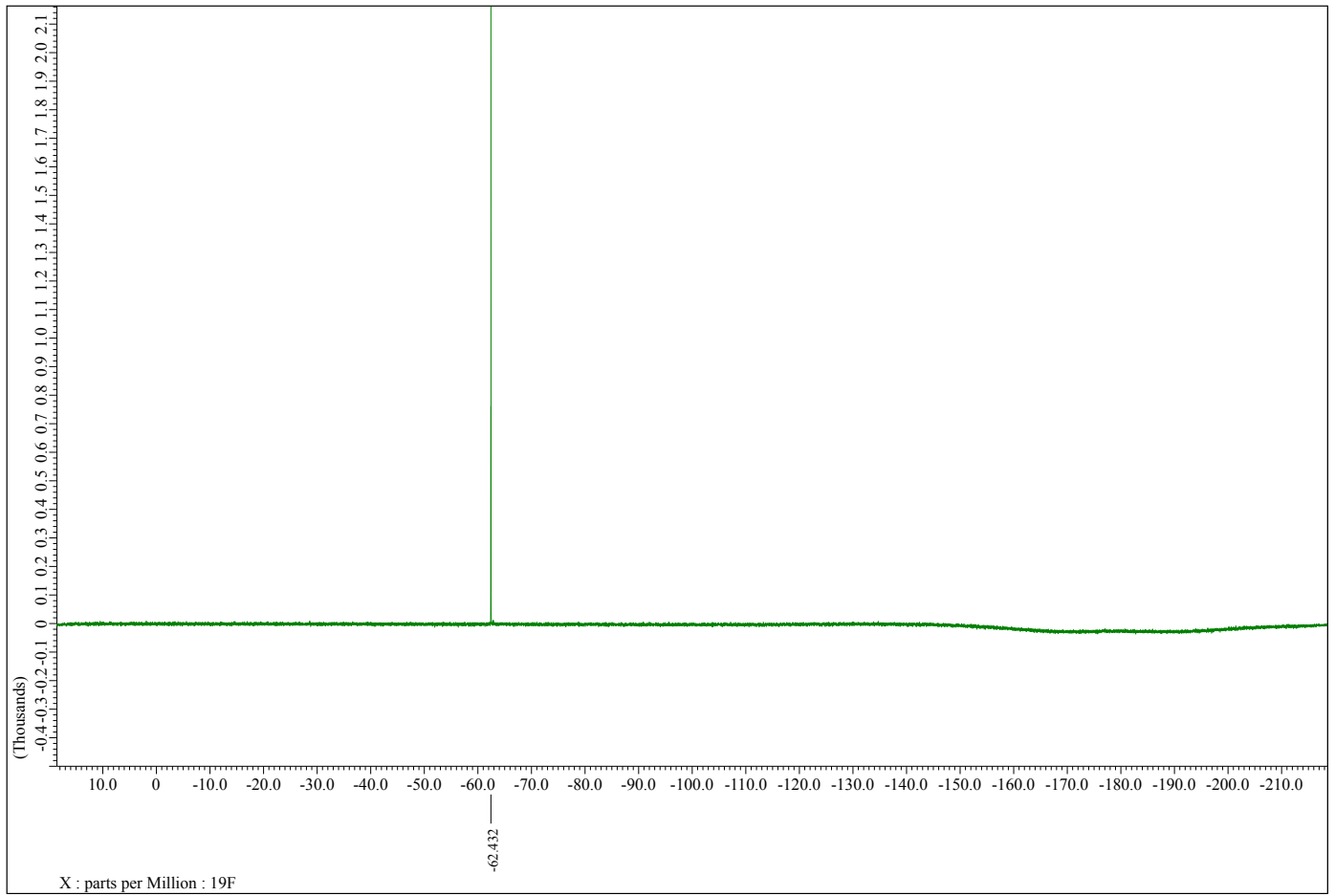


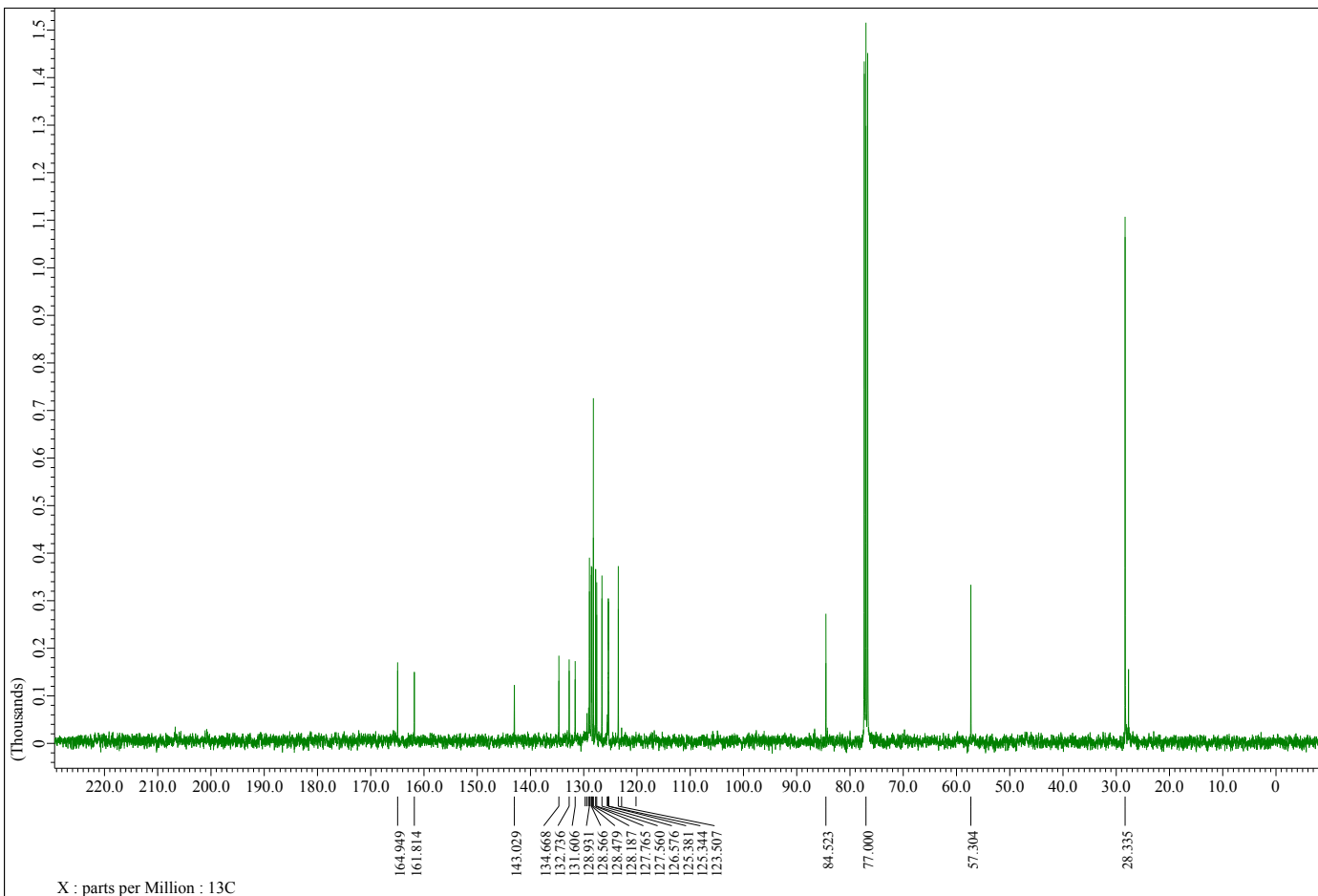
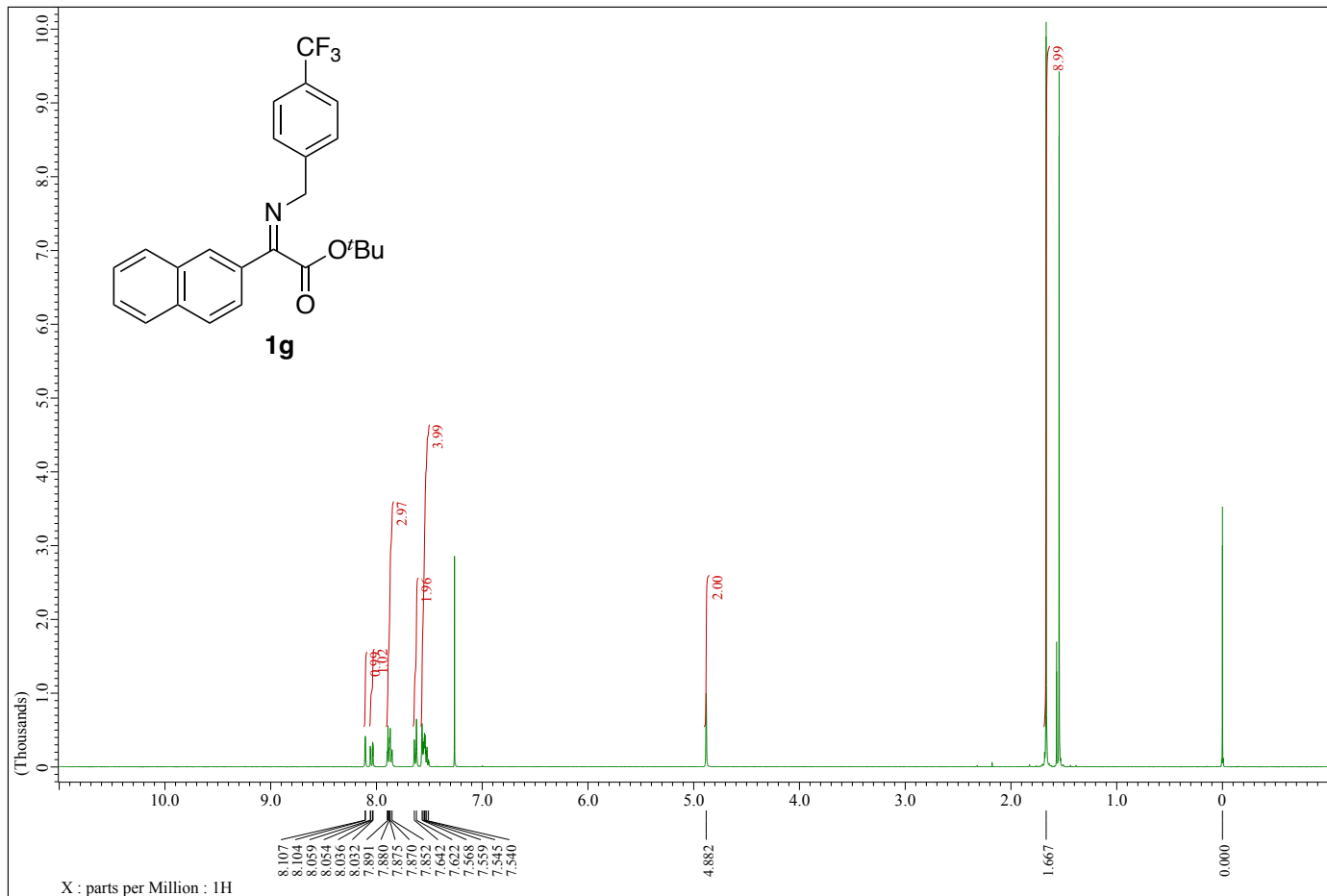


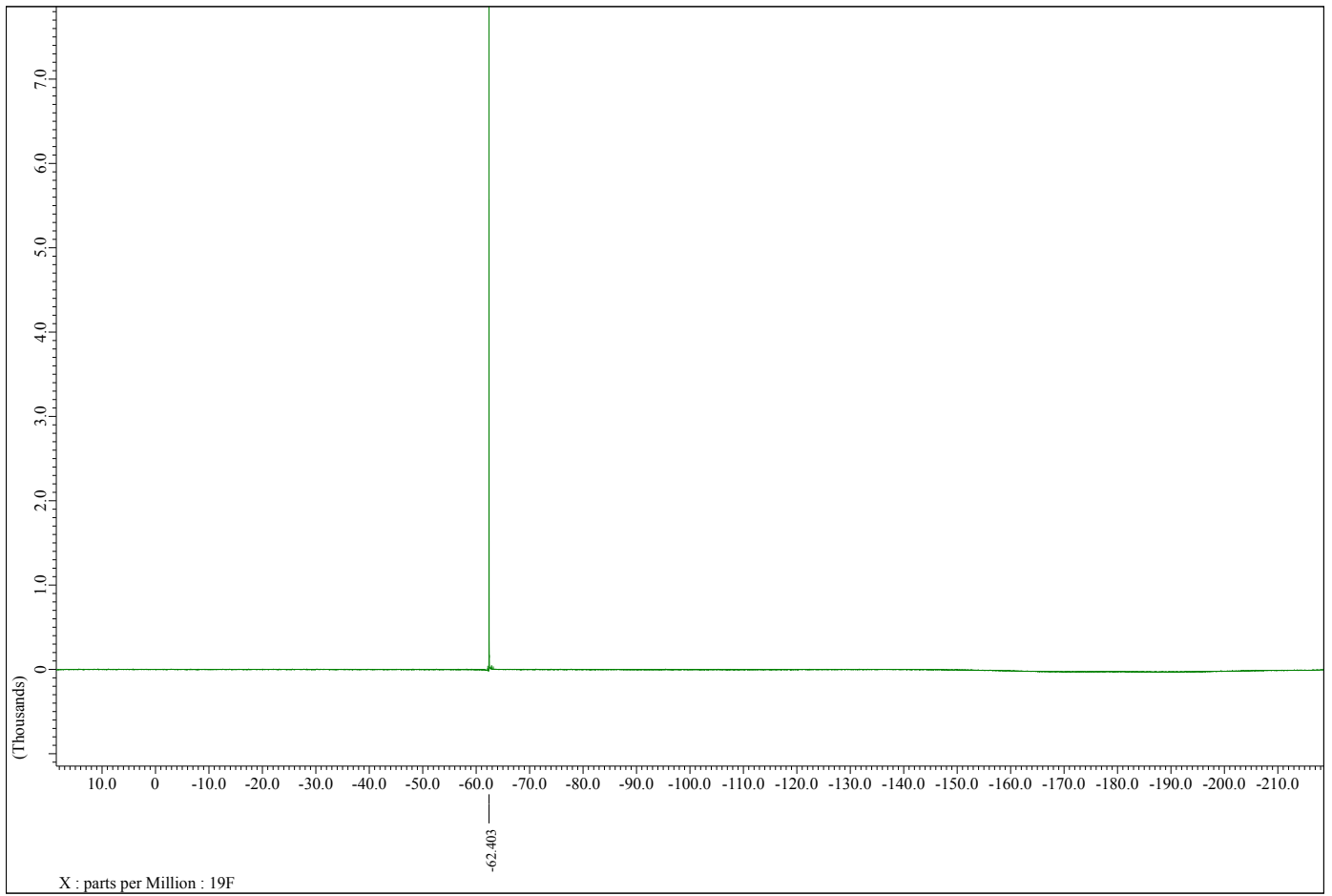


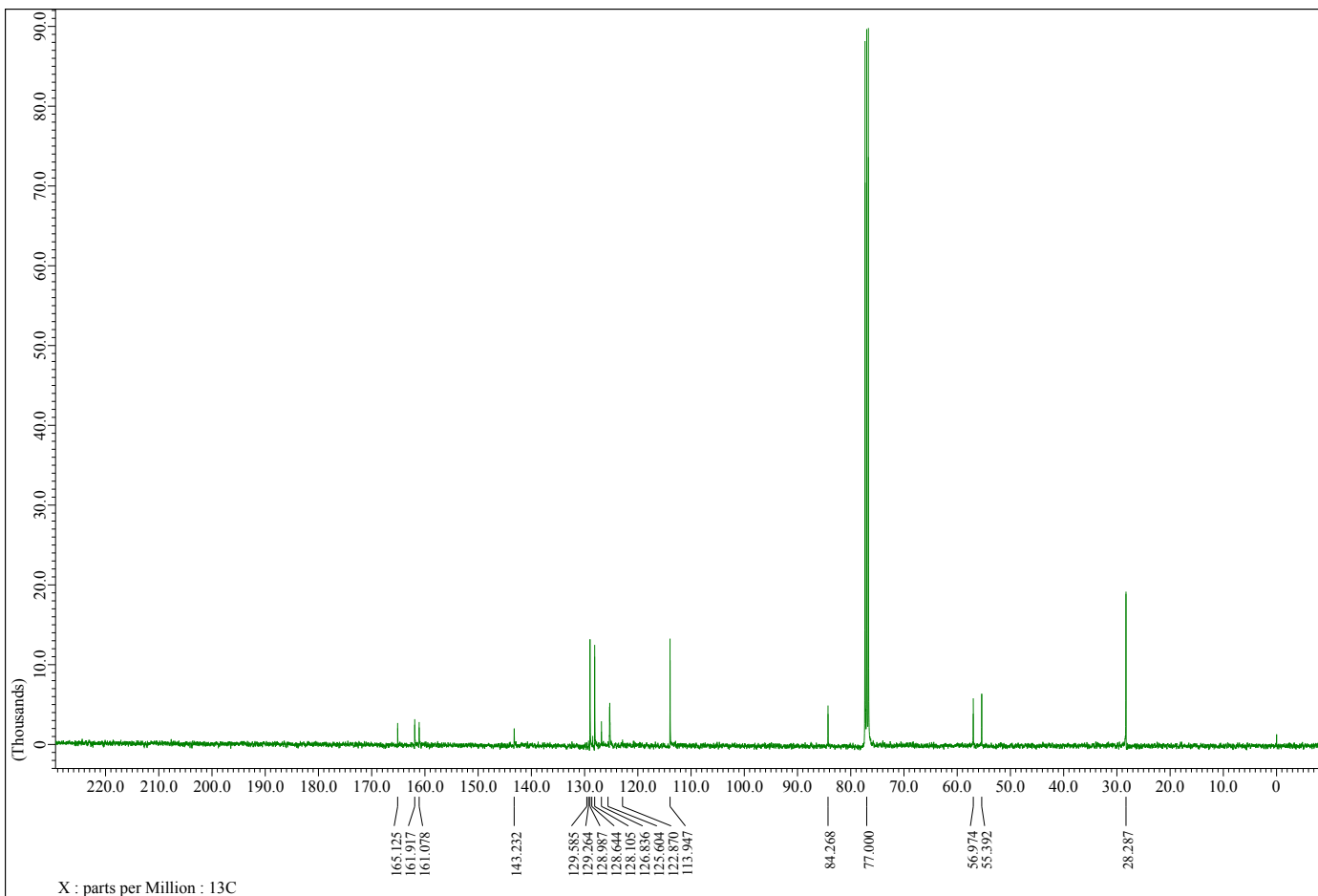
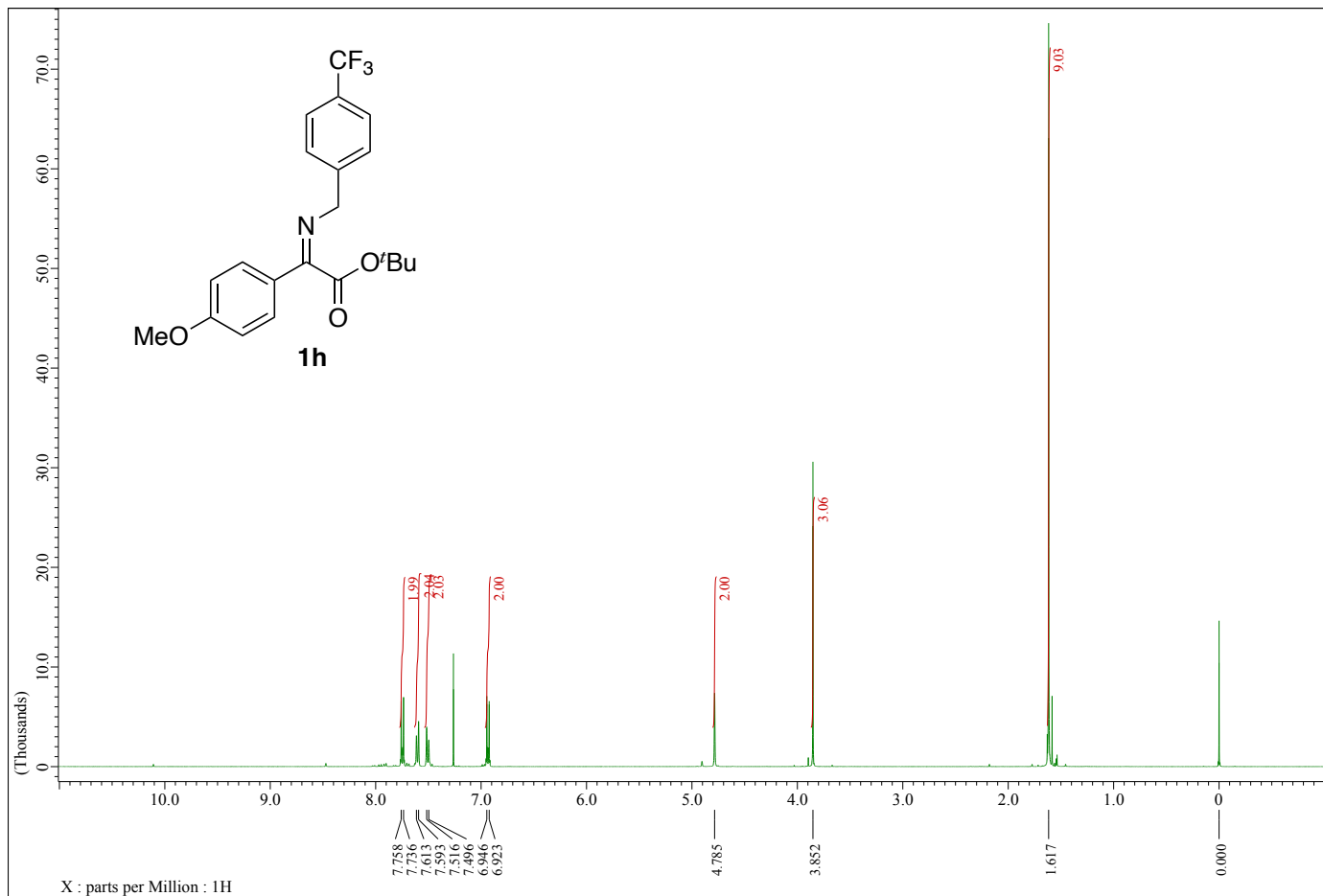


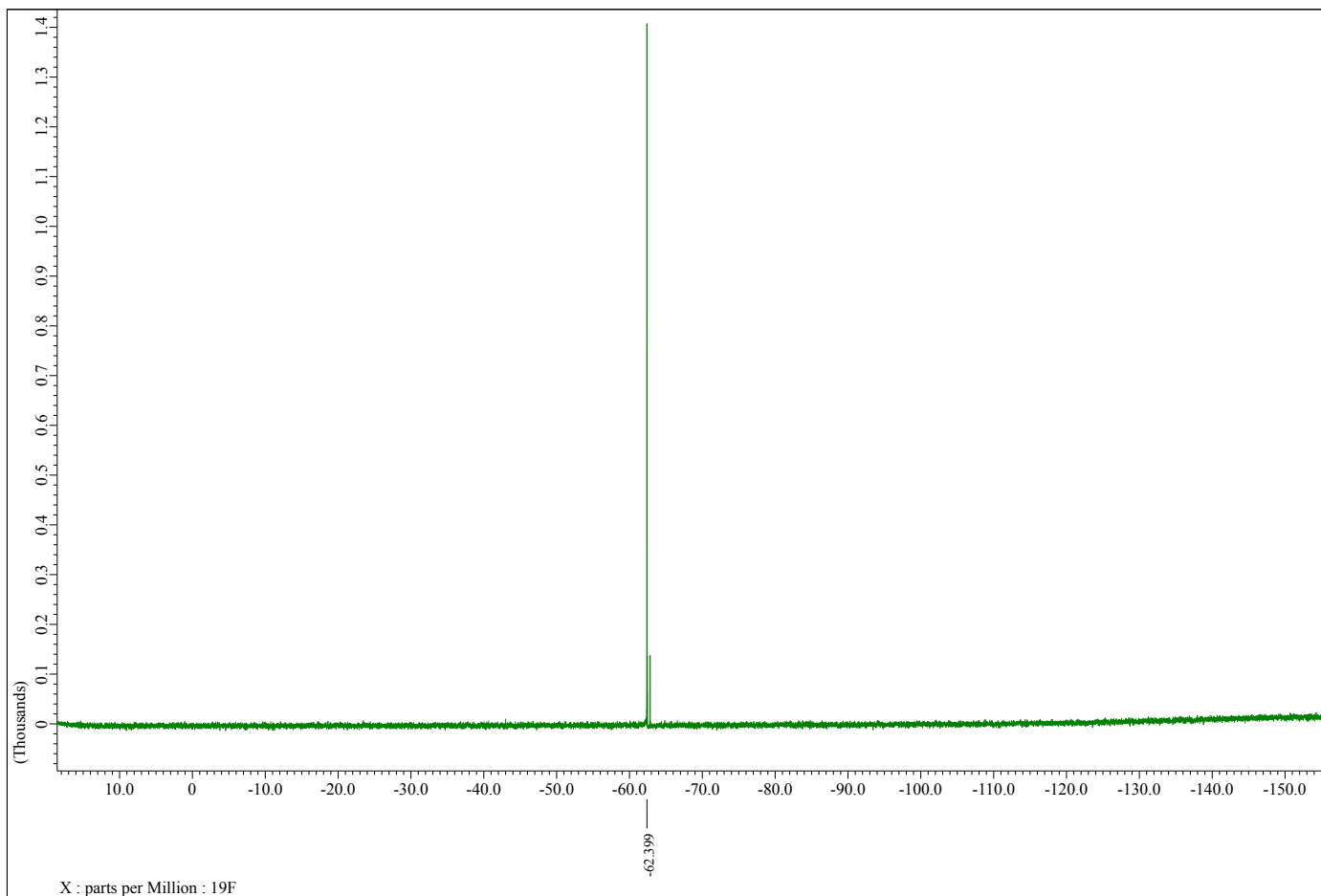


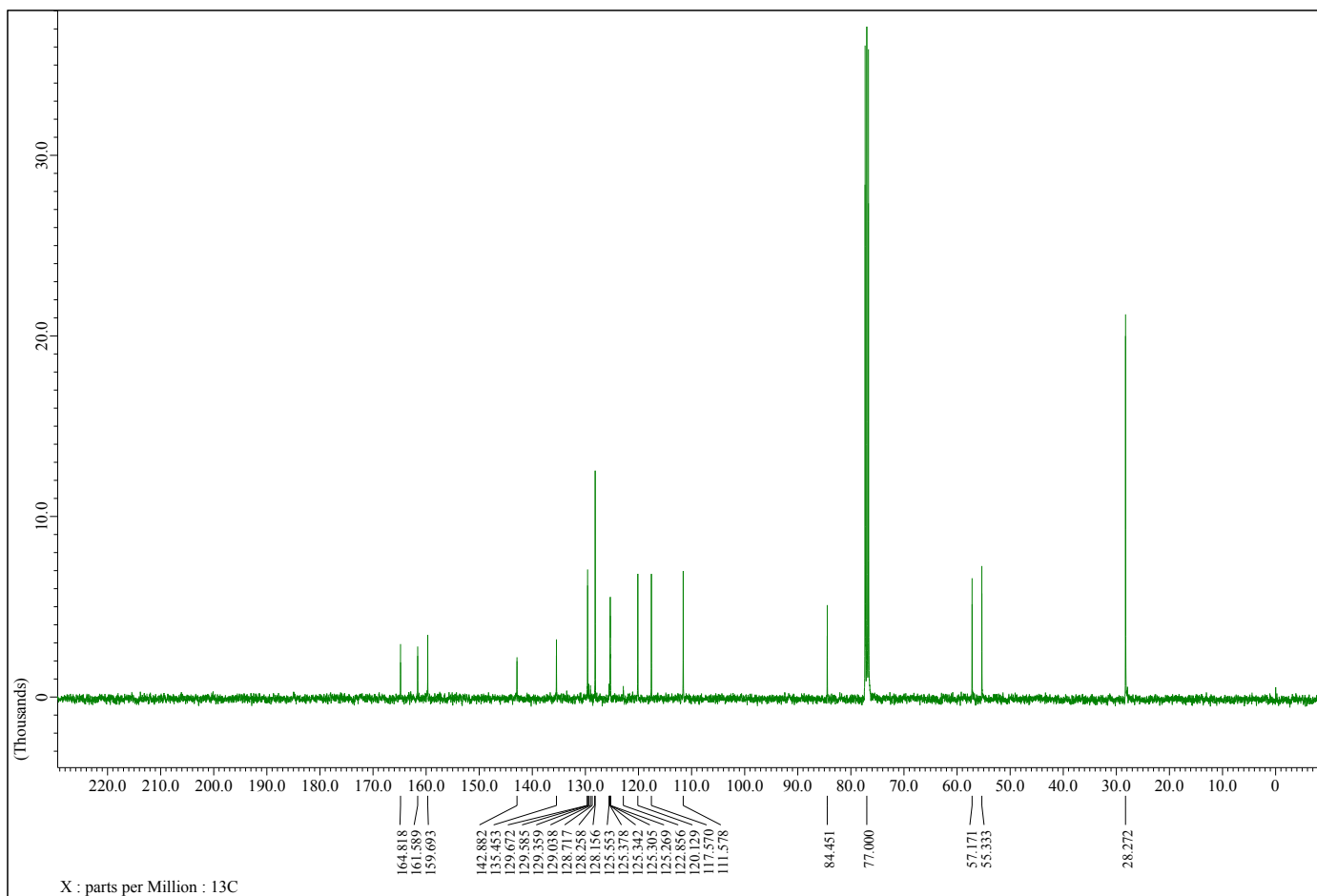
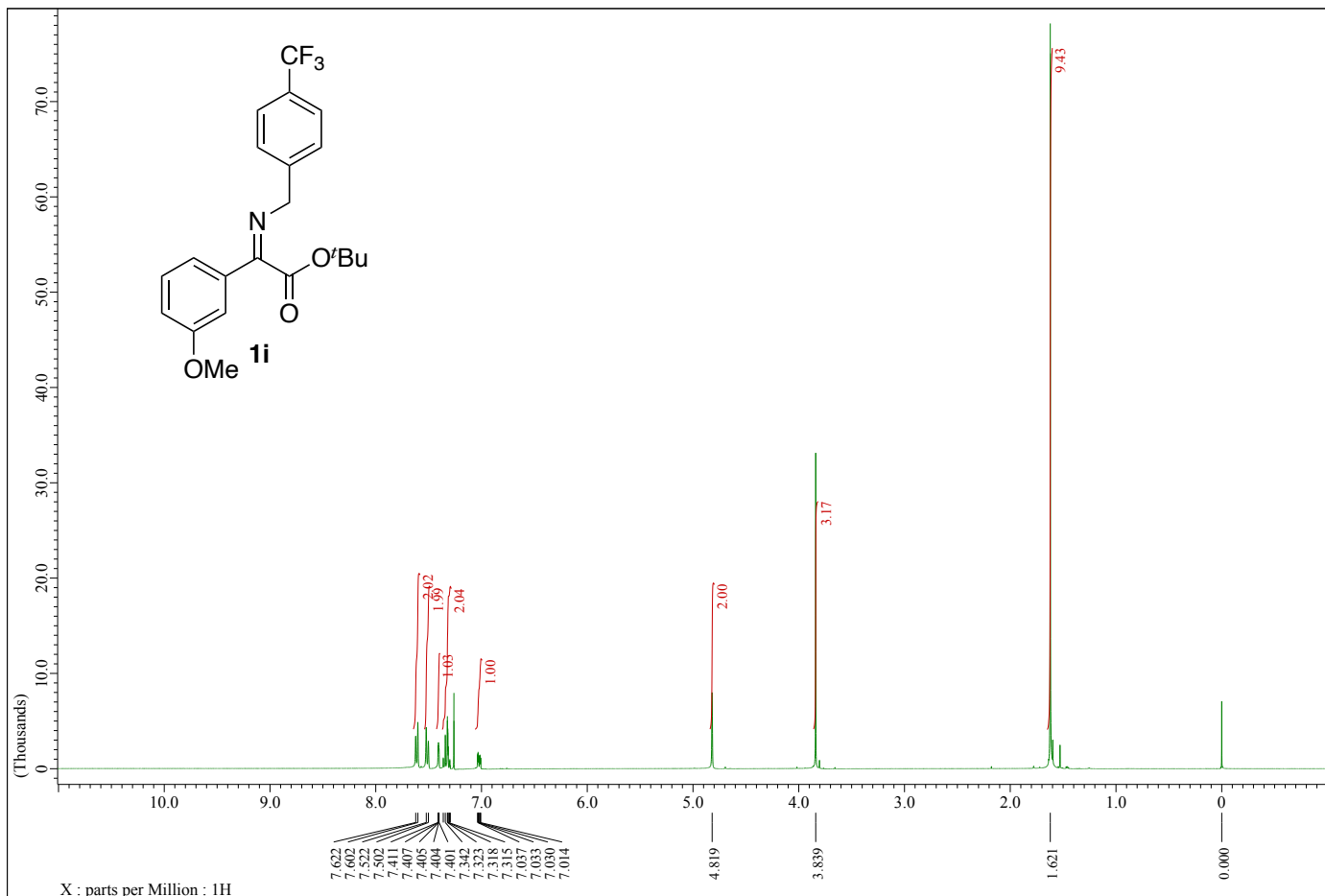




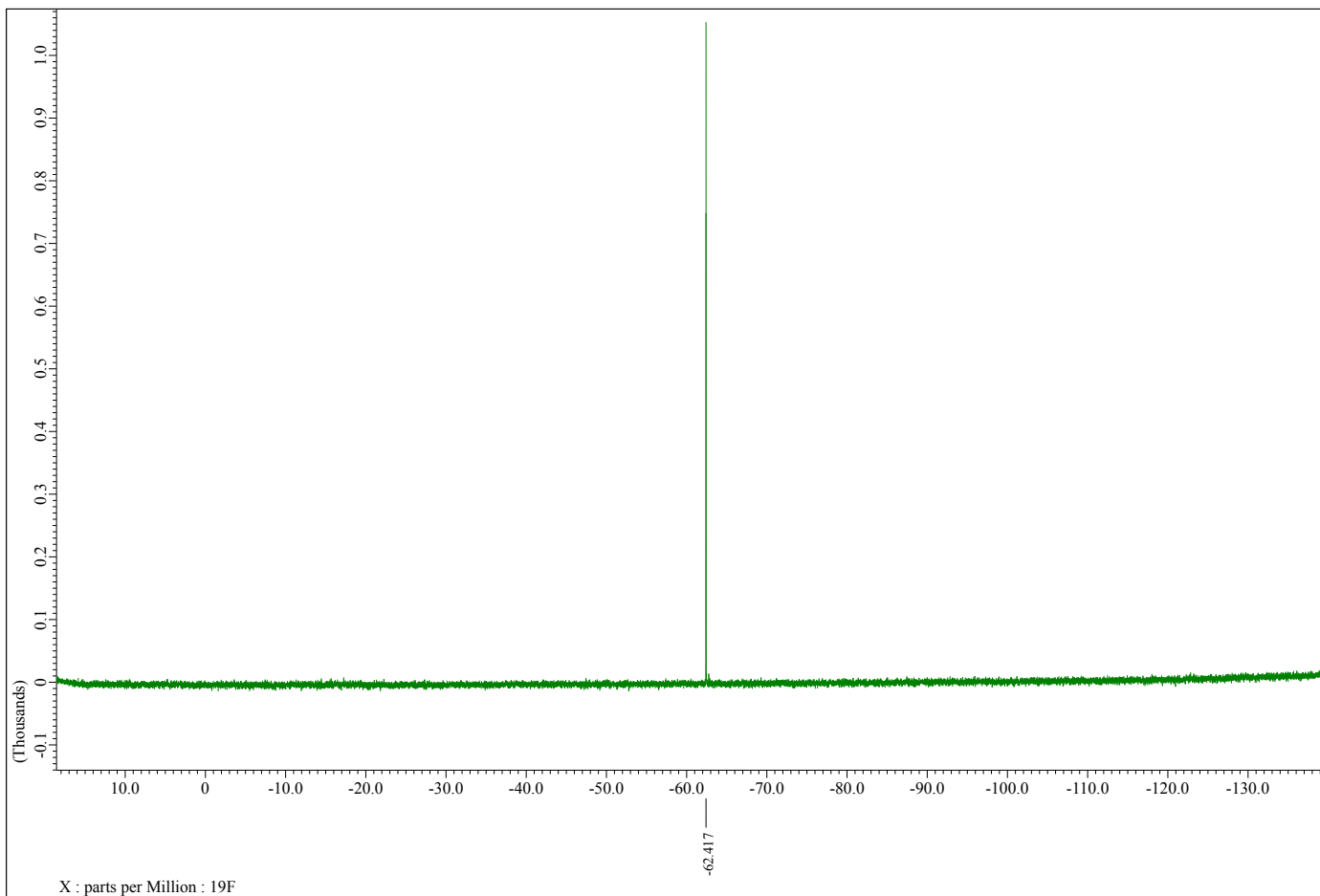


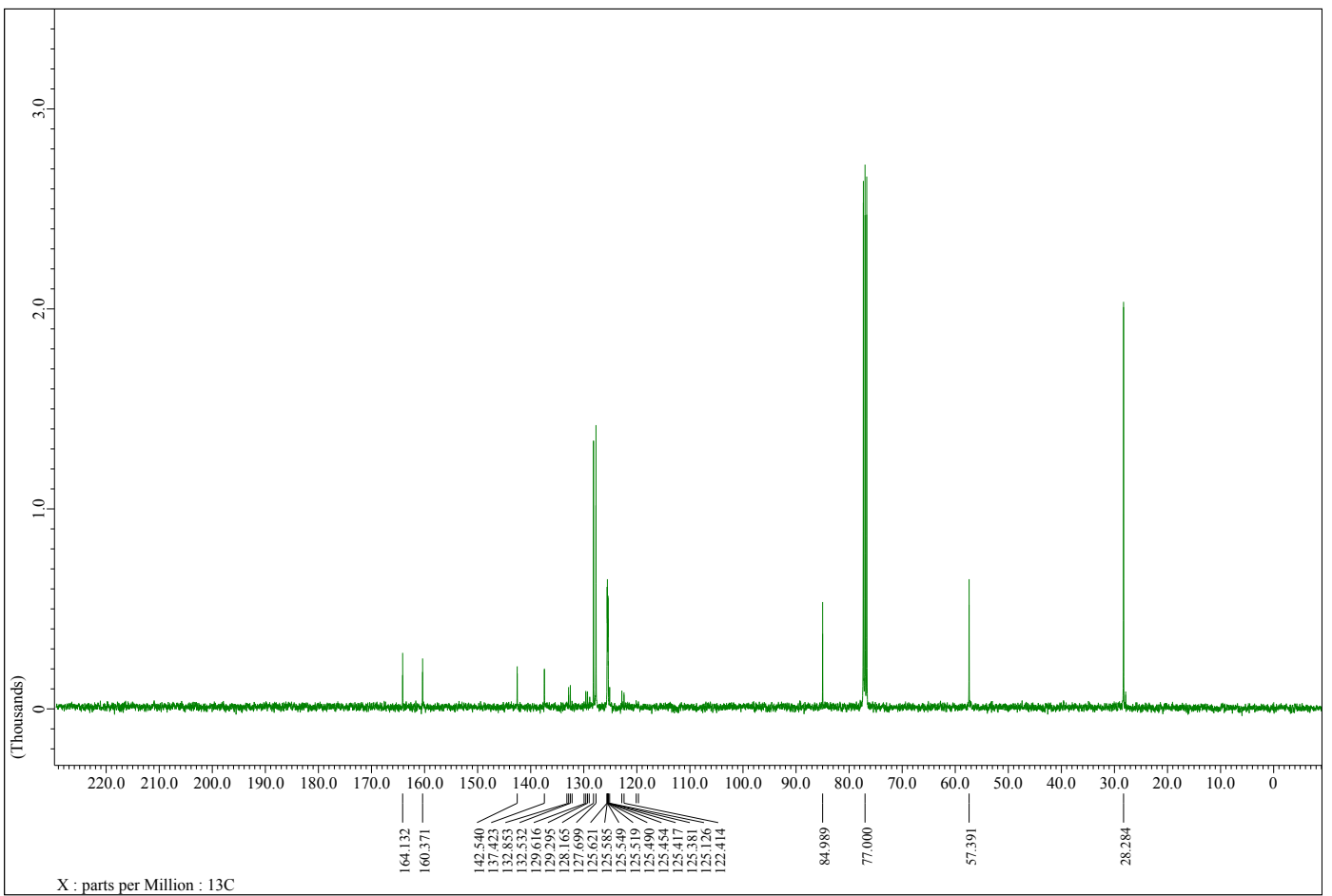
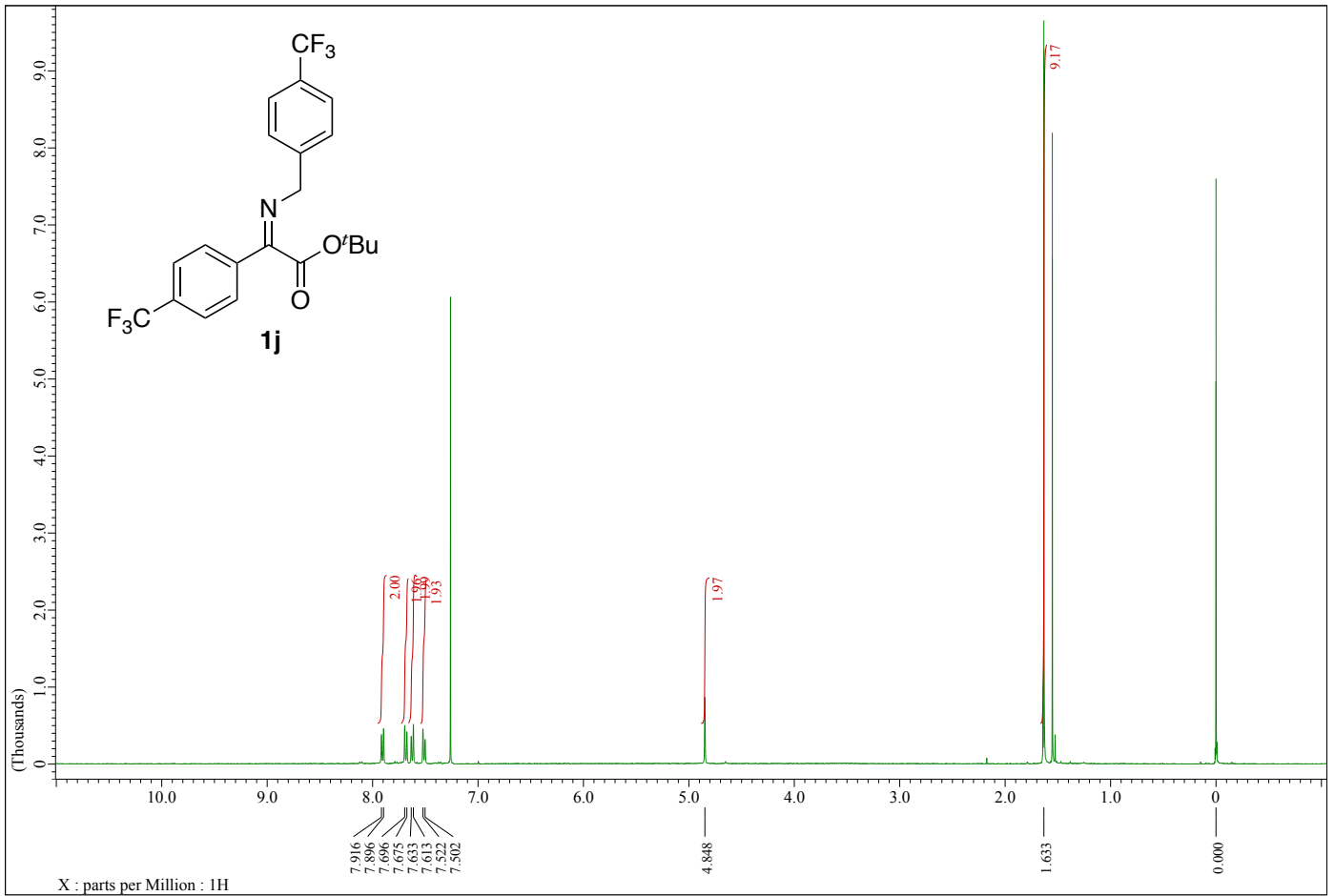


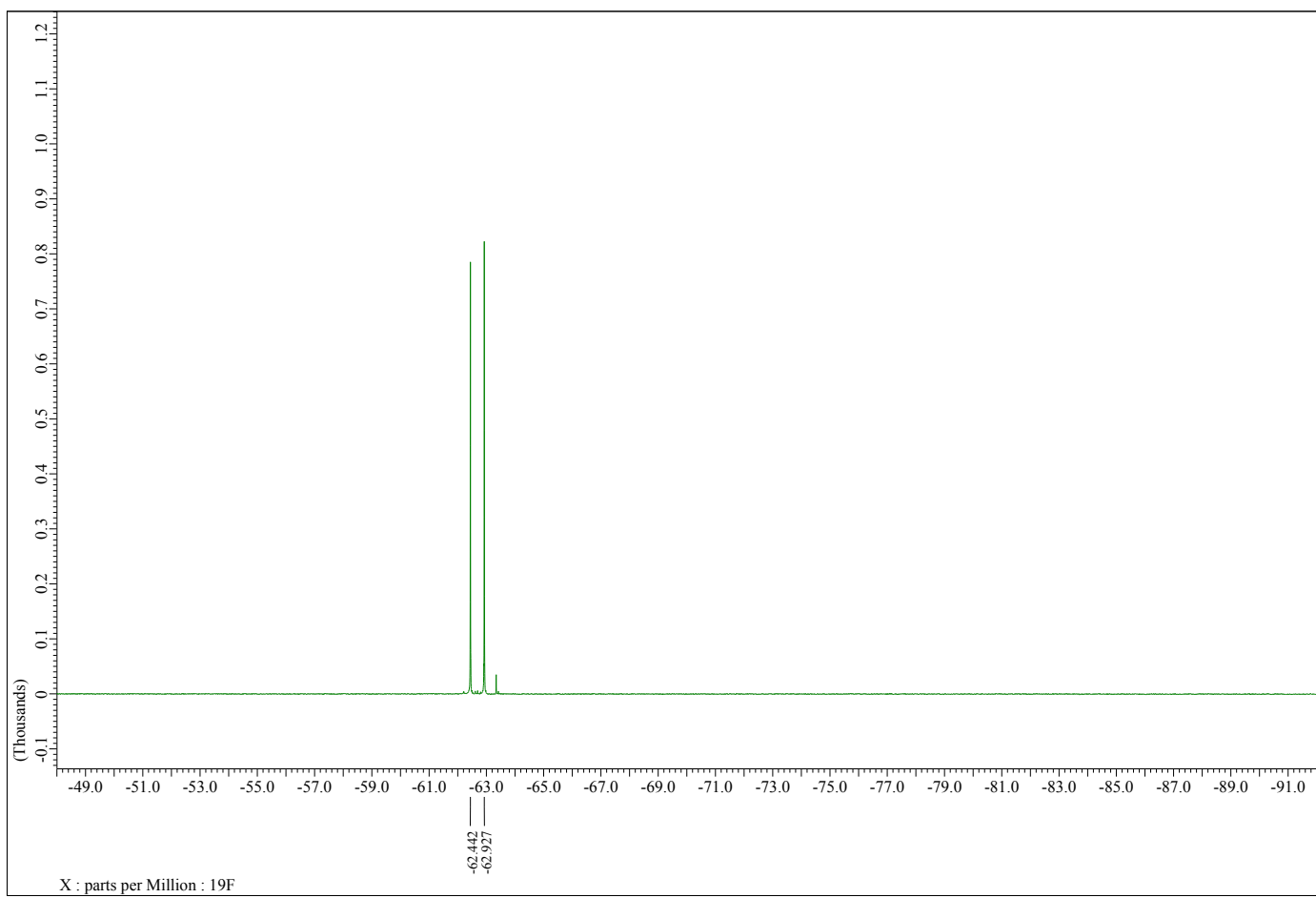


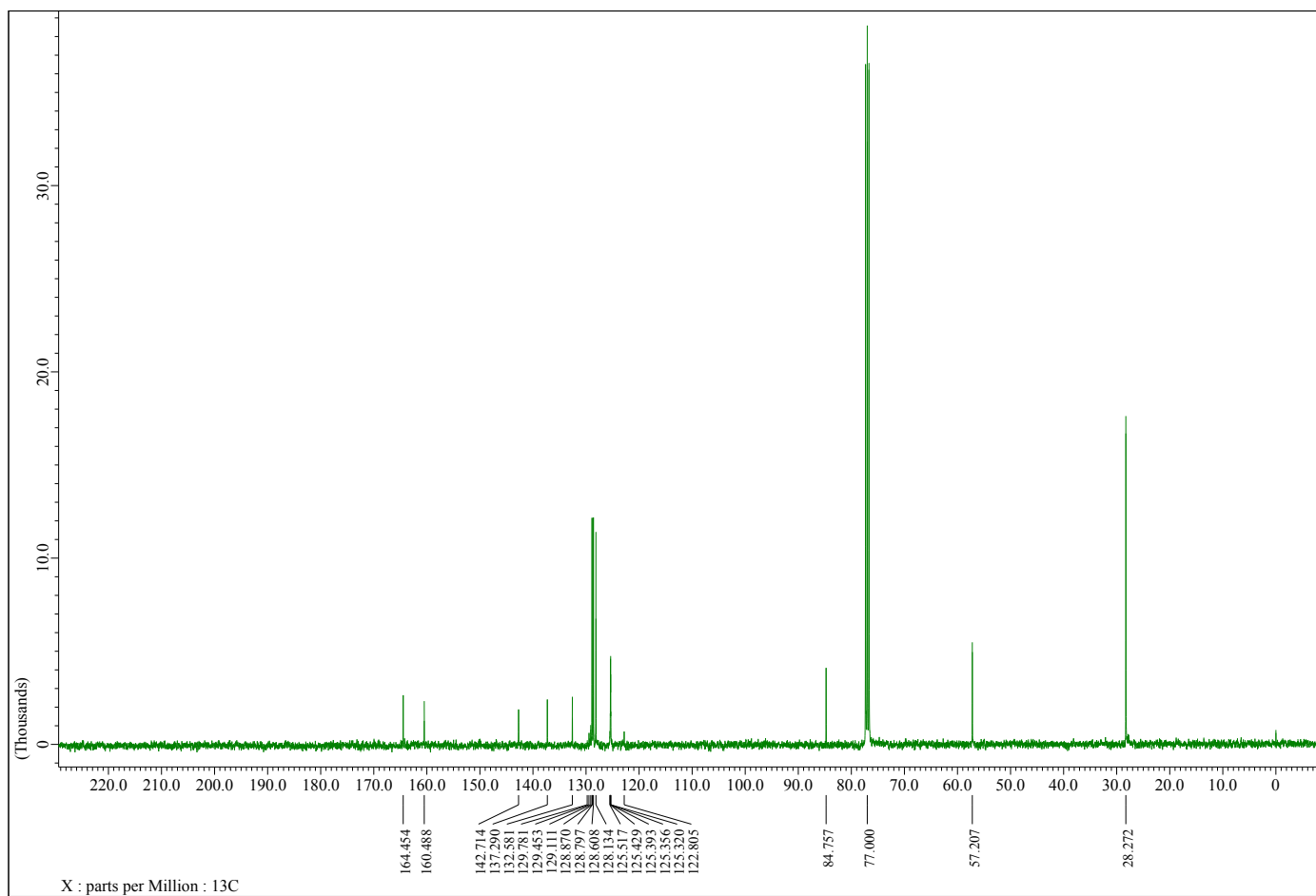
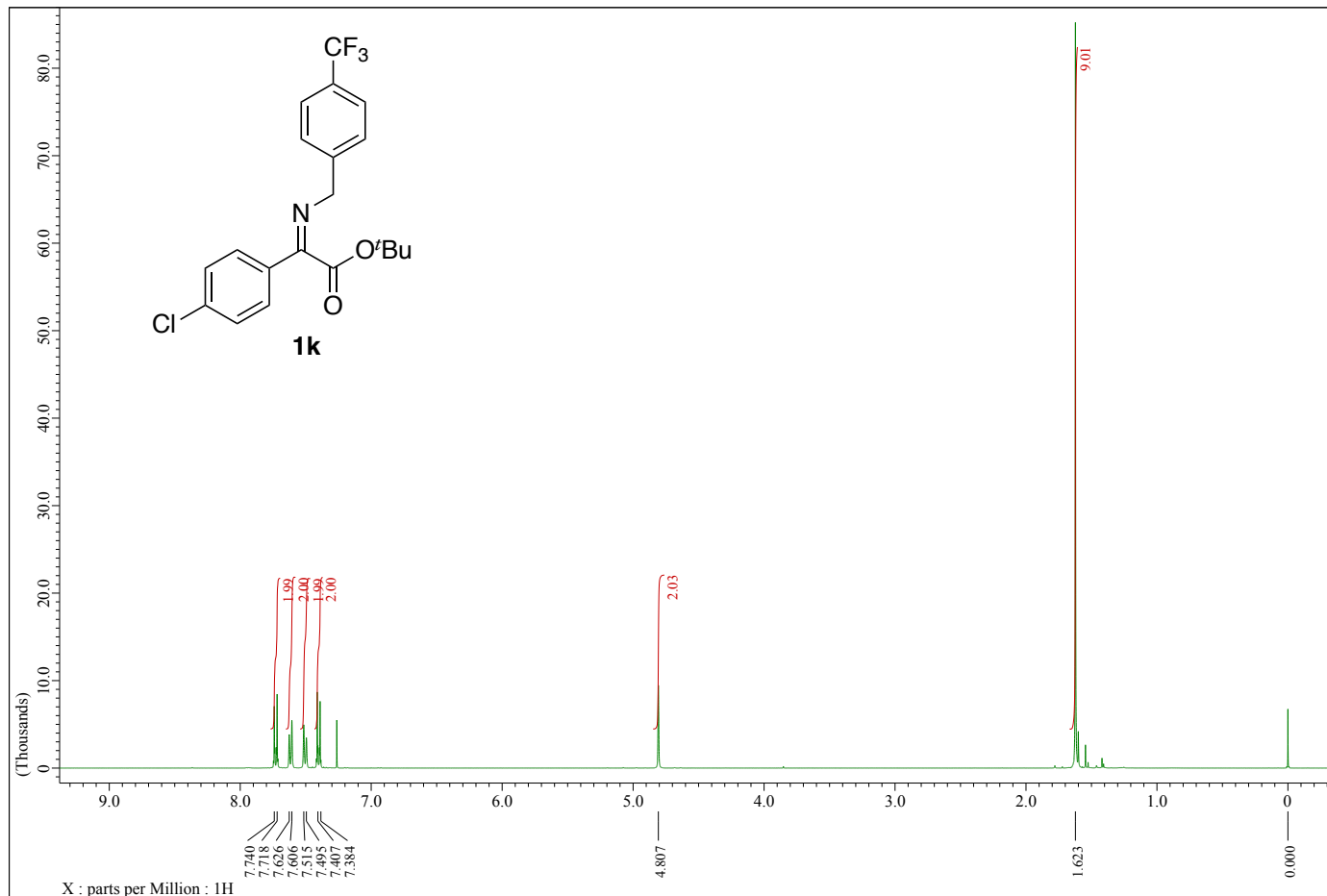


