

Supporting information

Synthesis of β,β -Disubstituted Indanones via Pd-Catalyzed Tandem Conjugate Addition/Cyclization Reaction of Arylboronic acids with α,β -Unsaturated Esters

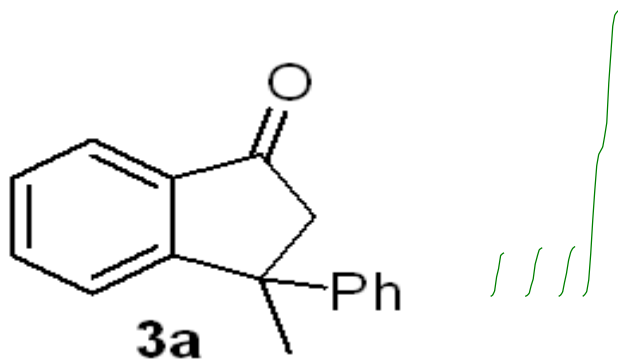
Ang Gao,[†] Xiu-Yan Liu,[†] Hao Li,[†] Chang-Hua Ding,^{*,†} and Xue-Long Hou^{*,†,‡}

[†]State Key Laboratory of Organometallic Chemistry, [‡]Shanghai–Hong Kong Joint Laboratory in Chemical Synthesis, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, China.

xlhou@sioc.ac.cn; dingch@sioc.ac.cn

Table of Contents

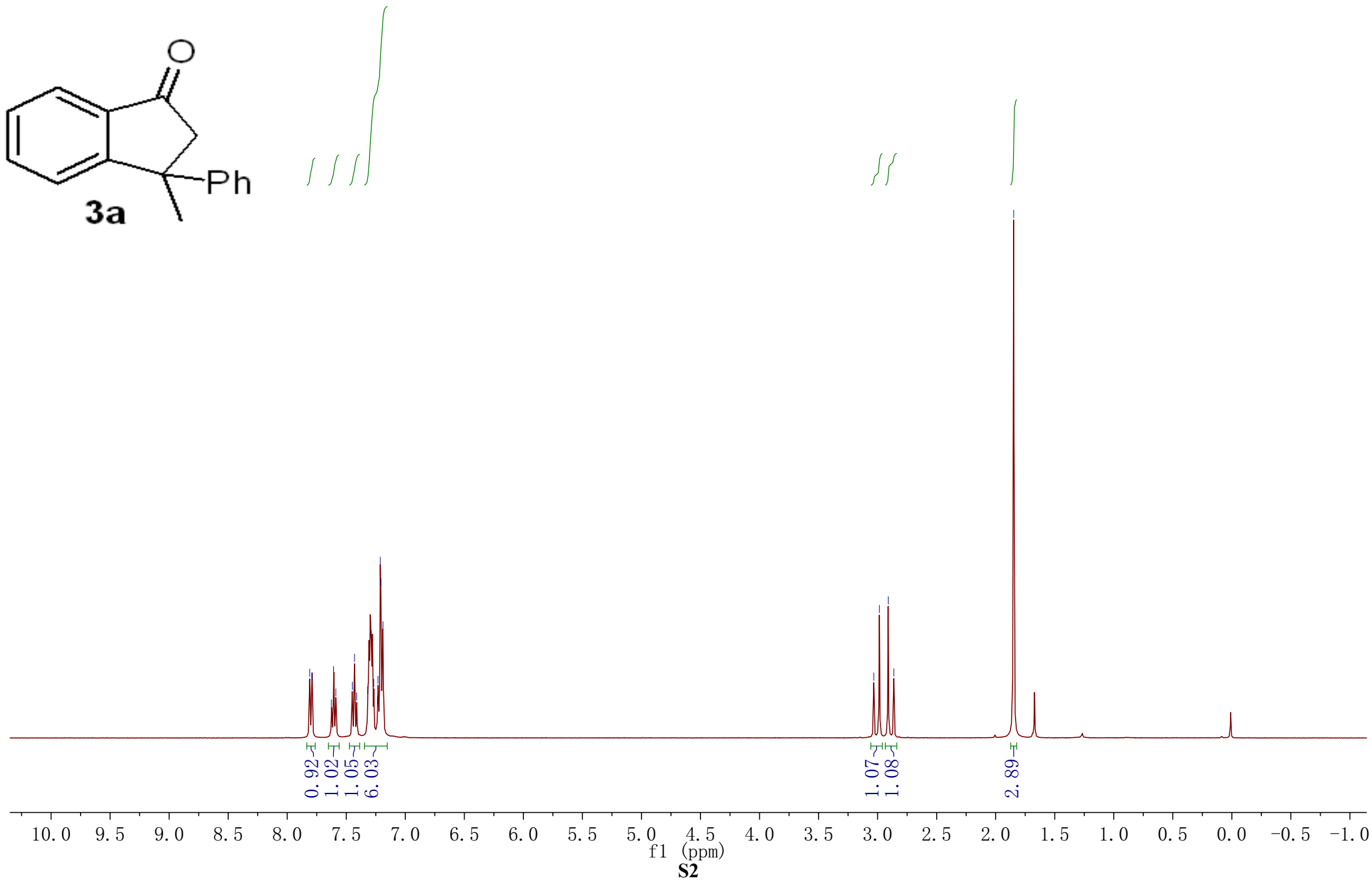
1. NMR Spectra	S2
-----------------------------	-----------

