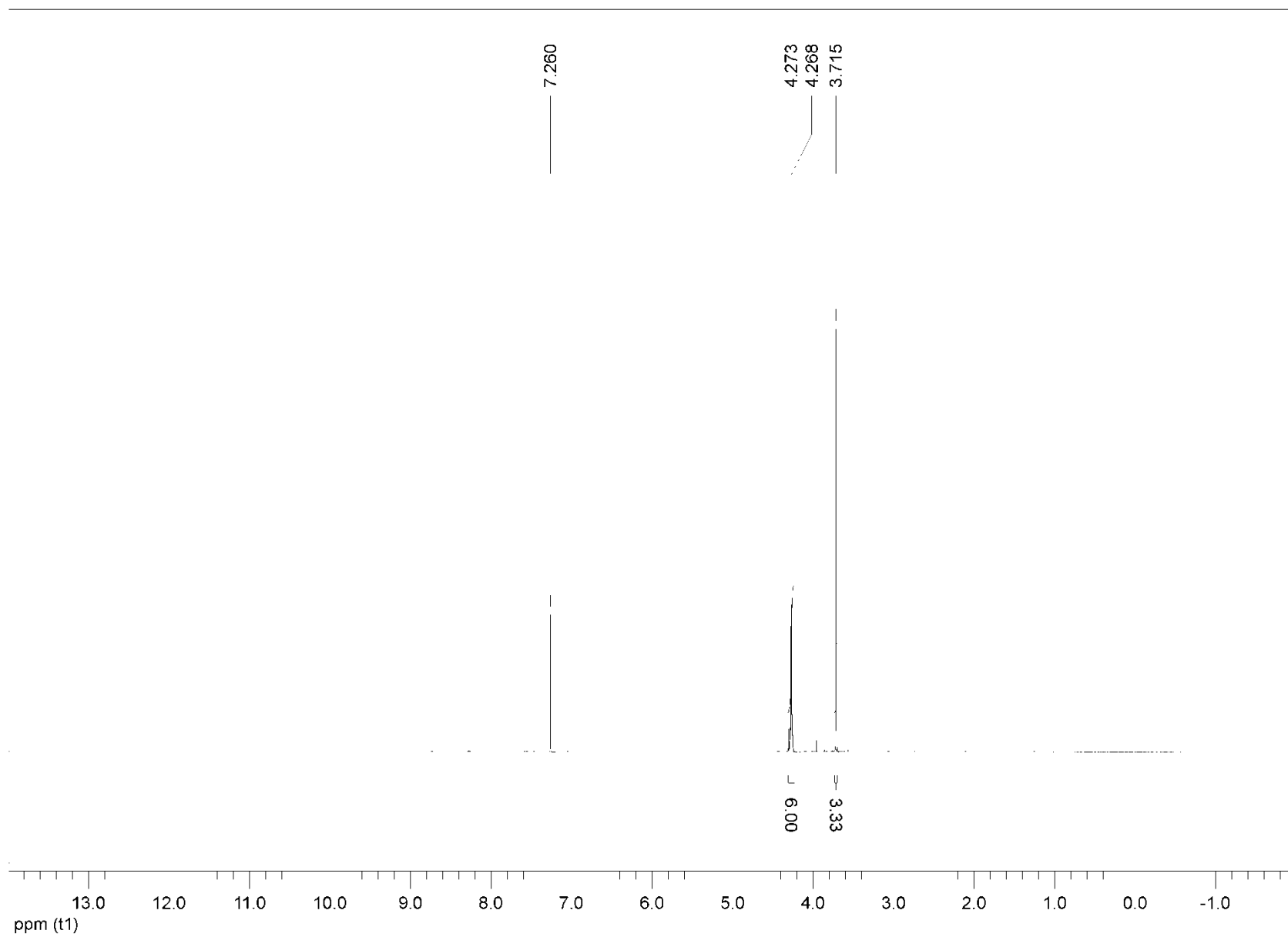


## Supplementary Material –Table of Contents

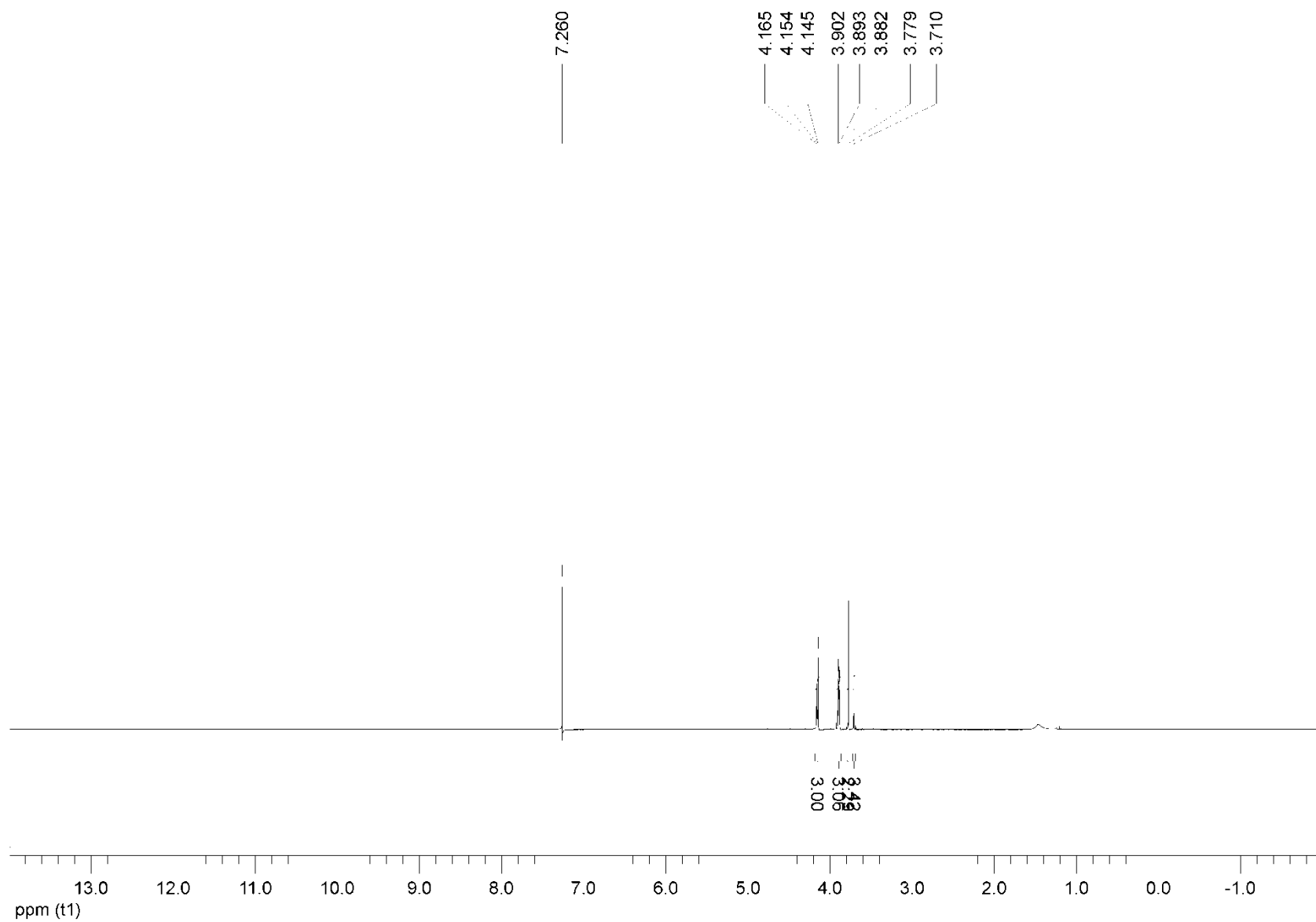
1. 4-Methoxycarbonylcubane Carboxylic Acid (20) –  $^1\text{H}$  NMR
2. (4-Methoxycarbonyl)cubylmethanol (11a) –  $^1\text{H}$  NMR
3. (4-Methoxycarbonyl)cubylmethyl p-nitrophenoxide (11b) –  $^1\text{H}$  NMR
4. (4-Methoxycarbonyl)cubylmethyl p-nitrophenoxide (11b) –  $^{13}\text{C}$  NMR
5. (4-Methoxycarbonyl)cubylmethyl p-nitrophenoxide (11b) – HR MS
6. (4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate (11c) –  $^1\text{H}$  NMR
7. (4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate (11c) –  $^{13}\text{C}$  NMR
8. (4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate(11c) – HR MS
9. (4-Methoxycarbonyl)cubylmethyl 2-nitrobenzoate (11d) –  $^1\text{H}$  NMR
10. (4-Methoxycarbonyl)cubylmethyl 2-nitrobenzoate (11d) –  $^{13}\text{C}$  NMR
11. (4-Methoxycarbonyl)cubylmethyl 2-nitrobenzoate (11d) – HR MS
12. (4-Methoxycarbonyl)cubylmethyl 2,2,2-trichloroacetate (11e) –  $^1\text{H}$  NMR
13. (4-Methoxycarbonyl)cubylmethyl 2,2,2-trichloroacetate (11e) –  $^{13}\text{C}$  NMR
14. (4-Methoxycarbonyl)cubylmethyl 2,2,2-trichloroacetate (11e) – HR MS
15. (4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f) –  $^1\text{H}$  NMR
16. (4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f) –  $^{13}\text{C}$  NMR
17. (4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f) – HR MS

Pages 18-32. Final Z matrices for 11a, 11c, 11f, 18a, 18c, 18f, 16a, 16c, 16f, 19a, 19c, 19f, 13a, 13c, 13f respectively

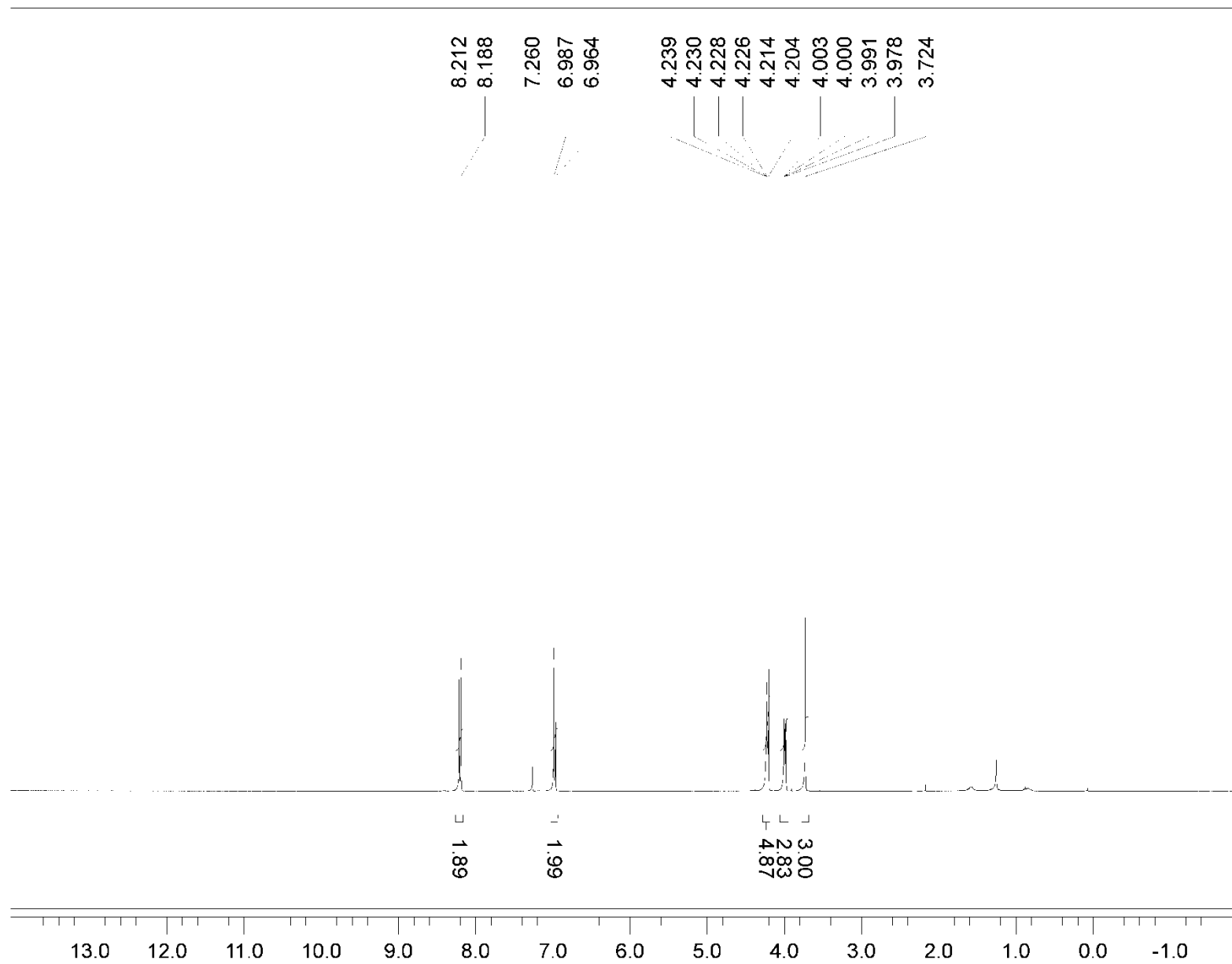
# 1. 4-Methoxycarbonylcubane Carboxylic Acid (20) – $^1\text{H}$ NMR