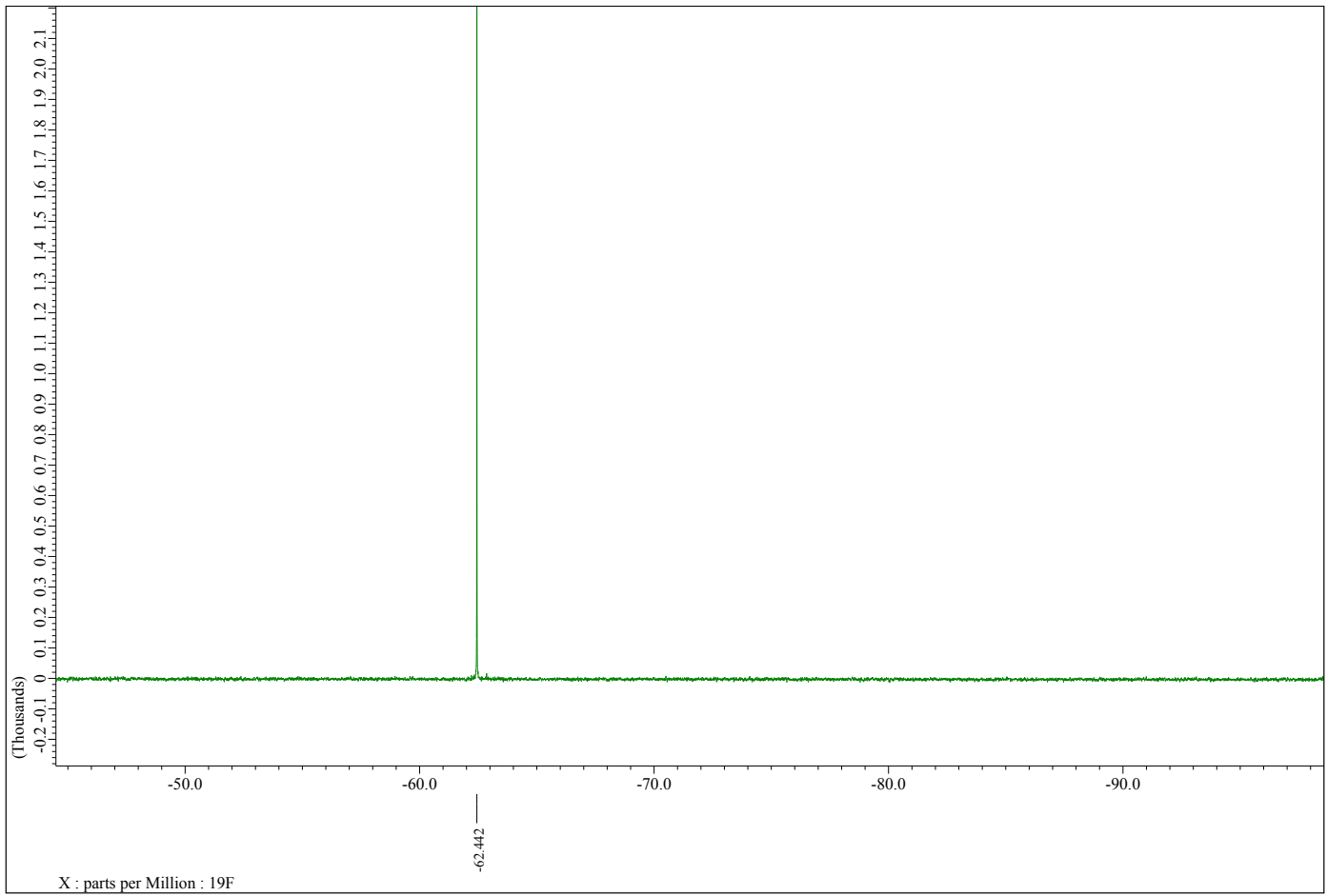


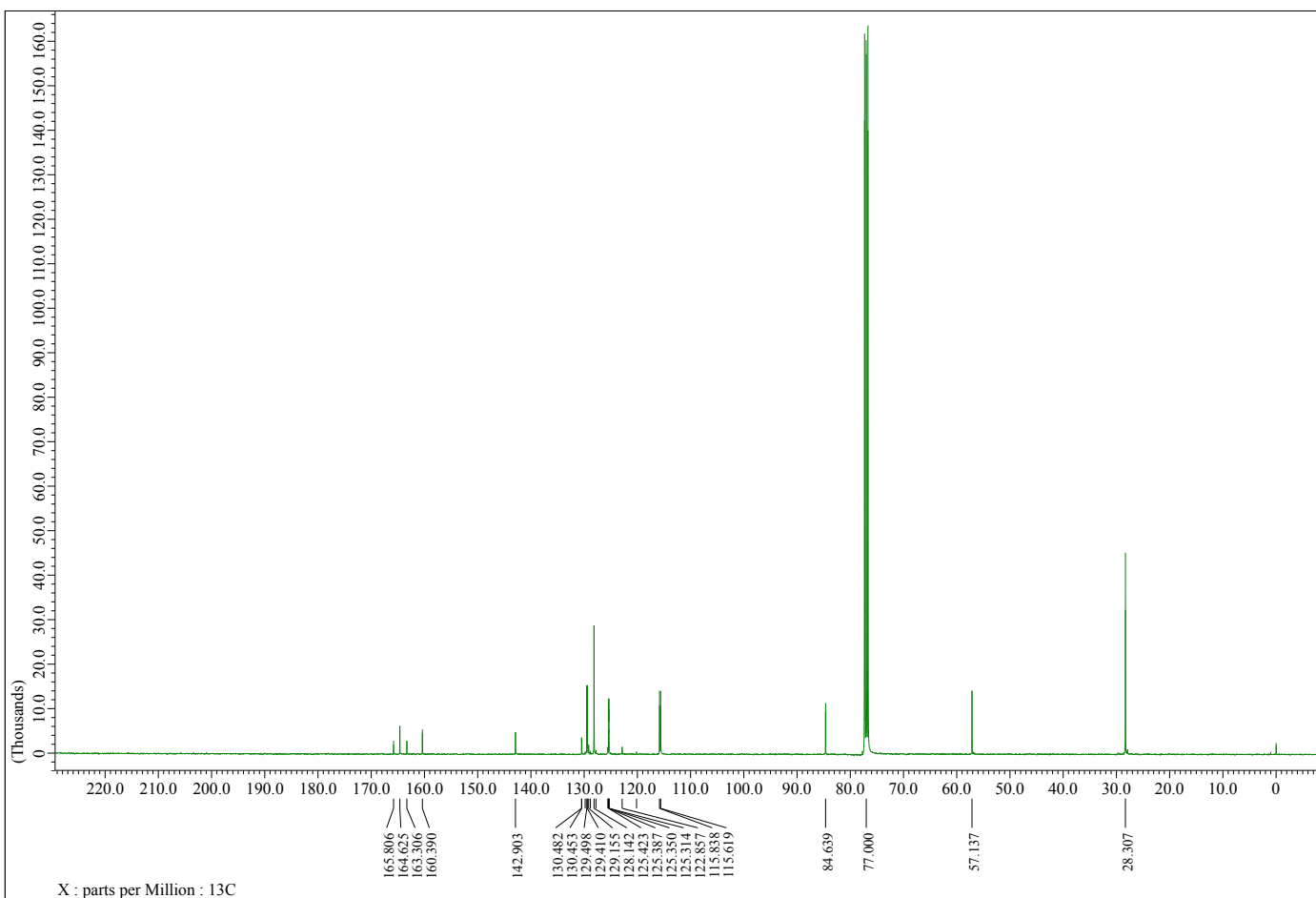
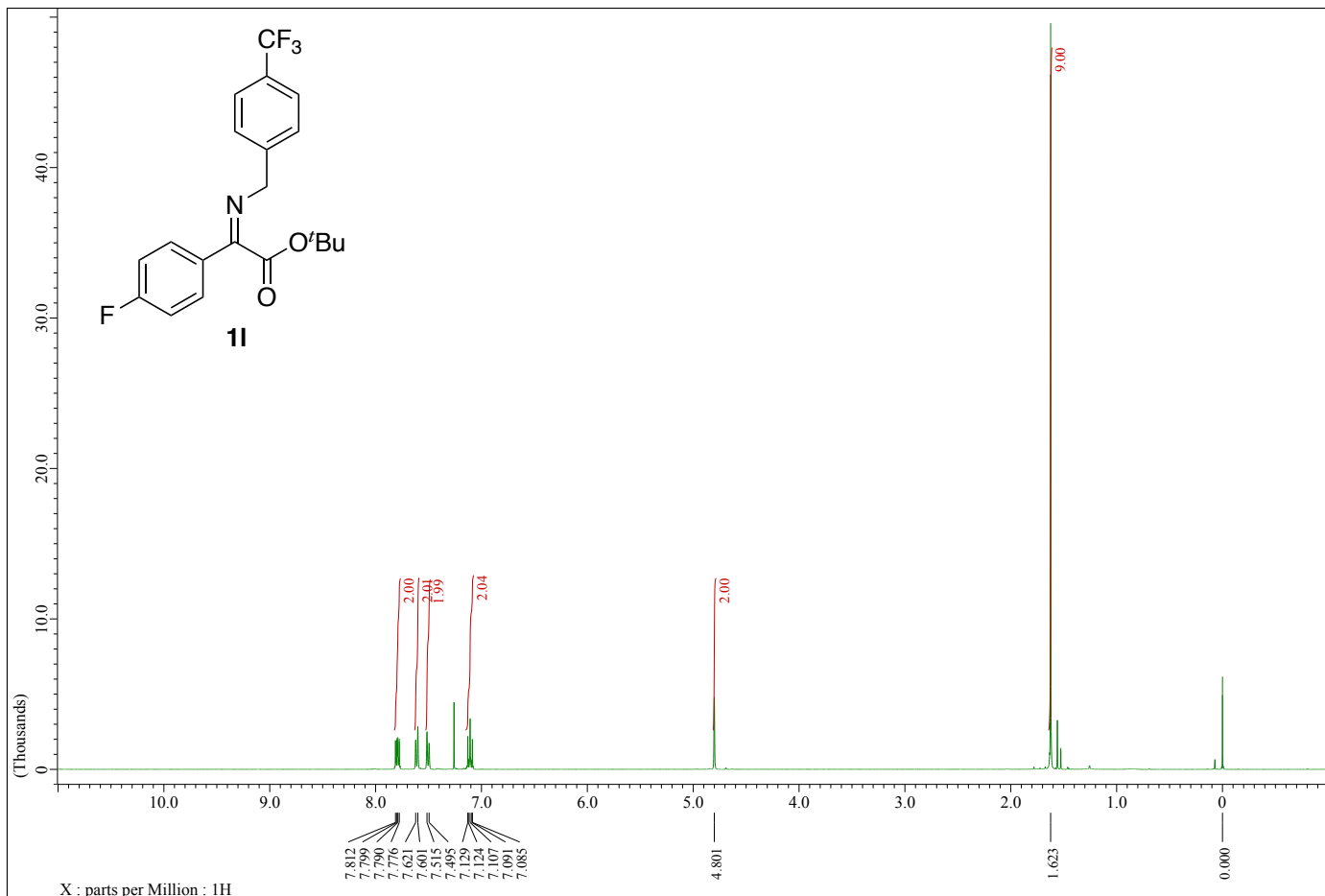


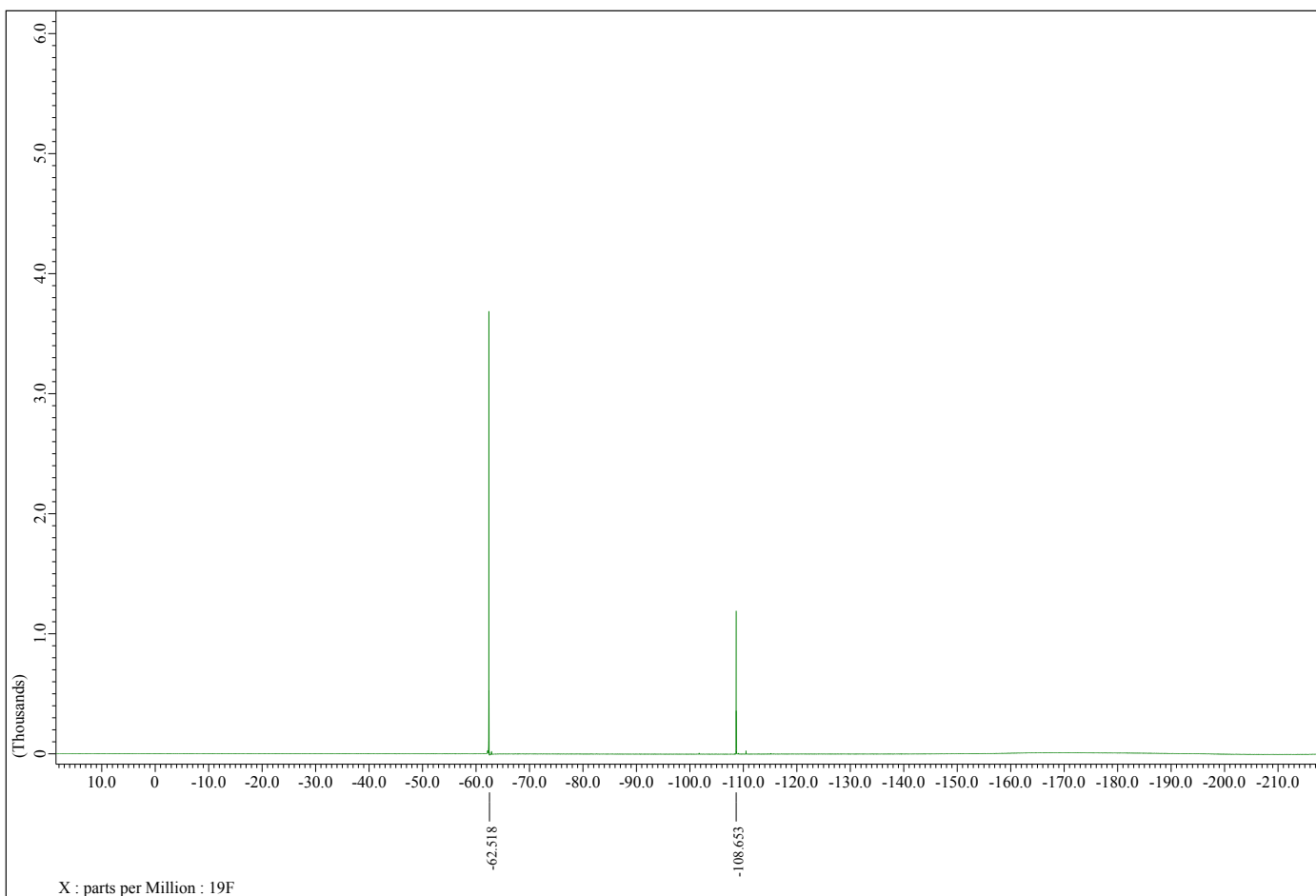


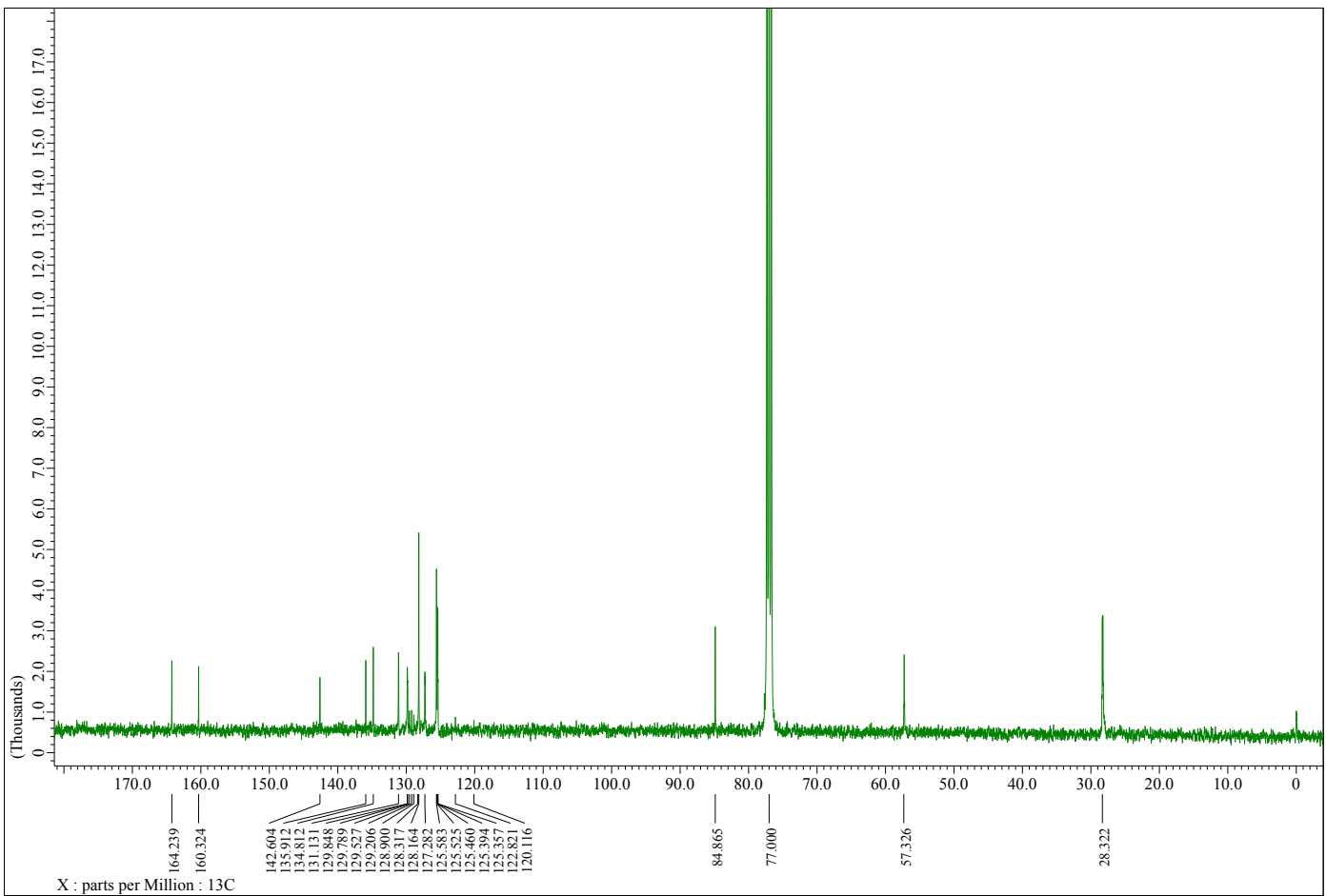
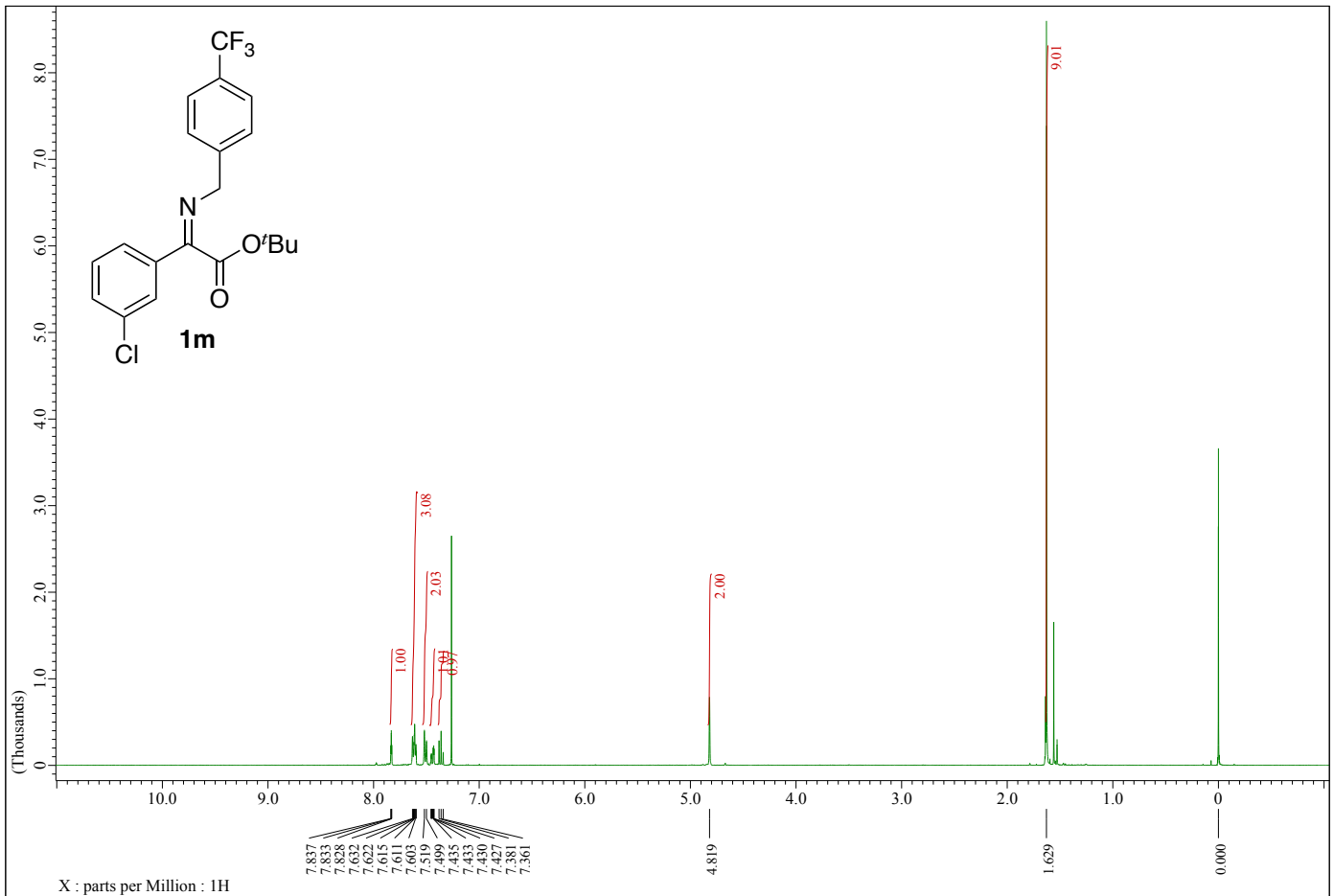




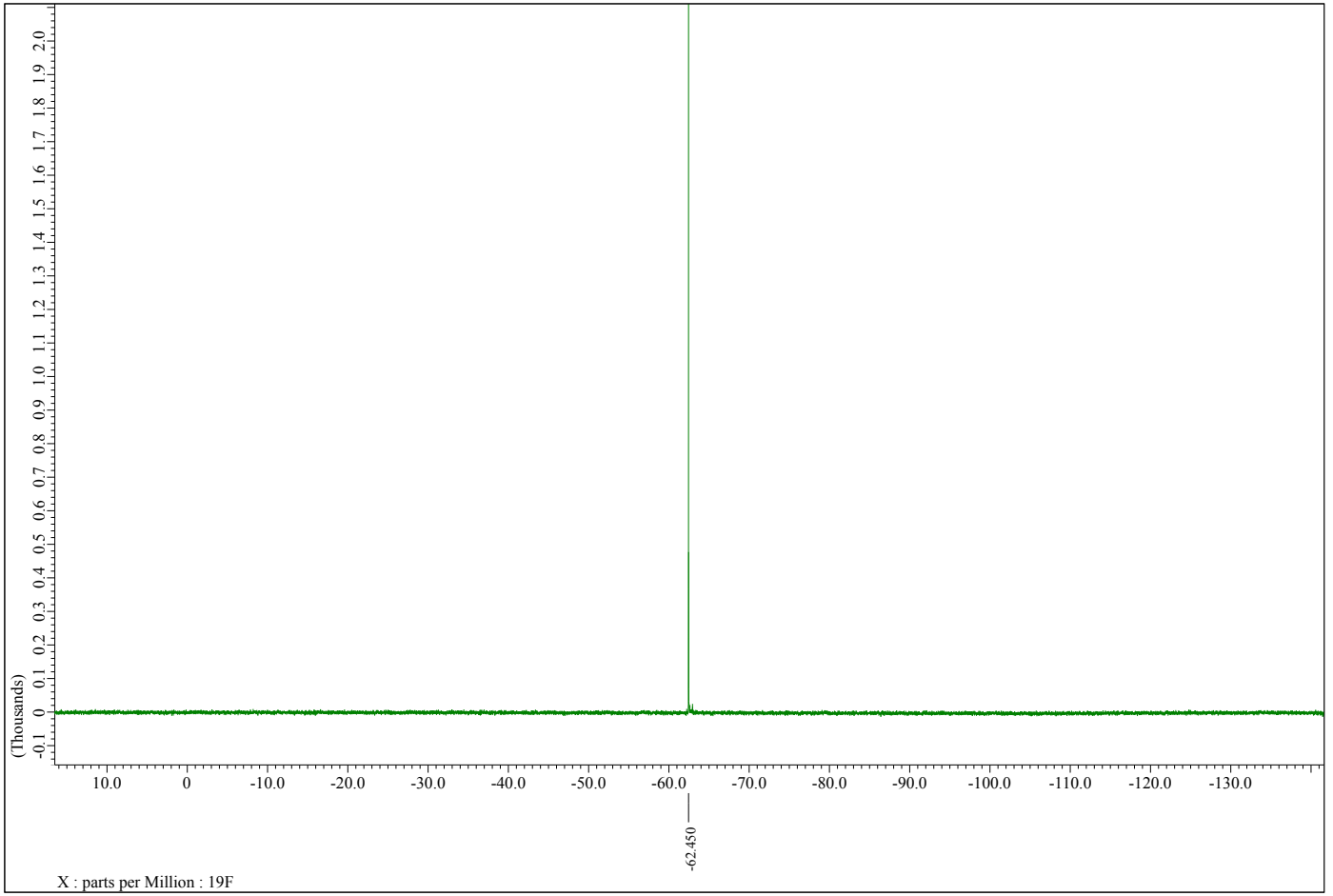


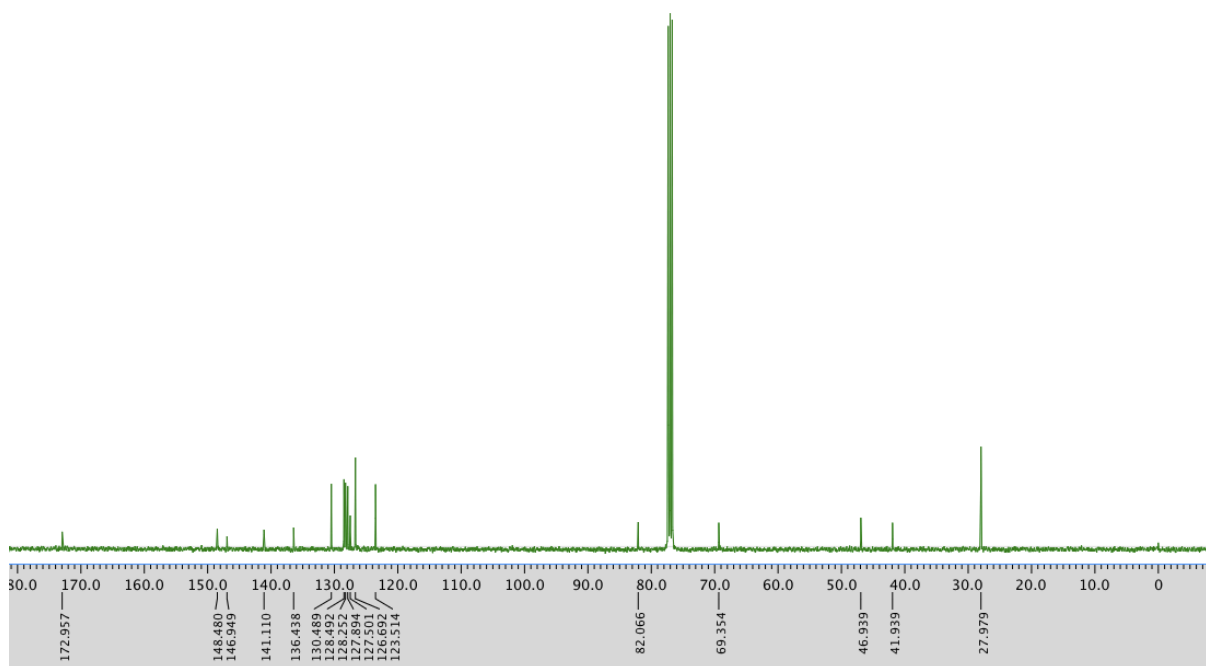
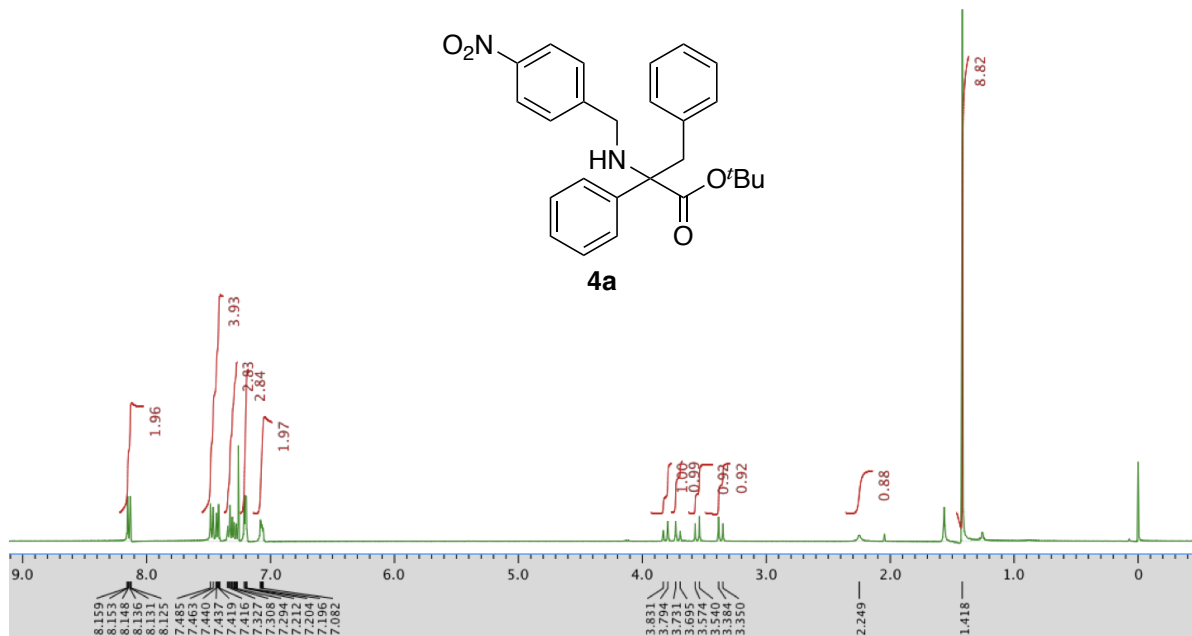
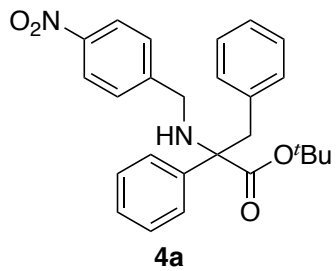


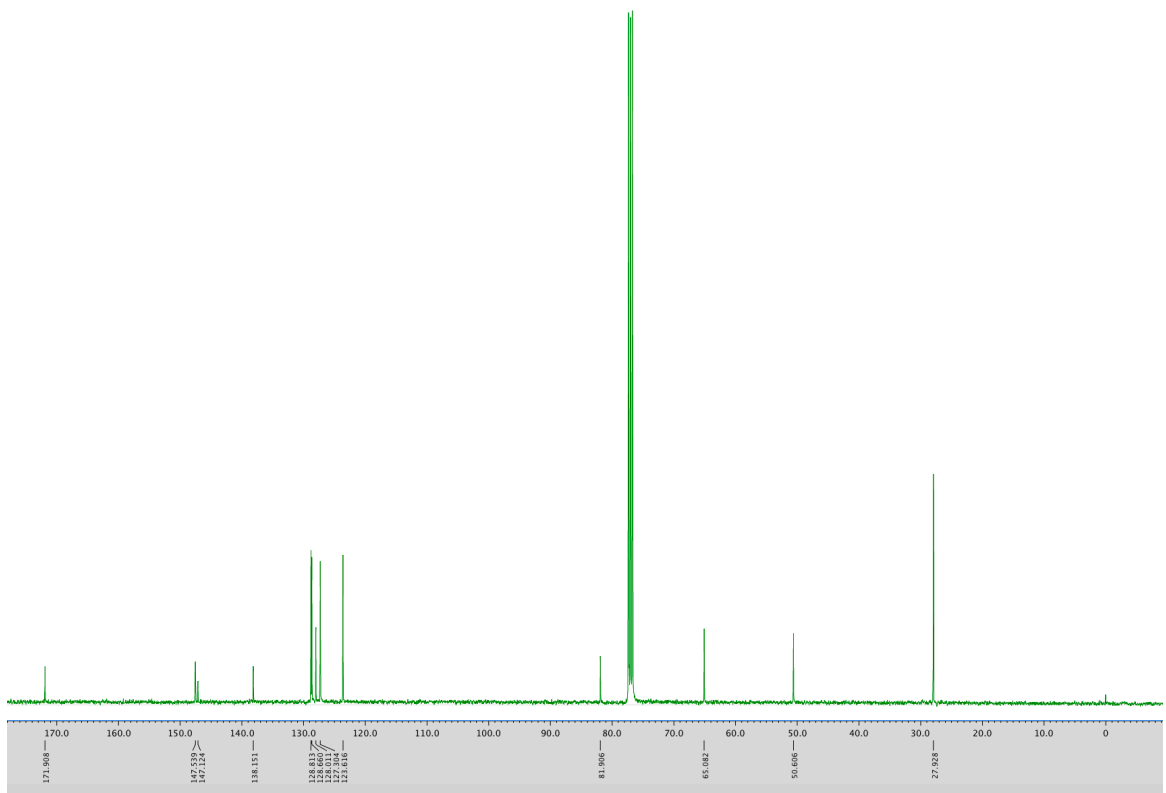
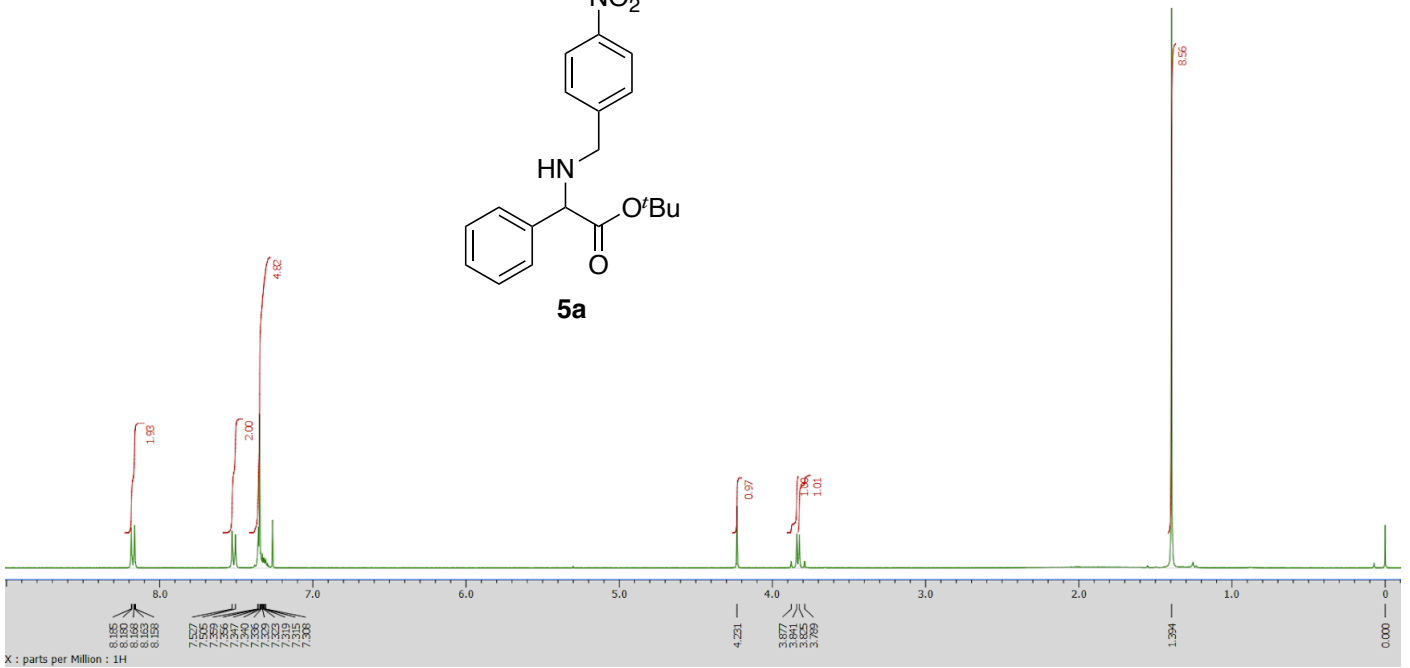
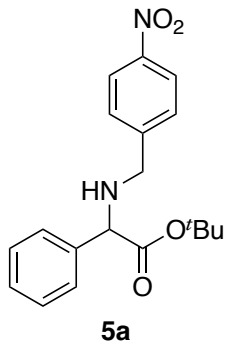


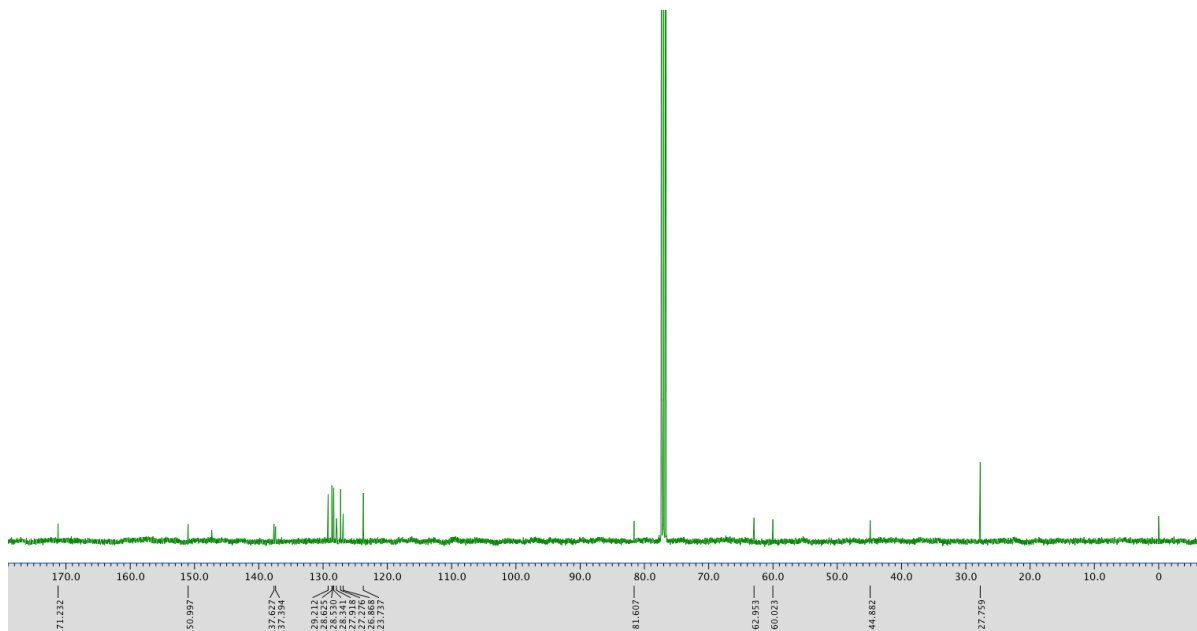
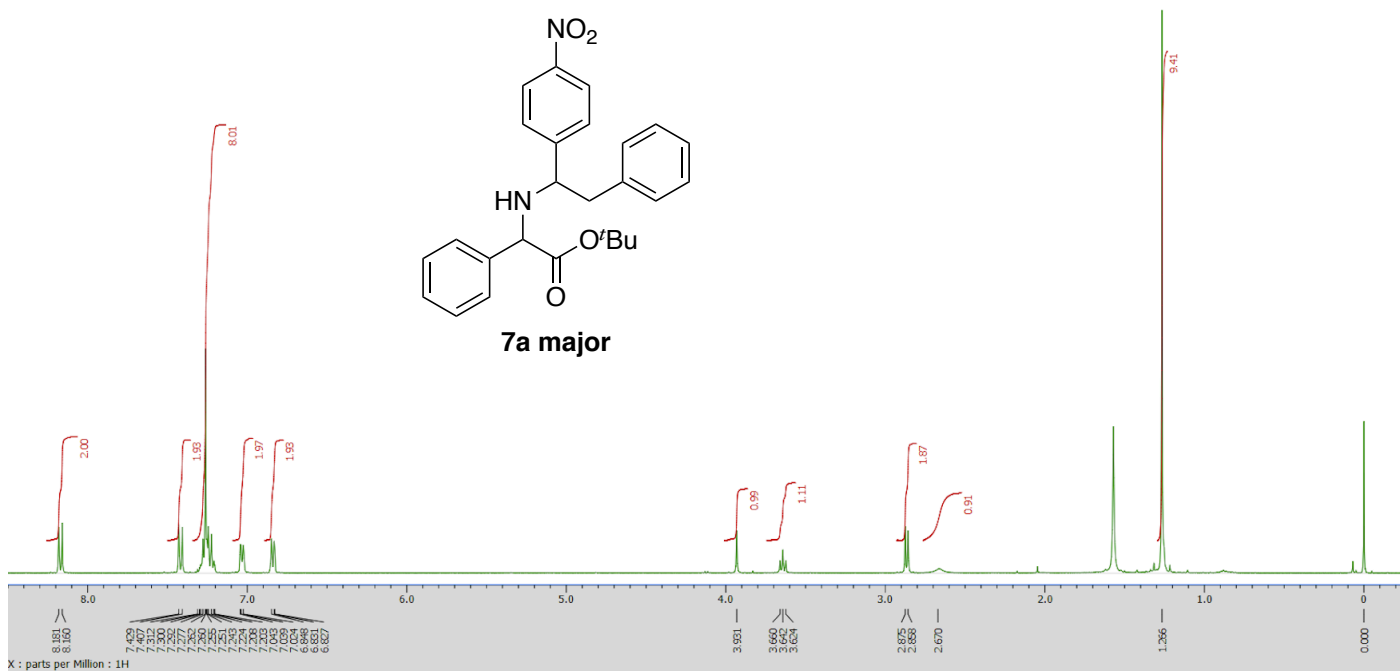
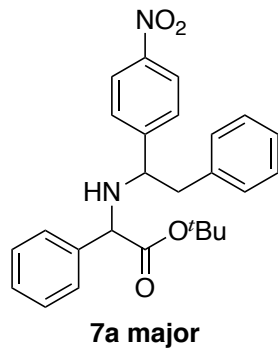