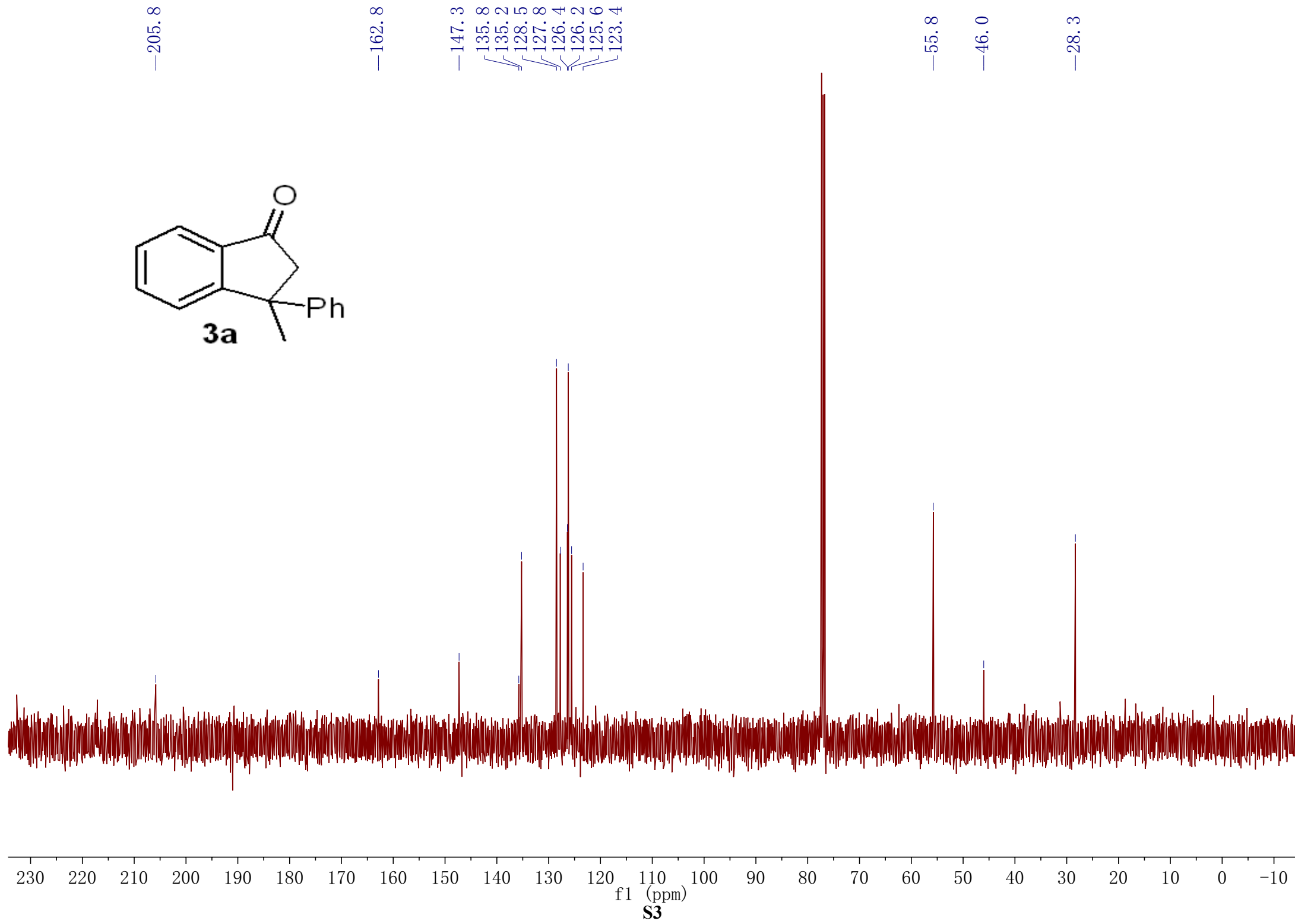
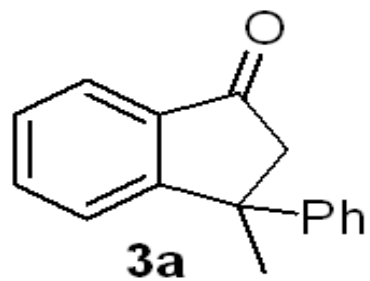


