Appendix
Spectral Data

Green Chemistry Using Bismuth(III) Salts: Synthesis of Cyclic Acetals and Allylation of Tetrahydropyranyl Ethers and Aldehydes

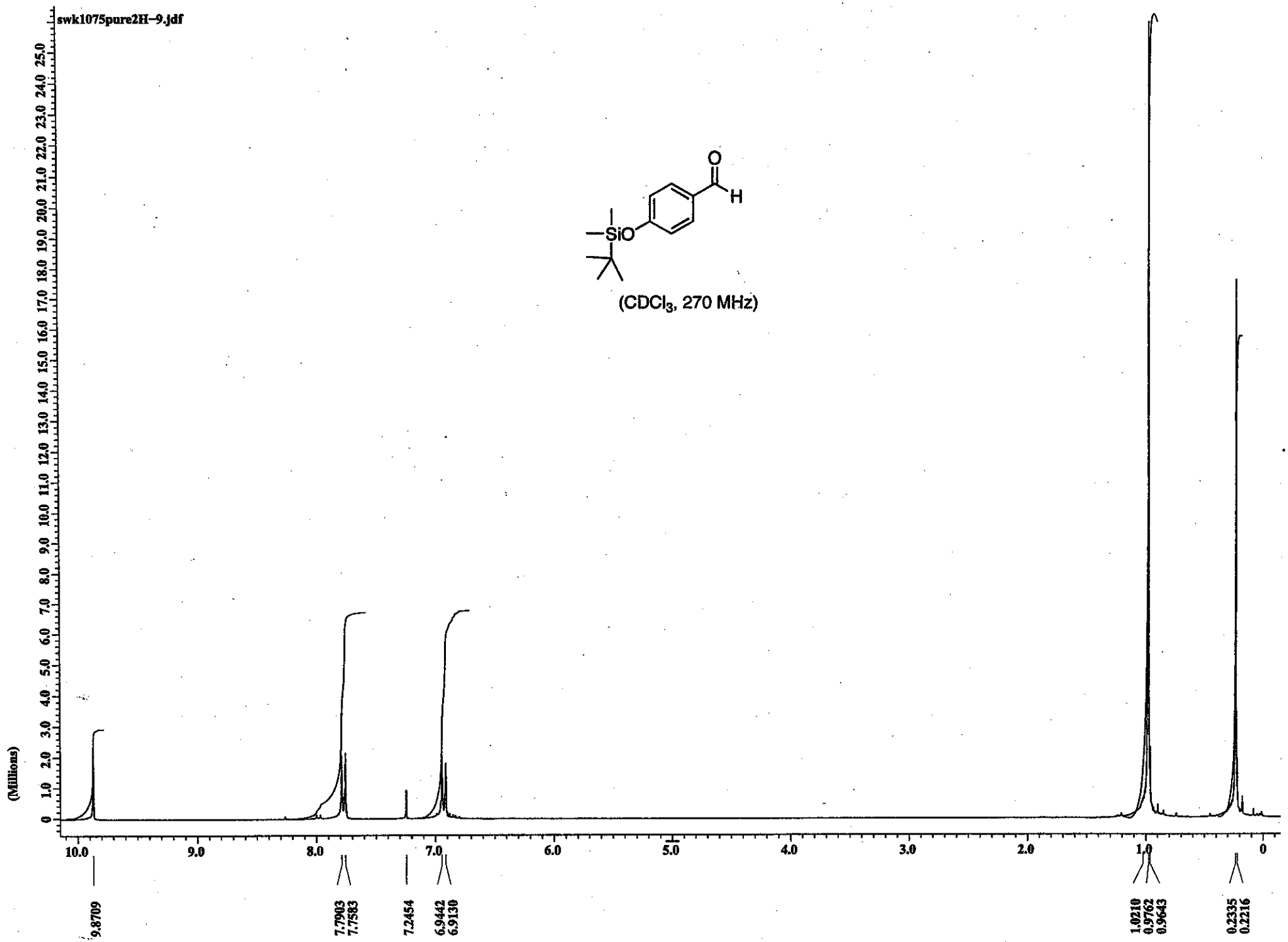
By

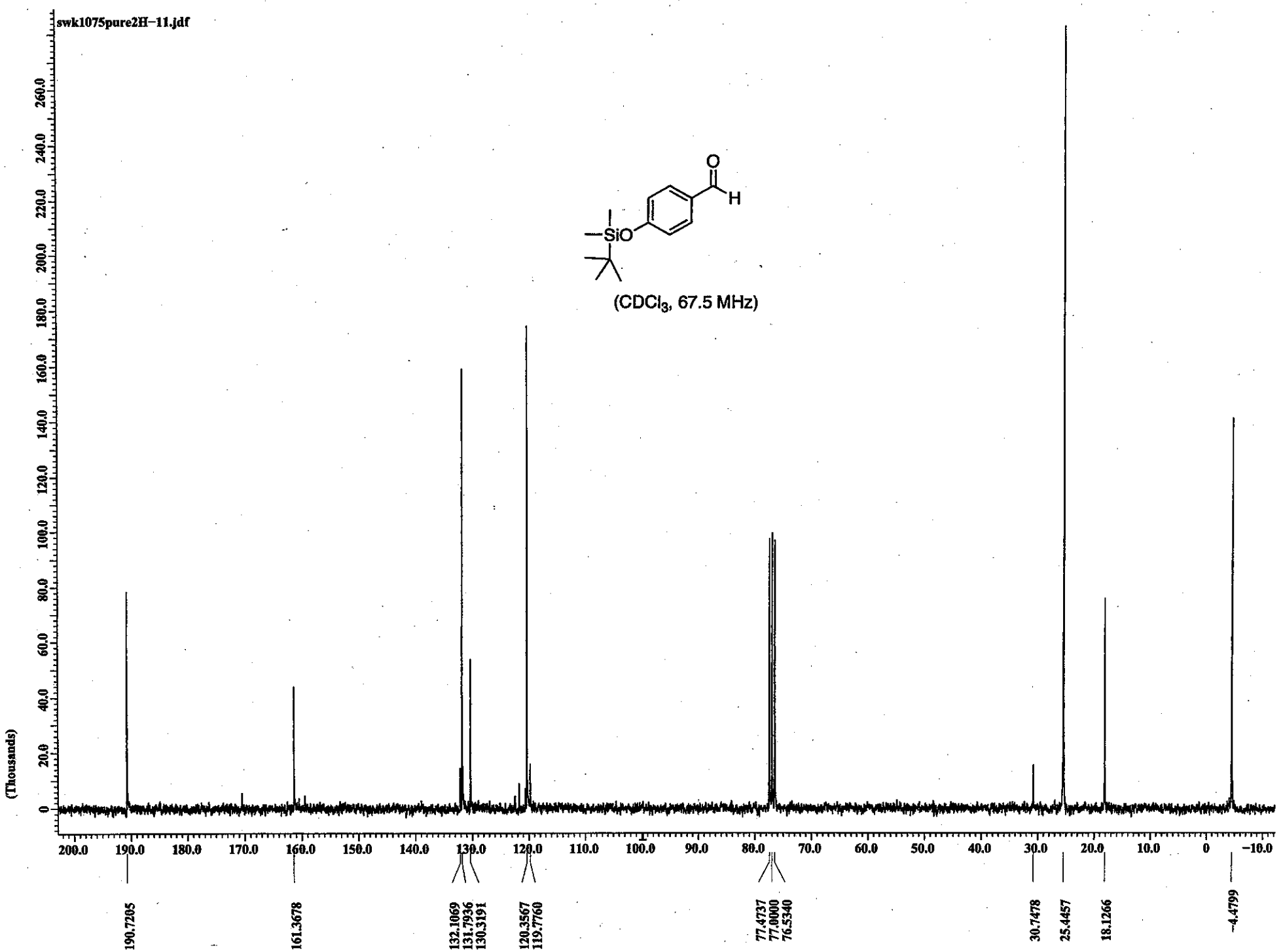
Scott W. Krabbe

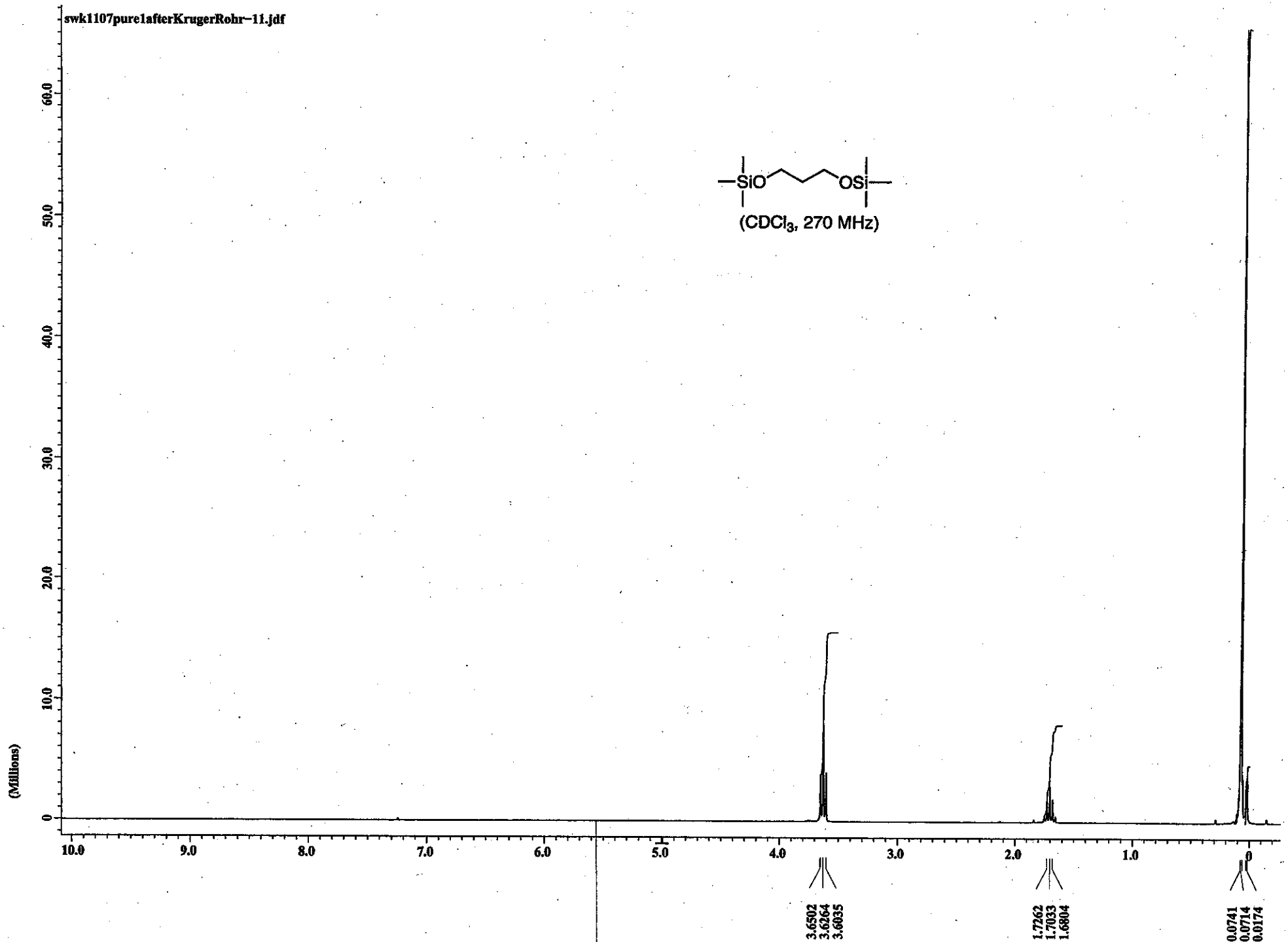
A Paper Submitted As Part of The Requirement For Research Honors In Chemistry

Illinois Wesleyan University, April 19, 2010

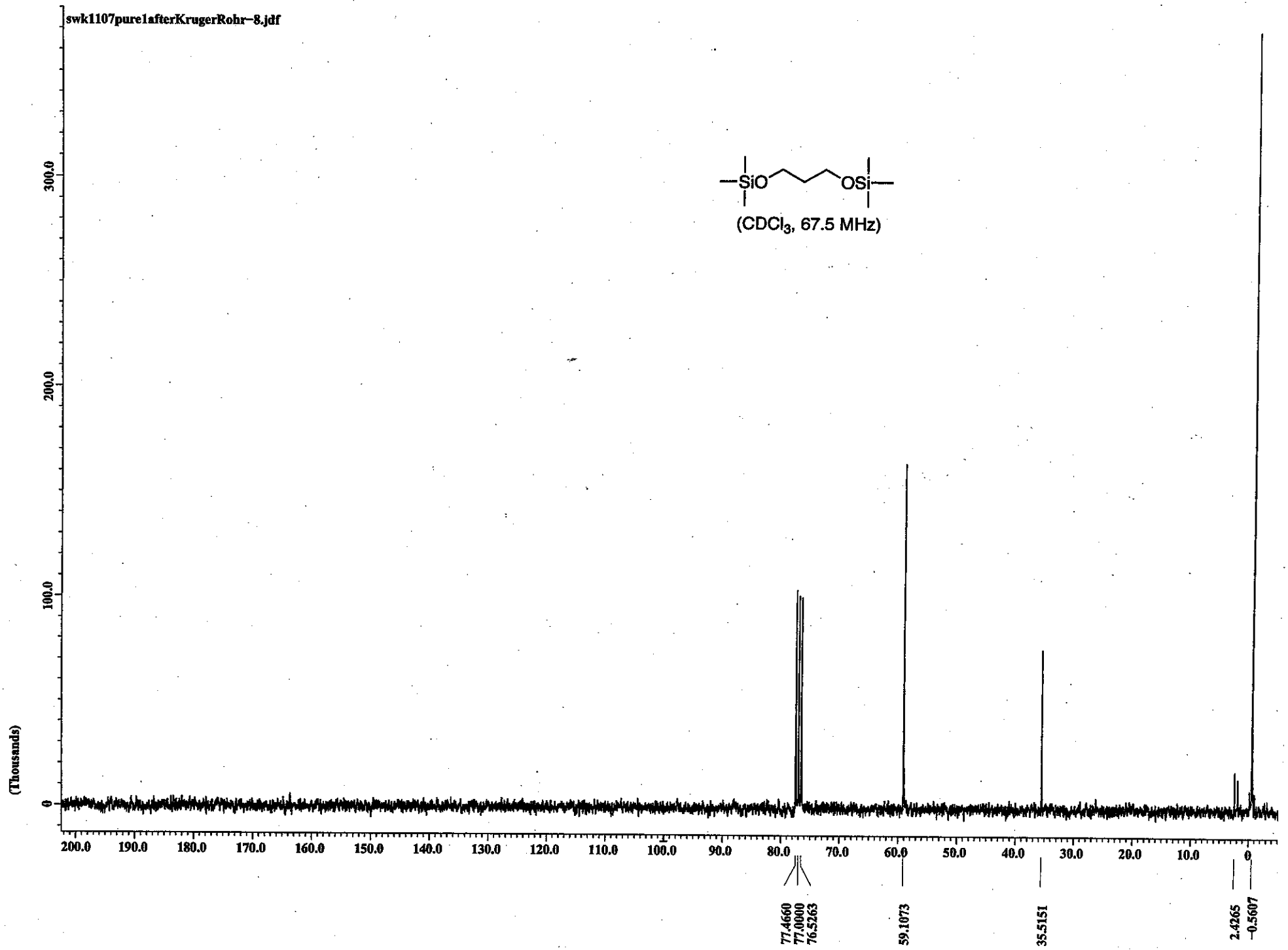
VI. Appendix: Spectral Data

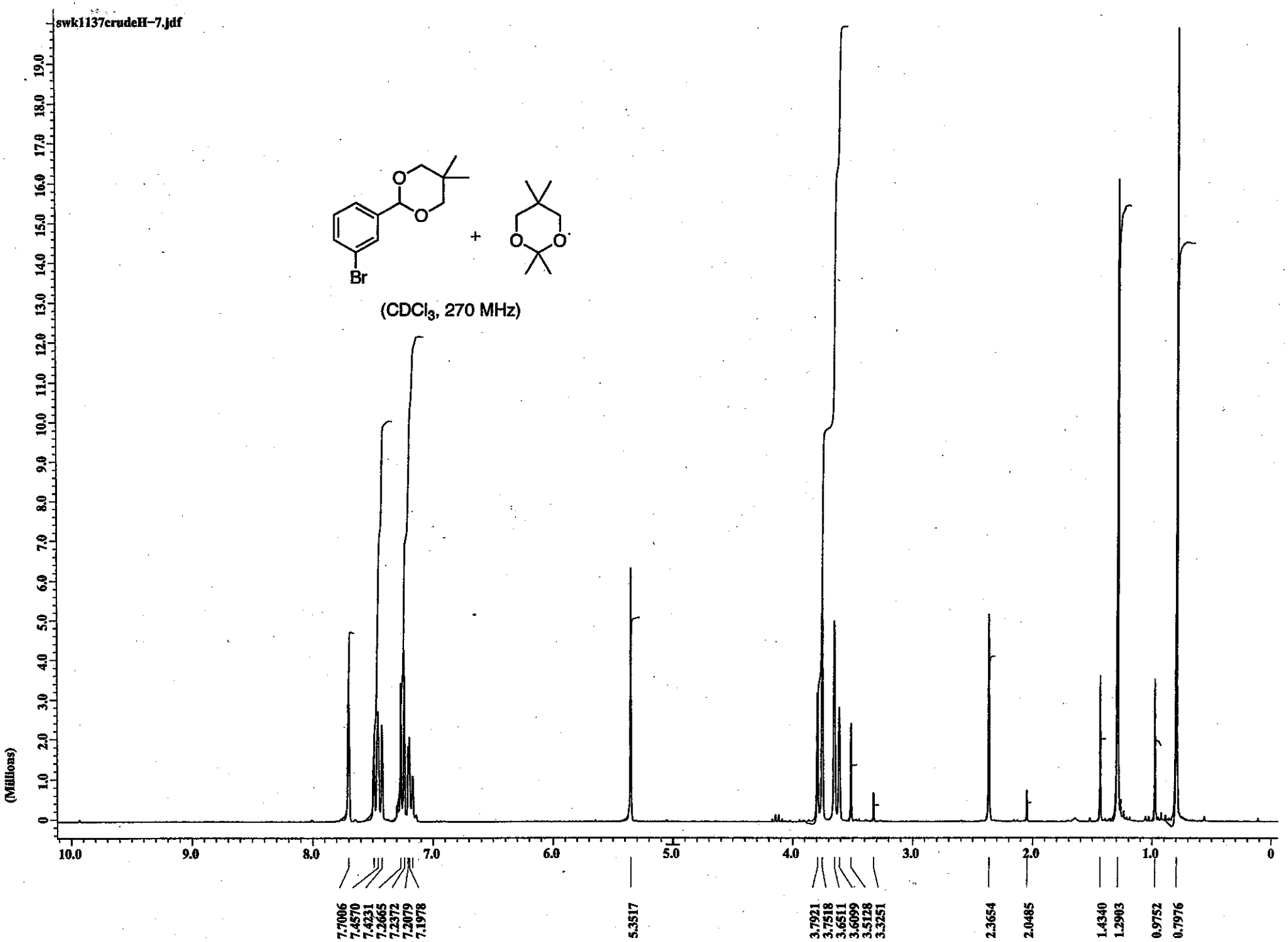

swk1075pure2H-9.jdf
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
22.0
23.0
24.0
25.0
O
H
SiO
(CDCl3, 270 MHz)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.8709
7.7903
7.7583
7.2454
6.9442
6.9130
1.0210
0.9762
0.9643
0.2335
0.2216
X : parts per Million : 1H

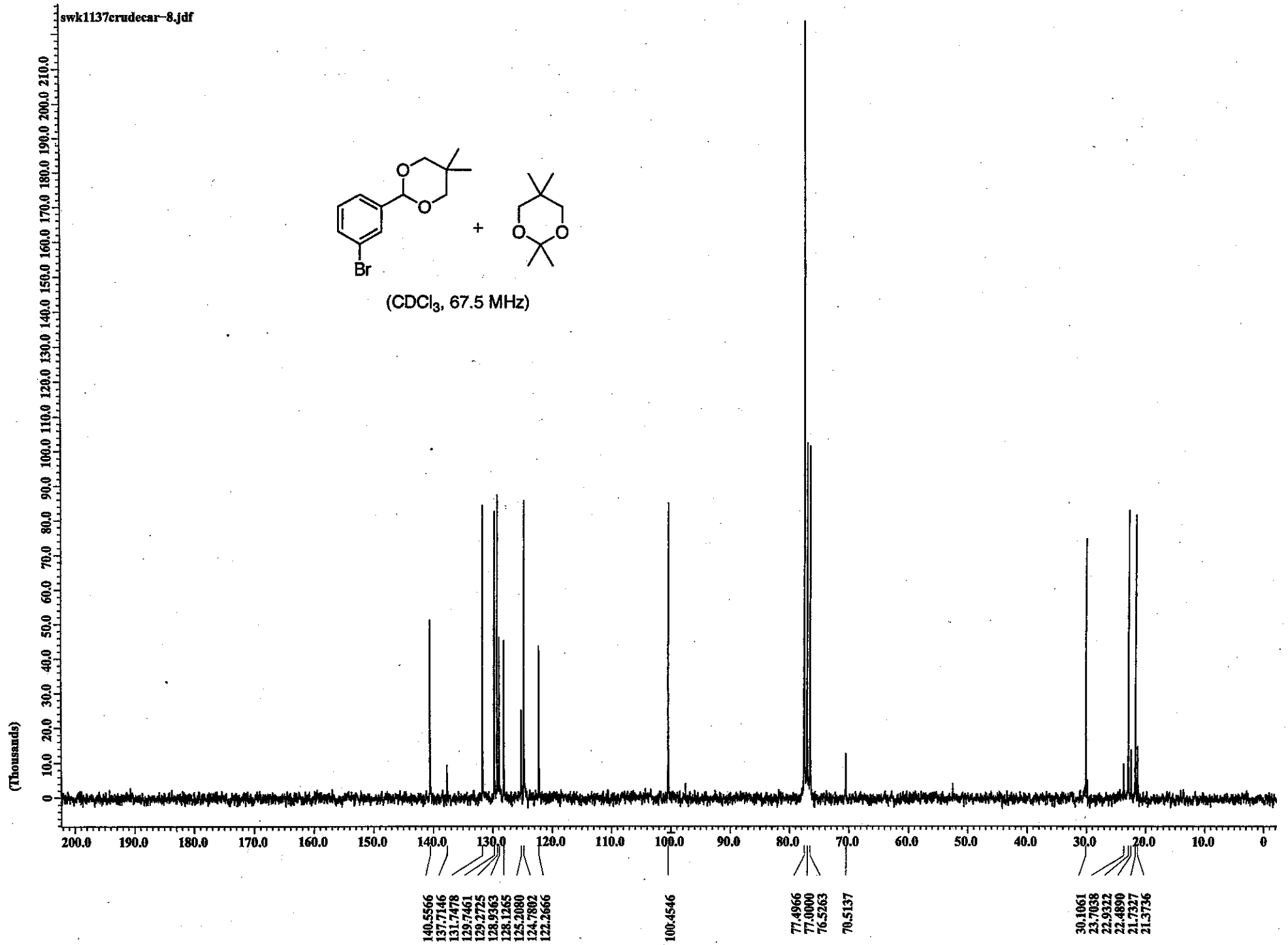

swk1075pure2H-11.jdf
(CDCl3, 67.5 MHz)
(Thousands)
0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
200.0
220.0
240.0
260.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
190.7205
161.3678
132.1069
131.7936
130.3191
120.3567
119.7760
77.4737
77.0000
76.5340
30.7478
25.4457
18.1266
-4.4799
X : parts per Million : 13C

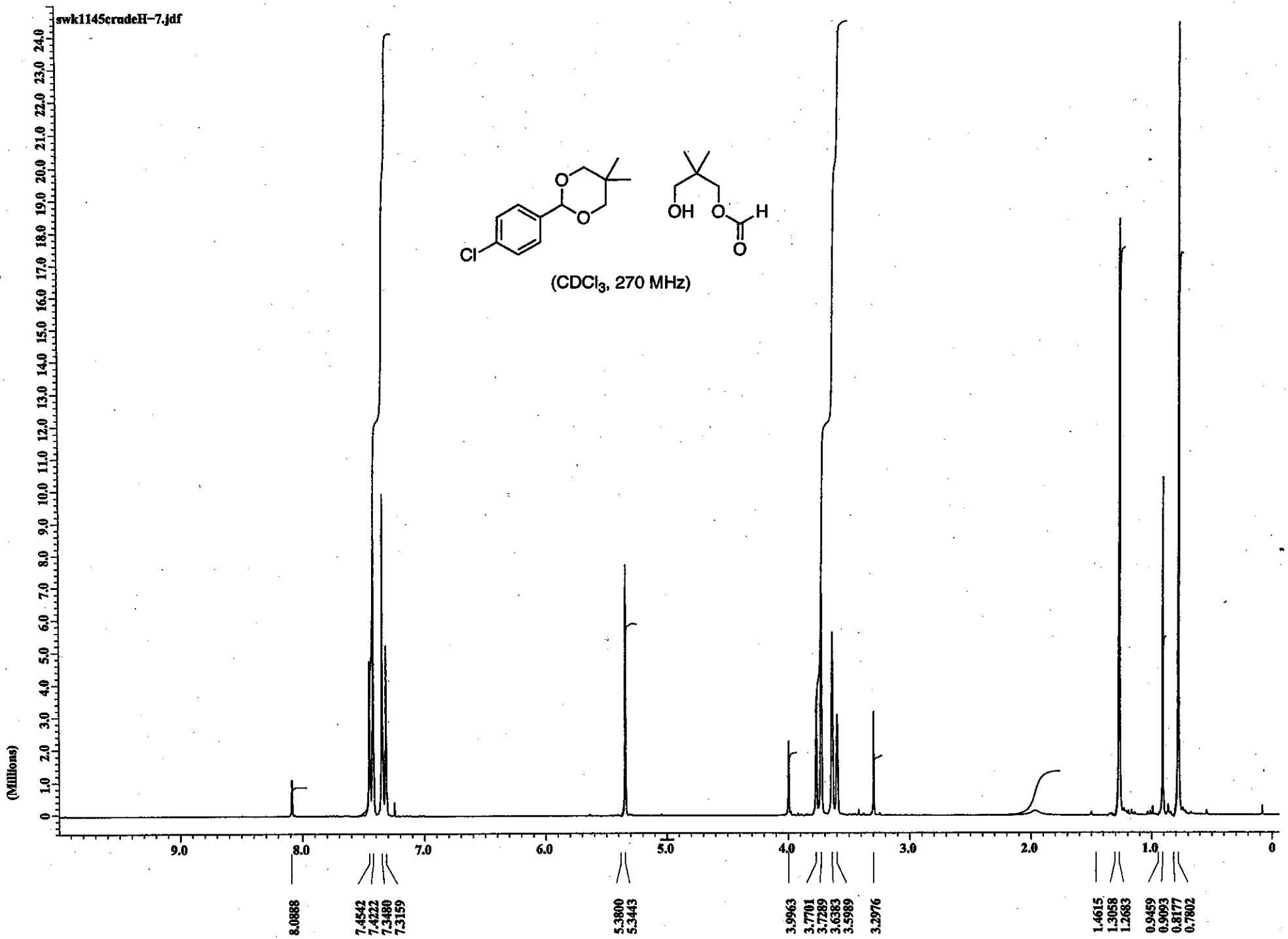


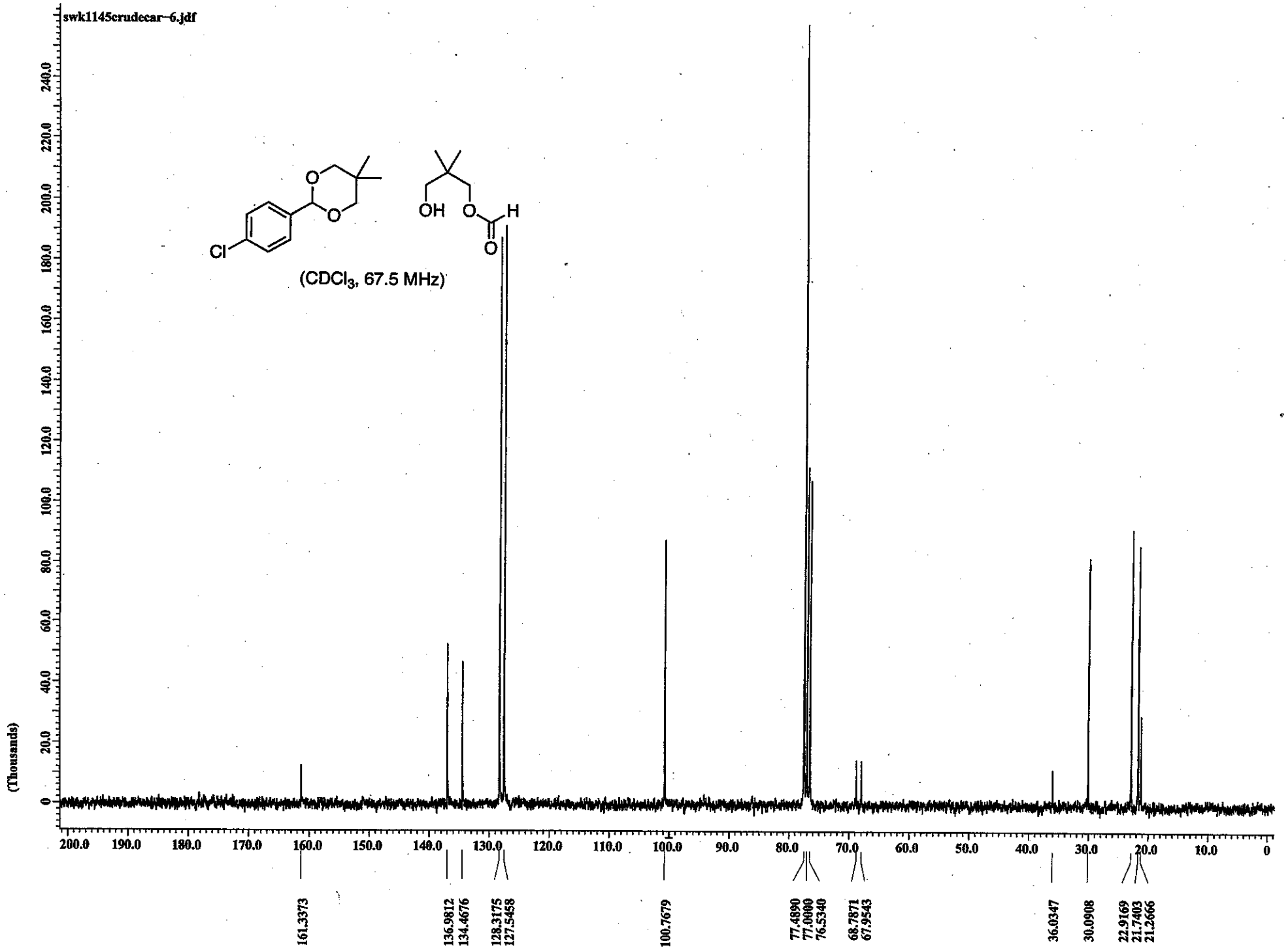
($CDCl_3$, 270 MHz)

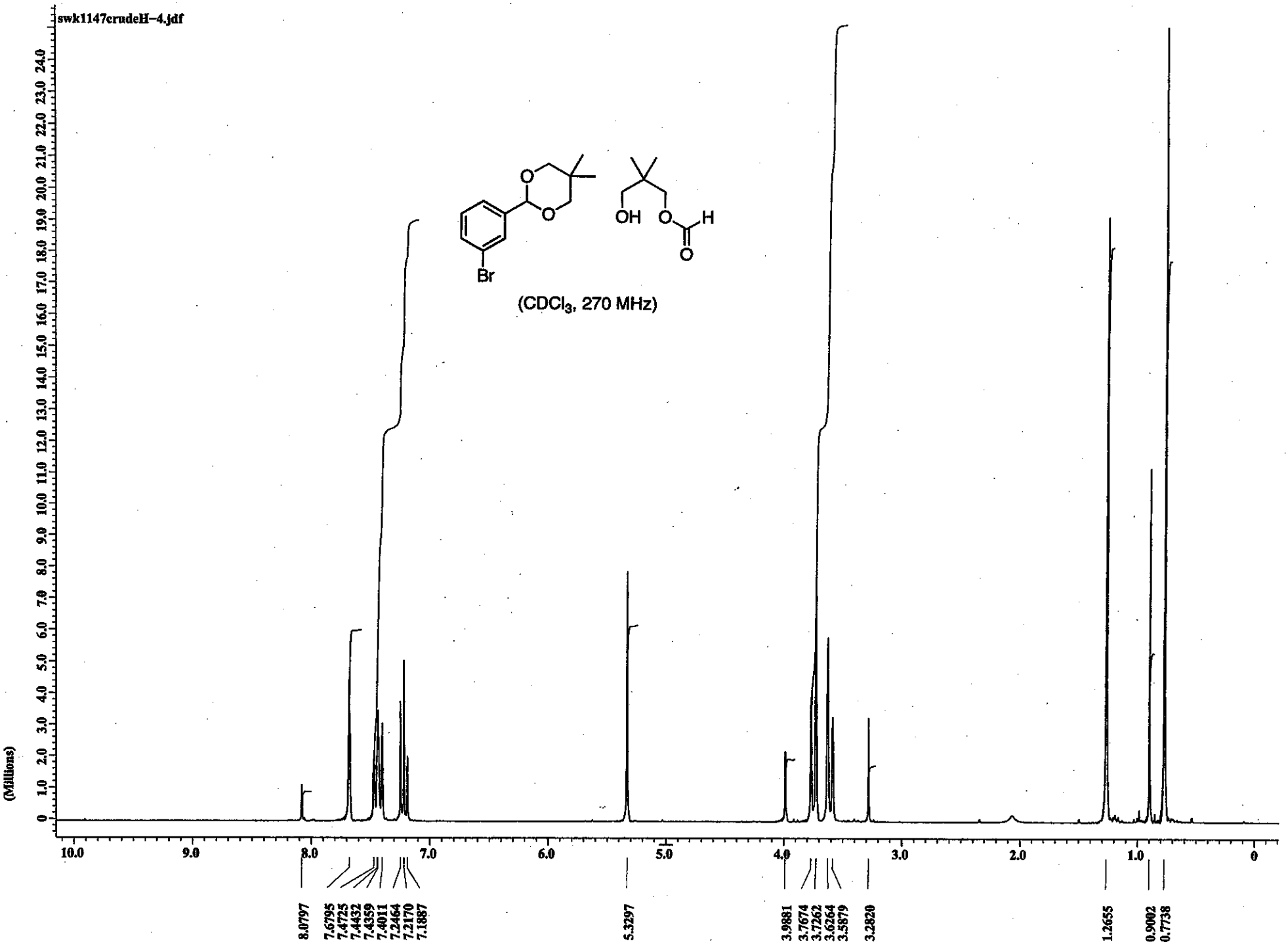

swk1107pure1afterKrugerRohr-8.jdf
(CDCl3, 67.5 MHz)
(Thousands)
300.0
200.0
100.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
77.4660
77.0900
76.5263
59.1073
35.5151
2.4265
-0.5607
X : parts per Million : 13C

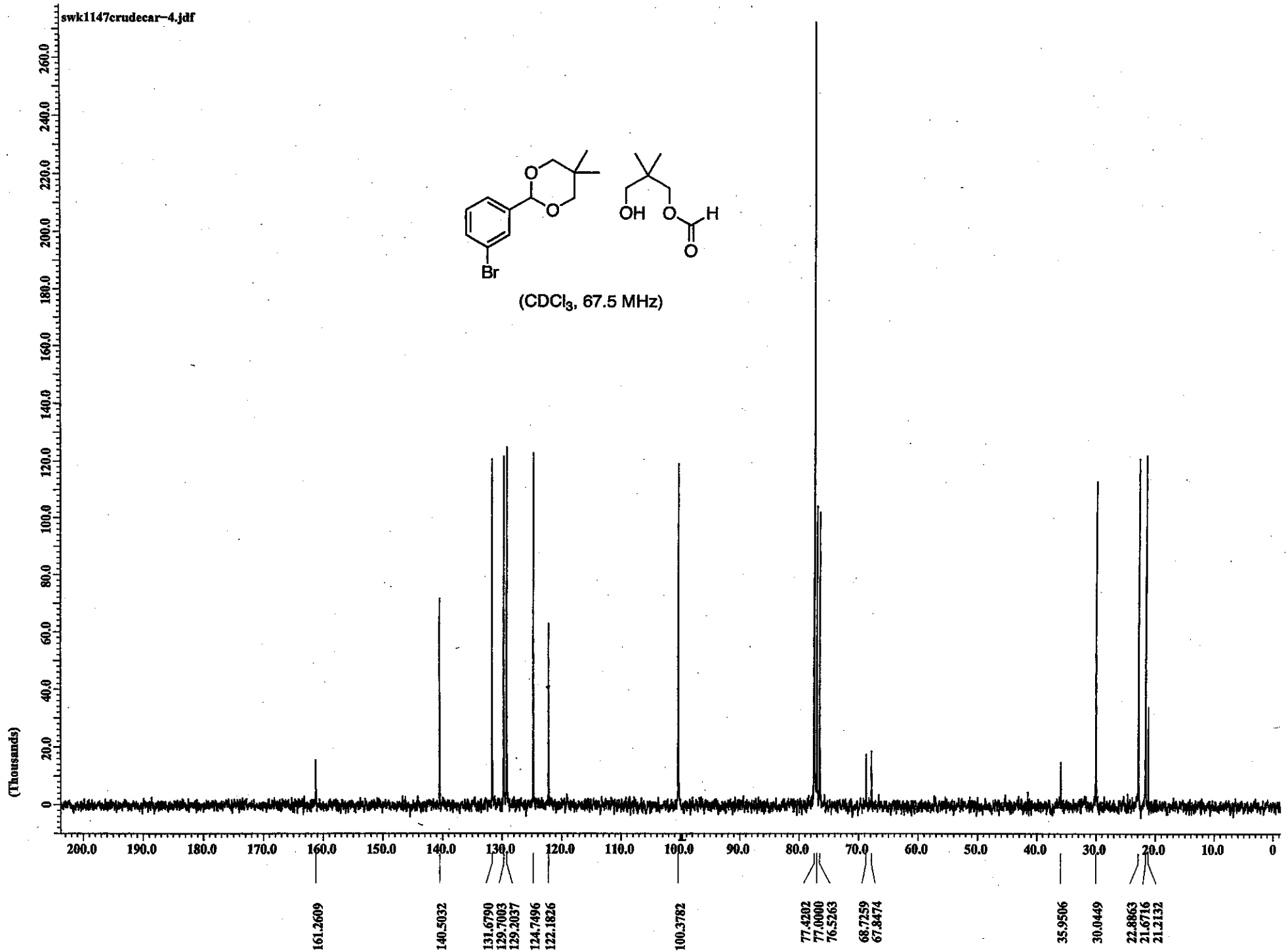

swk1137crudeH-7.jdf
Br
(CDCl3, 270 MHz)
(Millions)
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.7006
7.4570
7.4231
7.2665
7.2372
7.2079
7.1978
5.3517
3.7921
3.7518
3.6511
3.6099
3.5128
3.3251
2.3654
2.0485
1.4340
1.2903
0.9752
0.7976
X : parts per Million : 1H


swk1137crudecar-8.jdf
Br
+
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
140.5566
137.7146
131.7478
129.7461
129.2725
128.9363
128.1265
125.2080
124.7802
122.2666
100.4546
77.4966
77.0000
76.5263
70.5137
30.1061
23.7038
22.9322
22.4890
21.7327
21.3736
X : parts per Million : 13C

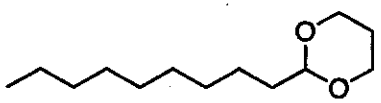

swk1145crudeH-7.jdf
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.0888
7.4542 7.4222 7.3480 7.3159
5.3800 5.3443
3.9963 3.7701 3.7289 3.6383 3.5989 3.2976
1.4615 1.3058 1.2683 0.9459 0.9093 0.8177 0.7802
Cl
O O
OH O H
O
(CDCl3, 270 MHz)
X : parts per Million : 1H


swk1145crudecar-6.jdf
(CDCl3, 67.5 MHz)
(Thousands)
240.0
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.3373
136.9812
134.4676
128.3175
127.5458
100.7679
77.4890
77.0000
76.5340
68.7871
67.9543
36.0347
30.0908
22.9169
21.7403
21.2666
X : parts per Million : 13C


swk1147crudeH-4.jdf
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
22.0
23.0
24.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
O
Br
OH
O
H
O
(CDCl3, 270 MHz)
8.0797
7.6795
7.4725
7.4432
7.4359
7.4011
7.2464
7.2170
7.1887
5.3297
3.9881
3.7674
3.7262
3.6264
3.5879
3.2820
1.2655
0.9002
0.7738
X : parts per Million : 1H


swk1147crudecar-4.jdf
(CDCl3, 67.5 MHz)
(Thousands)
X : parts per Million : 13C
161.2609
140.5032
131.6790
129.7003
129.2037
124.7496
122.1826
100.3782
77.4202
77.0000
76.5263
68.7259
67.8474
35.9506
30.0449
22.8863
21.6716
21.2132

swk1169crudeH-5.jdf



($CDCl_3$, 270 MHz)

(Millions)

0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0

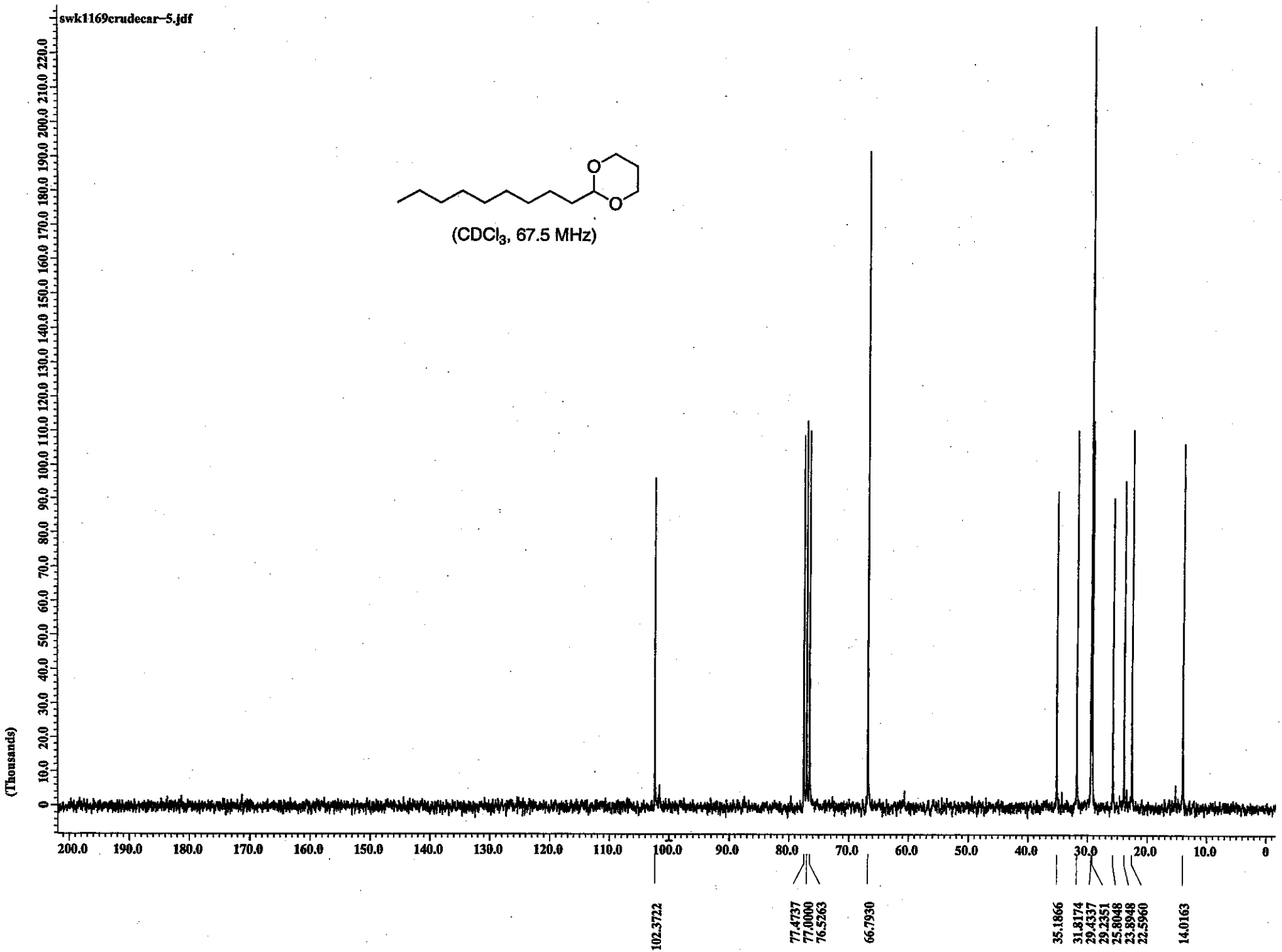
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0