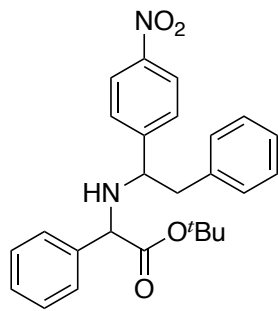




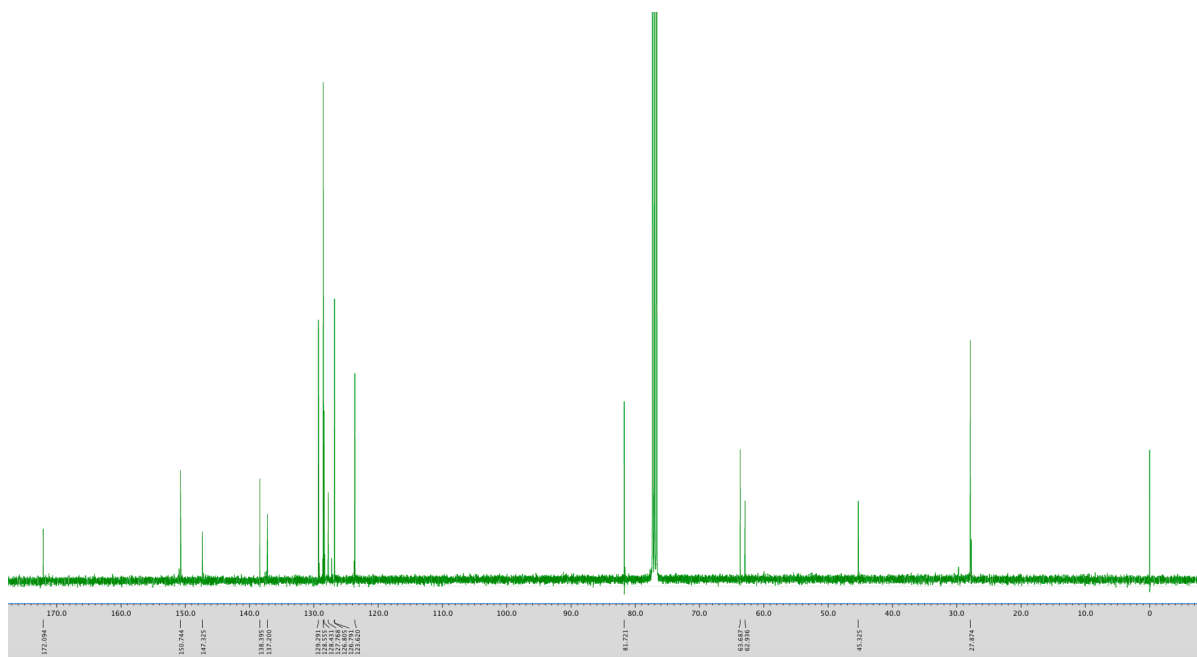
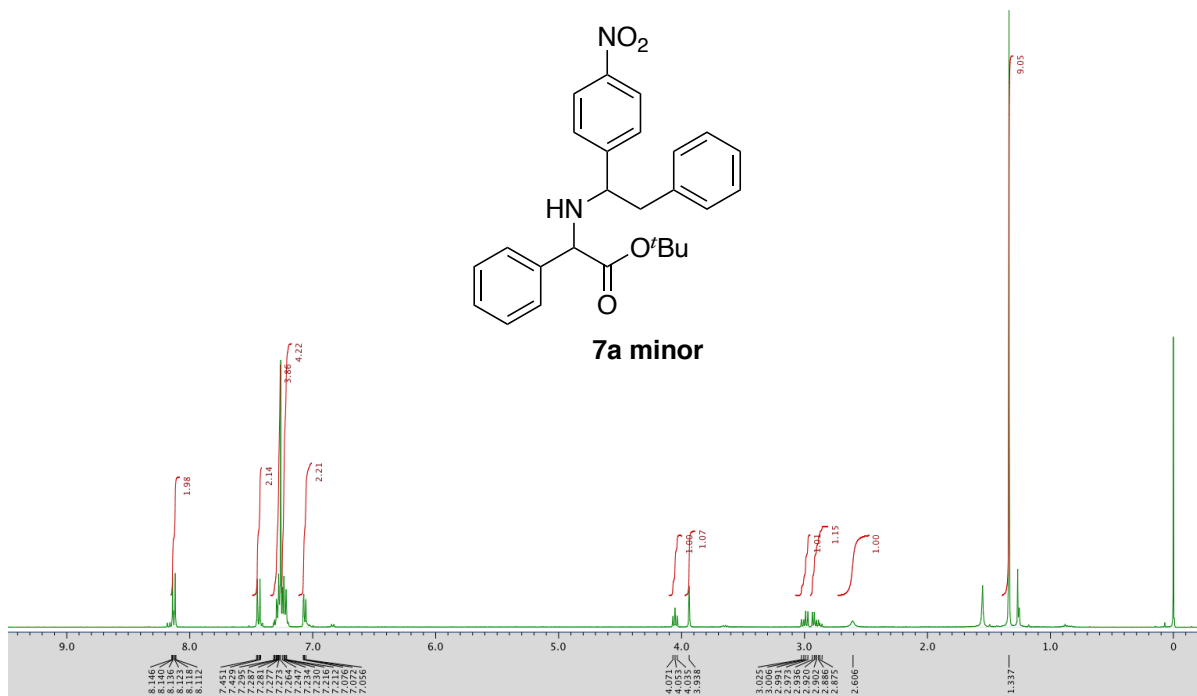


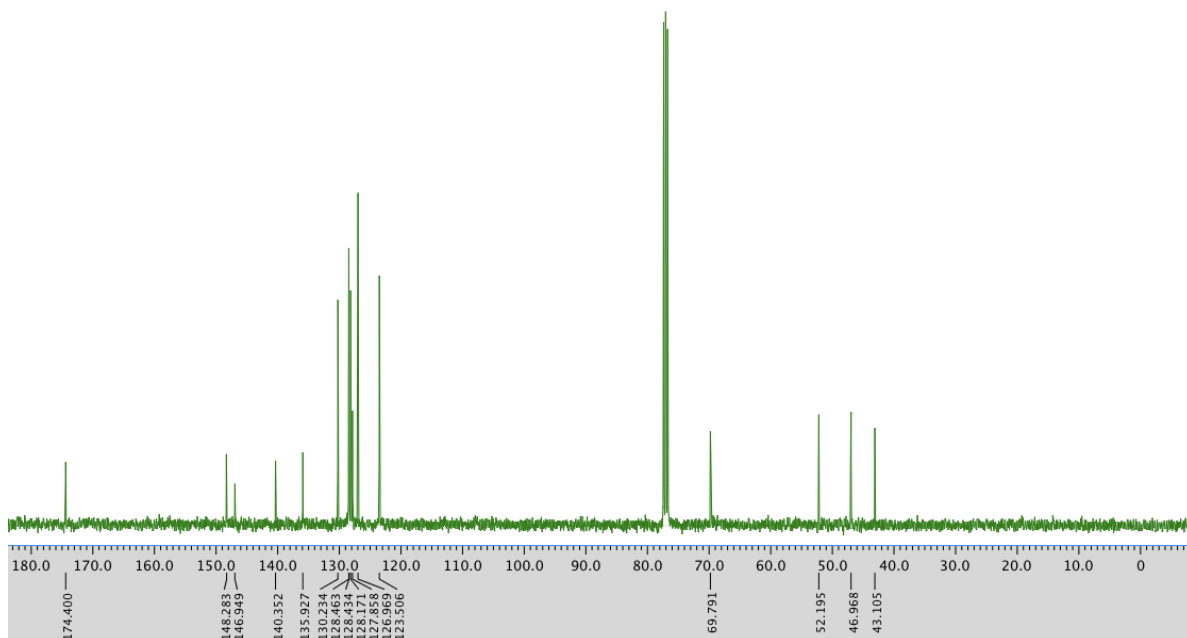
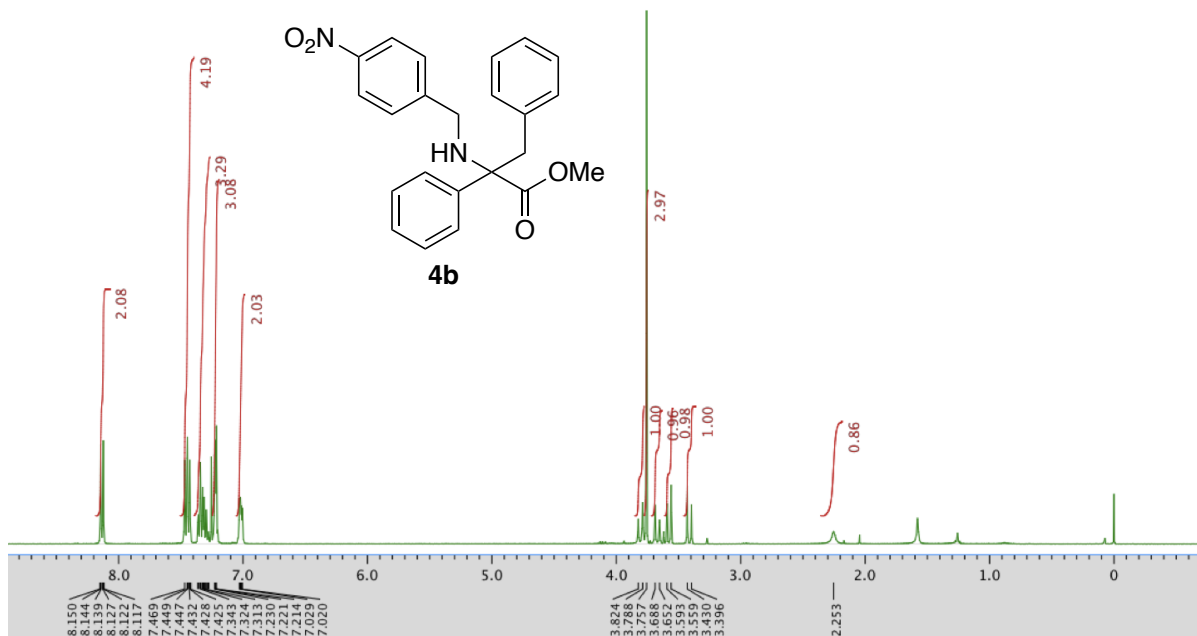




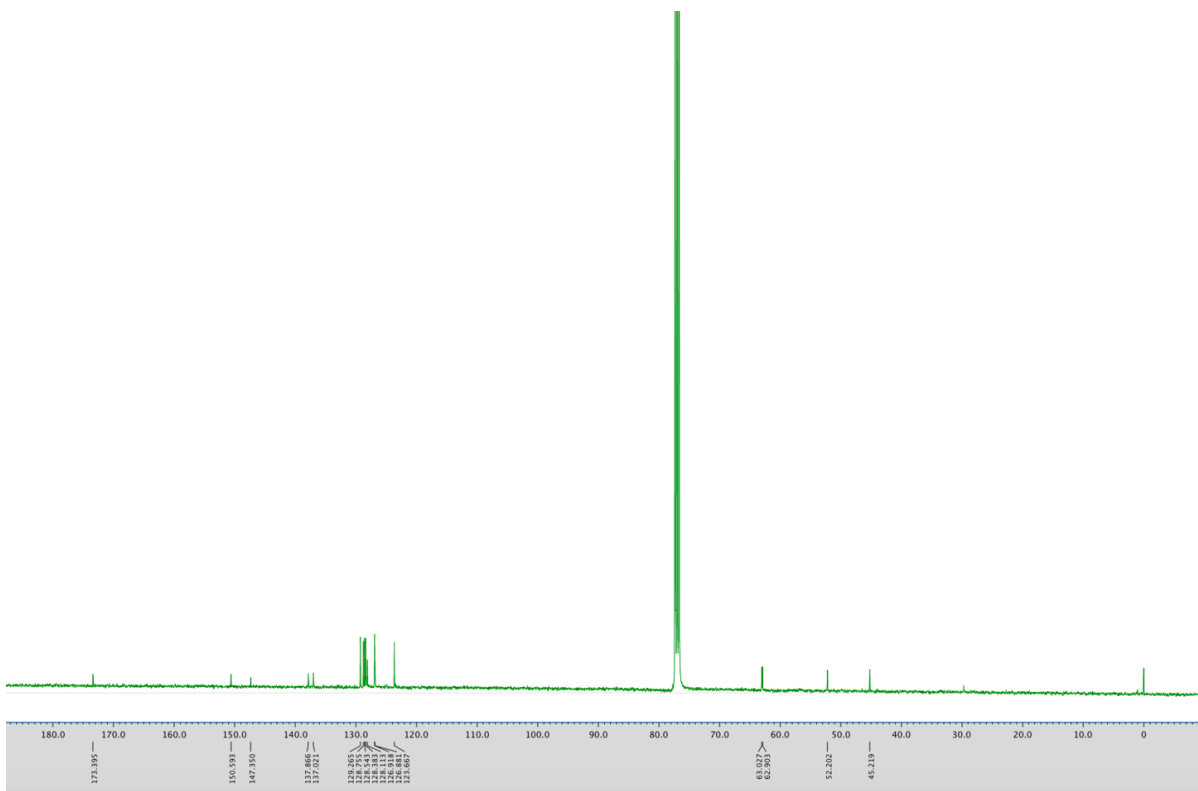
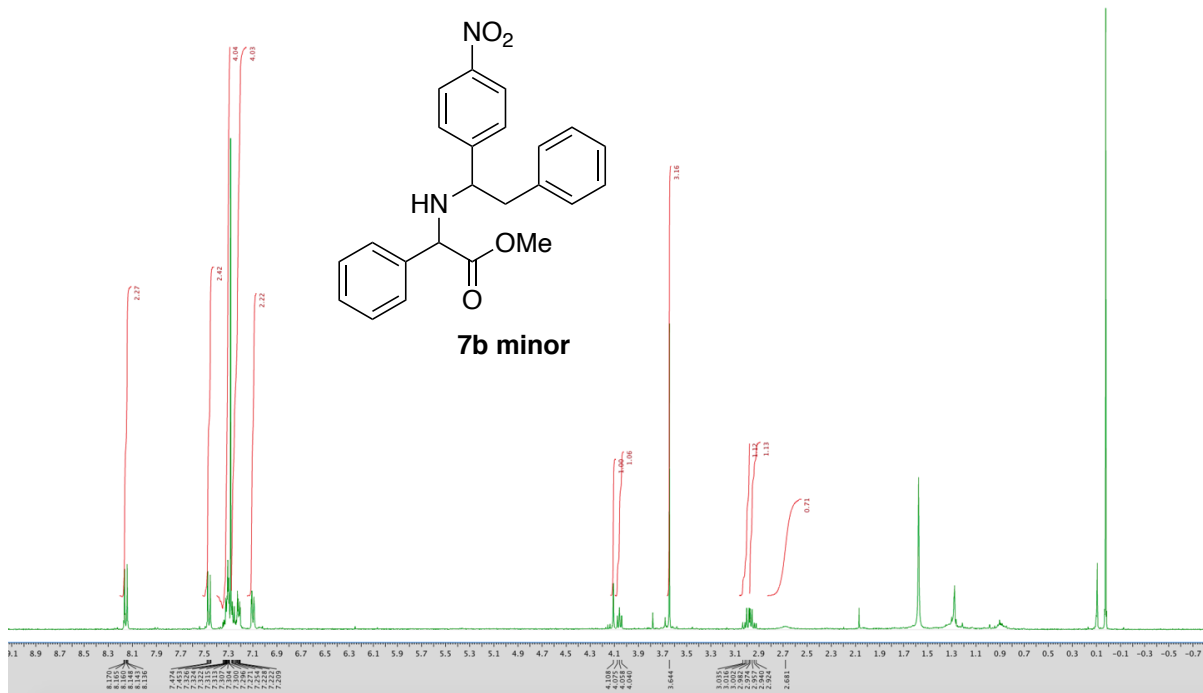


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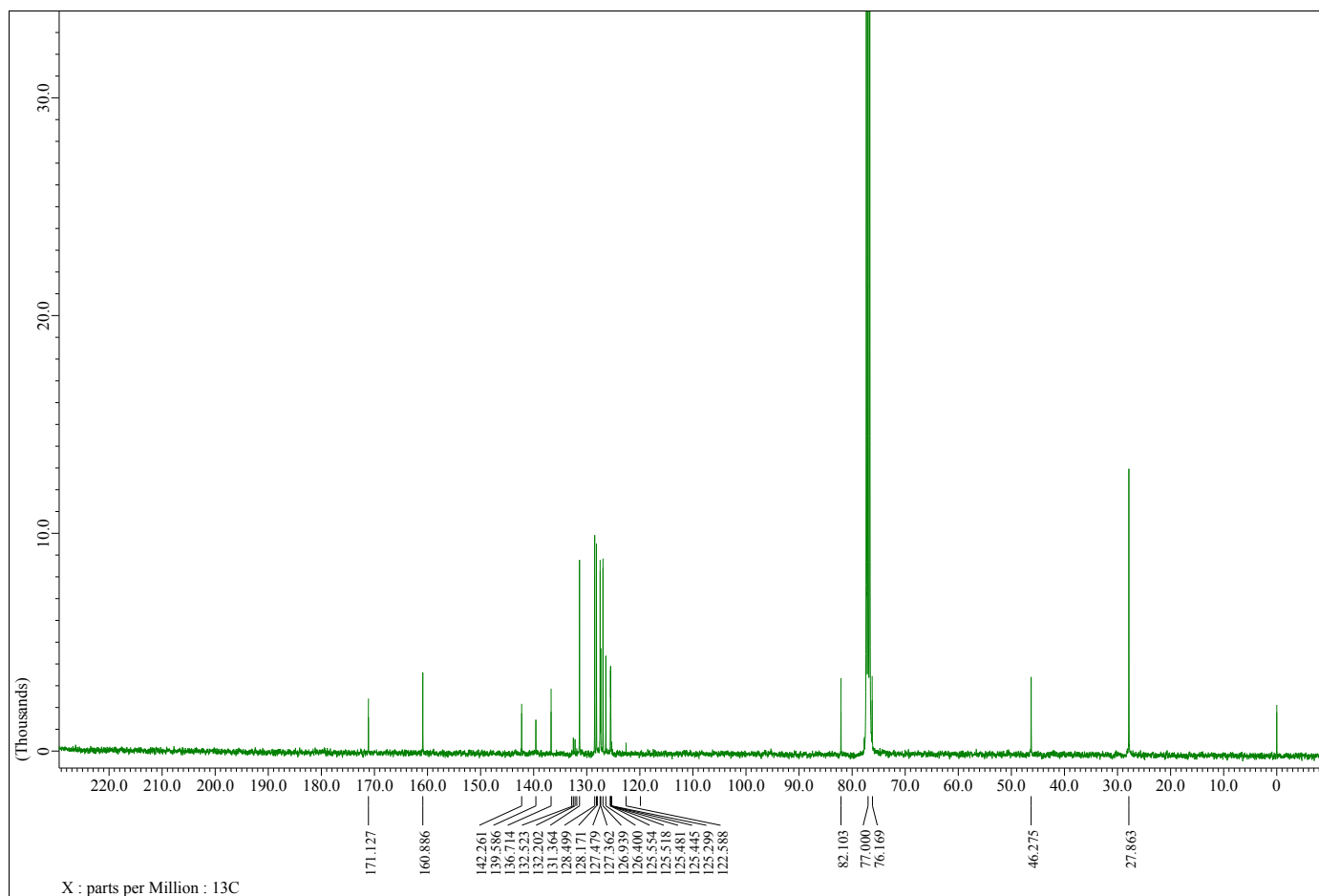
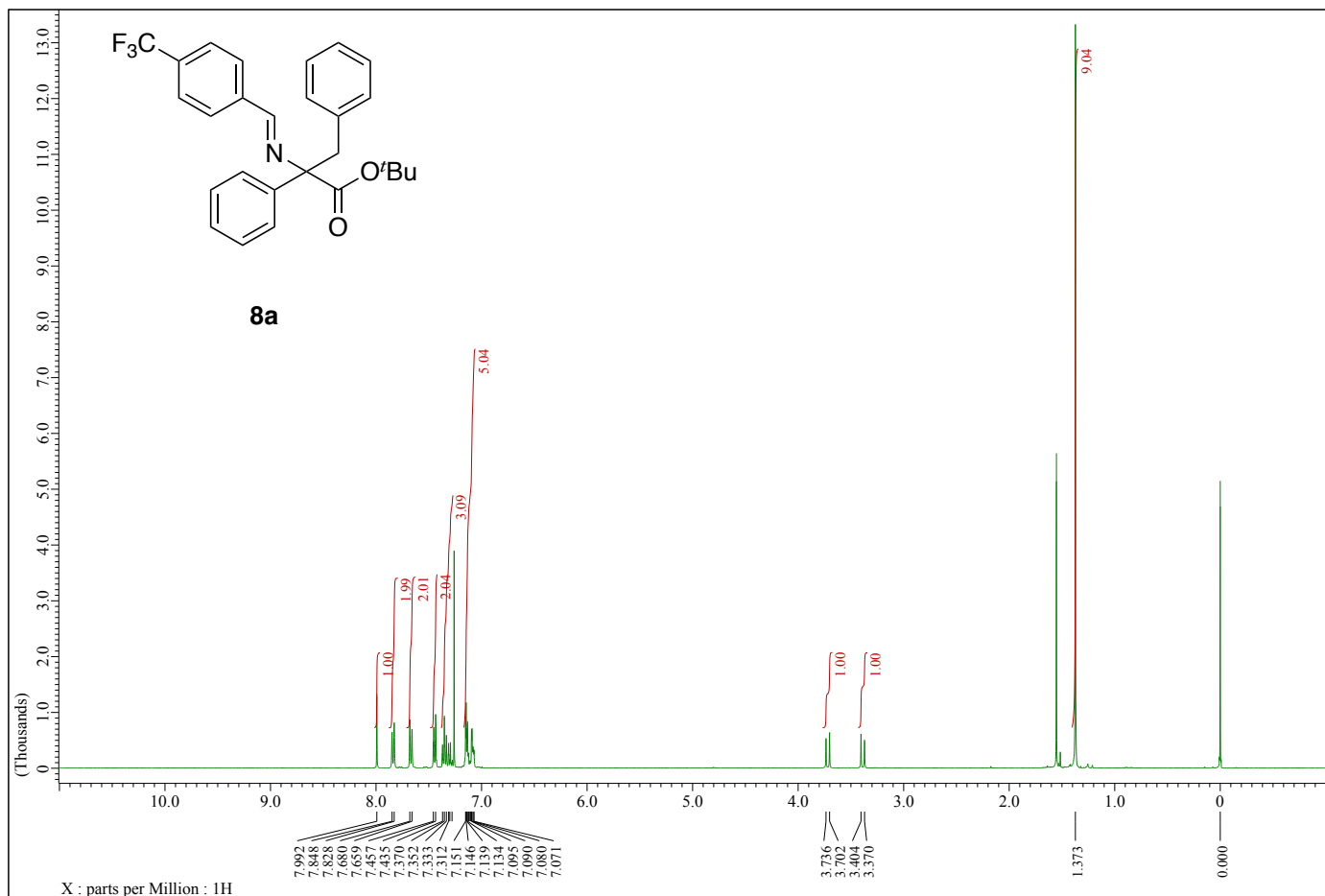


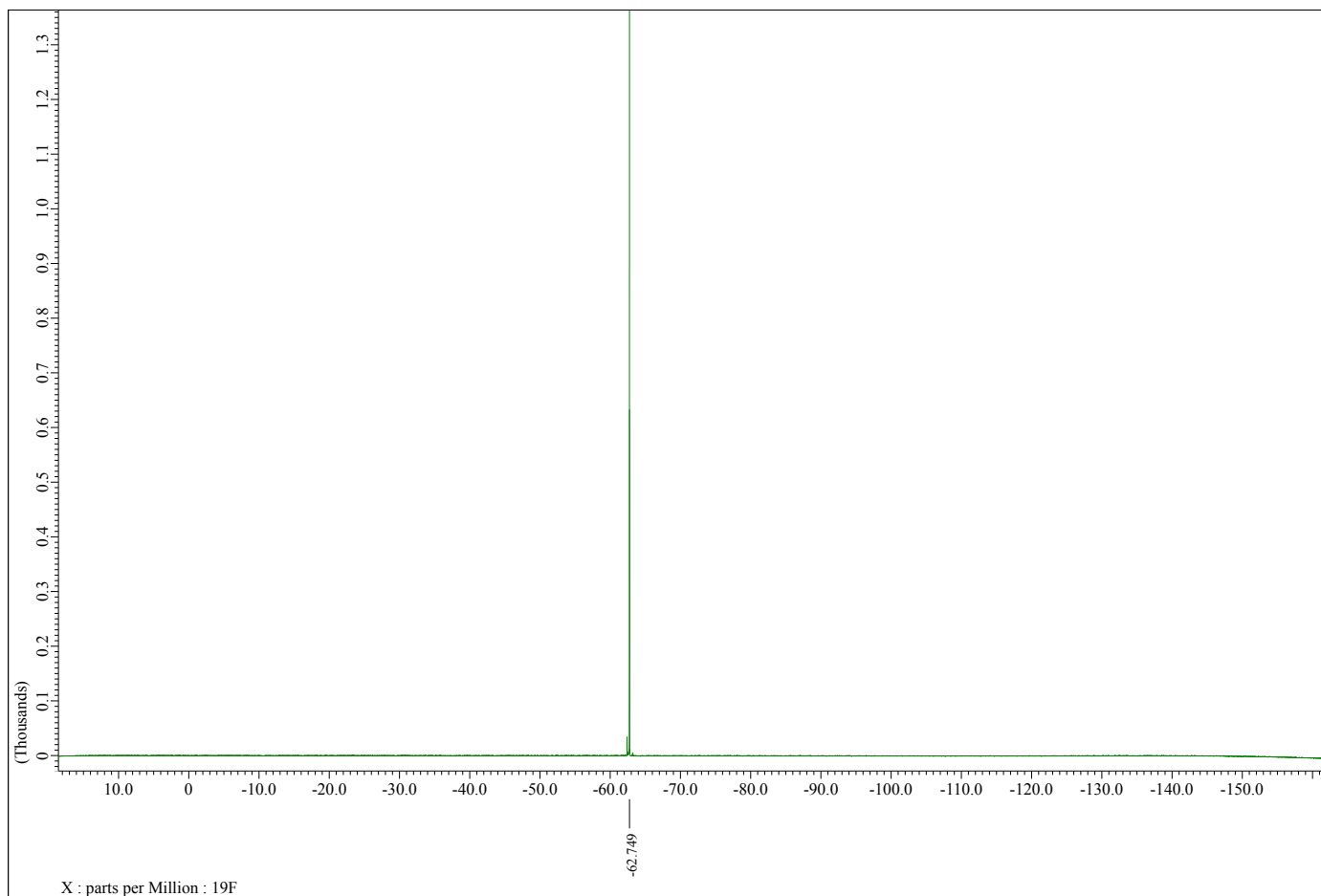


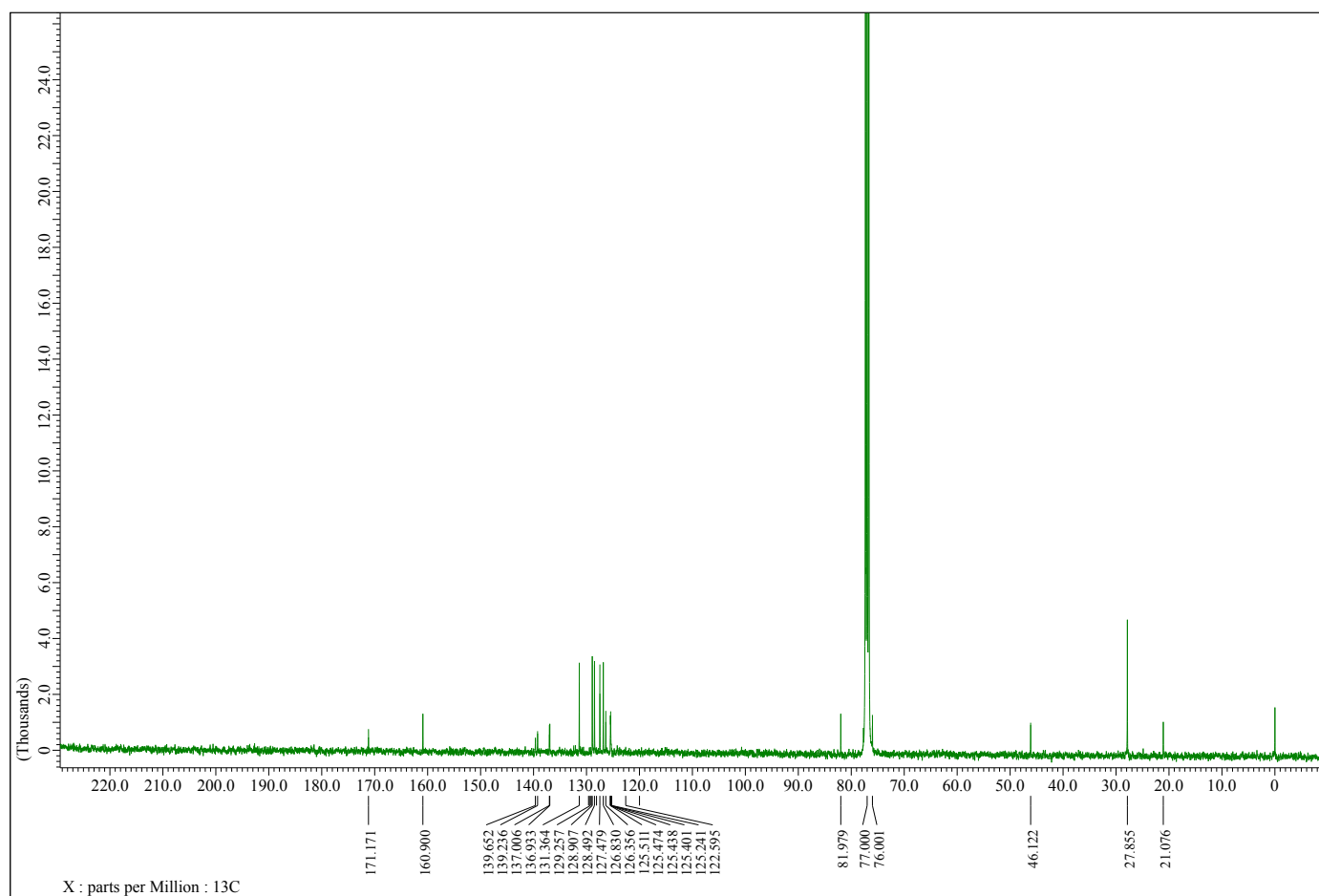
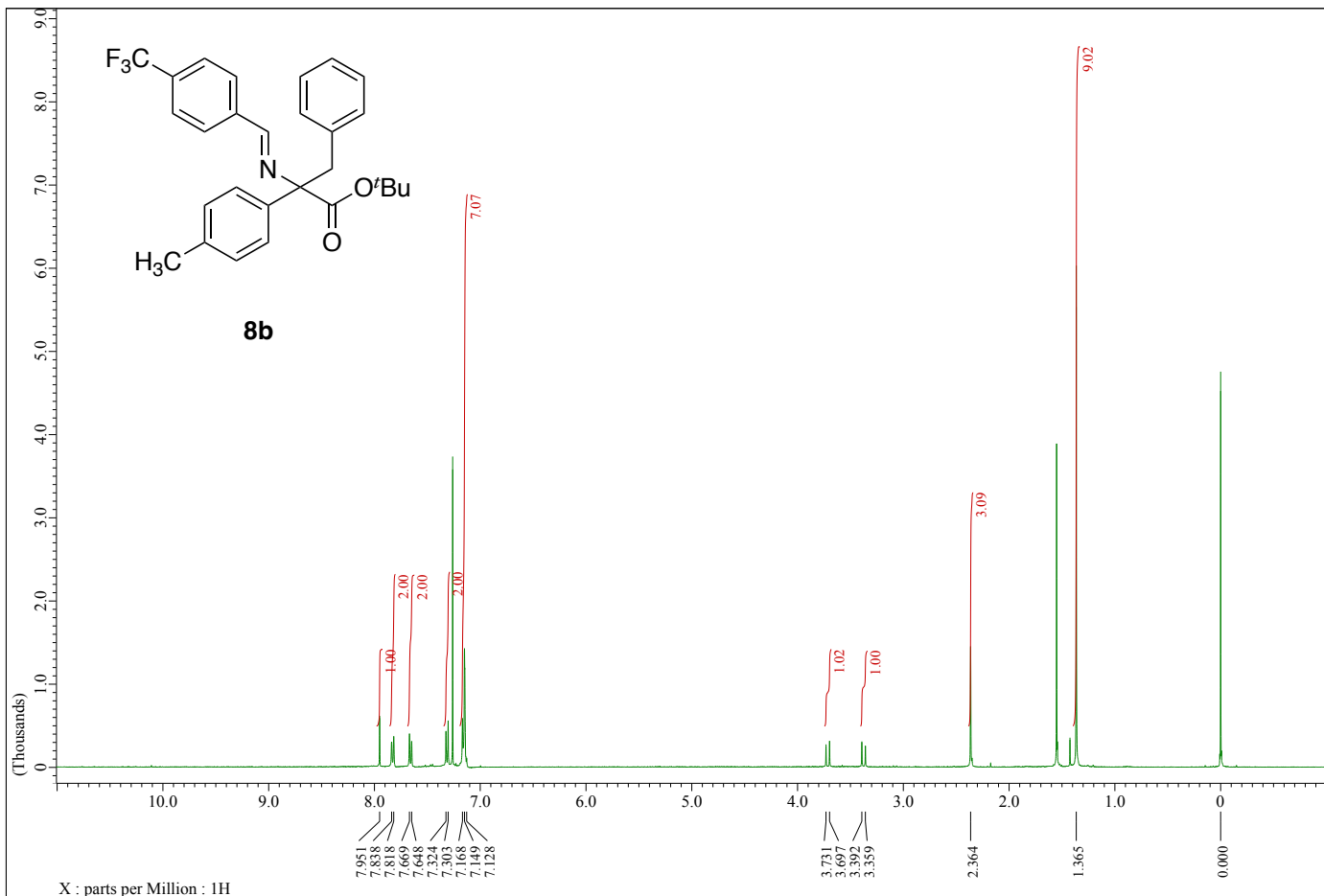


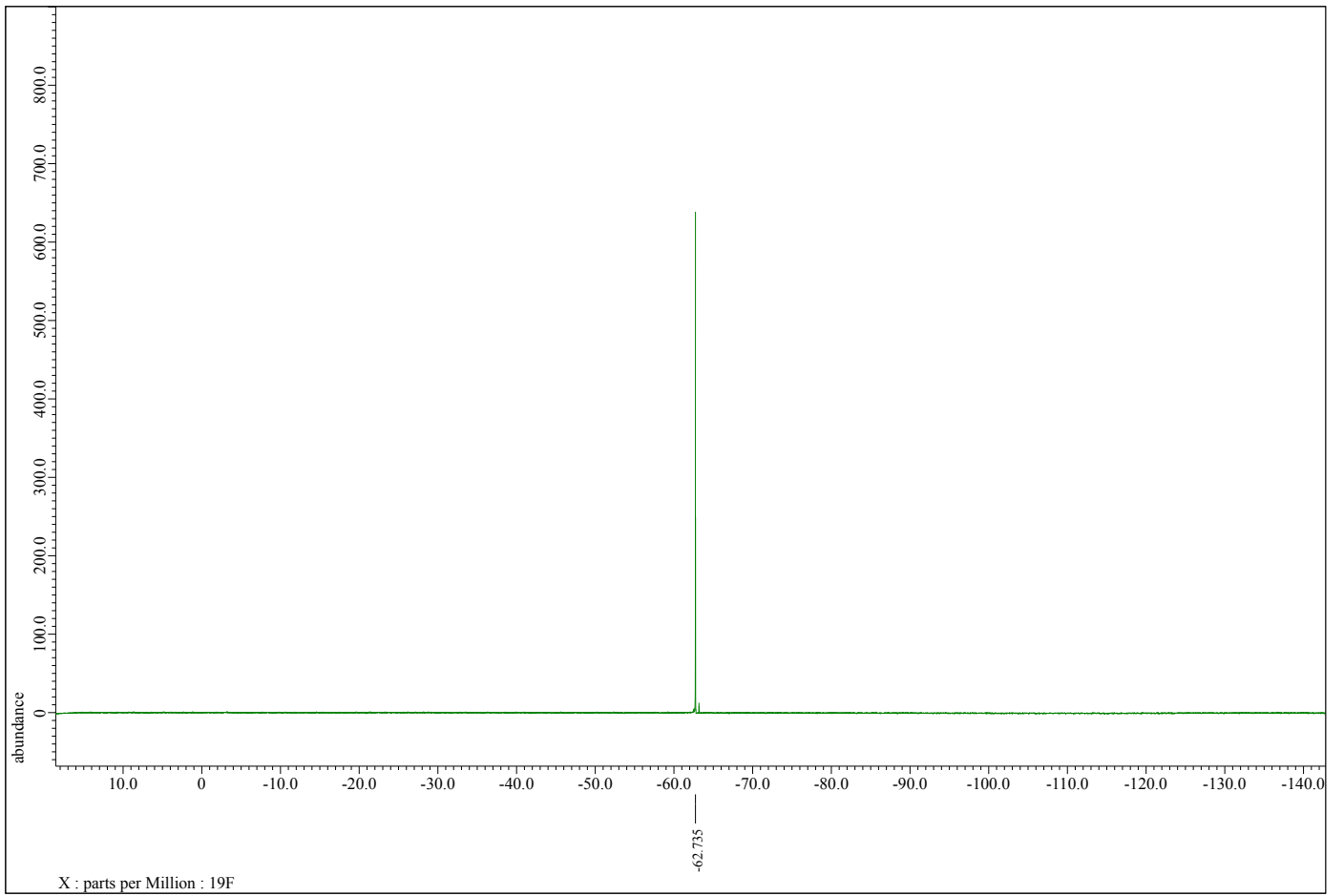


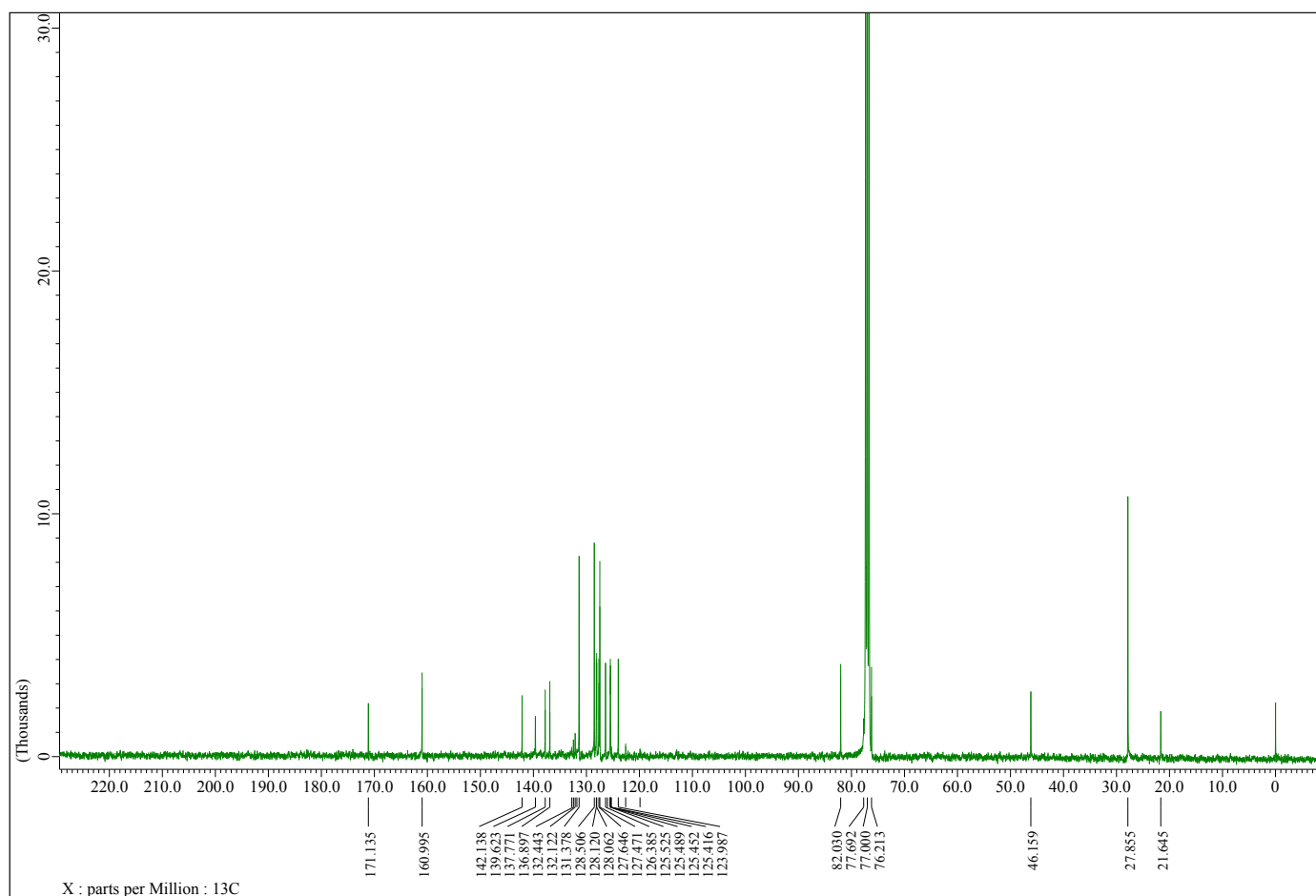
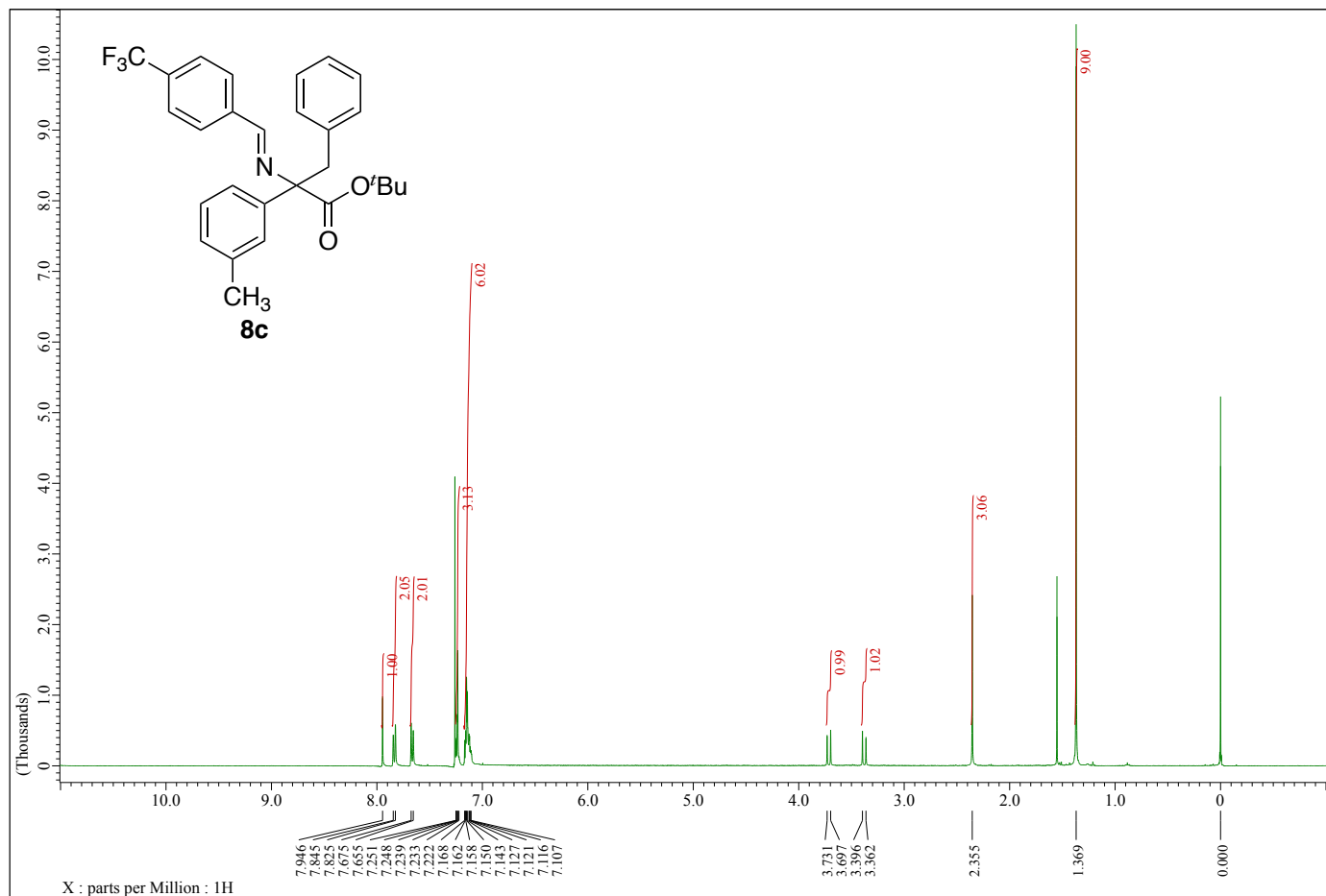


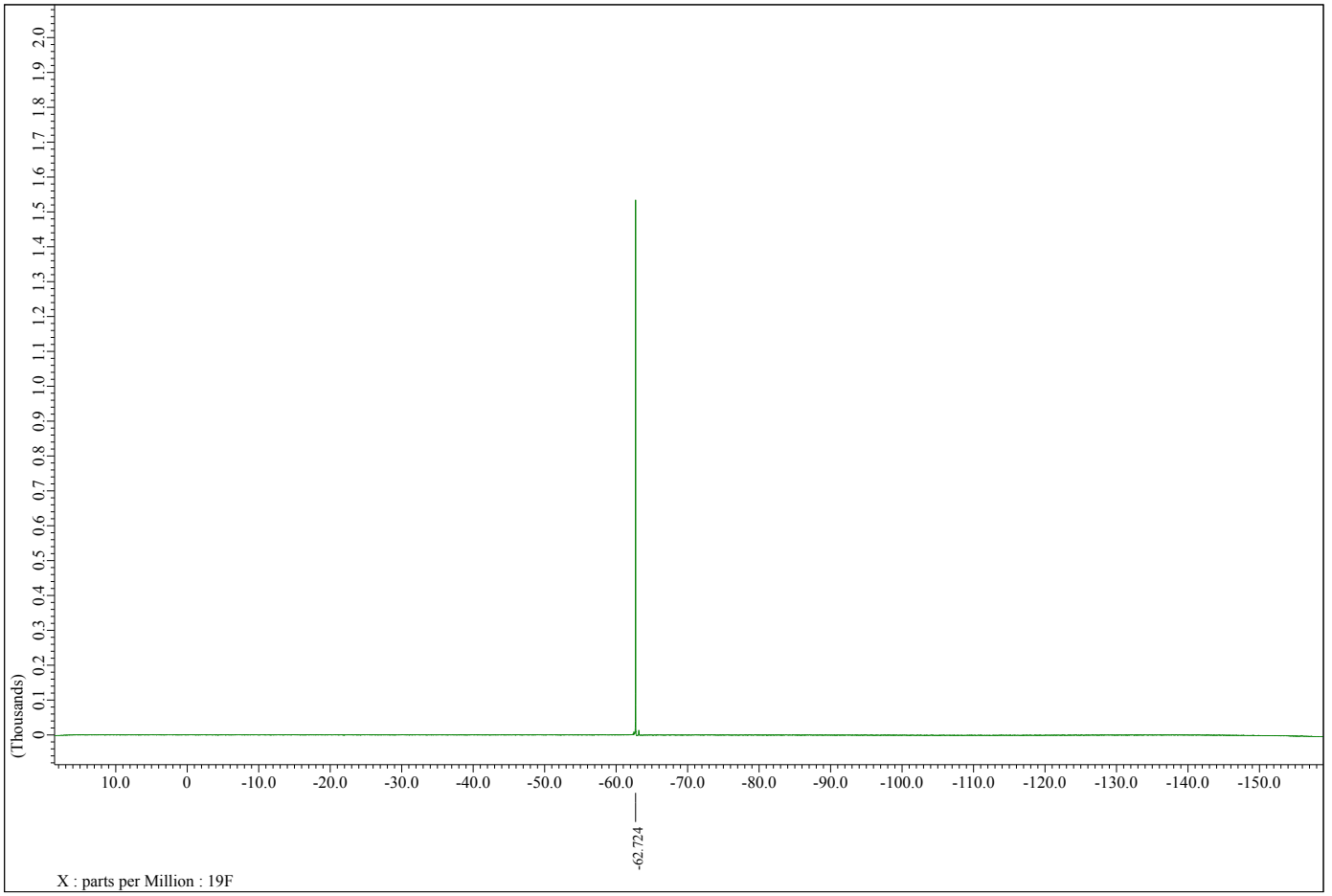


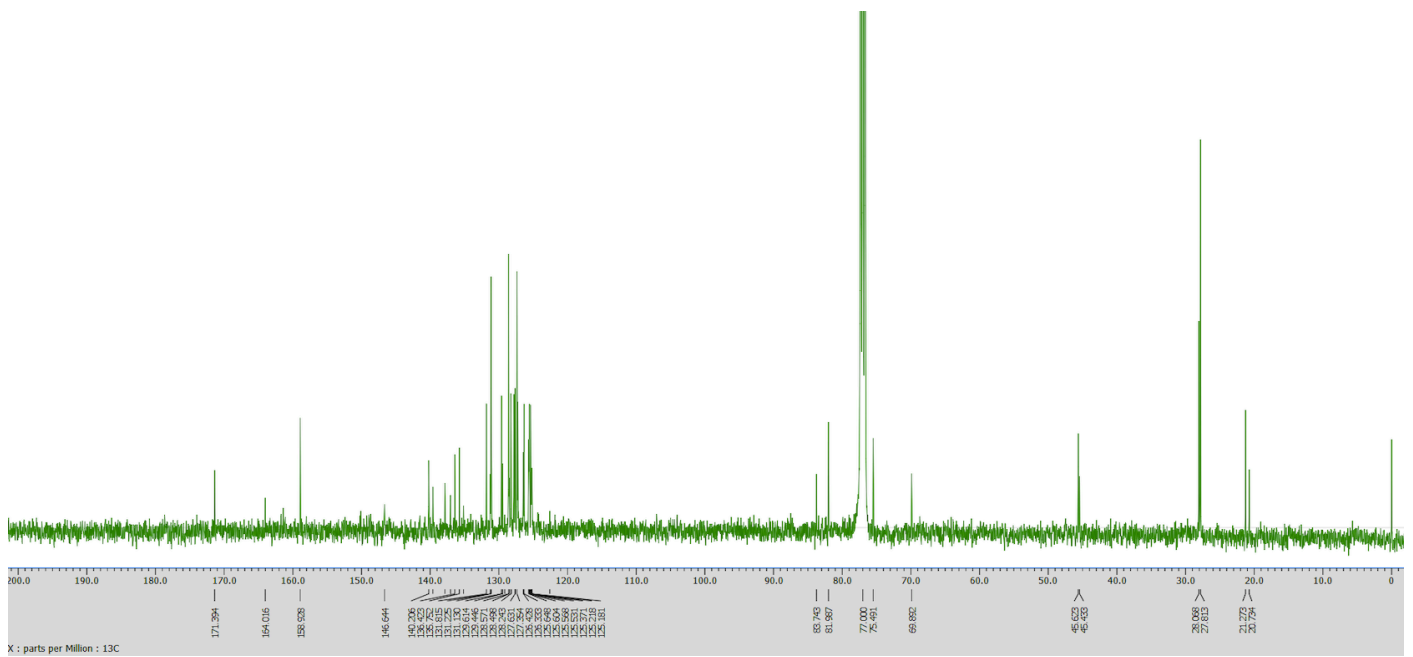
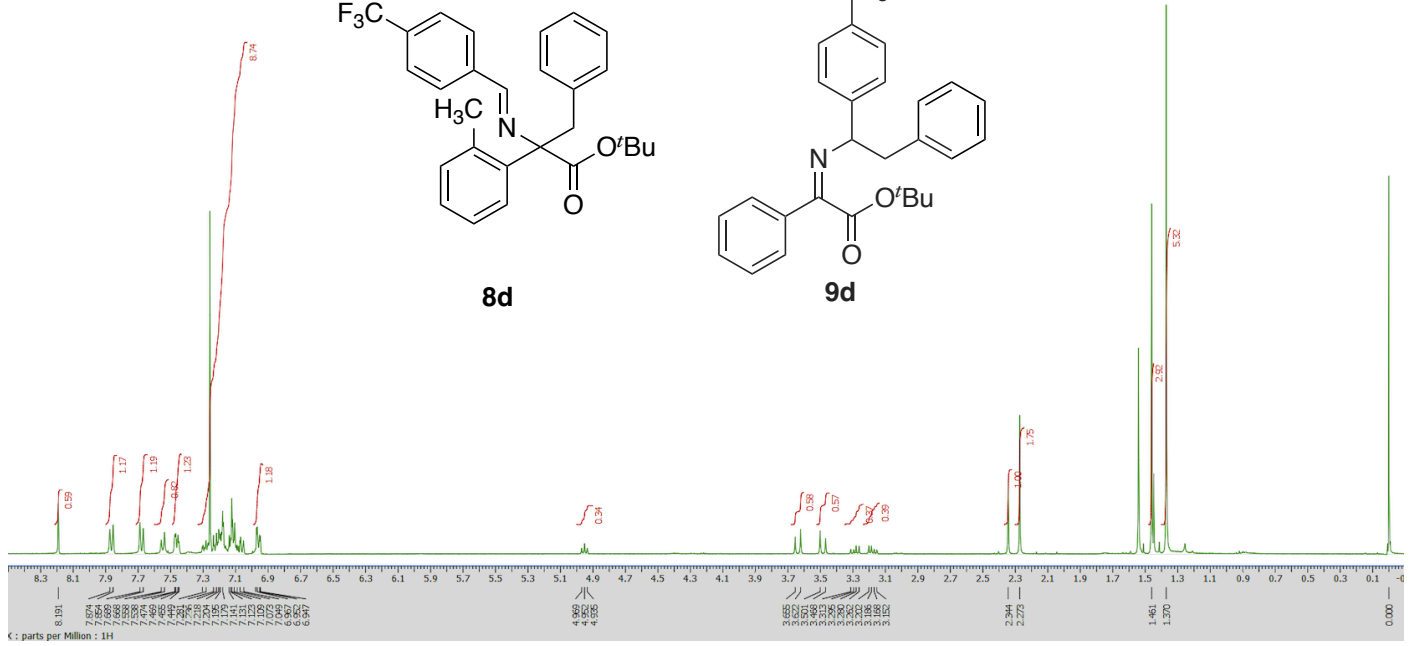
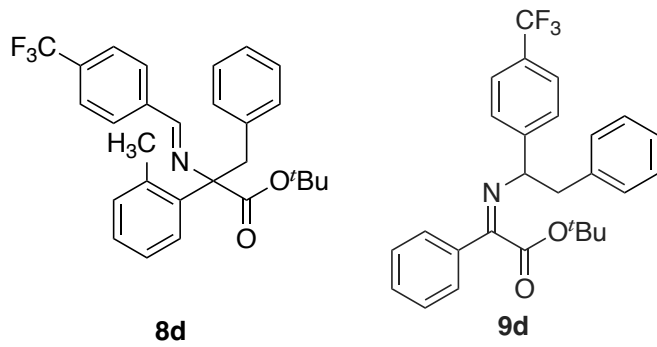