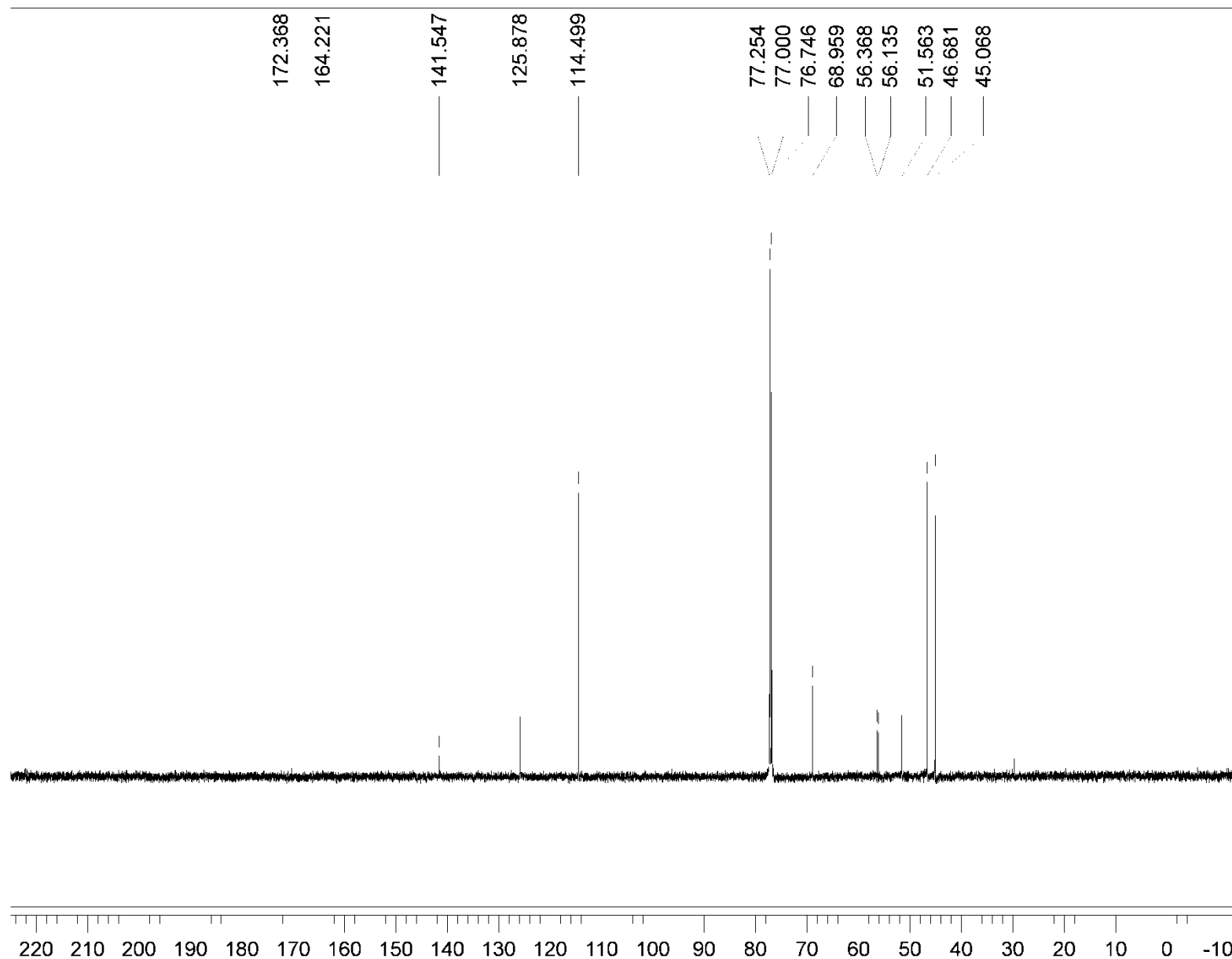
## 2. (4-Methoxycarbonyl)cubylmethanol (11a) – $^1\text{H}$ NMR



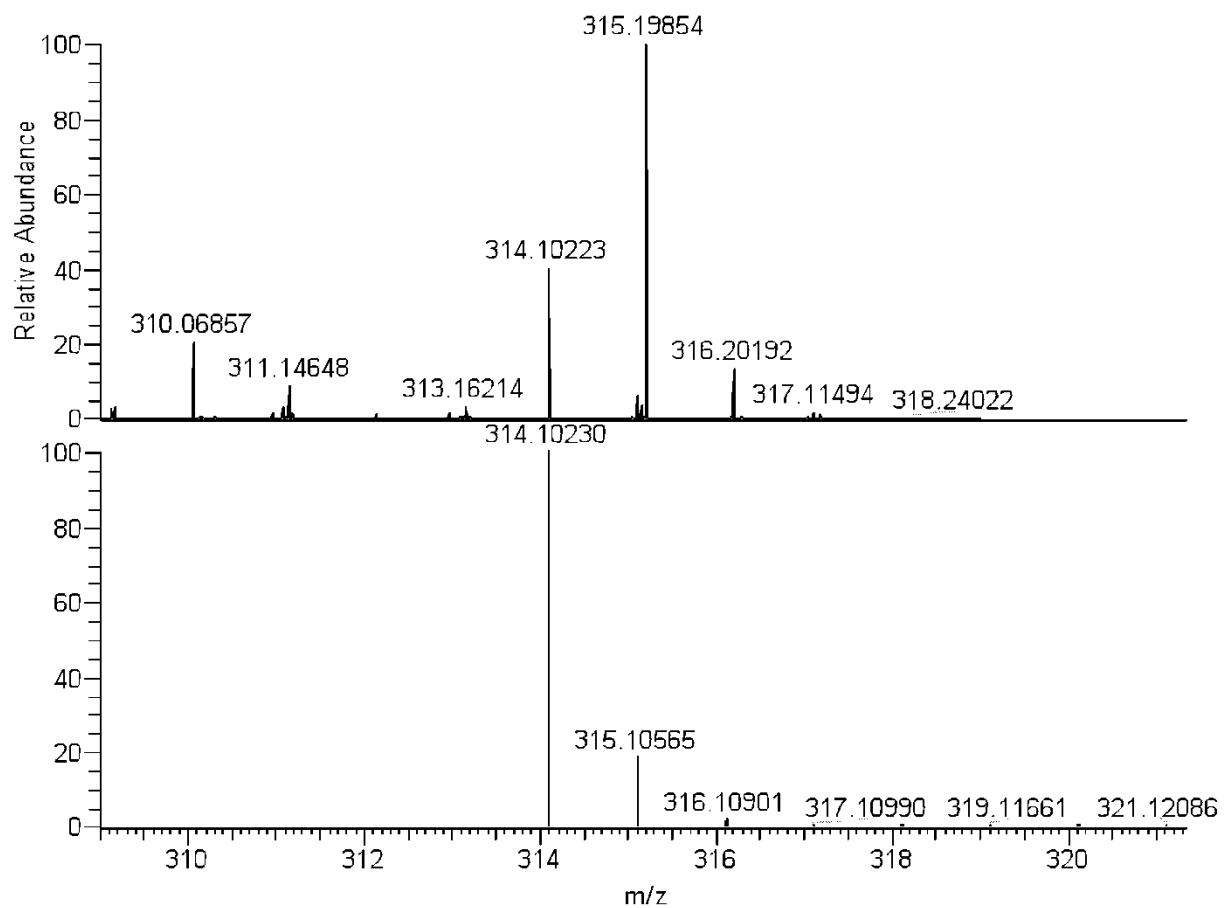
### 3. (4-Methoxycarbonyl)cubylmethyl p-nitrophenoxide (11b) – $^1\text{H}$ NMR



#### 4. (4-Methoxycarbonyl)cubylmethyl p-nitrophenoxide (11b) – $^{13}\text{C}$ NMR



## 5. (4-Methoxycarbonyl)cubylmethyl p-nitrophenoxide (11b) – HR MS



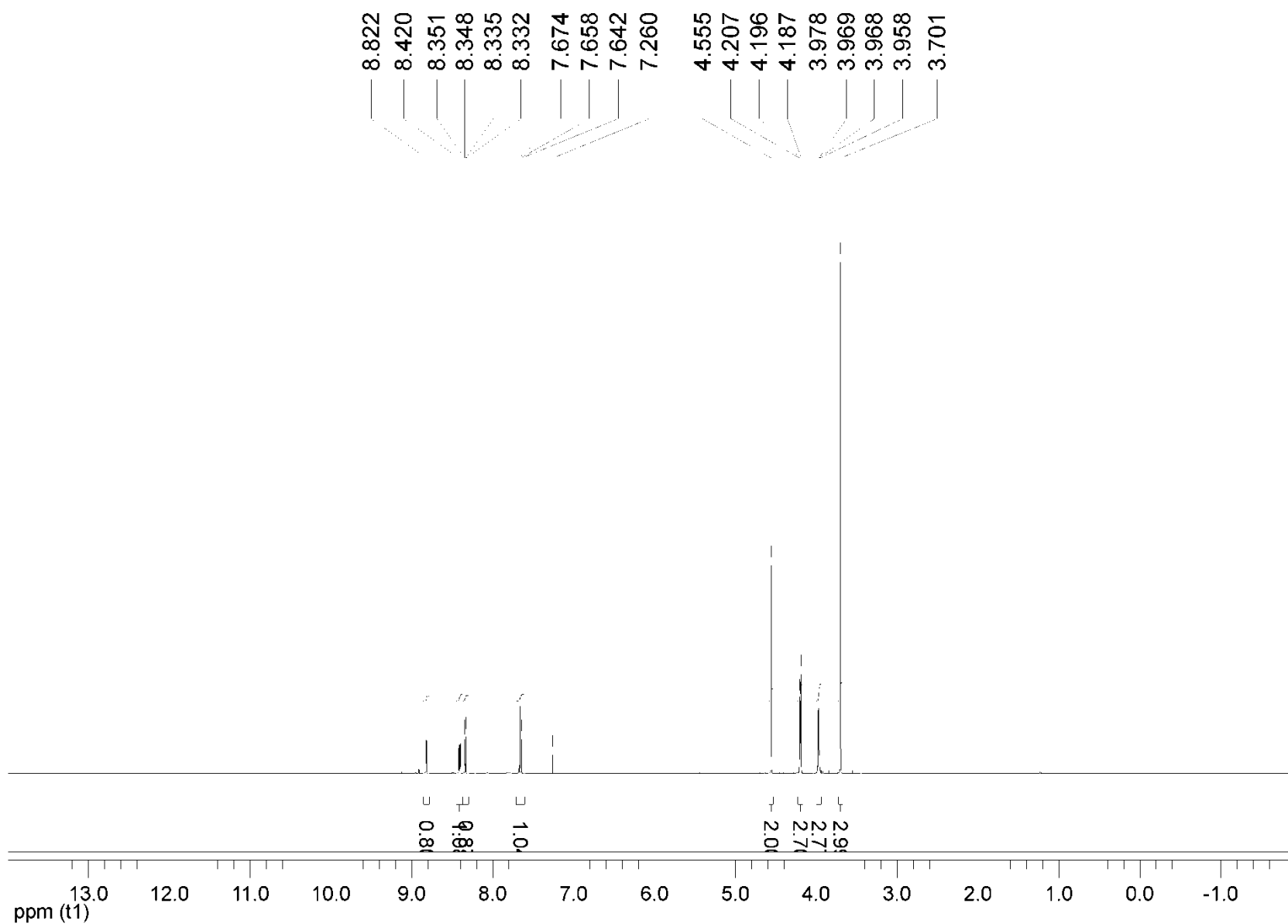
NL:  
1.08E6  
MSS-25-01-  
2011\_19SIM#1-01  
0.01-0.86 AV: 50 T:  
FTMS + p ESI SIM ms  
[ 309.00-319.00]