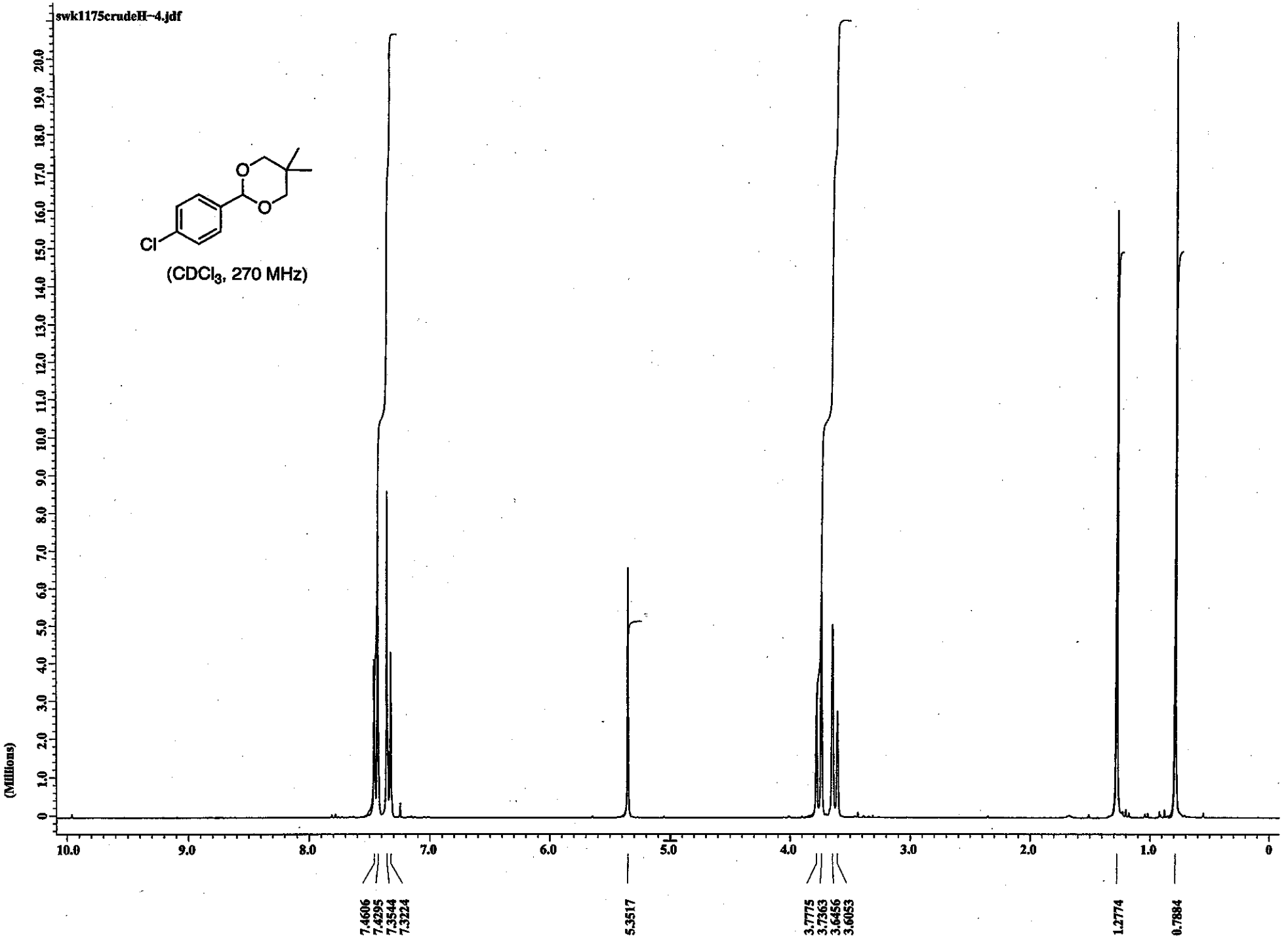
7.2454

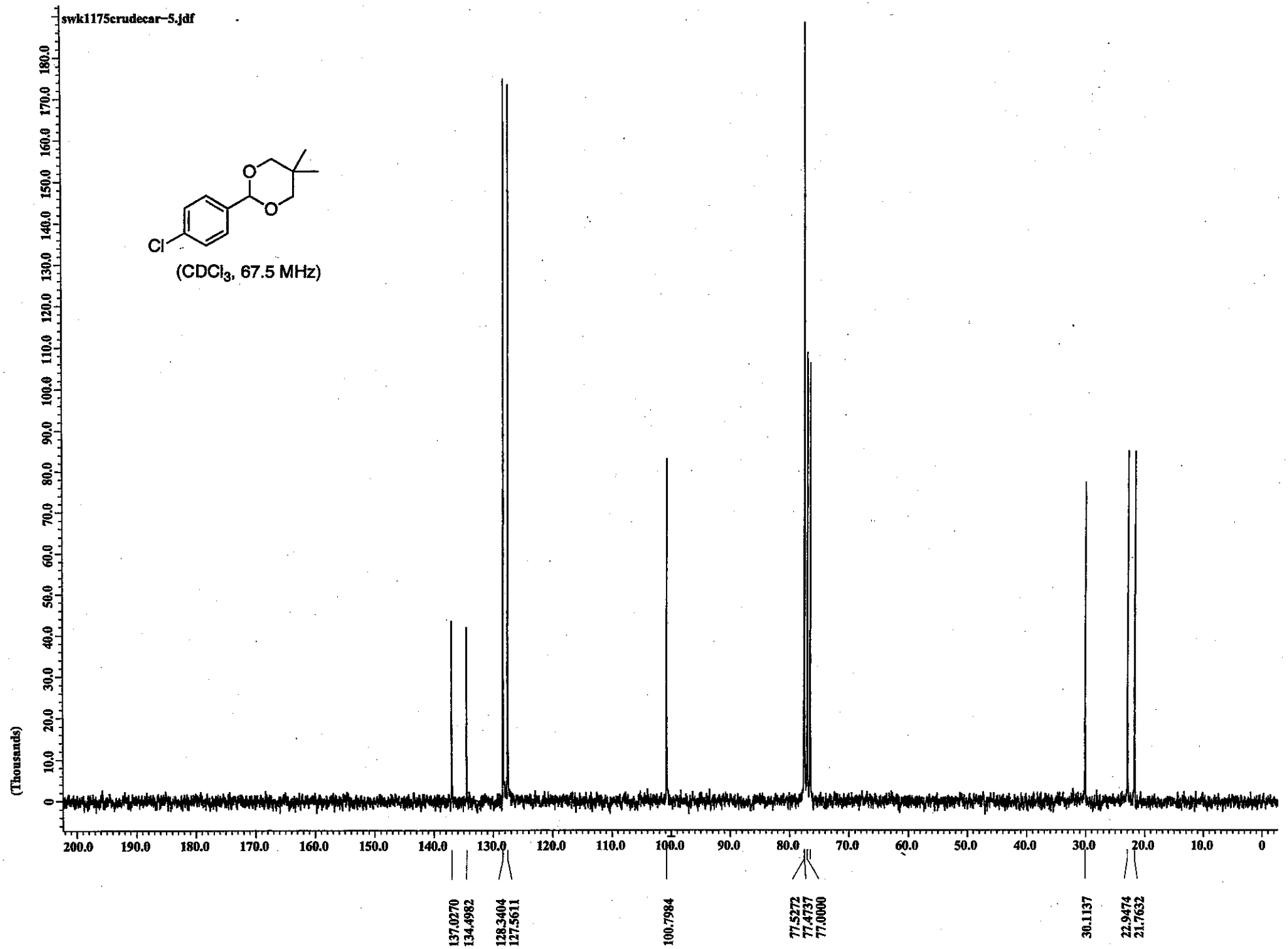
4.4679 4.4496 4.4304 4.0723 4.0540 4.0330 4.0146 3.7042 3.6960

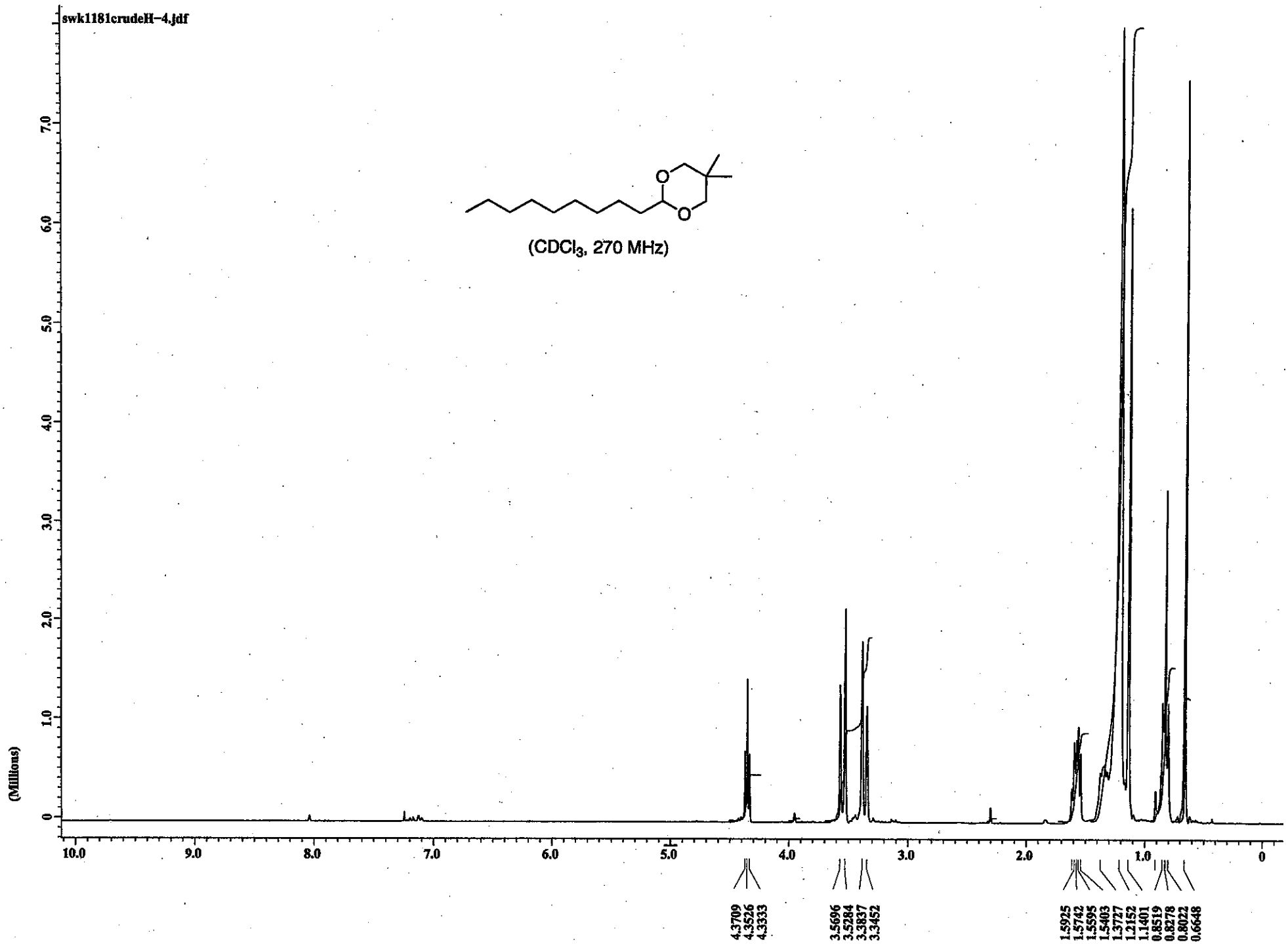
2.0439 2.0137 1.9954 1.9771 1.5421 1.5238 1.5101 1.4908 1.3003 1.2079 0.8452 0.8223 0.7967

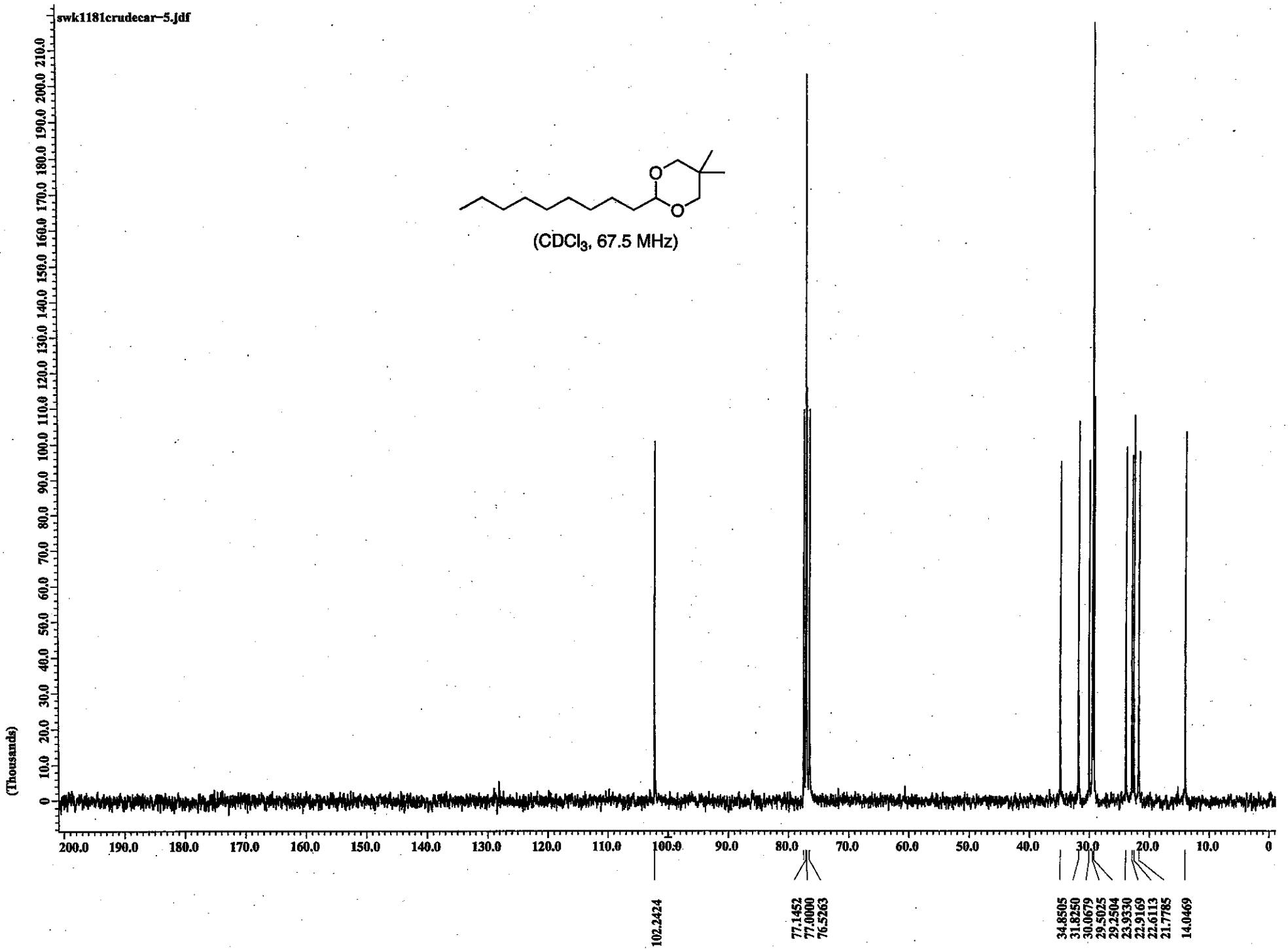
X : parts per Million : 1H

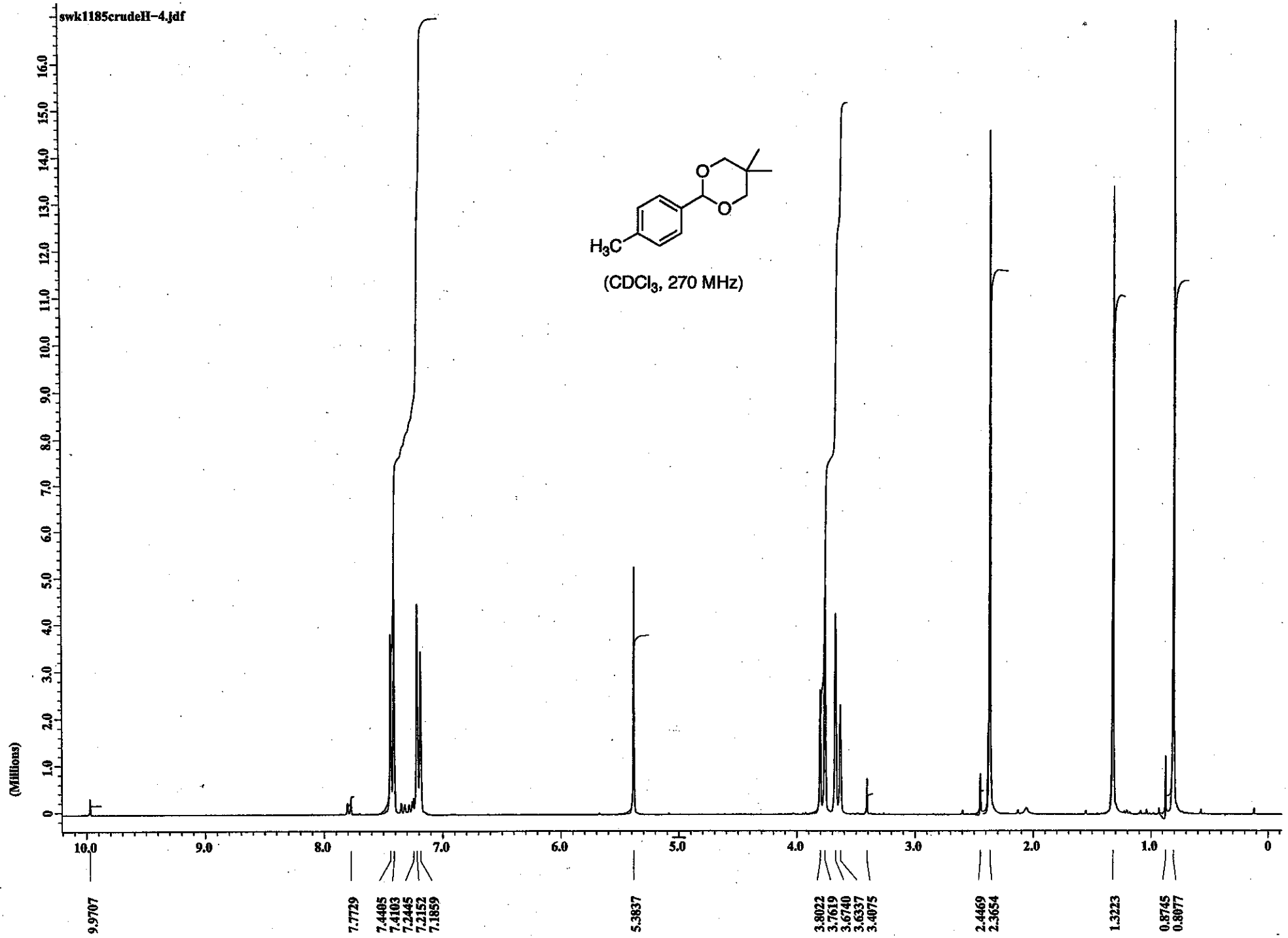

swk1169crudecar~5.jdf
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
210.0
220.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
102.3722
77.4737
77.0000
76.5263
66.7930
35.1866
31.8174
29.4337
29.2351
25.8048
23.8948
22.5960
14.0163
X : parts per Million : 13C

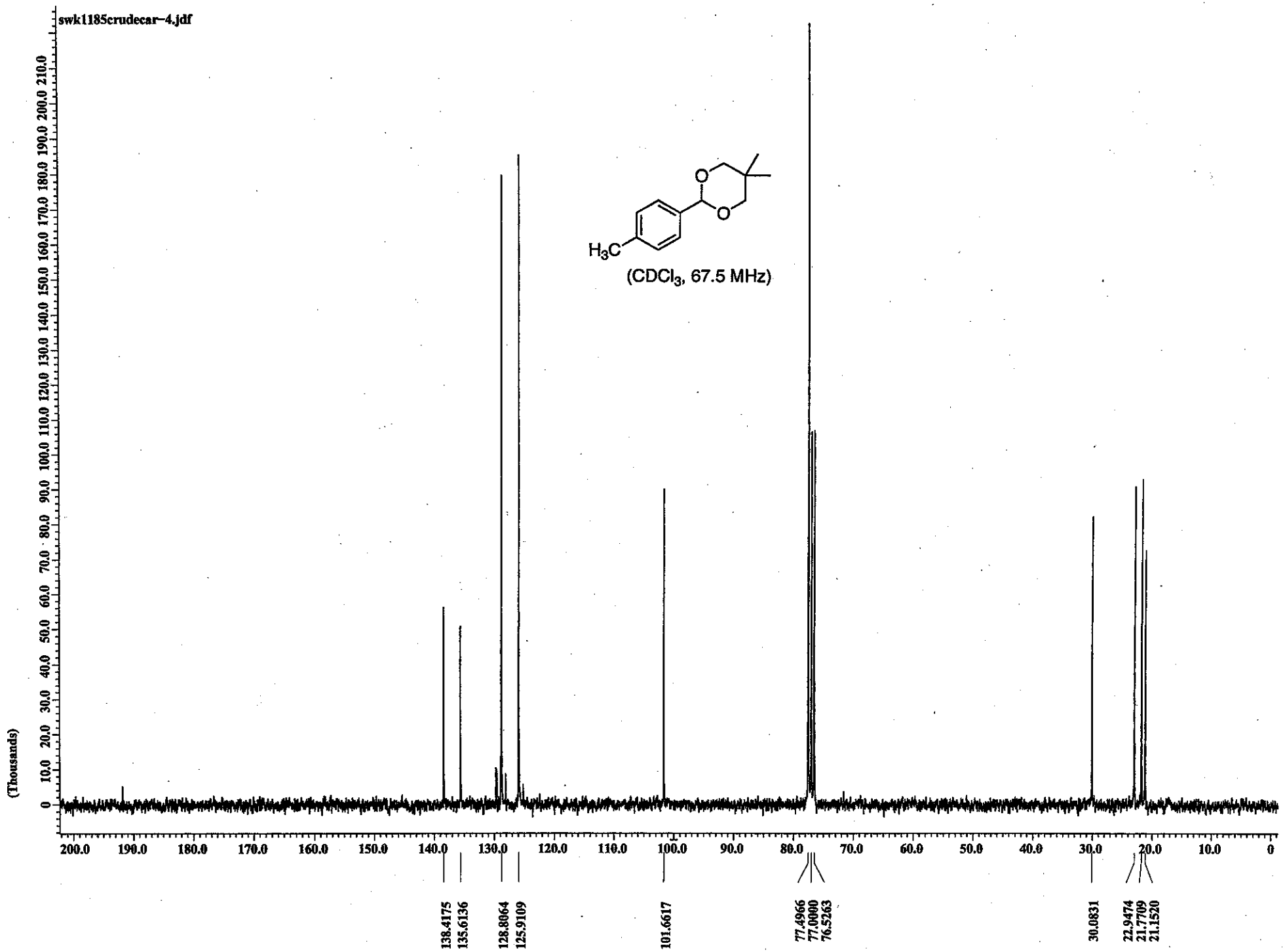

swk1175crudeH-4.jdf
(CDCl3, 270 MHz)
(Millions)
7.4606
7.4295
7.3544
7.3224
5.3517
3.7775
3.7363
3.6456
3.6053
1.2774
0.7884
X : parts per Million : 1H

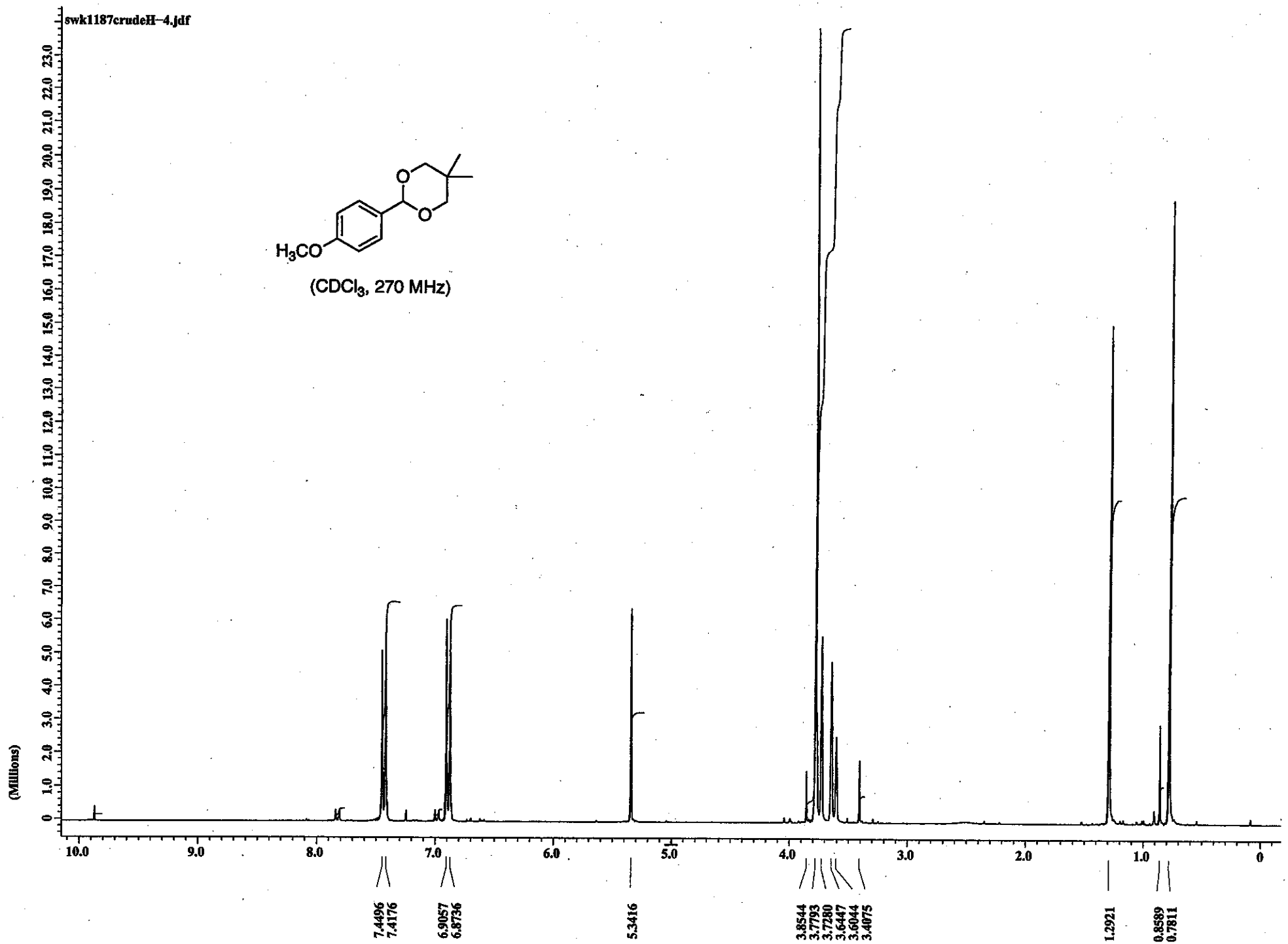

swk1175crudecar-5.jdf
Cl
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
137.0270
134.4982
128.3404
127.5611
100.7984
77.5272
77.4737
77.0000
30.1137
22.9474
21.7632
X : parts per Million : 13C

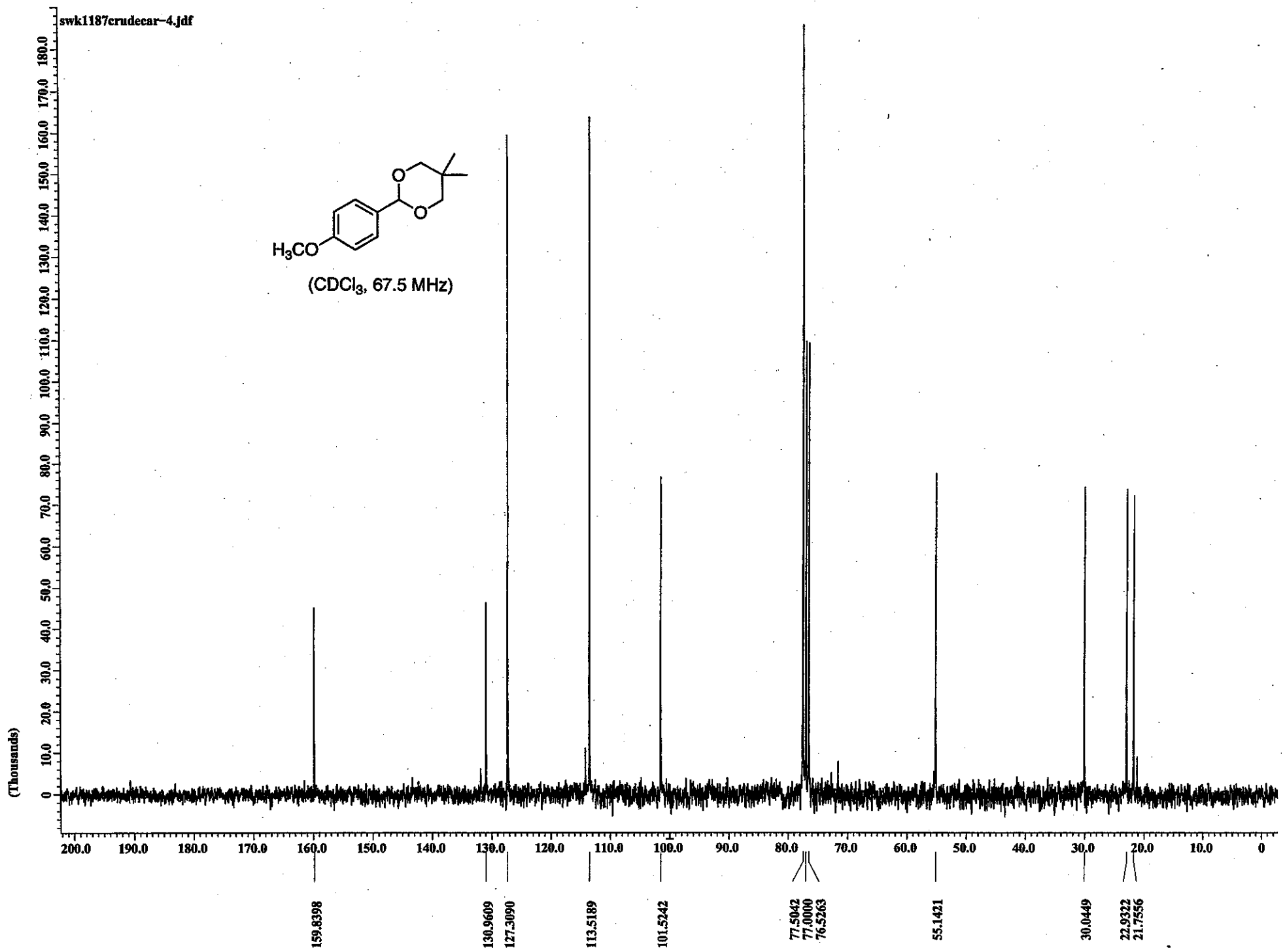

swk1181crudeH-4.jdf
(CDCl3, 270 MHz)
(Millions)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
4.3709
4.3526
4.3333
3.5696
3.5284
3.3837
3.3452
1.5925
1.5742
1.5595
1.5403
1.3727
1.2152
1.1401
0.8519
0.8278
0.8022
0.6648
X : parts per Million : 1H

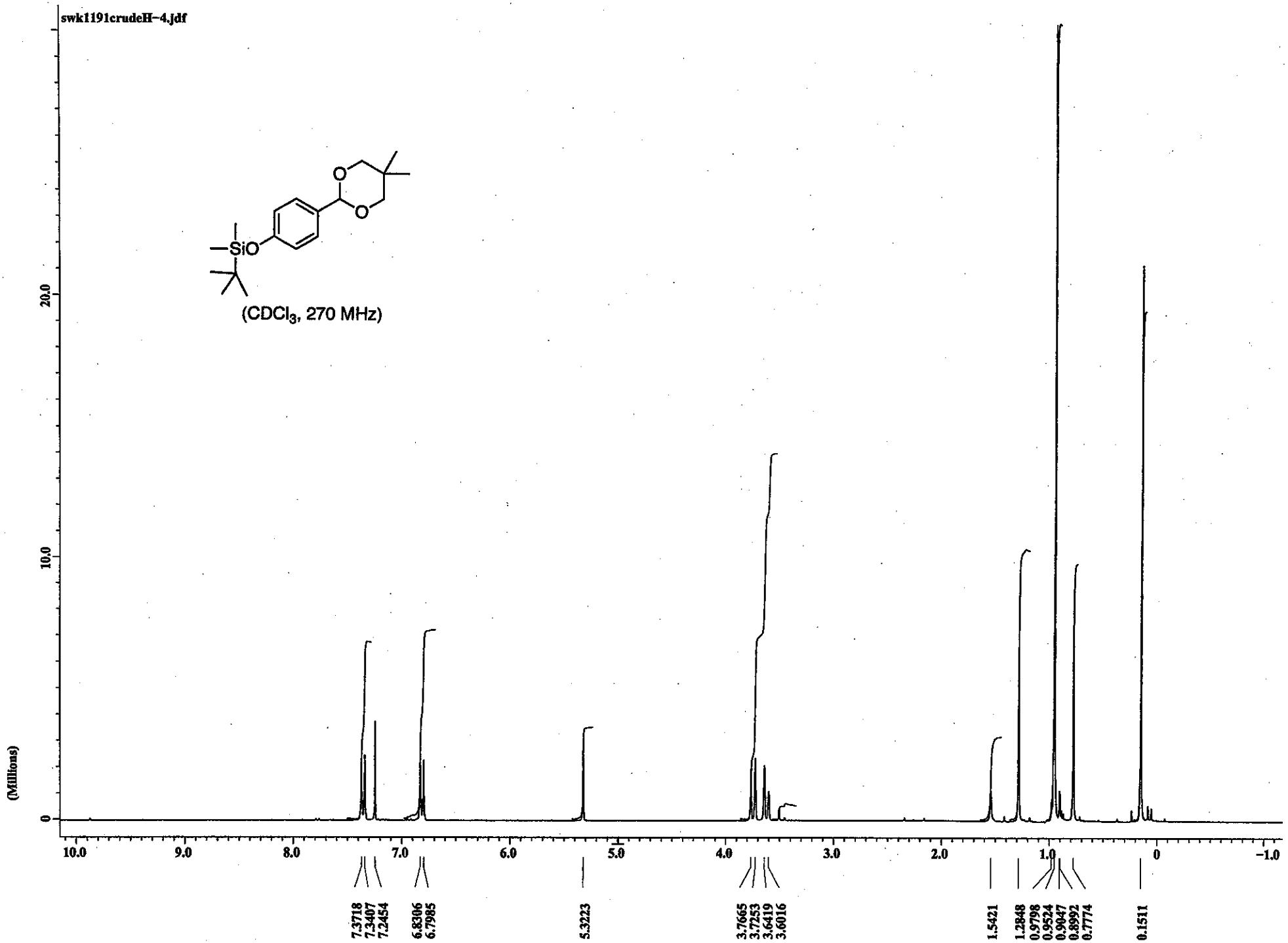

swk1181crudecar-5.jdf
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
102.2424
77.1452
77.0000
76.5263
34.8505
31.8250
30.0679
29.5025
29.2504
23.9330
22.9169
22.6113
21.7785
14.0469
X : parts per Million : 13C

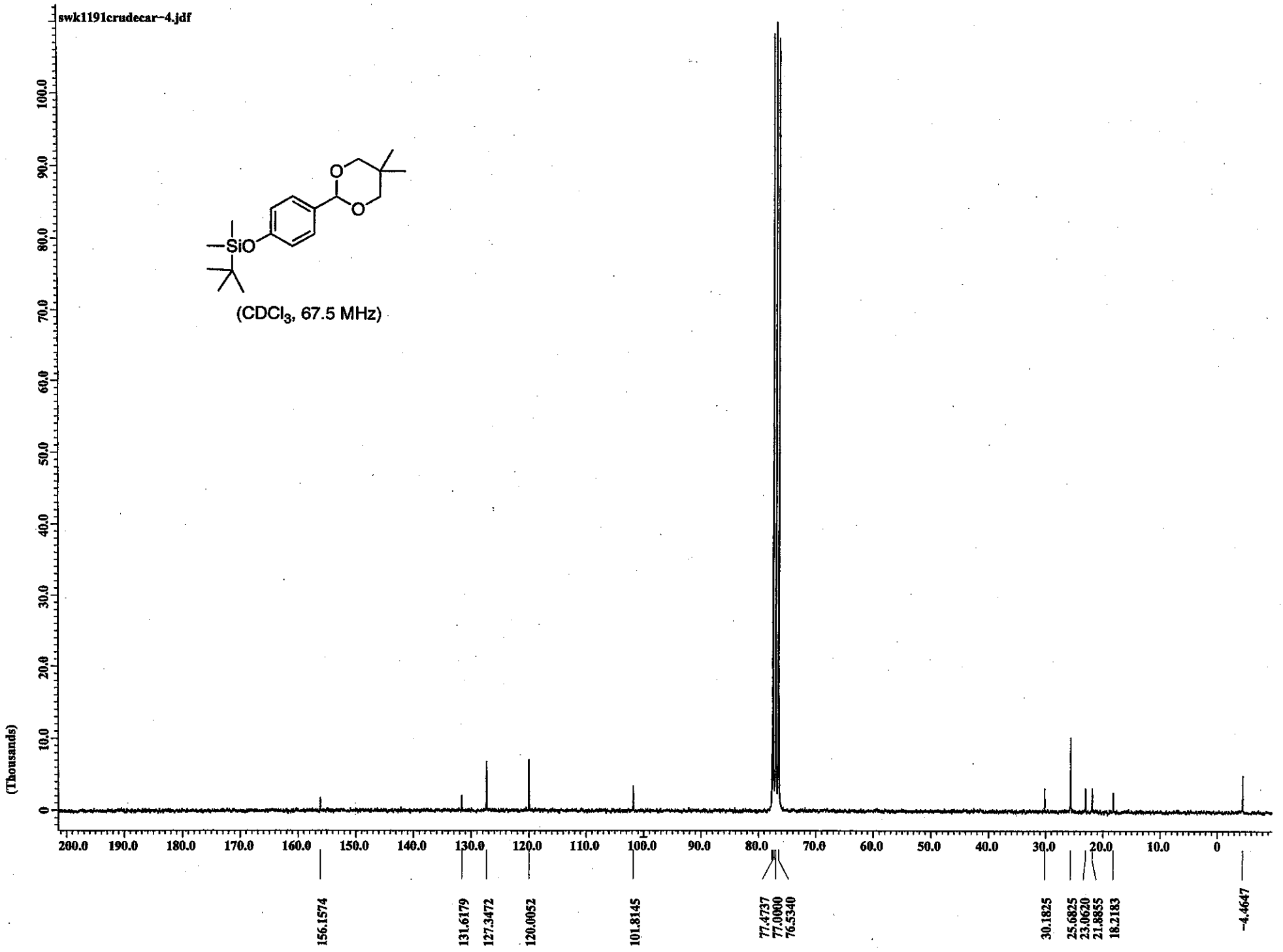

swk1185crudeH-4.jdf
(Millions)
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.9707
7.7729
7.4485
7.4103
7.2445
7.2152
7.1859
5.3837
3.8022
3.7619
3.6740
3.6337
3.4075
2.4469
2.3654
1.3223
0.8745
0.8077
X : parts per Million : 1H
O
O
H3C
(CDCl3, 270 MHz)

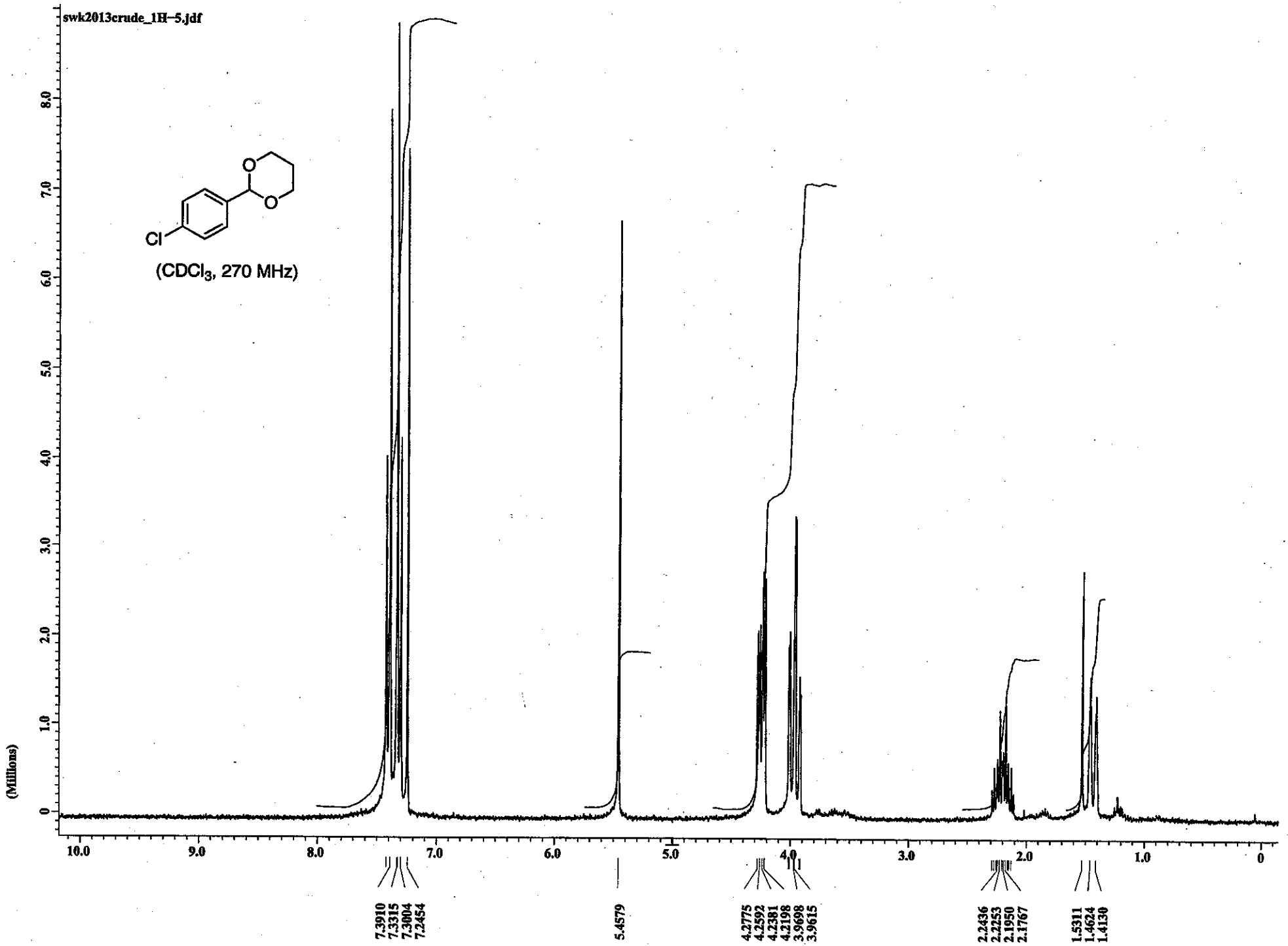

swk1185crudecar-4.jdf
(CDCl3, 67.5 MHz)
(Thousands)
138.4175
135.6136
128.8064
125.9109
101.6617
77.4966
77.0000
76.5263
30.0831
22.9474
21.7709
21.1520
X : parts per Million : 13C

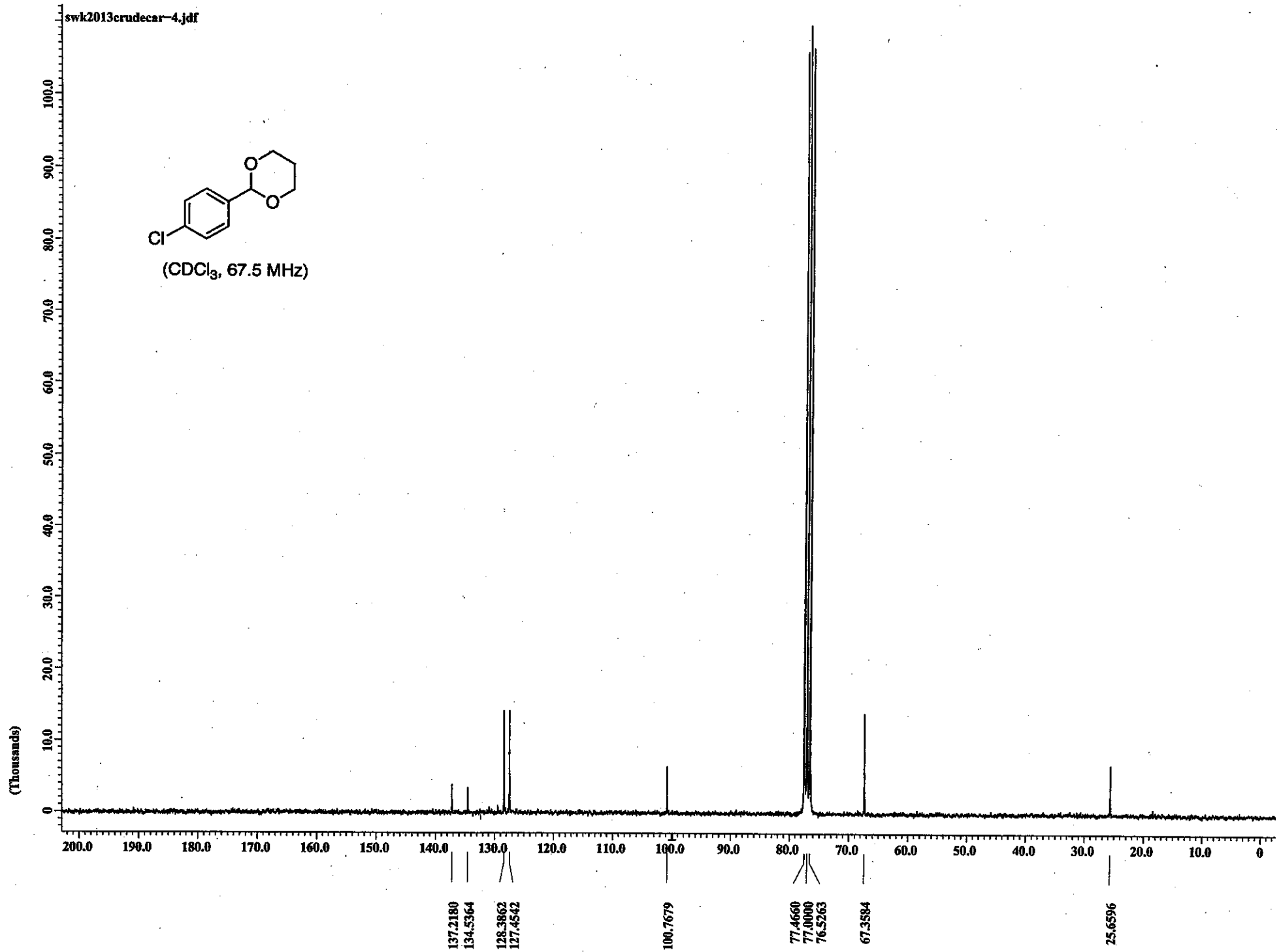

swk1187crudeH-4.jdf
H3CO
(CDCl3, 270 MHz)
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.4496
7.4176
6.9057
6.8736
5.3416
3.8544
3.7793
3.7280
3.6447
3.6044
3.4075
1.2921
0.8589
0.7811
X : parts per Million : 1H