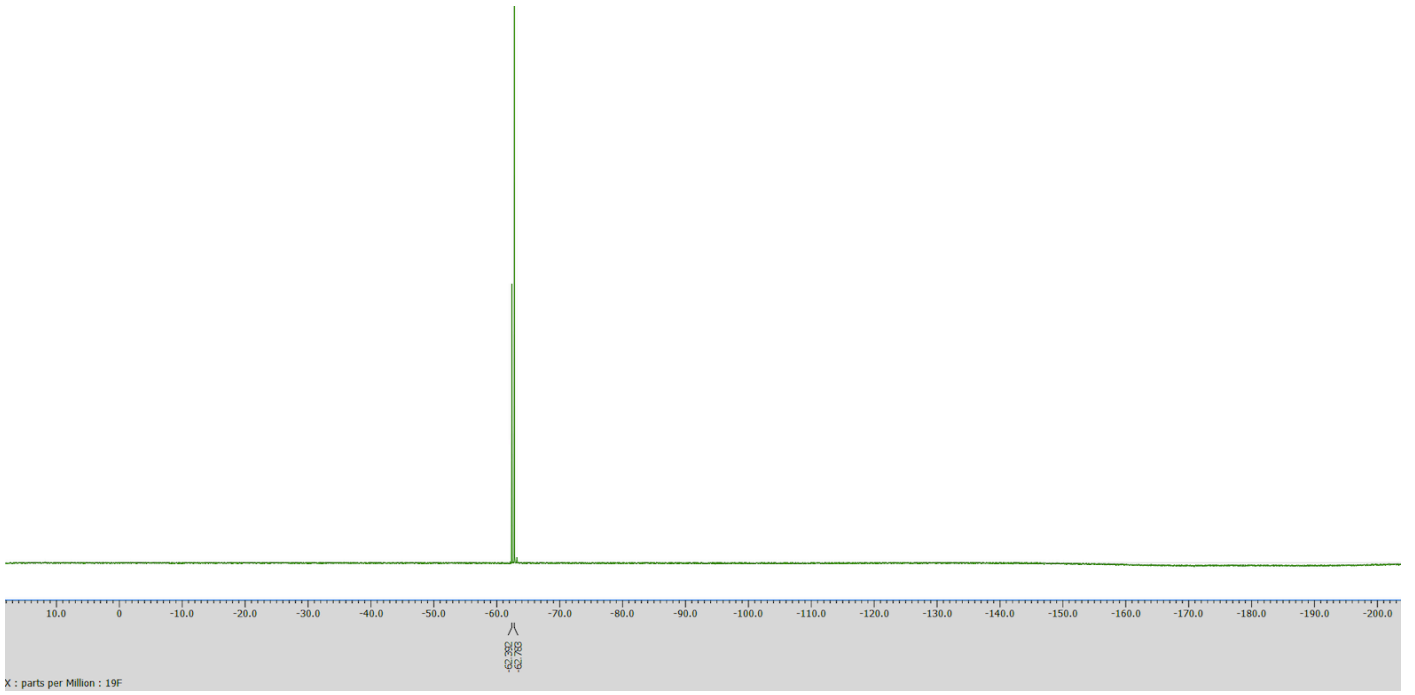




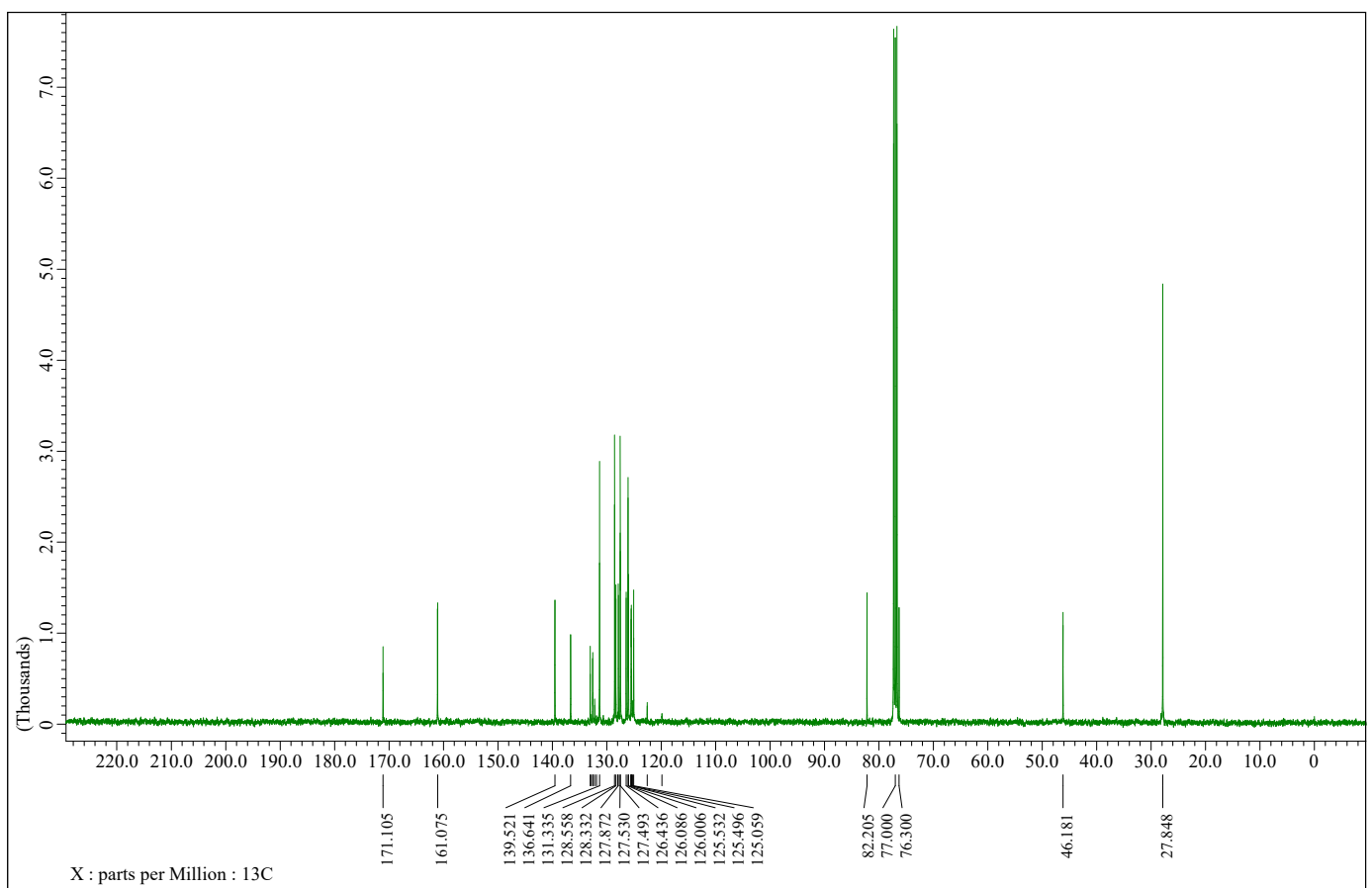
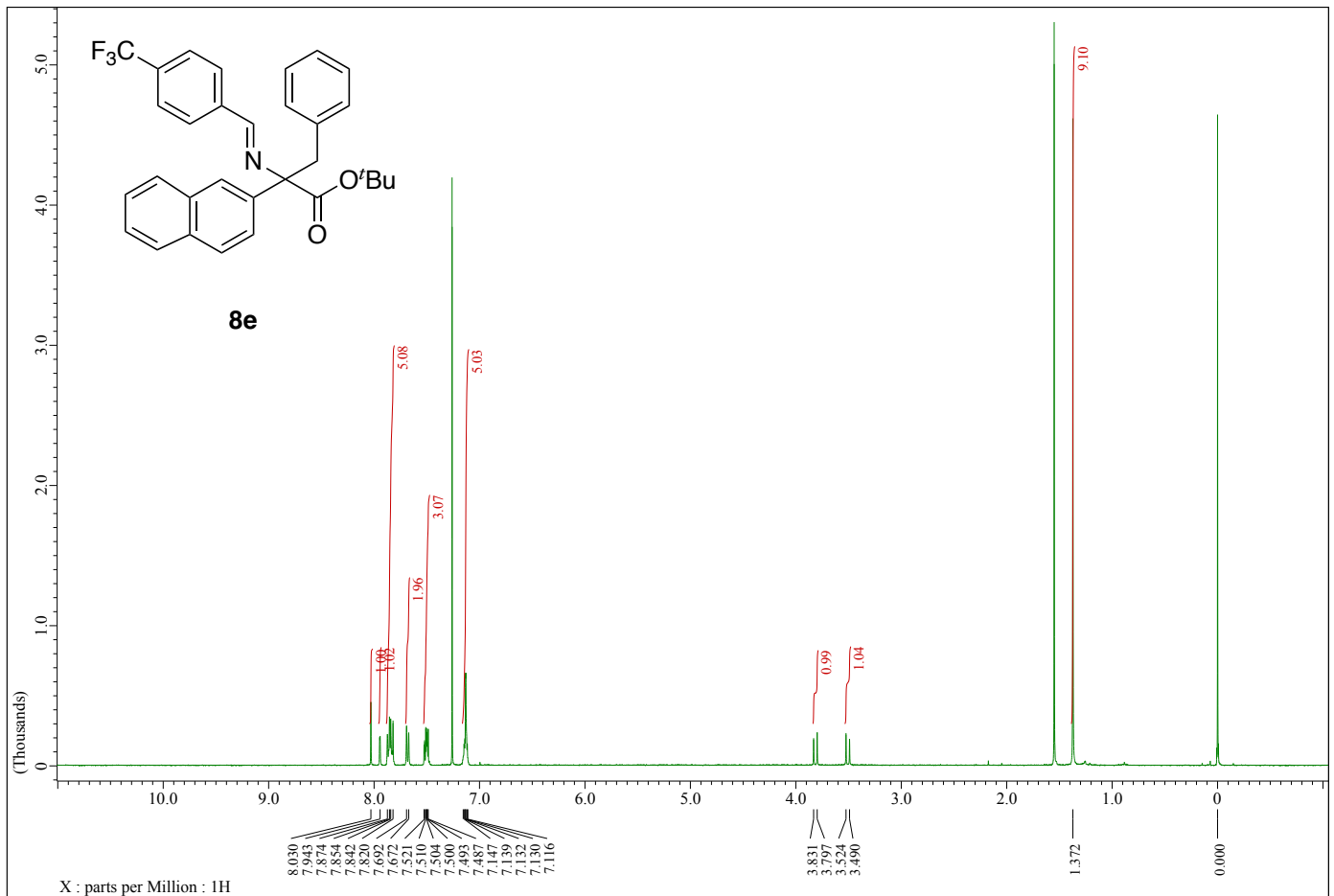


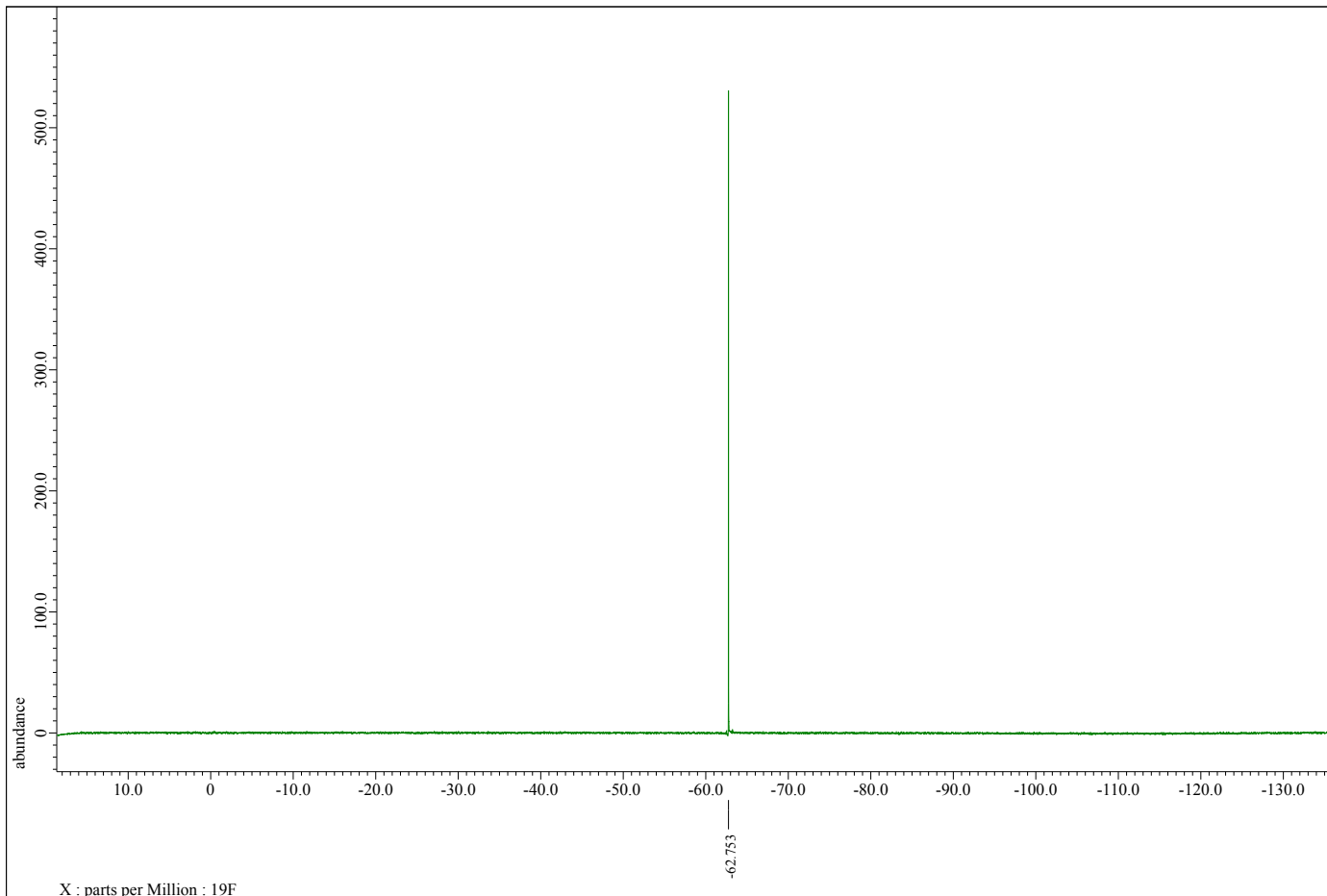


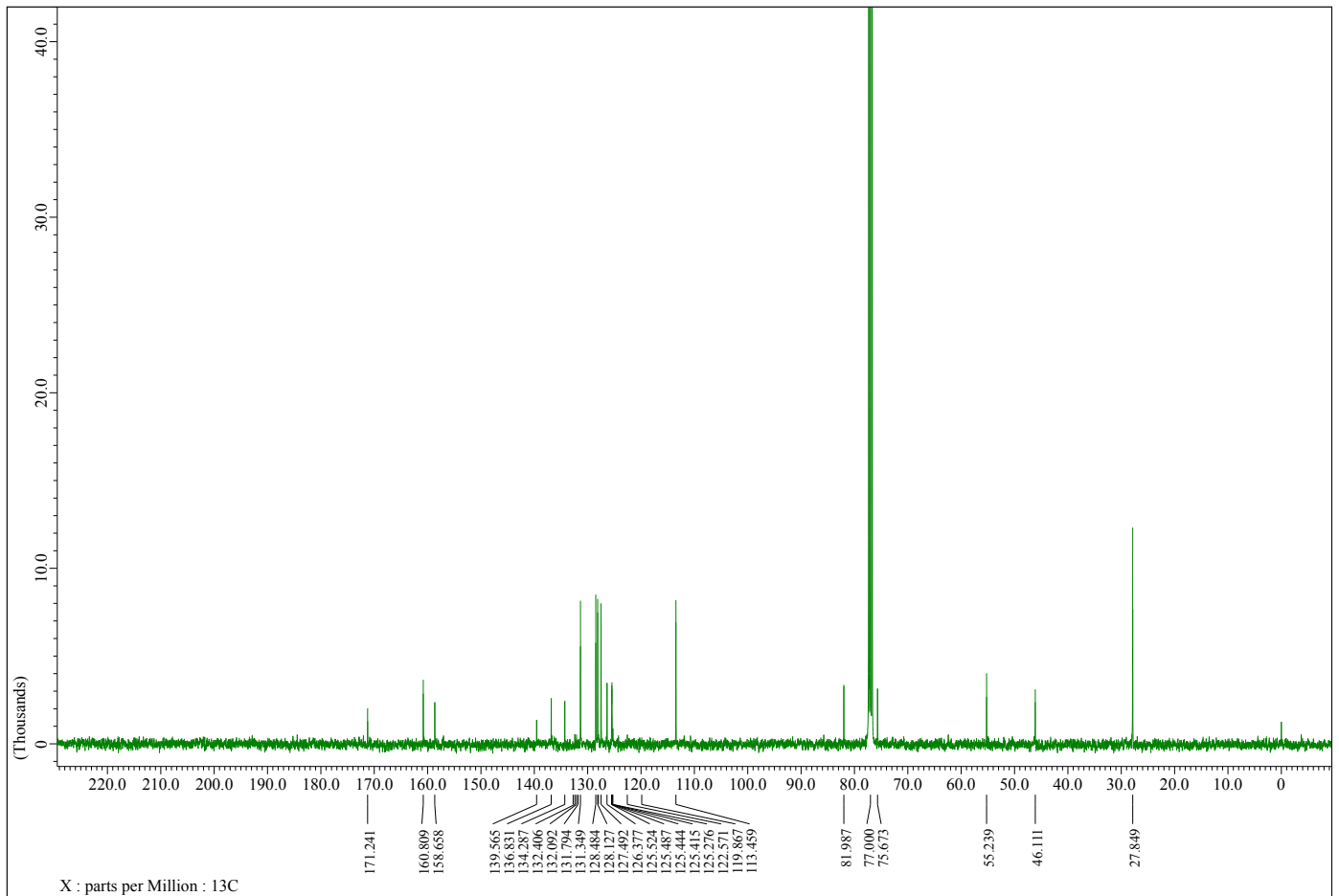
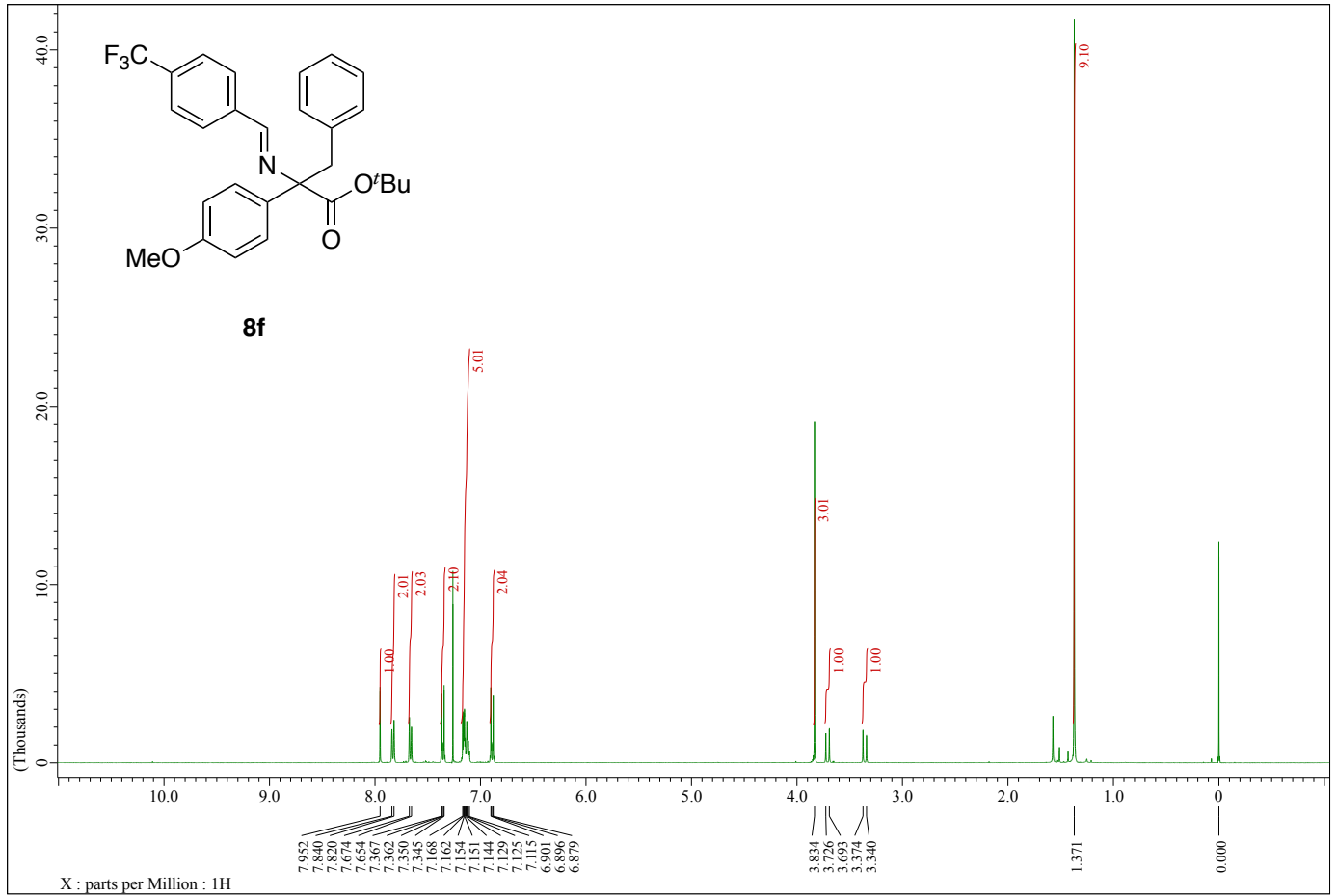


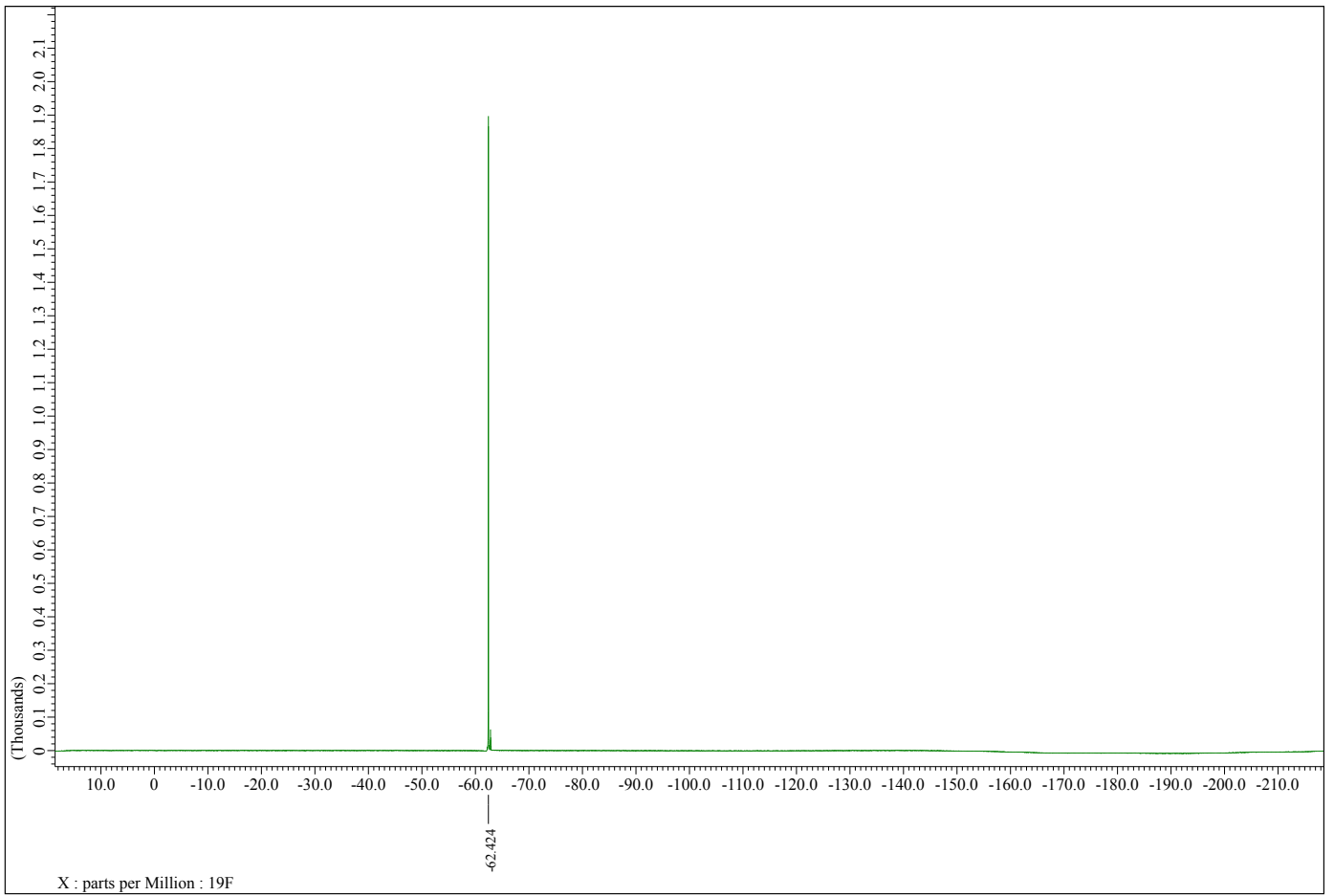


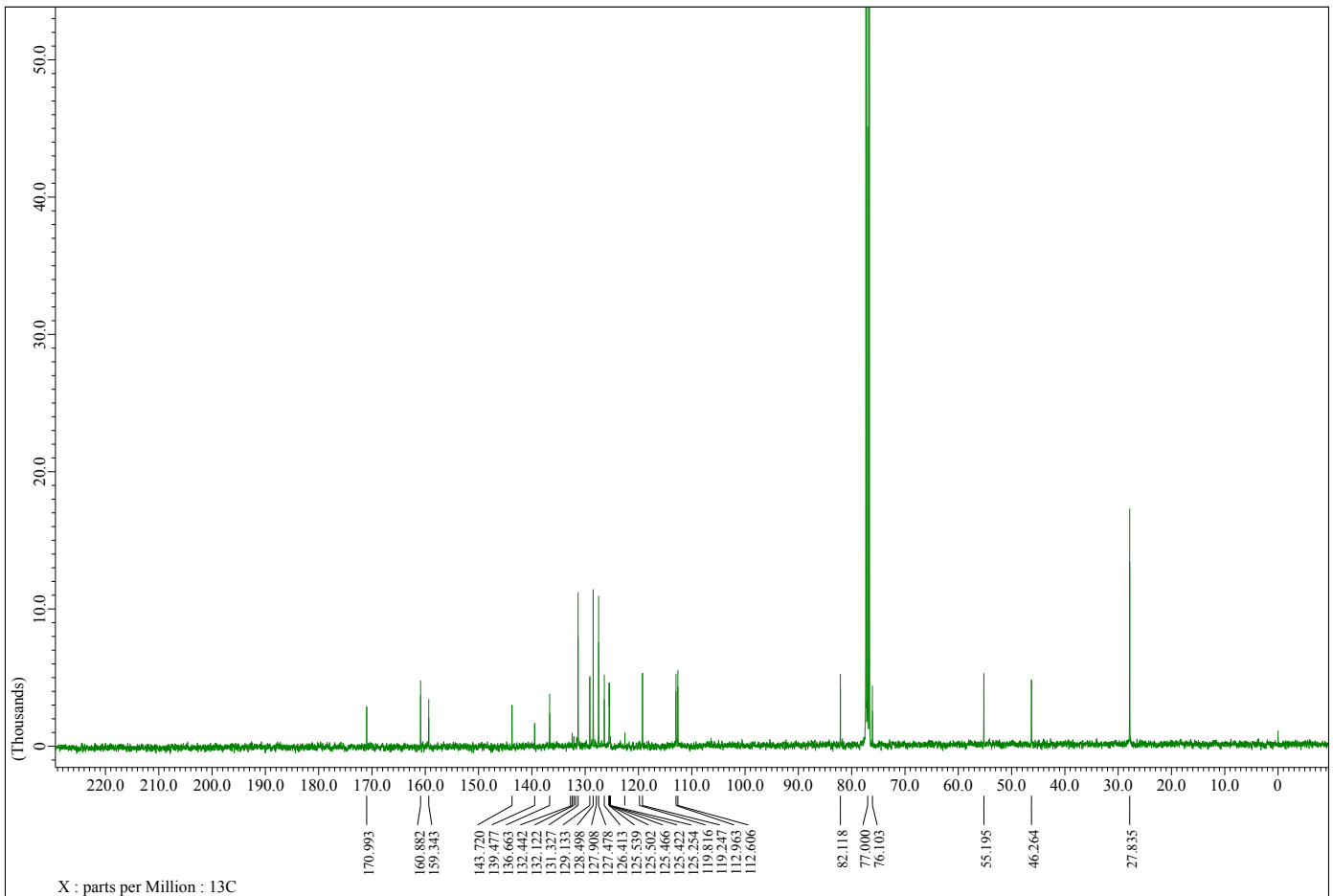
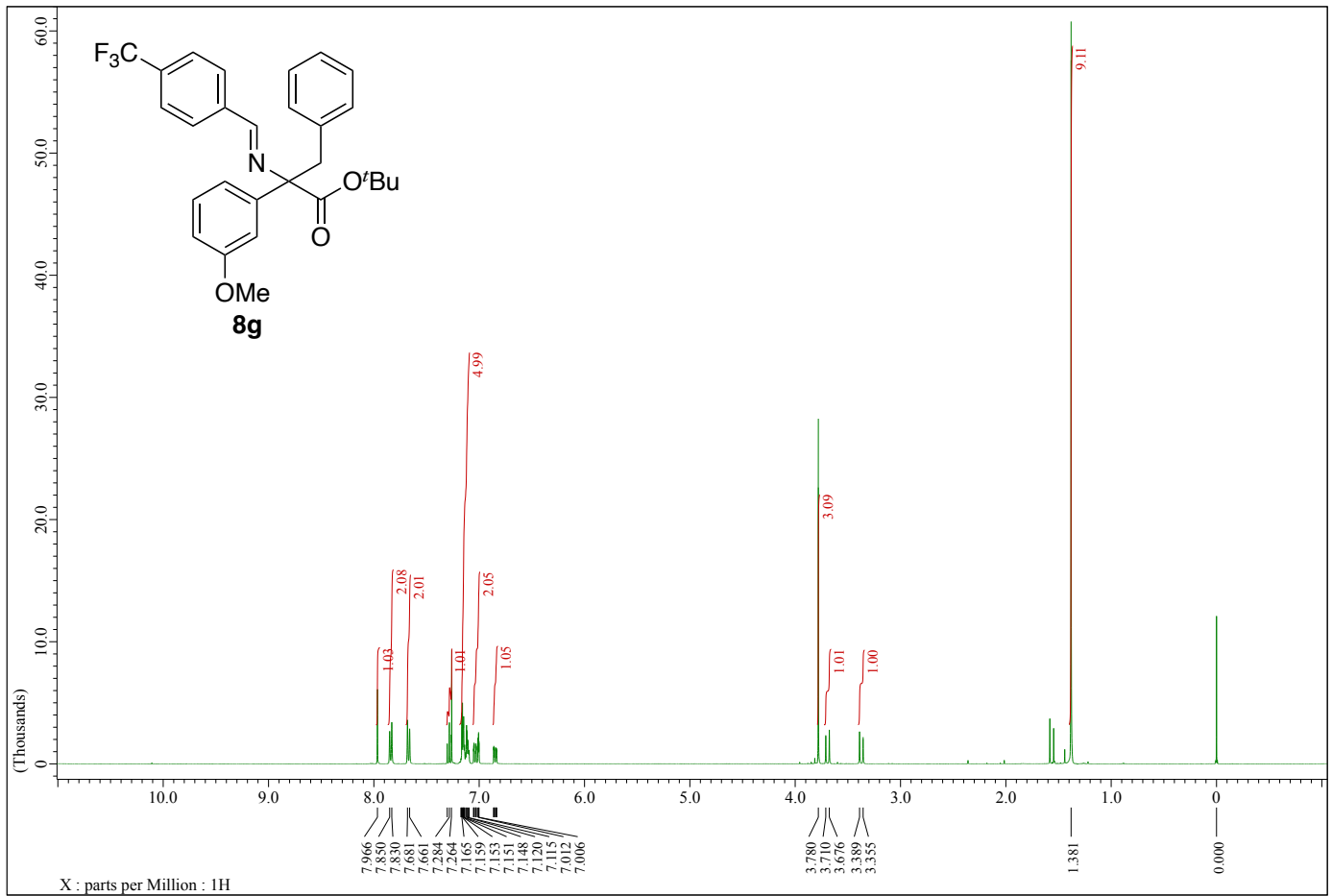


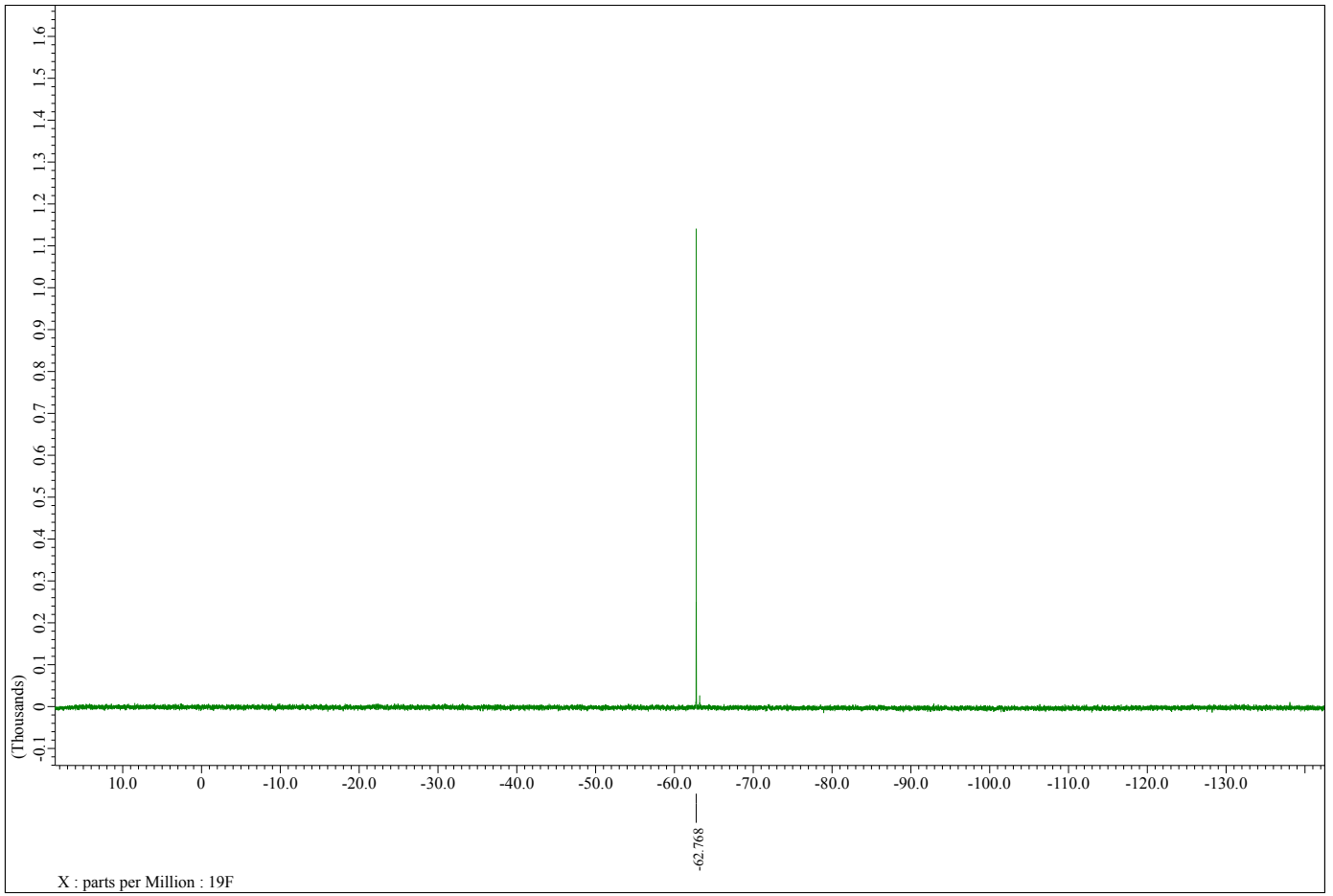


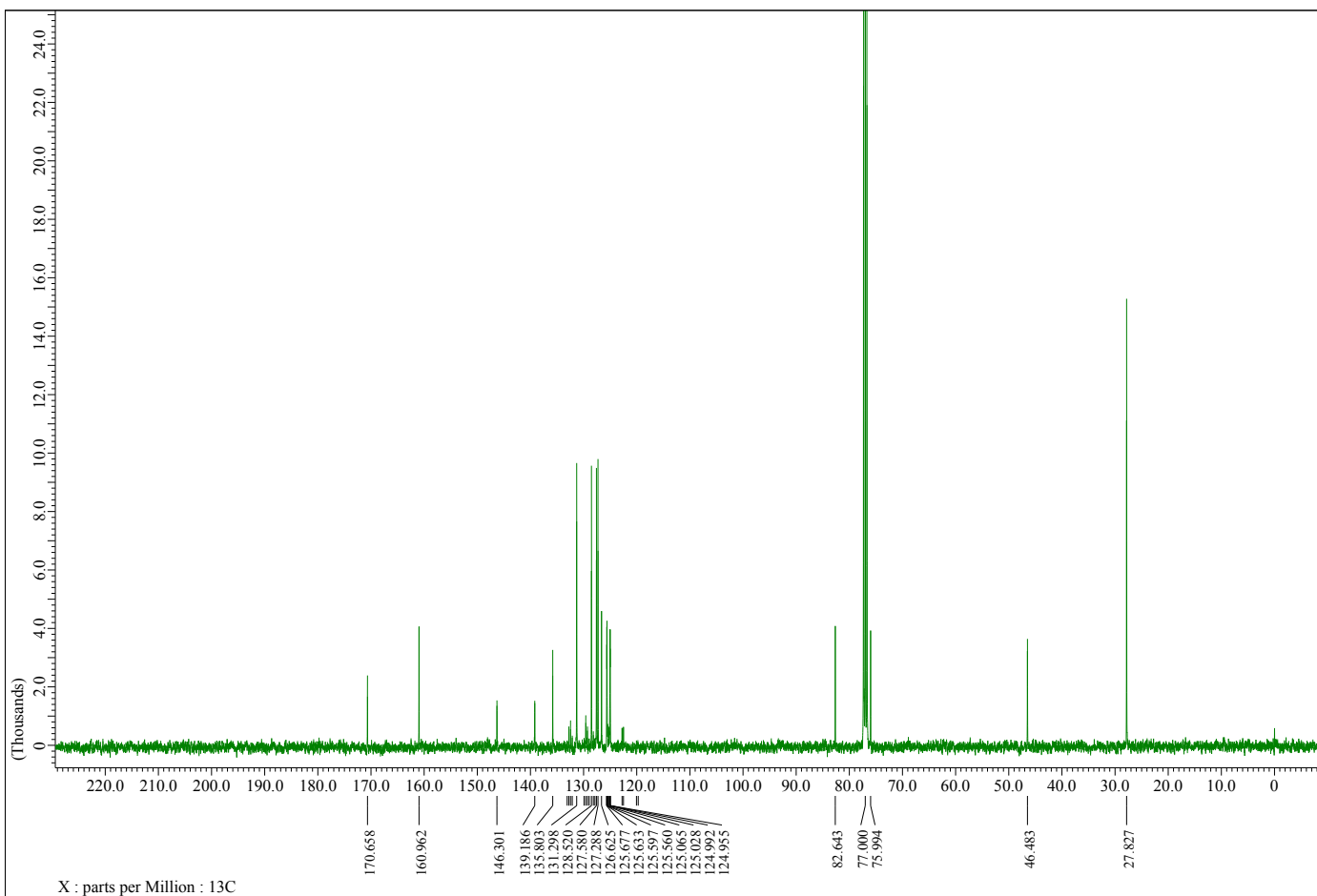
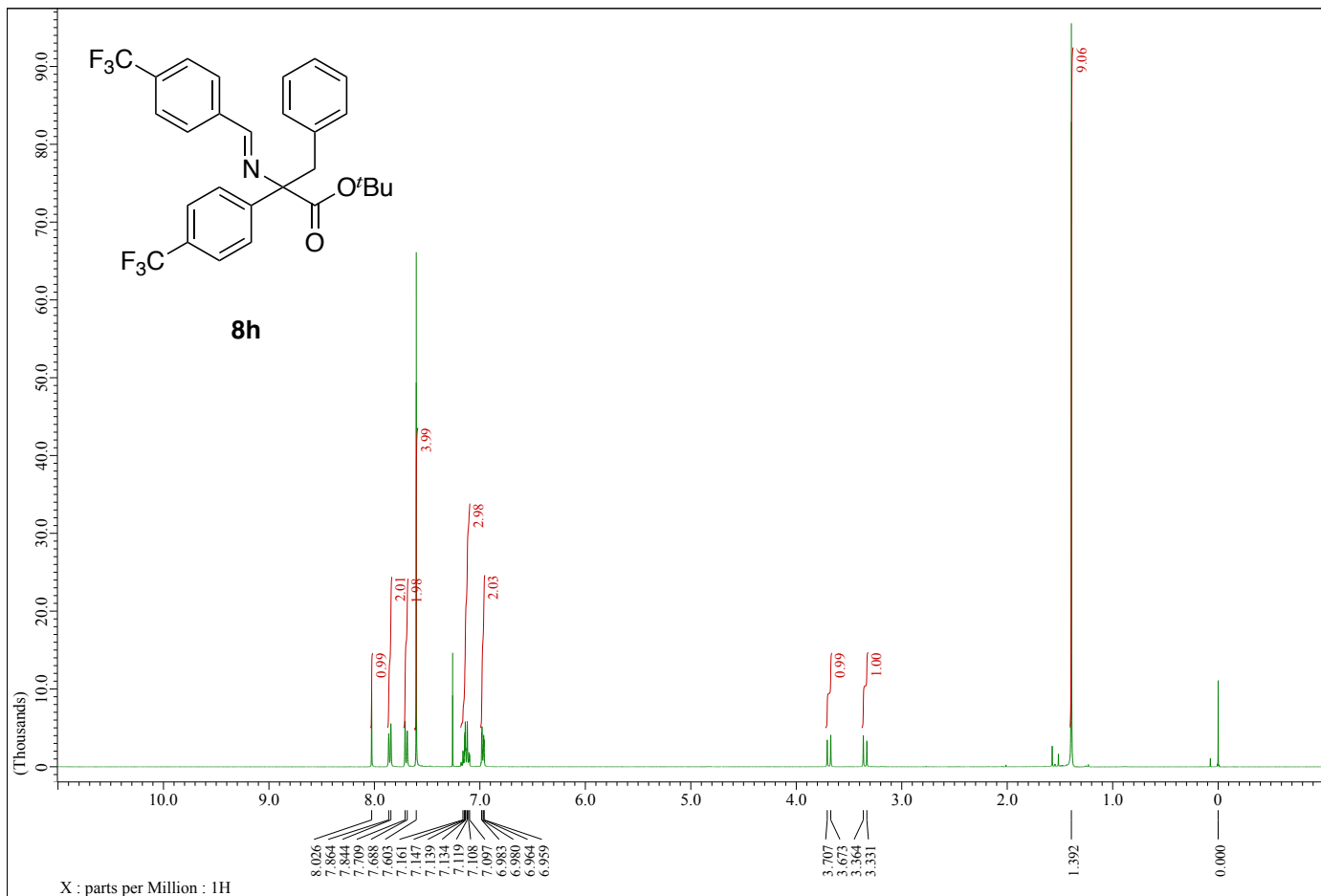