**Experimental peaks**

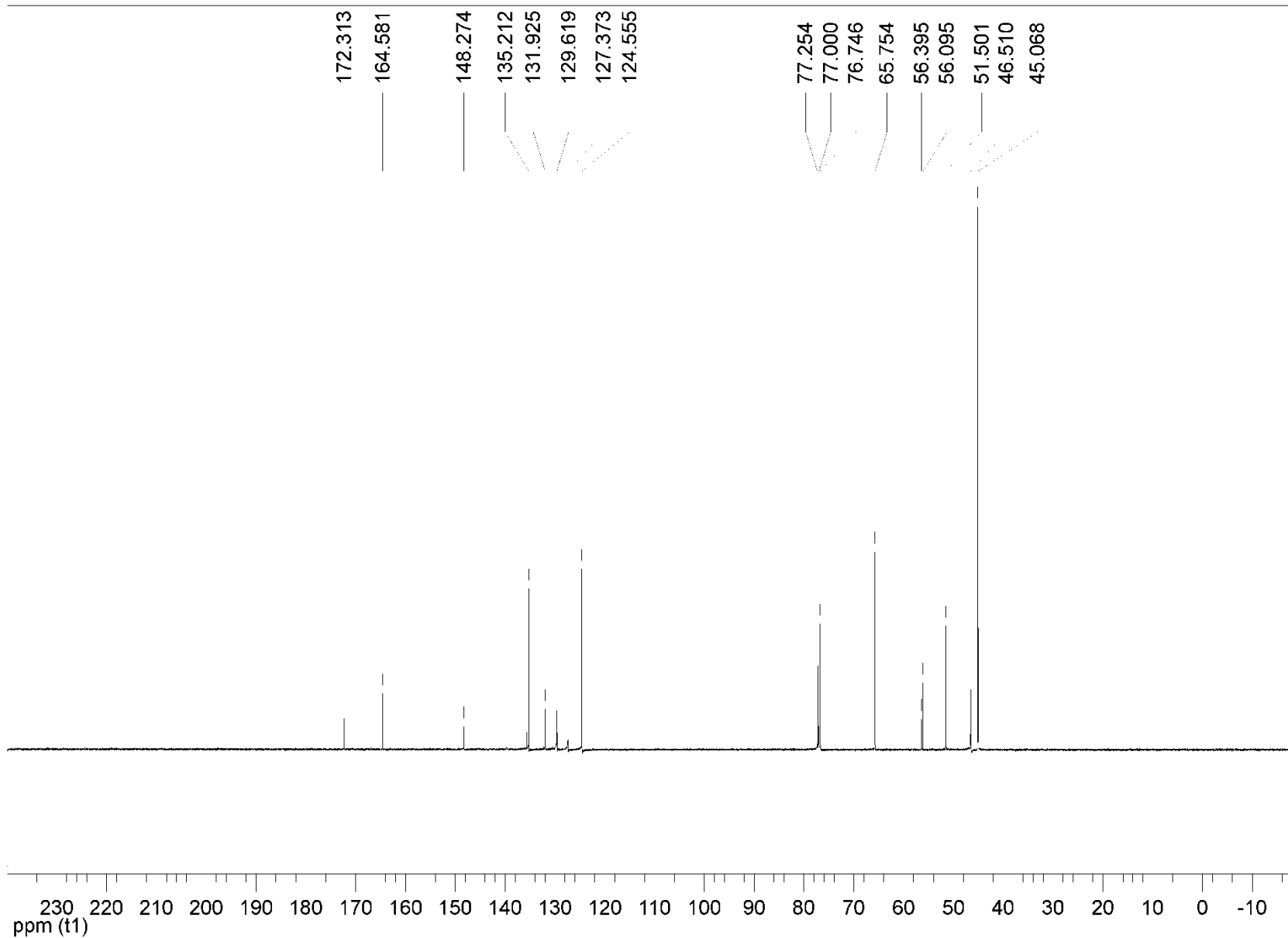
NL:  
8.18E5  
C<sub>17</sub>H<sub>15</sub>NO<sub>5</sub>H:  
C<sub>17</sub>H<sub>15</sub>N<sub>1</sub>O<sub>5</sub>  
pa Chrg 1