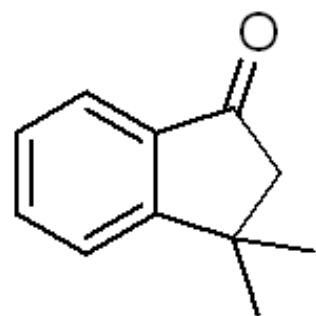
7.81
7.79
7.63
7.61
7.59
7.45
7.43
7.41
7.32
7.29
7.27
7.23
7.23
7.21
7.21
7.19

3.03
2.98
2.91
2.86

1.85







3b

7.69
7.67
7.62
7.60
7.58
7.49
7.47
7.37
7.35
7.33

0.87
0.98
1.05
1.12

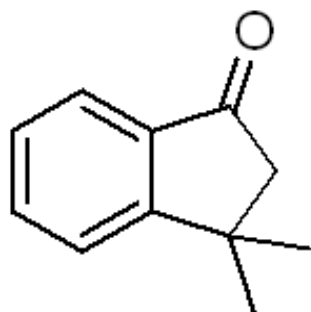
1.98

6.14

1.41

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)
S4



3b

—205.8

—163.8

—135.2

—134.9

—127.3

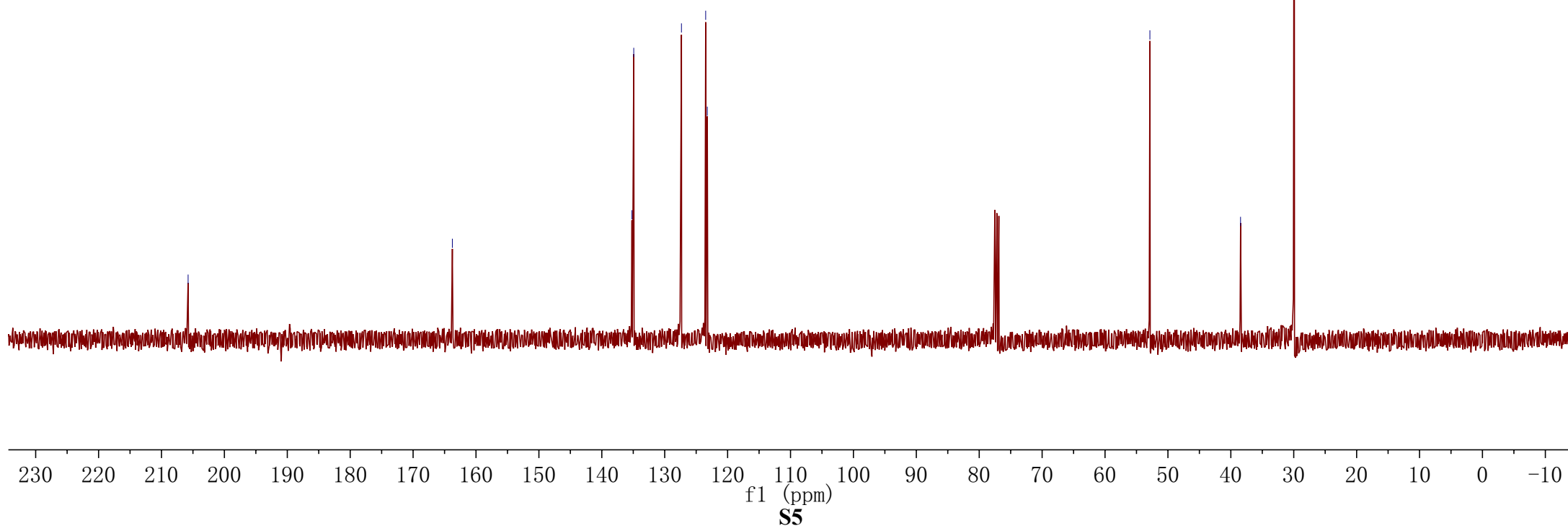
—123.5