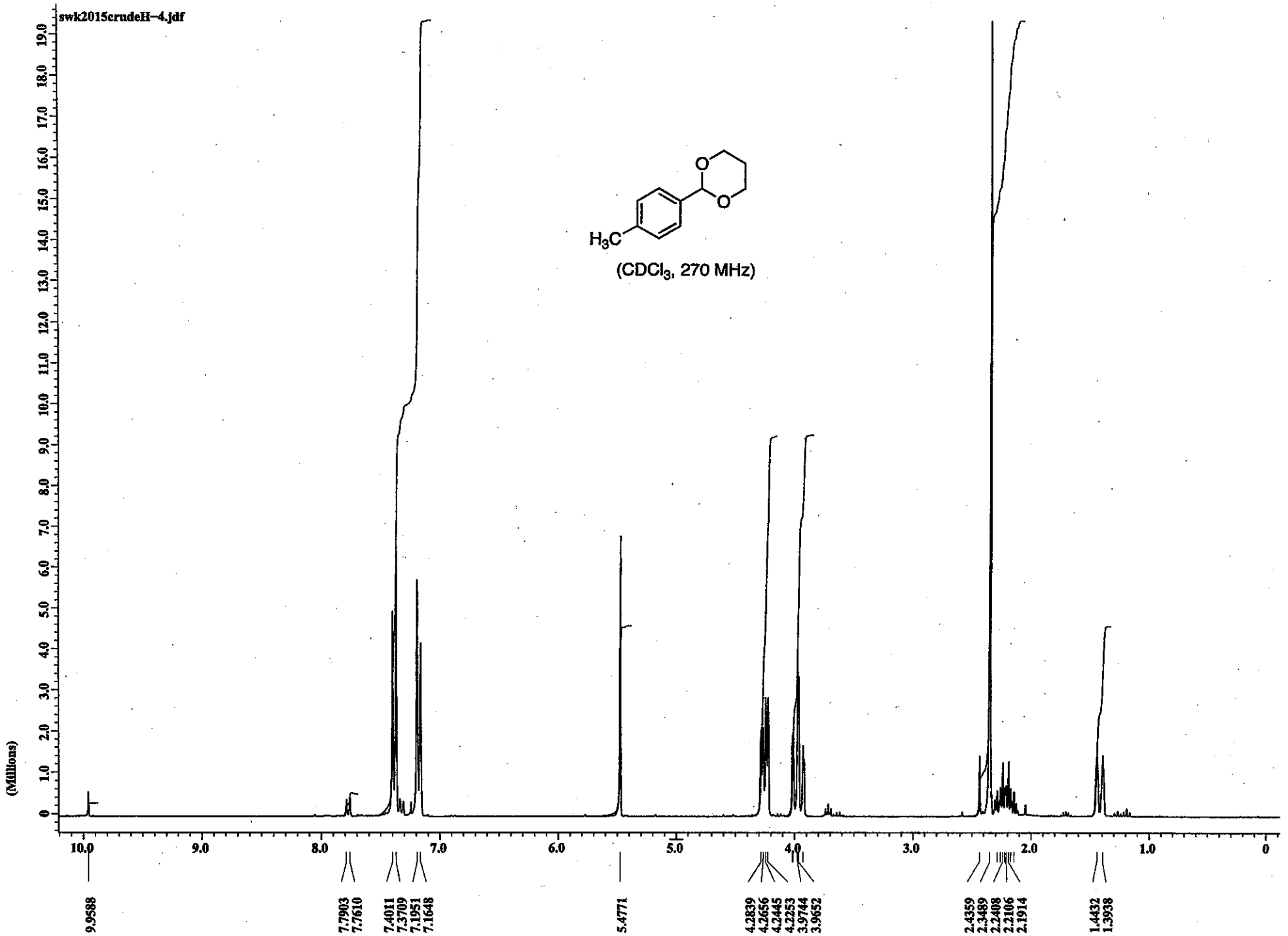

swk1187crudecar-4.jdf
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
O
O
H3CO
(CDCl3, 67.5 MHz)
159.8398
130.9609
127.3090
113.5189
101.5242
77.5042
77.0000
76.5263
55.1421
30.0449
22.9322
21.7556
X : parts per Million : 13C


swk1191crudeH-4.jdf
(CDCl3, 270 MHz)
(Millions)
20.0
10.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
7.3718
7.3407
7.2454
6.8306
6.7985
5.3223
3.7665
3.7253
3.6419
3.6016
1.5421
1.2848
0.9798
0.9524
0.9047
0.8992
0.7774
0.1511
X : parts per Million : 1H

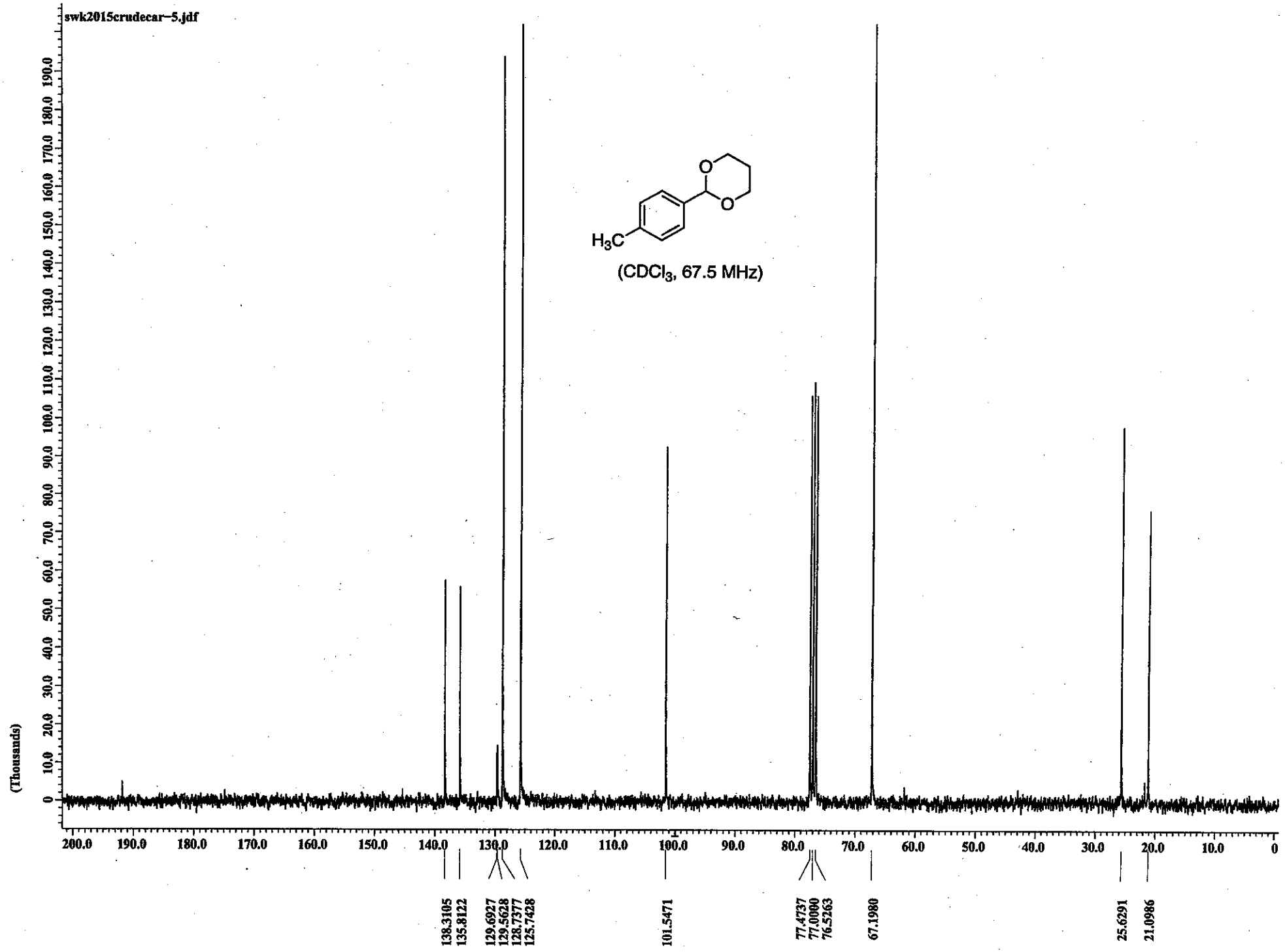

swk1191crudecar-4.jdf
(CDCl3, 67.5 MHz)
(Thousands)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
156.1574
131.6179
127.3472
120.0052
101.8145
77.4737
77.0000
76.5340
30.1825
25.6825
23.0620
21.8855
18.2183
-4.4647
X : parts per Million : 13C

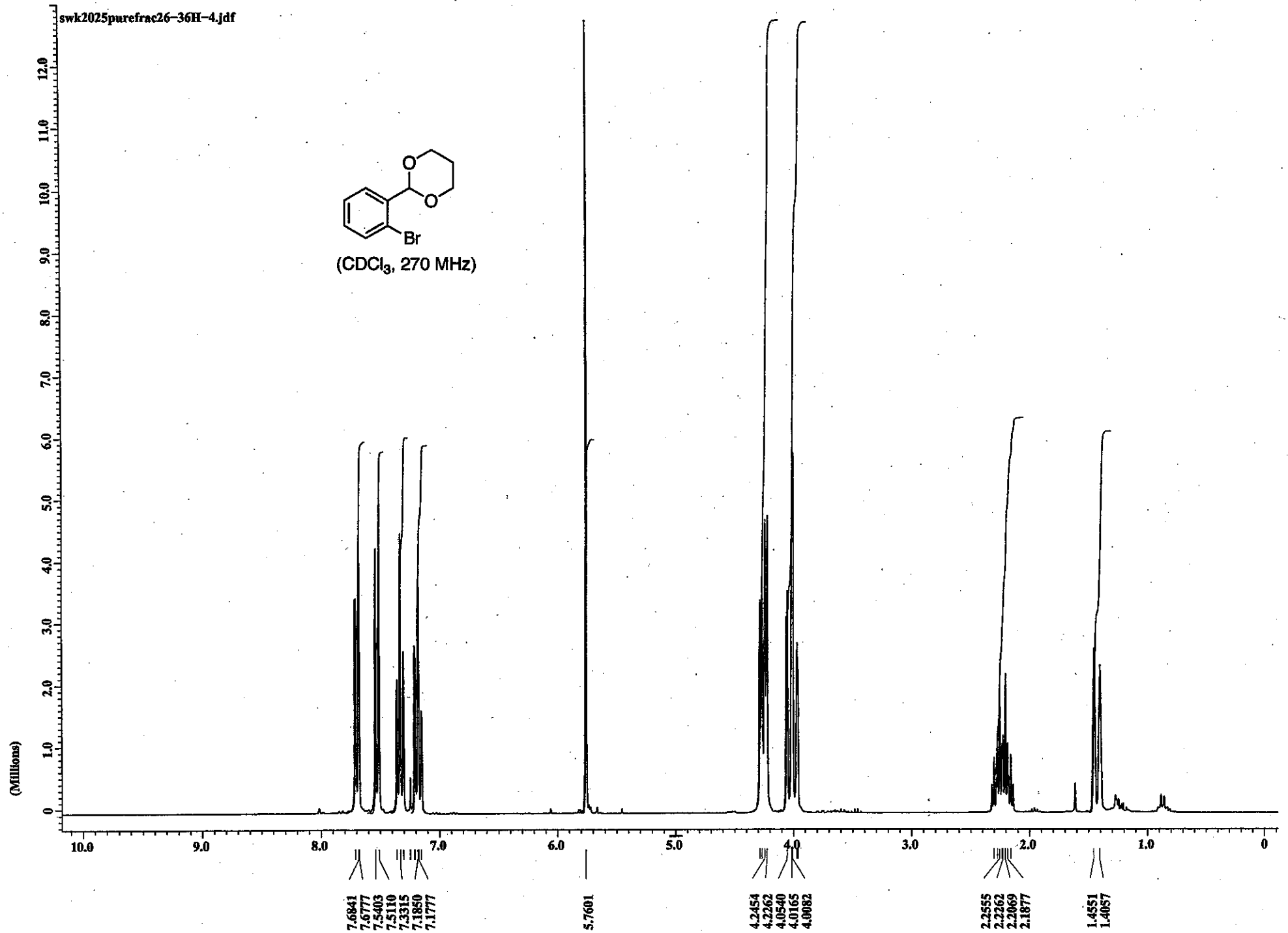

swk2013crude_1H-5.jdf
Cl
O
O
(CDCl3, 270 MHz)
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.3910
7.3315
7.3004
7.2454
5.4579
4.2775
4.2592
4.2381
4.2198
3.9698
3.9615
2.2436
2.2253
2.1950
2.1767
1.5311
1.4624
1.4130
X : parts per Million : 1H

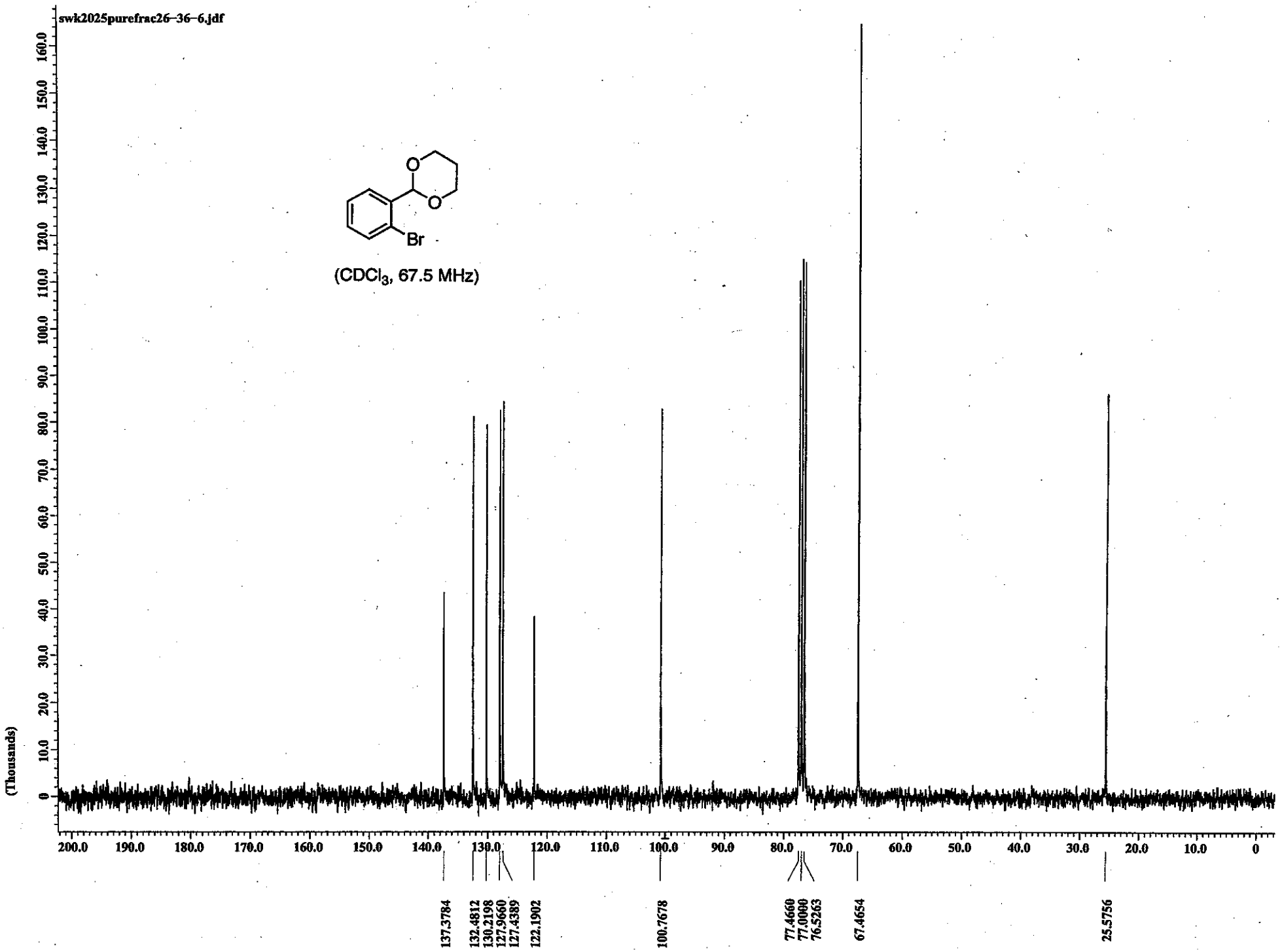

swk2013crudecar-4.jdf
Cl
O
O
(CDCl3, 67.5 MHz)
(Thousands)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
137.2180
134.5364
128.3862
127.4542
100.7679
77.4660
77.0000
76.5263
67.3584
25.6596
X : parts per Million : 13C



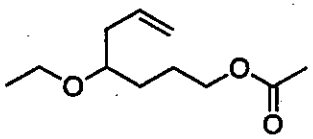
($CDCl_3$, 270 MHz)


swk2015crudecar-5.jdf
(Thousands)
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
O
O
H3C
(CDCl3, 67.5 MHz)
138.3105
135.8122
129.6927
129.5628
128.7377
125.7428
101.5471
77.4737
77.0000
76.5263
67.1980
25.6291
21.0986
X : parts per Million : 13C


swk2025purefrac26-36H-4.jdf
(CDCl3, 270 MHz)
Br
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6841
7.6777
7.5403
7.5110
7.3315
7.1850
7.1777
5.7601
4.2454
4.2262
4.0540
4.0165
4.0082
2.2555
2.2262
2.2069
2.1877
1.4551
1.4057
X : parts per Million : 1H


swk2025purefrac26-36-6.jdf
Br
(CDCl3, 67.5 MHz)
(Thousands)
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
137.3784
132.4812
130.2198
127.9660
127.4389
122.1902
100.7678
77.4660
77.0000
76.5263
67.4654
25.5756
X : parts per Million : 13C

swk2129frac34~54H~4.jdf

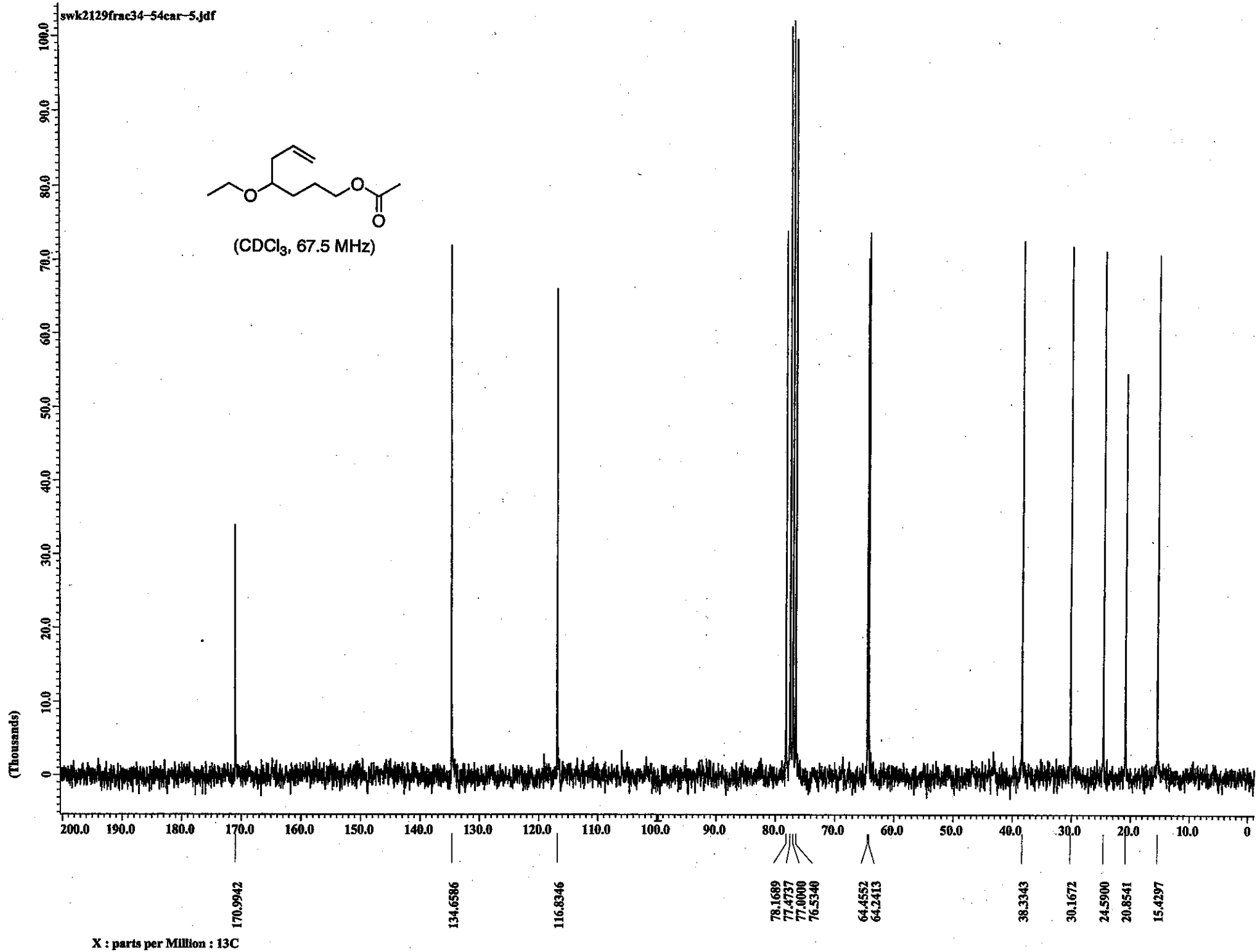


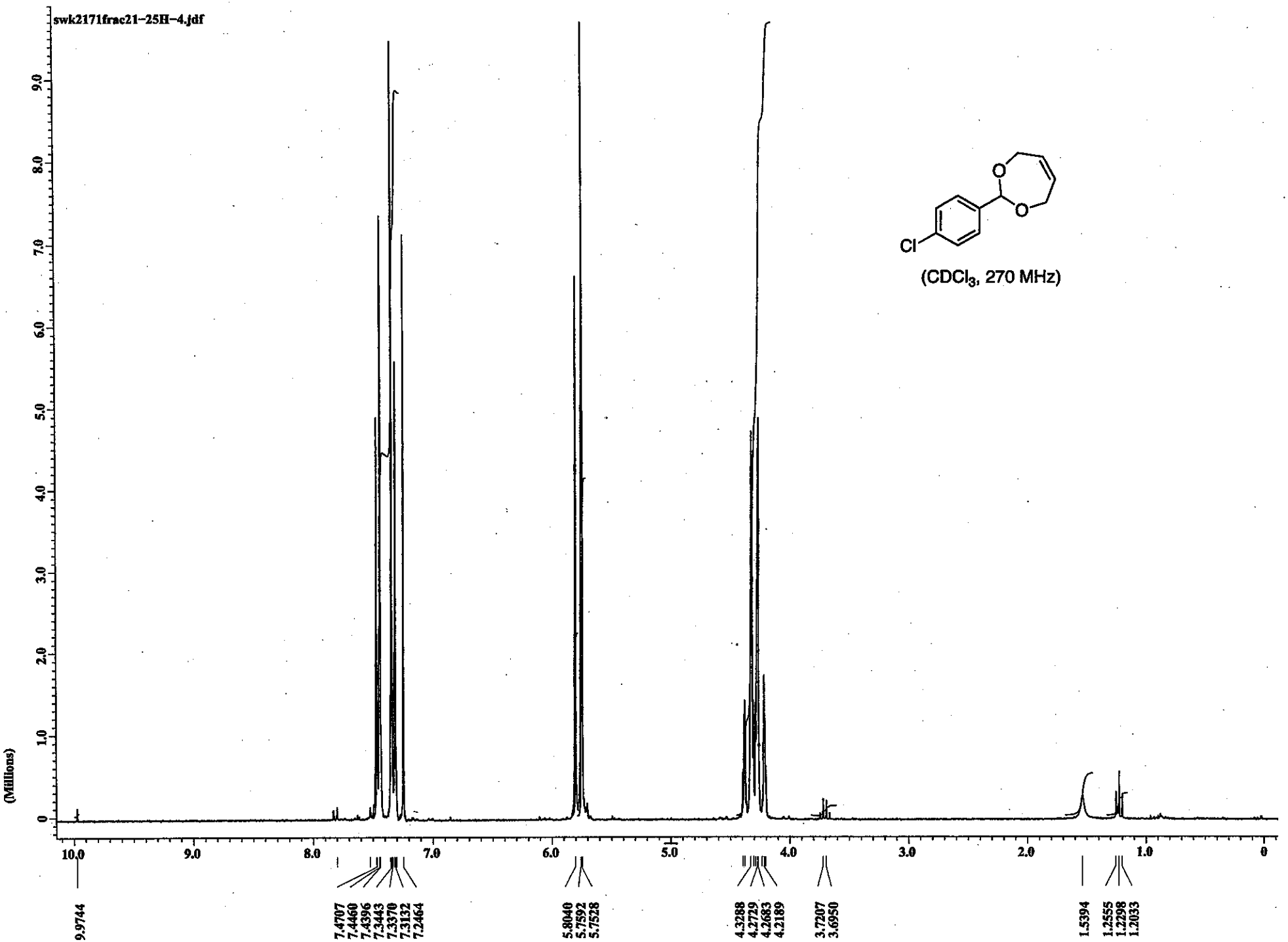
($CDCl_3$, 270 MHz)

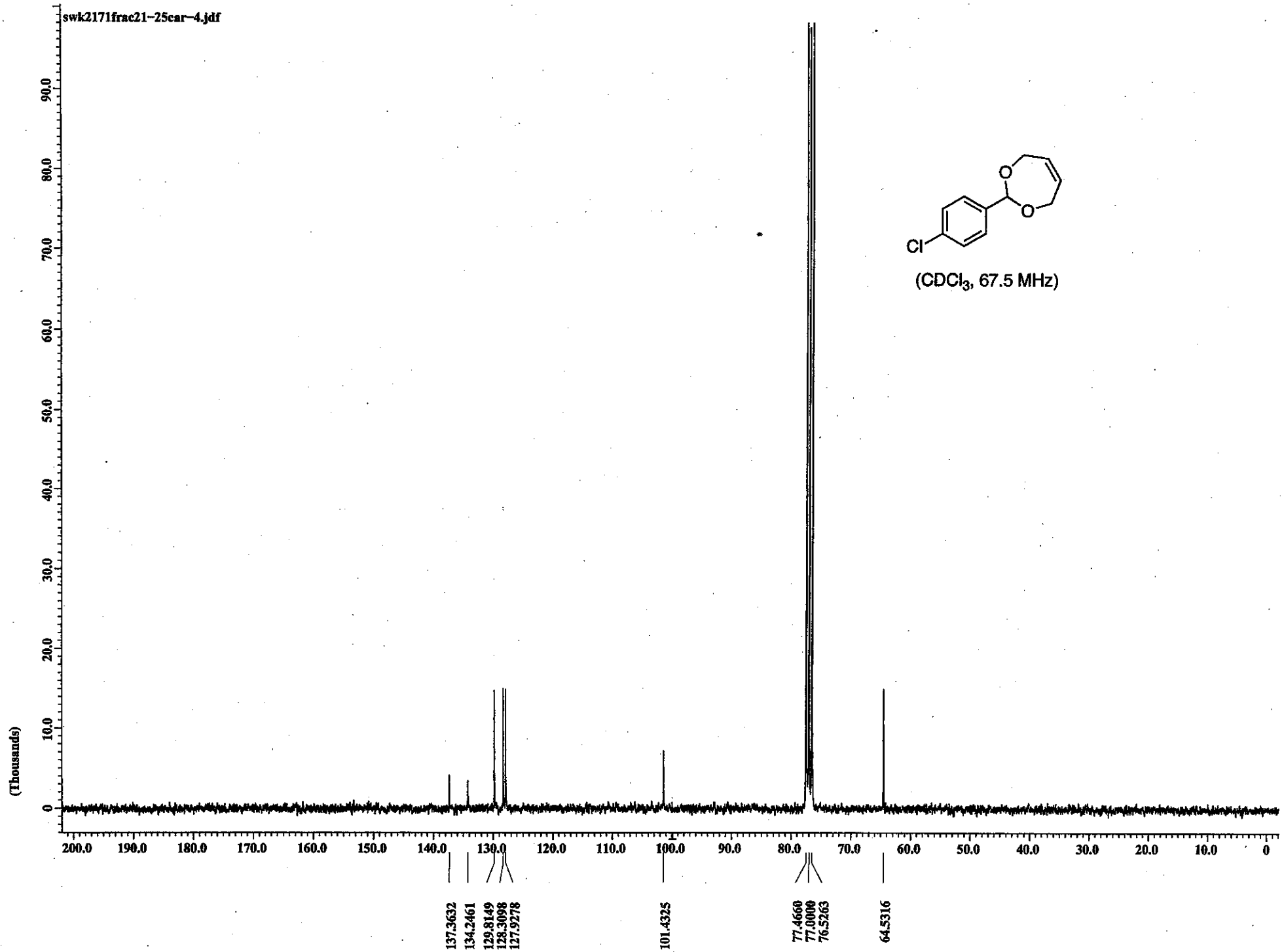
(Millions)

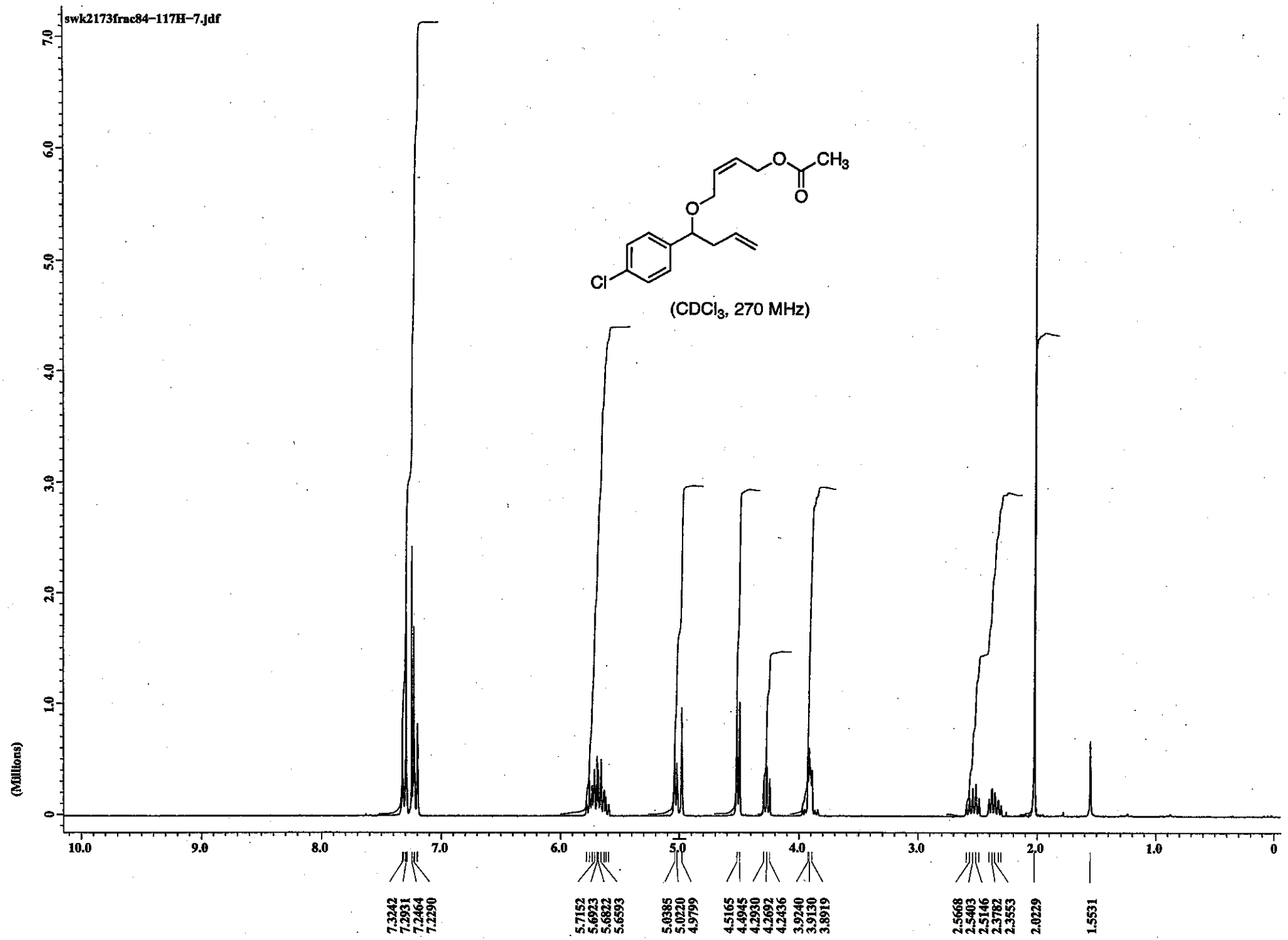
X : parts per Million : 1H

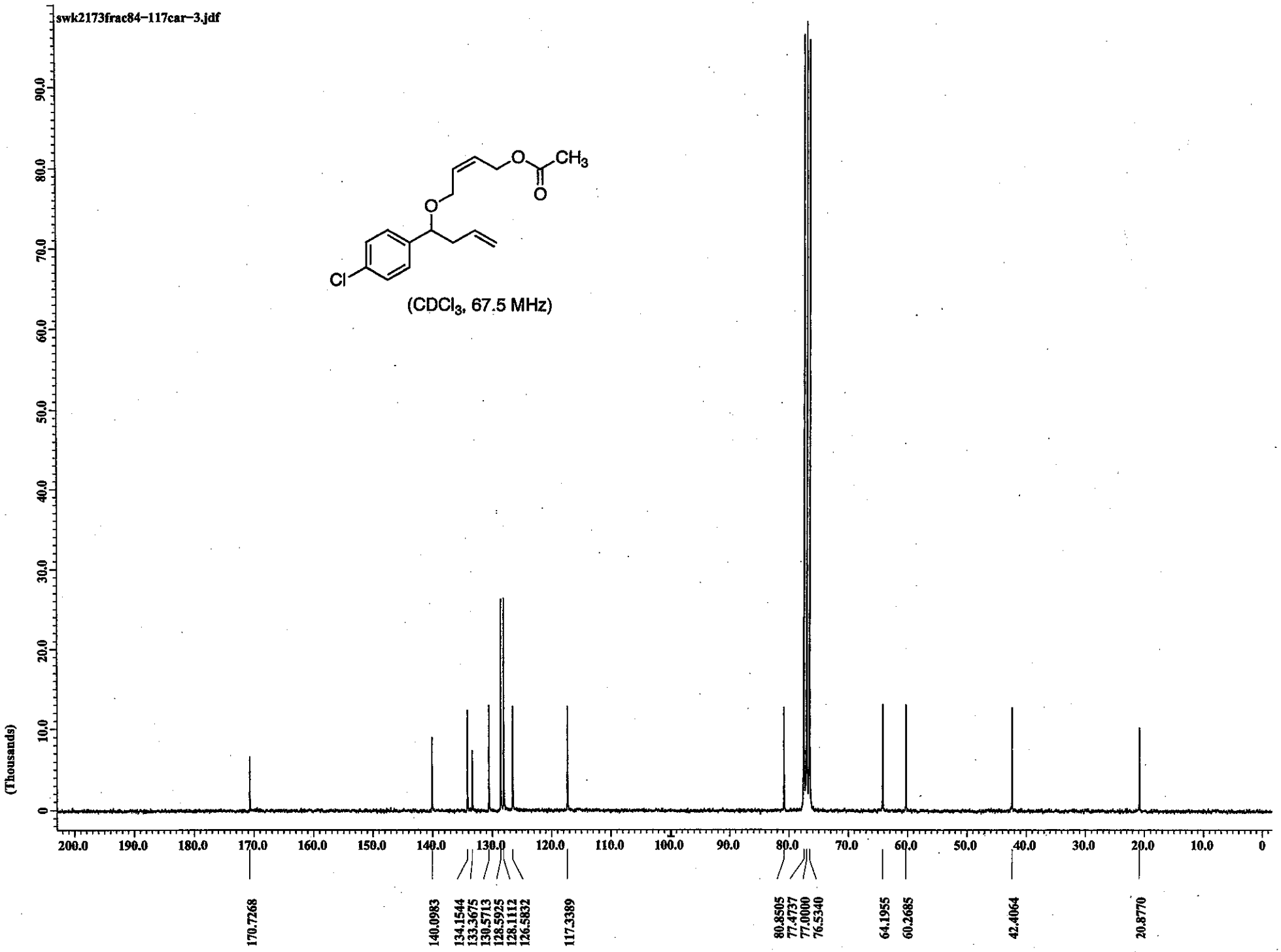
5.7976
5.7601
5.7344
5.6969
5.0385
4.9753
4.9707
4.0293
4.0055
3.9808
3.5073
3.4808
3.4048
3.3791
3.2500
2.2161
2.1905
2.1666
1.9789
1.6639
1.4817
1.4624
1.4469
1.4258
1.1474
1.1209
1.0952

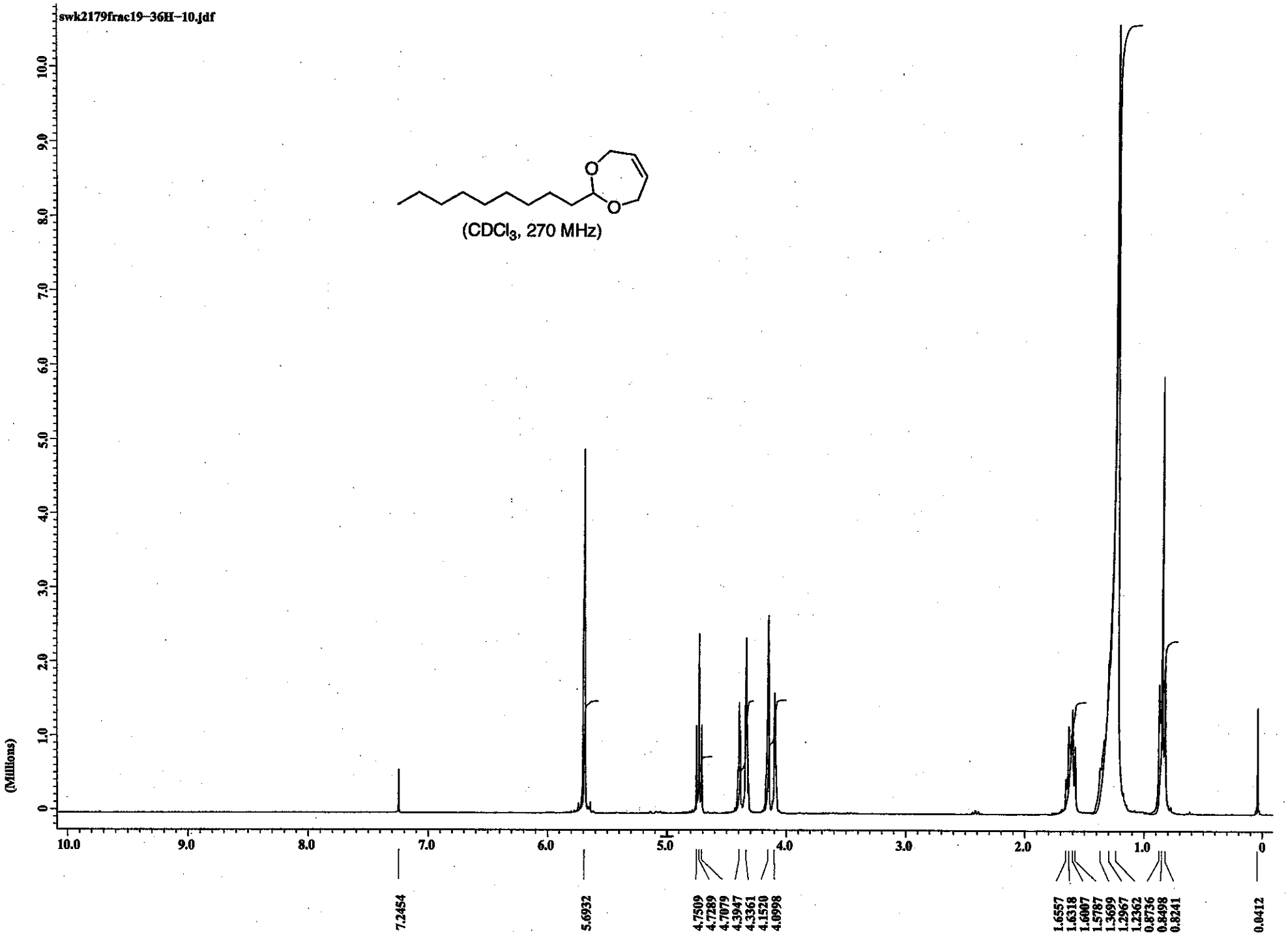

swk2129frac34-54car-5.jdf
(CDCl3, 67.5 MHz)
(Thousands)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.9942
134.6586
116.8346
78.1689
77.4737
77.0000
76.5340
64.4552
64.2413
38.3343
30.1672
24.5900
20.8541
15.4297
X : parts per Million : 13C

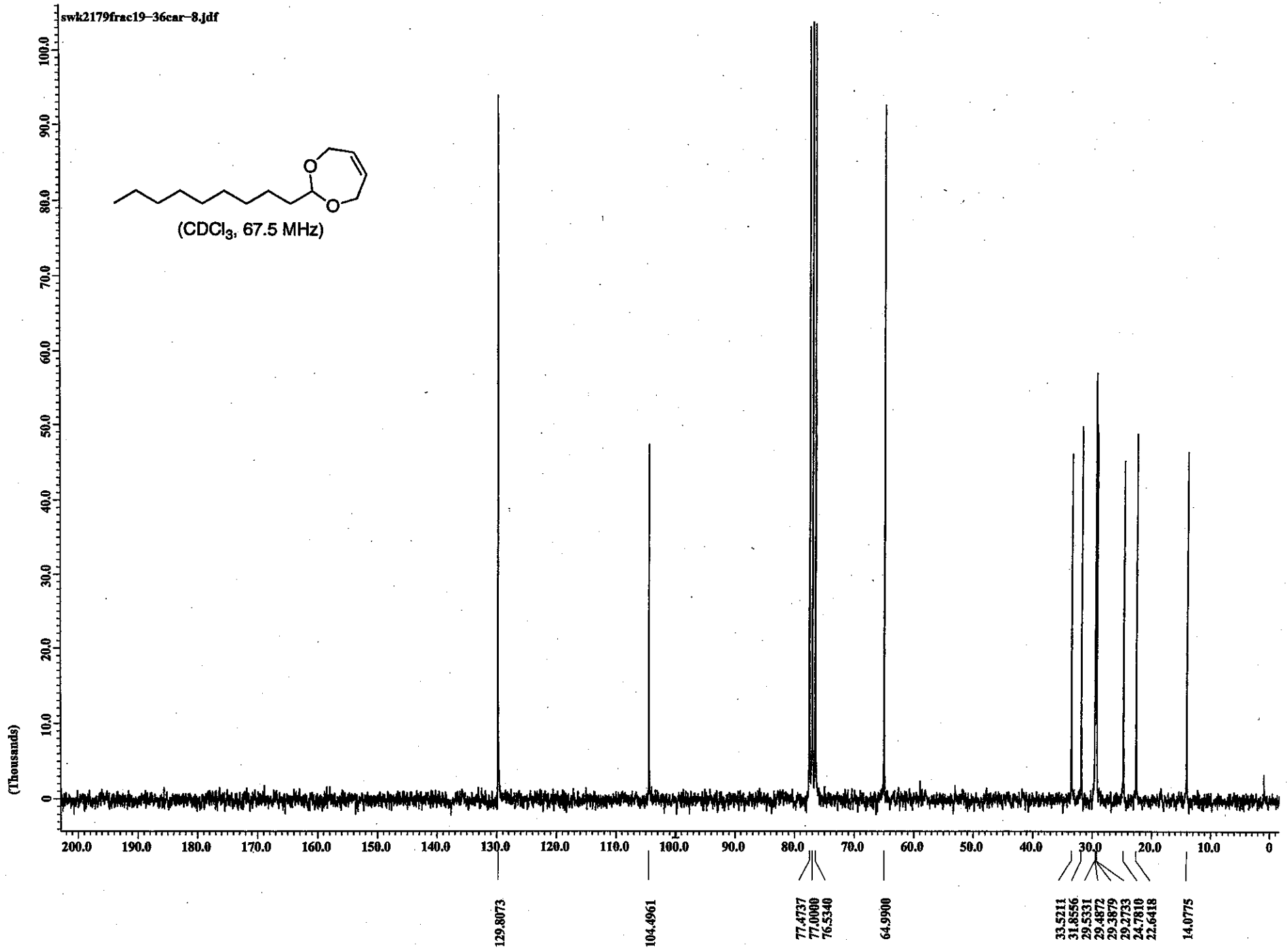

swk2171frac21-25H-4.jdf
(Millions)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.9744
7.4707
7.4460
7.4396
7.3443
7.3370
7.3132
7.2464
5.8040
5.7592
5.7528
4.3288
4.2729
4.2683
4.2189
3.7207
3.6950
1.5394
1.2555
1.2298
1.2033
X : parts per Million : 1H
O
O
Cl
(CDCl3, 270 MHz)