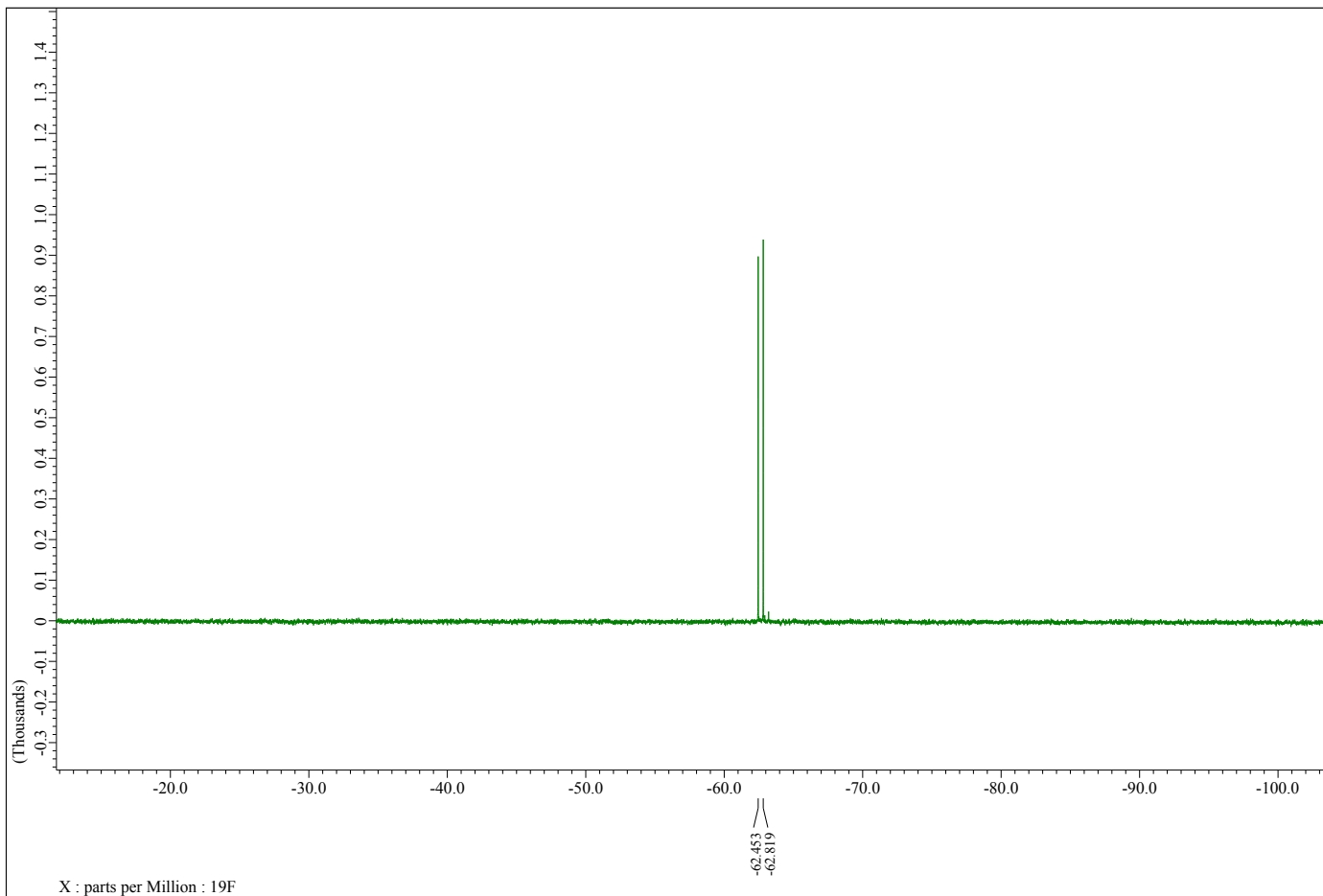




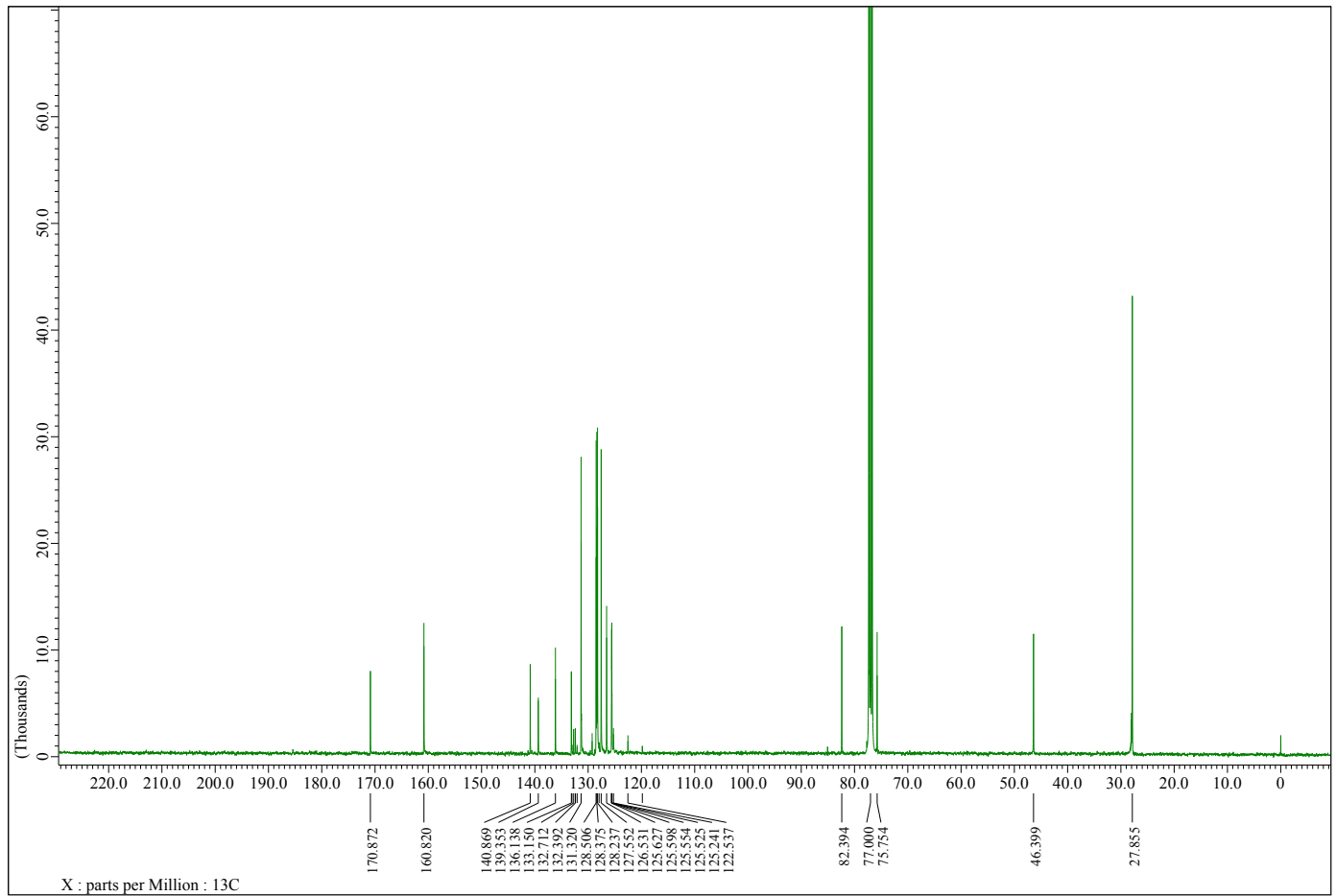
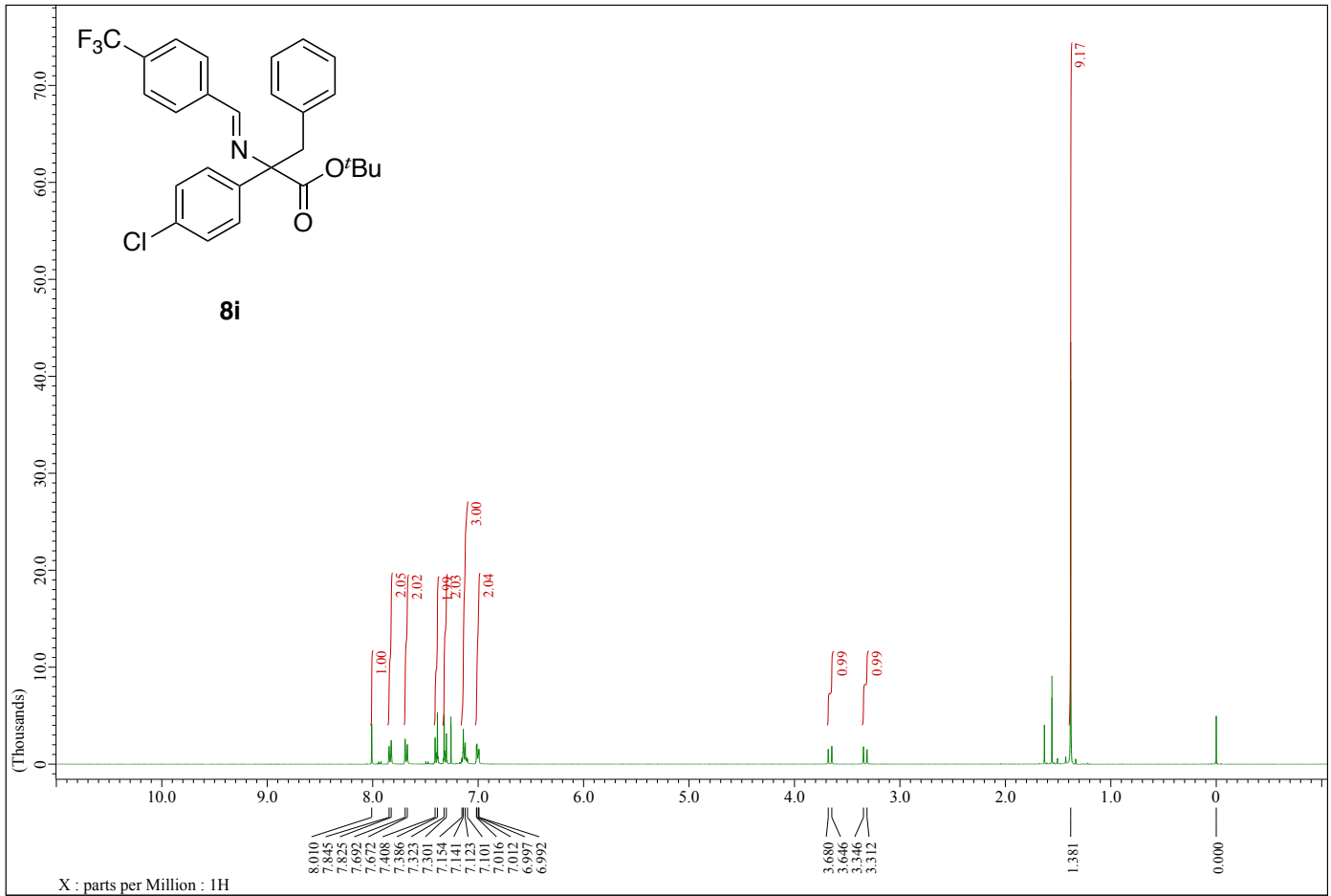


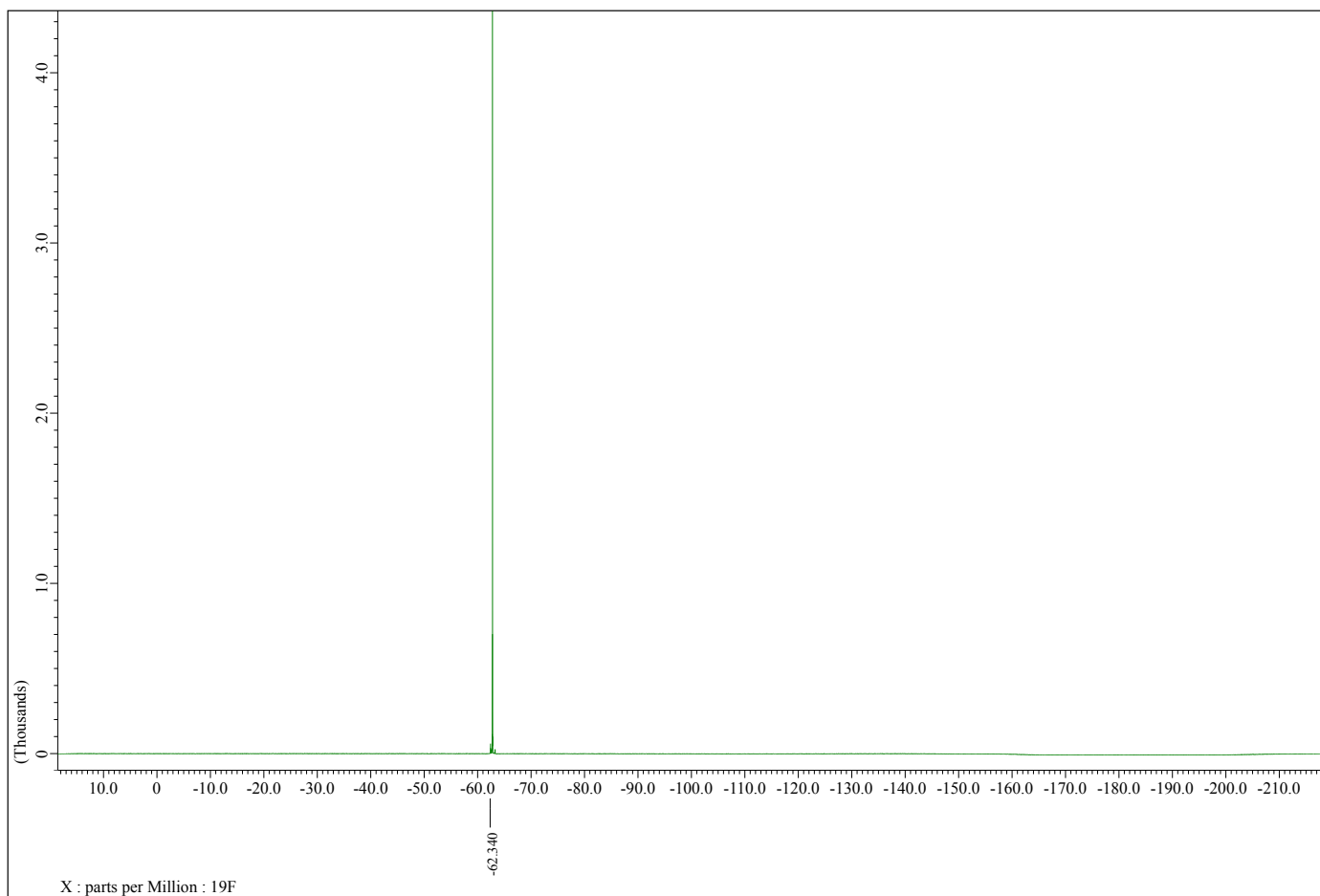


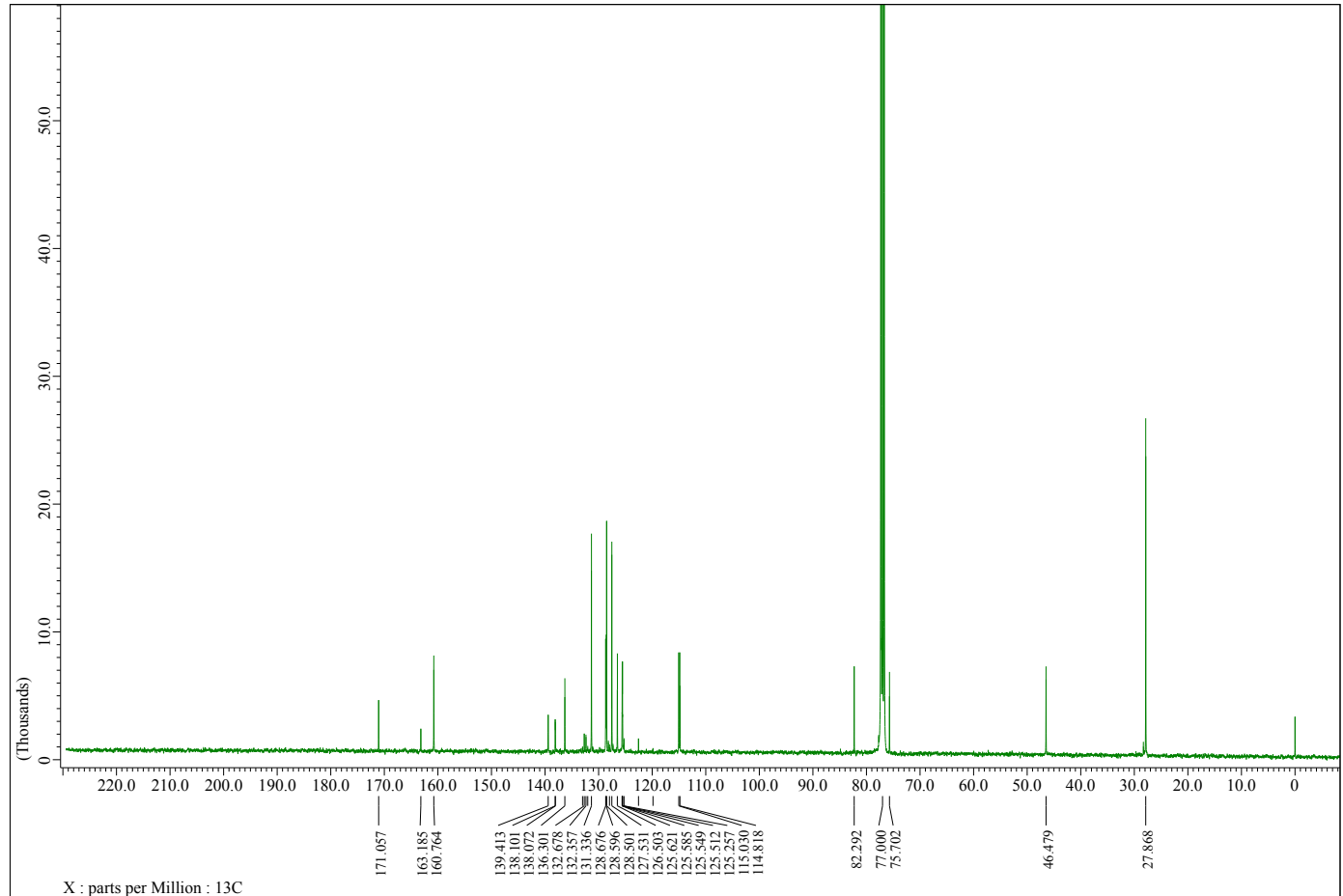
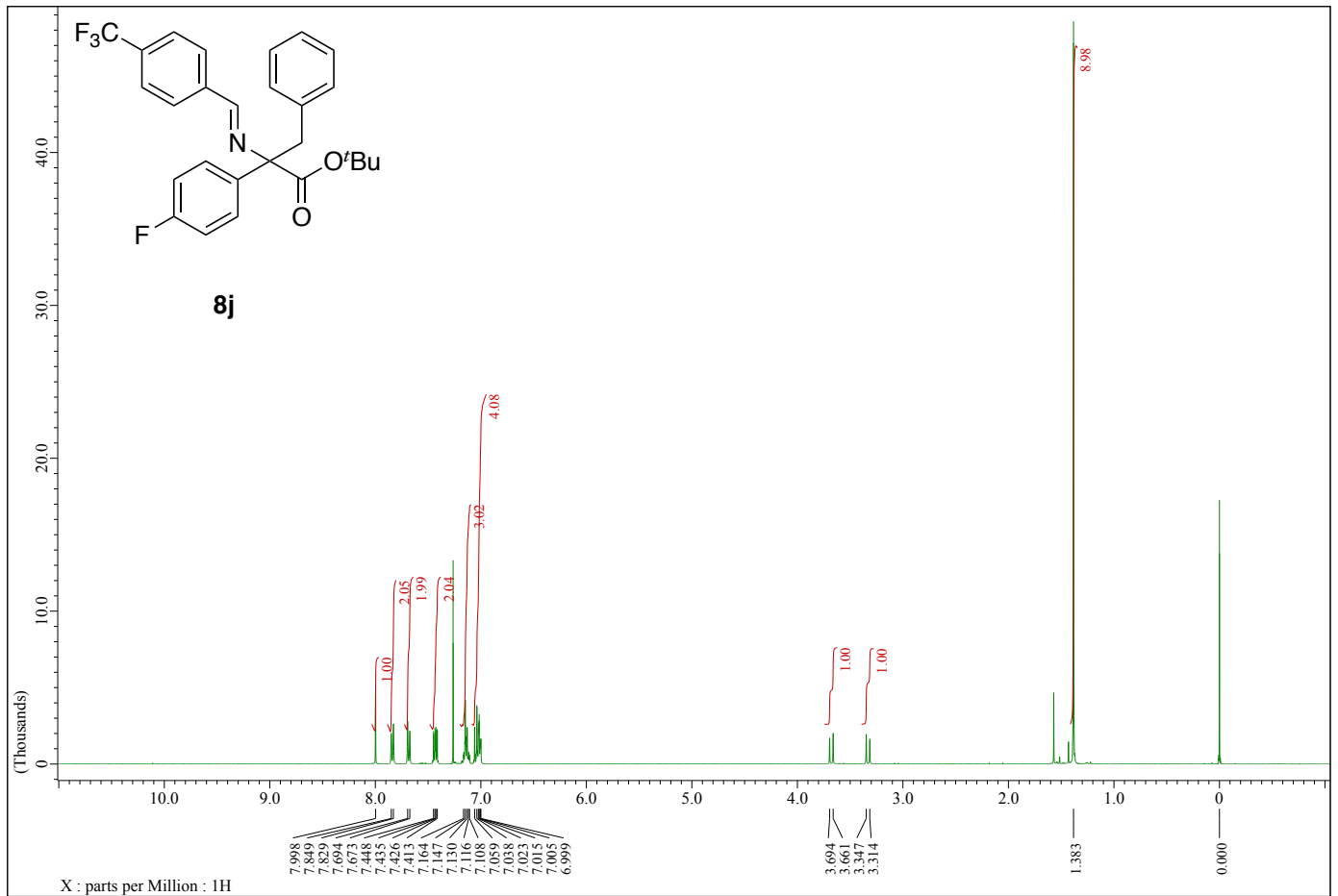


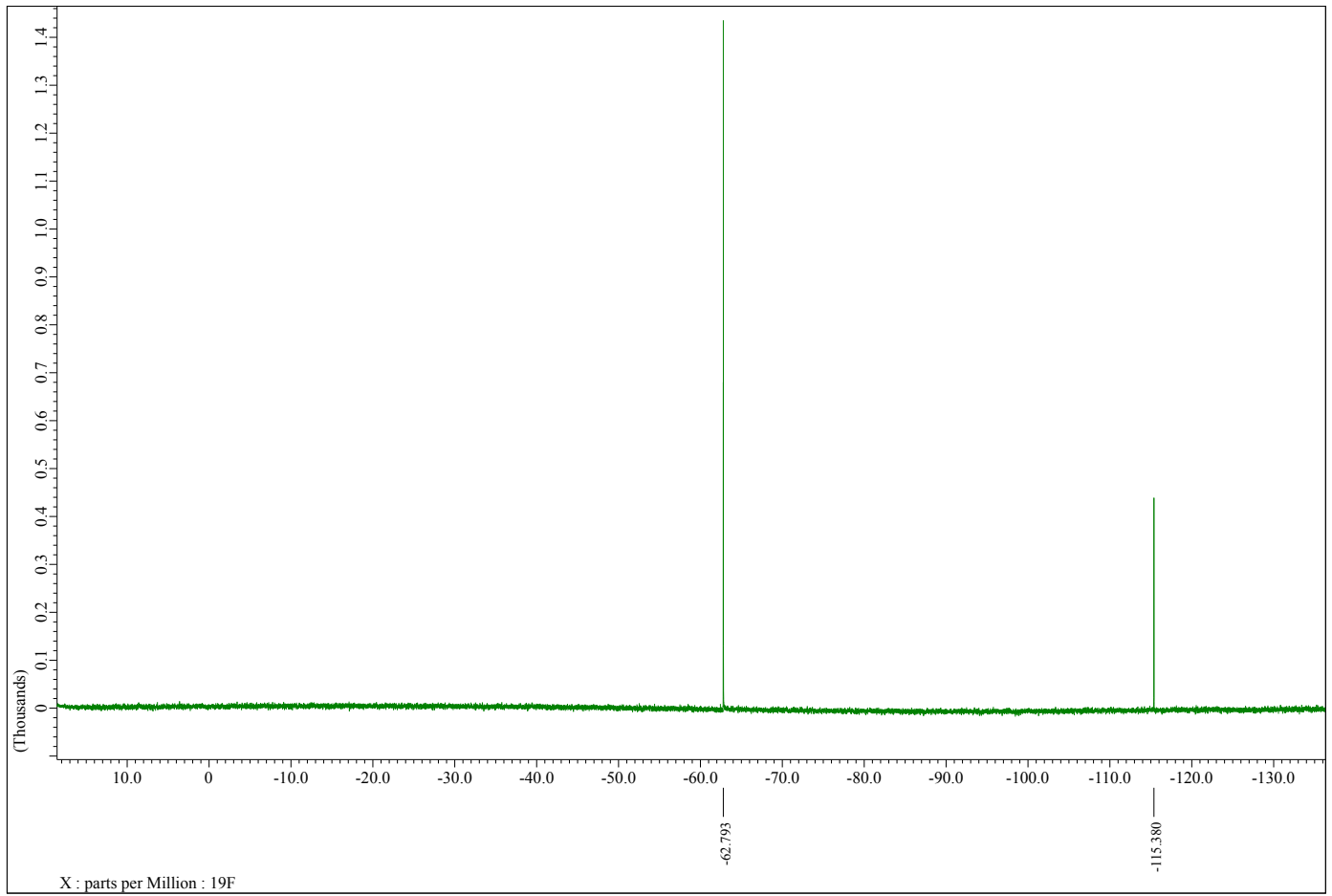


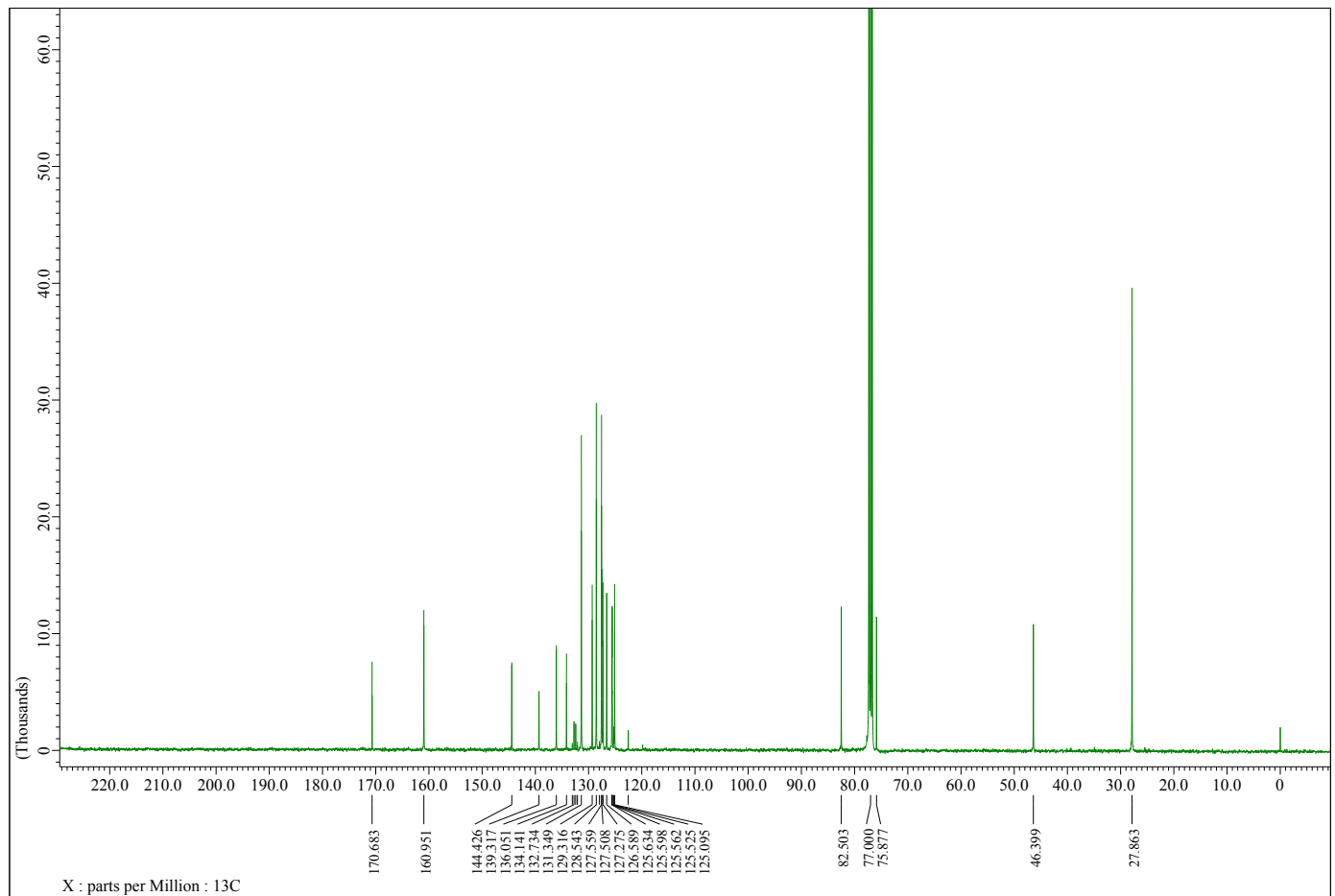
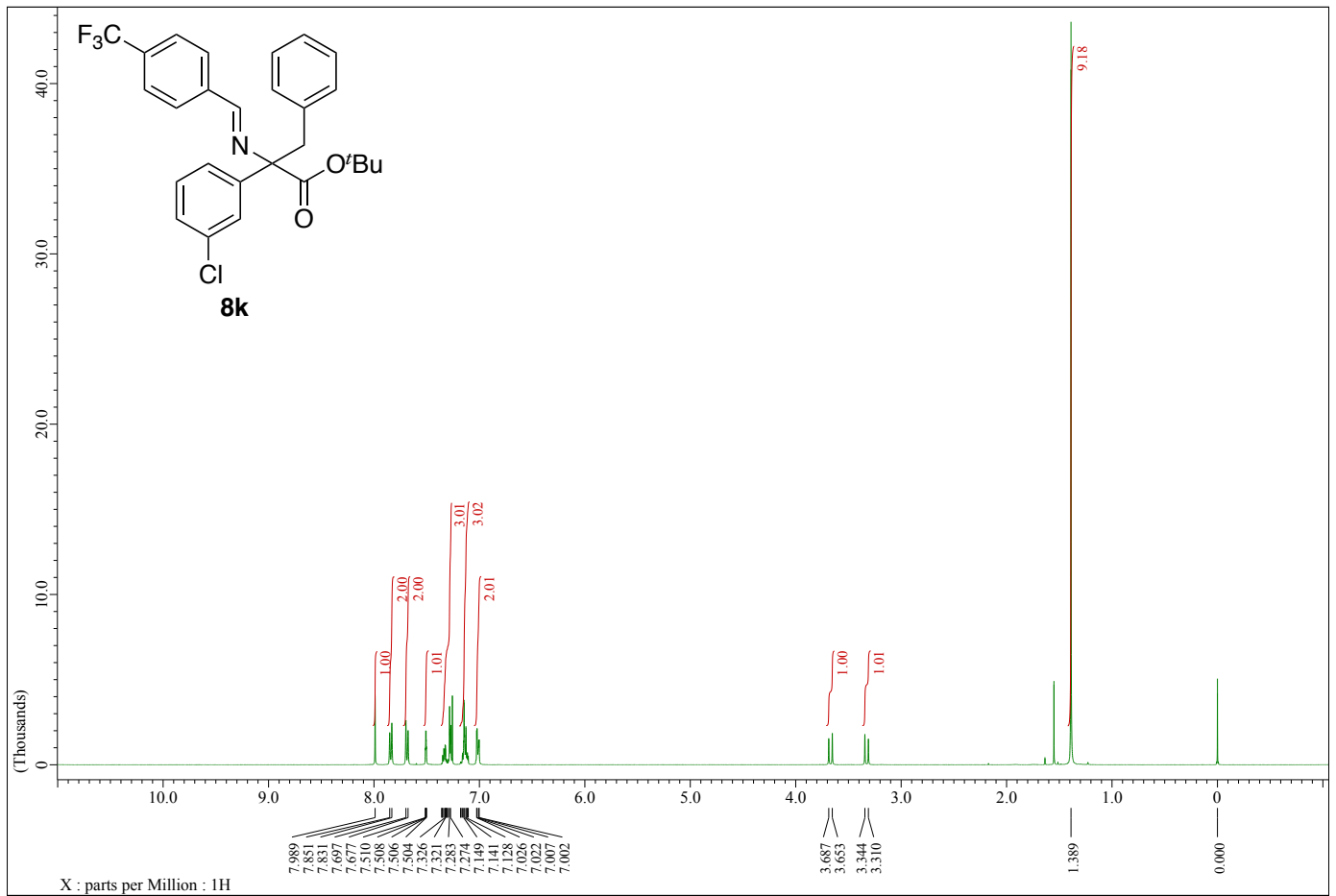


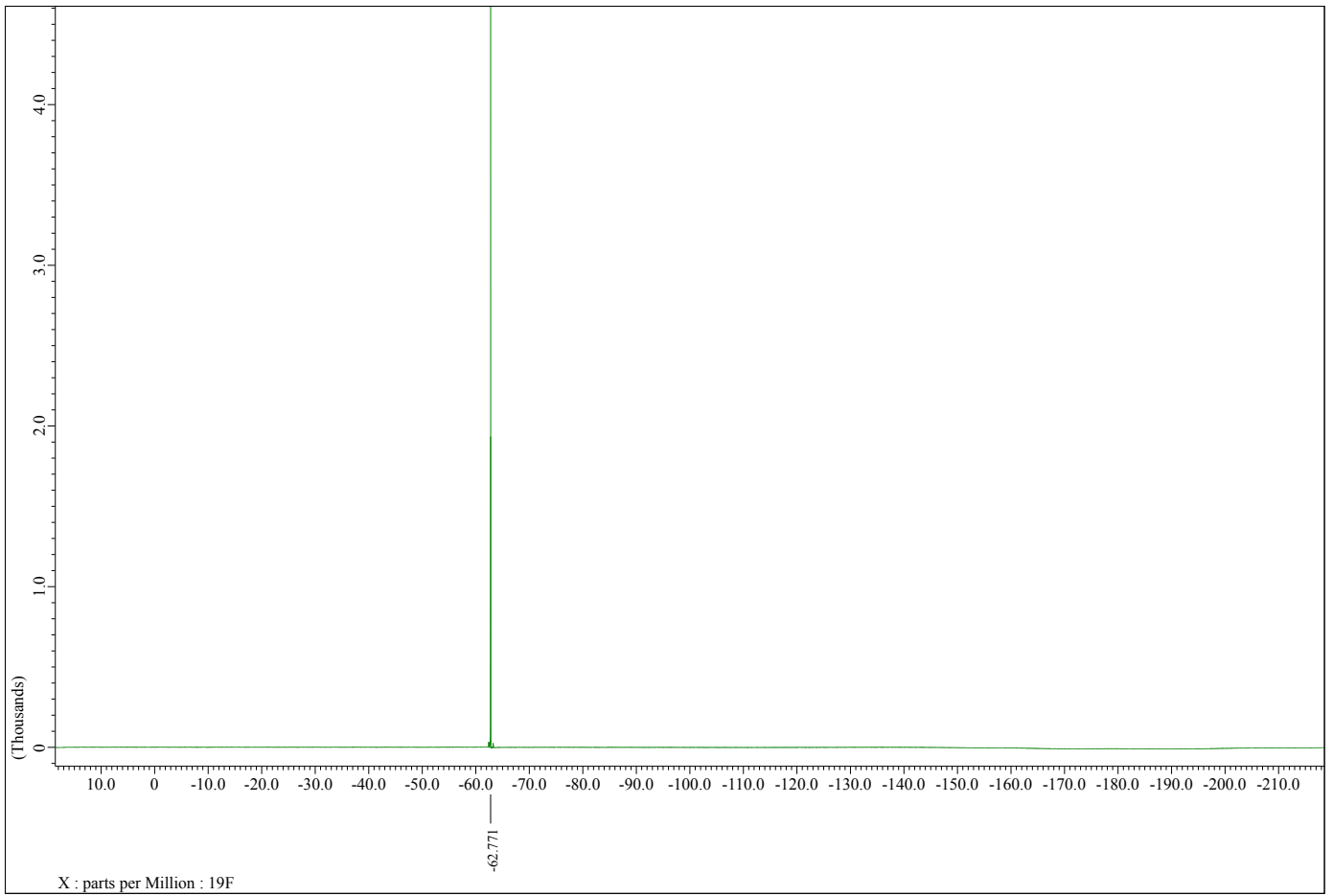


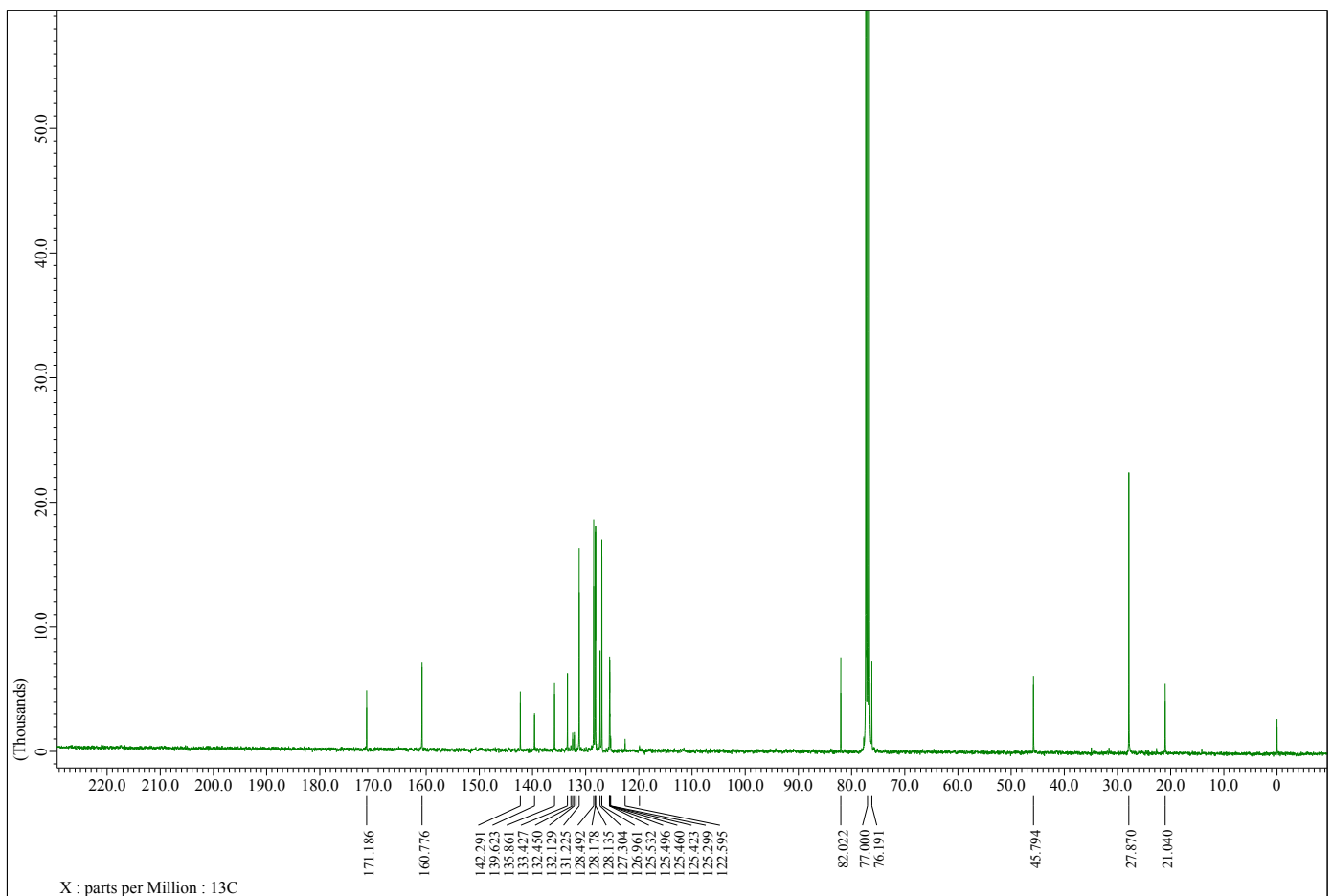
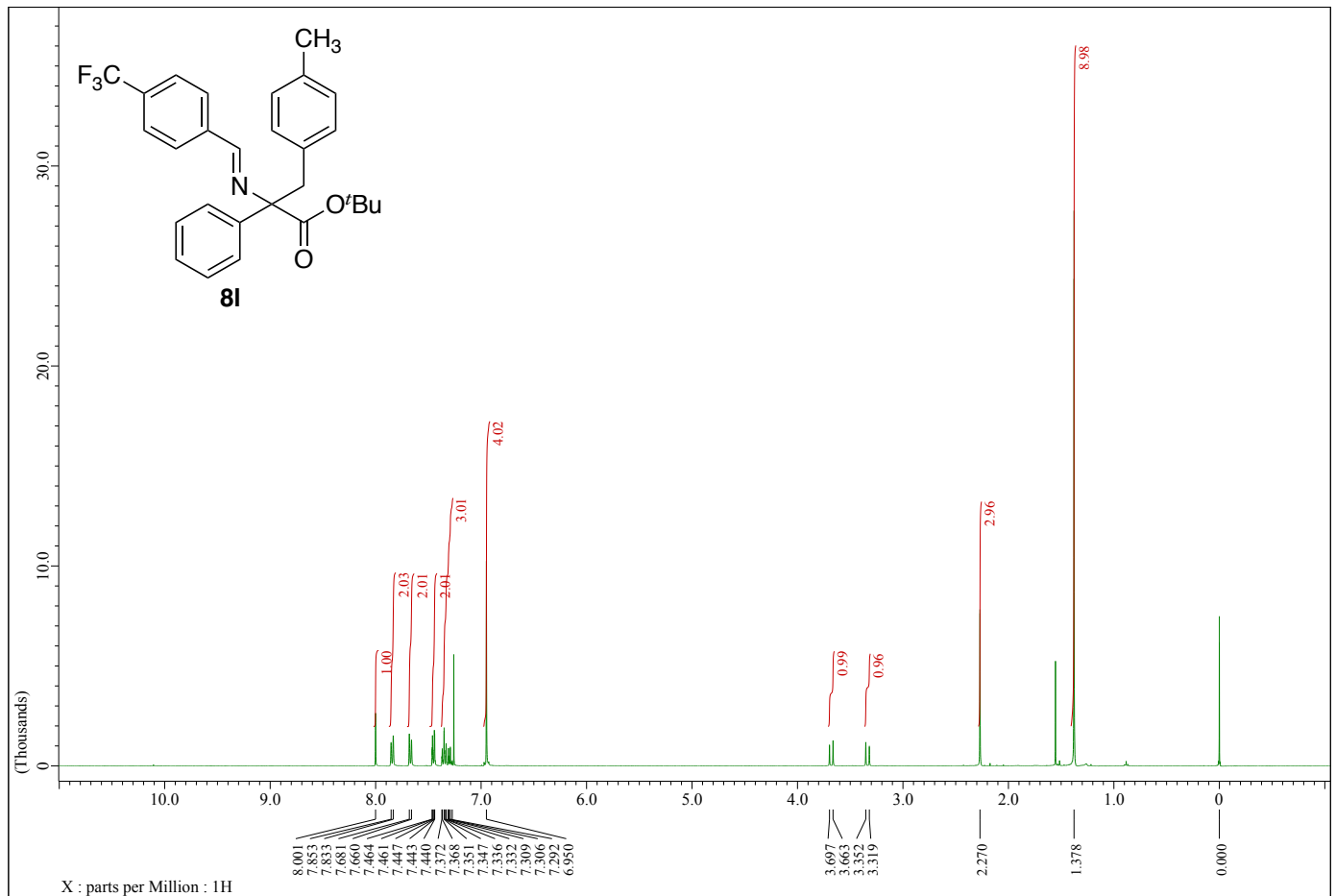


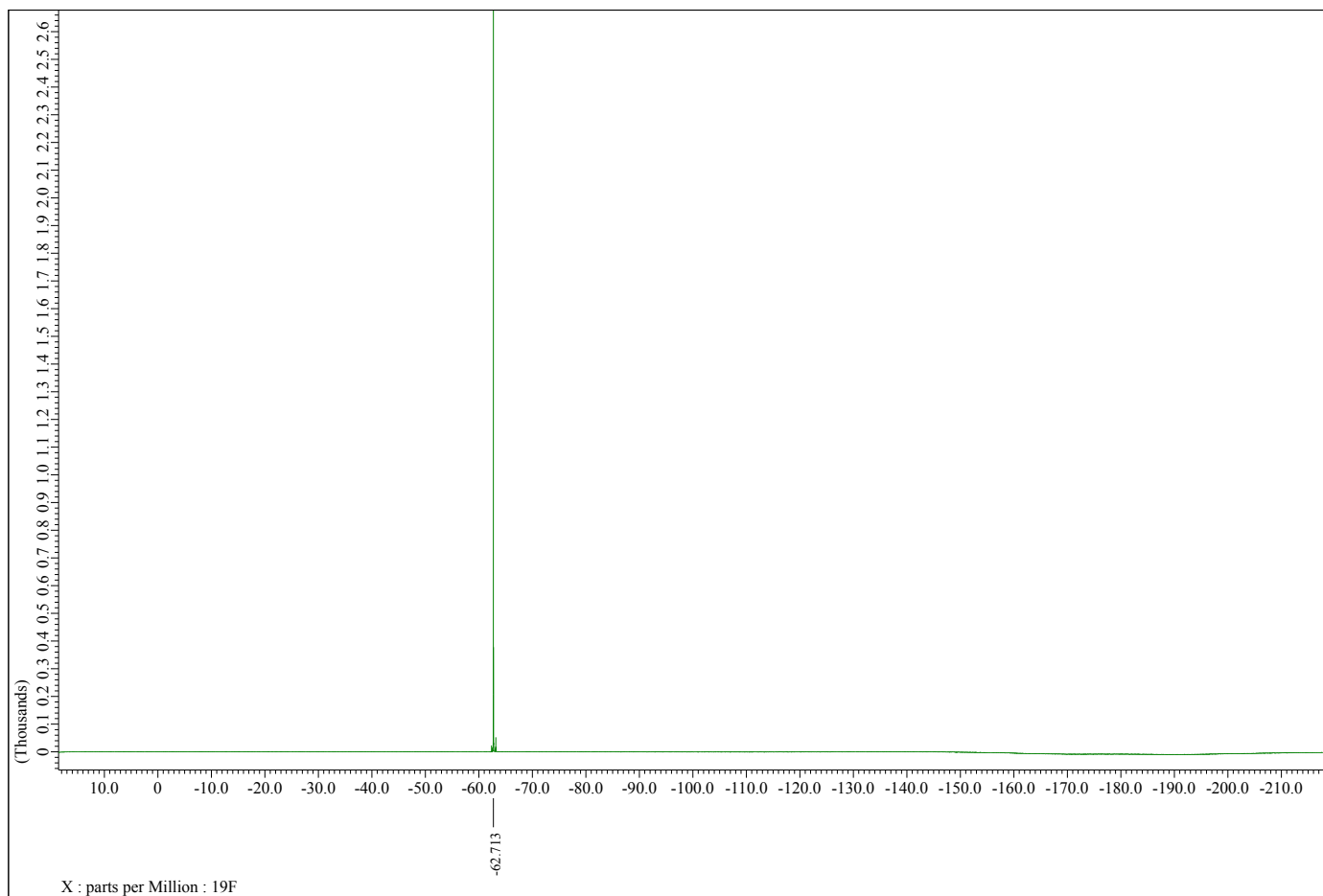




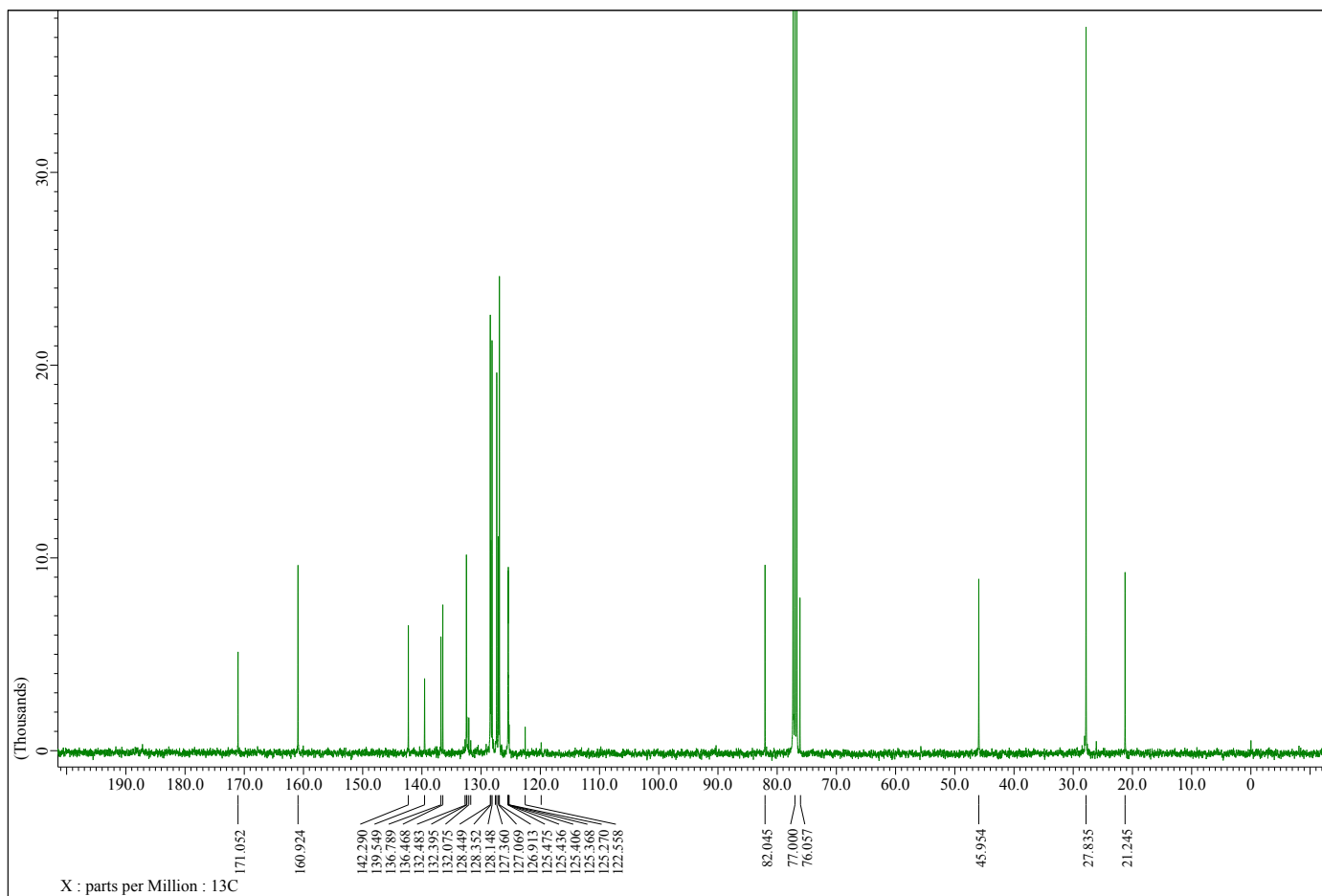
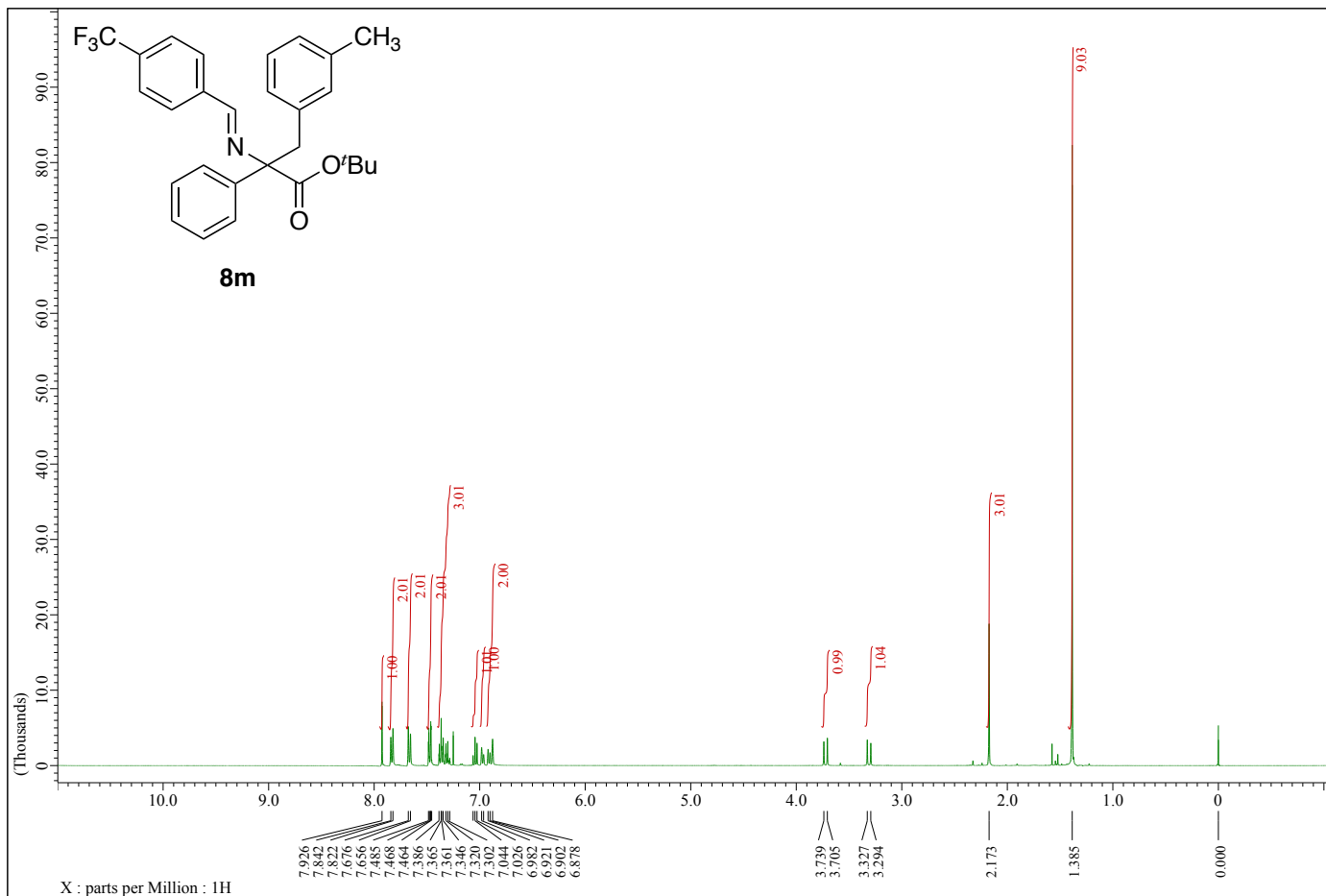