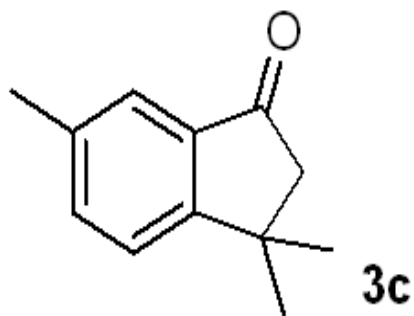
—123.2

—52.9

—38.5

—29.9





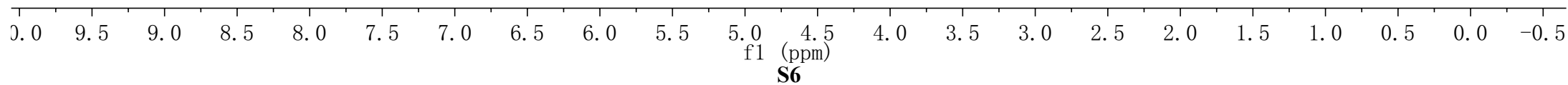
7.48
7.44
7.42
7.39
7.37

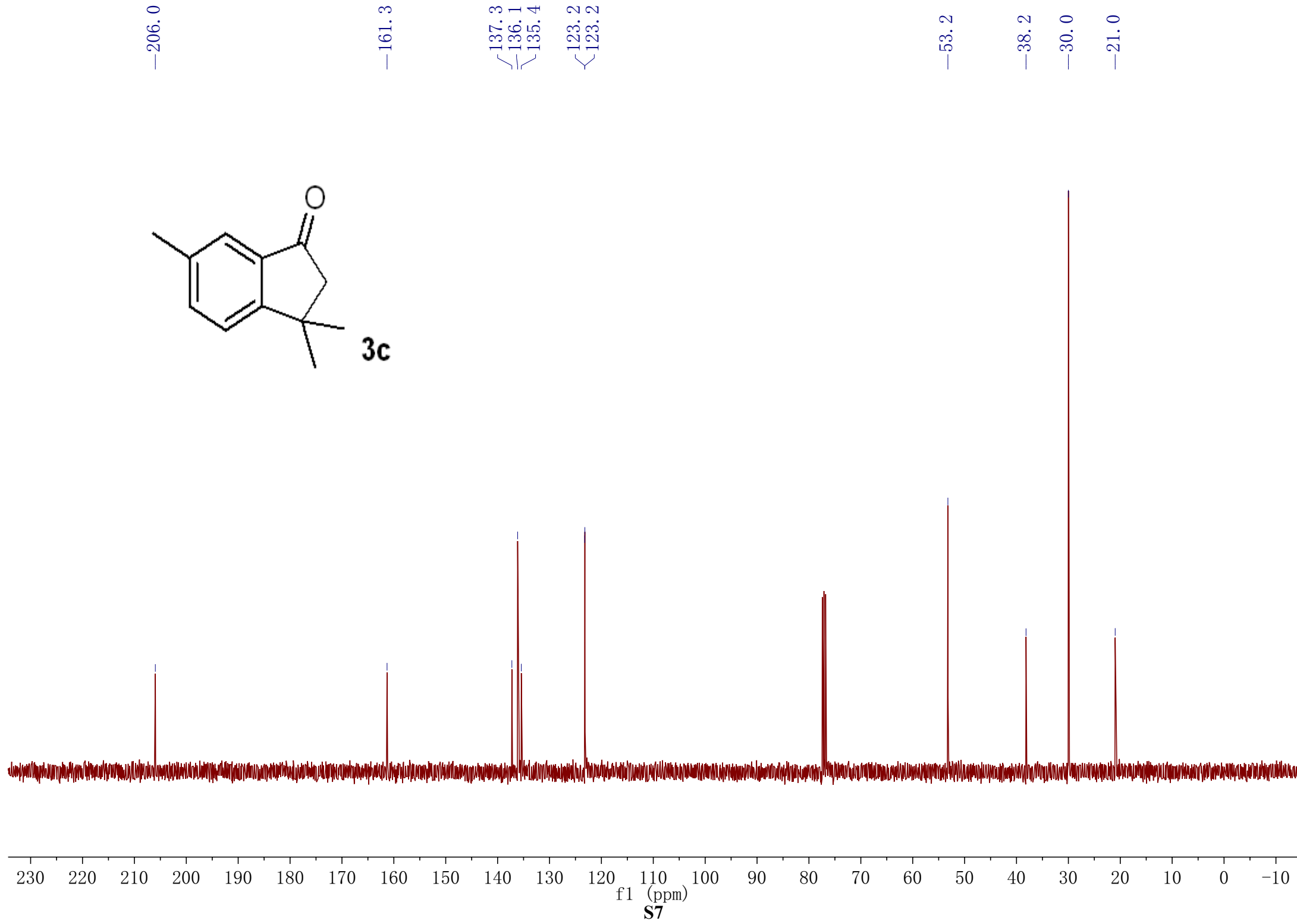
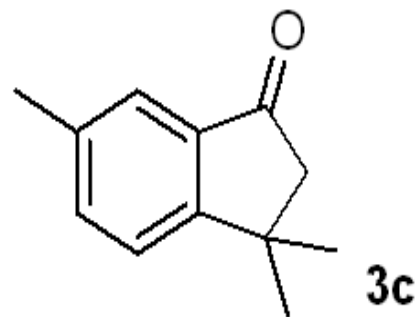