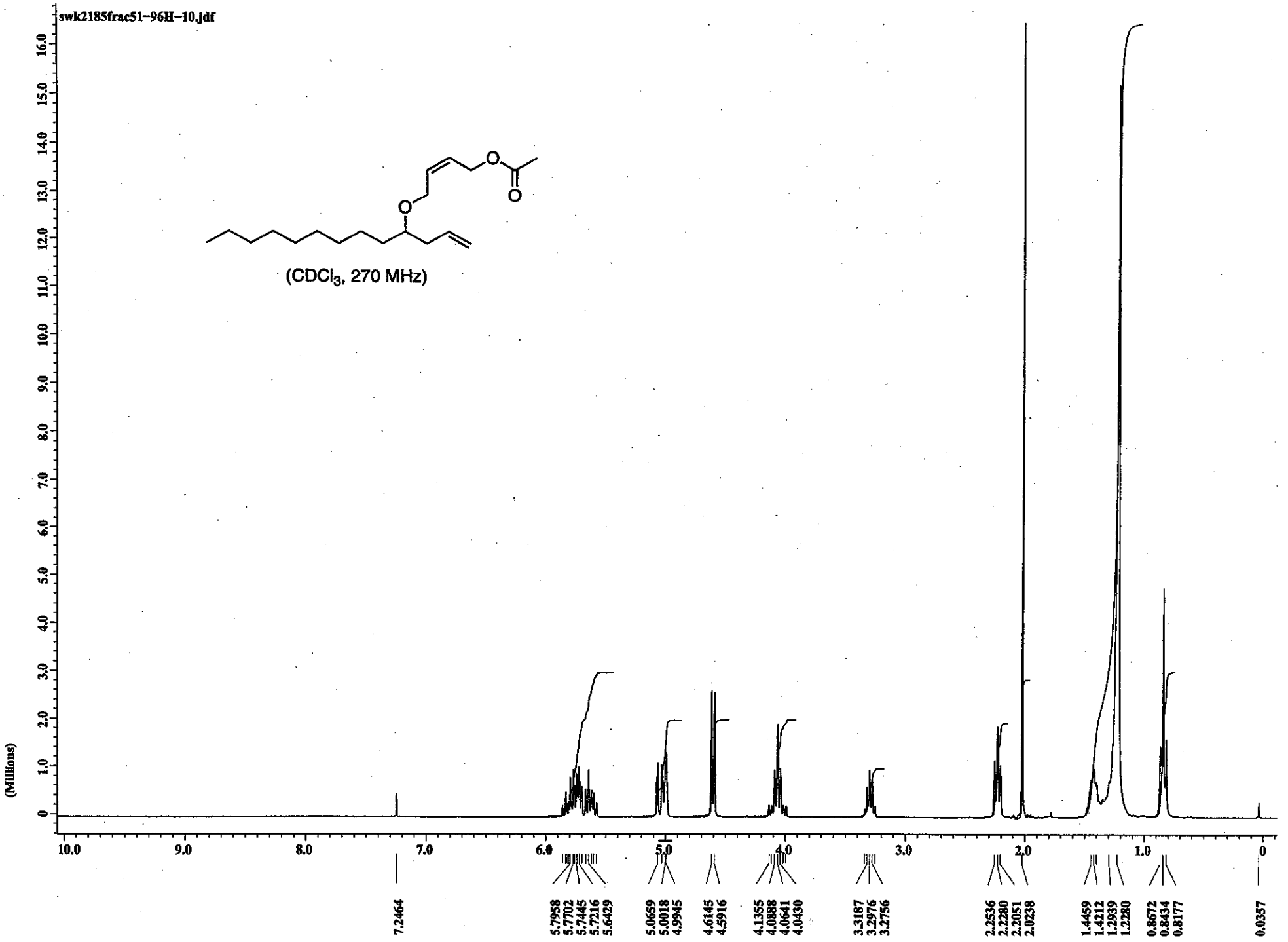

swk2171frac21-25car-4.jdf
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
137.3632
134.2461
129.8149
128.3098
127.9278
101.4325
77.4660
77.0000
76.5263
64.5316
O
O
Cl
(CDCl3, 67.5 MHz)
X : parts per Million : 13C

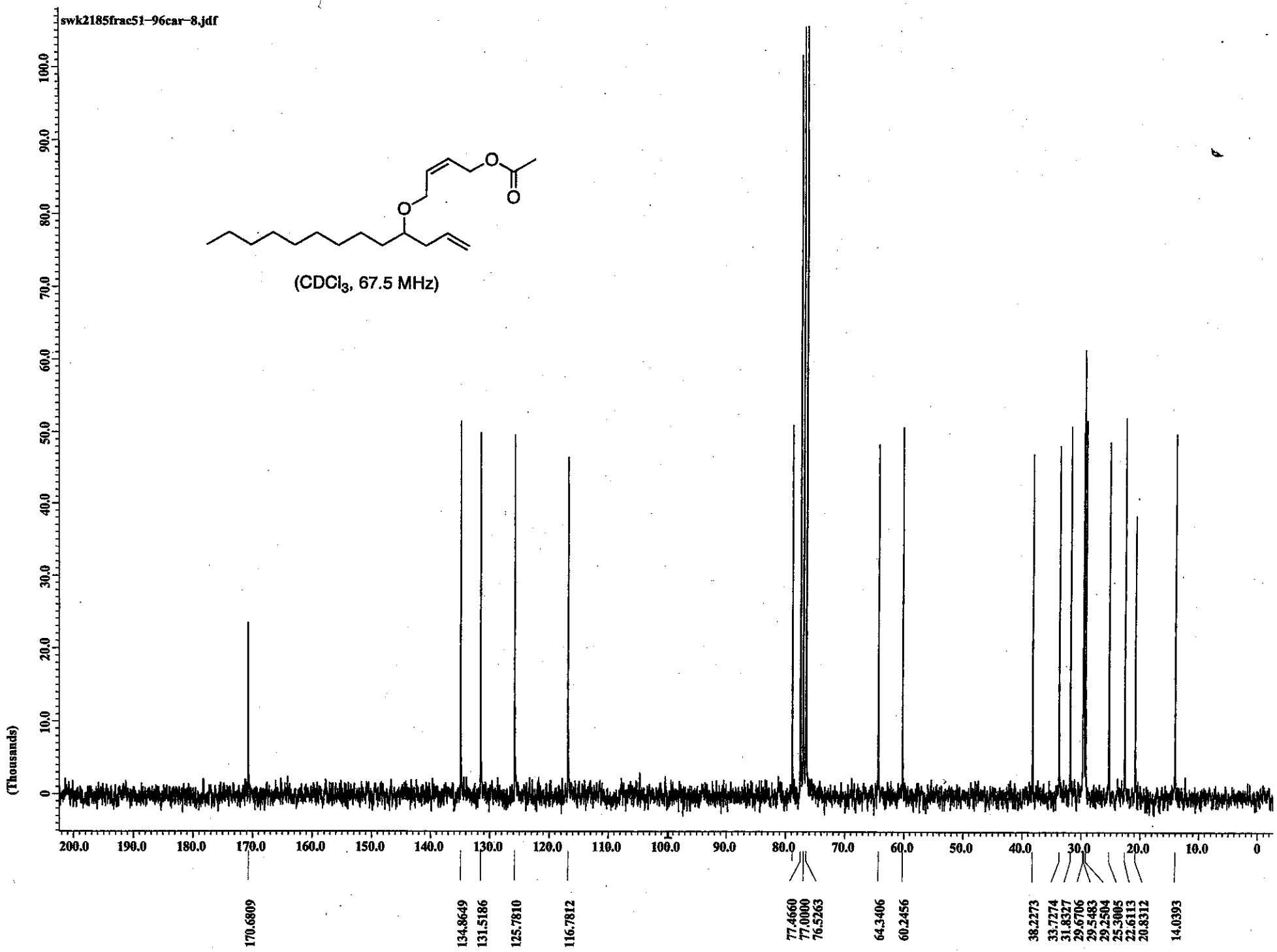

swk2173frac84-117H-7.jdf
(CDCl3, 270 MHz)
(Millions)
X : parts per Million : 1H
7.3242
7.2931
7.2464
7.2290
5.7152
5.6923
5.6822
5.6593
5.0385
5.0220
4.9799
4.5165
4.4945
4.2930
4.2692
4.2436
3.9240
3.9130
3.8919
2.5668
2.5403
2.5146
2.3782
2.3553
2.0229
1.5531

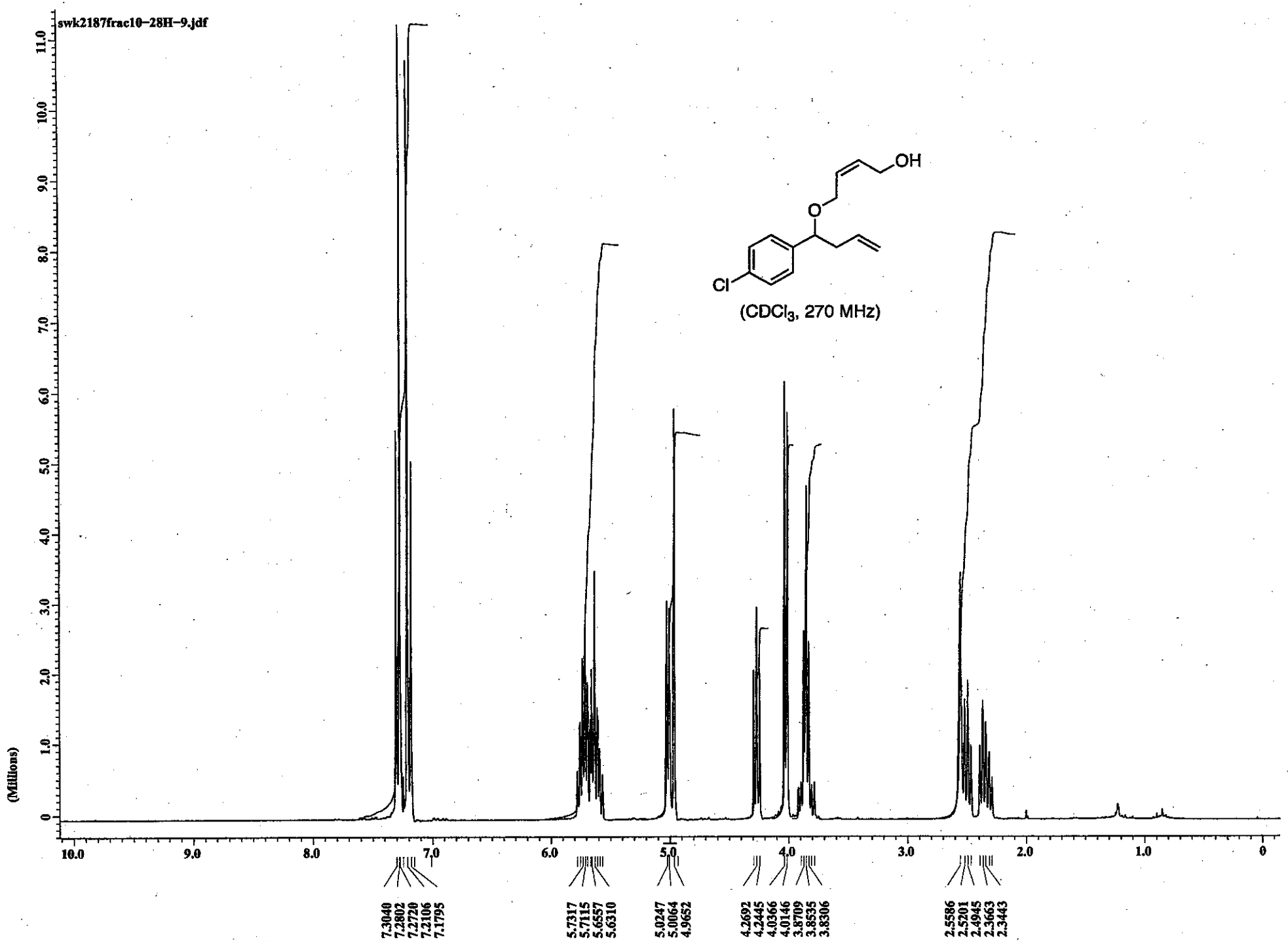

swk2173frac84-117car-3.jdf
(CDCl3, 67.5 MHz)
(Thousands)
X : parts per Million : 13C
170.7268
140.0983
134.1544
133.3675
130.5713
128.5925
128.1112
126.5832
117.3389
80.8505
77.4737
77.0000
76.5340
64.1955
60.2685
42.4064
20.8770

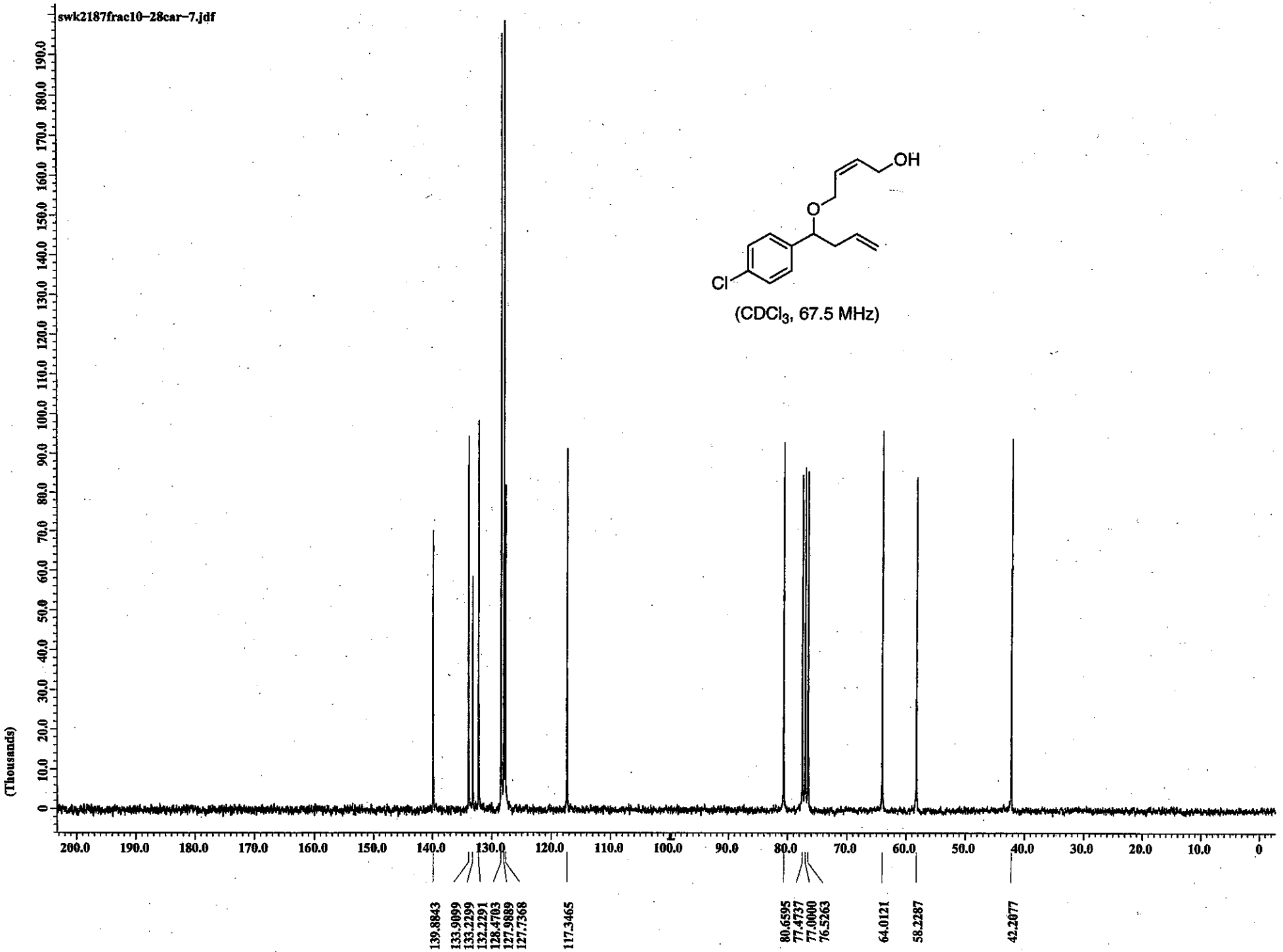

swk2179frac19-36H-10.jdf
(CDCl3, 270 MHz)
(Millions)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2454
5.6932
4.7509
4.7289
4.7079
4.3947
4.3361
4.1520
4.0998
1.6557
1.6318
1.6007
1.5787
1.3699
1.2967
1.2362
0.8736
0.8498
0.8241
0.0412
X : parts per Million : 1H


swk2179frac19–36car–8.jdf
(CDCl3, 67.5 MHz)
(Thousands)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
129.8073
104.4961
77.4737
77.0000
76.5340
64.9900
33.5211
31.8556
29.5331
29.4872
29.3879
29.2733
24.7810
22.6418
14.0775
X : parts per Million : 13C

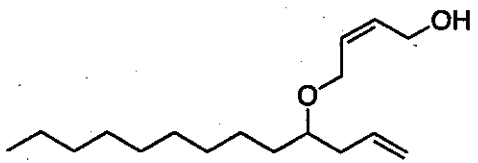

swk2185frac51-96H-10.jdf
(CDCl3, 270 MHz)
(Millions)
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2464
5.7958
5.7702
5.7445
5.7216
5.6429
5.0659
5.0018
4.9945
4.6145
4.5916
4.1355
4.0888
4.0641
4.0430
3.3187
3.2976
3.2756
2.2536
2.2280
2.2051
2.0238
1.4459
1.4212
1.2939
1.2280
0.8672
0.8434
0.8177
0.0357
X : parts per Million : 1H


swk2185frac51-96car-8.jdf
(CDCl3, 67.5 MHz)
(Thousands)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.6809
134.8649
131.5186
125.7810
116.7812
77.4660
77.0000
76.5263
64.3406
60.2456
38.2273
33.7274
31.8327
29.6706
29.5483
29.2504
25.3005
22.6113
20.8312
14.0393
X : parts per Million : 13C


swk2187frac10-28H-9.jdf
(Millions)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
OH
O
Cl
(CDCl3, 270 MHz)
7.3040
7.2802
7.2720
7.2106
7.1795
5.7317
5.7115
5.6557
5.6310
5.0247
5.0064
4.9652
4.2692
4.2445
4.0366
4.0146
3.8709
3.8535
3.8306
2.5586
2.5201
2.4945
2.3663
2.3443
X : parts per Million : 1H


swk2187frac10-28car-7.jdf
OH
O
Cl
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
139.8843
133.9099
133.2299
132.2291
128.4703
127.9889
127.7368
117.3465
80.6595
77.4737
77.0000
76.5263
64.0121
58.2287
42.2077
X : parts per Million : 13C

swk2189frac5-18H-4.jdf



($CDCl_3$, 270 MHz)

(Millions)

7.2454

5.7885
5.7619
5.7280
5.7244
5.6658

5.0687
5.0046
5.0000

4.1474
4.1255
4.0549
4.0339

3.3352
3.3141
3.2921

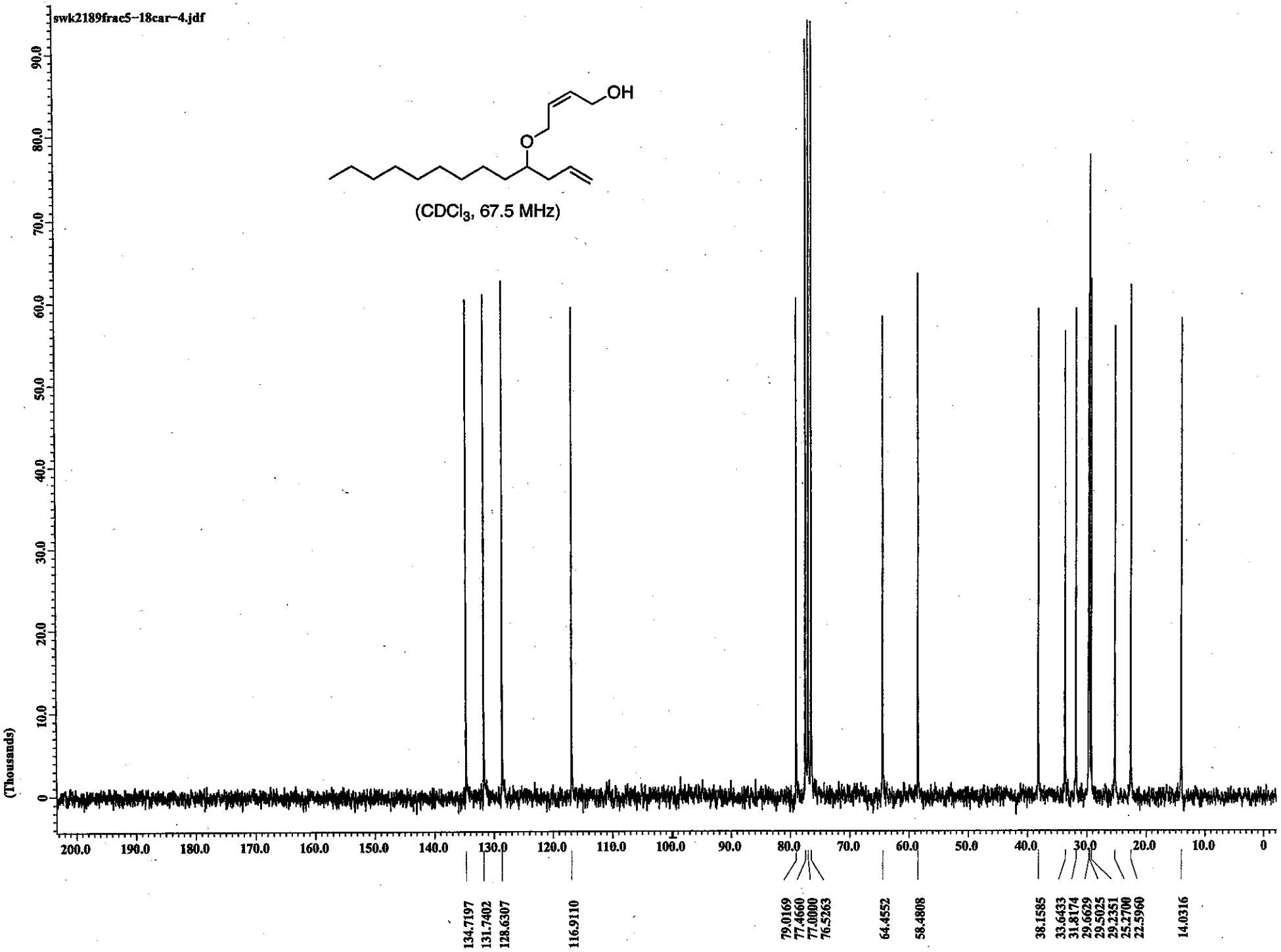
2.5604

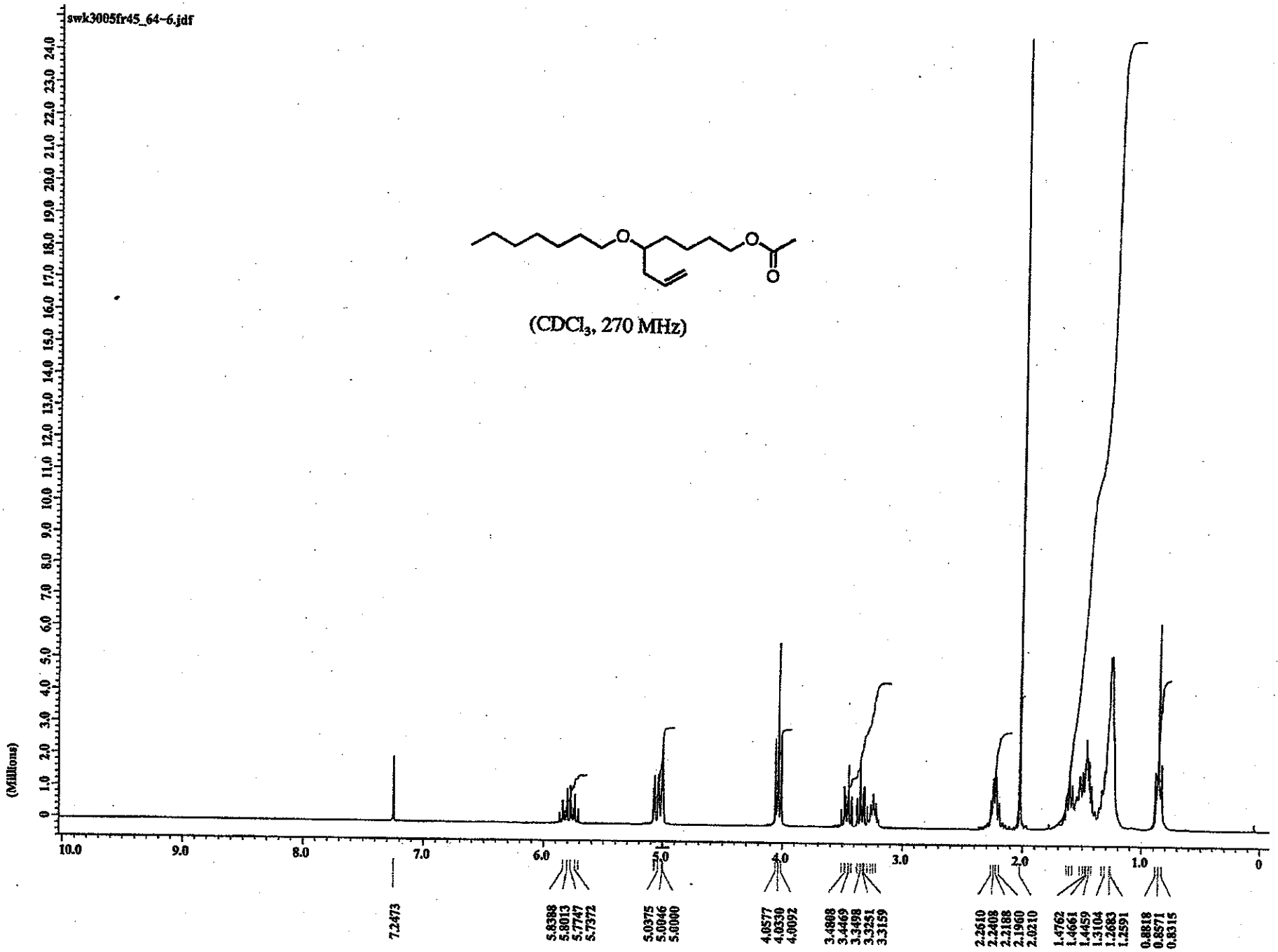
2.2564
2.2353
2.2308

1.4542
1.4304
1.2903
1.2262

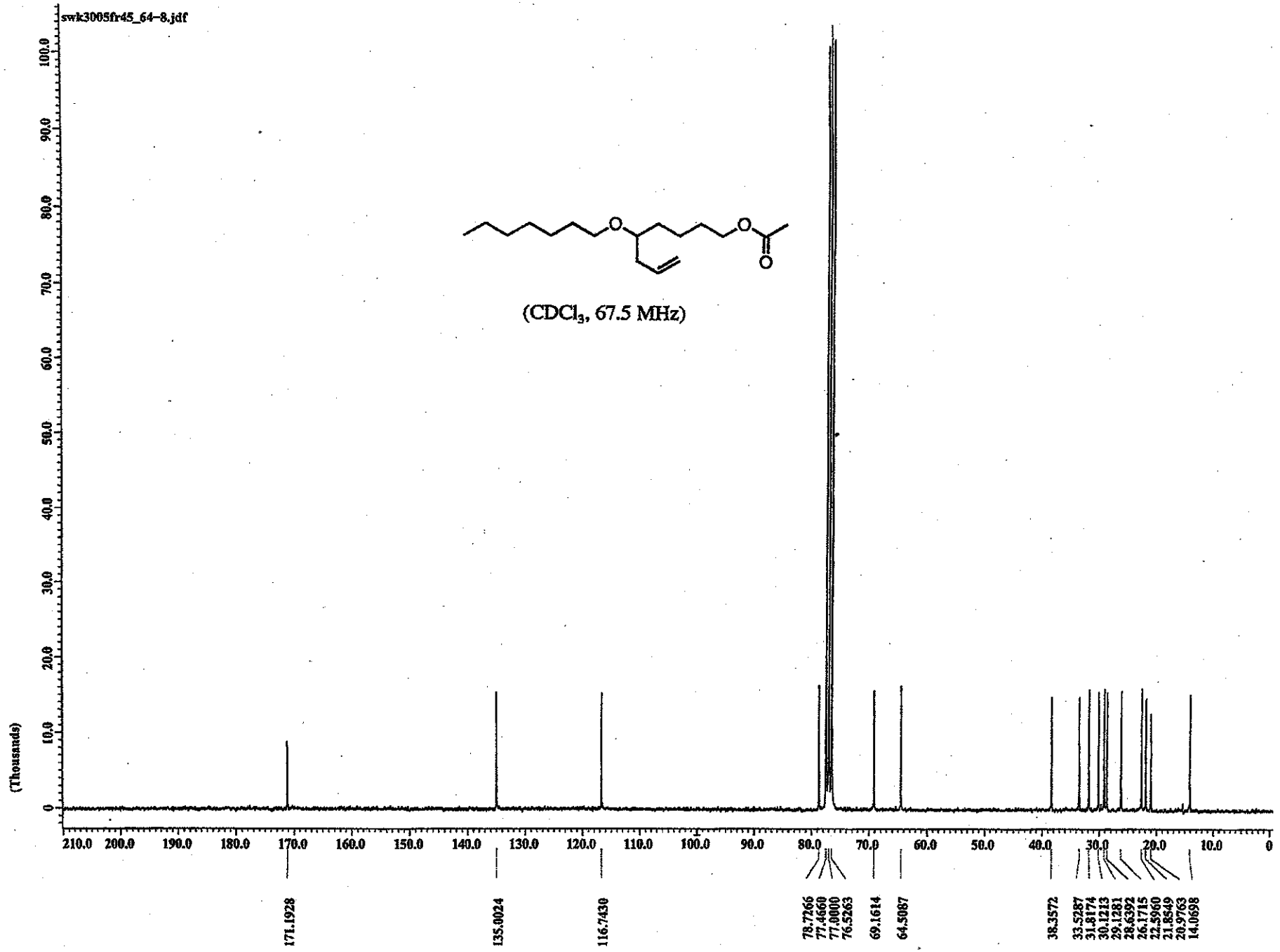
0.8644
0.8406
0.8159

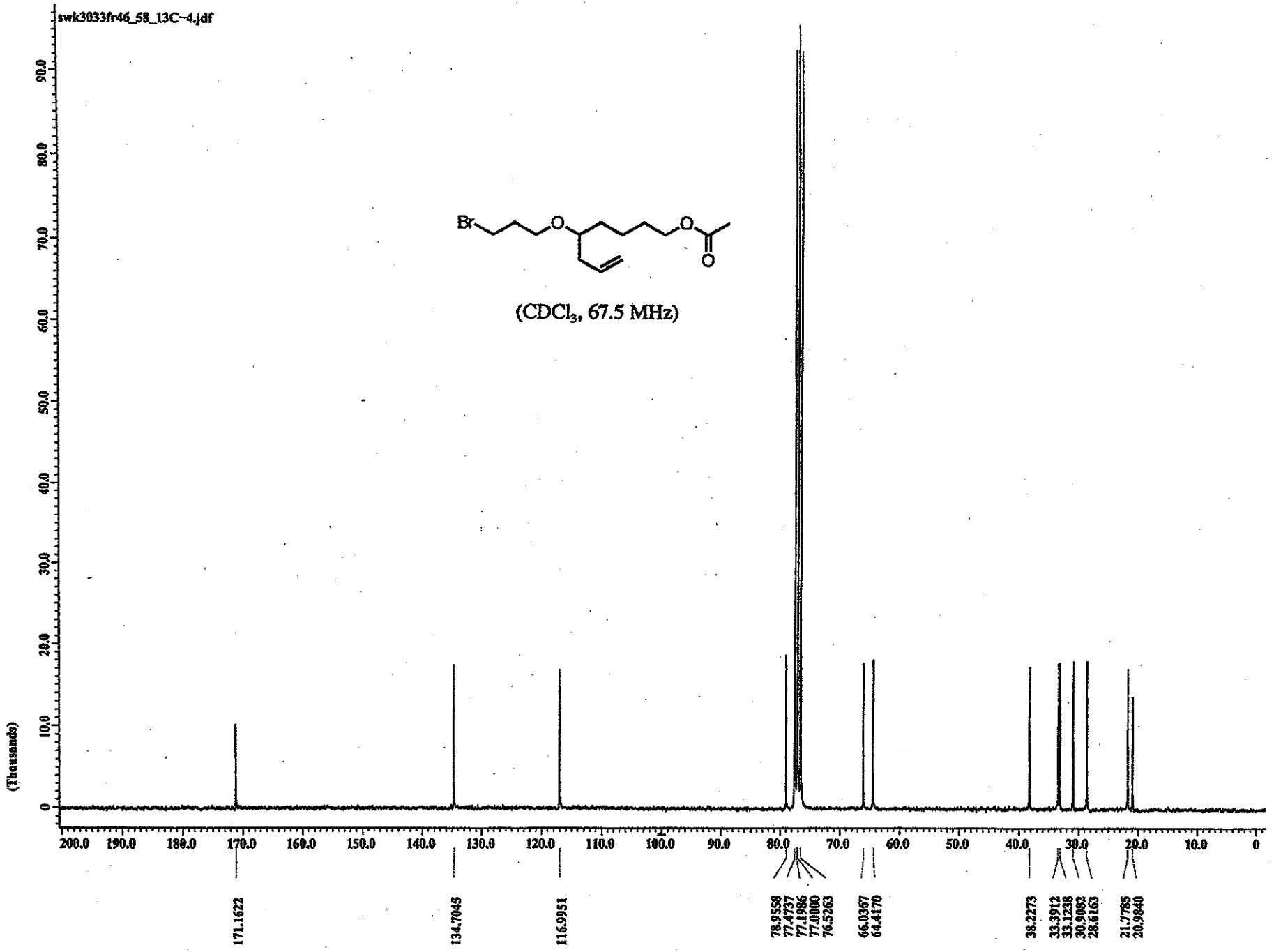
X : parts per Million : 1H

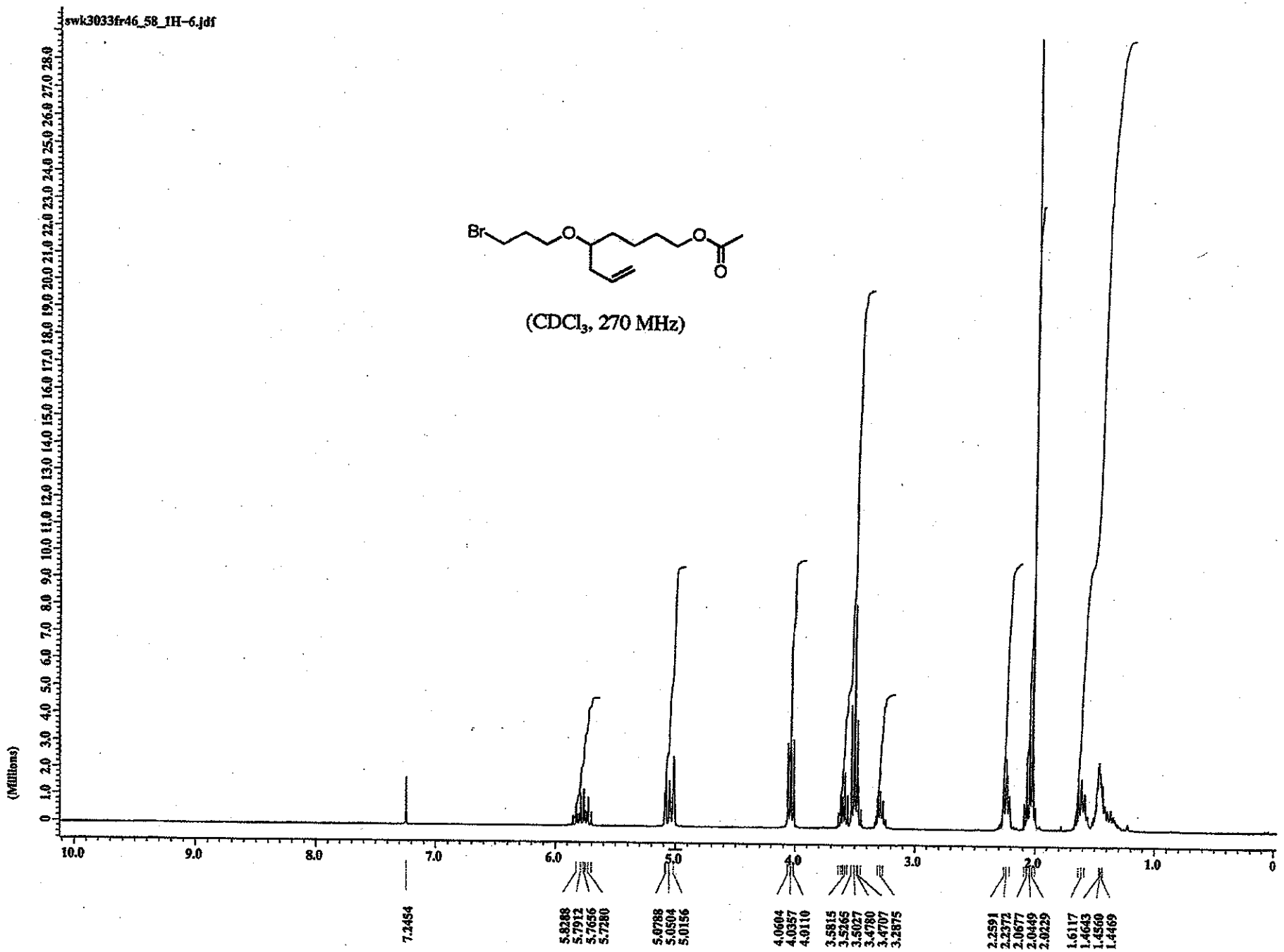

swk2189frac5-18car-4.jdf
OH
O
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
134.7197
131.7402
128.6307
116.9110
79.0169
77.4660
77.0000
76.5263
64.4552
58.4808
38.1585
33.6433
31.8174
29.6629
29.5025
29.2351
25.2700
22.5960
14.0316
X : parts per Million : 13C

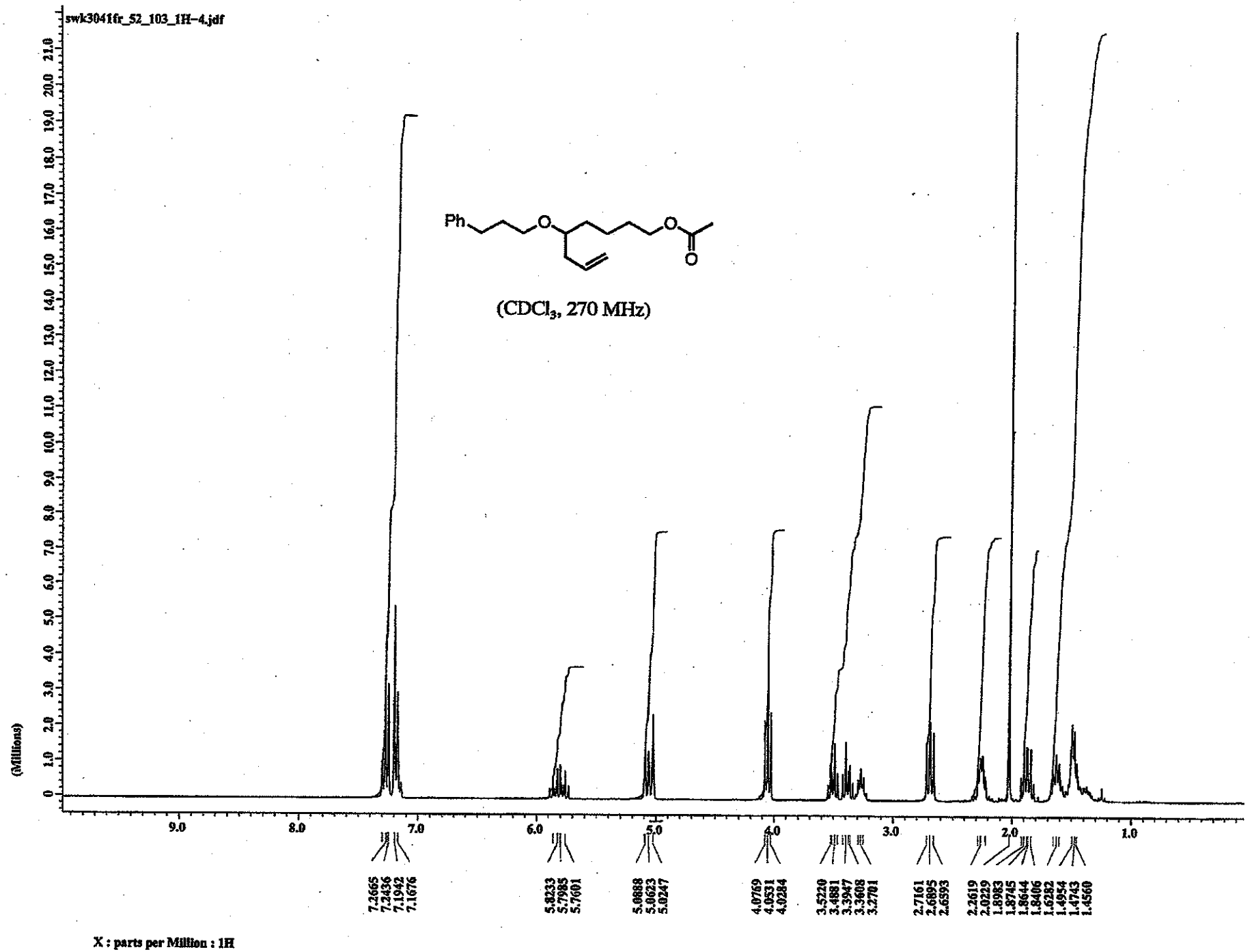


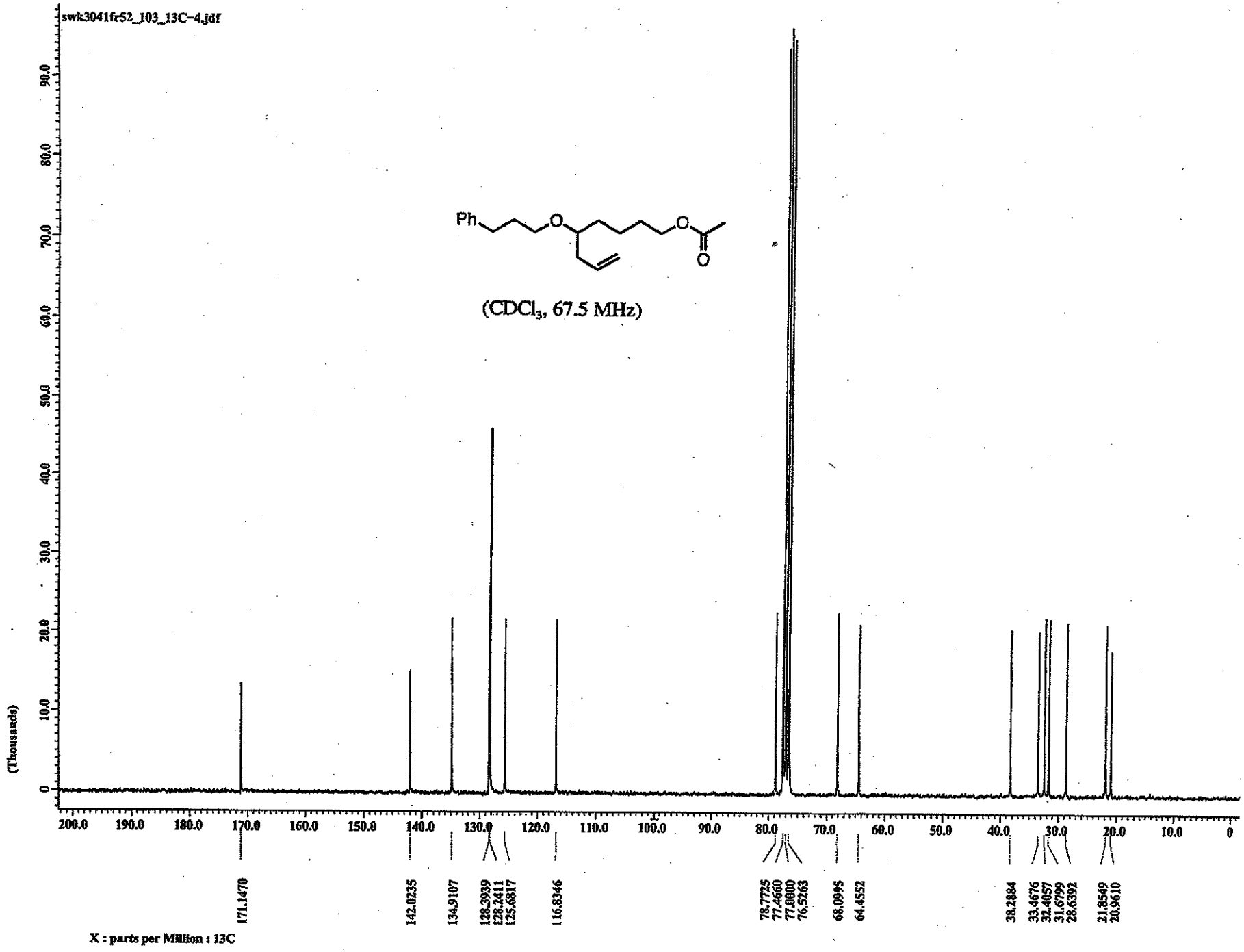
($CDCl_3$, 270 MHz)