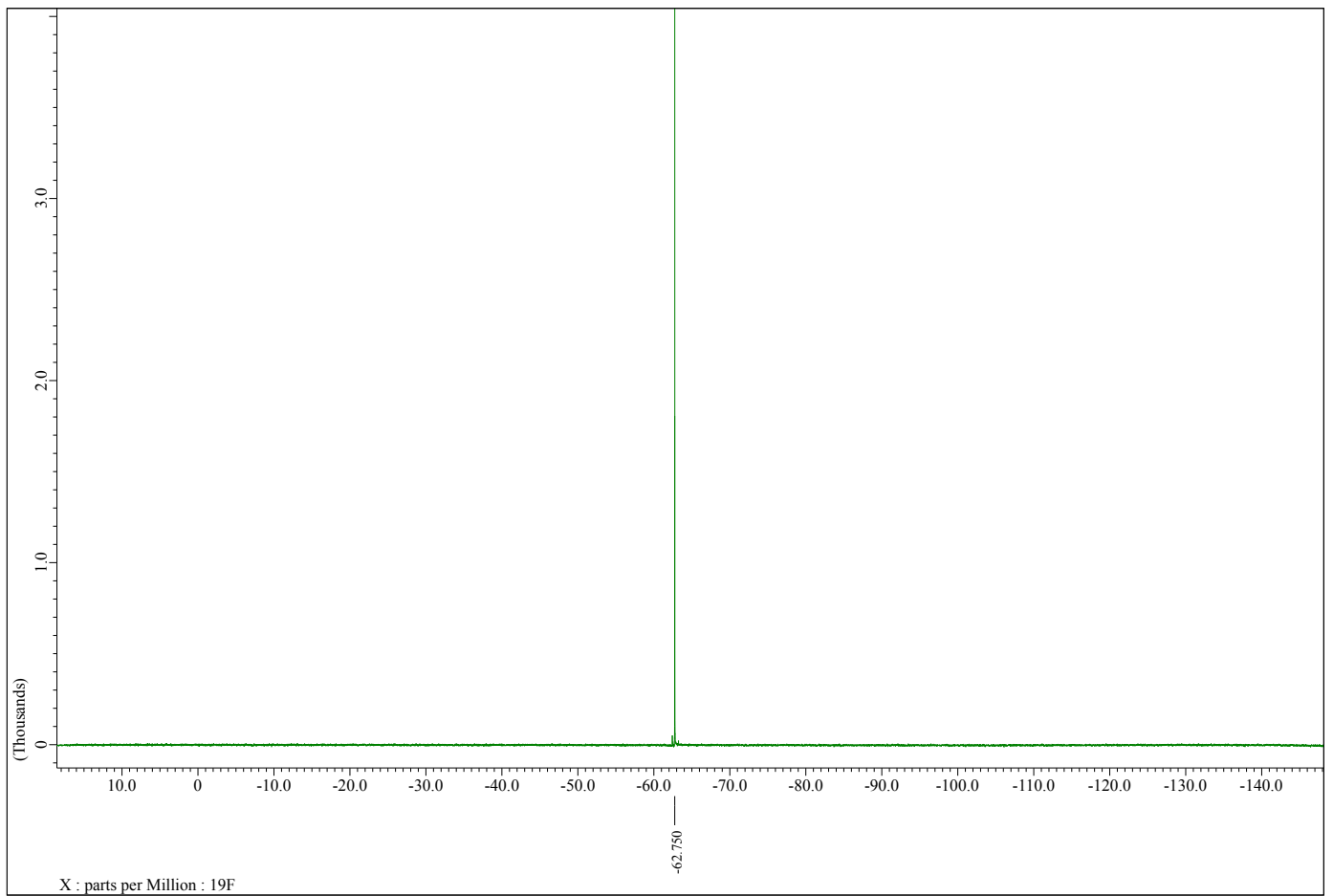


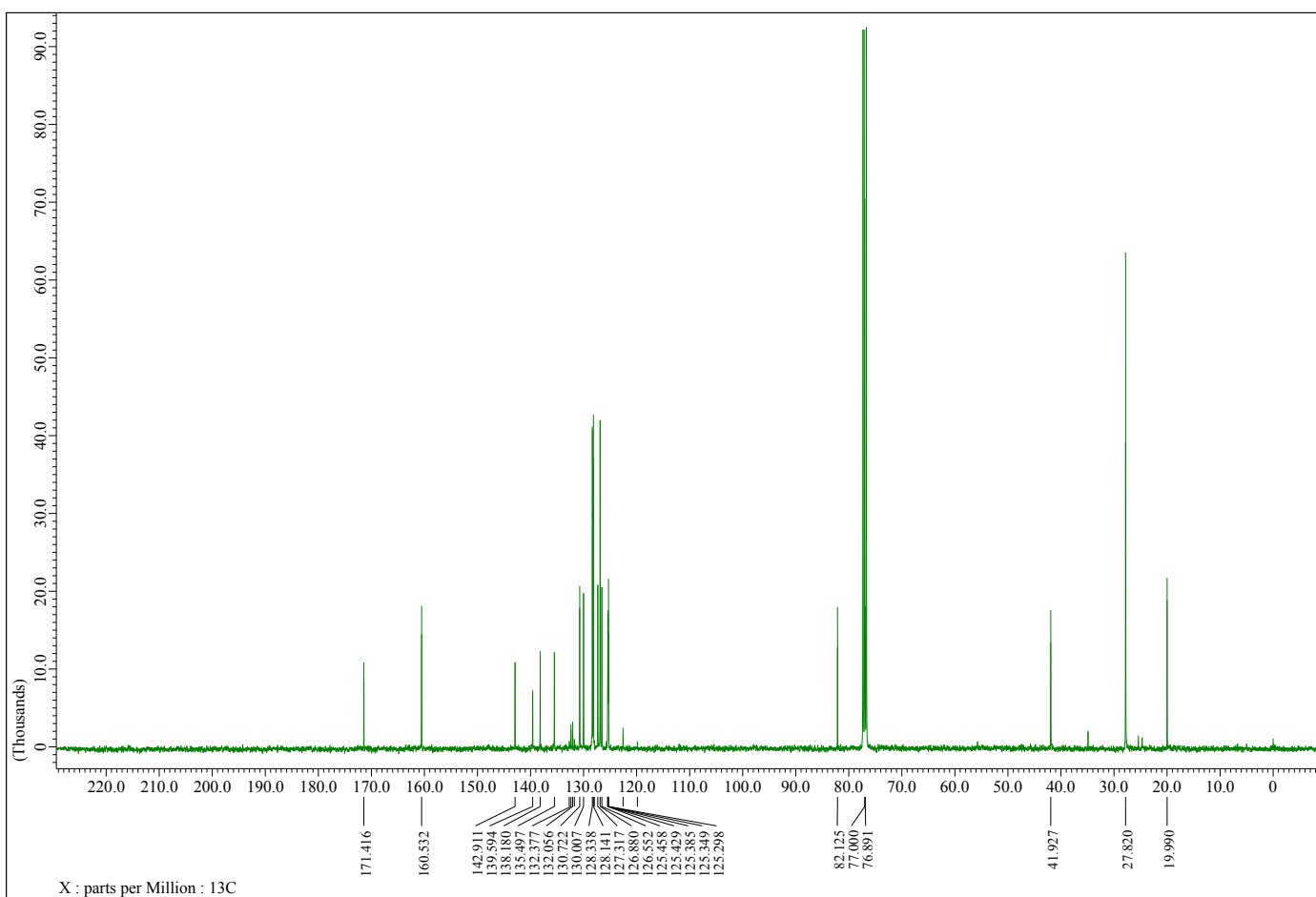
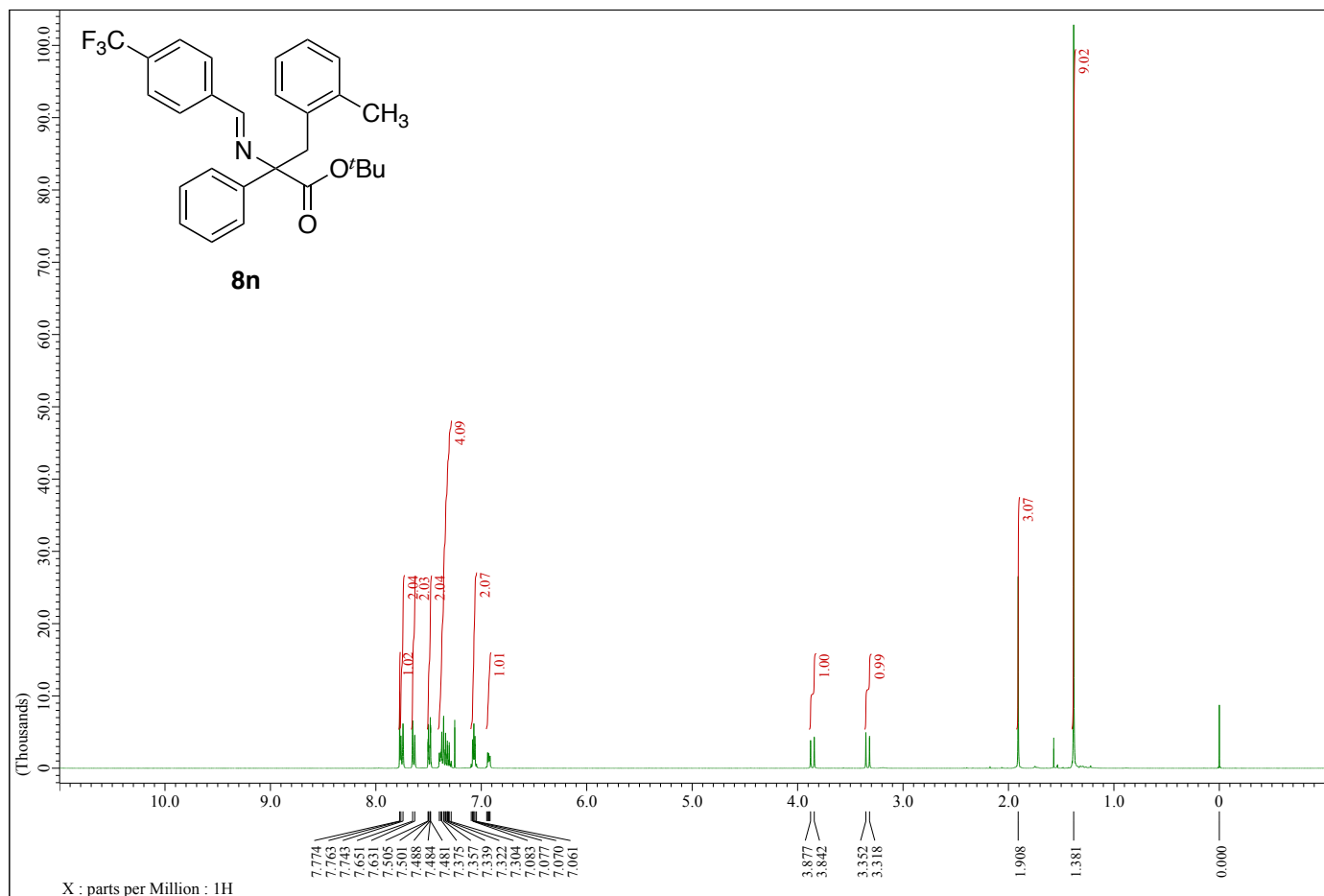


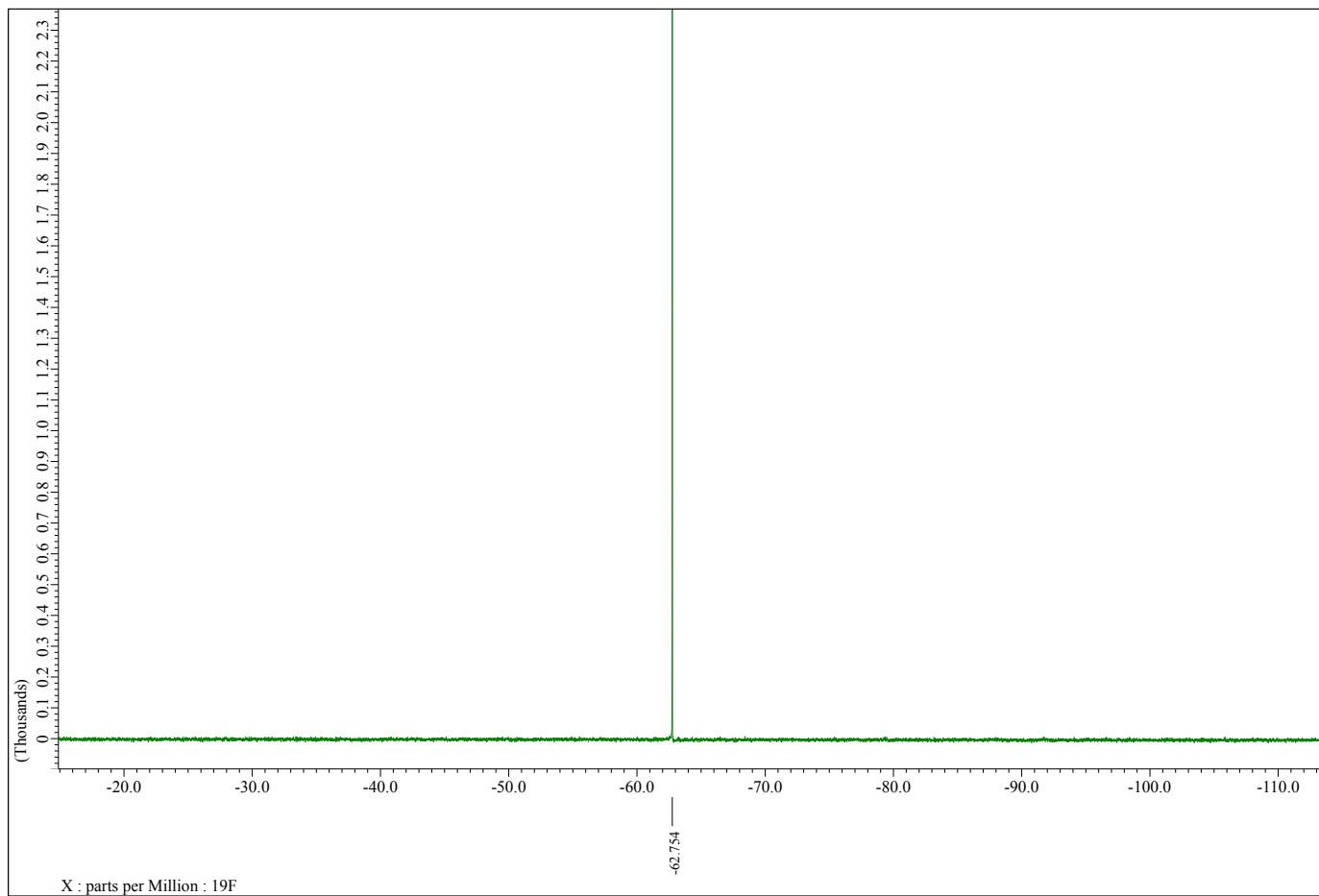


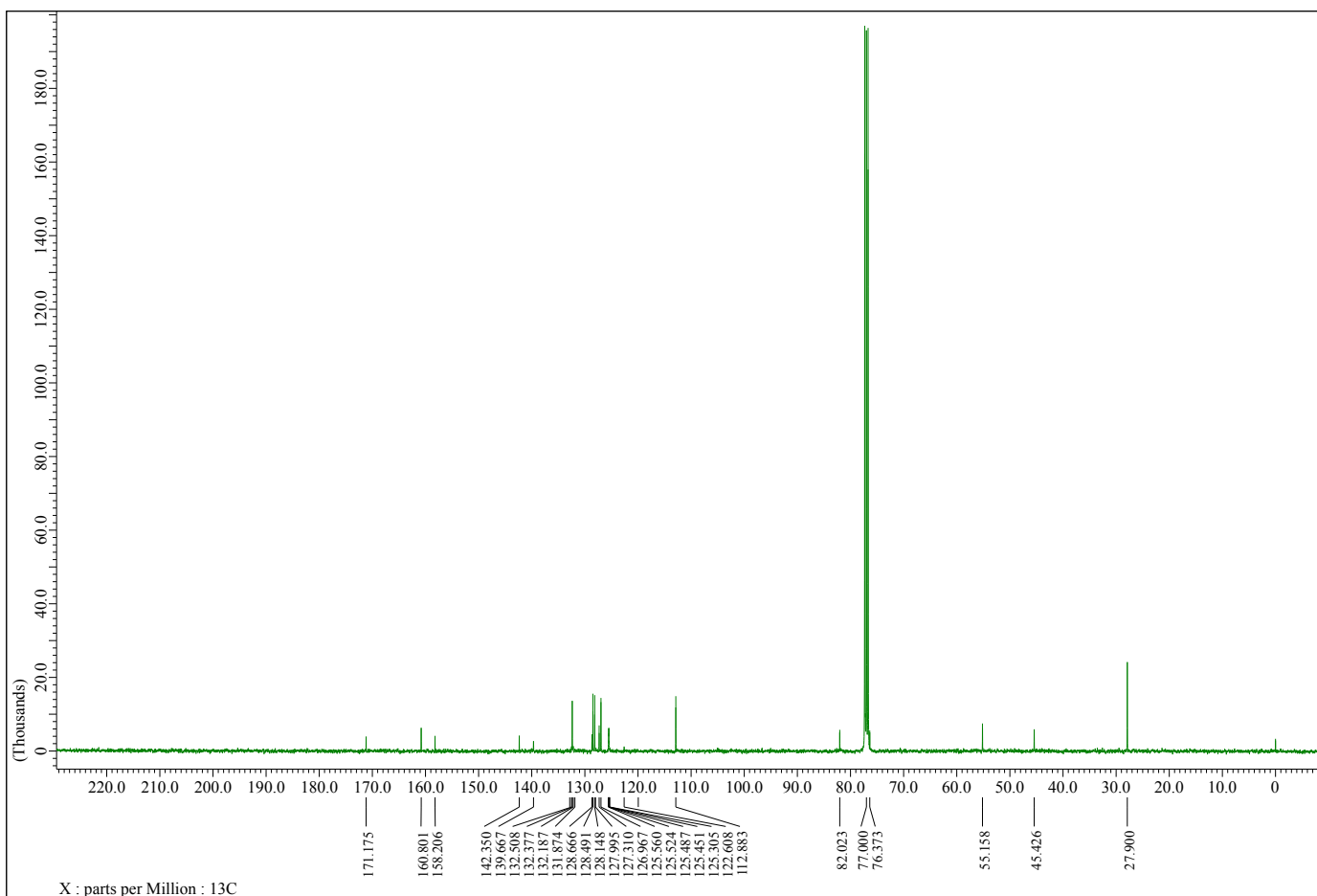
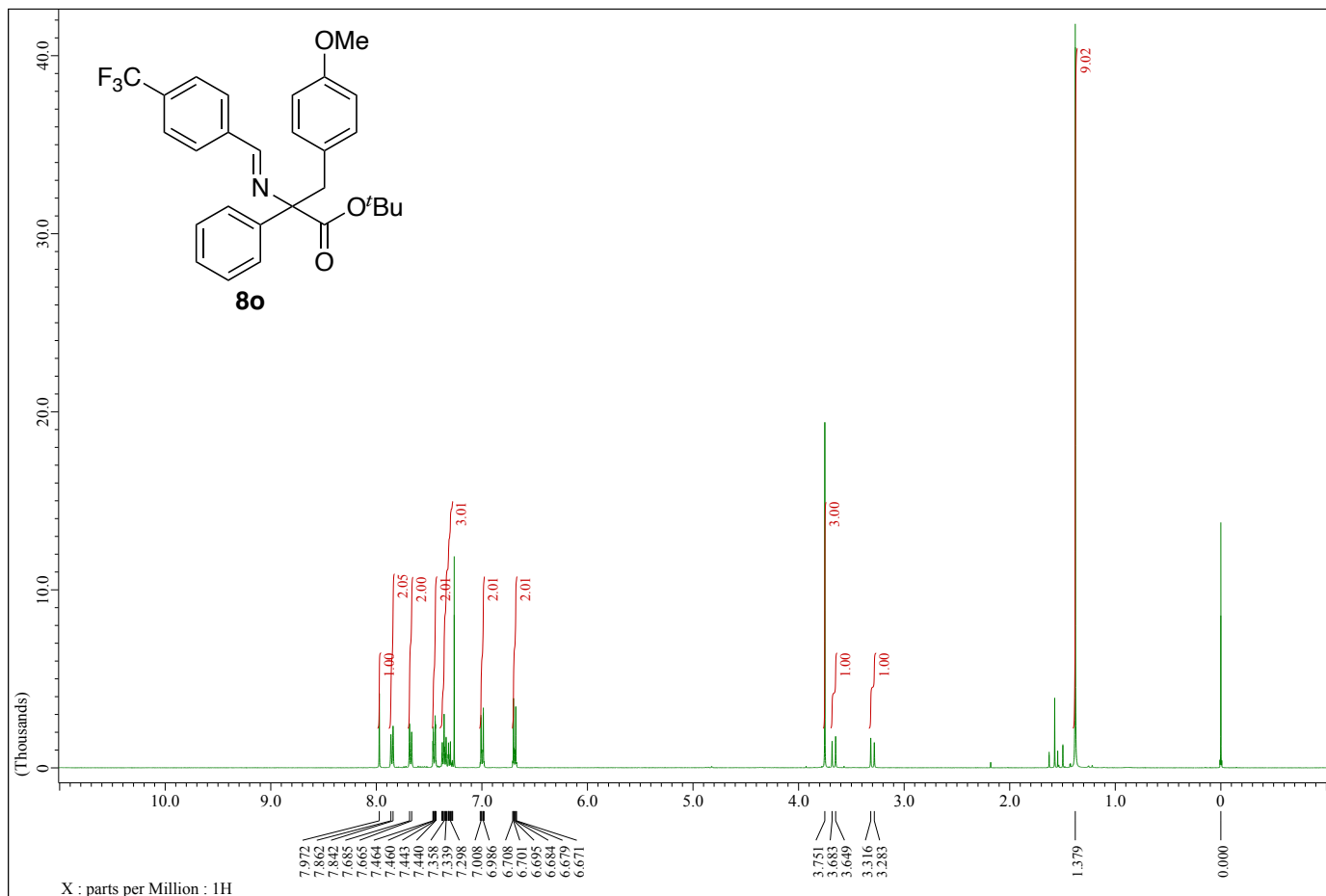


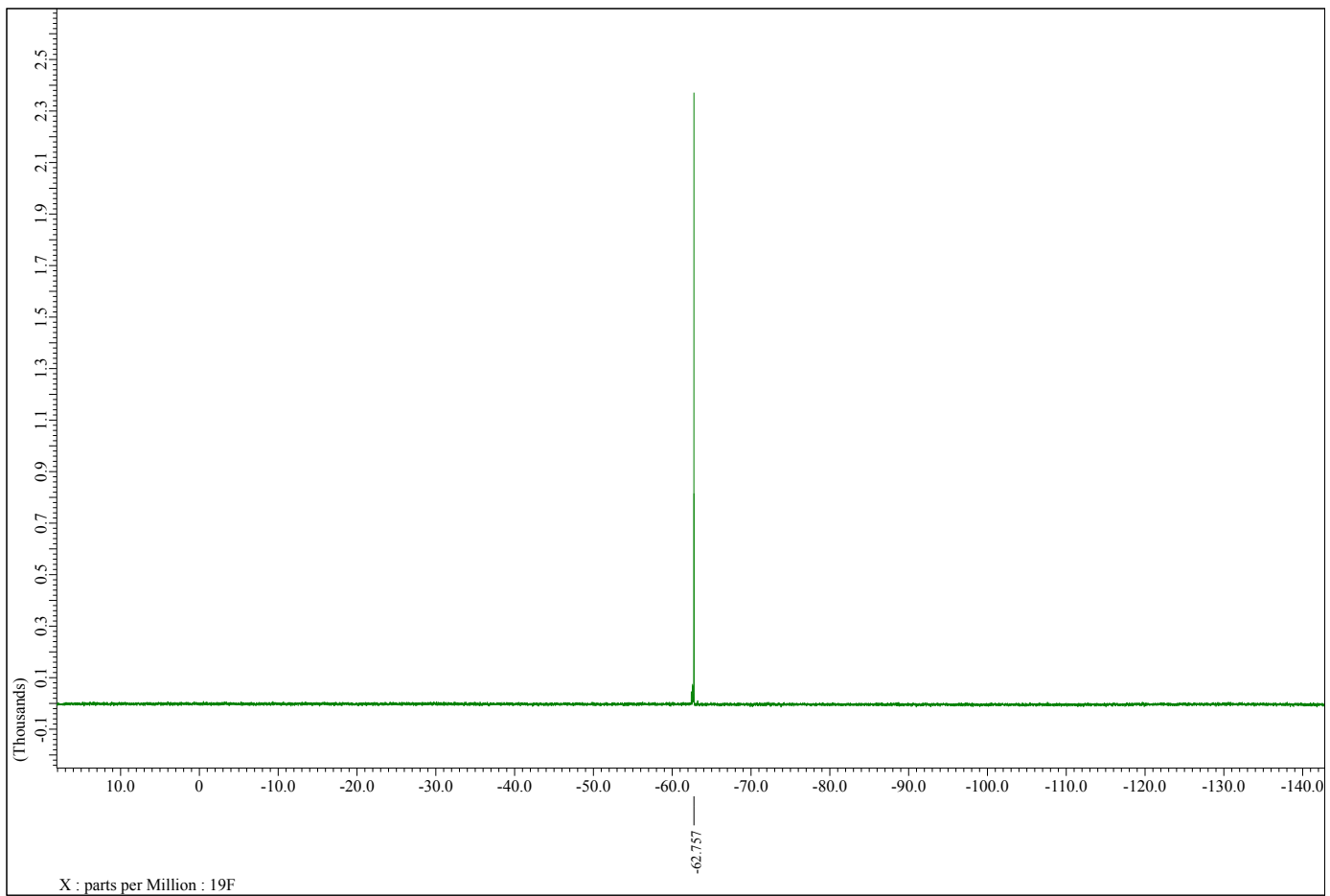


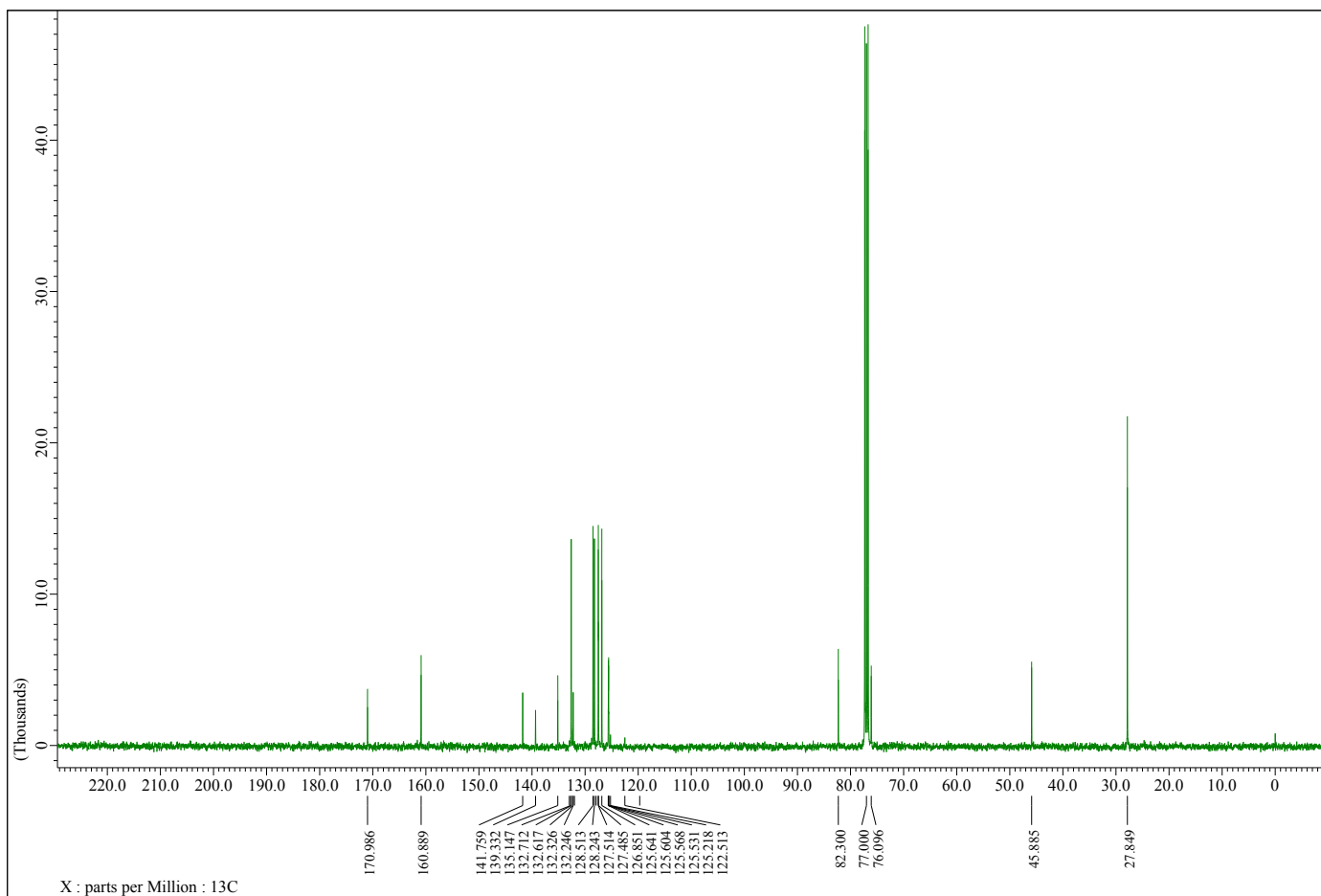
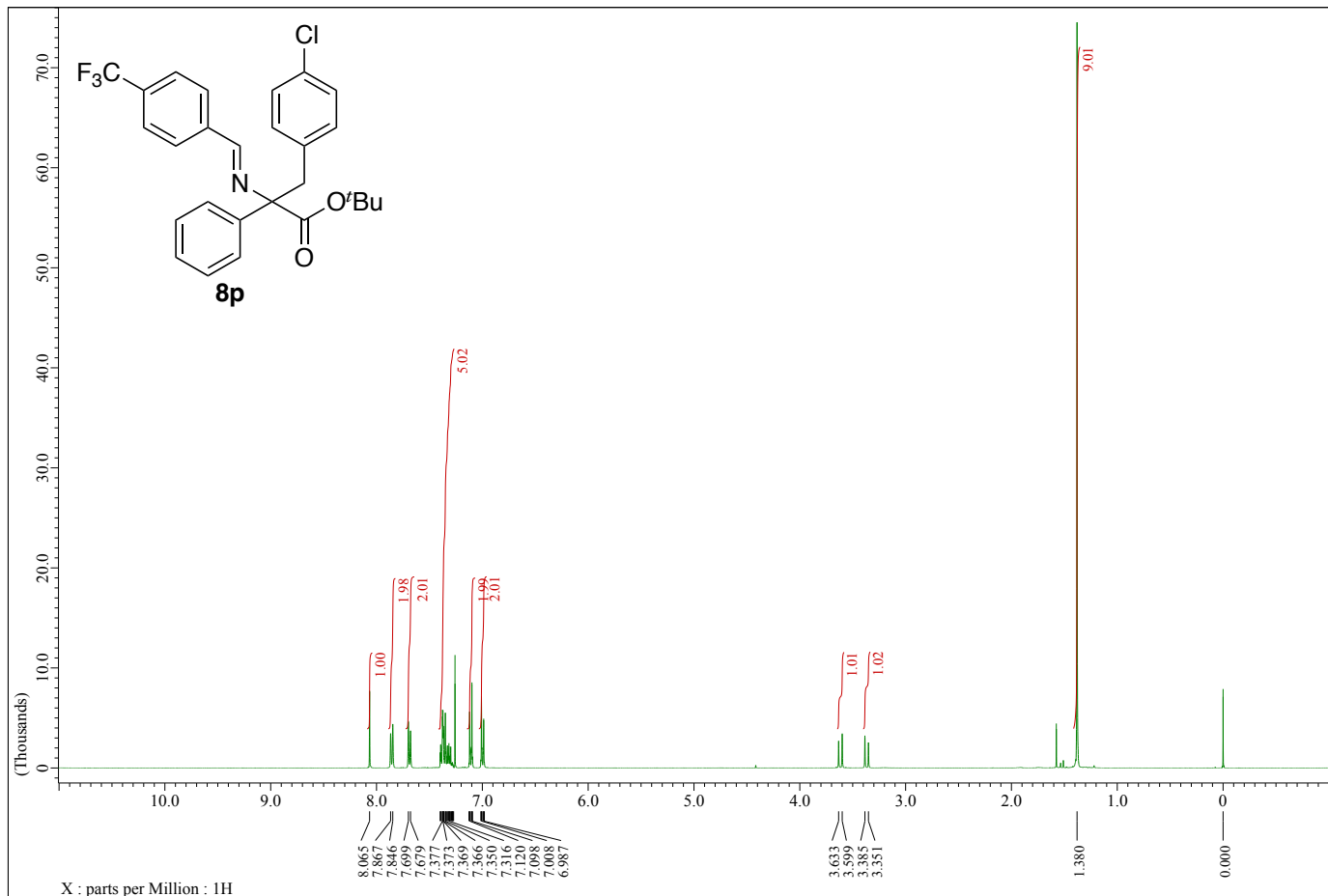


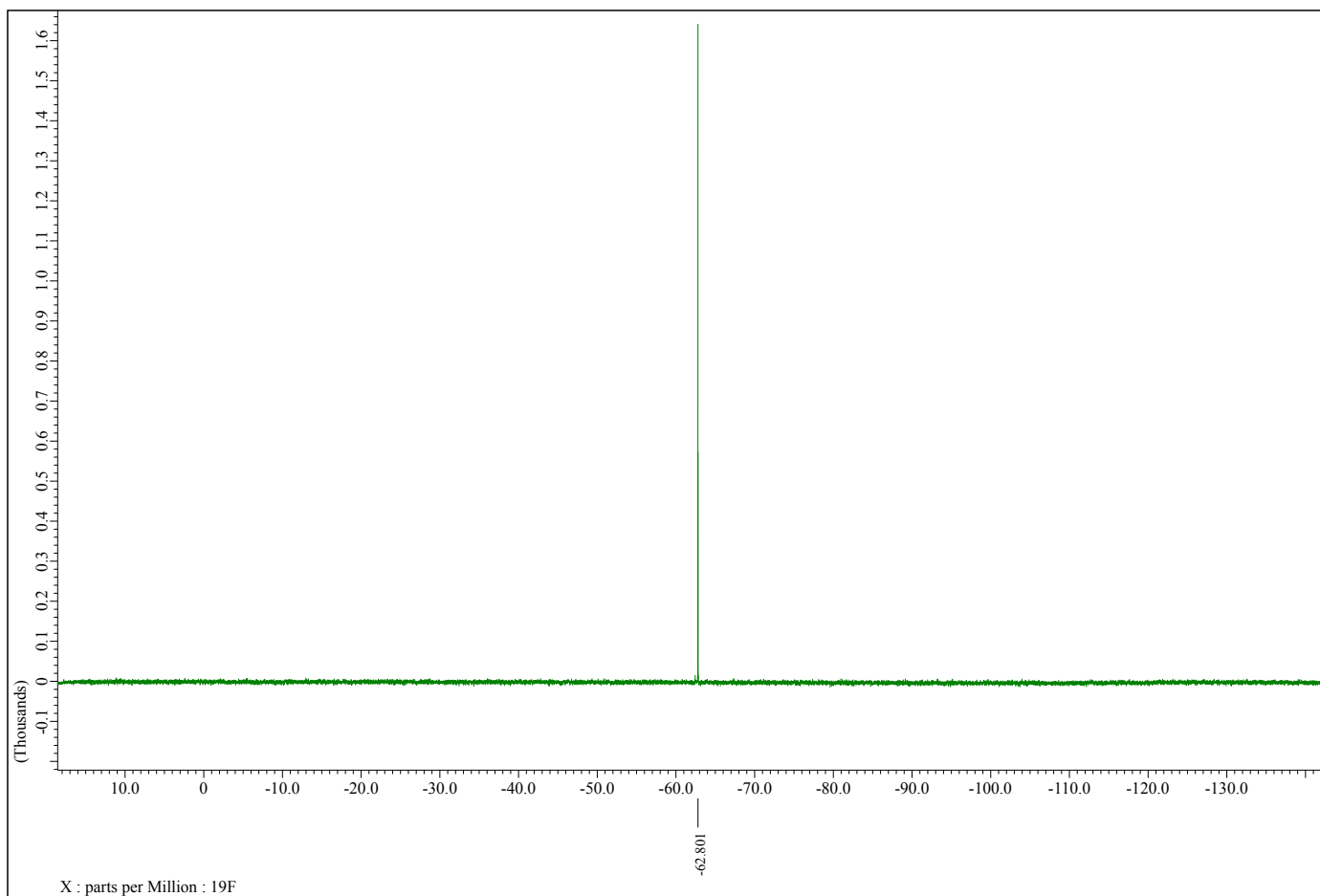




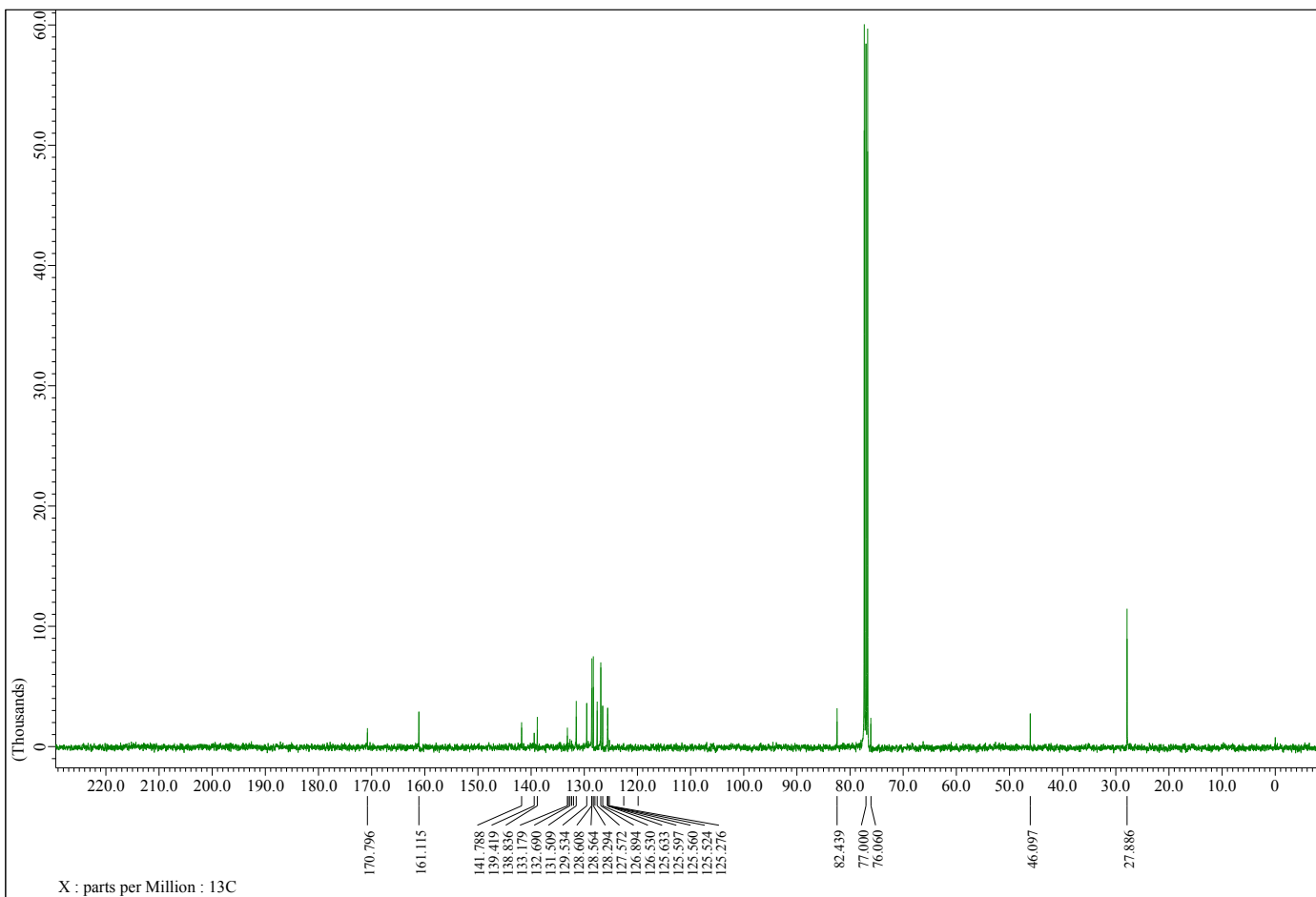
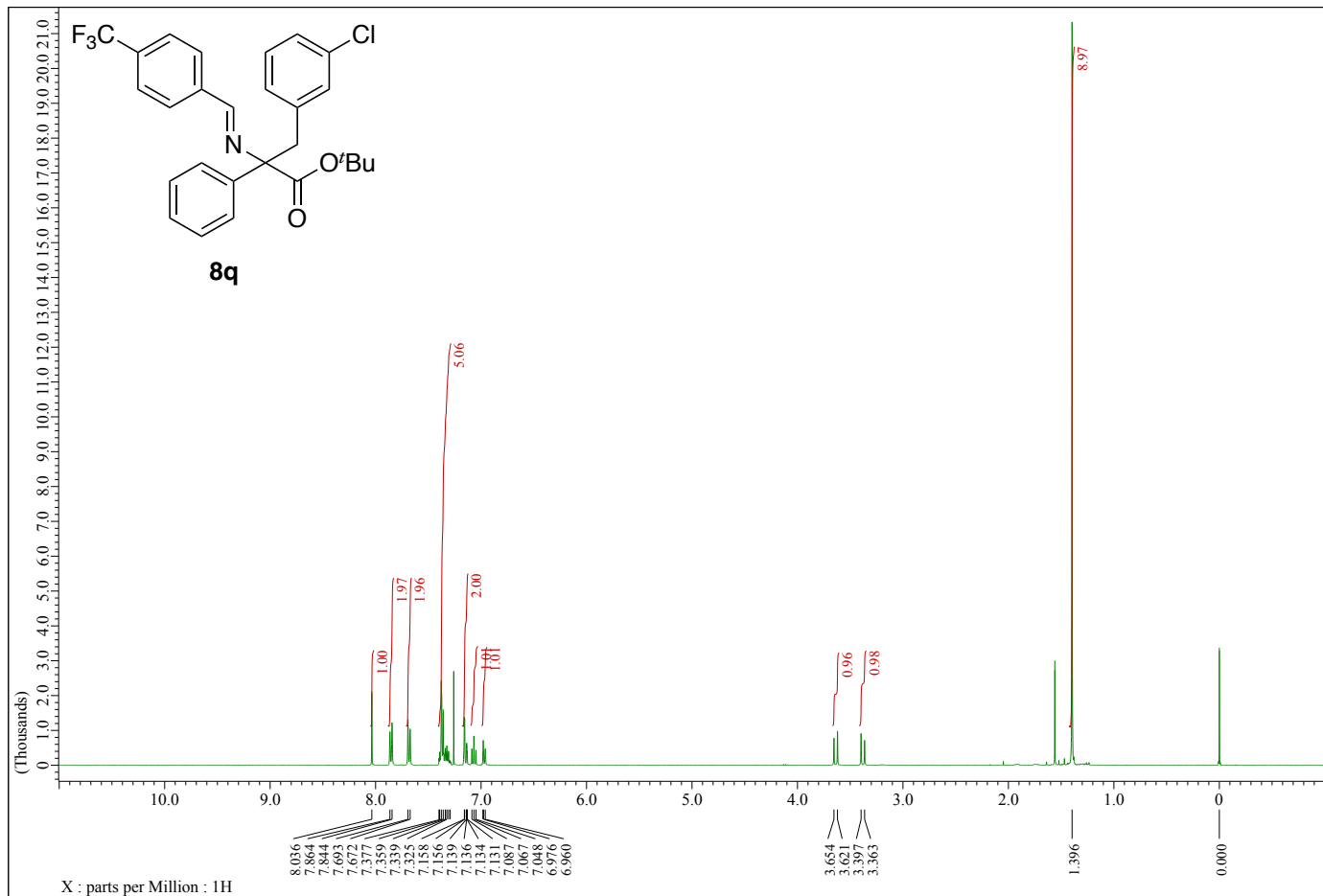