**Simulated peaks**

## 6. (4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate (11c) – $^1\text{H}$ NMR

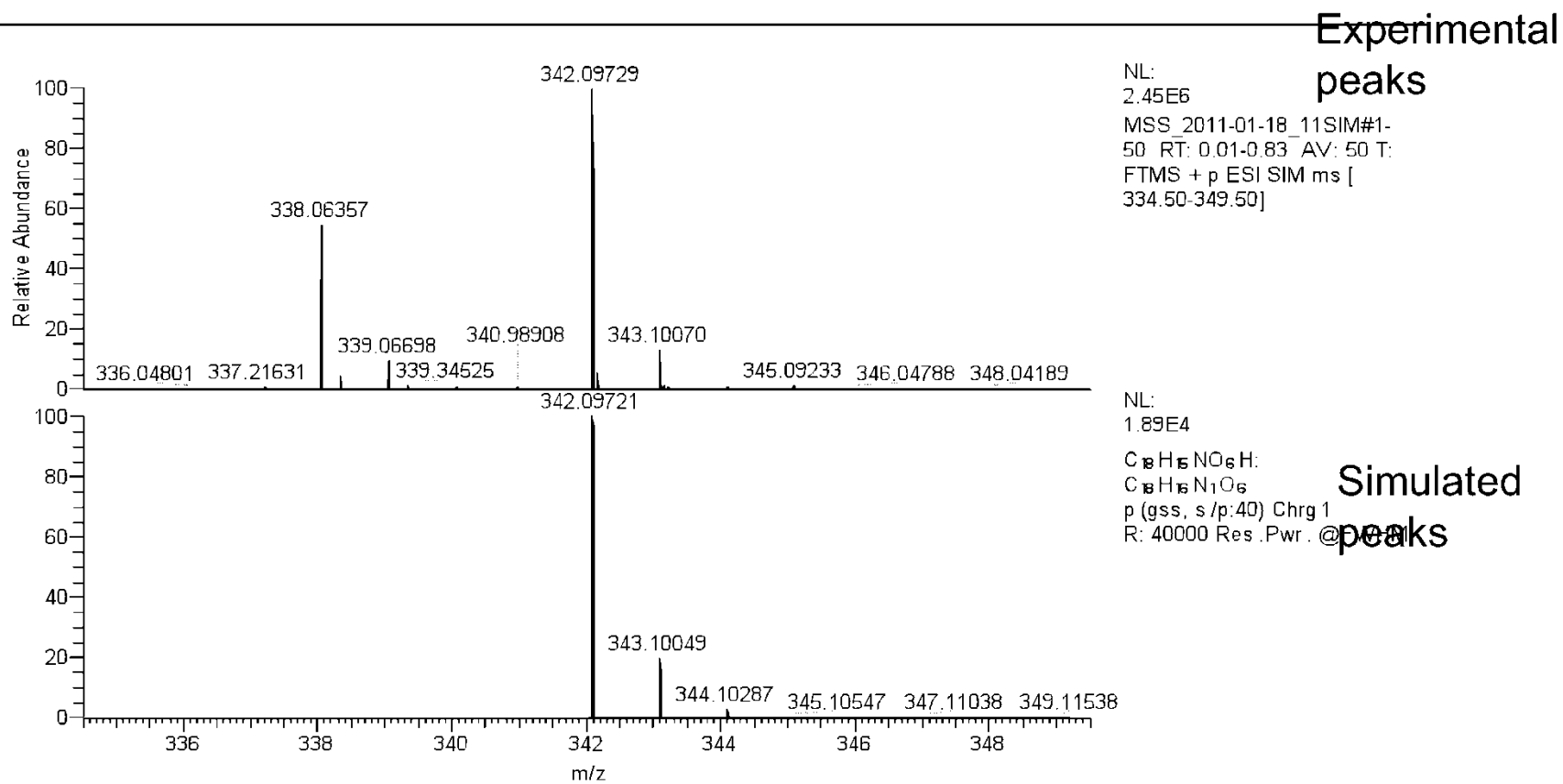


## 7. (4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate (11c) – $^{13}\text{C}$ NMR

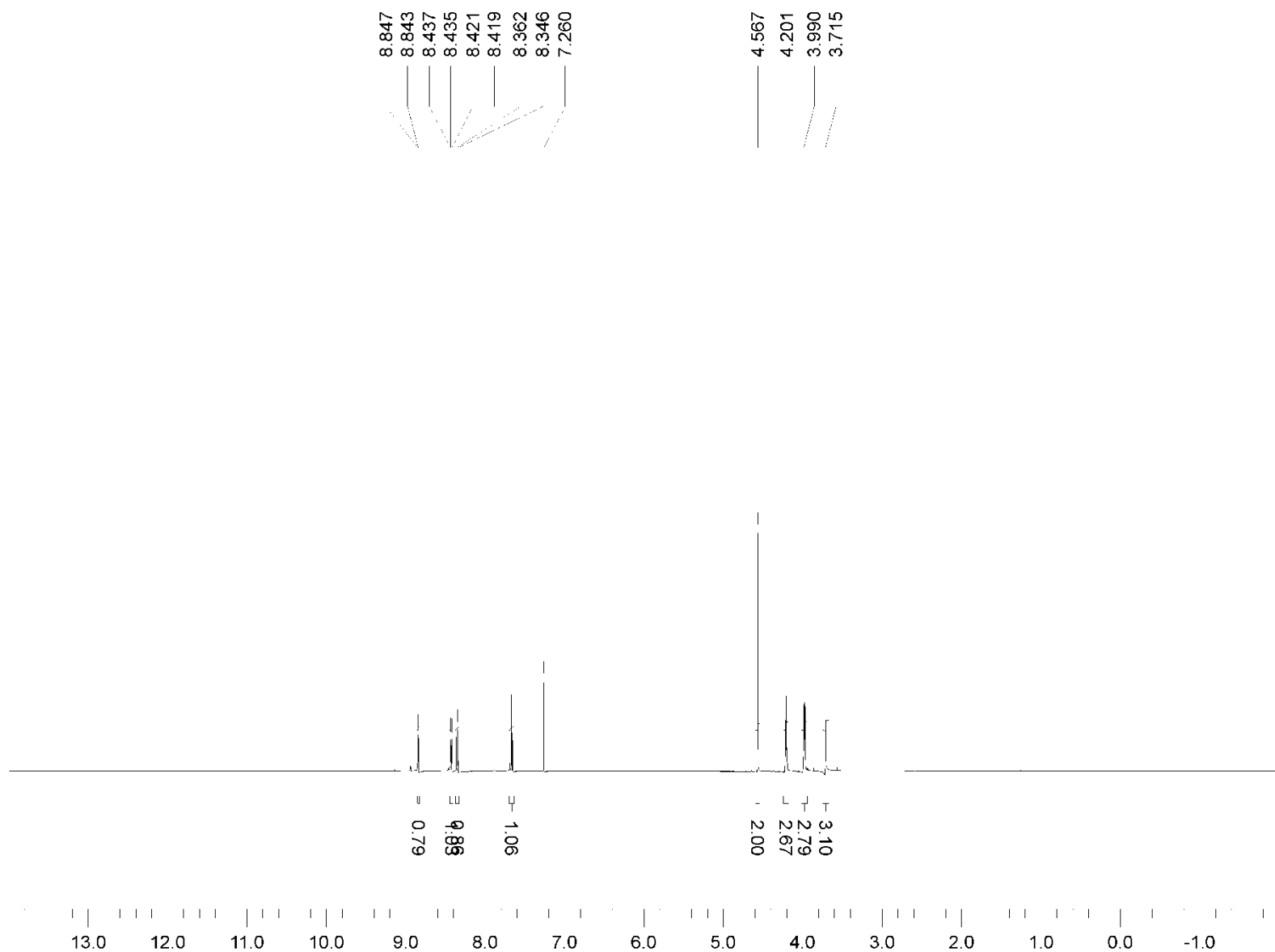




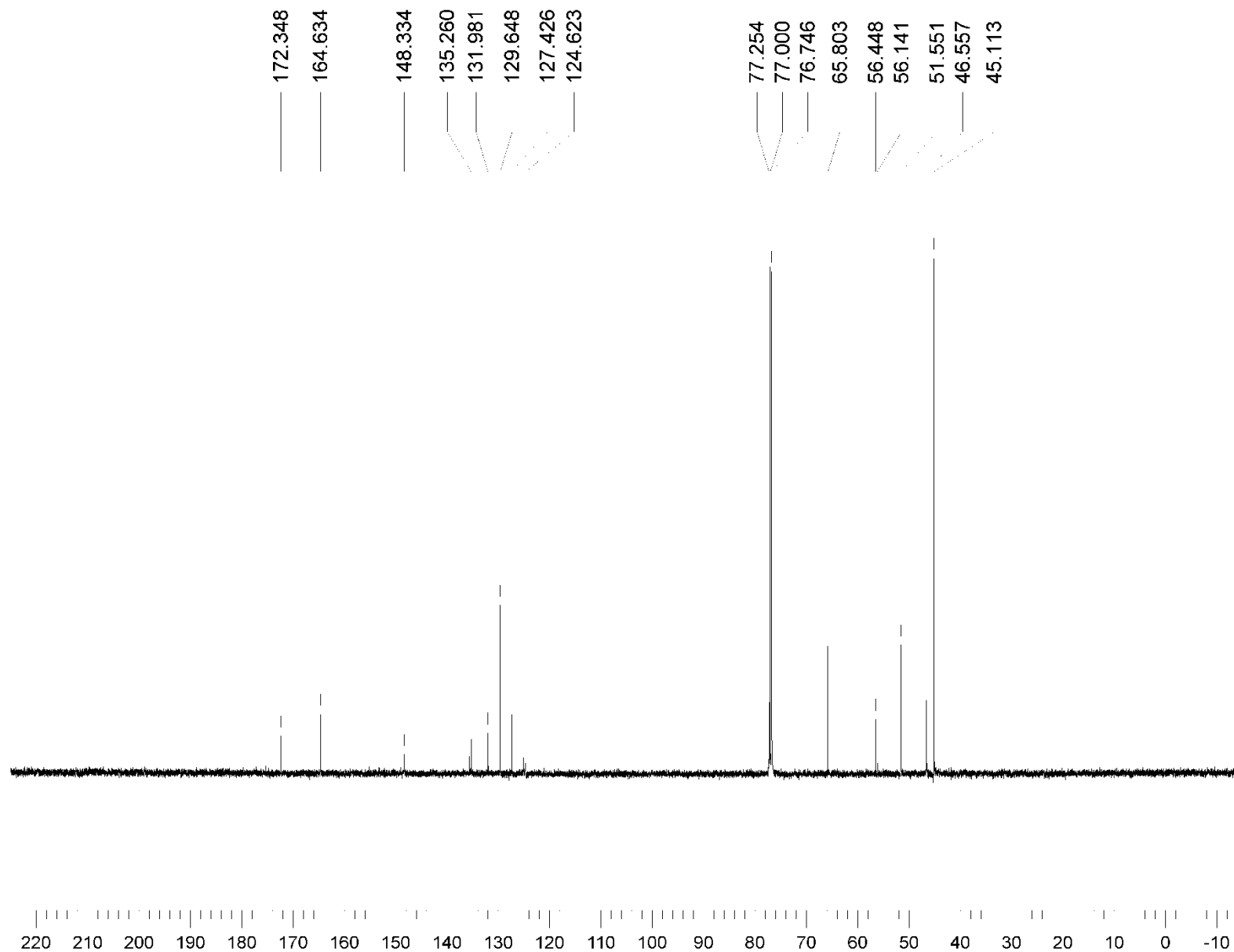
## 8. (4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate (11c) – HR MS



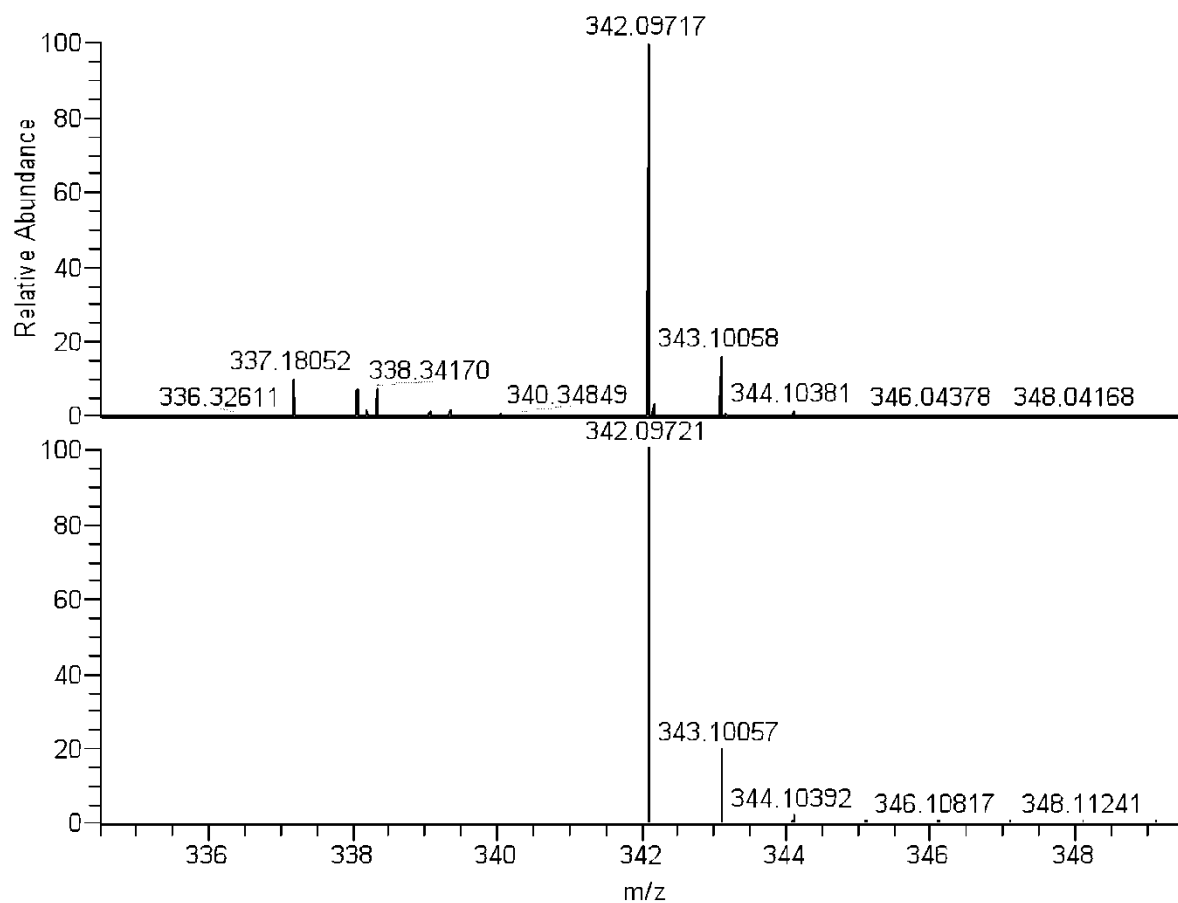
## 9. (4-Methoxycarbonyl)cubylmethyl 2-nitrobenzoate (11d) – $^1\text{H}$ NMR



### 10. (4-Methoxycarbonyl)cubylmethyl 2-nitrobenzoate (11d) – $^{13}\text{C}$ NMR



## 11. (4-Methoxycarbonyl)cubylmethyl 2-nitrobenzoate (11d) – HR MS



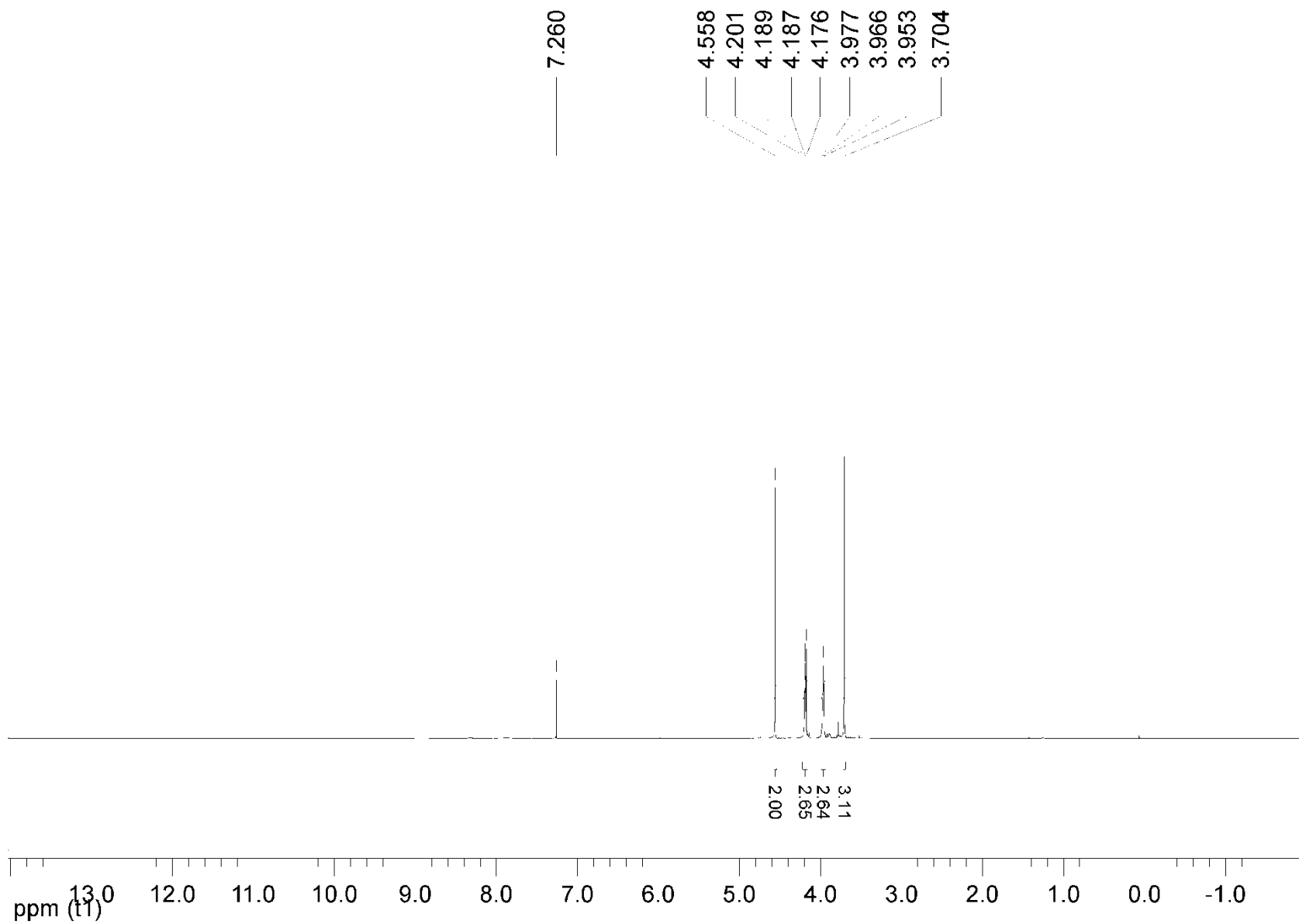
NL:  
5.01E6  
MSS-25-01-  
2011\_18SIM#1-001  
0.01-0.82 AV: 50 T:  
FTMS + p ESI SIM ms  
[ 334.50-349.50]