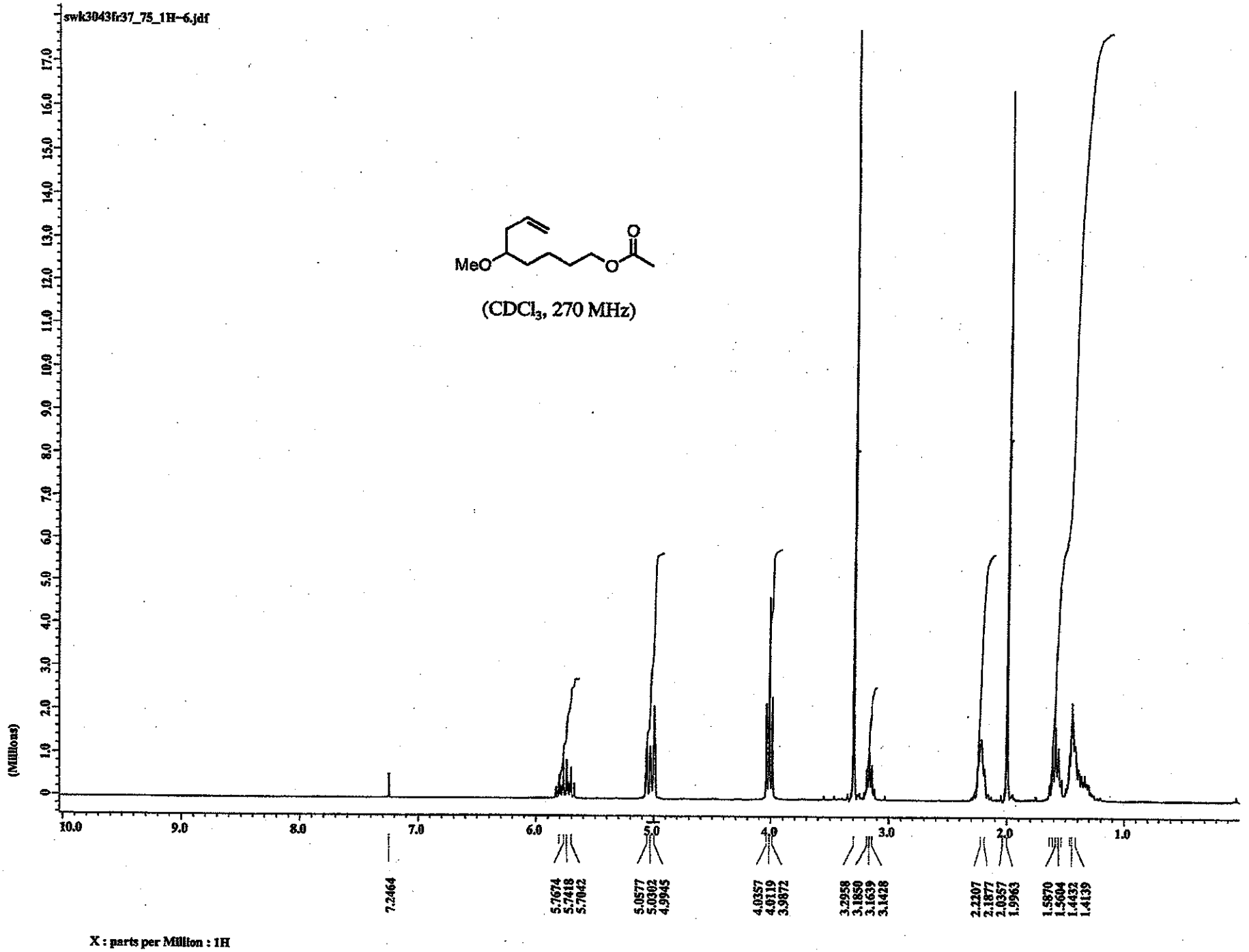

swk3005fr45_64-8.jdf
(CDCl3, 67.5 MHz)
(Thousands)
171.1928
135.0024
116.7430
78.7266
77.4660
77.0000
76.5263
69.1614
64.5087
38.3572
33.5287
31.8174
30.1213
29.1281
28.6392
26.1715
22.5960
21.8549
20.9763
14.0698
X : parts per Million : 13C

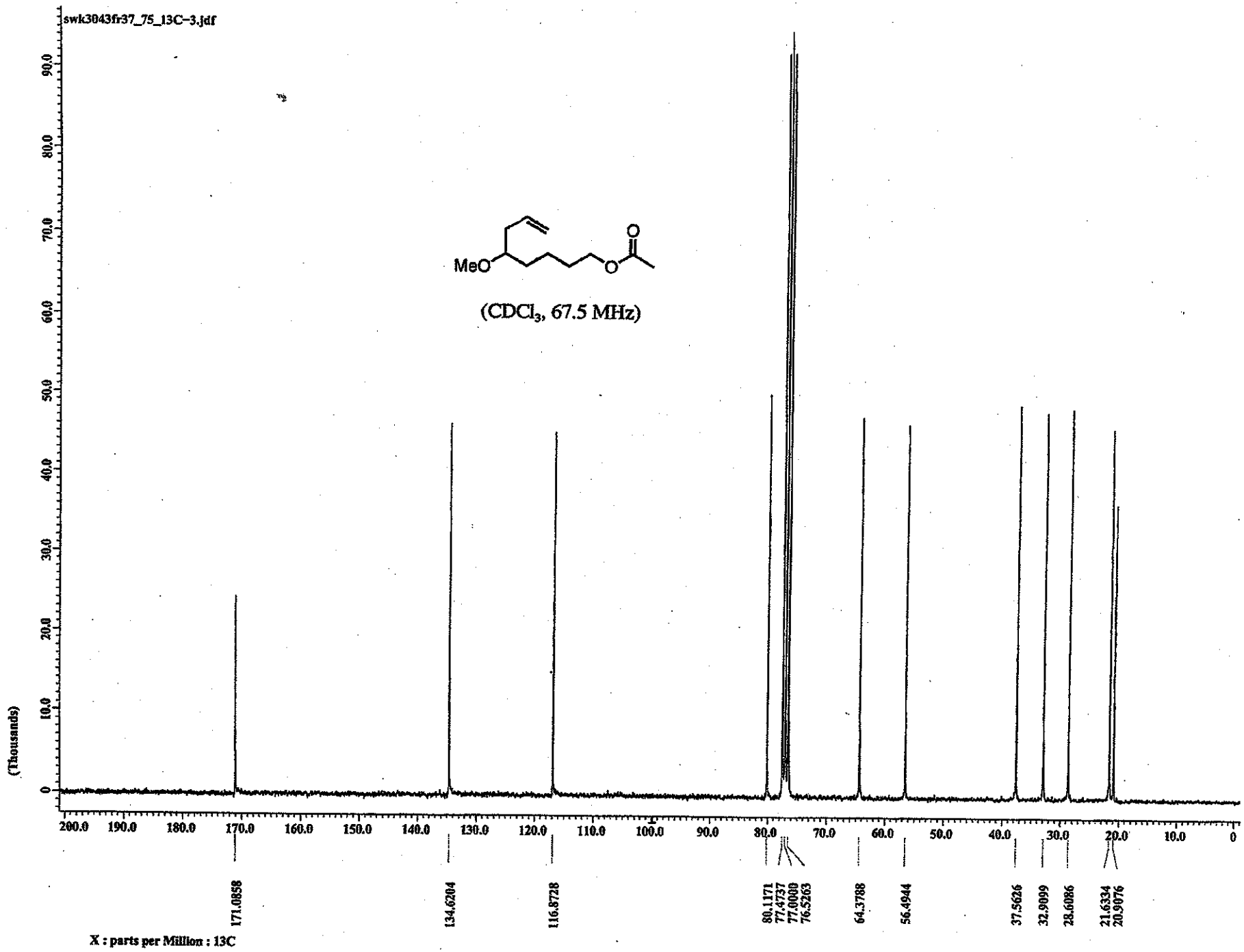

swk3033fr46_58_13C~4.jdf
Br
O
O
O
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.1622
134.7045
116.9951
78.9558
77.4737
77.1986
77.0000
76.5263
66.0367
64.4170
38.2273
33.3912
33.1238
30.9062
28.6163
21.7785
20.9840
X : parts per Million : 13C

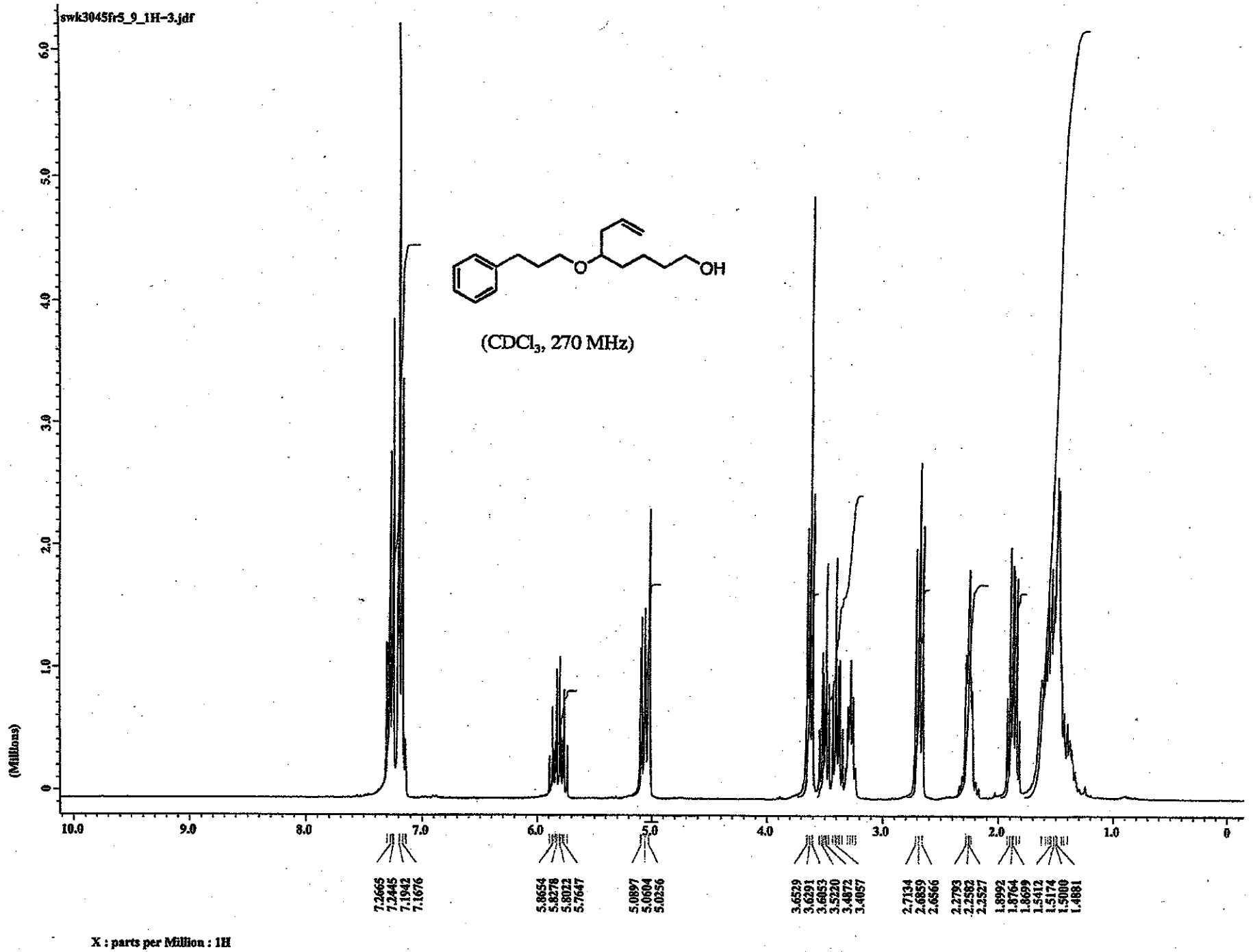

swk3033fr46_58_1H-6.jdf
Br
O
O
O
(CDCl3, 270 MHz)
(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0 21.0 22.0 23.0 24.0 25.0 26.0 27.0 28.0
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.2454
5.8288 5.7912 5.7656 5.7280
5.0788 5.0504 5.0156
4.0604 4.0357 4.0110
3.5815 3.5265 3.5027 3.4780 3.4707 3.2875
2.2591 2.2372 2.0677 2.0449 2.0229
1.6117 1.4643 1.4560 1.4469
X : parts per Million : 1H

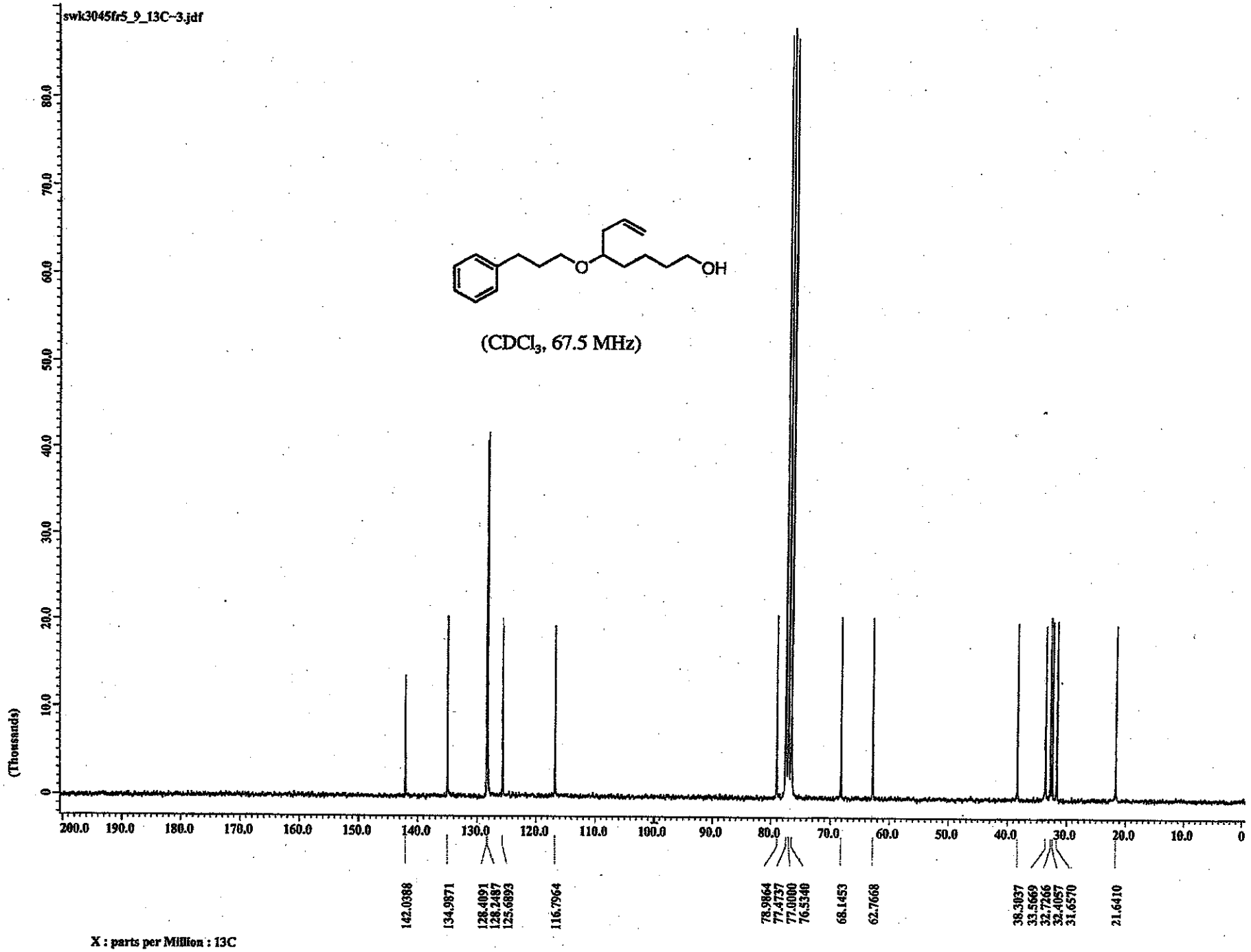

swk3041fr_52_103_1H-4.jdf
Ph
O
O
O
(CDCl3, 270 MHz)
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.2665
7.2436
7.1942
7.1676
5.8233
5.7985
5.7601
5.0888
5.0623
5.0247
4.0769
4.0531
4.0284
3.5220
3.4881
3.3947
3.3608
3.2701
2.7161
2.6895
2.6593
2.2619
2.0229
1.8983
1.8745
1.8644
1.8406
1.6282
1.4954
1.4743
1.4560
X : parts per Million : 1H

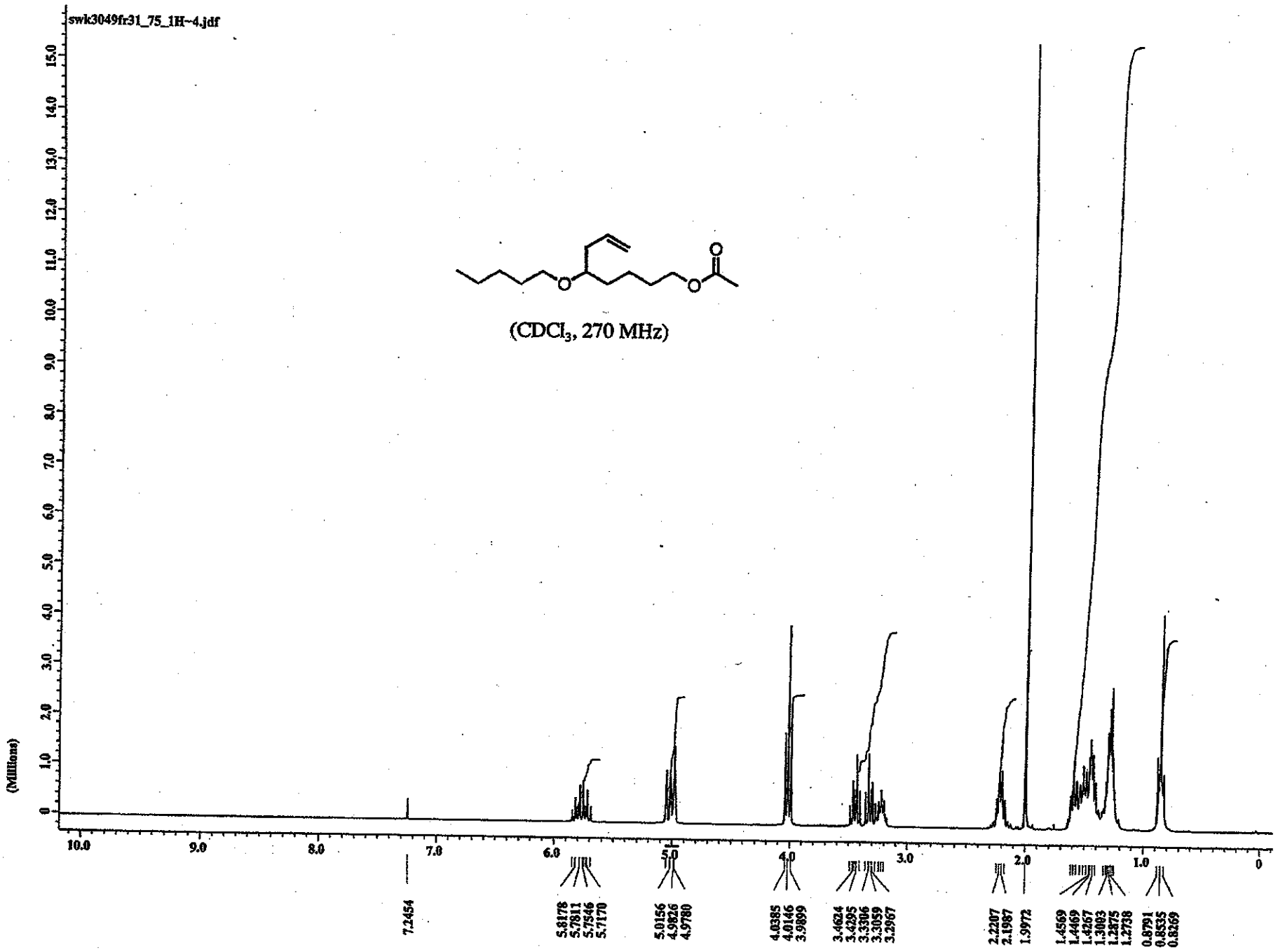

swk3041fr52_103_13C-4.jdf
Ph
O
O
O
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.1470
142.0235
134.9107
128.3939
128.2411
125.6817
116.8346
78.7725
77.4660
77.0800
76.5263
68.0995
64.4552
38.2884
33.4676
32.4057
31.6799
28.6392
21.8549
20.9610
X : parts per Million : 13C


swk3043fr37_75_1H~6.jdf
MeO
O
O
(CDCl3, 270 MHz)
(Millions)
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.2464
5.7674
5.7418
5.7042
5.0577
5.0302
4.9945
4.0357
4.0119
3.9872
3.2958
3.1850
3.1639
3.1428
2.2207
2.1877
2.0357
1.9963
1.5870
1.5604
1.4432
1.4139
X : parts per Million : 1H

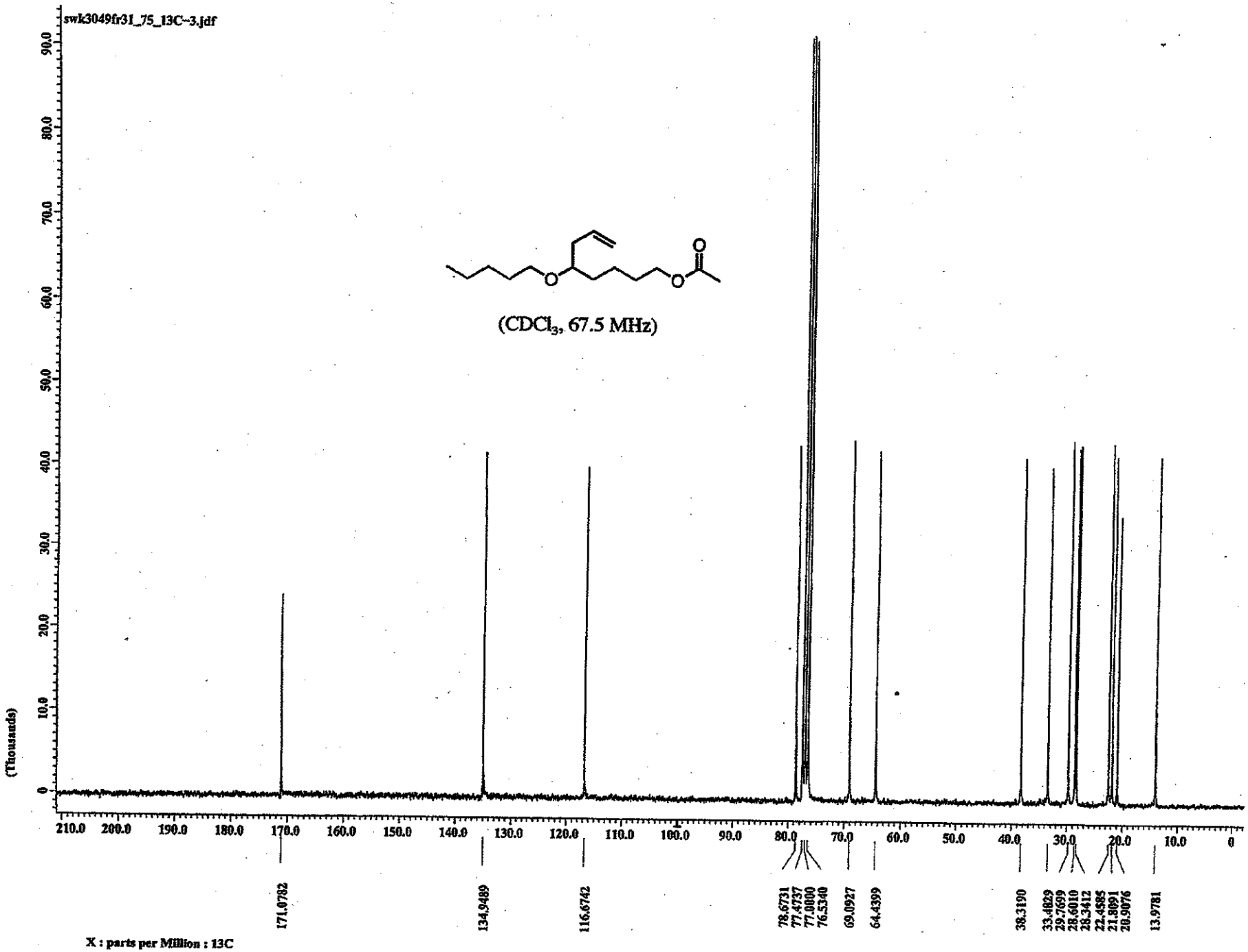

swk3043fr37_75_13C-3.jdf
MeO
O
O
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.0858
134.6204
116.8728
80.1171
77.4737
77.0000
76.5263
64.3788
56.4944
37.5626
32.9099
28.6086
21.6334
20.9076
X : parts per Million : 13C

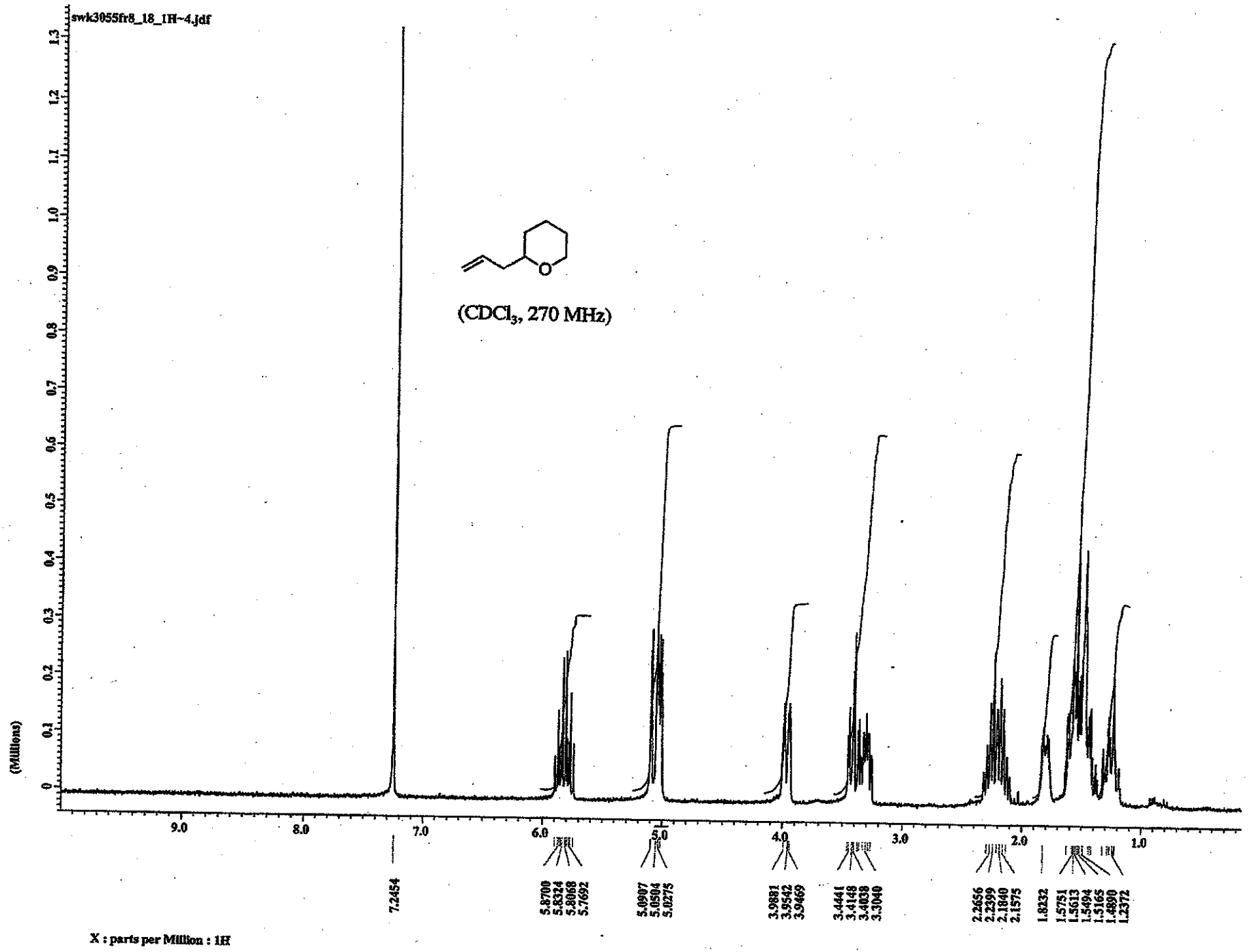

swk3045fr5_9_1H-3.jdf
OH
(CDCl3, 270 MHz)
(Millions)
X : parts per Million : 1H
7.2665
7.2445
7.1942
7.1676
5.8654
5.8278
5.8022
5.7647
5.0897
5.0604
5.0256
3.6529
3.6291
3.6053
3.5220
3.4872
3.4057
2.7134
2.6859
2.6566
2.2793
2.2582
2.2527
1.8992
1.8764
1.8699
1.5412
1.5174
1.5000
1.4881

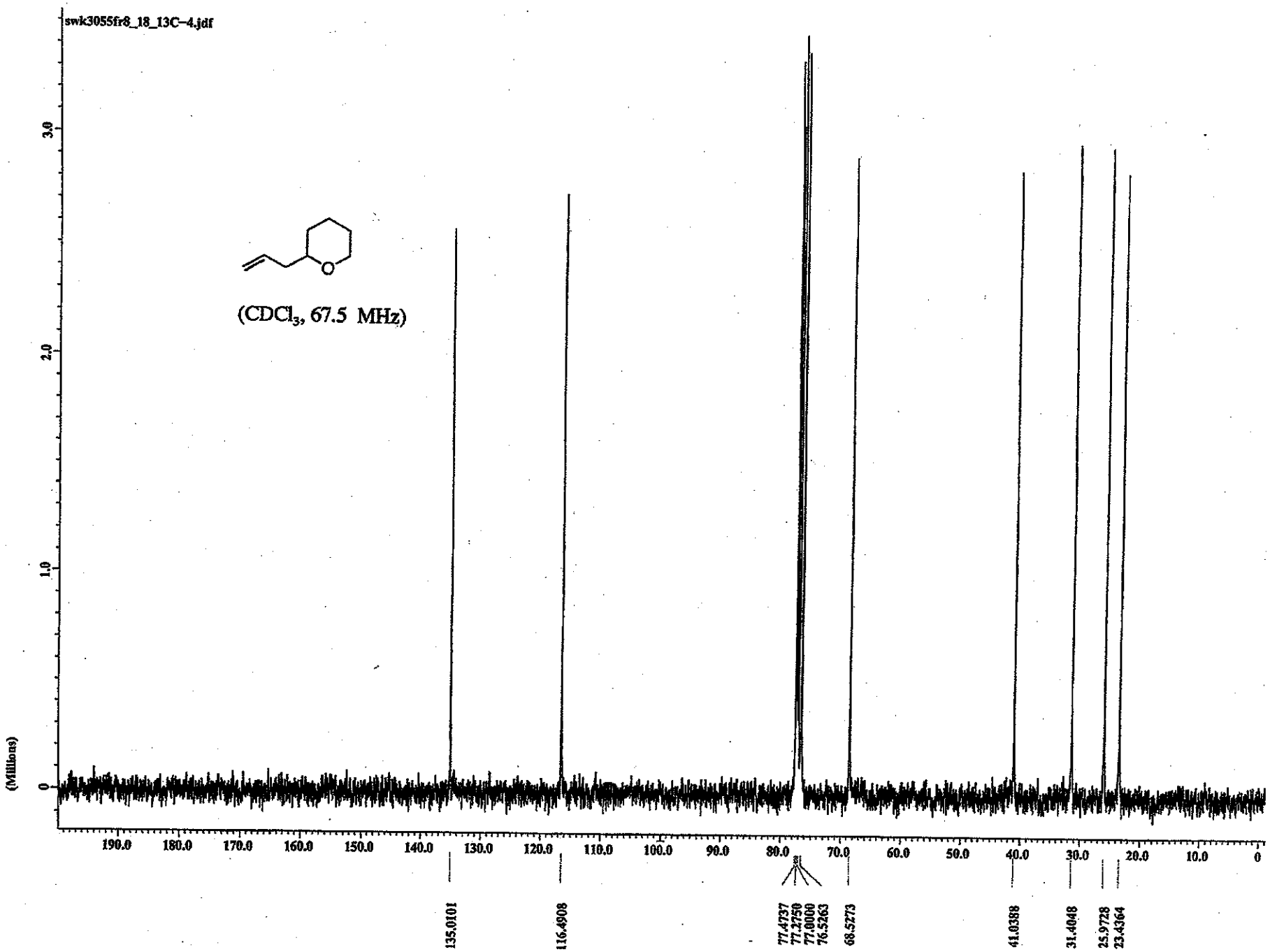

swk3045fr5_9_13C~3.jdf
OH
(CDCl3, 67.5 MHz)
(Thousands)
142.0388
134.9871
128.4091
128.2487
125.6893
116.7964
78.9864
77.4737
77.0000
76.5340
68.1453
62.7668
38.3037
33.5669
32.7266
32.4057
31.6570
21.6410
X : parts per Million : 13C

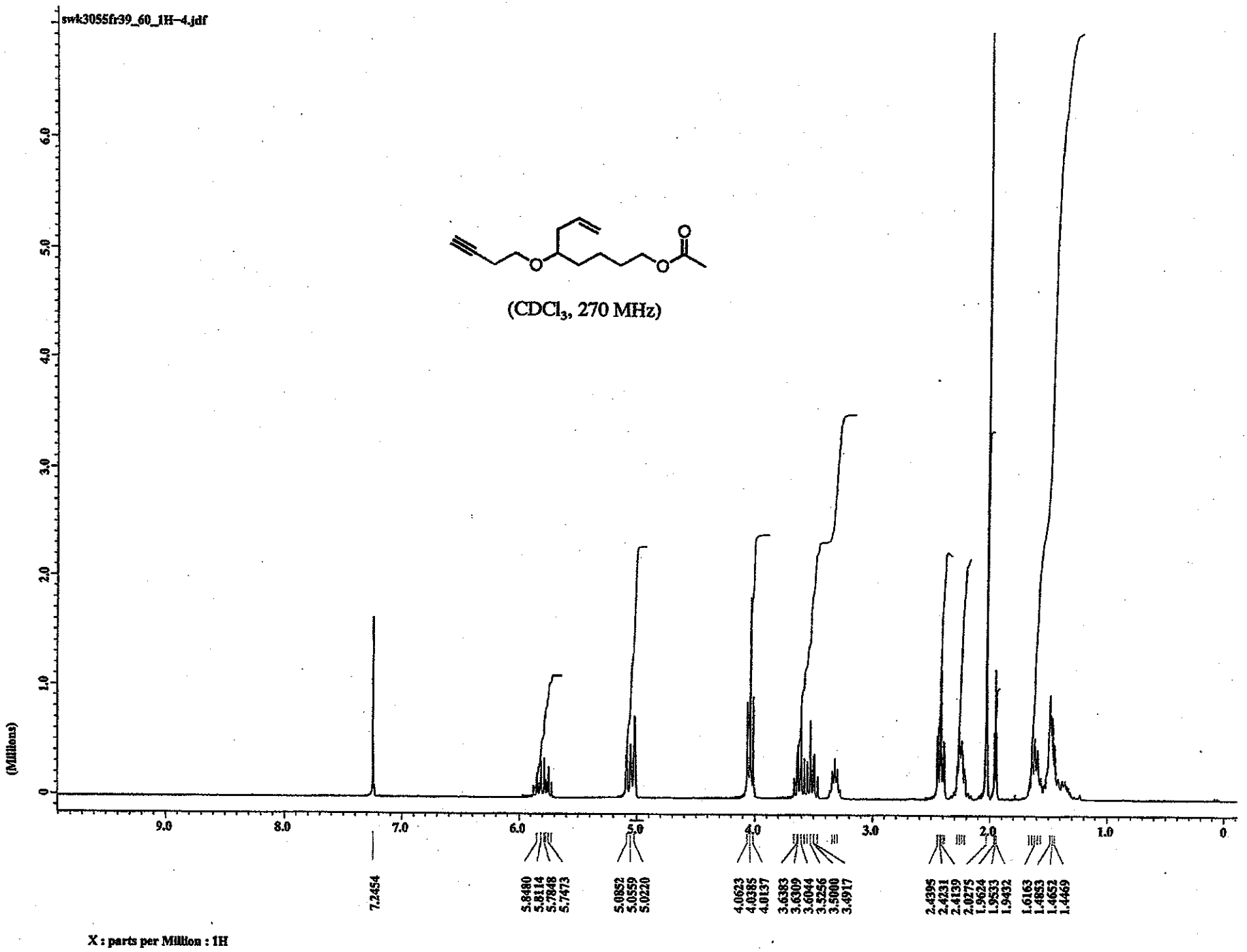


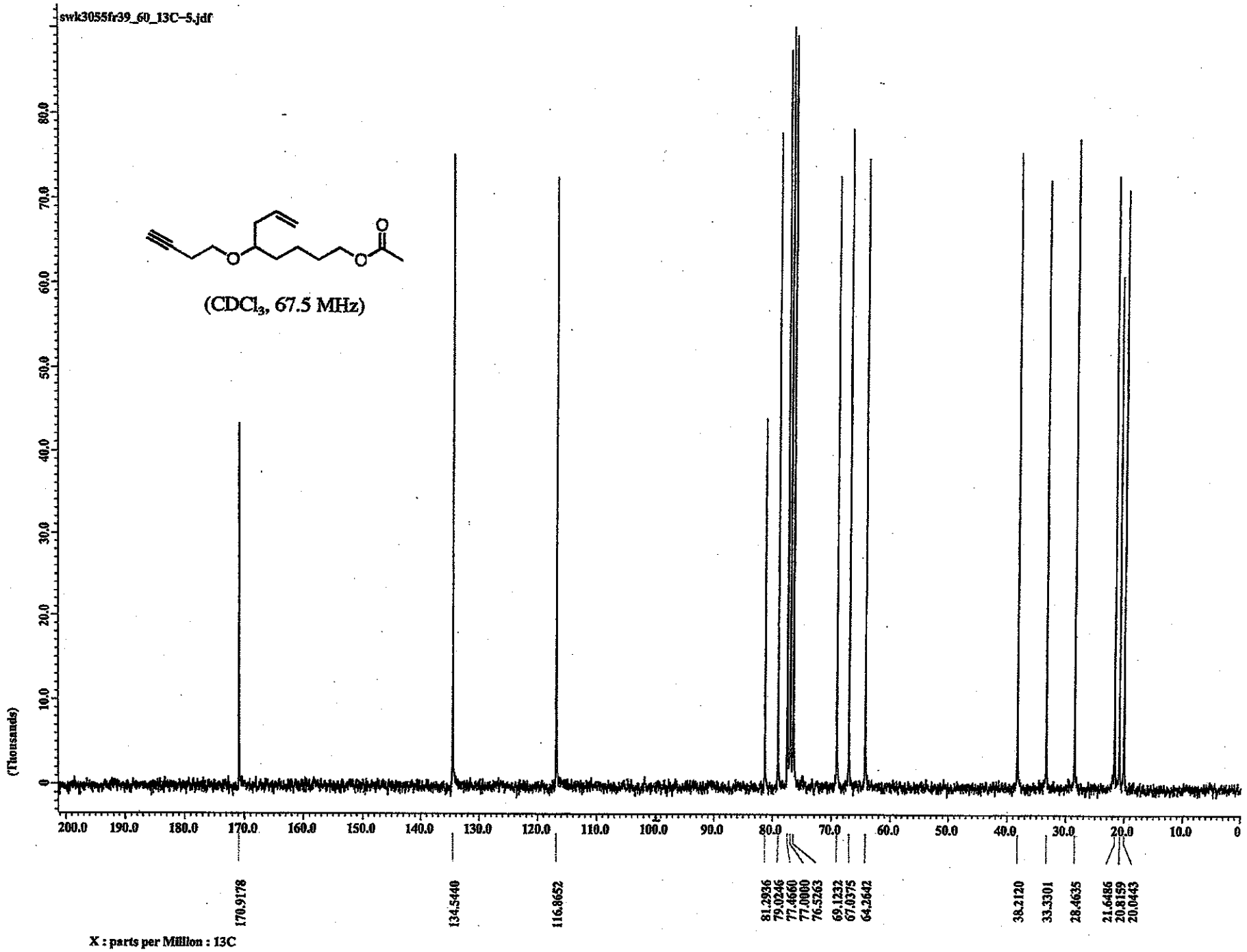
($CDCl_3$, 270 MHz)

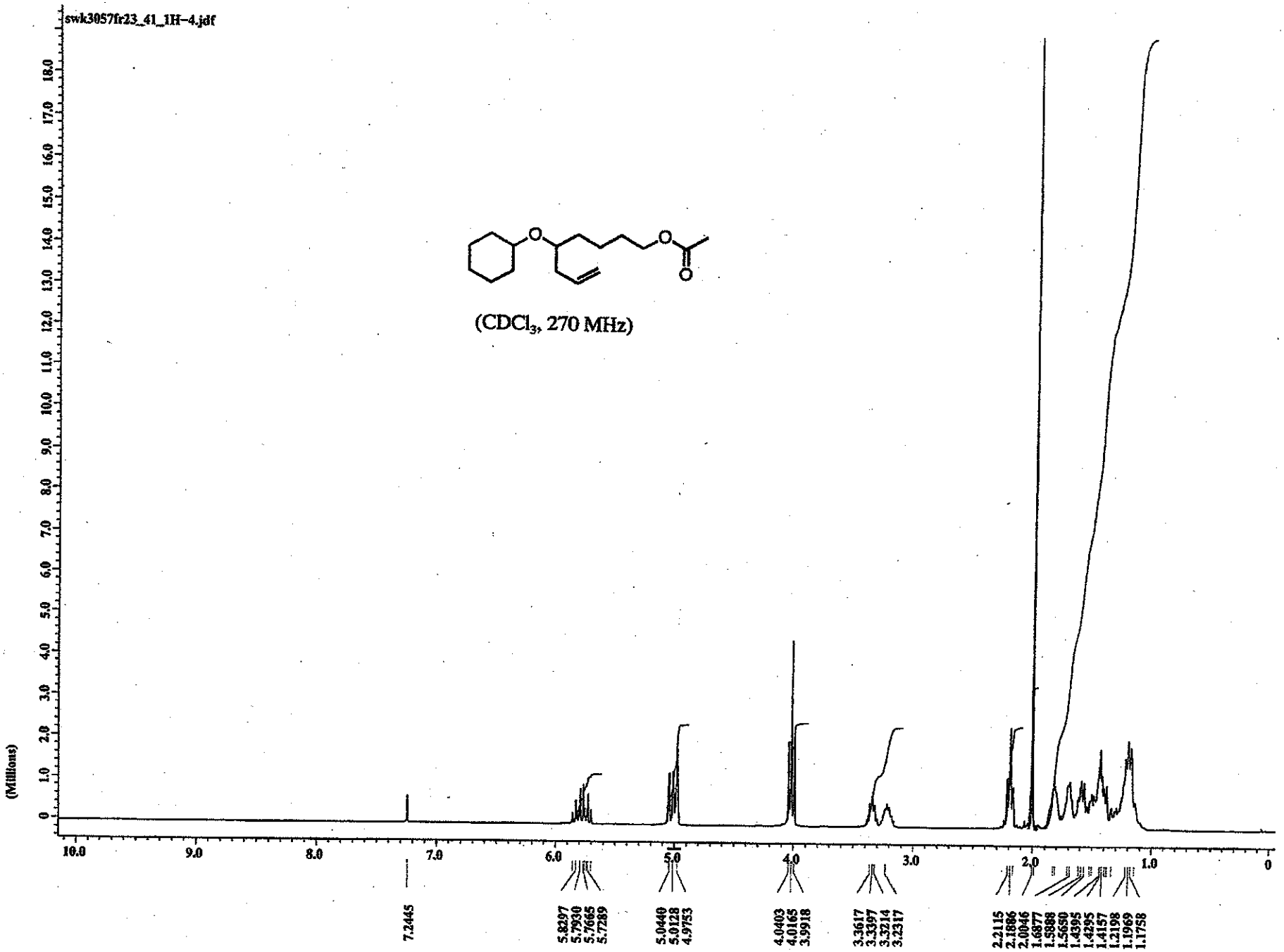

swk3049fr31_75_13C~3.jdf
(CDCl3, 67.5 MHz)
(Thousands)
X : parts per Million : 13C
171.0782
134.9489
116.6742
78.6731
77.4737
77.0000
76.5340
69.0927
64.4399
38.3190
33.4829
29.7699
28.6010
28.3412
22.4585
21.8091
20.9076
13.9781


swk3055fr8_18_1H~4.jdf
(CDCl3, 270 MHz)
(Millions)
X : parts per Million : 1H
7.2454
5.8700
5.8324
5.8068
5.7692
5.0907
5.0594
5.0275
3.9881
3.9542
3.9469
3.4441
3.4148
3.4038
3.3040
2.2656
2.2399
2.1840
2.1575
1.8332
1.5751
1.5613
1.5494
1.5165
1.4890
1.2372

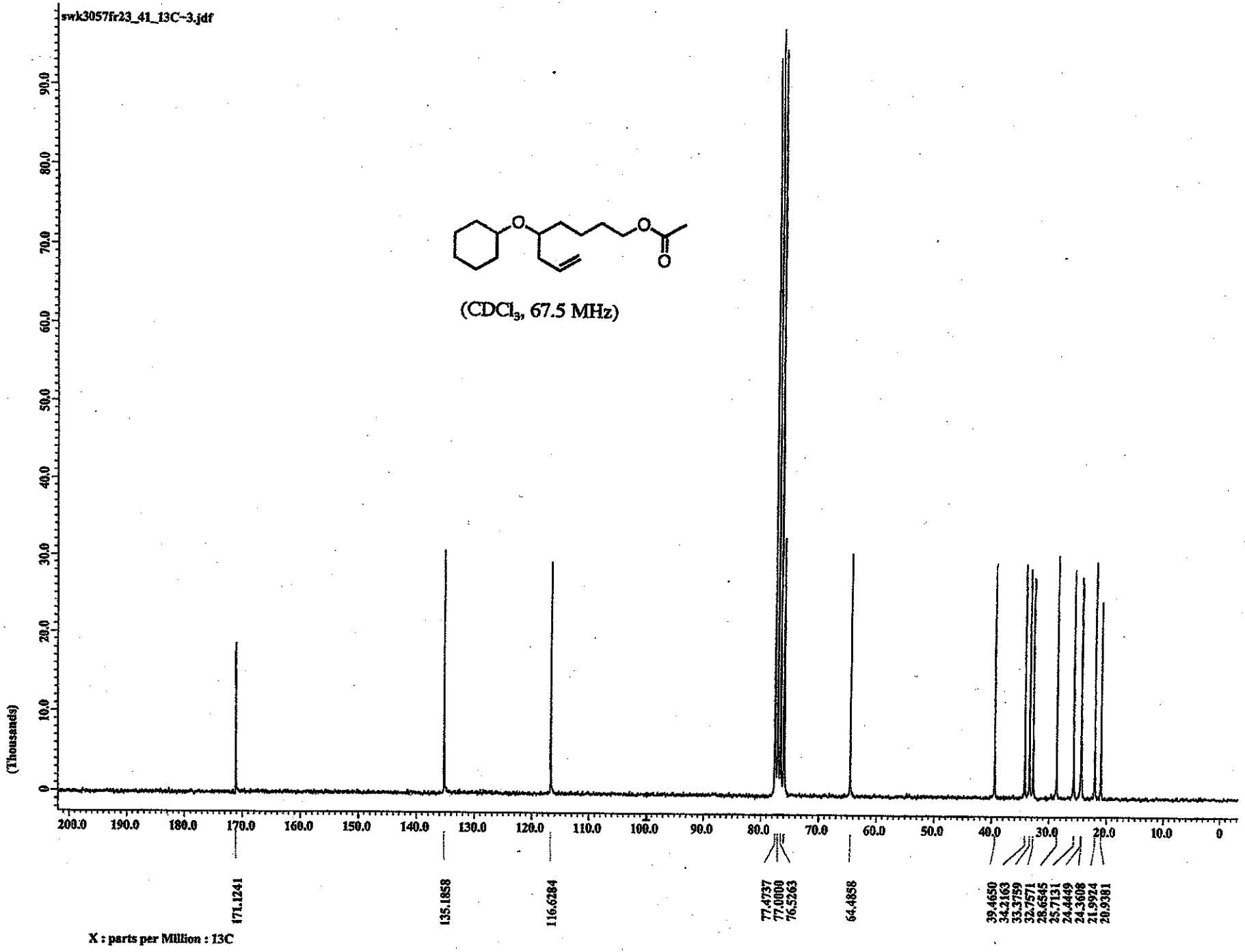

swk3055fr8_18_13C-4.jdf
(CDCl3, 67.5 MHz)
(Millions)
3.0
2.0
1.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
135.0101
116.4908
77.4737
77.2750
77.0000
76.5263
68.5273
41.0388
31.4048
25.9728
23.4364
X : parts per Million : 13C