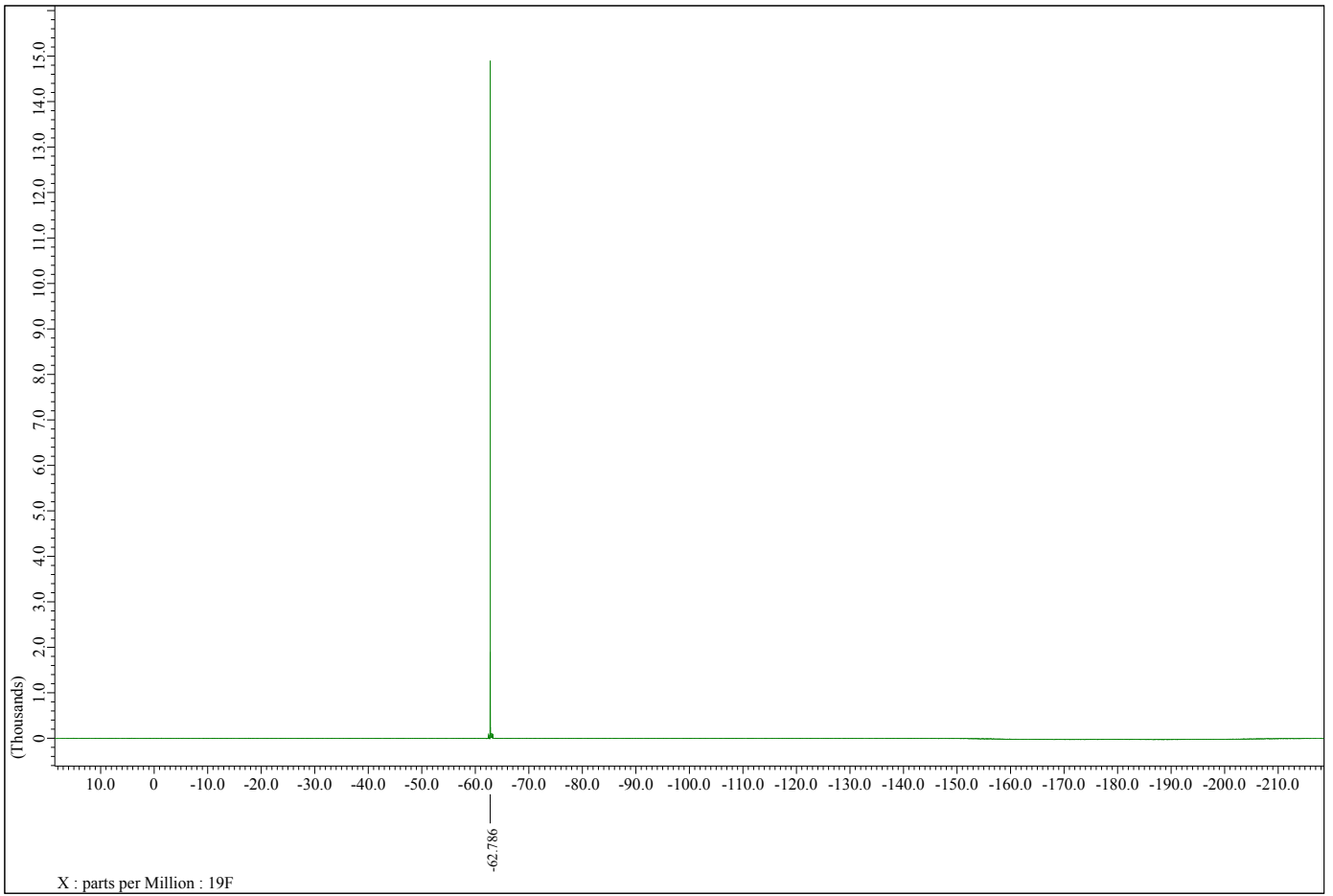


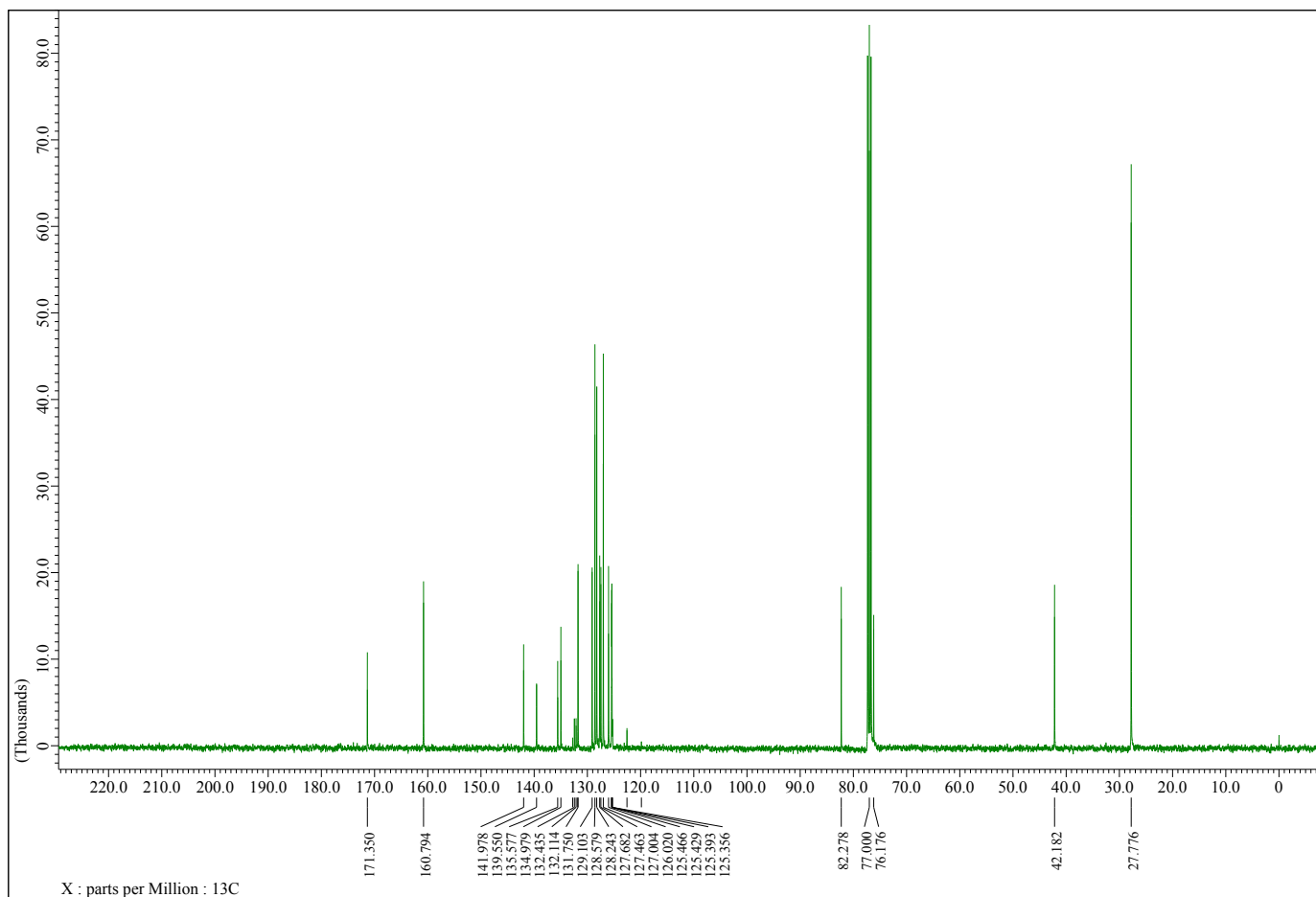
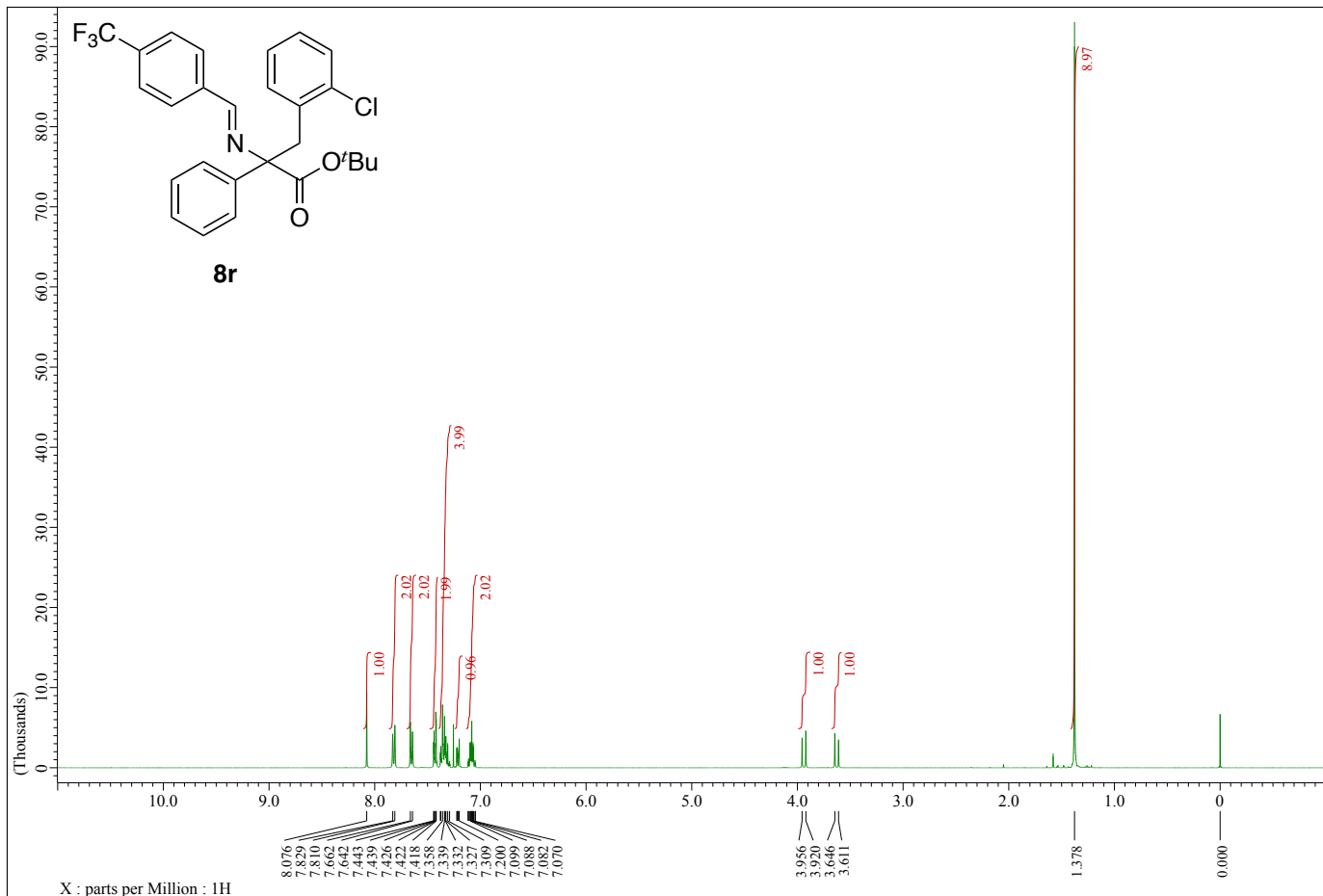


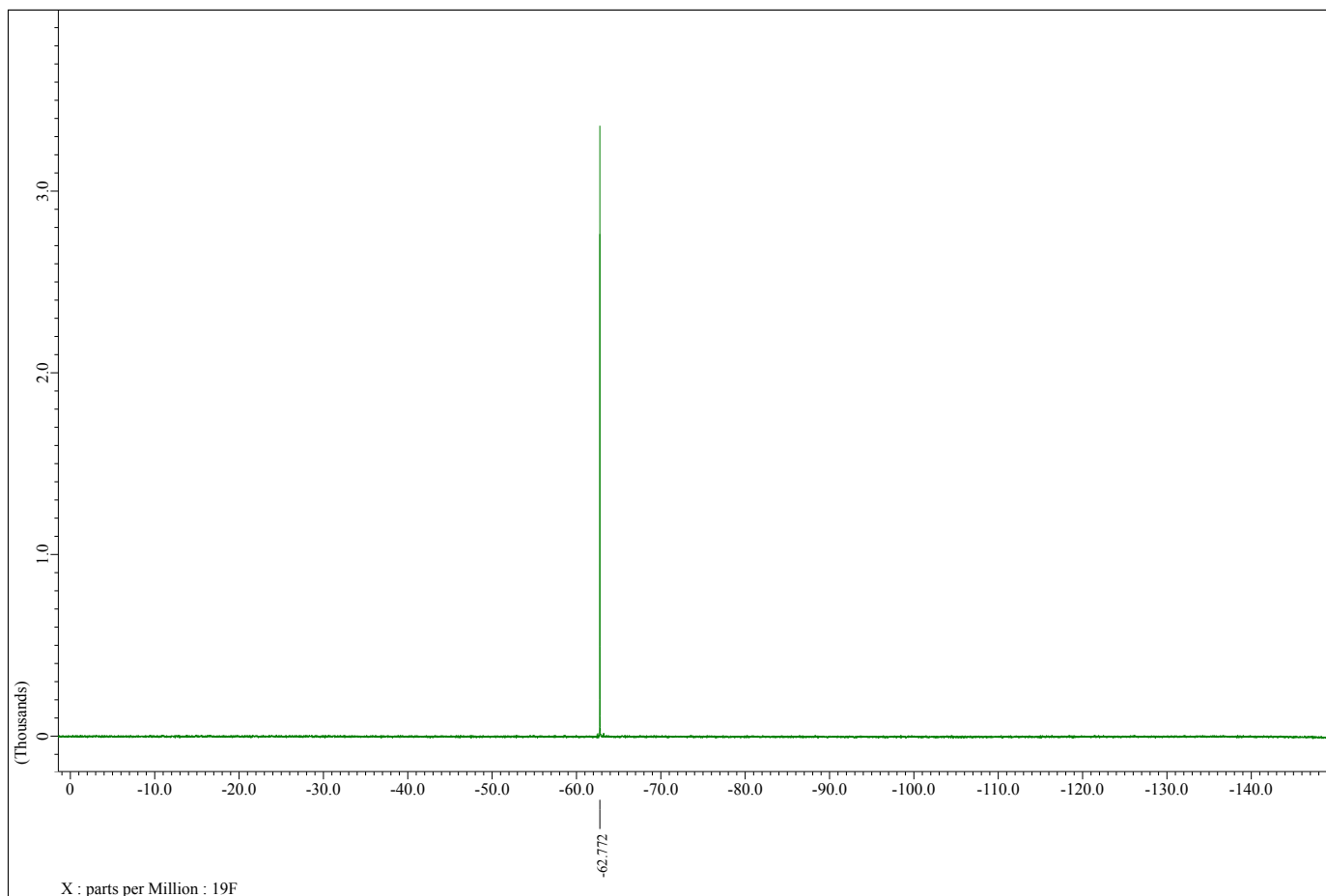


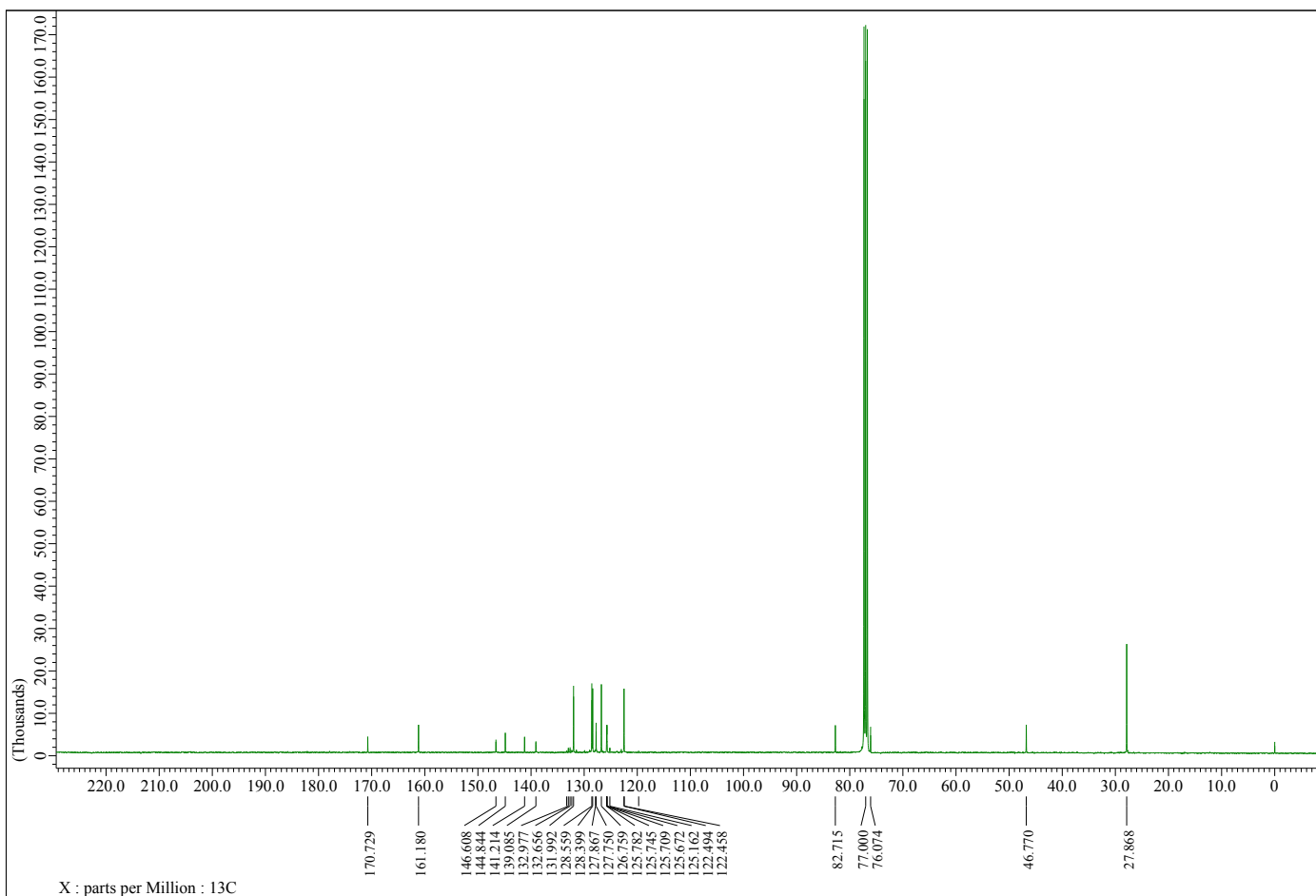
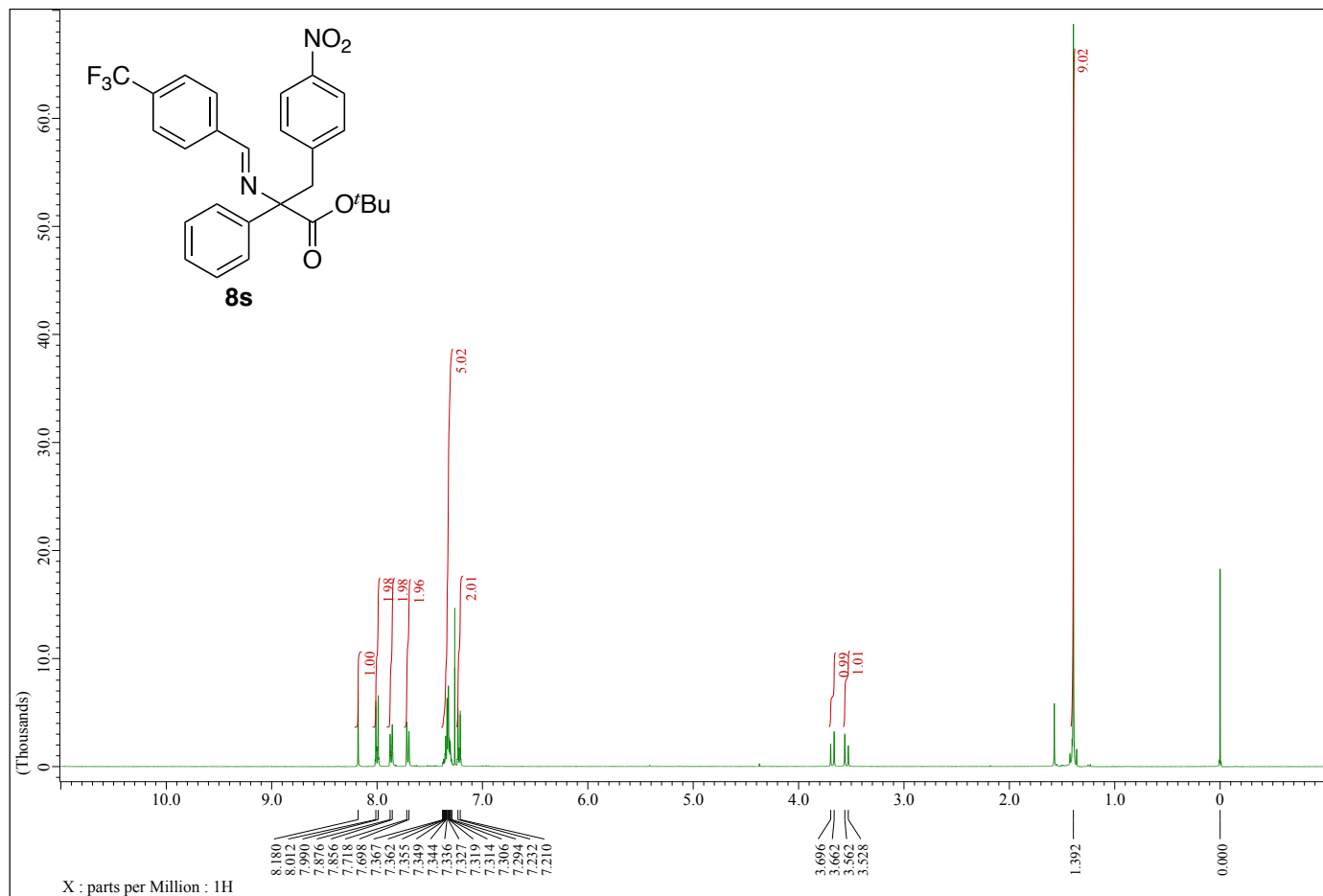


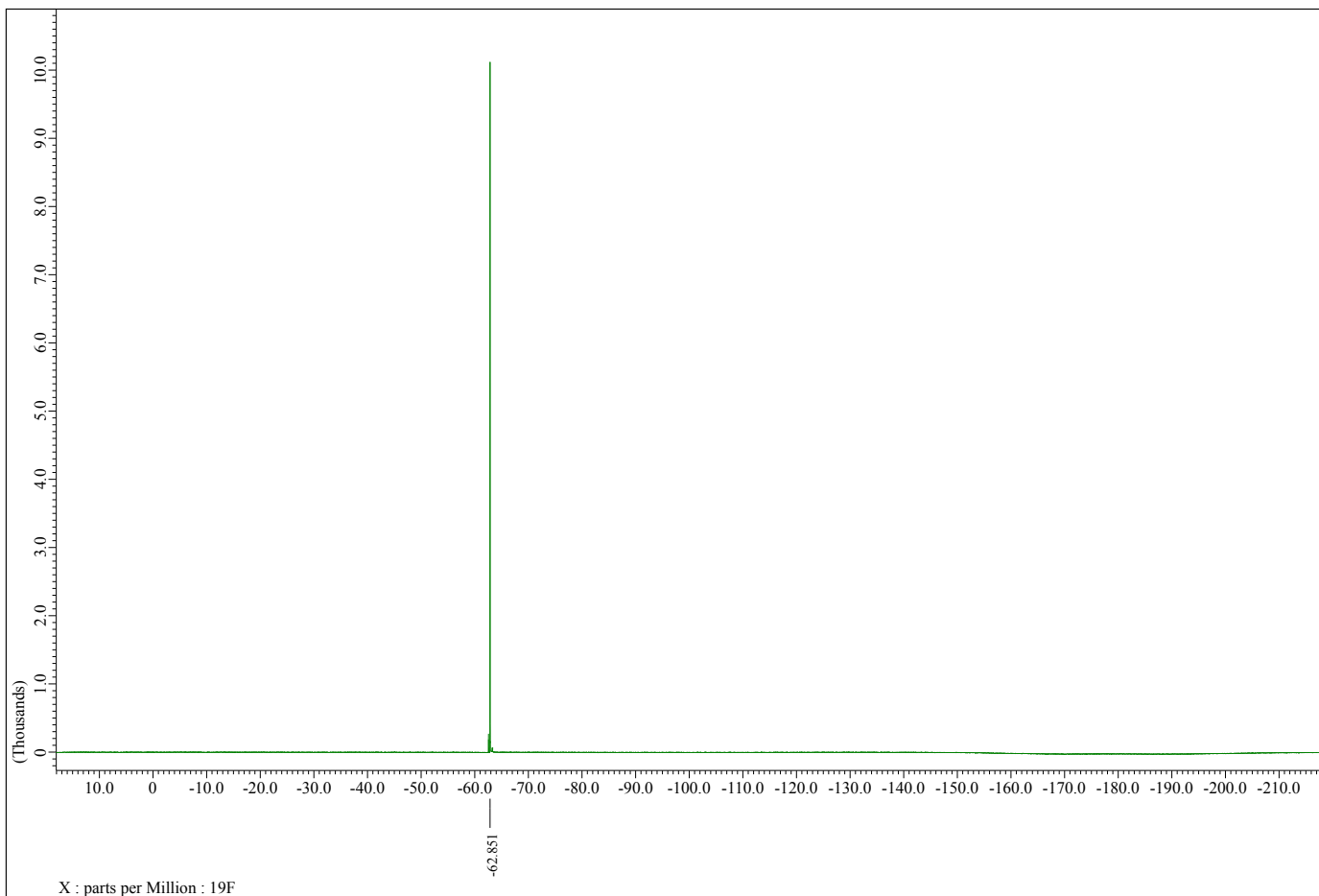


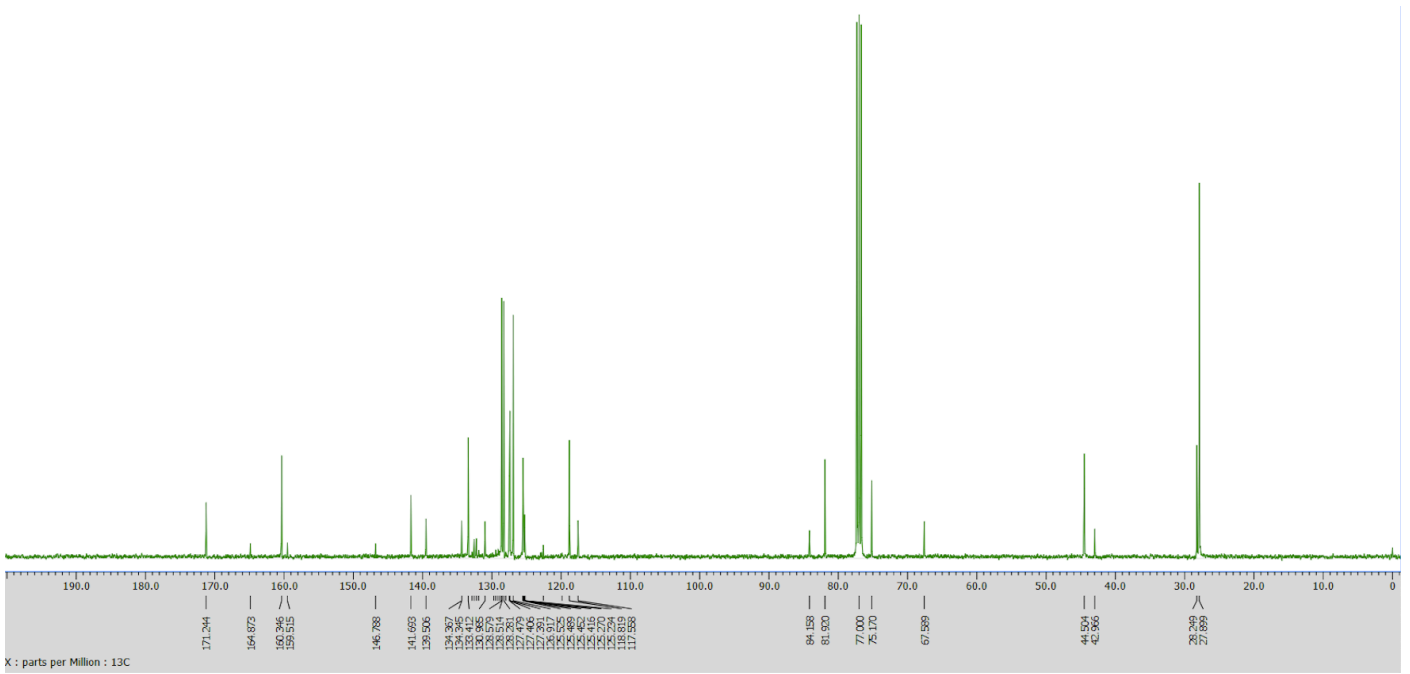
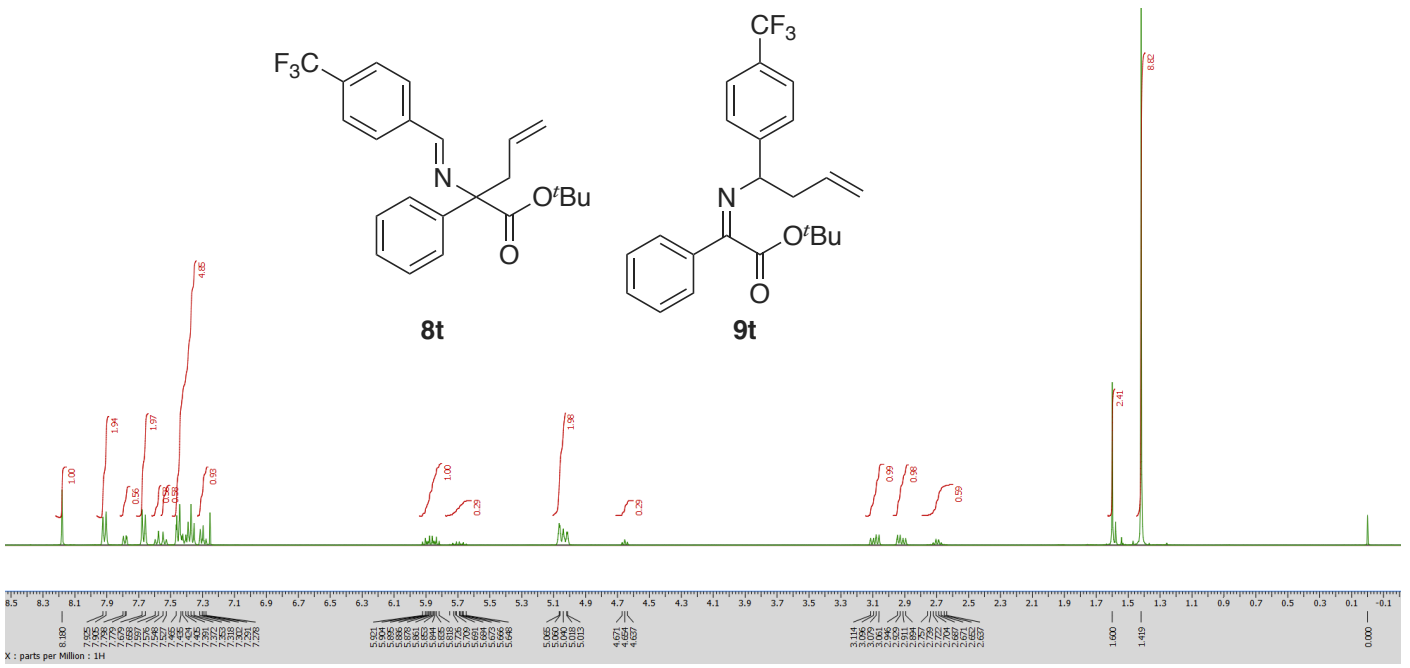
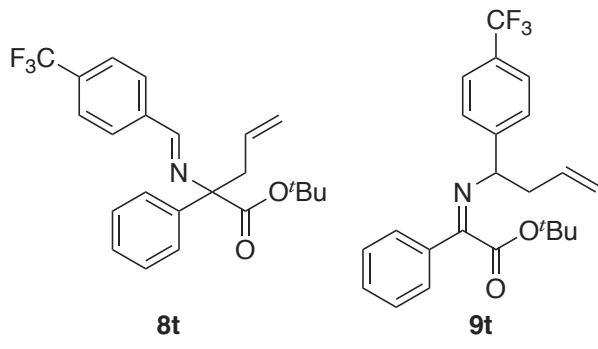


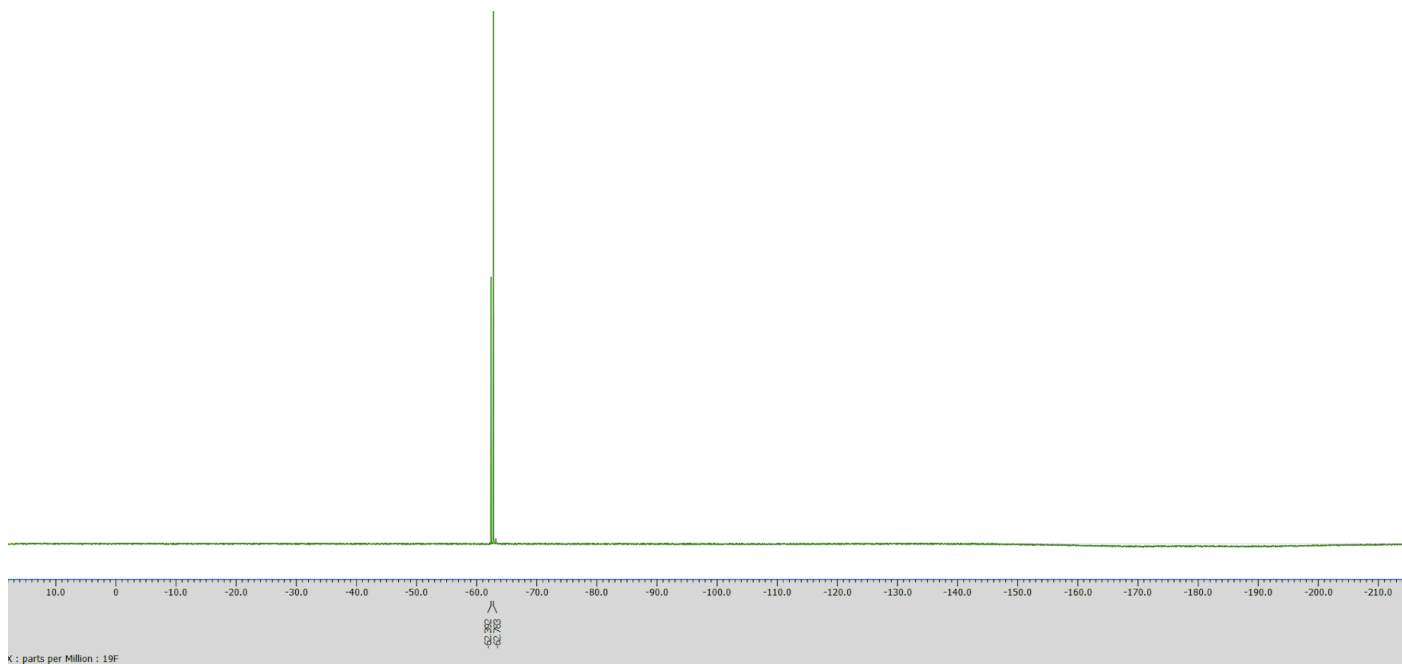




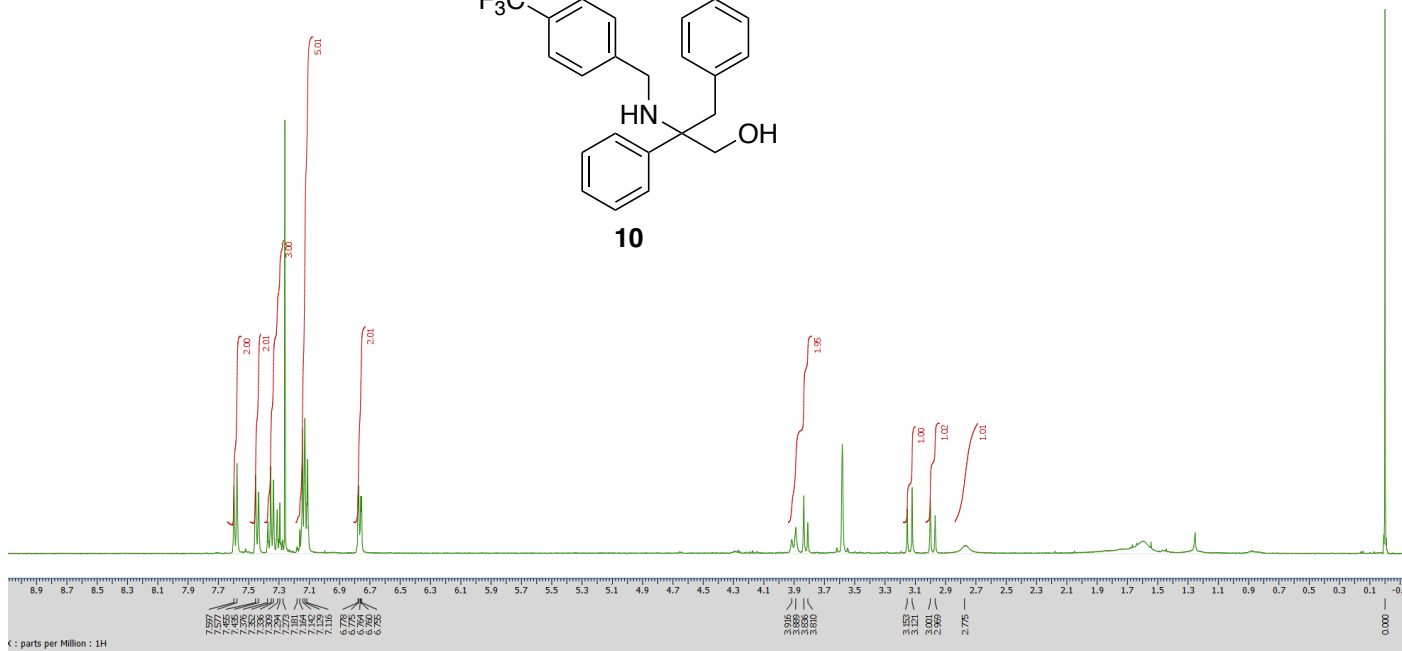
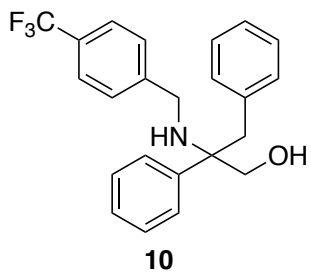


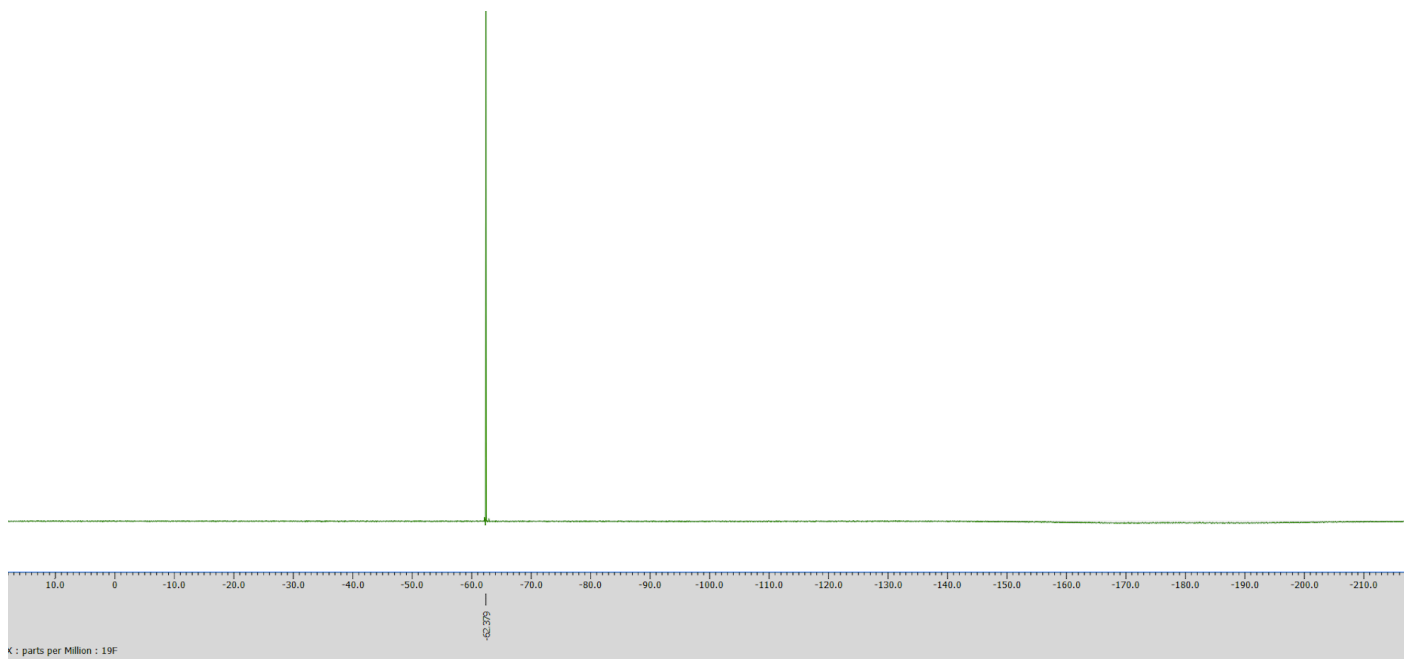
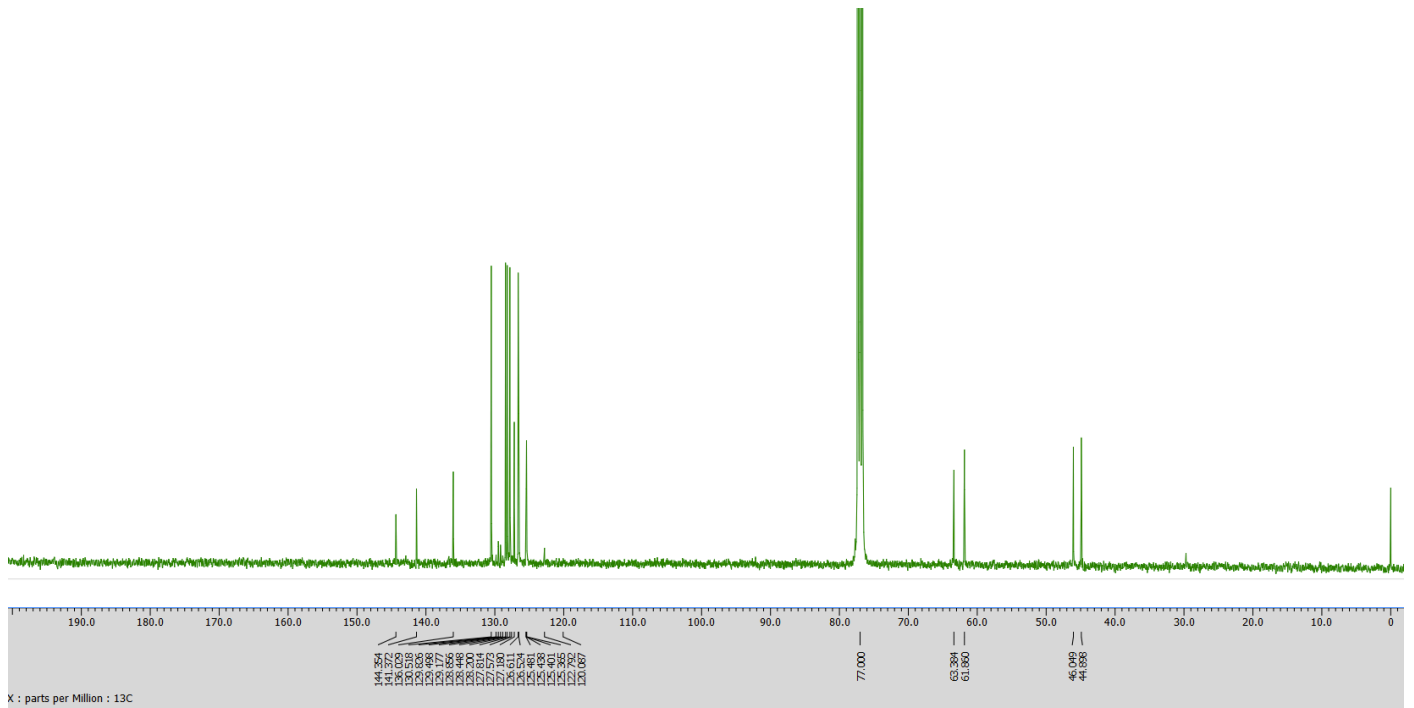


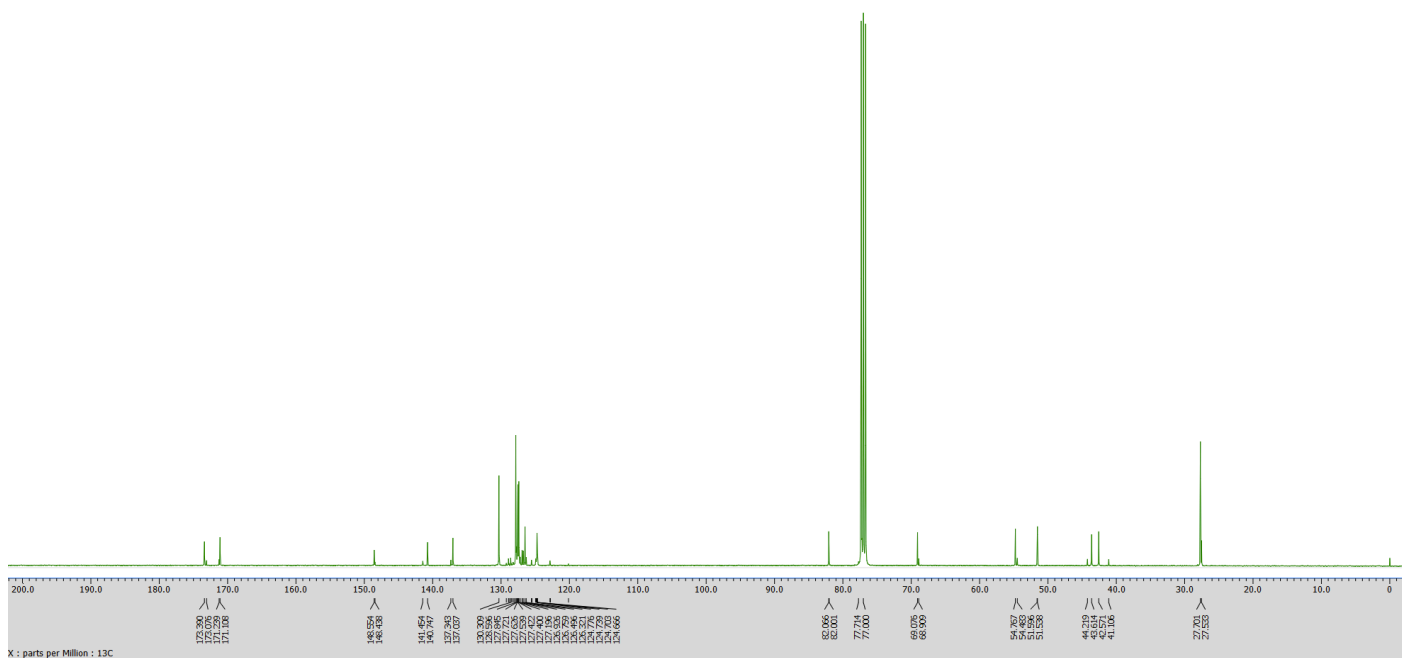
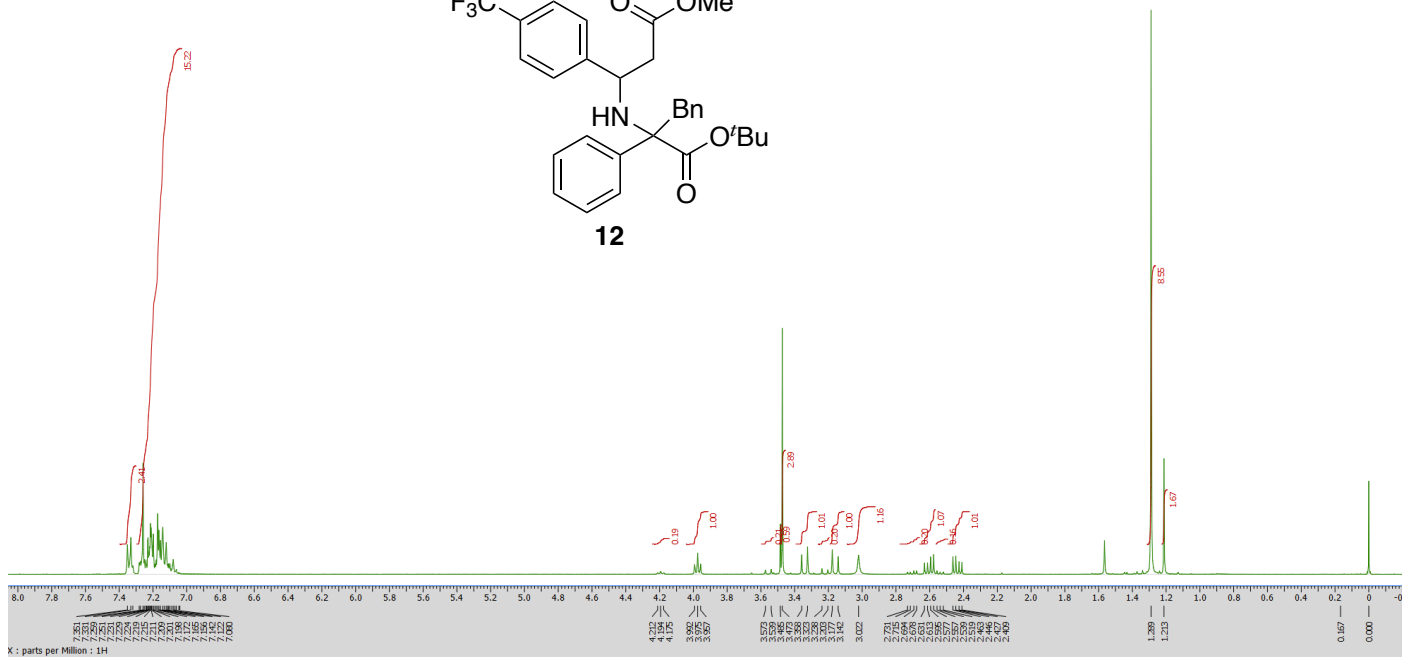
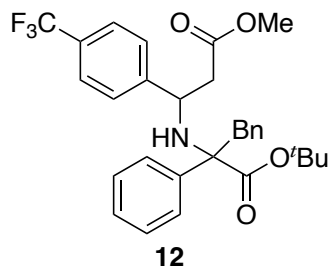