**Experimental peaks**

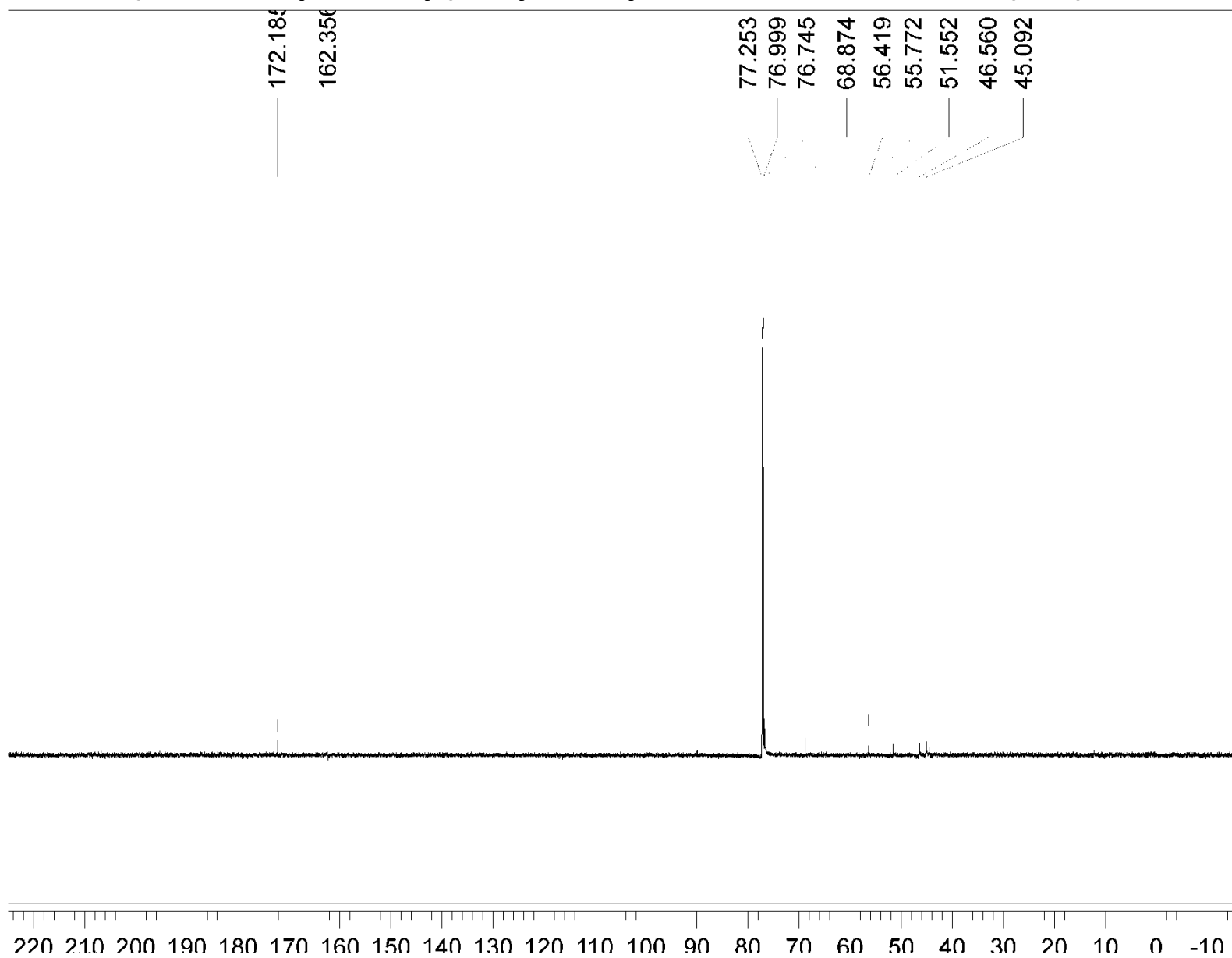
NL:  
8.08E5  
C<sub>18</sub>H<sub>15</sub>NO<sub>6</sub>H:  
C<sub>18</sub>H<sub>15</sub>N<sub>1</sub>O<sub>6</sub>  
pa Chrg 1

**Simulated peaks**

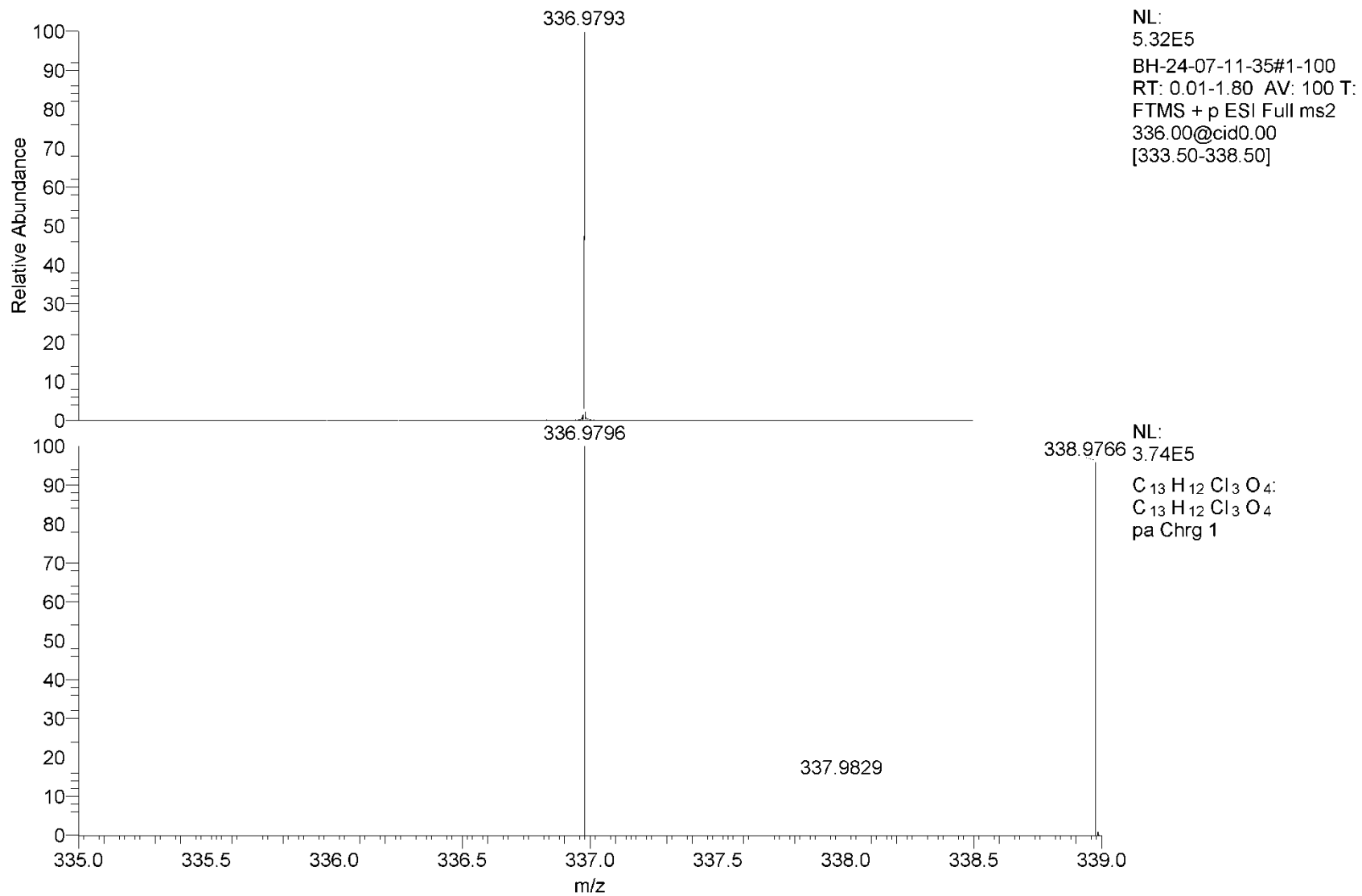
## 12. (4-Methoxycarbonyl)cubylmethyl 2,2,2-trichloroacetate (11e) – $^1\text{H}$ NMR



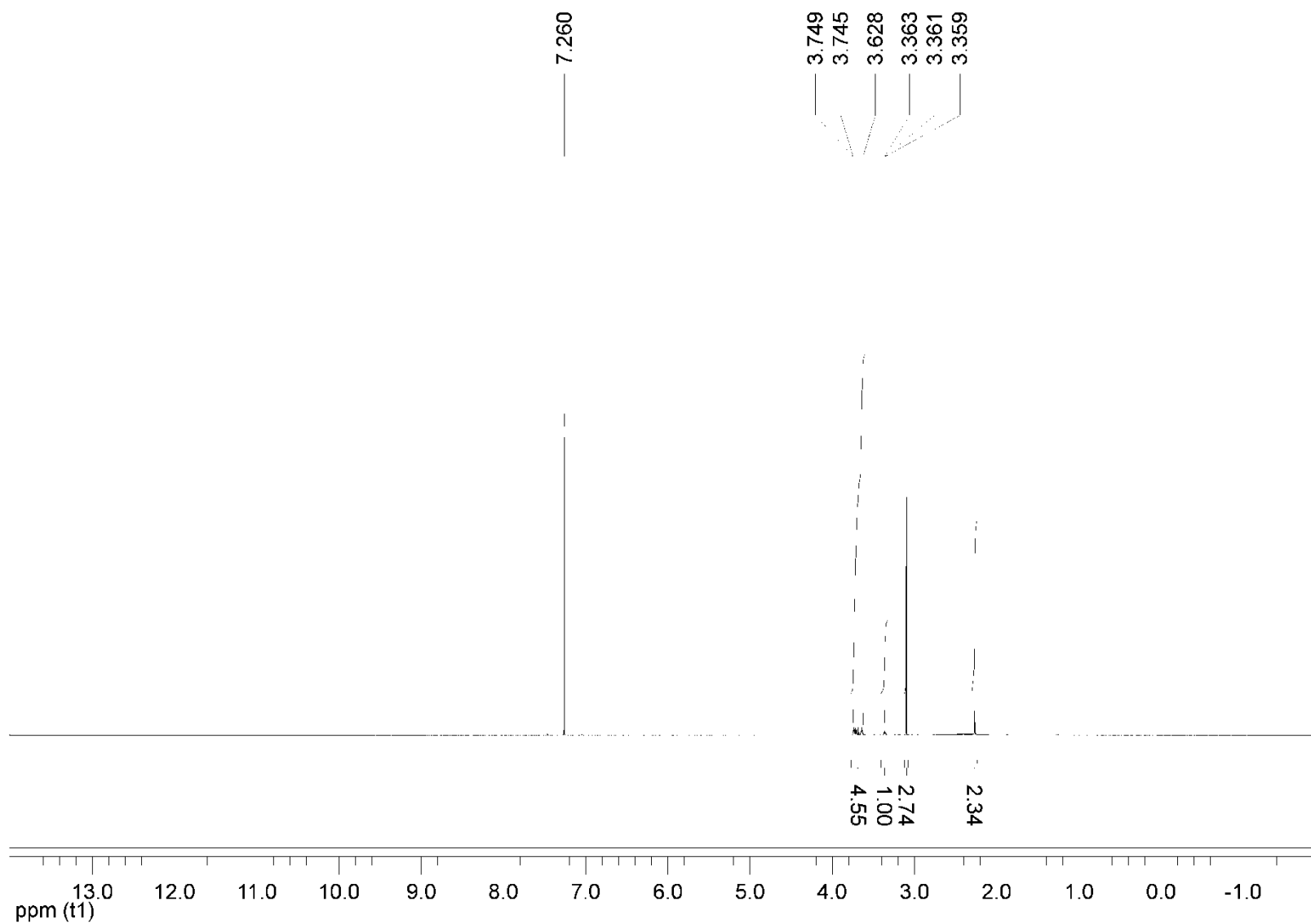
### 13. (4-Methoxycarbonyl)cubylmethyl 2,2,2-trichloroacetate (11e) – $^{13}\text{C}$ NMR