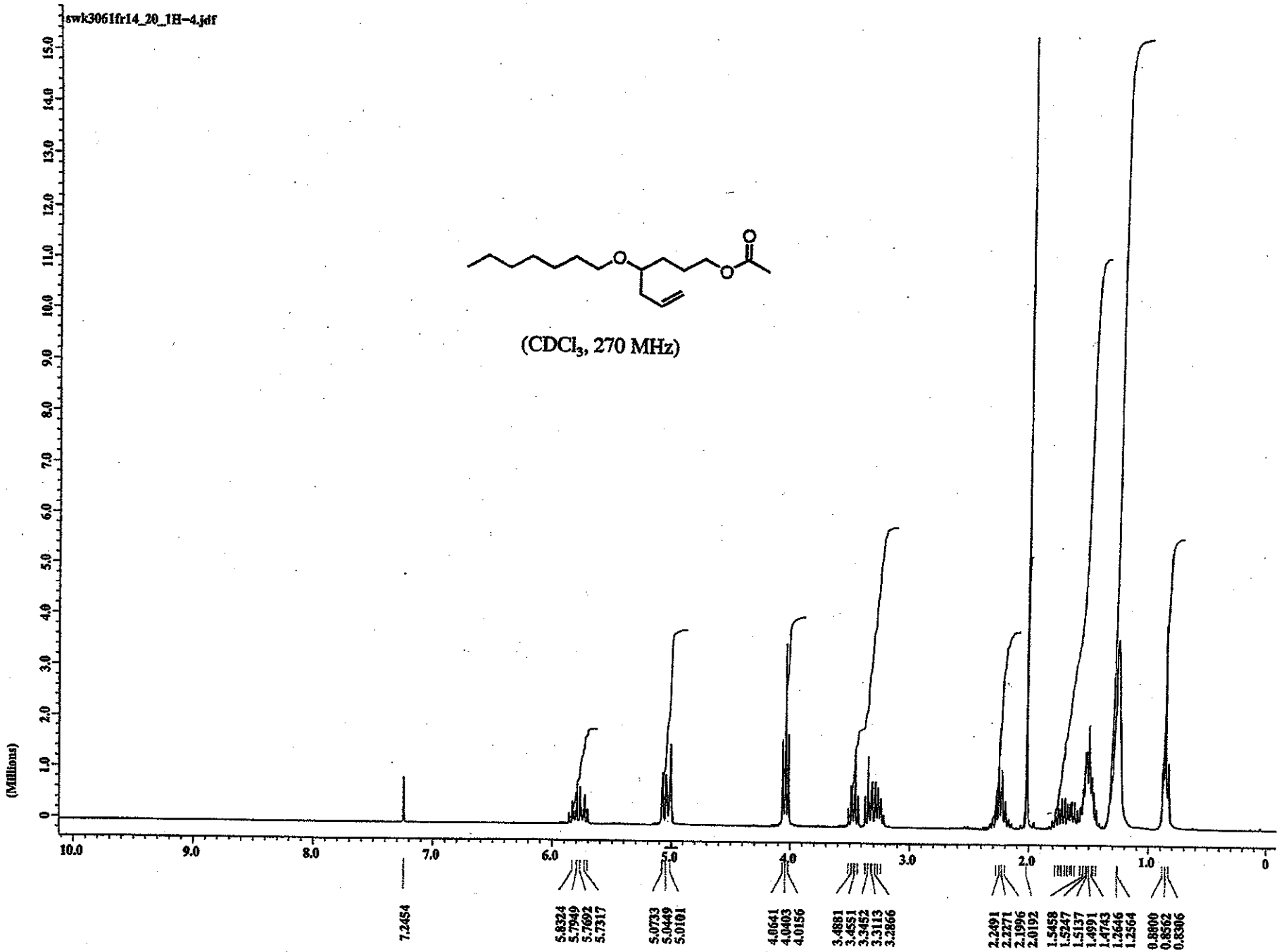

swk3055fr39_60_1H-4.jdf
(CDCl3, 270 MHz)
(Millions)
X : parts per Million : 1H
7.2454
5.8480
5.8114
5.7848
5.7473
5.0852
5.0559
5.0220
4.0623
4.0385
4.0137
3.6383
3.6309
3.6044
3.5256
3.5000
3.4917
2.4395
2.4231
2.4139
2.0275
1.9624
1.9533
1.9432
1.6163
1.4853
1.4652
1.4469


swk3055fr39_60_13C-5.jdf
(CDCl3, 67.5 MHz)
(Thousands)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.9178
134.5440
116.8652
81.2936
79.0246
77.4660
77.0060
76.5263
69.1232
67.0375
64.2642
38.2120
33.3301
28.4635
21.6486
20.8159
20.0443
X : parts per Million : 13C

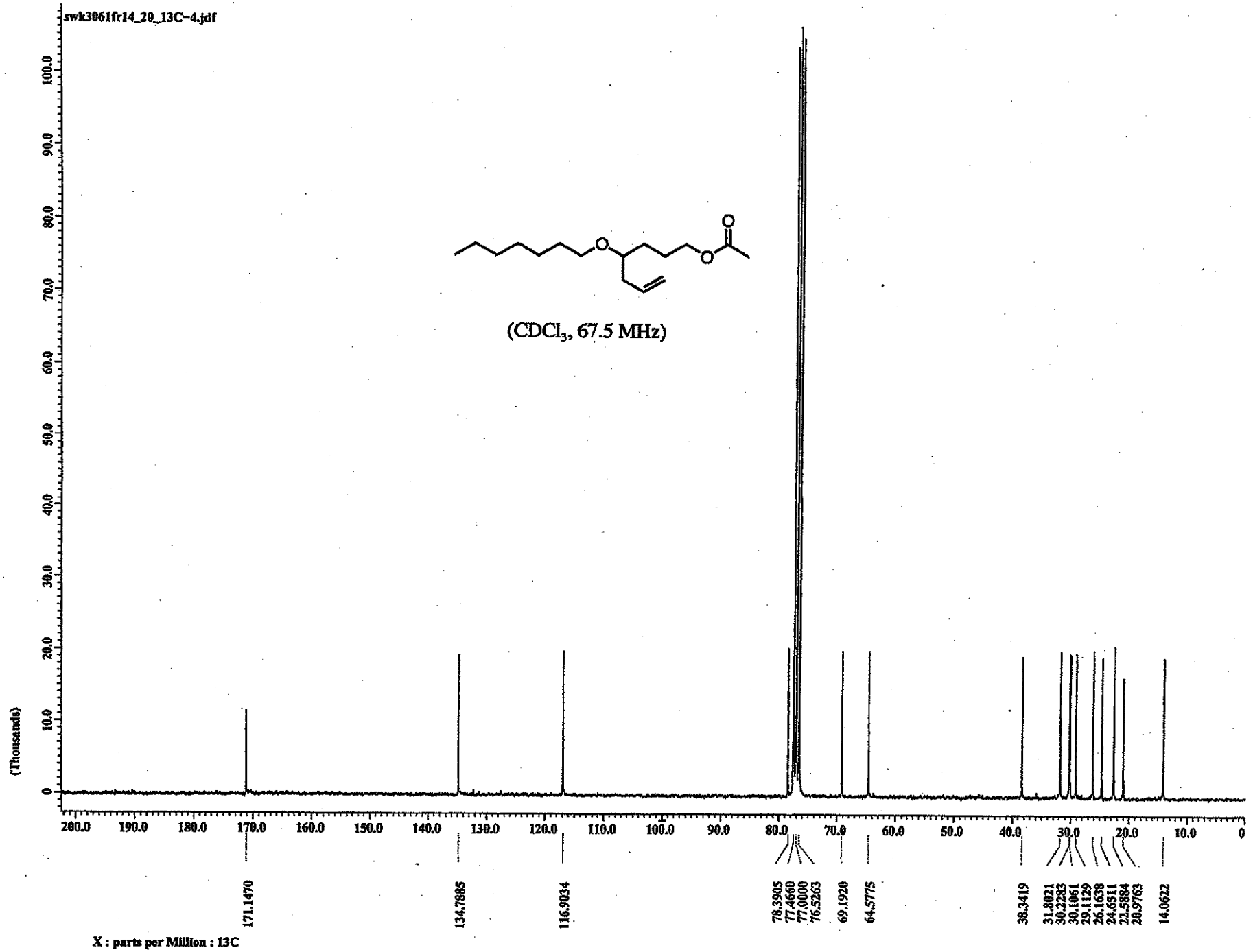


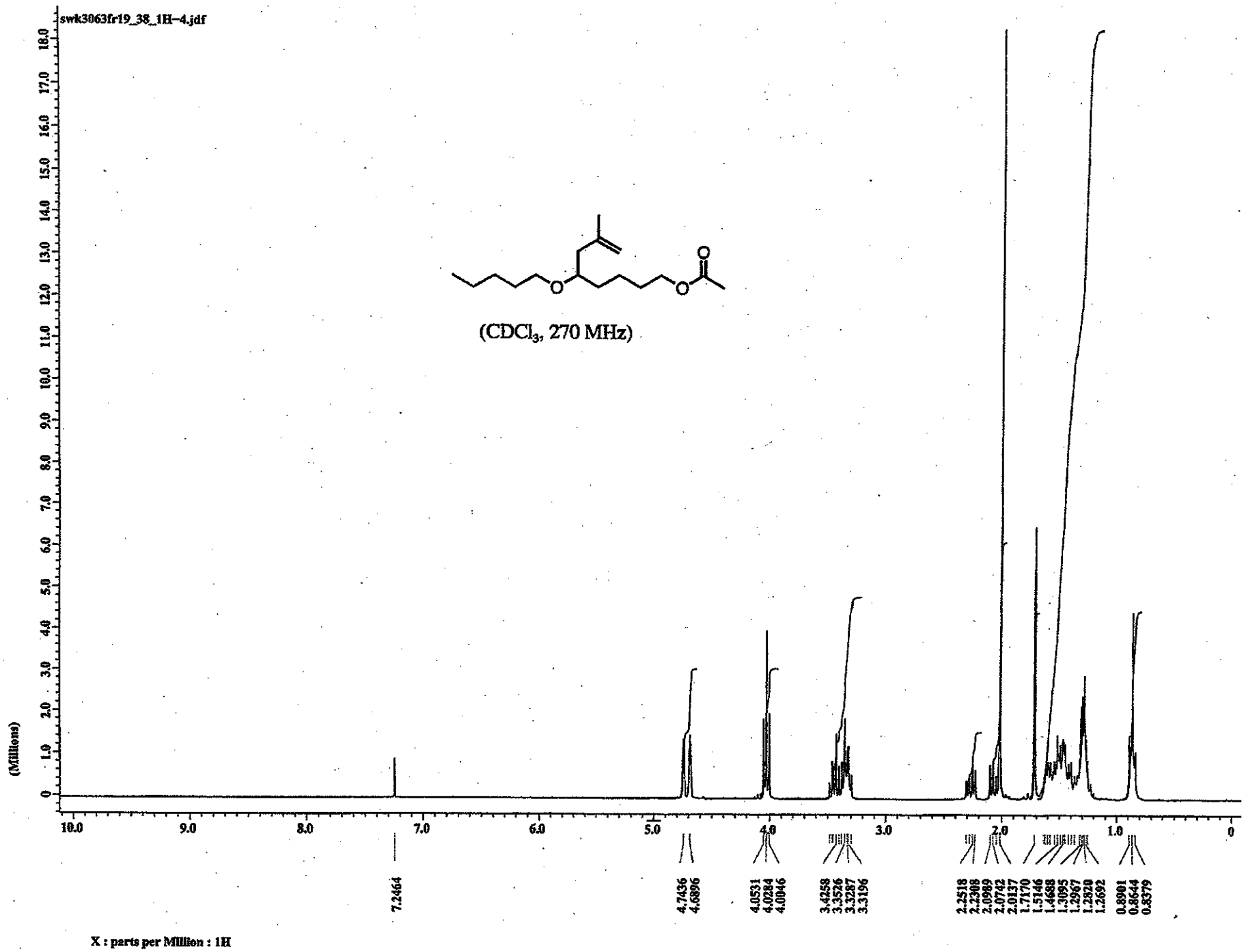
(CDCl$_3$, 270 MHz)

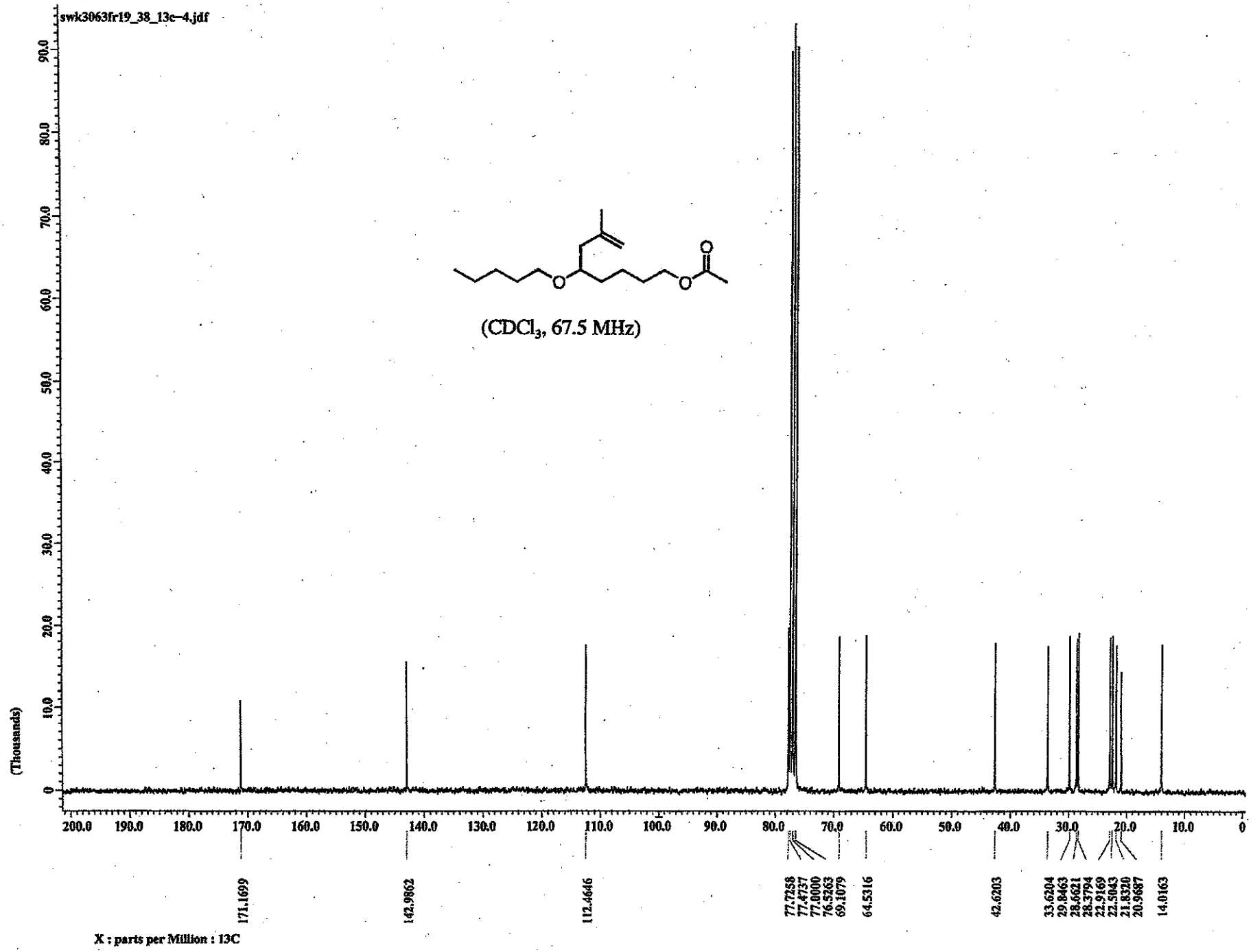

swk3057fr23_41_13C~3.jdf
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.1241
135.1858
116.6284
77.4737
77.0000
76.5263
64.4858
39.4650
34.2163
33.3759
32.7571
28.6545
25.7131
24.4449
24.3608
21.9924
20.9381
X : parts per Million : 13C

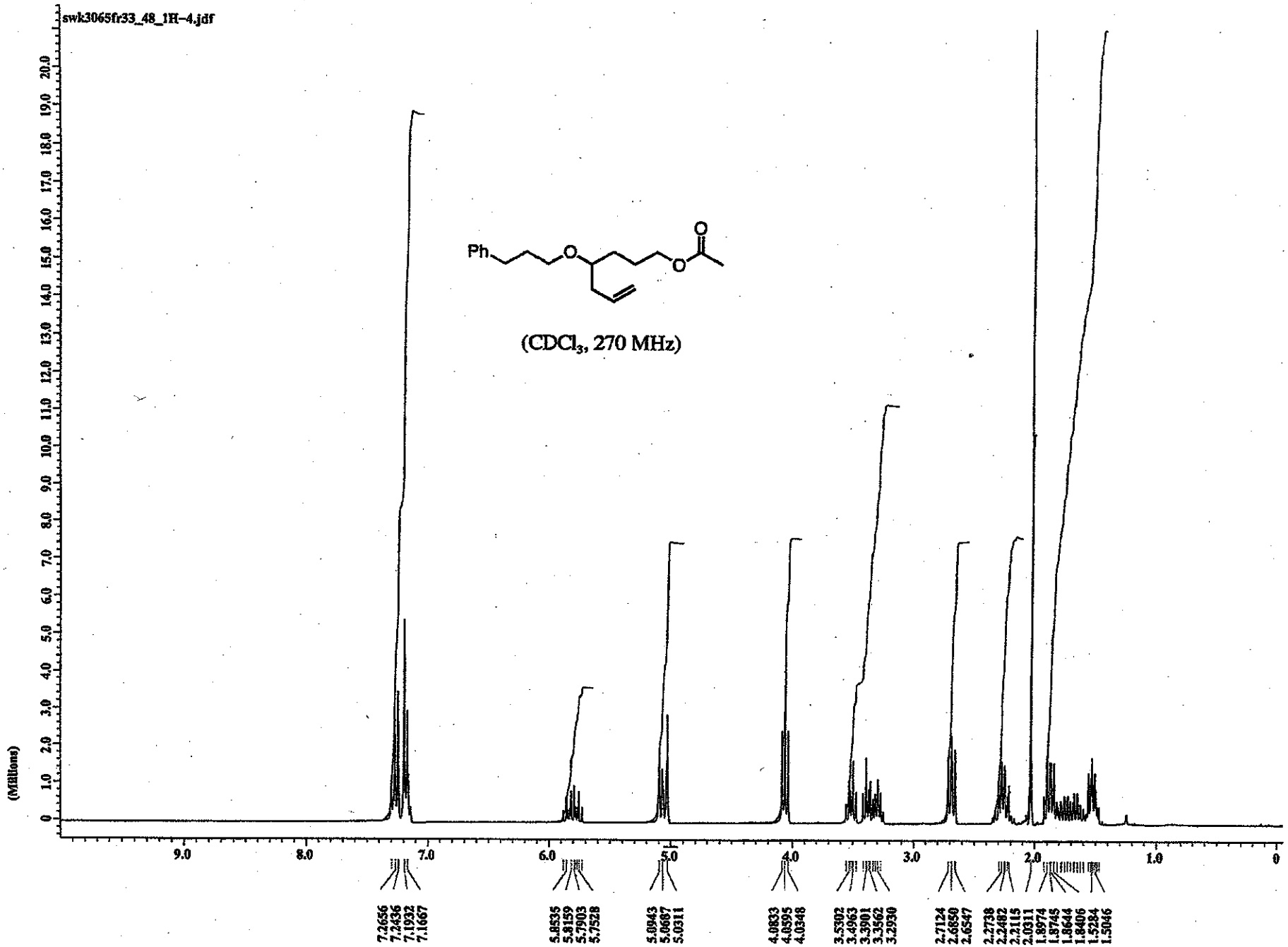


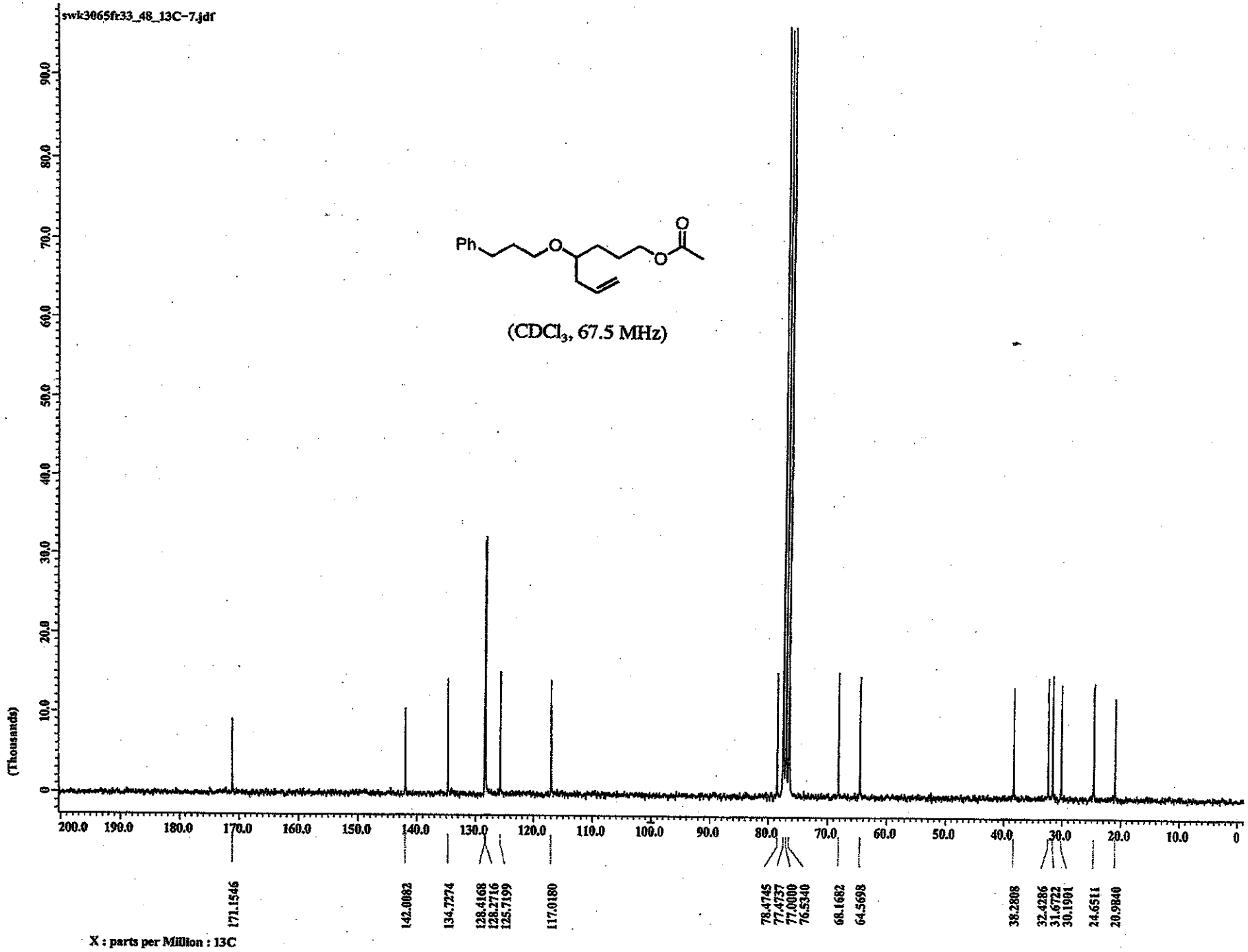
(CDCl$_3$, 270 MHz)

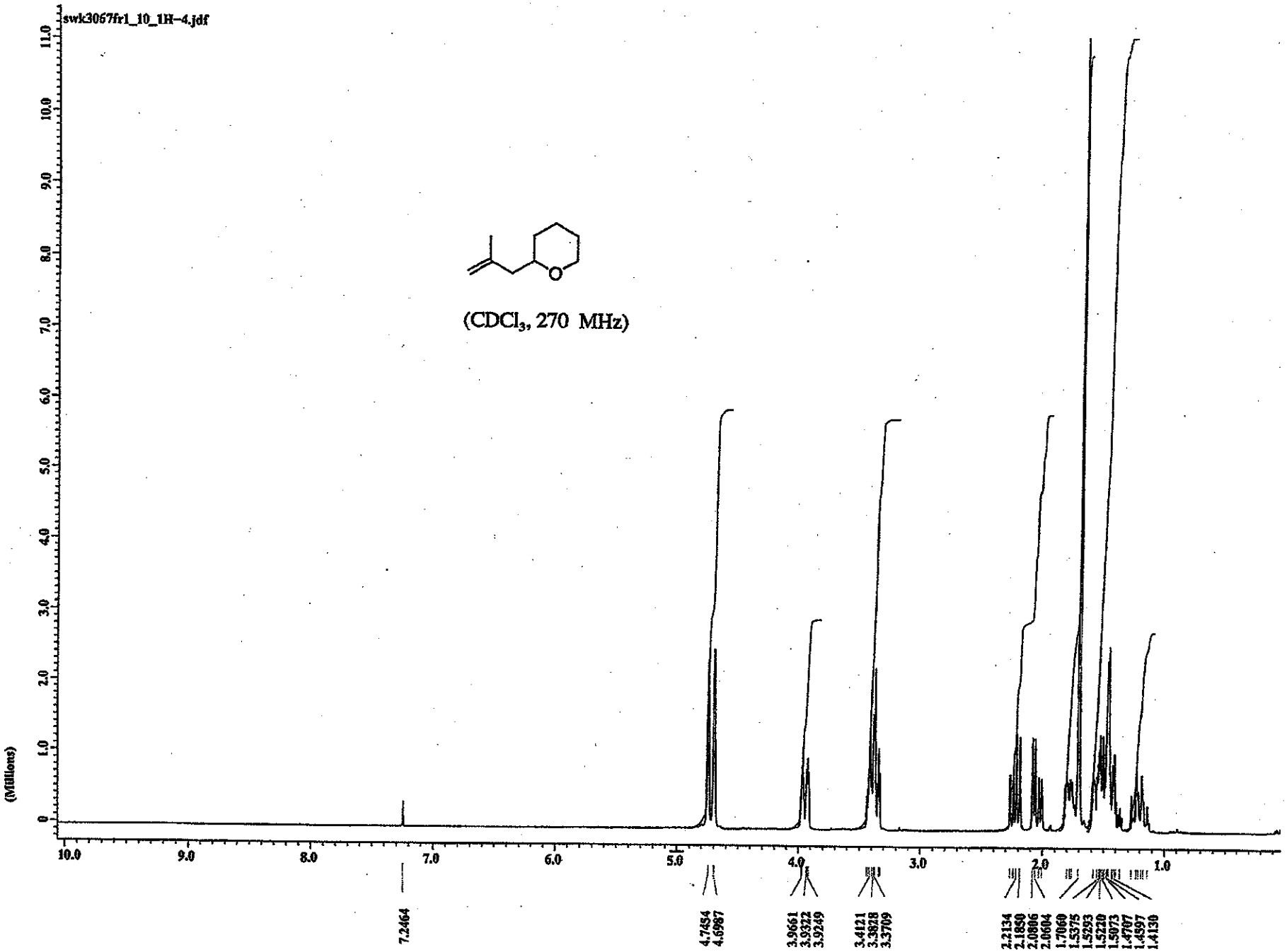

swk3061fr14_20_13C-4.jdf
(CDCl3, 67.5 MHz)
(Thousands)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.1470
134.7885
116.9034
78.3905
77.4660
77.0000
76.5263
69.1920
64.5775
38.3419
31.8021
30.2283
30.1061
29.1129
26.1638
24.6511
22.5884
20.9763
14.0622
X : parts per Million : 13C

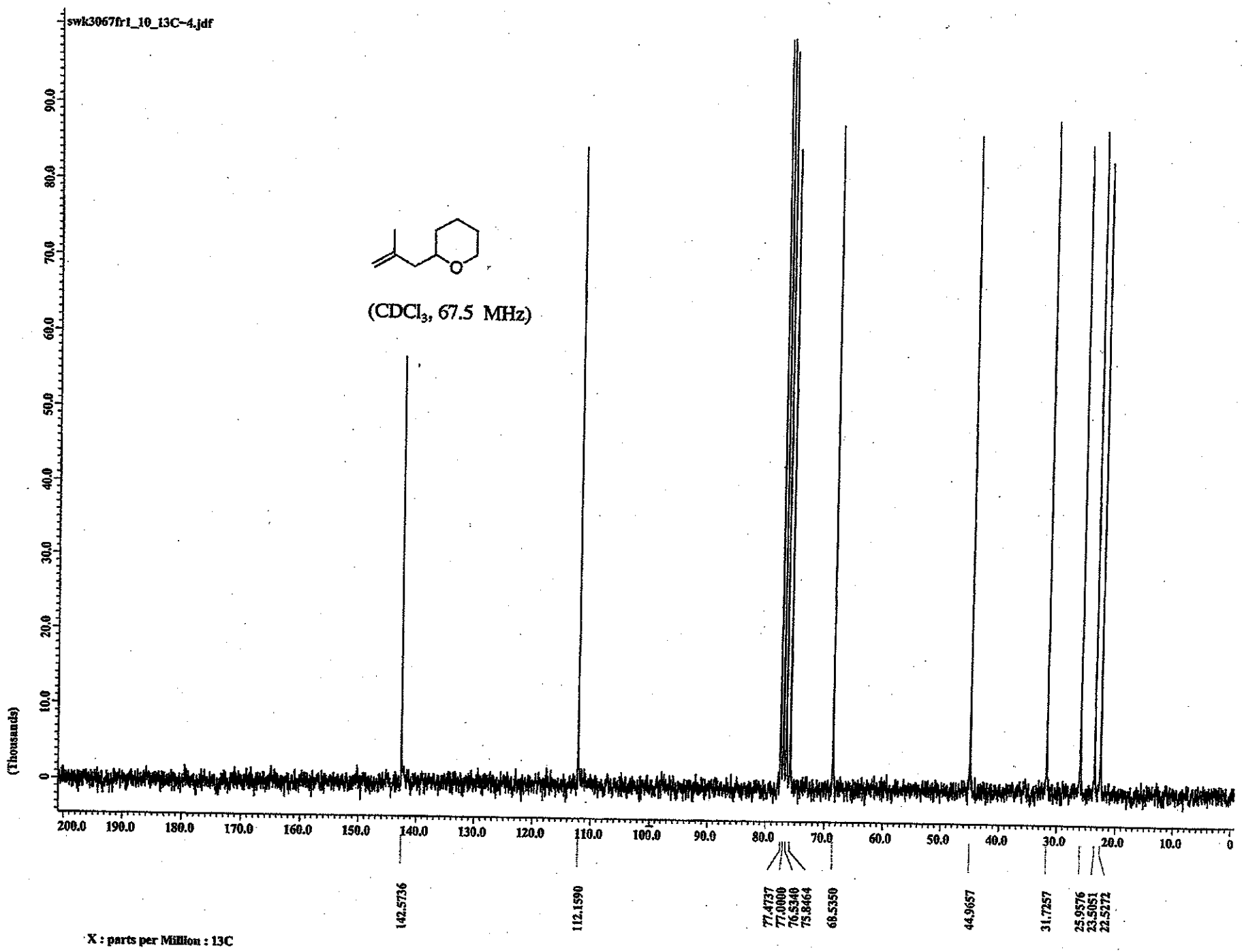

swk3063fr19_38_1H-4.jdf
(CDCl3, 270 MHz)
(Millions)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2464
4.7436
4.6896
4.0531
4.0284
4.0046
3.4258
3.3526
3.3287
3.3196
2.2518
2.2308
2.0989
2.0742
2.0137
1.7170
1.5146
1.4688
1.3095
1.2967
1.2820
1.2692
0.8901
0.8644
0.8379
X : parts per Million : 1H

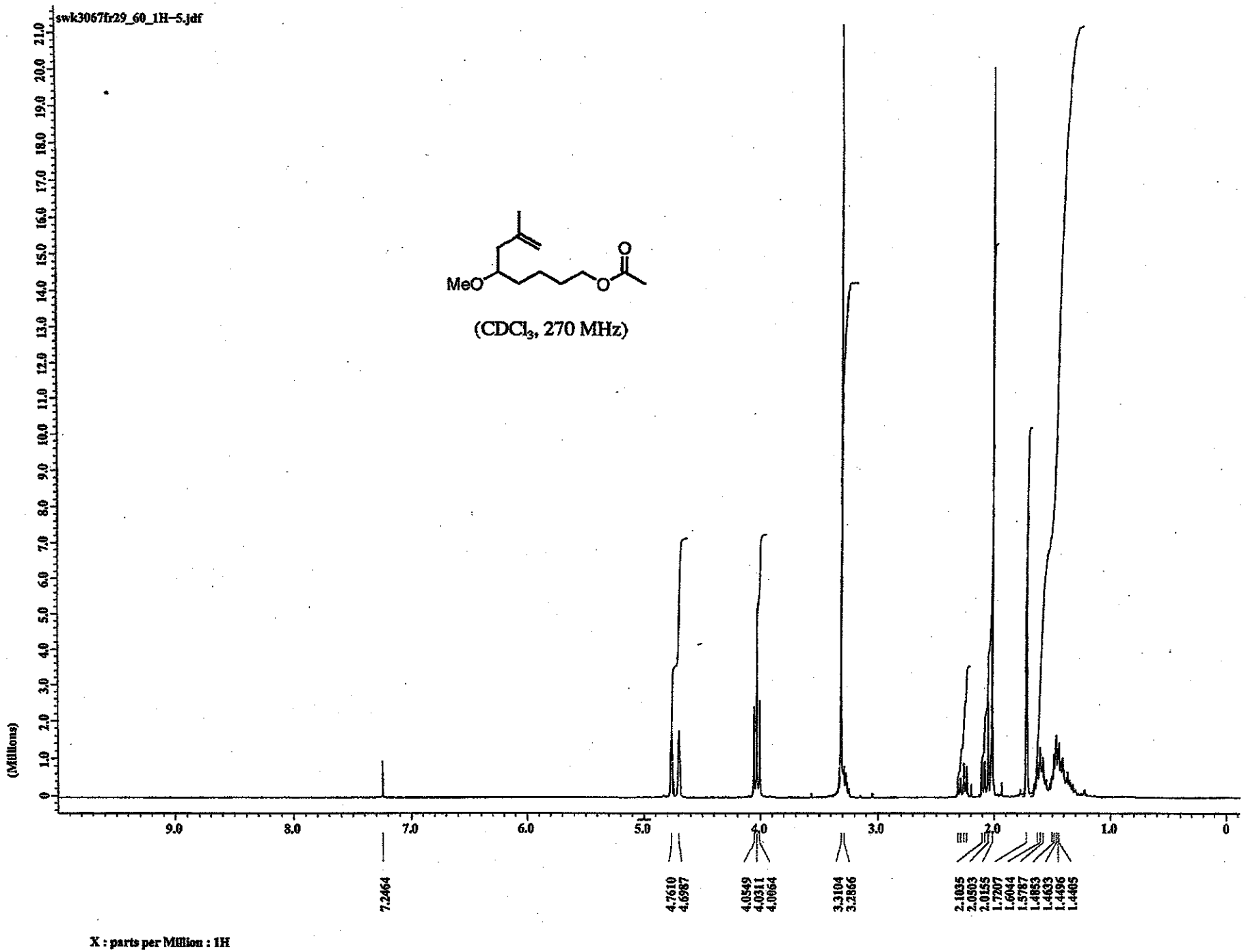

swk3063fr19_38_13c-4.jdf
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.1699
142.9862
112.4646
77.7258
77.4737
77.0000
76.5263
69.1079
64.5316
42.6203
33.6204
29.8463
28.6621
28.3794
22.9169
22.5043
21.8320
20.9687
14.0163
X : parts per Million : 13C

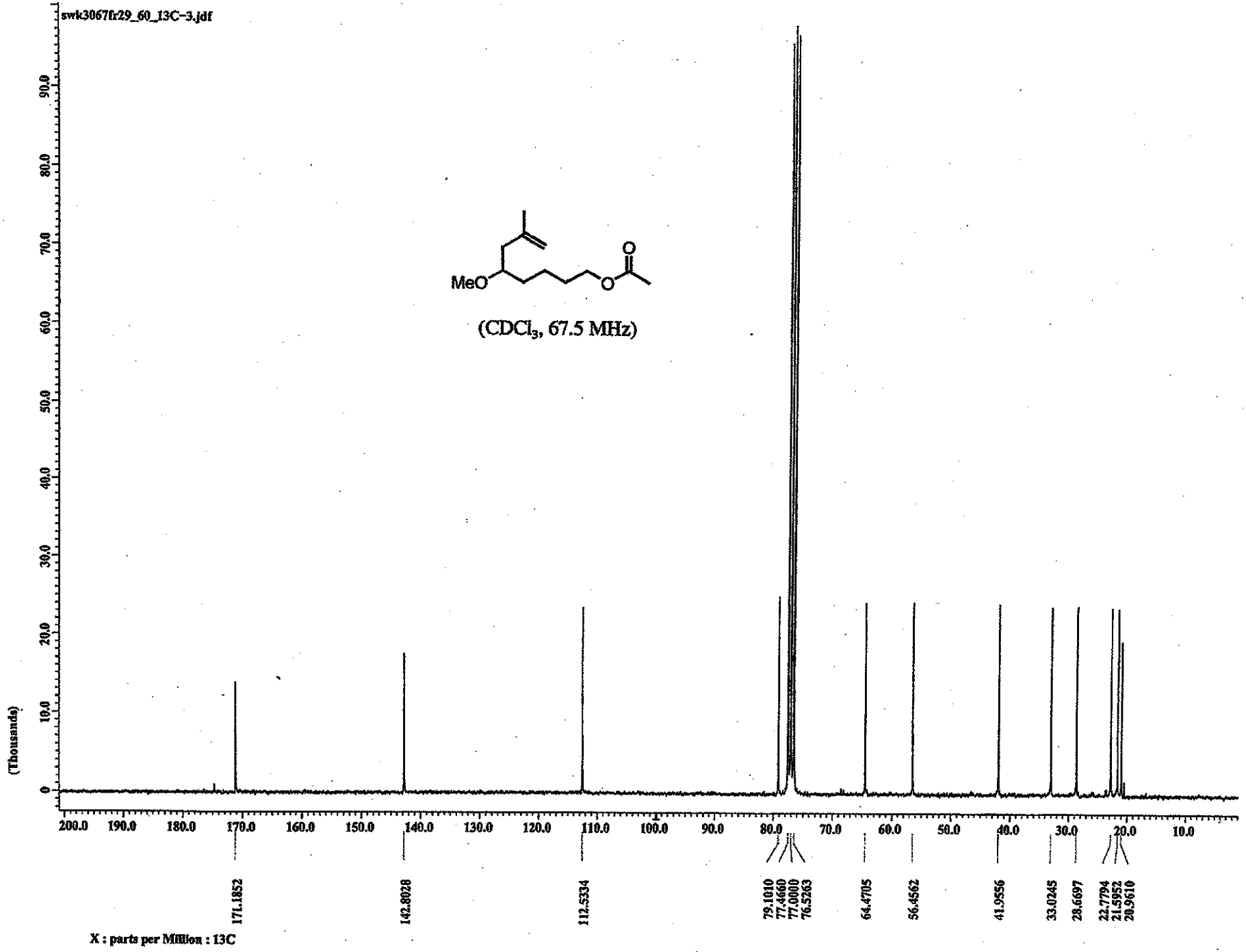

swk3065fr33_48_1H-4.jdf
Ph
O
O
O
(CDCl3, 270 MHz)
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2656
7.2436
7.1932
7.1667
5.8535
5.8159
5.7903
5.7528
5.0943
5.0687
5.0311
4.0833
4.0595
4.0348
3.5302
3.4963
3.3901
3.3562
3.2930
2.7124
2.6850
2.6547
2.2738
2.2482
2.2115
2.0311
1.8974
1.8745
1.8644
1.8406
1.5284
1.5046
X : parts per Million : 1H

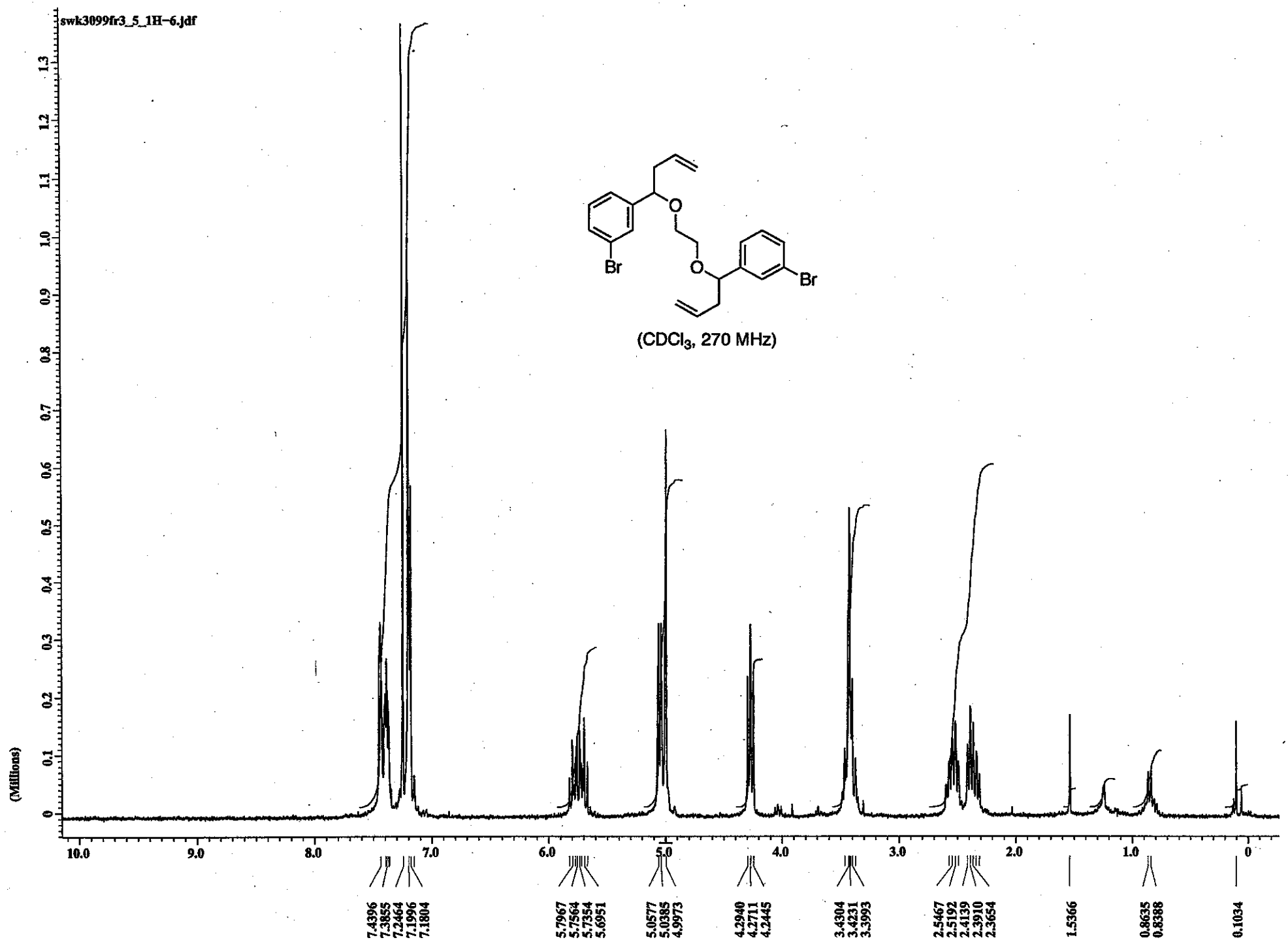

swk3065fr33_48_13C-7.jdf
Ph
O
O
O
(CDCl3, 67.5 MHz)
(Thousands)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.1546
142.0082
134.7274
128.4168
128.2716
125.7199
117.0180
78.4745
77.4737
77.0000
76.5340
68.1682
64.5698
38.2808
32.4286
31.6722
30.1901
24.6511
20.9840
X : parts per Million : 13C