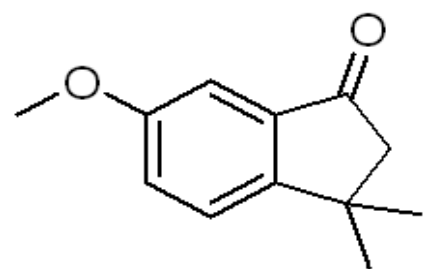
2.57
2.39



1.39



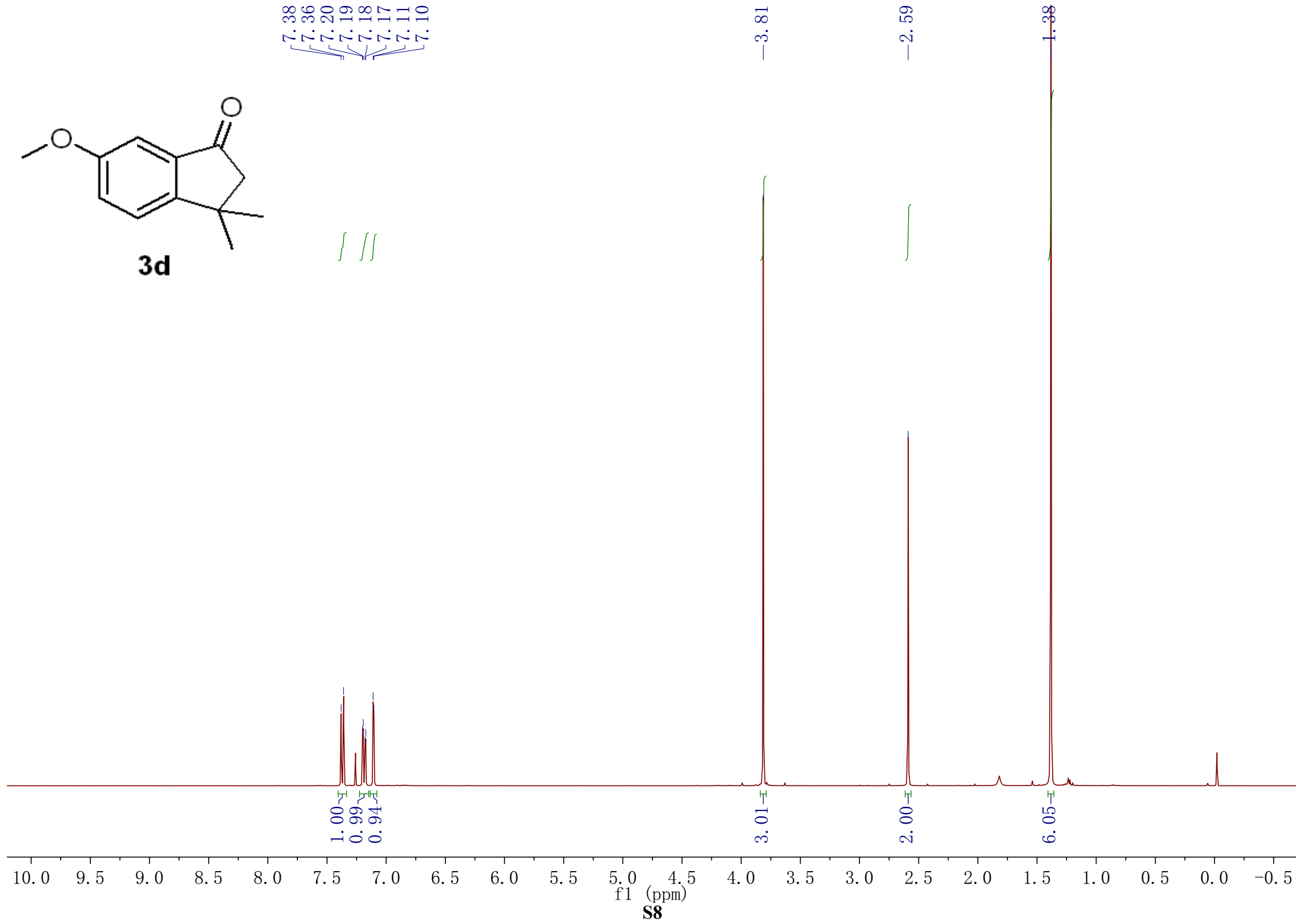


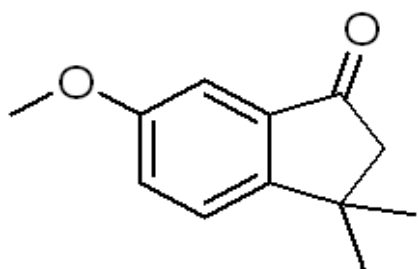


3d

7.38
7.36
7.20
7.19
7.18
7.17
7.11
7.10

7.38