## 14. (4-Methoxycarbonyl)cubylmethyl 2,2,2-trichloroacetate (11e) – HR MS

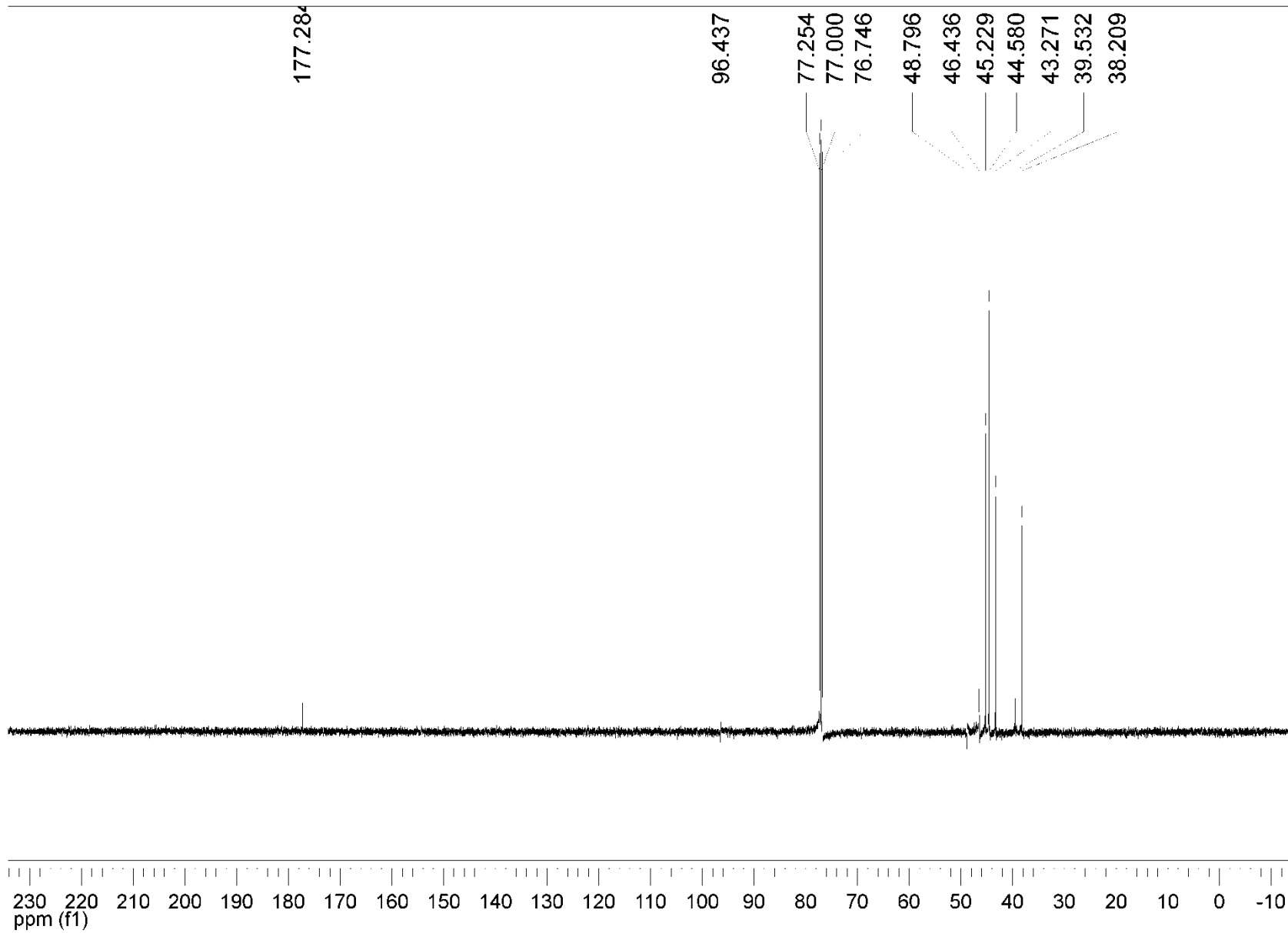


## 15. (4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f) – $^1\text{H}$ NMR



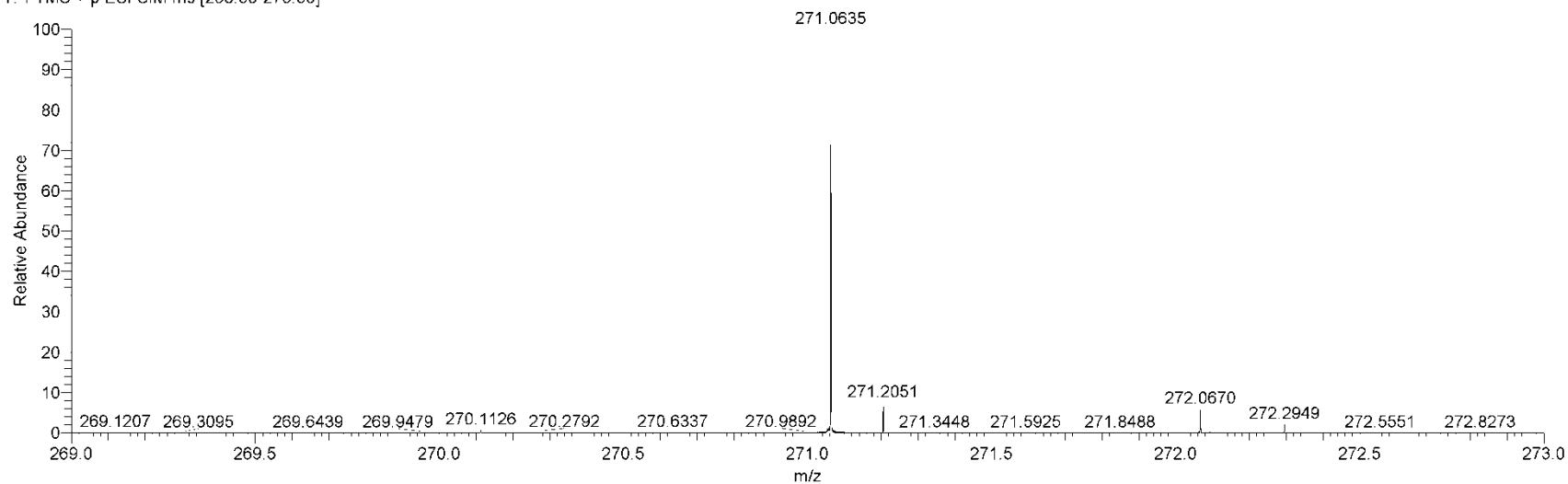


### 16. (4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f) – $^{13}\text{C}$ NMR

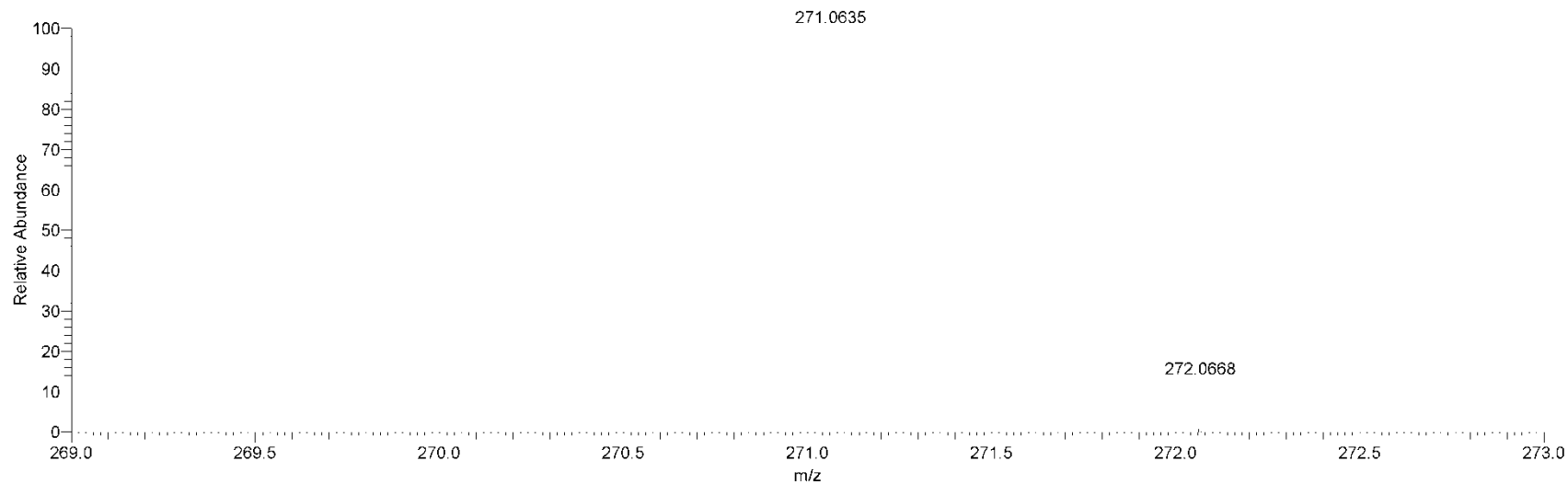


## 17. (4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f) – HR MS

12-06-05-14\_120606073223 #1-49 RT: 0.01-0.85 AV: 49 NL: 4.44E6  
T: FTMS + p ESI SIM ms [268.50-273.50]

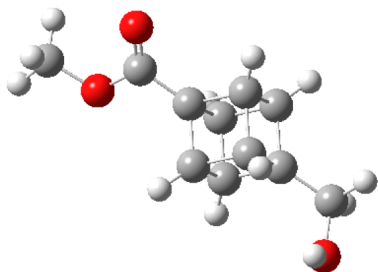


C12H14O5S +H: C12 H15 O5 S1 pa Chrg 1,3



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(4-Methoxycarbonyl)cubylmethanol 11a

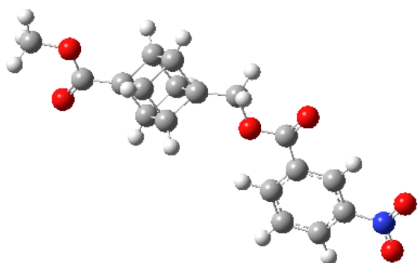


ZPE -423.936843 a.u.

Symbol	X	Y	Z				
H	-3.8937250	-0.6448520	-1.4364870	C	-1.9666860	0.1113280	0.2024260
O	-4.0705650	-0.9008670	-0.5252880	C	-1.0261940	1.0538120	1.0436570
O	2.7937070	-0.8744400	0.1112420	H	-1.3633060	1.7557990	1.8052110
C	-0.1926230	-0.7056600	-0.8533450	C	-0.2397610	1.4397280	-0.2586840
H	0.1641060	-1.4057380	-1.6057180	H	0.0757260	2.4418470	-0.5386610
O	2.8583260	1.3213290	-0.4078320	C	-0.9774810	-1.0881460	0.4464580
C	-3.4591480	0.0605090	0.3398360	H	-1.2804980	-2.0960480	0.7219920
H	-3.7339330	-0.2442880	1.3541420	C	2.2233040	0.3292320	-0.1331840
H	-3.8855510	1.0607550	0.1698020	C	4.2296010	-0.9233850	0.0272730
C	-1.1681760	0.4965500	-1.1047280	H	4.4991970	-1.9530280	0.2525230
H	-1.6054320	0.7551260	-2.0694170	H	4.6785590	-0.2417570	0.7512170
C	-0.0495780	-0.1489800	1.2909390	H	4.5632110	-0.6498260	-0.9748380
H	0.4230190	-0.4040250	2.2370580				
C	0.7445570	0.2513230	-0.0159490				

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(4-Methoxycarbonyl)cubylmethyl 3-nitrobenzoate (11c)



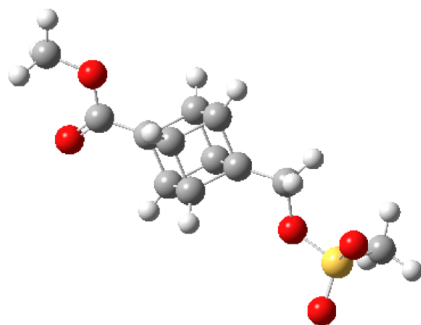
ZPE -1200.801675 a.u.