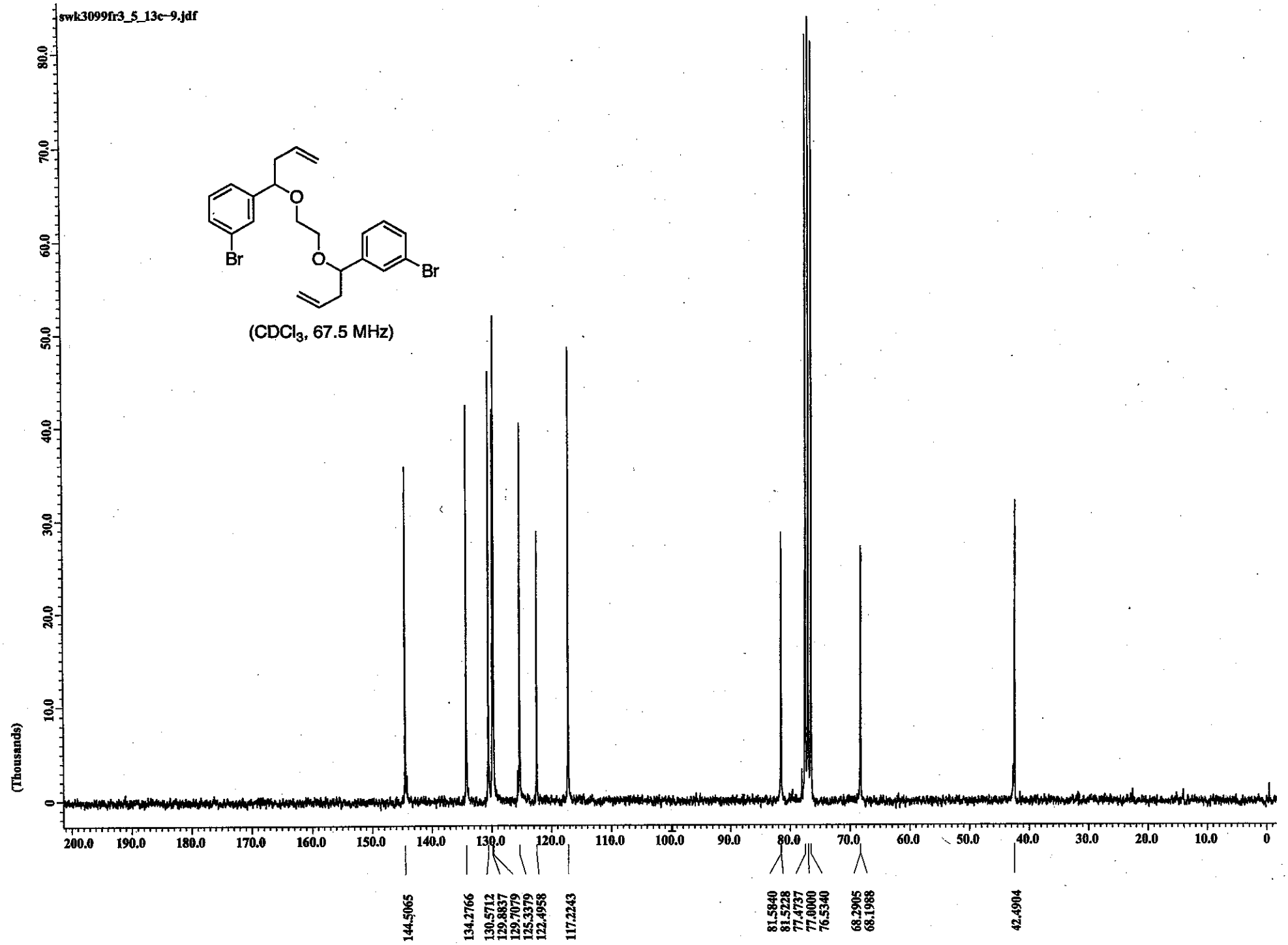

swk3067fr1_10_1H-4.jdf
(CDCl3, 270 MHz)
(Millions)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.2464
4.7454
4.6987
3.9661
3.9322
3.9249
3.4121
3.3828
3.3709
2.2134
2.1850
2.0806
2.0604
1.7060
1.5375
1.5293
1.5220
1.5073
1.4707
1.4597
1.4130
X : parts per Million : 1H

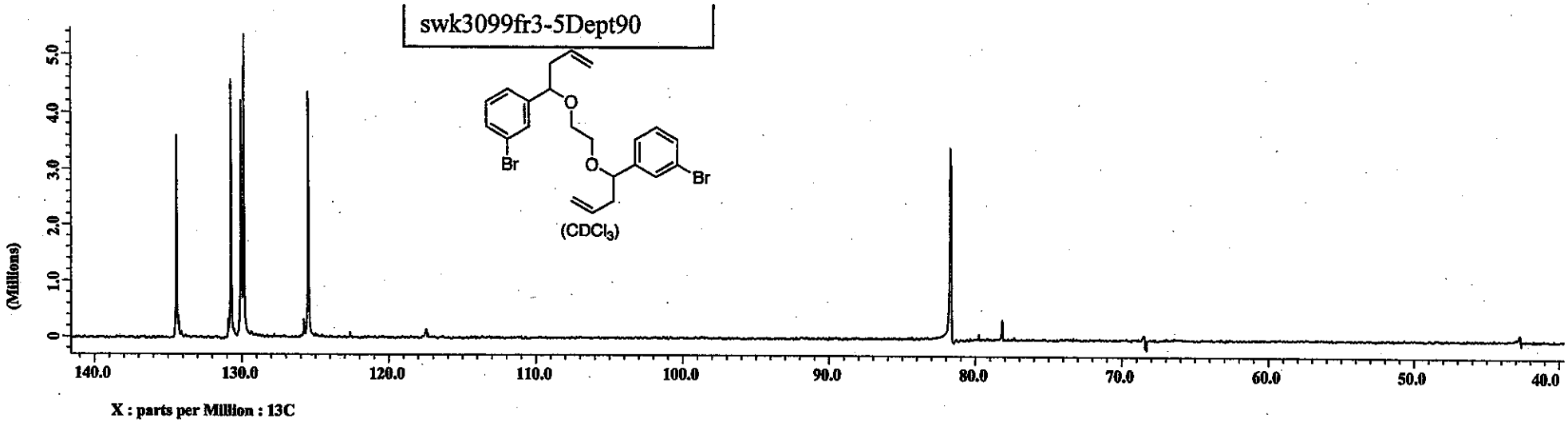

swk3067fr1_10_13C-4.jdf
(CDCl3, 67.5 MHz)
(Thousands)
X : parts per Million : 13C
142.5736
112.1590
77.4737
77.0000
76.5340
75.8464
68.5350
44.9657
31.7257
25.9576
23.5051
22.5272

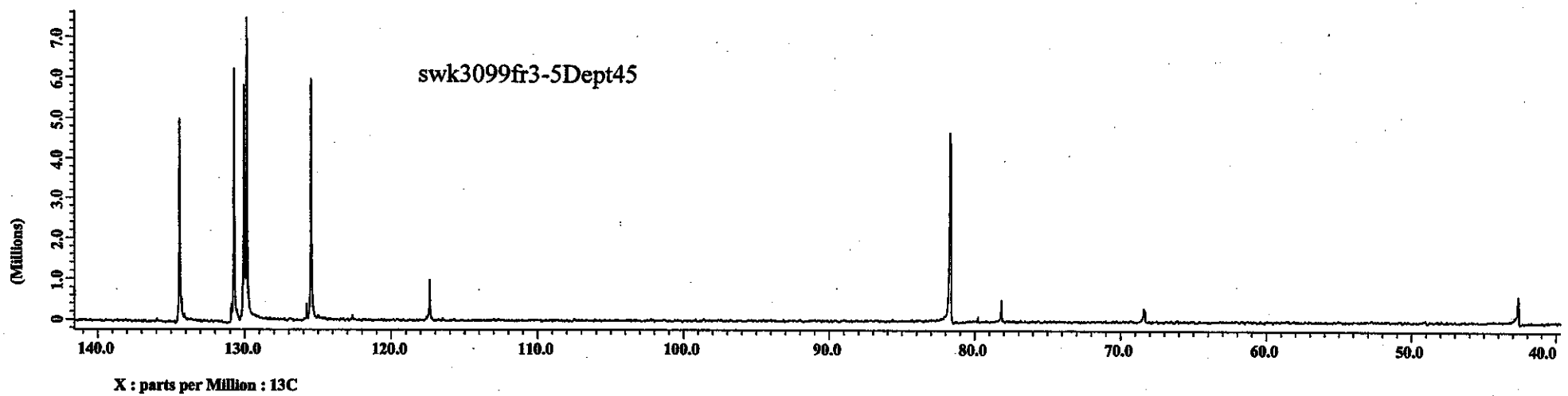

swk3067fr29_60_1H-5.jdf
MeO
O
O
(CDCl3, 270 MHz)
(Millions)
21.0
20.0
19.0
18.0
17.0
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2464
4.7610
4.6987
4.0549
4.0311
4.0064
3.3104
3.2866
2.1035
2.0503
2.0155
1.7207
1.6044
1.5787
1.4853
1.4633
1.4496
1.4405
X : parts per Million : 1H

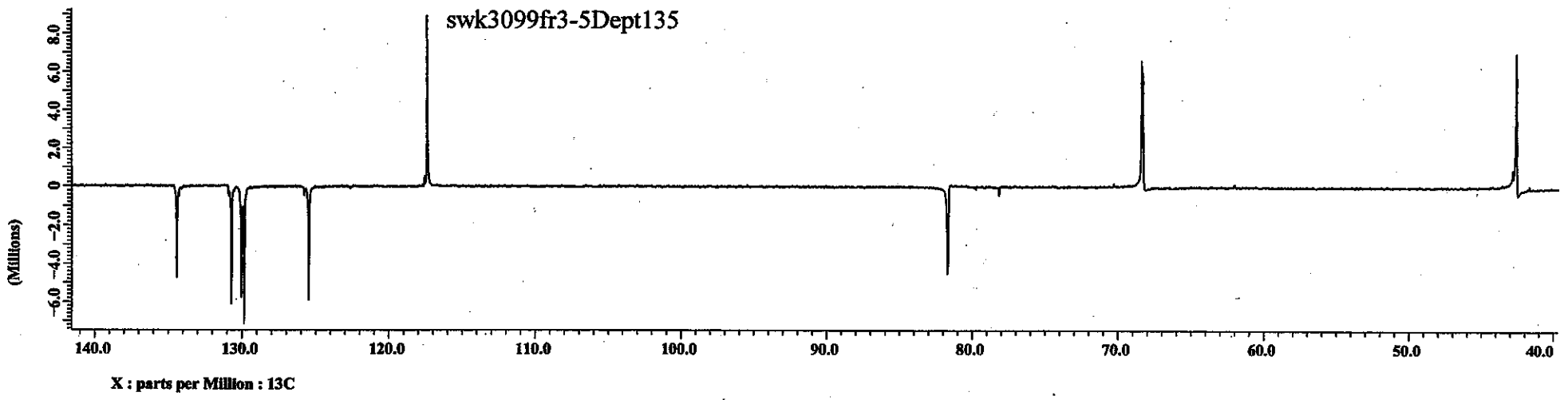

swk3067fr29_60_13C-3.jdf
MeO
O
O
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
171.1852
142.8028
112.5334
79.1010
77.4660
77.0000
76.5263
64.4705
56.4562
41.9556
33.0245
28.6697
22.7794
21.5952
20.9610
X : parts per Million : 13C

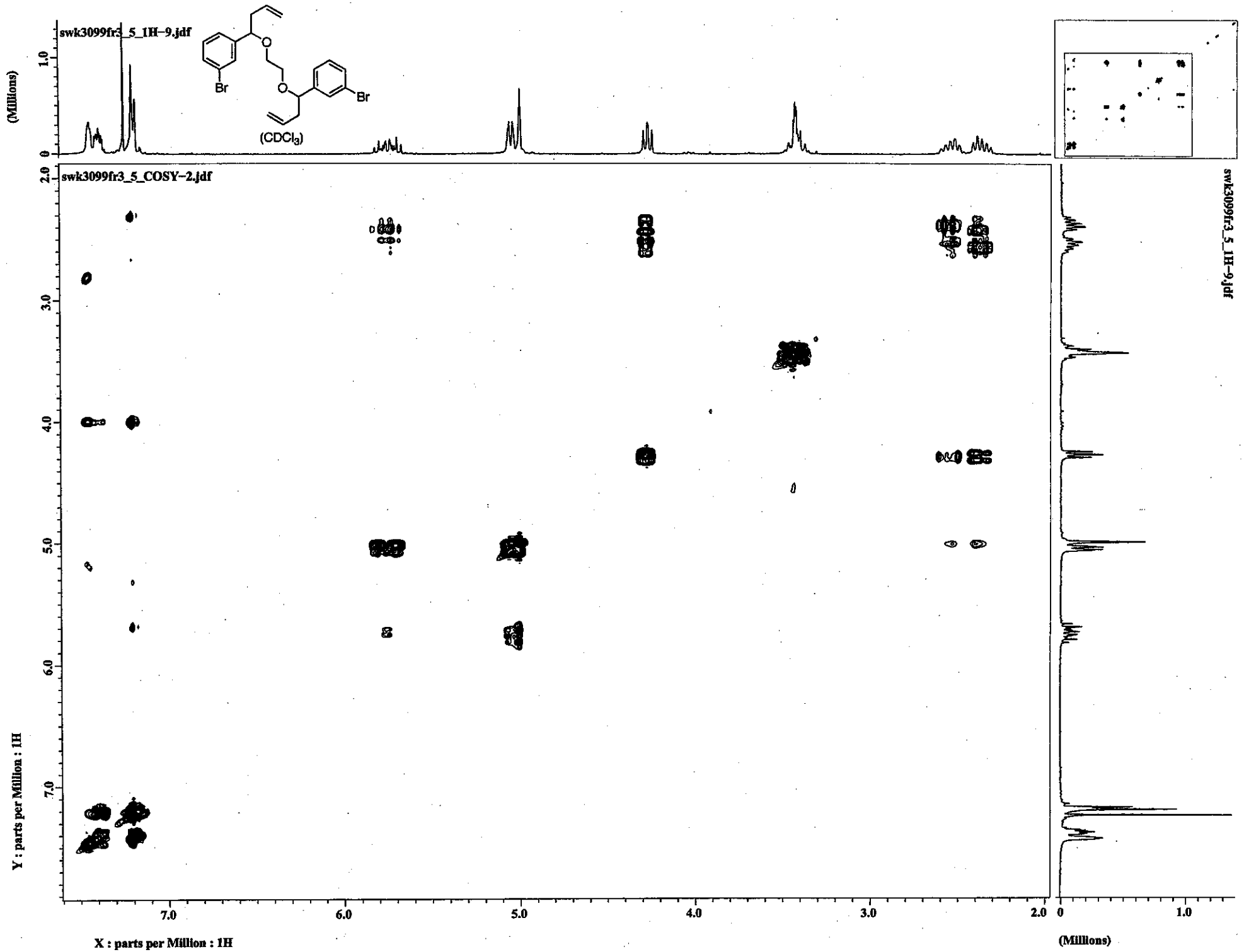

swk3099fr3_5_1H-6.jdf
Br
O
O
Br
(CDCl3, 270 MHz)
(Millions)
X : parts per Million : 1H
7.4396
7.3855
7.2464
7.1996
7.1804
5.7967
5.7564
5.7354
5.6951
5.0577
5.0385
4.9973
4.2940
4.2711
4.2445
3.4304
3.4231
3.3993
2.5467
2.5192
2.4139
2.3910
2.3654
1.5366
0.8635
0.8388
0.1034

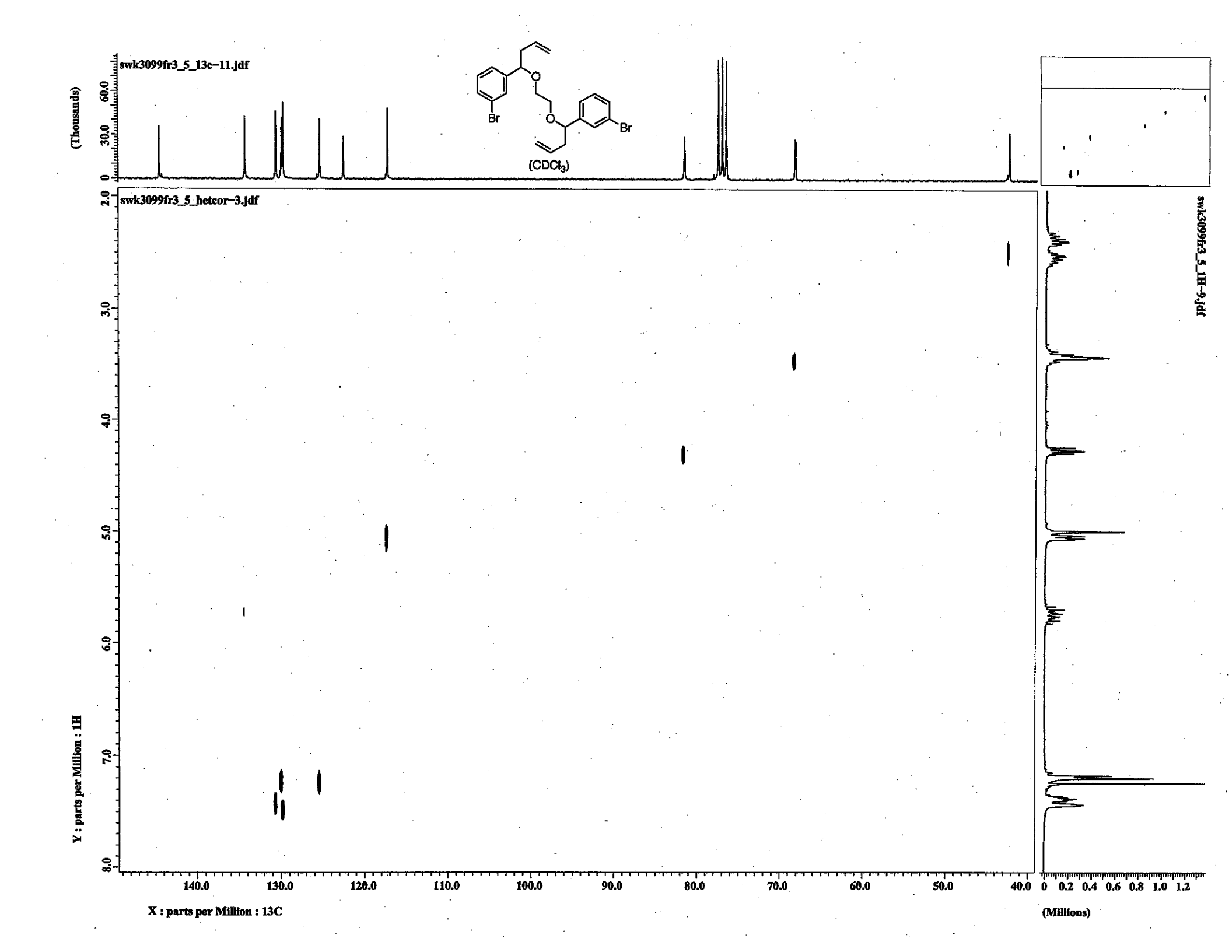

swk3099fr3_5_13c-9.jdf
Br
O
O
Br
(CDCl3, 67.5 MHz)
(Thousands)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
144.5065
134.2766
130.5712
129.8837
129.7079
125.3379
122.4958
117.2243
81.5840
81.5228
77.4737
77.0000
76.5340
68.2905
68.1988
42.4904
X : parts per Million : 13C

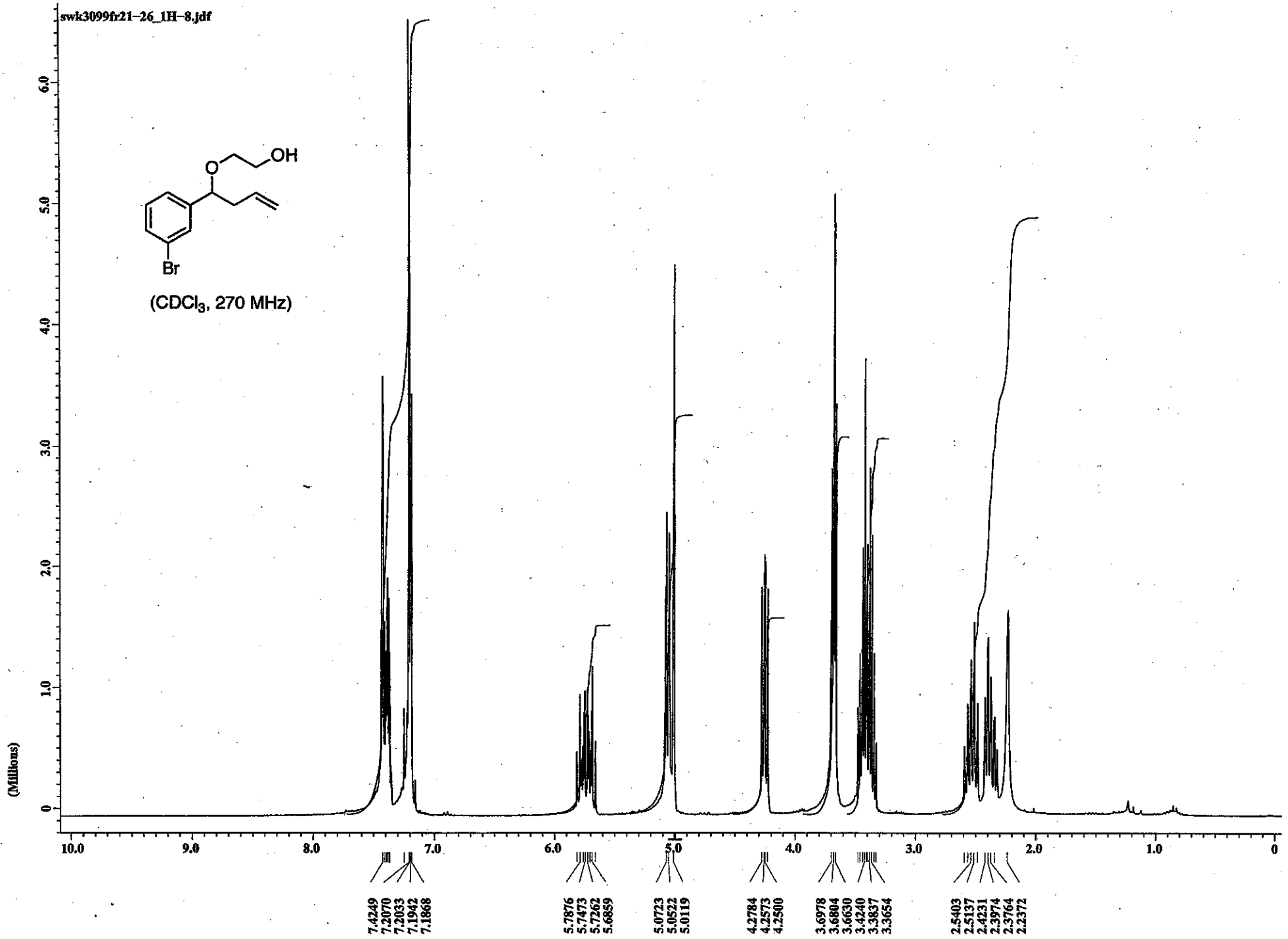

swk3099fr3-5Dept90
Br
O
O
Br
(CDCl3)
(Millions)
0
1.0
2.0
3.0
4.0
5.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C

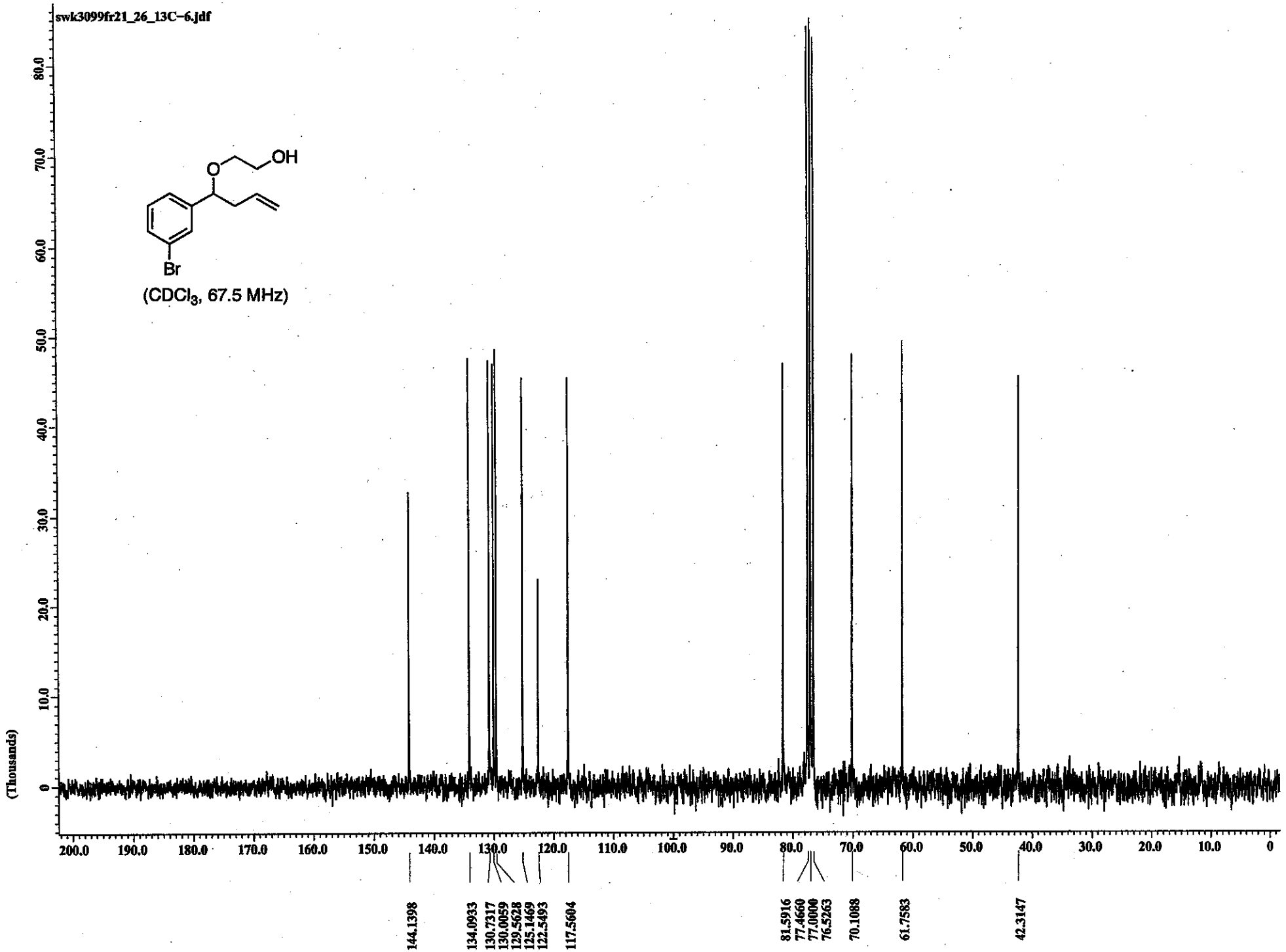

swk3099fr3-5Dept45
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C

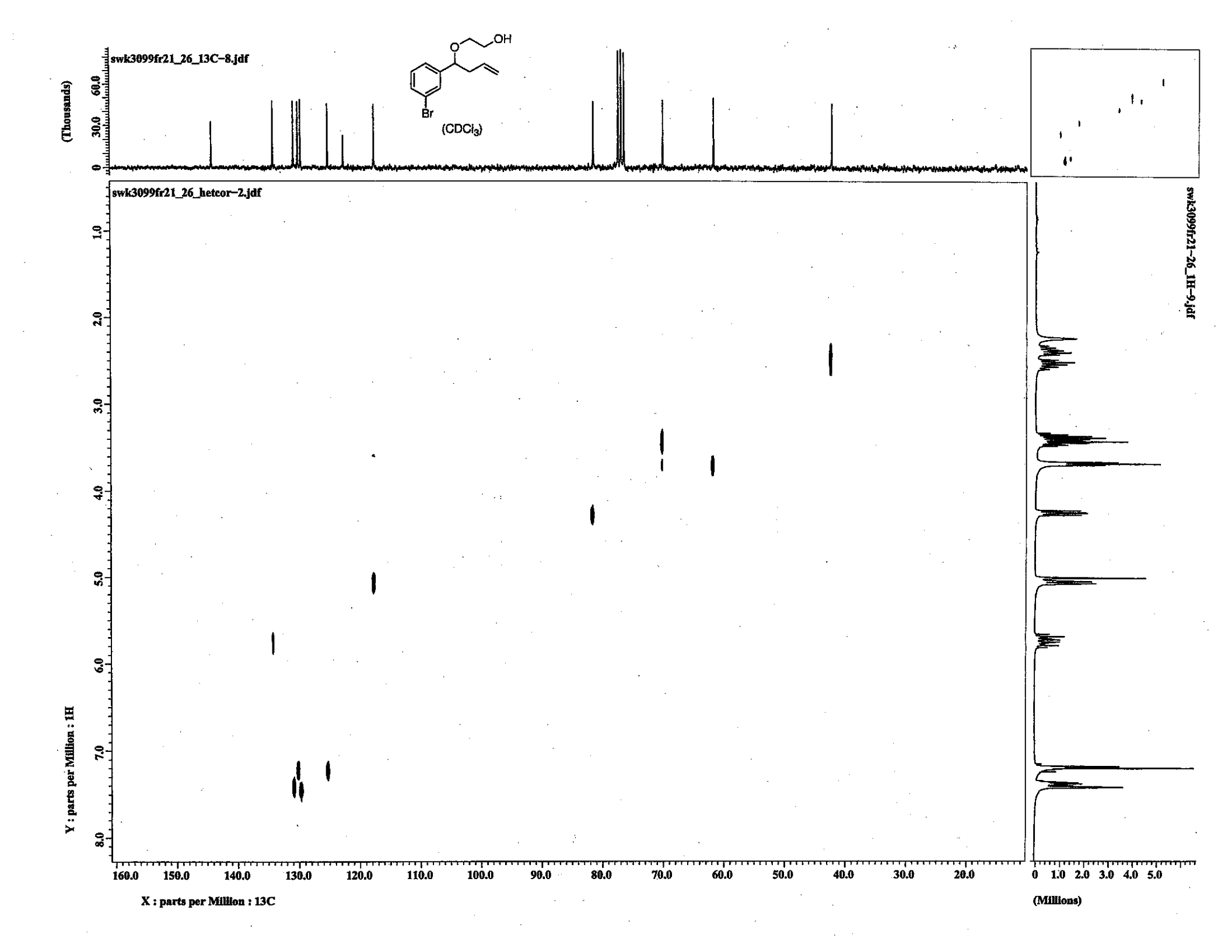

swk3099fr3-5Dept135
(Millions)
−6.0
−4.0
−2.0
0
2.0
4.0
6.0
8.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C

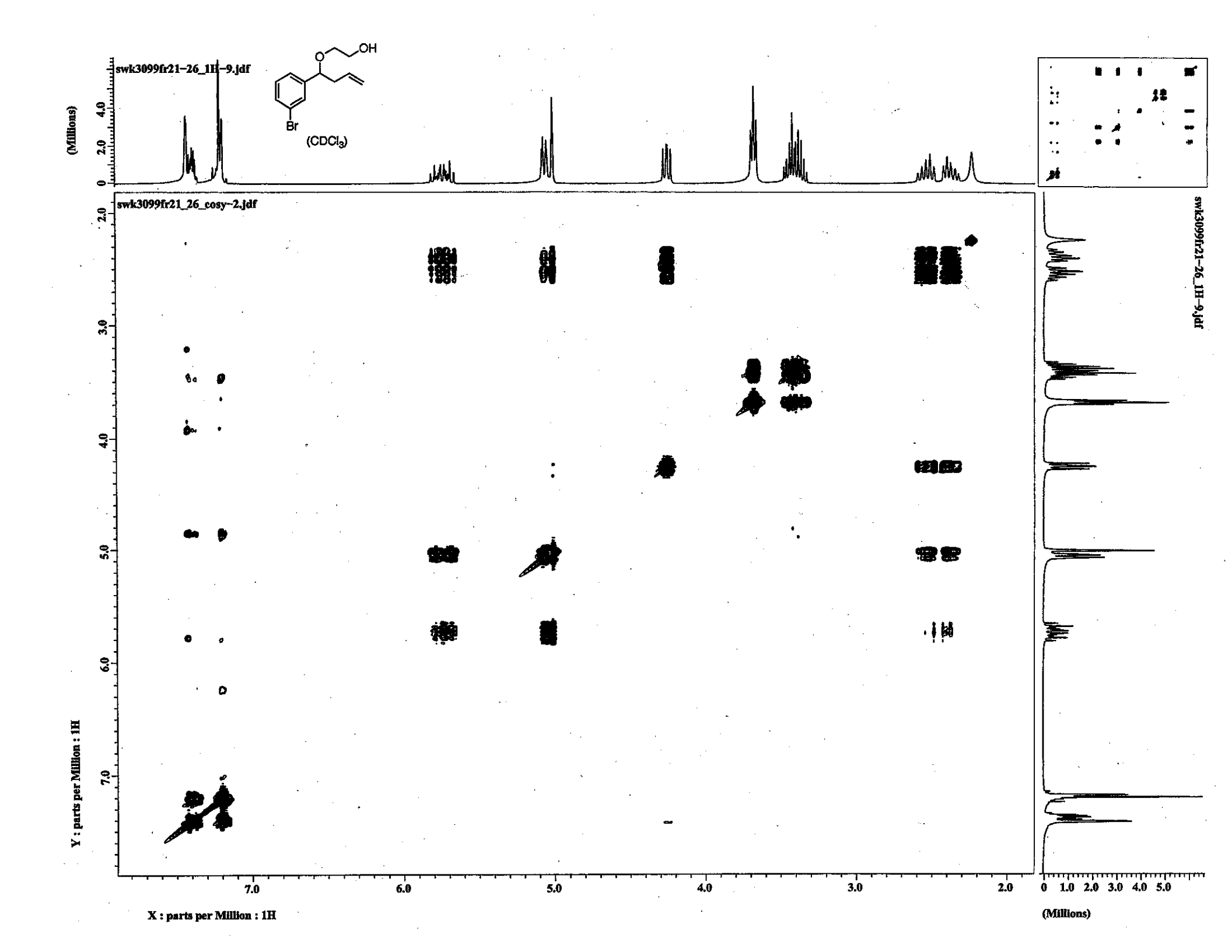

swk3099fr3_5_1H-9.jdf
(Millions)
1.0
0
Br
O
O
Br
(CDCl3)
swk3099fr3_5_COSY-2.jdf
2.0
3.0
4.0
5.0
6.0
7.0
Y : parts per Million : 1H
7.0
6.0
5.0
4.0
3.0
2.0
X : parts per Million : 1H
swk3099fr3_5_1H-9.jdf
0
1.0
(Millions)

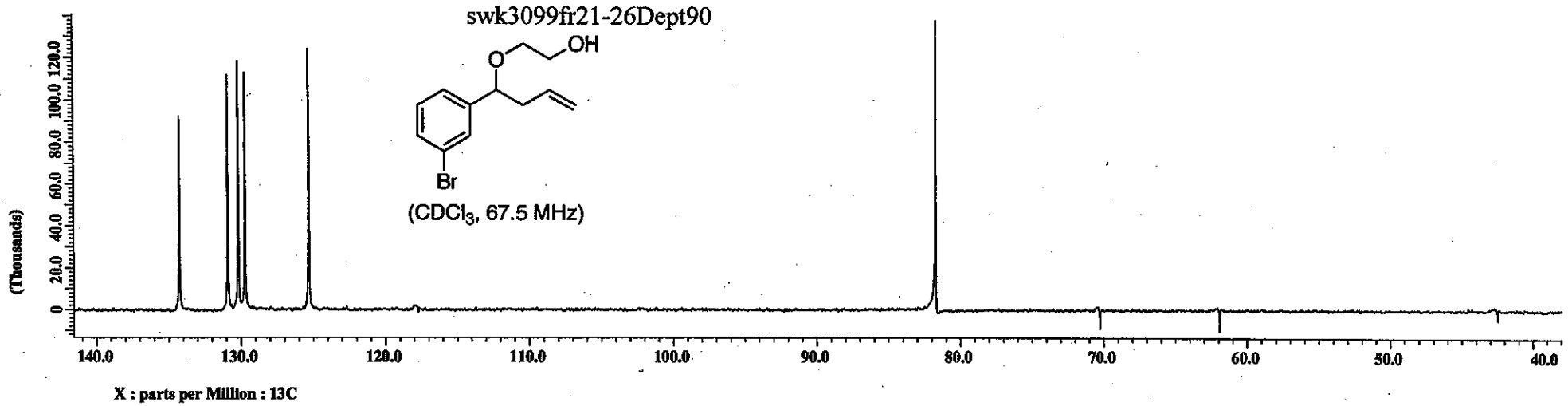

swk3099fr3_5_13c-11.jdf
(Thousands)
60.0
30.0
0
Br
O
O
Br
(CDCl3)
swk3099fr3_5_hetcor-3.jdf
2.0
3.0
4.0
5.0
6.0
7.0
8.0
Y : parts per Million : 1H
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C
swk3099fr3_5_1H-9.jdf
0
0.2
0.4
0.6
0.8
1.0
1.2
(Millions)

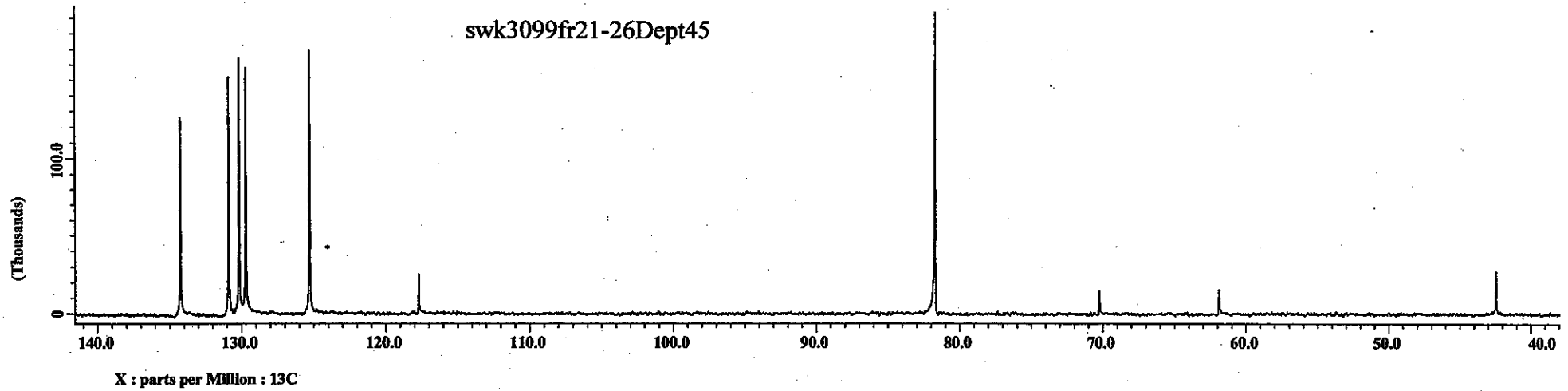

swk3099fr21-26_1H-8.jdf
OH
O
Br
(CDCl3, 270 MHz)
(Millions)
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4249
7.2070
7.2033
7.1942
7.1868
5.7876
5.7473
5.7262
5.6859
5.0723
5.0522
5.0119
4.2784
4.2573
4.2500
3.6978
3.6804
3.6630
3.4240
3.3837
3.3654
2.5403
2.5137
2.4231
2.3974
2.3764
2.2372
X : parts per Million : 1H

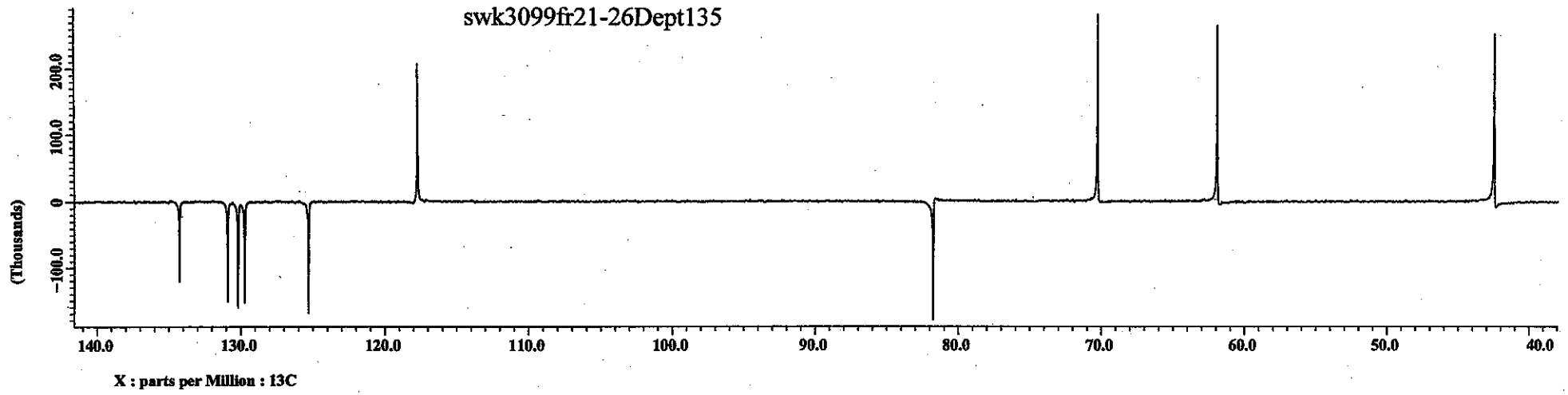

swk3099fr21_26_13C-6.jdf
OH
O
Br
(CDCl3, 67.5 MHz)
(Thousands)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
144.1398
134.0933
130.7317
130.0059
129.5628
125.1469
122.5493
117.5604
81.5916
77.4660
77.0000
76.5263
70.1088
61.7583
42.3147
X : parts per Million : 13C

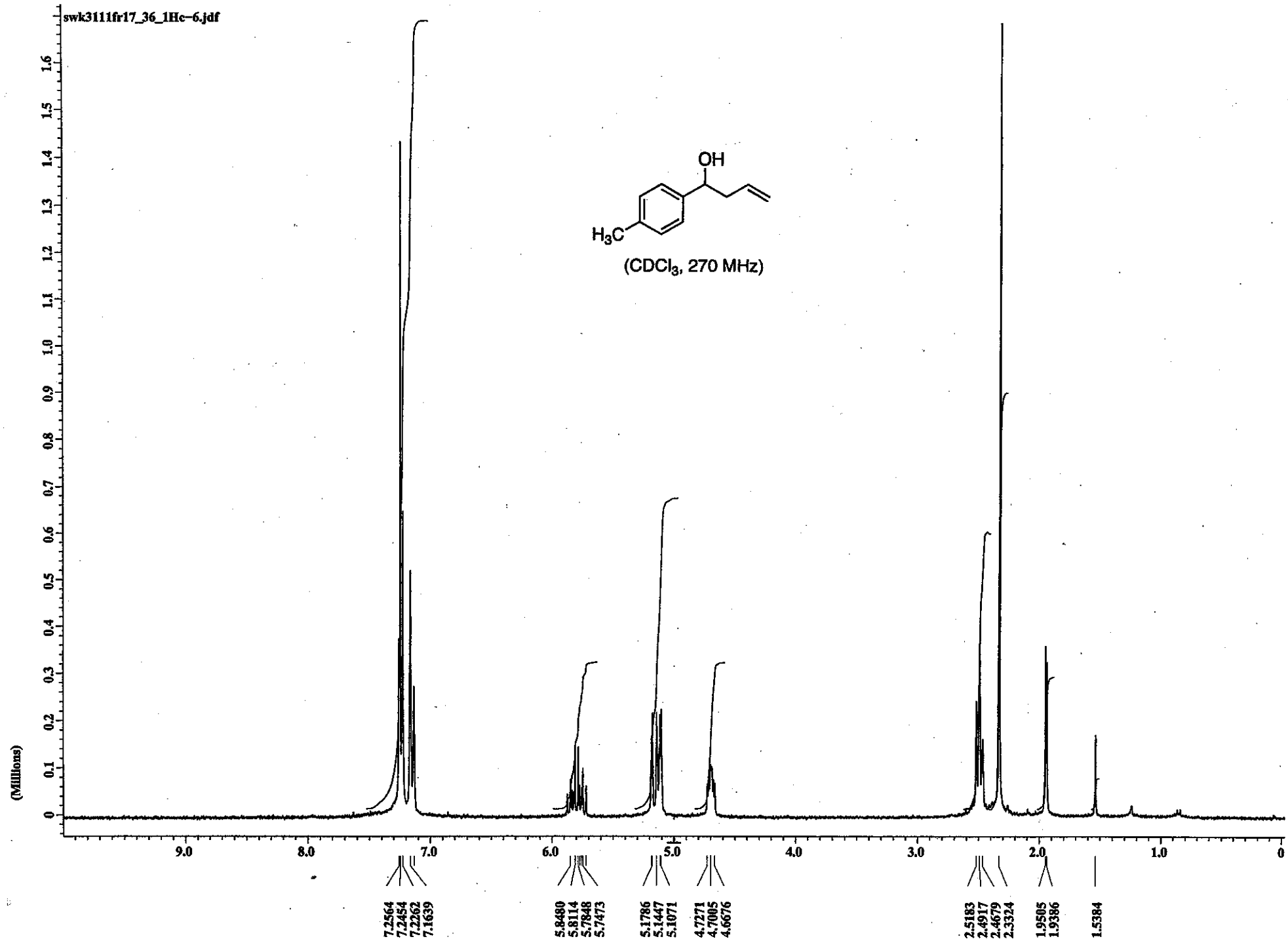

swk3099fr21_26_13C-8.jdf
(Thousands)
60.0
30.0
0
OH
O
Br
(CDCl3)
swk3099fr21_26_hetcor-2.jdf
swk3099fr21-26_1H-9.jdf
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
Y : parts per Million : 1H
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
X : parts per Million : 13C
0
1.0
2.0
3.0
4.0
5.0
(Millions)