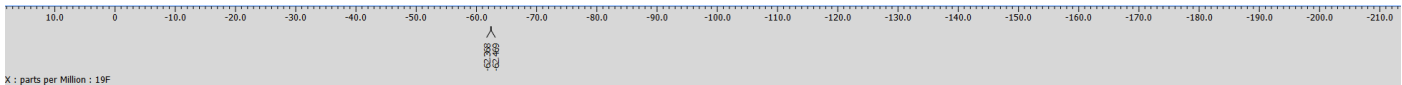


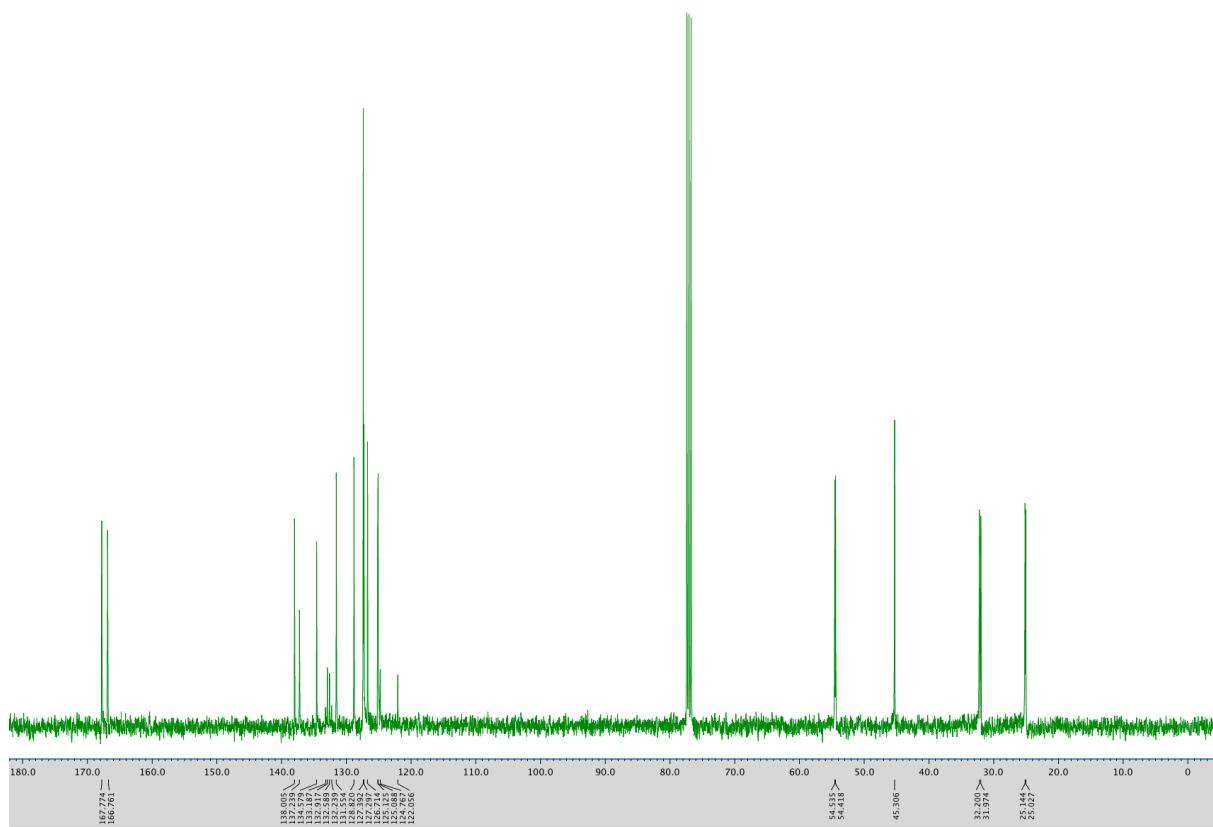
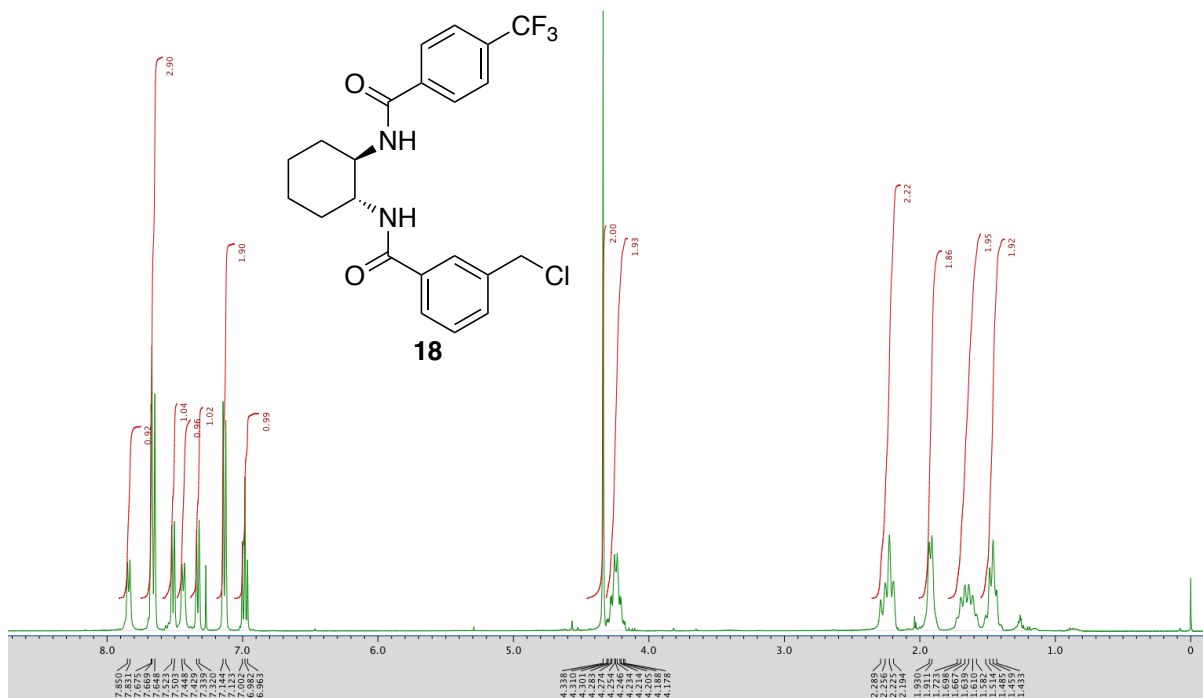


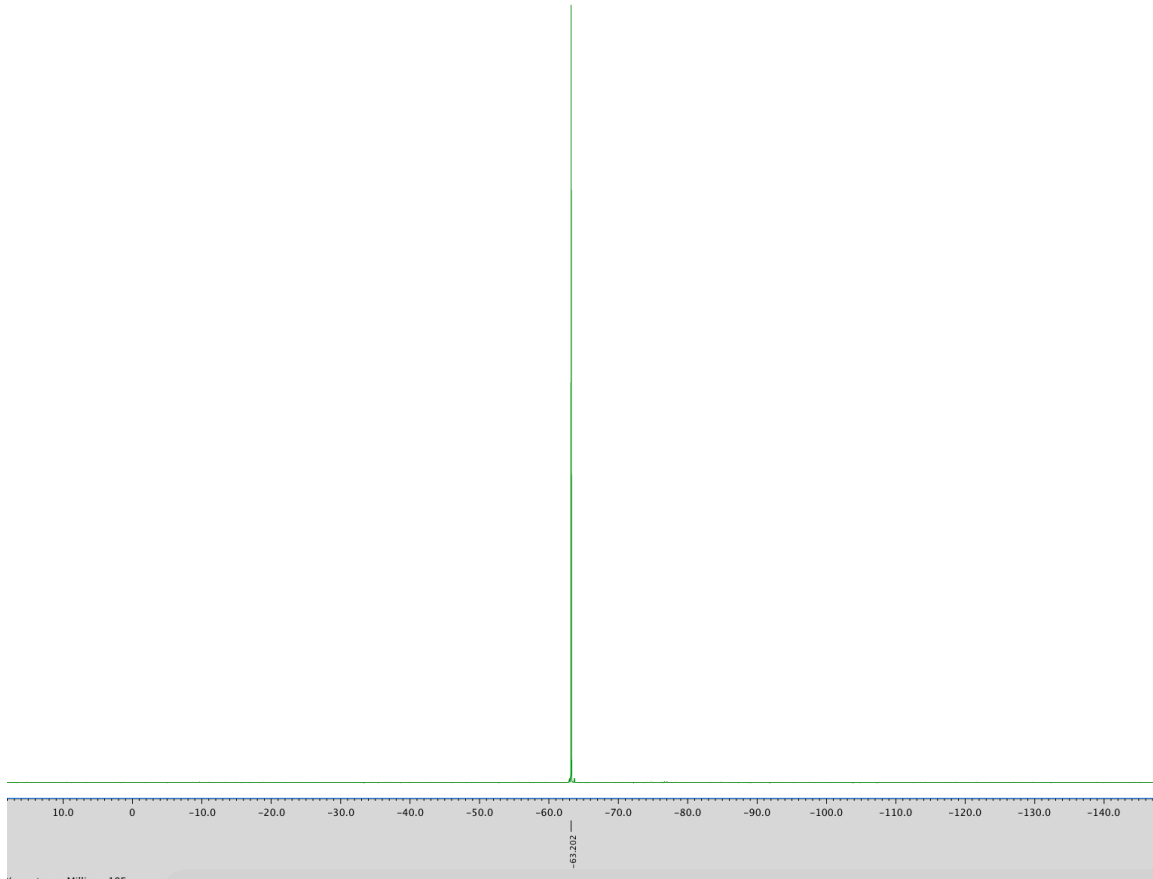


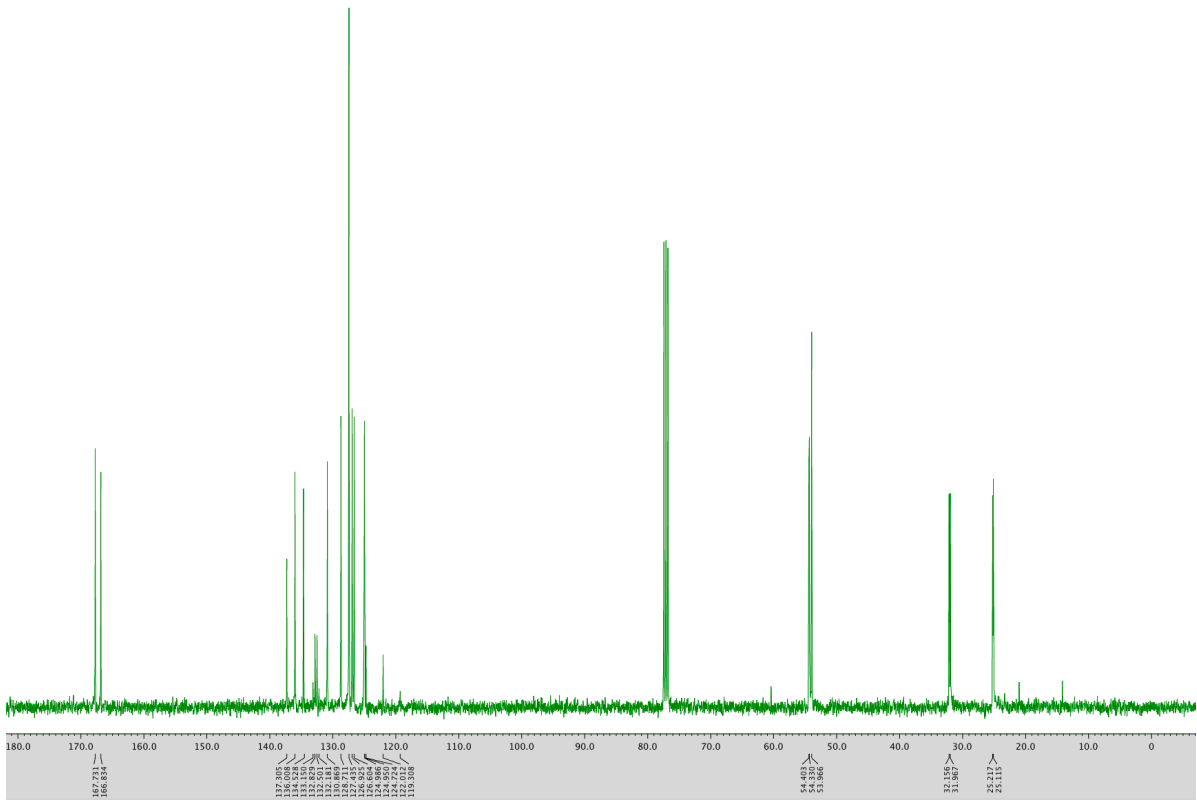
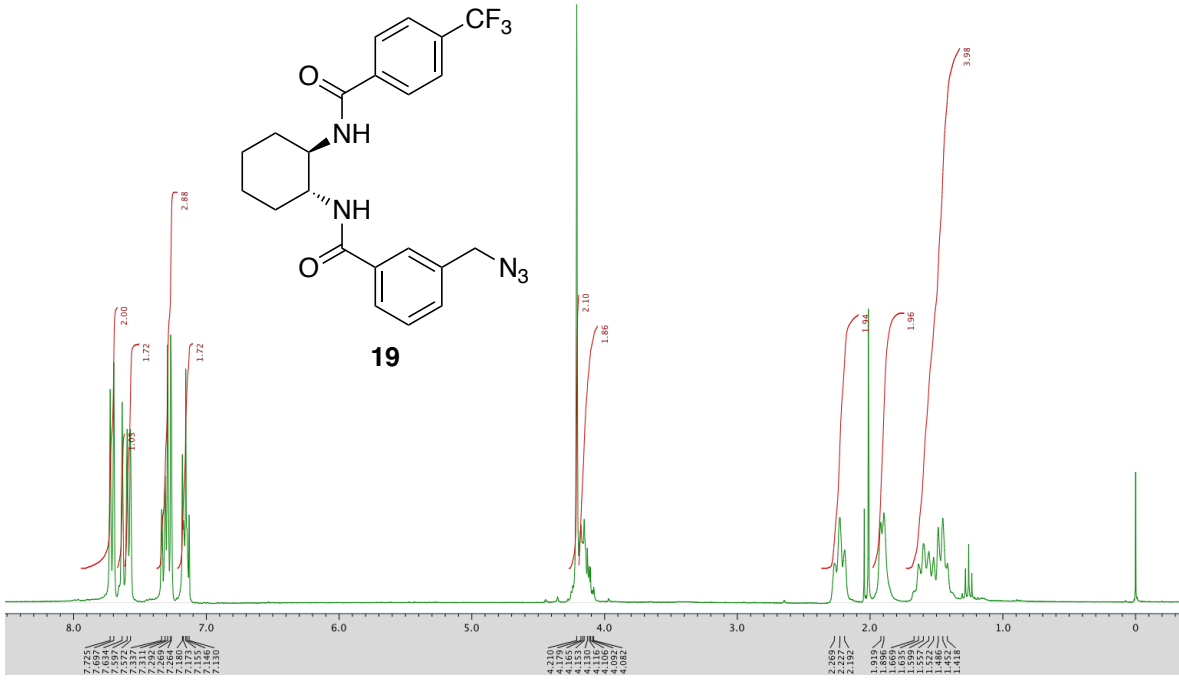


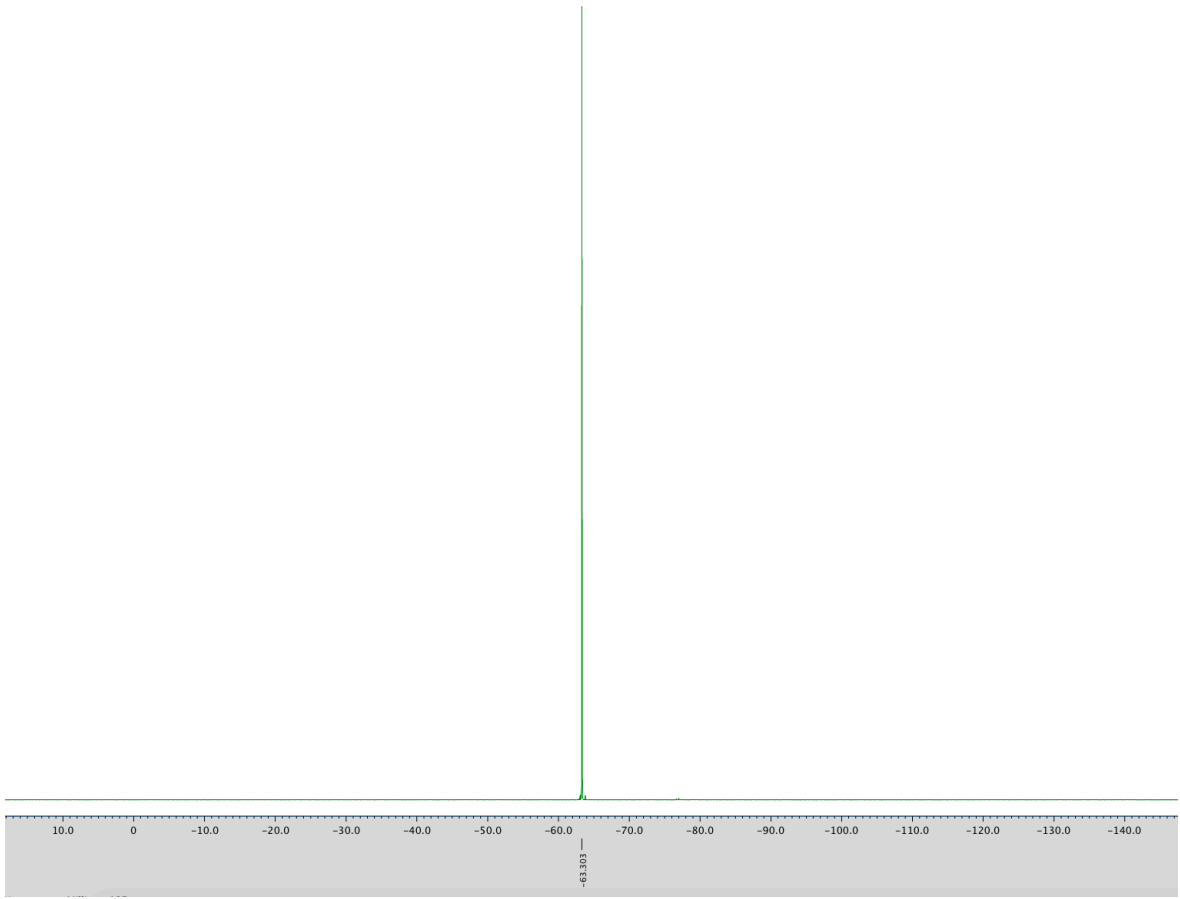




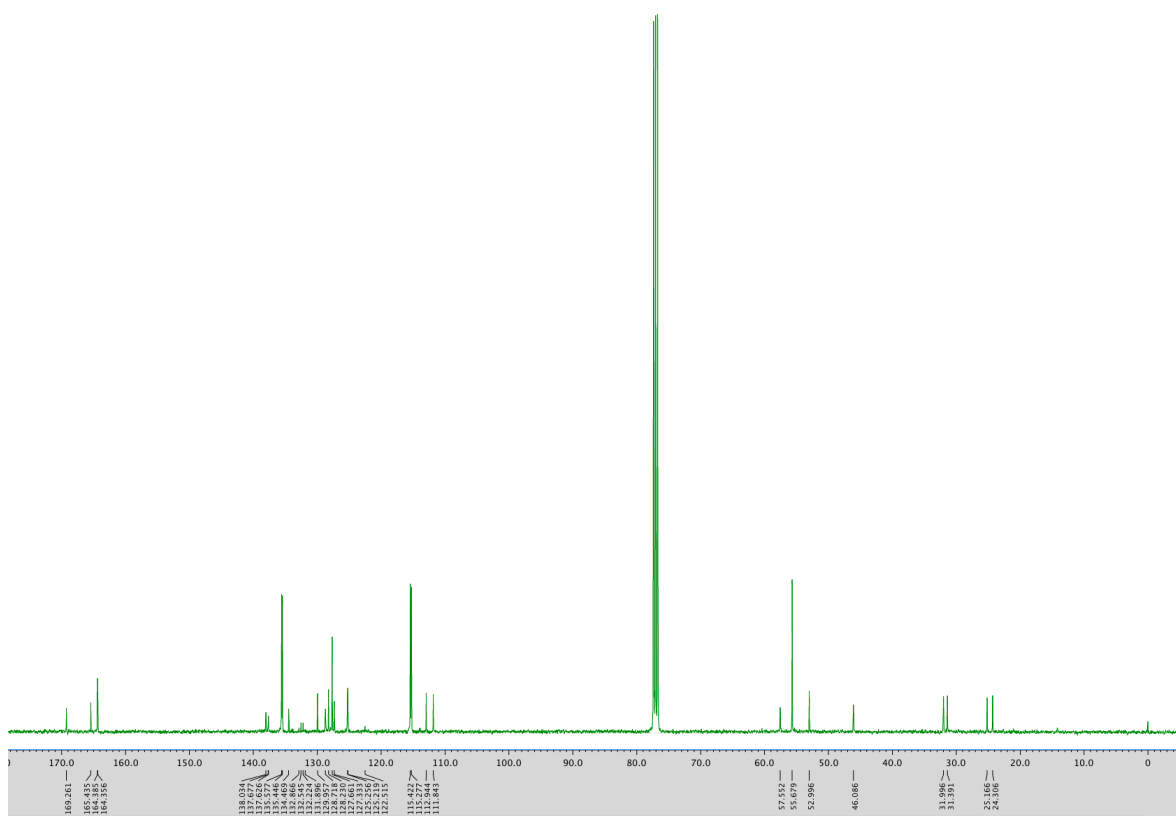
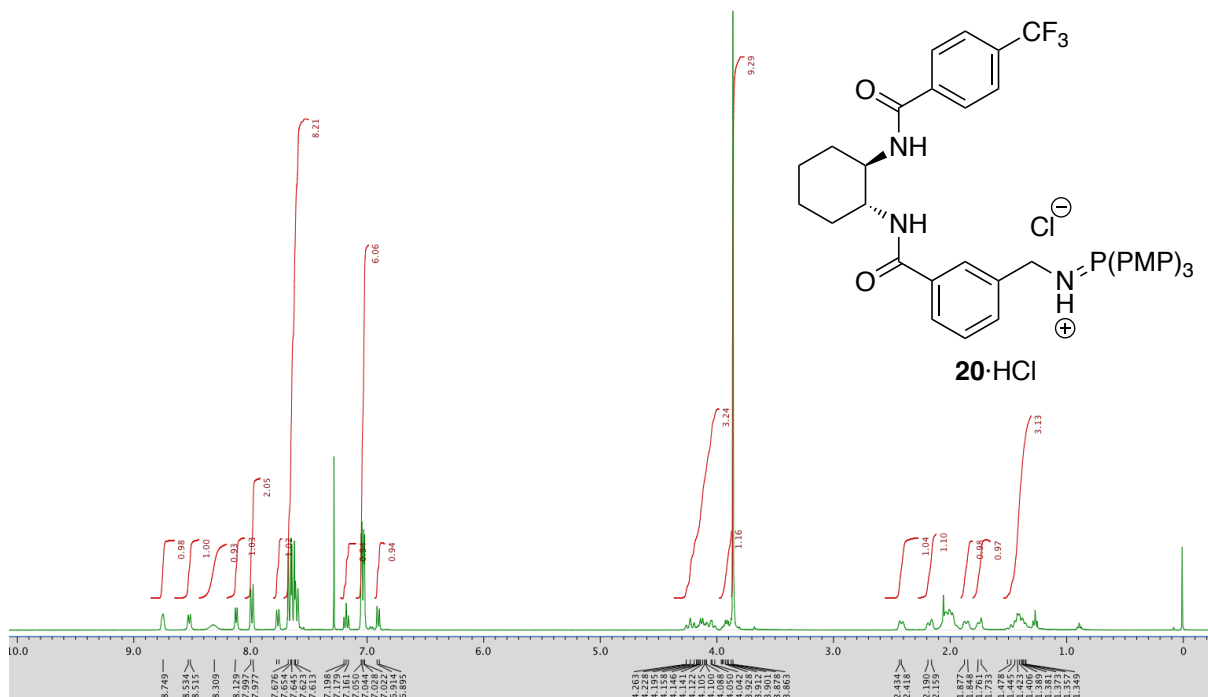


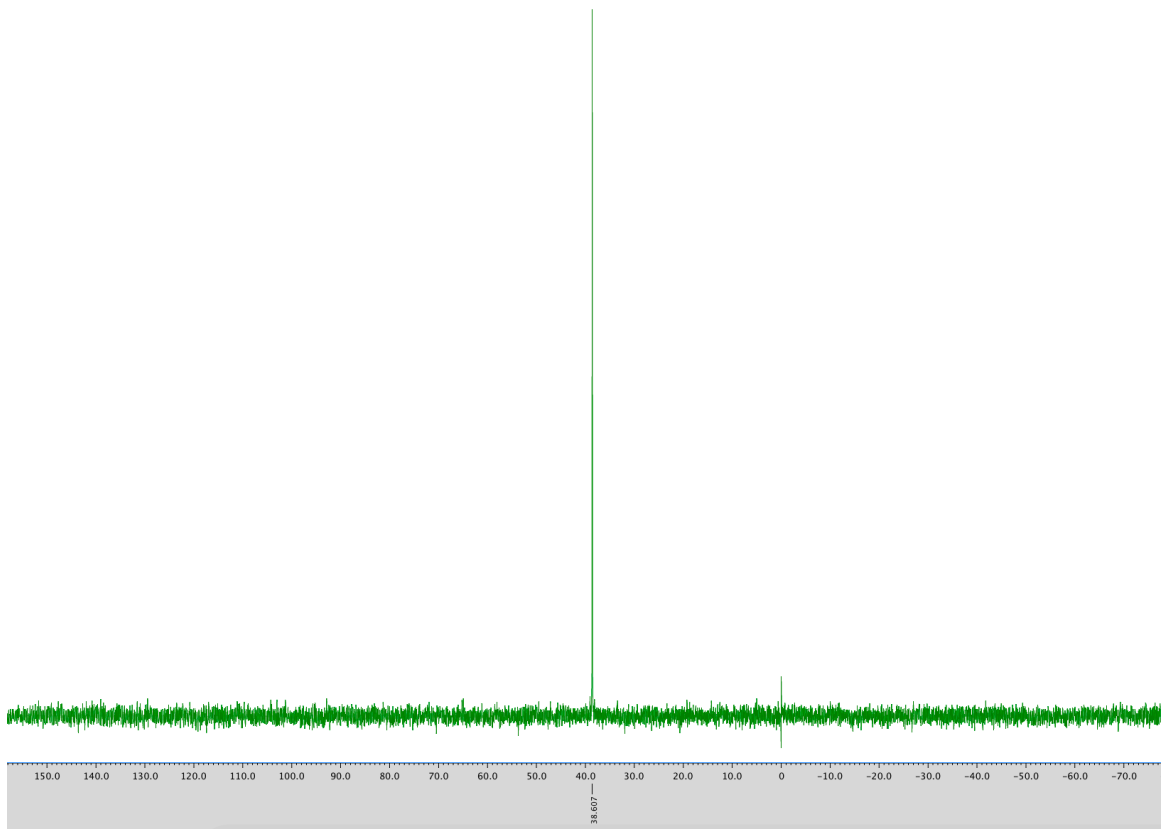
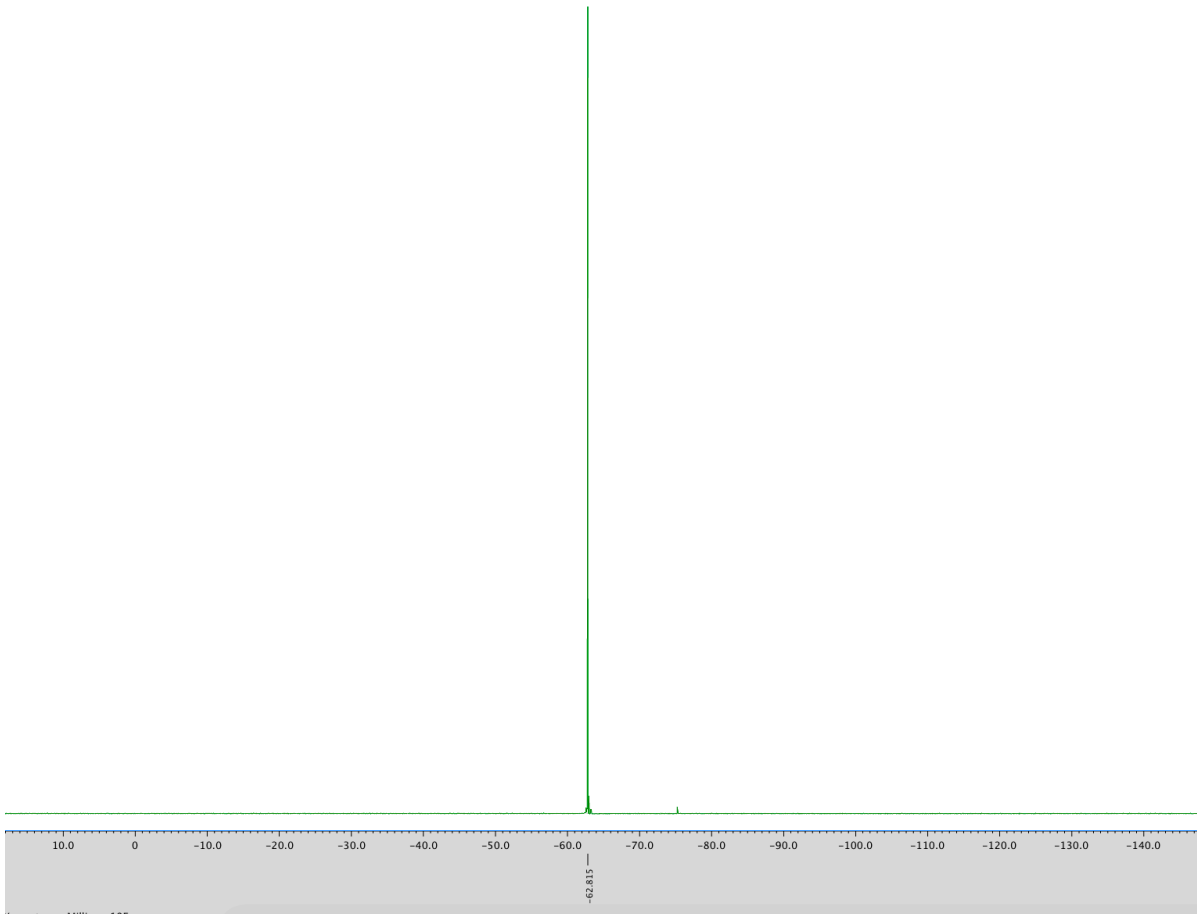


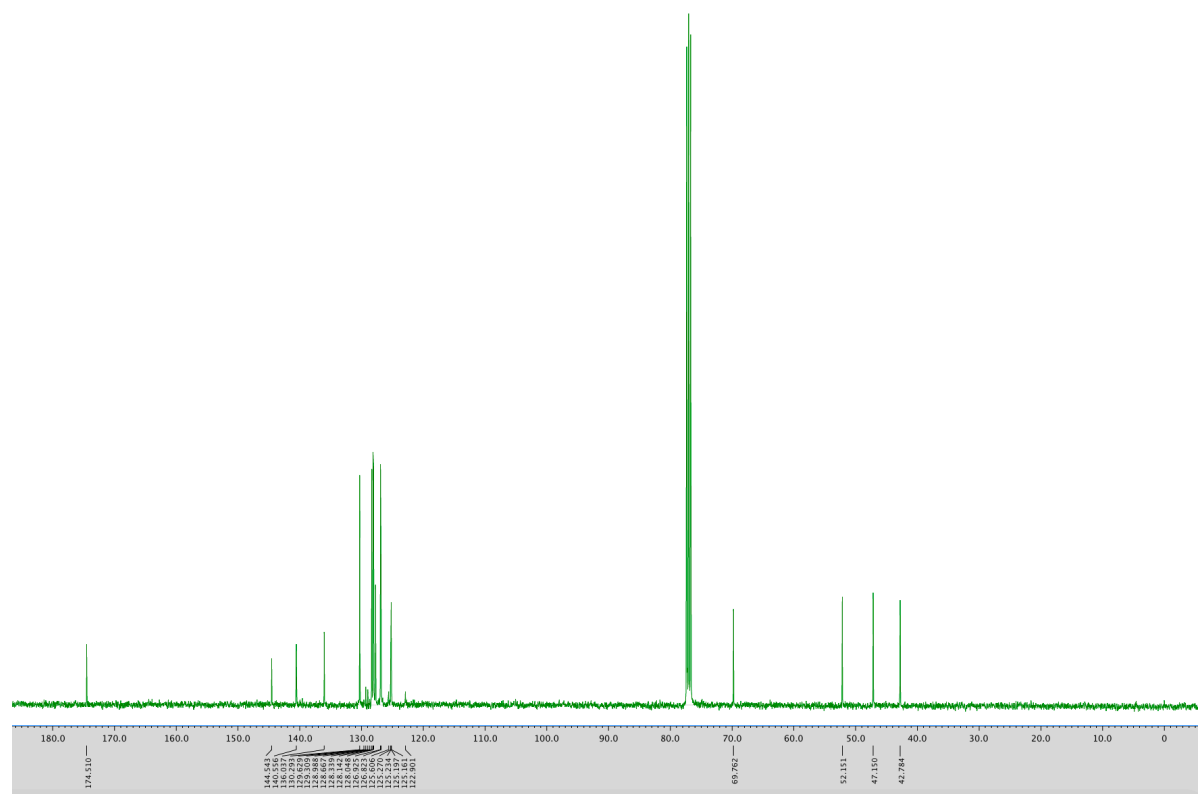
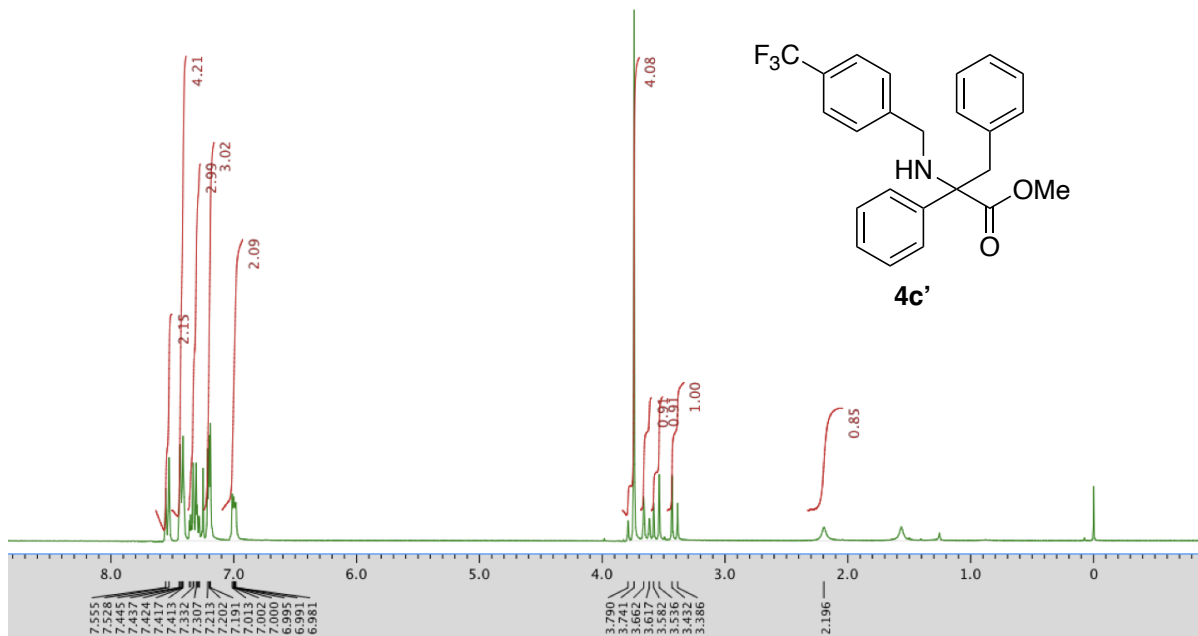


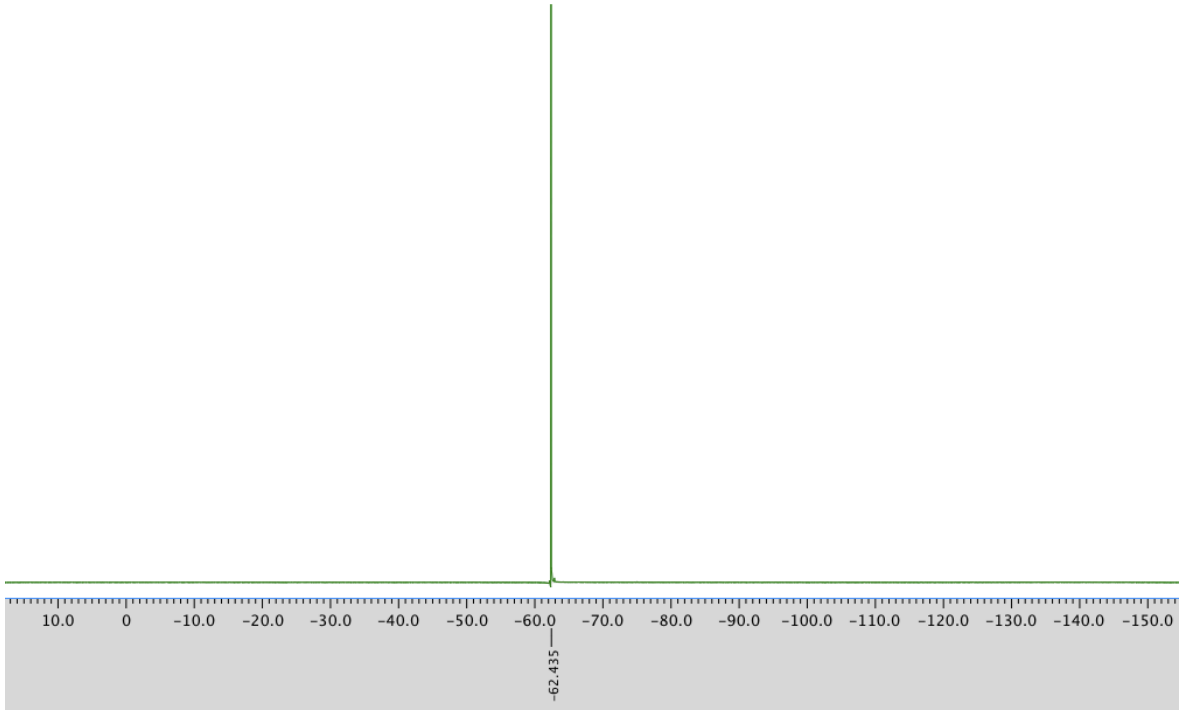


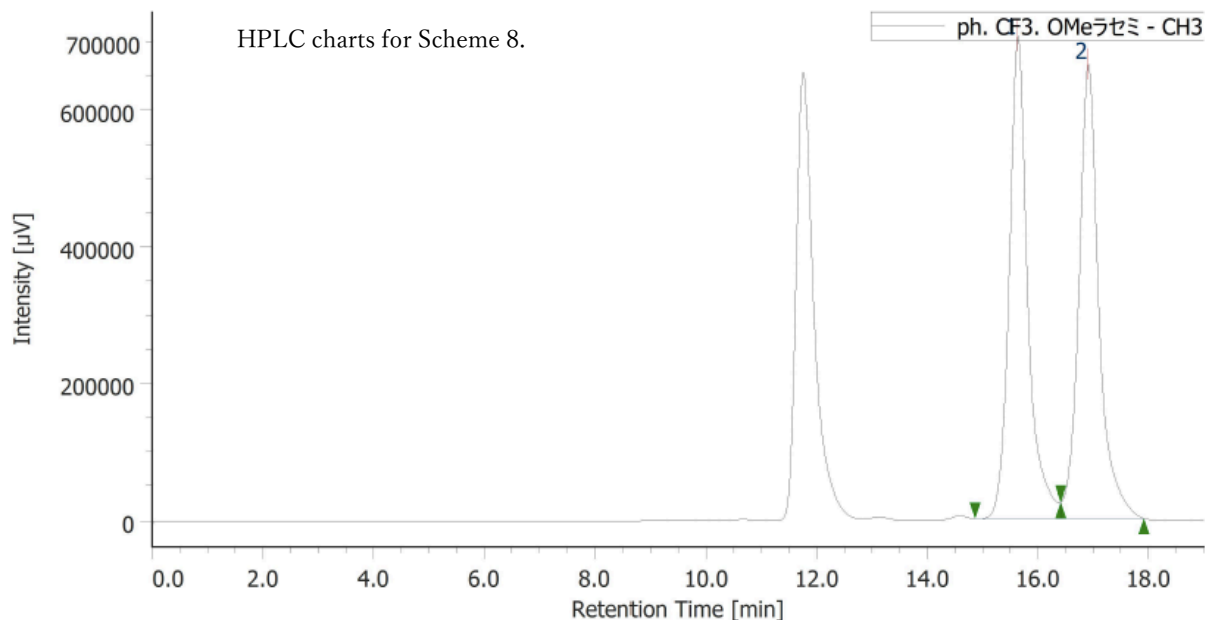




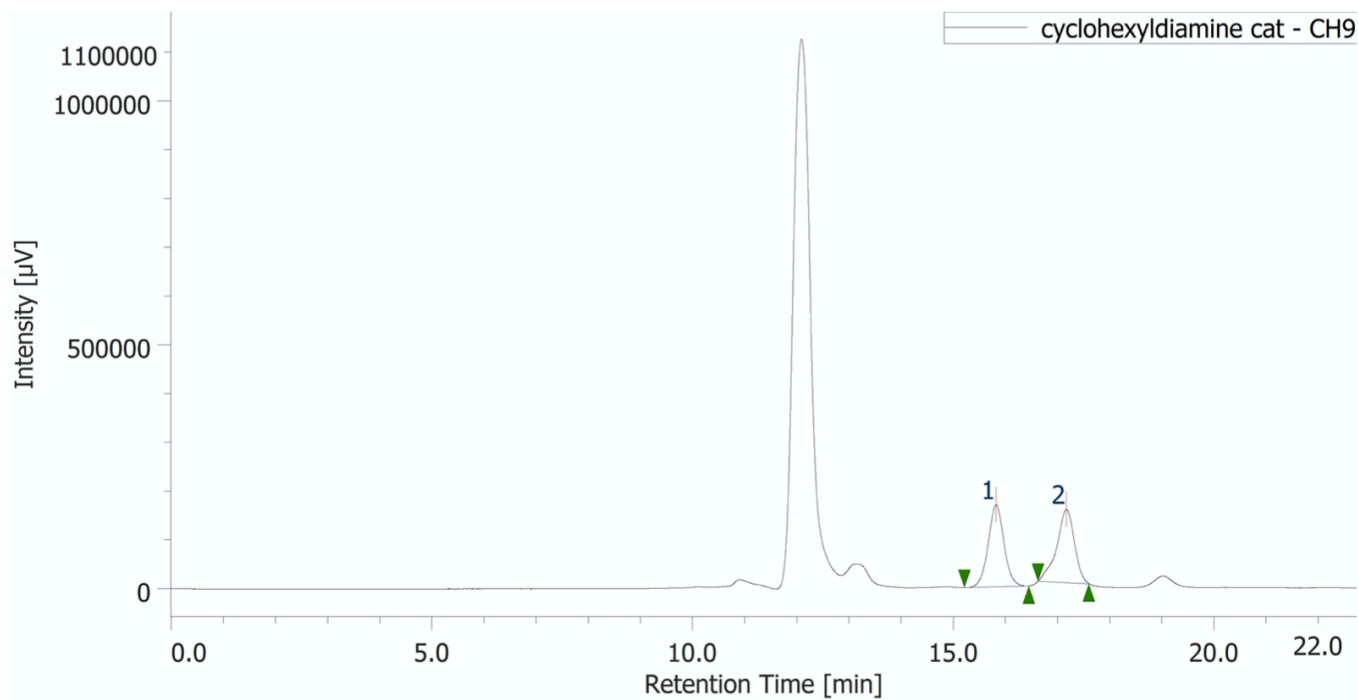








#	ピーク名	CH	tR [min]	area [μV·sec]	height [μV]	area%	height%
1	Unknown	3	15.633	16421893	704913	49.700	51.497
2	Unknown	3	16.908	16620101	663922	50.300	48.503



#	ピーク名	CH	tR [min]	面積 [μV·sec]	高さ [μV]	面積%	高さ%	定量値	NTP	分離度	シンメトリー係数	警告
1	Unknown	9	15.818	3539934	167938	50.012	52.820	N/A	13581	2.394	1.026	
2	Unknown	9	17.167	3538247	150003	49.988	47.180	N/A	13708	N/A	0.863	

## 2. Calculation results

APT charges for 14

		1
1	C	0.057578
2	C	-0.204254
3	C	0.006295
4	C	-0.234990
5	C	0.474475
6	C	-0.202360
7	C	-1.789996
8	C	2.548976
9	O	-1.175909
10	O	-1.896817
11	C	0.949861
12	C	-0.016011
13	C	-0.070054
14	C	-0.059340
15	N	1.548022
16	C	-1.702556
17	C	1.748612
18	C	-0.674597
19	C	0.832251
20	C	-2.168591
21	C	0.761228
22	C	-0.913810
23	N	4.445701
24	O	-2.085545
25	O	-1.660953
26	H	-0.004974
27	H	0.020504
28	H	0.027881
29	H	0.079067

30	H	0.074195
31	H	-0.009525
32	H	-0.015410
33	H	-0.013511
34	H	-0.018141
35	H	0.037196
36	H	-0.013053
37	H	-0.014754
38	H	-0.027899
39	H	0.047621
40	H	0.011192
41	H	0.081102
42	H	0.085323
43	H	0.090914
44	H	0.045056

Sum of APT charges = -1.00000

APT charges with hydrogens summed into heavy atoms:

1		
1	C	0.052603
2	C	-0.183750
3	C	0.034176
4	C	-0.155923
5	C	0.474475
6	C	-0.128165
7	C	-1.789996
8	C	2.548976
9	O	-1.175909
10	O	-1.896817
11	C	0.949861
12	C	-0.054456
13	C	-0.064052
14	C	-0.054372

15 N 1.548022  
 16 C -1.691364  
 17 C 1.748612  
 18 C -0.593496  
 19 C 0.917574  
 20 C -2.168591  
 21 C 0.852142  
 22 C -0.868754  
 23 N 4.445701  
 24 O -2.085545  
 25 O -1.660953

Electronic spatial extent (au):  $\langle R^{**2} \rangle =$  12639.6273

Charge= -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -13.5830 Y= 5.0781 Z= 0.5726 Tot=  
 14.5125

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -298.7349 YY= -141.7707 ZZ= -155.3366  
 XY= -2.2532 XZ= -8.7809 YZ= 0.8714

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -100.1208 YY= 56.8434 ZZ= 43.2775  
 XY= -2.2532 XZ= -8.7809 YZ= 0.8714

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= -868.3300 YYY= 55.8687 ZZZ= 0.7060 XYY=  
 -44.2275

XXY= 63.6739 XXZ= 25.6566 XZZ= 10.1374 YZZ=  
 17.1797

YYZ= -7.1366 XYZ= 6.4813

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -18644.1341 YYYY= -4890.0285 ZZZZ= -434.4642 XXXY=  
 202.0320

XXXZ= -226.6219 YYYYX= -110.7852 YYYYZ= 31.6756 ZZZX=  
 4.1115



ZZZY= 5.5002 XXYY= -2866.3736 XXZZ= -2041.6761 YYZZ= -  
996.3062  
XXYZ= -25.0263 YYXZ= -24.8568 ZZXY= -56.1882  
N-N= 2.030127132297D+03 E-N=-6.747352665266D+03 KE= 1.135174893490D+03

APT charges for 15

1

1	C	0.132016
2	C	-0.297806
3	C	0.112695
4	C	-0.256308
5	C	0.749801
6	C	-0.369664
7	C	-1.802282
8	C	2.324376
9	O	-1.237073
10	O	-1.706005
11	C	0.918701
12	C	0.002765
13	C	-0.053537
14	C	-0.052689
15	N	1.209611
16	C	-1.162417
17	C	1.255011
18	C	-0.448009
19	C	0.369335
20	C	-0.972621
21	C	0.390596
22	C	-0.671160
23	C	2.949834
24	F	-0.847072
25	F	-1.002019
26	F	-0.860207
27	H	-0.000581
28	H	0.018222
29	H	0.016665
30	H	0.074784

31	H	0.094243
32	H	-0.021044
33	H	-0.020534
34	H	-0.018871
35	H	-0.027412
36	H	0.038027
37	H	-0.021607
38	H	-0.021826
39	H	-0.030169
40	H	0.037062
41	H	-0.010711
42	H	0.075974
43	H	0.050864
44	H	0.050215
45	H	0.040826

Sum of APT charges = -1.00000

APT charges with hydrogens summed into heavy atoms:

1		
1	C	0.131435
2	C	-0.279584
3	C	0.129360
4	C	-0.181523
5	C	0.749801
6	C	-0.275421
7	C	-1.802282
8	C	2.324376
9	O	-1.237073
10	O	-1.706005
11	C	0.918701
12	C	-0.057684
13	C	-0.064529
14	C	-0.067622

15 N 1.209611  
 16 C -1.173128  
 17 C 1.255011  
 18 C -0.372034  
 19 C 0.420199  
 20 C -0.972621  
 21 C 0.440811  
 22 C -0.630334  
 23 C 2.949834  
 24 F -0.847072  
 25 F -1.002019  
 26 F -0.860207

Electronic spatial extent (au):  $\langle R^2 \rangle = 14287.9823$

Charge = -1.0000 electrons

Dipole moment (field-independent basis, Debye):

X = 2.4449 Y = 5.2320 Z = 0.0468 Tot = 5.7753

Quadrupole moment (field-independent basis, Debye-Ang):

XX = -237.1129 YY = -152.4060 ZZ = -162.9796  
 XY = -11.0577 XZ = -5.1864 YZ = 0.2003

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX = -52.9467 YY = 31.7602 ZZ = 21.1866  
 XY = -11.0577 XZ = -5.1864 YZ = 0.2003

Octapole moment (field-independent basis, Debye-Ang<sup>2</sup>):

XXX = -43.4763 YYY = 70.7153 ZZZ = -0.2681 XYY = 43.9035

XXY = 52.2995 XXZ = 15.5042 XZZ = 30.5530 YZZ = 18.9064

YYZ = -4.3204 XYZ = 4.7761

Hexadecapole moment (field-independent basis, Debye-Ang<sup>3</sup>):

XXXX = -15347.7890 YYYY = -5187.0152 ZZZZ = -496.3790 XXXY = 71.3648 -

XXXZ=	-158.3663	YYYYX=	-240.2914	YYYYZ=	26.3293	ZZZX=	
-1.9766							
ZZZY=	1.6191	XXYY=	-2961.9583	XXZZ=	-2326.4079	YYZZ=	-
1037.7977							
XXYZ=	-46.1228	YYXZ=	-6.8933	ZZXY=	-66.7223		
N-N=	2.205285503500D+03	E-N=-	7.419783988978D+03	KE=	1.266903673763D+03		
Exact polarizability:	737.070	84.562	455.238	-14.079	1.397	233.400	
Approx polarizability:	794.079	81.974	488.514	-20.042	2.232	258.874	