Symbol	X	Y	Z
O	-0.7079680	-0.7139900	0.0000670
O	-2.2410840	-2.3665080	0.0001330
O	6.4187280	0.0195840	-0.0004350
O	5.5891610	2.1190670	0.0005000
O	-7.5588230	1.0418520	0.0000080
C	-2.9875560	-0.0948980	0.0000230
C	0.3542500	-1.7065090	0.0001160
H	0.2402850	-2.3401480	-0.8846270
H	0.2402870	-2.3400600	0.8849300
C	3.5691270	-0.7508000	1.1107970
H	4.1426460	-1.0395080	1.9887210
C	3.5691310	-0.7509320	-1.1106820
H	4.1426390	-1.0397520	-1.9885750
C	-4.3334640	-0.4664070	-0.0000020
H	-4.6134960	-1.5106480	0.0000170
C	2.1879370	-0.0065080	-1.1124560
H	1.6340290	0.2885490	-2.0017990
C	-1.9674120	-1.1895520	0.0000810
C	5.4109410	0.9230870	0.0000400

N	-6.7291510	0.1412010	-0.0000730
C	1.6609450	-0.9871080	0.0000750
C	-2.6373870	1.2602080	-0.0000080
H	-1.5920010	1.5384370	0.0000100
C	2.1879370	-0.0063770	1.1124920
H	1.6340320	0.2887780	2.0018030
C	2.7053870	0.9735230	-0.0000380
H	2.5865440	2.0541860	-0.0000930
C	-5.2982300	0.5300850	-0.0000510
O	-6.9929300	-1.0526990	-0.0001690
C	3.0520390	-1.7268380	0.0001150
H	3.1848580	-2.8075330	0.0001830
C	-4.9710000	1.8833480	-0.0000790
H	-5.7588640	2.6238840	-0.0001140
C	4.0880700	0.2459220	-0.0000150
C	-3.6267510	2.2413010	-0.0000590
H	-3.3506100	3.2887640	-0.0000840
C	7.7535260	0.5599670	-0.0003170
H	7.9177880	1.1712050	-0.8888620
H	8.4163750	-0.3025610	-0.0007190
H	7.9179240	1.1704840	0.8886960

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(4-Methoxycarbonyl)cubylmethyl methanesulphonate (11f)

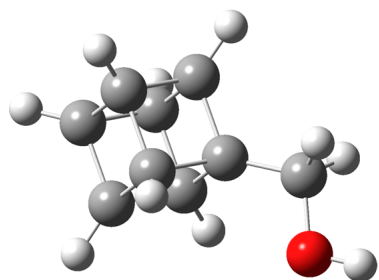


ZPE -1239.774056 a.u.

Symbol	X	Y	Z	Symbol	X	Y	Z
O	-4.6537220	-0.5521610	-0.0949580	O	2.4476830	0.2701310	0.1583990
O	-4.3022270	1.6682410	0.1093060	C	-3.8667240	0.5437760	0.0226480
C	1.6342670	-0.9382350	0.0515610	C	-1.7398140	-0.7764520	1.0942140
H	1.8538450	-1.5916480	0.9050310	H	-2.2634000	-1.2473870	1.9233410
H	1.8946660	-1.4622620	-0.8710070	C	-1.6749060	-0.6065950	-1.1203640
C	-6.0730390	-0.3115390	-0.1149390	H	-2.1461040	-0.9438390	-2.0407820
H	-6.5332410	-1.2927570	-0.2093330	C	-0.9933580	-1.5324720	-0.0563580
H	-6.3409170	0.3213680	-0.9622210	H	-0.8896700	-2.6135230	-0.1366740
H	-6.3910360	0.1748720	0.8083600	C	0.2044740	-0.5138070	0.0557690
O	4.2839690	-0.9600470	-1.0558090	C	-2.4288890	0.1687000	0.0317390
O	4.4053650	1.5361420	-0.6309510	C	-0.4875600	0.4132380	-1.0084380
C	4.7710960	-0.1055080	1.4126380	H	0.0192550	0.8880420	-1.8456100
H	4.4015280	-1.0573540	1.7910310	C	-0.5522060	0.2428130	1.2089100
H	4.4985090	0.7206070	2.0664640	H	-0.1006570	0.5832240	2.1388530
H	5.8501130	-0.1463730	1.2675210	C	-1.2358450	1.1718570	0.1438980
S	4.0438590	0.1990050	-0.2046060	H	-1.3481660	2.2498470	0.2231610

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Cubylmethanol (18a)

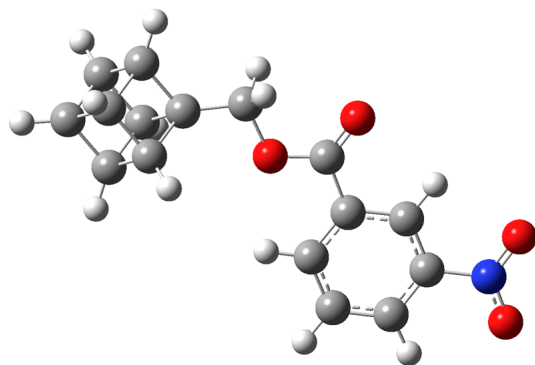


ZPE -423.936477 a.u.

Symbol	X	Y	Z
H	3.7482230	-0.3135370	0.0002980
O	2.8159250	-0.5496930	-0.0000470
C	-0.8914980	-1.3716580	0.0000020
H	-1.0099300	-2.4536960	0.0000000
C	2.0351230	0.6513160	-0.0000100
H	2.2609790	1.2591220	-0.8894720
H	2.2609800	1.2590450	0.8895020
C	-0.1544000	-0.5459770	1.1128980
H	0.3252630	-0.9659740	1.9953500
C	-1.3245820	0.5025520	-1.1120010
H	-1.7950840	0.9239580	-1.9990500
C	-2.0638300	-0.3253180	0.0000040
C	0.5868340	0.2825670	0.0000000
C	-0.5866240	1.3310040	0.0000010
H	-0.4549970	2.4132250	0.0000030
C	-1.3245750	0.5025480	1.1120070
H	-1.7950670	0.9239600	1.9990590
C	-0.1544060	-0.5459720	-1.1128960
H	0.3252480	-0.9659700	-1.9953510
H	-3.1252720	-0.5689560	0.0000070

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Cubylmethyl 3-nitrobenzoate (18c)

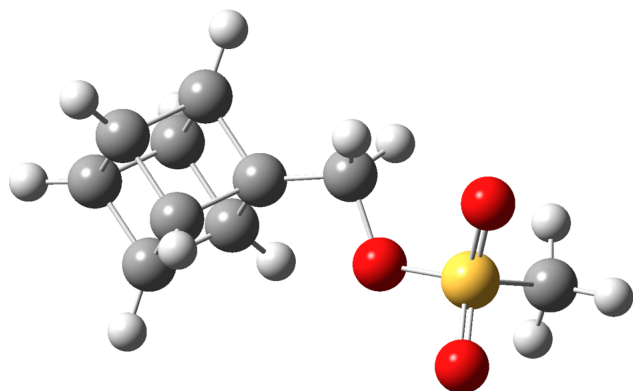


ZPE -972.896739 a.u.

Symbol	X	Y	Z				
O	0.6533600	-0.4654750	-0.0000070	C	3.0406090	-0.4901000	0.0000360
O	-0.7013360	-2.2676210	0.0000770	C	-1.4655070	1.2990490	-0.0001050
O	-6.3392490	0.5838030	-0.0000460	H	-0.4531820	1.6803310	-0.0001290
C	-1.6766300	-0.0845100	-0.0000300	C	3.4633960	0.5378930	1.1134430
C	1.8157760	-1.3411010	0.0000430	H	2.8751800	0.7725650	1.9994180
H	1.7671910	-1.9828930	-0.8848800	C	3.8822560	1.5629370	-0.0000220
H	1.7671600	-1.9828330	0.8850070	H	3.6344270	2.6229640	-0.0000660
C	4.9164620	-0.0588070	1.1117150	C	-4.0384970	0.3029040	-0.0000400
H	5.4986370	-0.2995110	1.9993190	O	-5.5649100	-1.4429170	0.0000630
C	4.9165100	-0.0588890	-1.1115940	C	4.4984130	-1.0860650	0.0000890
H	5.4987230	-0.2996580	-1.9991560	H	4.7340350	-2.1498340	0.0001340
C	-2.9777270	-0.5908820	0.0000030	C	-3.8500740	1.6823270	-0.0001150
H	-3.1502410	-1.6581750	0.0000610	H	-4.7092460	2.3388190	-0.0001460
C	3.4634430	0.5378110	-1.1134280	C	5.3366760	0.9686490	0.0000310
H	2.8752660	0.7724170	-1.9994460	C	-2.5491460	2.1749390	-0.0001470
C	-0.5486040	-1.0687390	0.0000190	H	-2.3809890	3.2450720	-0.0002050
N	-5.4226930	-0.2284910	-0.0000050	H	6.2548310	1.5533590	0.0000290

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Cubylmethyl mesylate (18f)



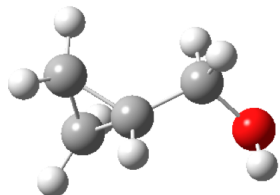
ZPE -1011.869219 a.u.

Symbol	X	Y	Z				
C	-0.2663140	-0.6204440	0.5912320	C	3.0442400	0.5061880	1.0718040
H	-0.4586000	-1.6841670	0.4031660	H	3.5325040	0.8818740	1.9691010
H	-0.4840680	-0.4033880	1.6396070	C	2.3888780	-0.9137050	0.9296810
O	-2.9705340	-0.1741280	1.4610730	H	2.3407490	-1.6700430	1.7127110
O	-3.2533600	1.4433450	-0.4702700	C	1.1355270	-0.2609710	0.2324630
C	-3.3446570	-1.1520590	-0.9800710	C	3.7307840	0.3263830	-0.3300800
H	-2.8748240	-2.0799250	-0.6576350	C	1.7955860	1.1580400	0.3765060
H	-3.0936630	-0.9114960	-2.0112350	H	1.2740050	2.0525950	0.7112860
H	-4.4243700	-1.2055800	-0.8449560	C	1.8233890	-0.4433740	-1.169797
S	-2.7587890	0.1904040	0.0654260	H	1.3271880	-0.8184070	-2.0637120
O	-1.1531290	0.1804210	-0.2512480	C	2.4795570	0.9754220	-1.0244110
C	3.0722240	-1.0929640	-0.4725110	H	2.5099650	1.7314680	-1.8063560
H	3.5833400	-1.9936370	-0.8082580	H	4.7692990	0.5620380	-0.5558760



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Cyclopropylmethanol 16a

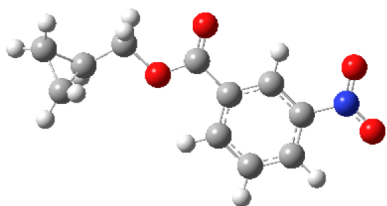


ZPE -232.382001 a.u.

Symbol	X	Y	Z
H	-2.2237540	0.4981180	0.8502650
O	-2.0252380	0.3543670	-0.0804620
C	-0.9467410	-0.5806620	-0.1775630
H	-0.7781710	-0.7126380	-1.2492600
H	-1.2517090	-1.5544790	0.2302760
C	0.3231300	-0.1145580	0.4910200
C	1.6614540	-0.5362520	-0.0710170
C	1.2076770	0.8982400	-0.1889070
H	0.2652410	-0.0512900	1.5753690
H	1.6627010	-1.1437380	-0.9692340
H	2.4577630	-0.7713960	0.6247310
H	1.7002750	1.6435650	0.4238530
H	0.8964470	1.2563120	-1.1634990

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Cyclopropylmethyl 3-nitrobenzoate 16c



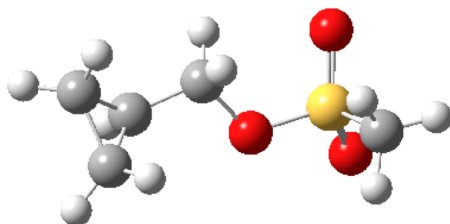
ZPE -781.342374 a.u.