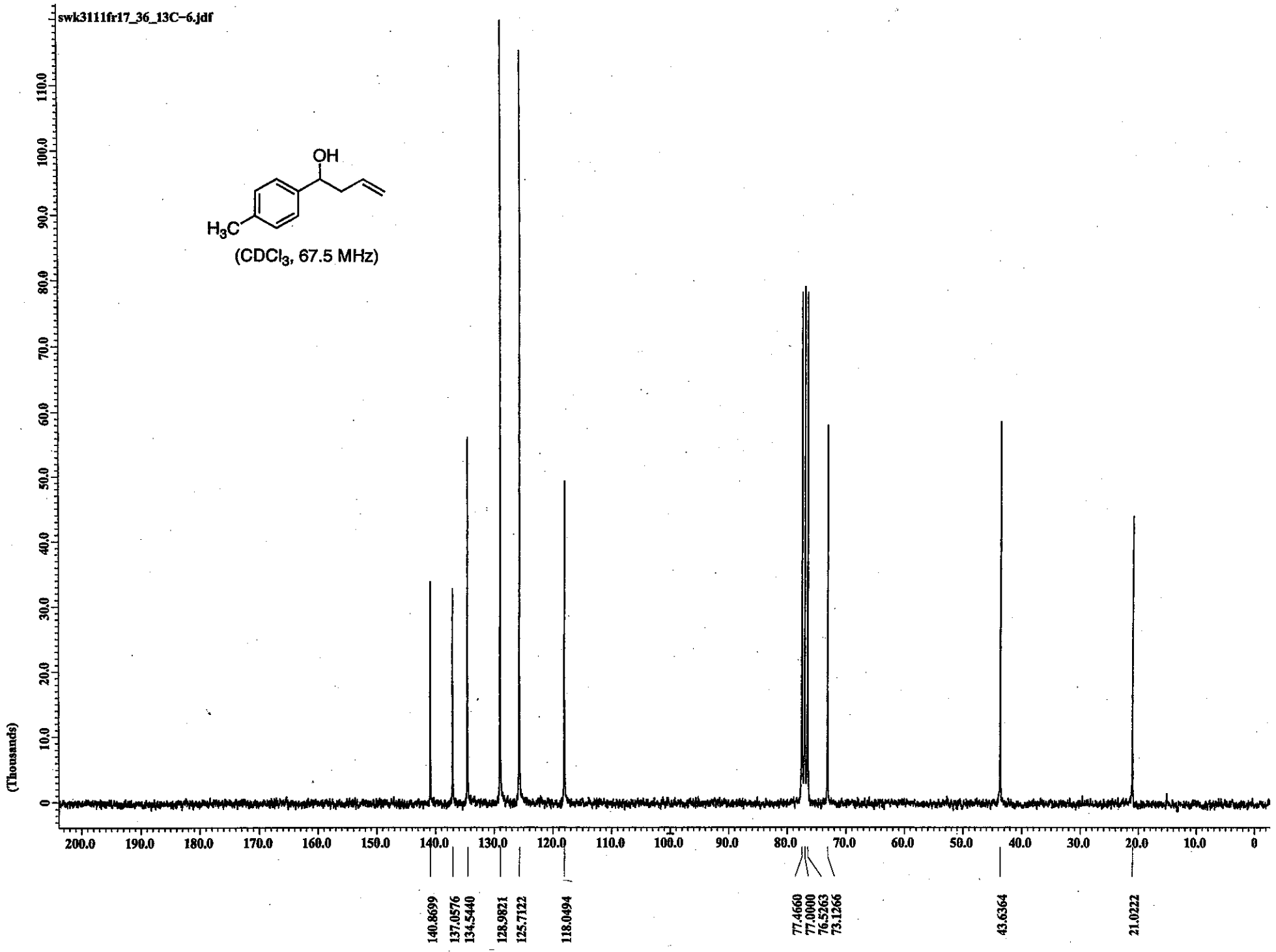

swk3099fr21-26_1H-9.jdf
(Millions)
OH
O
Br
(CDCl3)
swk3099fr21_26_cosy-2.jdf
swk3099fr21-26_1H-9.jdf
Y : parts per Million : 1H
X : parts per Million : 1H
(Millions)

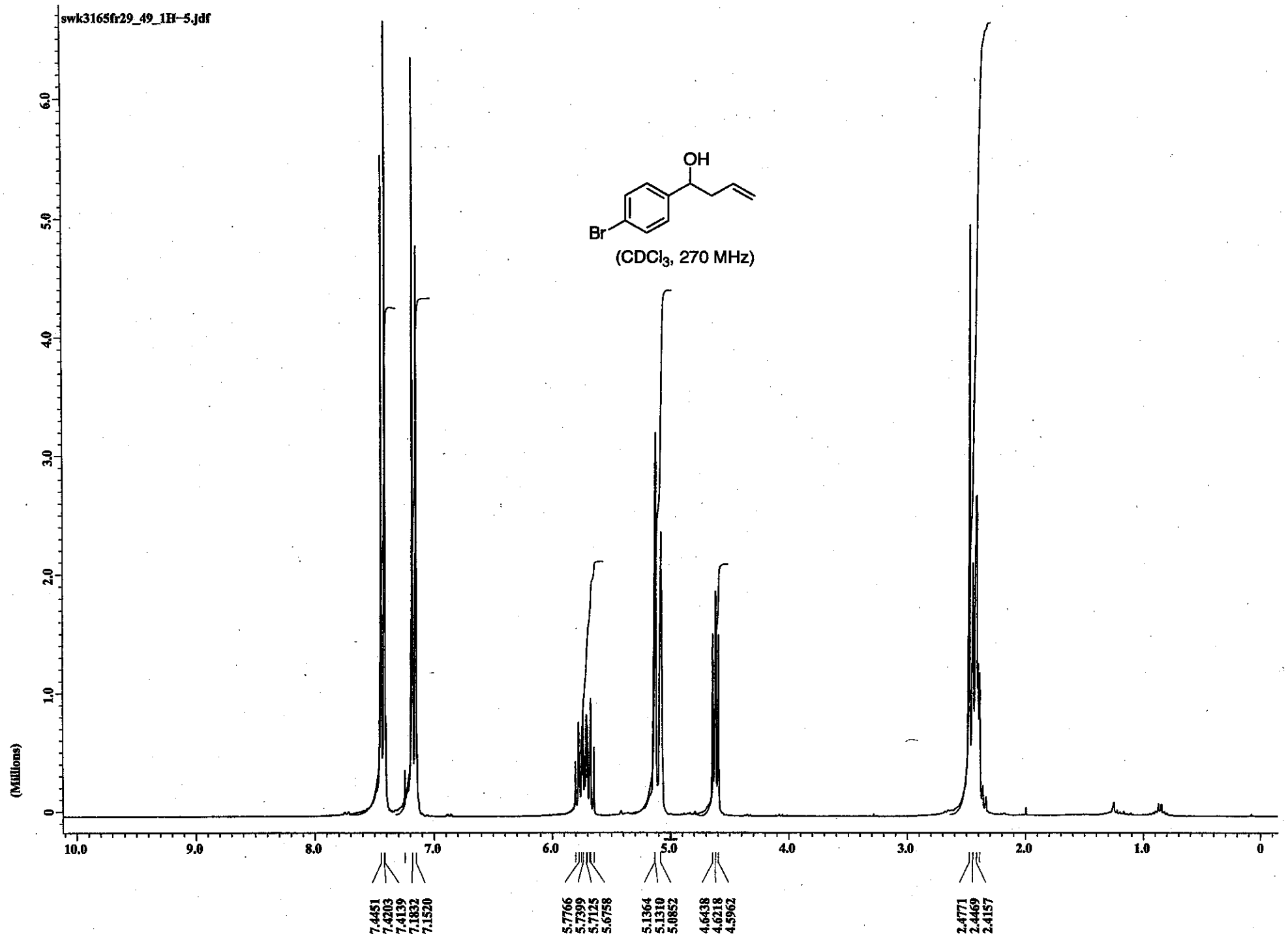

swk3099fr21-26Dept90
OH
O
Br
(CDCl3, 67.5 MHz)
(Thousands)
0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C

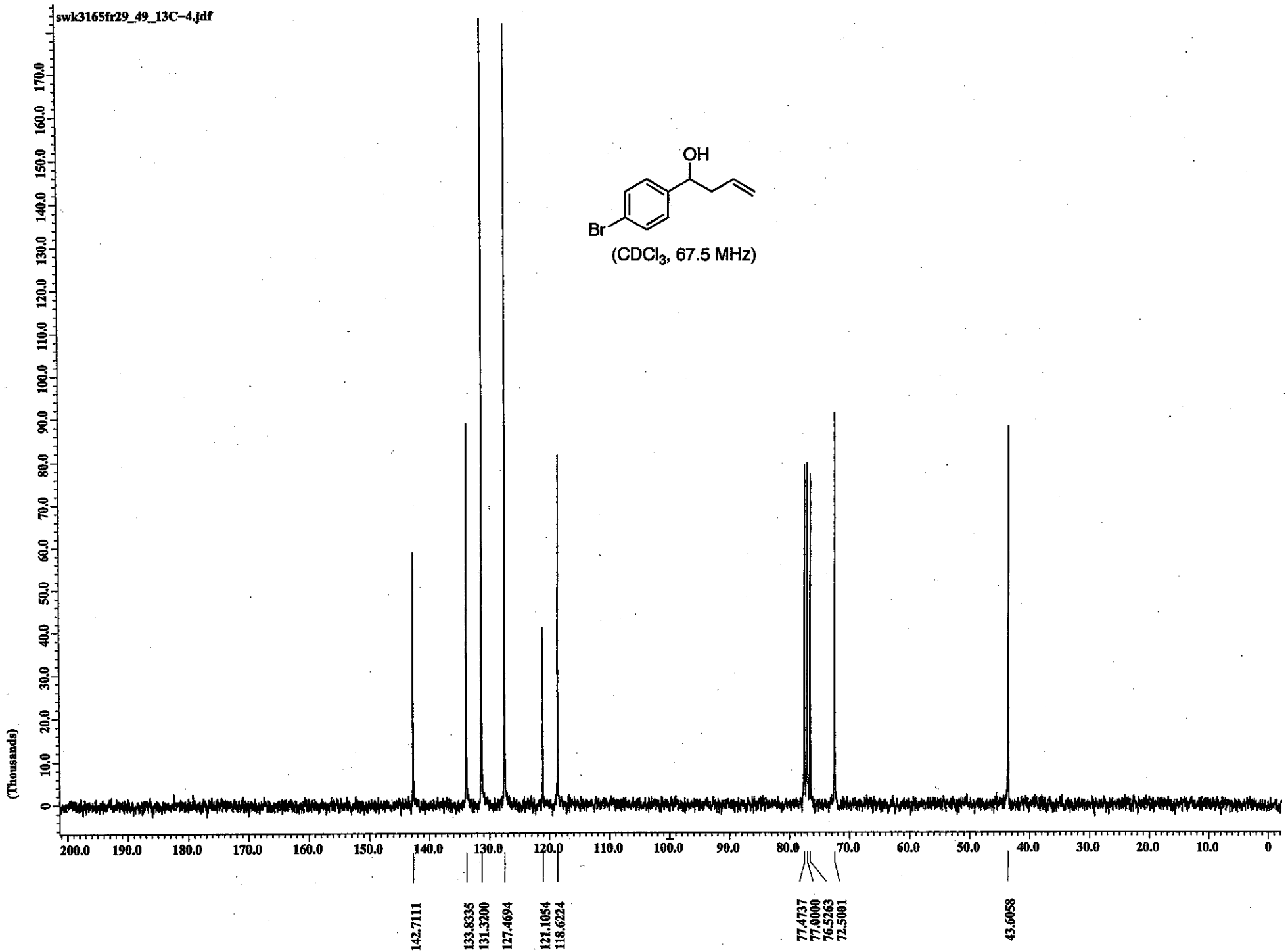

swk3099fr21-26Dept45
(Thousands)
0
100.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C

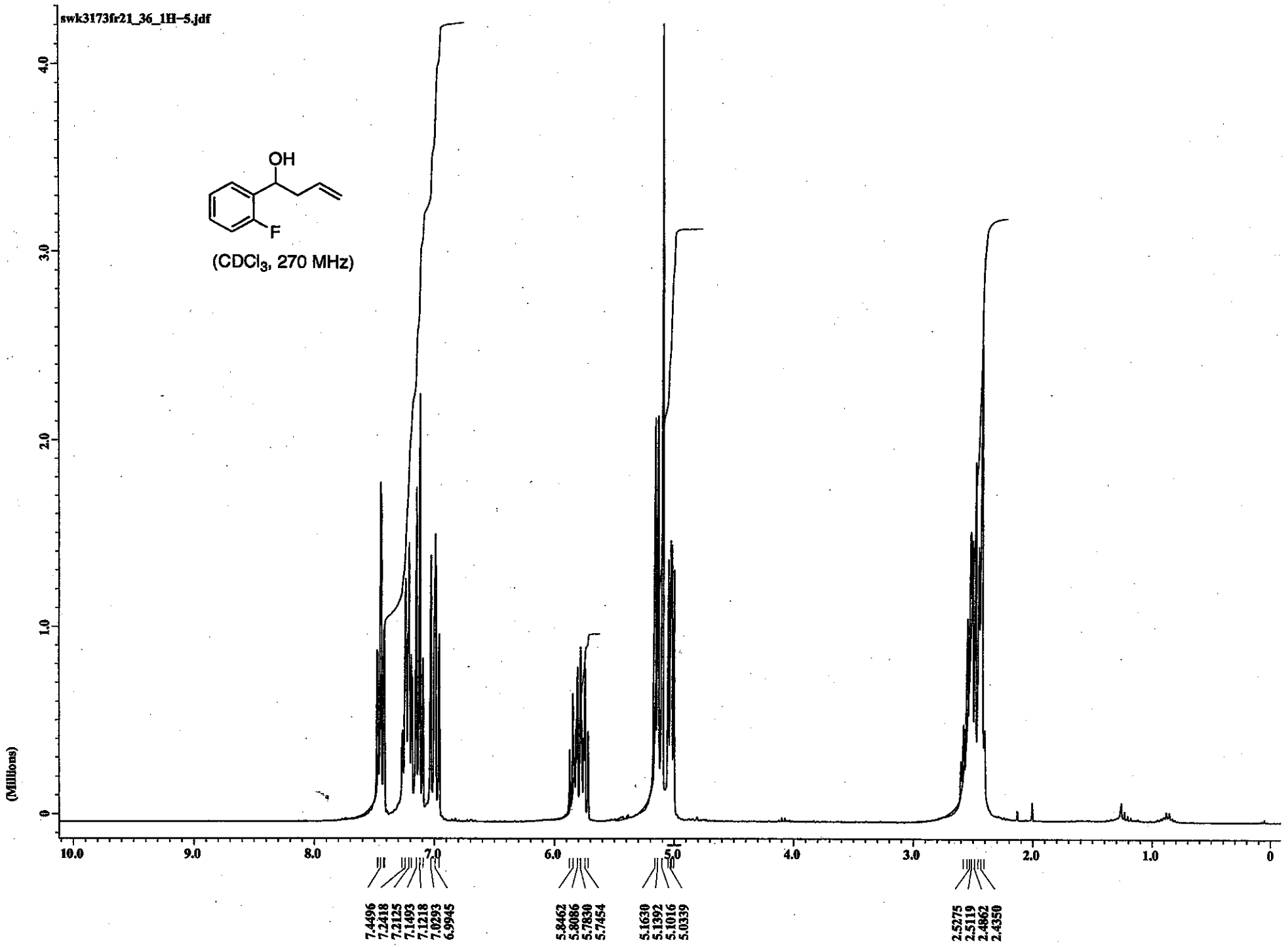

swk3099fr21-26Dept135
(Thousands)
-100.0
0
100.0
200.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
X : parts per Million : 13C

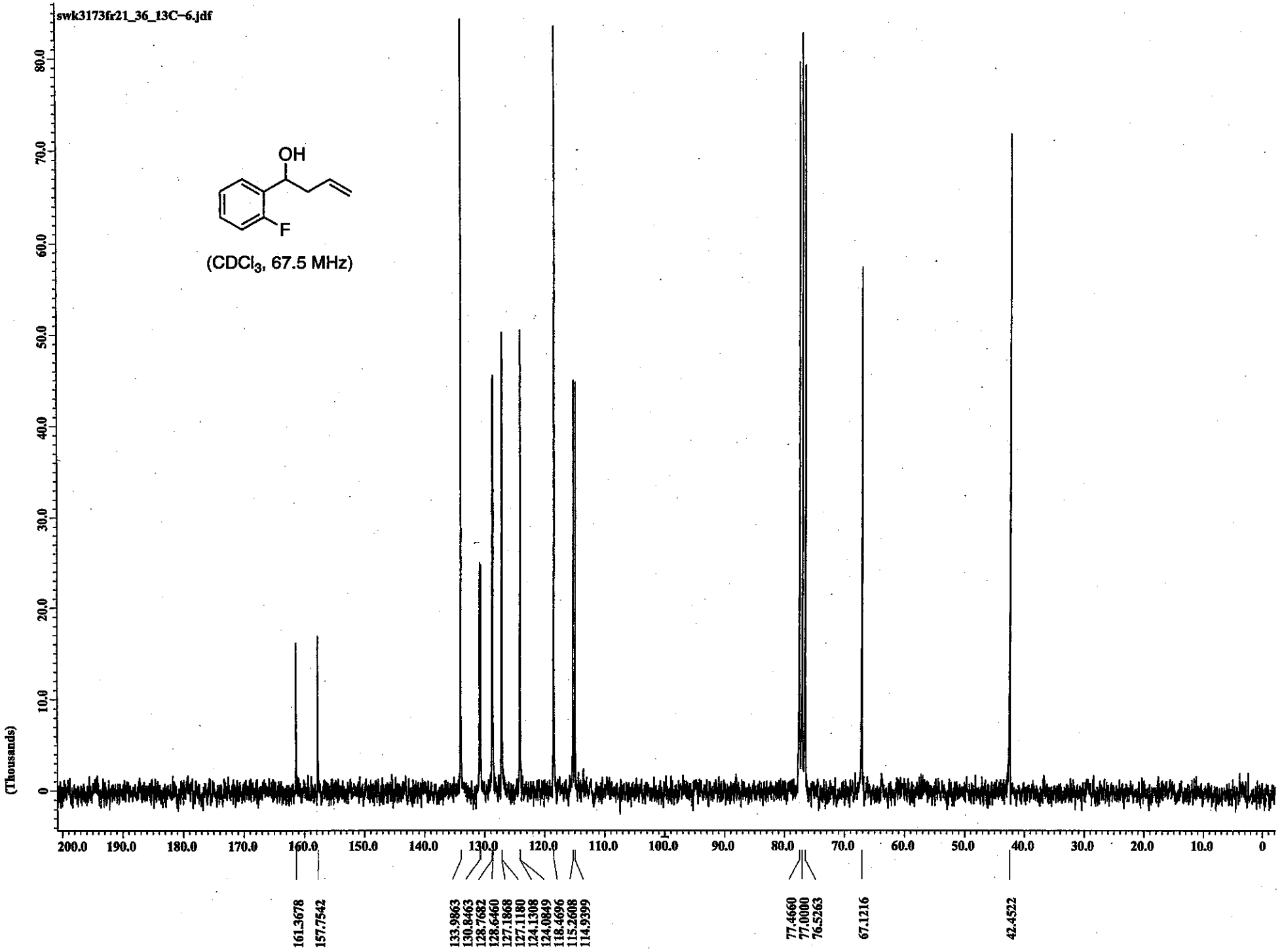

swk3111fr17_36_1Hc-6.jdf
OH
H3C
(CDCl3, 270 MHz)
(Millions)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2564
7.2454
7.2262
7.1639
5.8480
5.8114
5.7848
5.7473
5.1786
5.1447
5.1071
4.7271
4.7005
4.6676
2.5183
2.4917
2.4679
2.3324
1.9585
1.9386
1.5384
X : parts per Million : 1H


swk3111fr17_36_13C-6.jdf
OH
H3C
(CDCl3, 67.5 MHz)
(Thousands)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
140.8699
137.0576
134.5440
128.9821
125.7122
118.0494
77.4660
77.0000
76.5263
73.1266
43.6364
21.0222
X : parts per Million : 13C

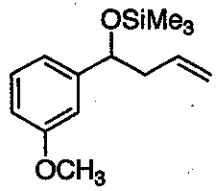

swk3165fr29_49_1H-5.jdf
OH
Br
(CDCl3, 270 MHz)
(Millions)
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4451
7.4203
7.4139
7.1832
7.1520
5.7766
5.7399
5.7125
5.6758
5.1364
5.1310
5.0852
4.6438
4.6218
4.5962
2.4771
2.4469
2.4157
X : parts per Million : 1H


swk3165fr29_49_13C-4.jdf
OH
Br
(CDCl3, 67.5 MHz)
(Thousands)
142.7111
133.8335
131.3200
127.4694
121.1054
118.6224
77.4737
77.0000
76.5263
72.5001
43.6058
X : parts per Million : 13C


swk3173fr21_36_1H-5.jdf
OH
F
(CDCl3, 270 MHz)
(Millions)
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4496
7.2418
7.2125
7.1493
7.1218
7.0293
6.9945
5.8462
5.8086
5.7830
5.7454
5.1630
5.1392
5.1016
5.0339
2.5275
2.5119
2.4862
2.4350
X : parts per Million : 1H


swk3173fr21_36_13C-6.jdf
OH
F
(CDCl3, 67.5 MHz)
(Thousands)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.3678
157.7542
133.9863
130.8463
128.7682
128.6460
127.1868
127.1180
124.1308
124.0849
118.4696
115.2608
114.9399
77.4660
77.0000
76.5263
67.1216
42.4522
X : parts per Million : 13C

swk3183fr7-9Car-4.jdf



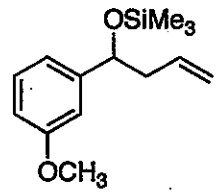
($CDCl_3$, 67.5 MHz)

(Thousands)

159.4808
146.5999
135.2545
129.0051
118.2633
116.7812
112.4188
111.3415
77.4737
77.0000
76.5340
74.7539
55.1192
45.0345
0.1117

X : parts per Million : 13C

swk3183fr7-9H-4.jdf



($CDCl_3$, 270 MHz)

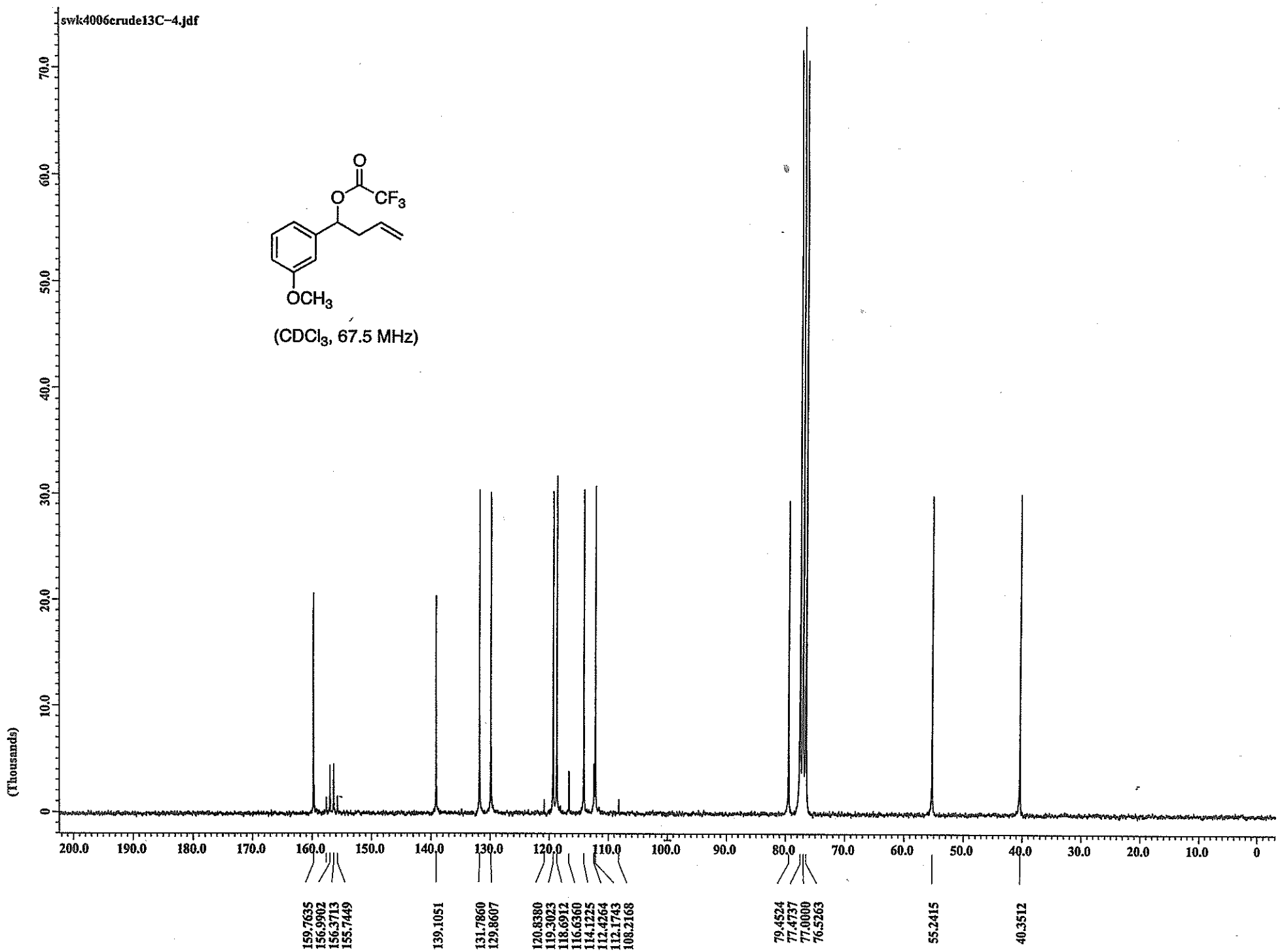
(Millions)

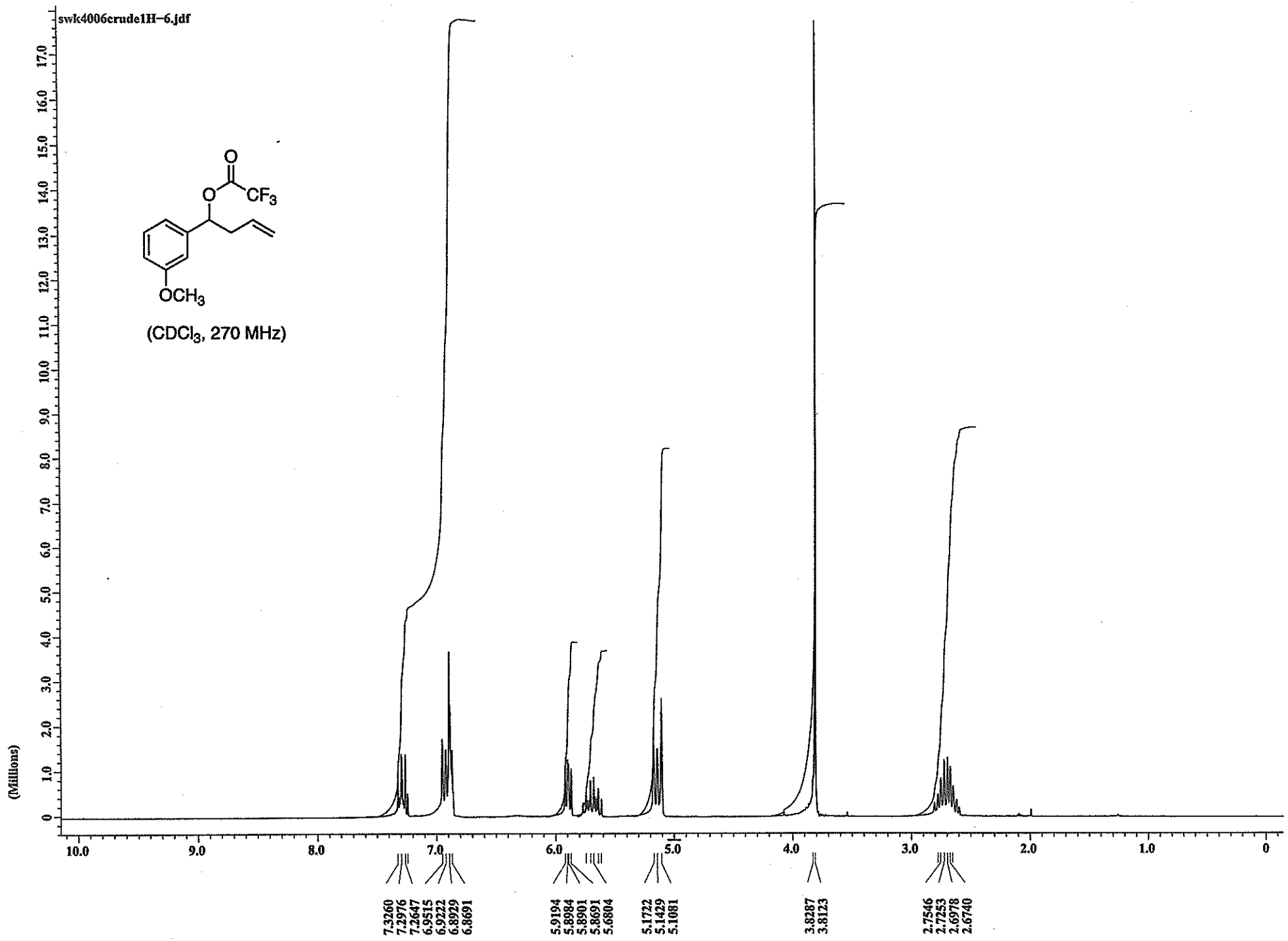
50.0
40.0
30.0
20.0
10.0
0

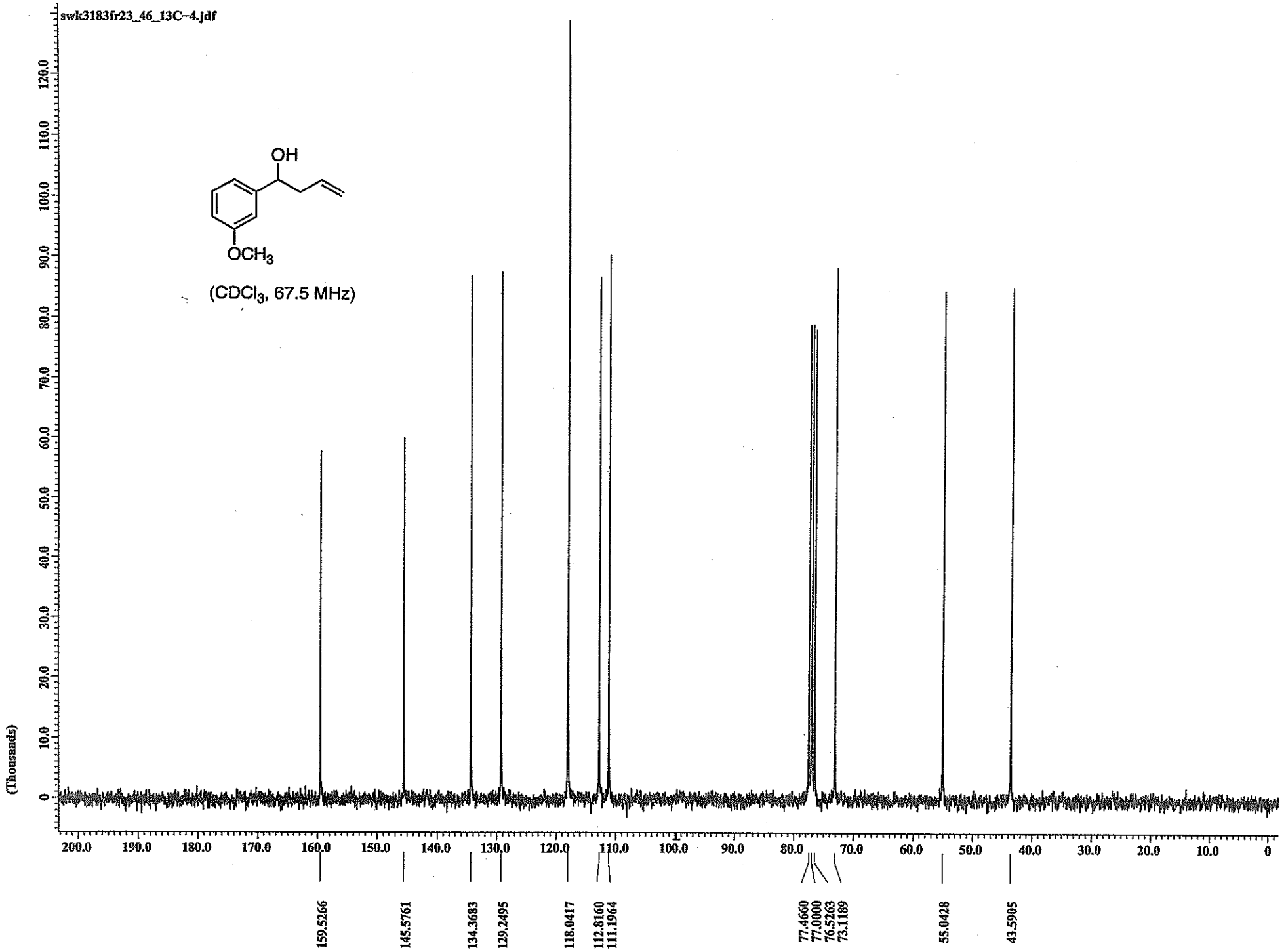
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0

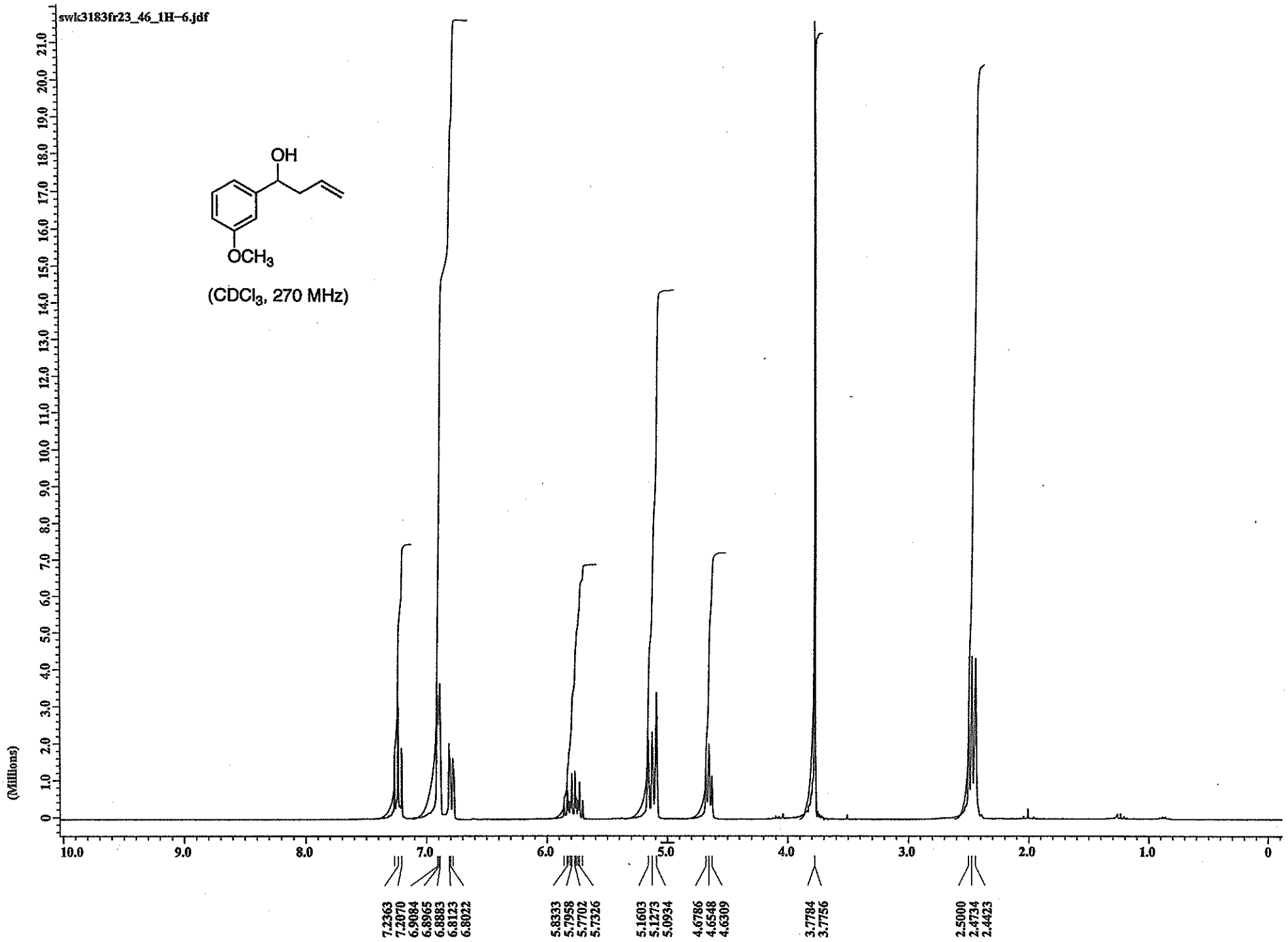
7.2454
7.2180
7.1887
6.8910
6.8645
6.7958
6.7885
5.8288
5.7912
5.7647
5.7271
5.0714
5.0073
5.0037
4.6703
4.6502
4.6429
3.8443
3.8031
3.7765
2.4734
2.4460
2.4194
2.3928
1.2628
0.0943
0.0824
0.0650
0.0531
0.0403

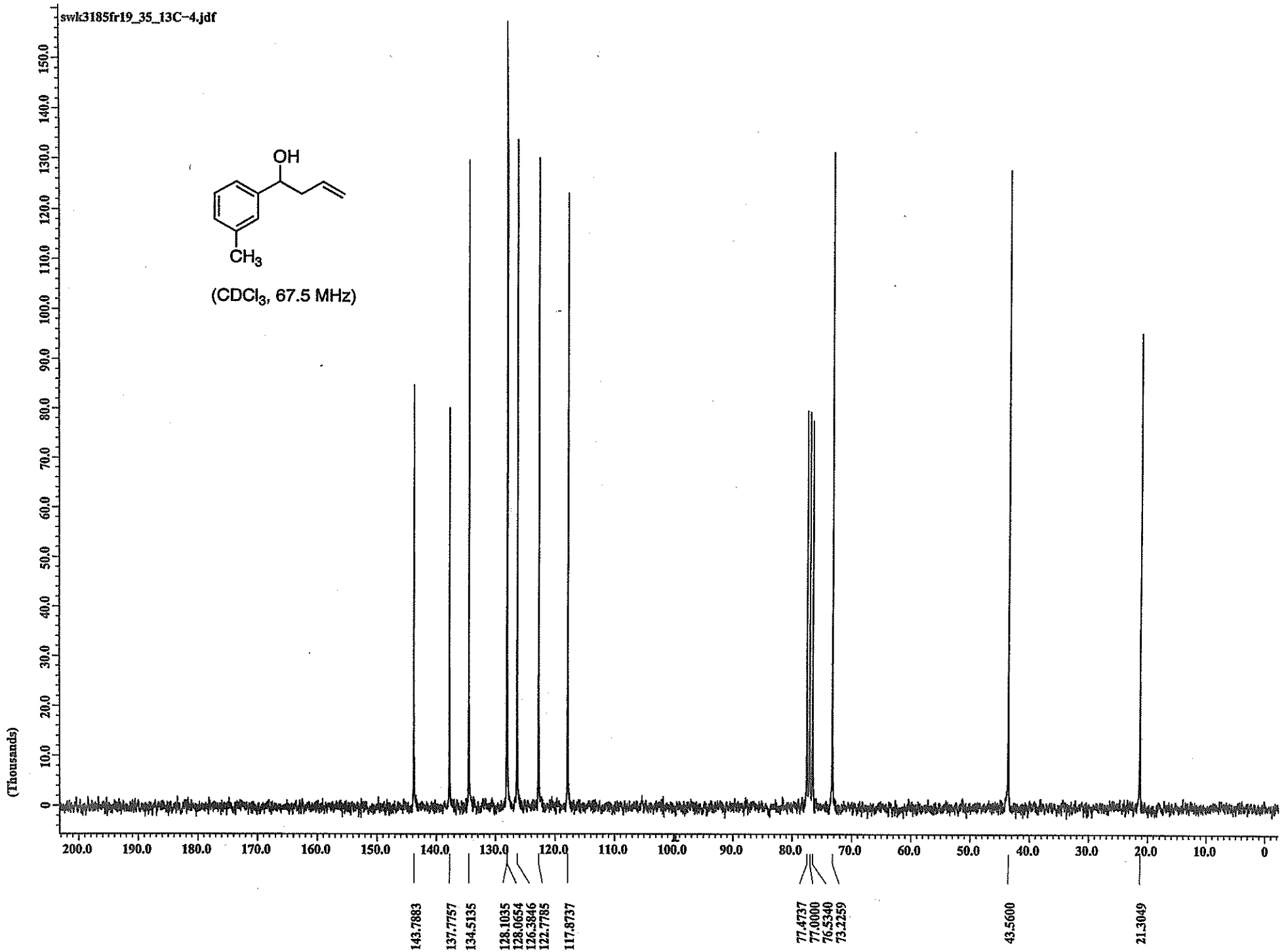
X : parts per Million : 1H

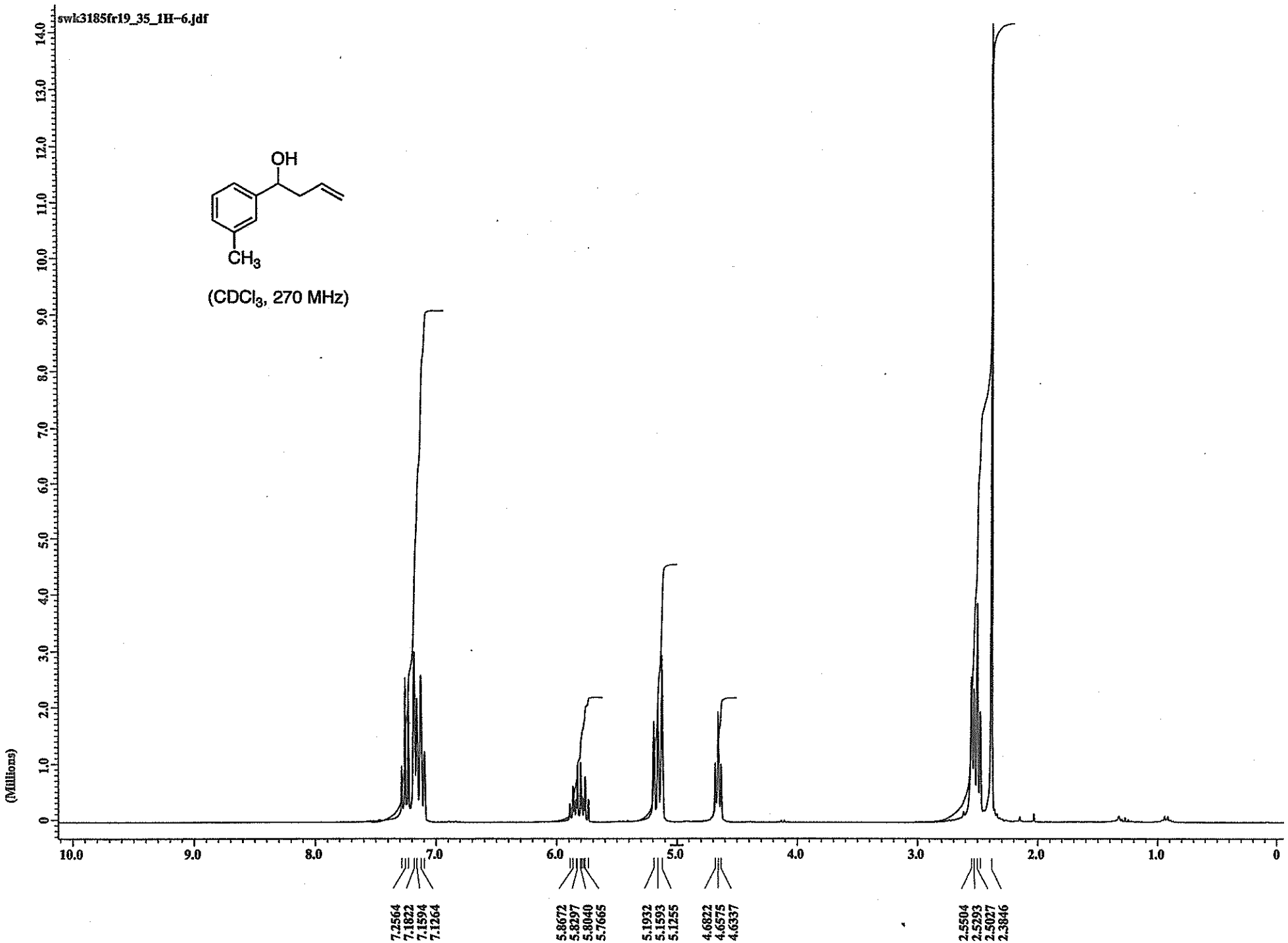

swk4006crude13C-4.jdf
O
O
CF3
OCH3
(CDCl3, 67.5 MHz)
(Thousands)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.7635
156.9902
156.3713
155.7449
139.1051
131.7860
129.8607
120.8380
119.3023
118.6912
116.6360
114.1225
112.4264
112.1743
108.2168
79.4524
77.4737
77.0000
76.5263
55.2415
40.3512
X : parts per Million : 13C


swk4006crude1H-6.jdf
O
O
CF3
OCH3
(CDCl3, 270 MHz)
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.3260
7.2976
7.2647
6.9515
6.9222
6.8929
6.8691
5.9194
5.8984
5.8901
5.8691
5.6804
5.1722
5.1429
5.1081
3.8287
3.8123
2.7546
2.7253
2.6978
2.6740
X : parts per Million : 1H


swk3183fr23_46_13C-4.jdf
OH
OCH3
(CDCl3, 67.5 MHz)
(Thousands)
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.5266
145.5761
134.3683
129.2495
118.0417
112.8160
111.1964
77.4660
77.0000
76.5263
73.1189
55.0428
43.5905
X : parts per Million : 13C


swlc3183fr23_46_1H-6.jdf
OH
OCH3
(CDCl3, 270 MHz)
(Millions)
X : parts per Million : 1H
7.2363
7.2070
6.9084
6.8965
6.8883
6.8123
6.8022
5.8333
5.7958
5.7702
5.7326
5.1603
5.1273
5.0934
4.6786
4.6548
4.6309
3.7784
3.7756
2.5000
2.4734
2.4423


swk3185fr19_35_13C-4.jdf
OH
CH3
(CDCl3, 67.5 MHz)
(Thousands)
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
143.7883
137.7757
134.5135
128.1035
128.0654
126.3846
122.7785
117.8737
77.4737
77.0000
76.5340
73.2259
43.5600
21.3049
X : parts per Million : 13C


swk3185fr19_35_1H-6.jdf
OH
CH3
(CDCl3, 270 MHz)
(Millions)
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
H
7.2564
7.1822
7.1594
7.1264
5.8672
5.8297
5.8040
5.7665
5.1932
5.1593
5.1255
4.6822
4.6575
4.6337
2.5504
2.5293
2.5027
2.3846
X : parts per Million : 1H