Symbol	X	Y	Z
O	-1.9266260	-0.0386580	-0.2466630
O	-0.7944190	-1.9790770	-0.0566660
O	5.1280740	0.2147660	0.1512470
C	0.4266690	0.0764990	-0.1055990
C	-3.1804070	-0.7779430	-0.2875340
H	-3.2587650	-1.3767220	0.6232670
H	-3.1437710	-1.4617130	-1.1388190
C	1.6584100	-0.5725030	-0.0018830
H	1.7061900	-1.6510660	0.0558870
C	-0.8060850	-0.7724960	-0.1317900
N	4.1251980	-0.4880360	0.1336360
C	0.3772320	1.4732070	-0.1798820
H	-0.5828350	1.9654360	-0.2598940

C	2.8136940	0.1948820	0.0245950
O	4.1260290	-1.7090190	0.1991610
C	2.7861950	1.5849910	-0.0477880
H	3.7140230	2.1396190	-0.0229630
C	1.5529570	2.2203230	-0.1503600
H	1.5095250	3.3012320	-0.2072100
C	-4.3024950	0.2075950	-0.4029600
C	-5.6563760	-0.1669050	0.1549020
C	-4.8321180	0.9008640	0.8279820
H	-4.3042040	0.7833940	-1.3227840
H	-5.7529640	-1.1237030	0.6553620
H	-6.5335370	0.1319210	-0.4052840
H	-5.1492930	1.9320370	0.7329420
H	-4.3712980	0.6606380	1.7793030

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Cyclopropylmethyl mesylate 16f

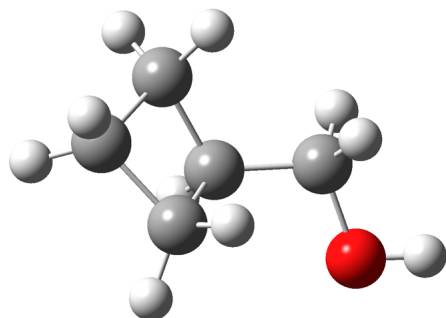


ZPE -820.314193 a.u.

Symbol	X	Y	Z
C	0.9797770	-0.4836610	-0.3541410
H	1.0206790	0.0488150	-1.3109200
H	0.7127750	-1.5246660	-0.5398460
O	-1.7470670	-1.3006410	-0.7426990
O	-2.3632940	0.0065650	1.3396950
C	-1.9741530	1.3405470	-0.9121300
H	-1.3357700	1.3161330	-1.7939930
H	-1.7872960	2.2240710	-0.3049820
H	-3.0230680	1.2813970	-1.2005730
S	-1.6316690	-0.1119000	0.0940070
O	-0.0592140	0.1201550	0.4811320
C	2.2756270	-0.3560800	0.3851760
C	3.5611020	-0.2868740	-0.4079500
C	3.0604100	0.9292800	0.3292370
H	2.3083900	-0.9076160	1.3183610
H	3.4942060	-0.2887980	-1.4900850
H	4.4221590	-0.8136900	-0.0161780
H	3.5828870	1.2421050	1.2246000
H	2.6517750	1.7447490	-0.2566750

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Cyclobutylmethanol 19a

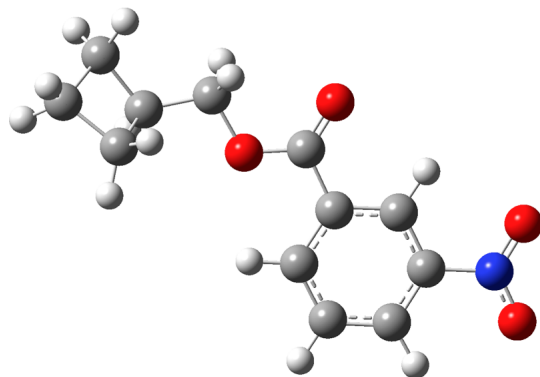


ZPE -271.679792 a.u.

Symbol	X	Y	Z
C	-0.7259180	-1.0873020	0.1353260
C	0.0261580	0.1726810	-0.3773110
C	-1.2225260	1.0216830	-0.0051160
C	-2.0548930	-0.2898350	0.0342750
H	-0.6318450	-2.0025670	-0.4503960
H	-0.4625290	-1.3104600	1.1735060
H	0.1505620	0.1262890	-1.4637430
H	-1.5306640	1.8023510	-0.7036060
H	-1.1237490	1.4652850	0.9906670
H	-2.5669870	-0.4713350	-0.9138160
H	-2.7772000	-0.4034010	0.8448890
C	1.3501110	0.5478410	0.2493050
H	1.6432220	1.5567010	-0.0764770
H	1.2512610	0.5614780	1.3446310
O	2.3300700	-0.4145980	-0.1533580
H	3.1697730	-0.1979640	0.2623390

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Cyclobutylmethyl 3-nitrobenzoate 19c

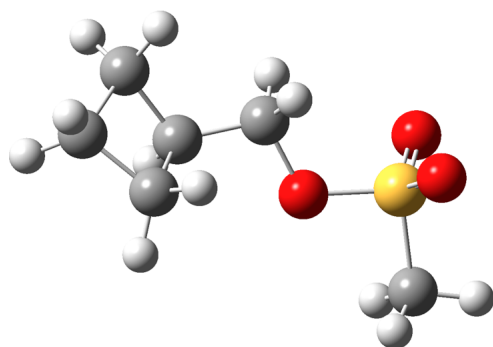


ZPE -820.639927 a.u.

Symbol	X	Y	Z				
C	4.3007930	0.9547800	0.8076960	C	0.3890910	-0.8453520	-0.1071890
C	3.9159260	0.0470400	-0.3946610	C	-0.8204640	0.0366540	-0.1147010
C	5.3498100	-0.5562320	-0.3458120	C	-0.7361620	1.4263920	-0.2571180
C	5.7954080	0.6720430	0.4946160	C	-2.0679620	-0.5745220	0.0249490
H	3.9620100	1.9917610	0.7861110	C	-1.8923460	2.2040090	-0.2596420
H	3.9937310	0.5073750	1.7575190	H	0.2352320	1.8899510	-0.3655750
H	3.7863720	0.6457980	-1.3013900	C	-3.2031360	0.2226150	0.0191920
H	5.8521270	-0.7363000	-1.2978710	H	-2.1429590	-1.6474910	0.1345000
H	5.3781720	-1.4783810	0.2423530	C	-3.1407870	1.6063980	-0.1211640
H	6.2346090	1.4523950	-0.1311740	H	-1.8217120	3.2793300	-0.3699890
H	6.4617890	0.4880160	1.3387040	O	0.3447800	-2.0472730	0.0113710
C	2.7624220	-0.9169910	-0.2605030	H	-4.0541150	2.1850950	-0.1199390
H	2.7229040	-1.6226820	-1.0948980	N	-4.5309860	-0.4203630	0.1669300
H	2.8201740	-1.4928910	0.6669870	O	-5.5154670	0.3080720	0.1546650
O	1.5298570	-0.1470830	-0.2488700	O	-4.5625430	-1.6362700	0.2918570

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Cyclobutylmethyl mesylate 19f

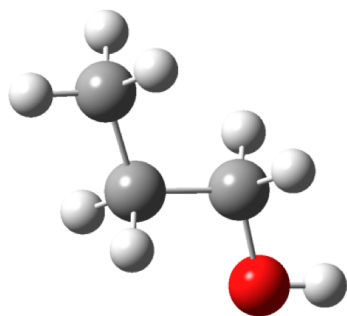


ZPE -859.614170 a.u.

Symbol	X	Y	Z		X	Y	Z
C	2.5187790	1.1139070	0.2131120	C	0.6003230	-0.6950360	0.0132150
C	1.9151800	-0.1403520	-0.4779140	H	0.3797240	-1.6667840	-0.4379640
C	3.2001360	-0.9271940	-0.0862570	H	0.5921110	-0.7893000	1.1031910
C	3.9133340	0.4333820	0.1466580	O	-0.4438100	0.2487020	-0.3802440
H	2.3947720	2.0734970	-0.2906970	S	-1.9666520	-0.1018220	0.1149890
H	2.1612270	1.2116420	1.2420560	O	-2.4029420	-1.3415610	-0.5157090
H	1.8661100	-0.0005830	-1.5616290	O	-2.0424900	0.0272570	1.5649280
H	3.6194170	-1.6054940	-0.8313230	C	-2.7712940	1.2972030	-0.6658090
H	3.0658550	-1.4773810	0.8496680	H	-2.6119880	1.2305010	-1.7397990
H	4.4792870	0.7490990	-0.7328190	H	-2.3530120	2.2113980	-0.2503080
H	4.5577730	0.5177960	1.0230070	H	-3.8296610	1.2081200	-0.4230370

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**n-Propanol 13a**

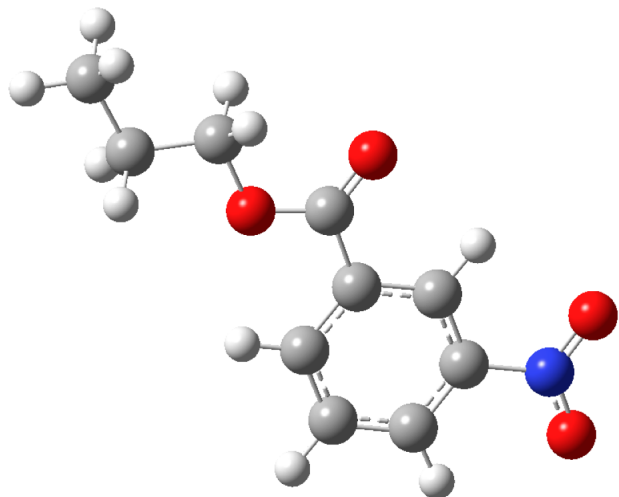


**ZPE -194.311332 a.u.**

<b>Symbol</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
C	0.5234850	-0.5241610	0.0000200
H	0.4152690	-1.1687850	-0.8781780
H	0.4153210	-1.1688010	0.8782040
C	1.9013300	0.1436090	-0.0000260
H	2.0415420	0.7740840	-0.8837390
H	2.0415630	0.7741590	0.8836310
H	2.6978020	-0.6044240	-0.0000050
C	-0.6145940	0.4842270	0.0000430
H	-0.5440860	1.1285680	-0.8880500
H	-0.5441280	1.1284660	0.8882020
O	-1.8508310	-0.2349560	-0.0000100
H	-2.5779550	0.3943350	-0.0002080

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**N-Propyl m-nitrobenzoate 13c**



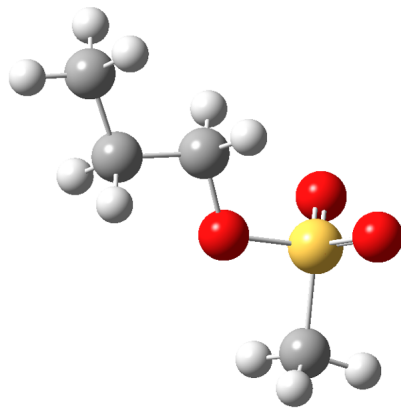
**ZPE -743.271441 a.u.**

Symbol	X	Y	Z
C	-4.5548290	0.5478910	0.0002310
H	-4.4270980	1.1874180	-0.8788840
H	-4.4269280	1.1869420	0.8796660
C	-5.9557910	-0.0723240	0.0001980
H	-6.1169000	-0.6967760	-0.8835380
H	-6.1167700	-0.6971680	0.8836790
H	-6.7231430	0.7049250	0.0004260
C	-3.4715070	-0.5154800	-0.0001550
H	-3.5275580	-1.1565350	-0.8836170
H	-3.5273720	-1.1570010	0.8829770
O	-2.1854230	0.1572520	-0.0001210
C	-1.0966150	-0.6329760	-0.0001230
O	-1.1407760	-1.8406280	-0.0001540
C	0.1760850	0.1550260	-0.0000820
C	0.1931890	1.5544310	-0.0001140



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**n-Propyl mesylate 13f**



**ZPE -782.245253 a.u.**

Symbol	X	Y	Z	
C	-2.5200210	0.6247960	0.0000310	
H	-2.4761760	1.2736630	-0.8798160	
H	-2.4761470	1.2735480	0.8799600	
C	-3.8243560	-0.1794800	-0.0000010	
H	-3.9002320	-0.8193320	-0.8840190	
H	-3.9001930	-0.8194640	0.8839240	
H	-4.6881630	0.4889640	0.0000670	
C	-1.3042390	-0.2846260	-0.0000480	
H	-1.2758980	-0.9166340	-0.8919420	
H	-1.2758580	-0.9167290	0.8917770	
O	-0.1229570	0.5724880	-0.0000320	
S	1.3292850	-0.1888130	0.0000120	
O	1.4950930	-0.9053760	1.2583340	
O	1.4951050	-0.9054960	-1.2582410	
C	2.3426410	1.2897890	-0.0000550	
H	2.1229600	1.8582720	0.9010090	
H	3.3760910	0.9447440	-0.0000240	
H	2.1229770	1.8581730	-0.9011850	