7.36
7.20
7.19
7.18
7.17
7.11
7.10





3d

—205.6

~159.3

~156.7

—136.4

124.3

124.1

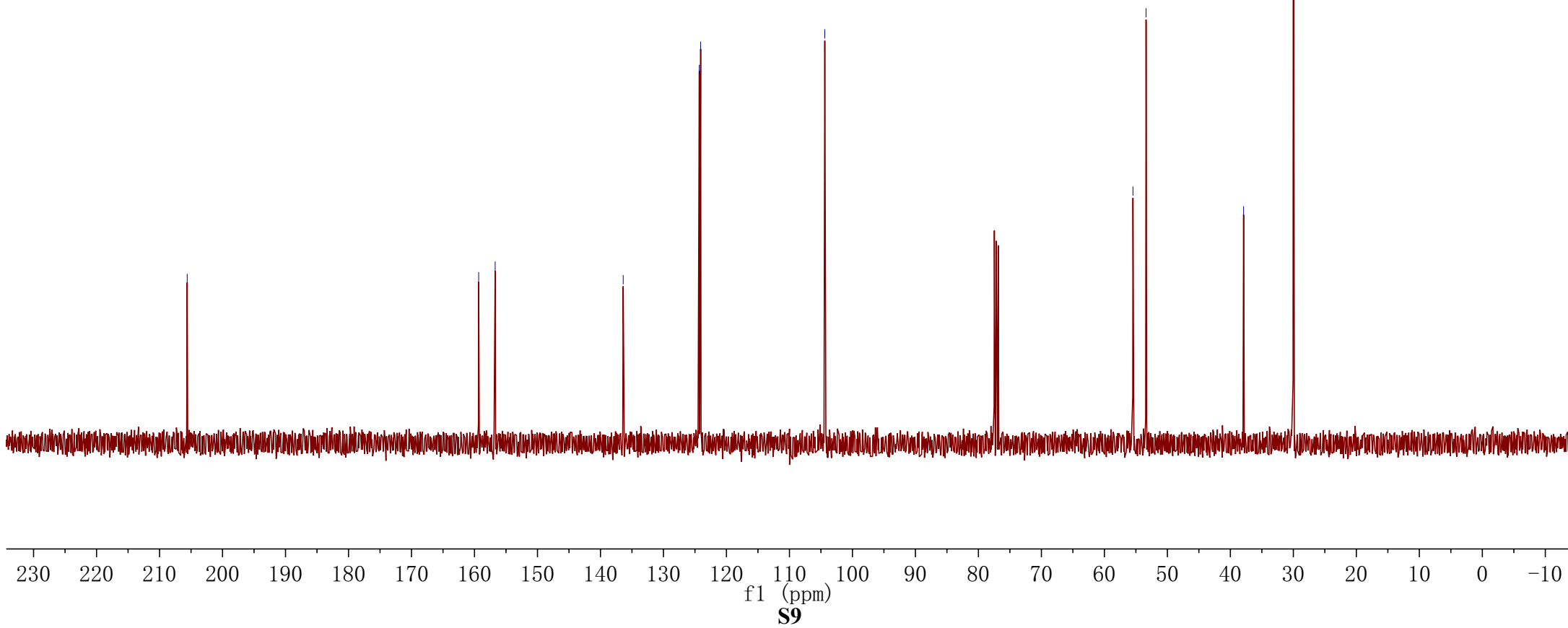
—104.4

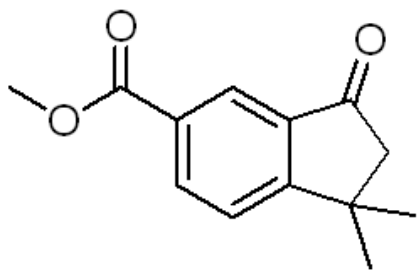
~55.5

~53.4

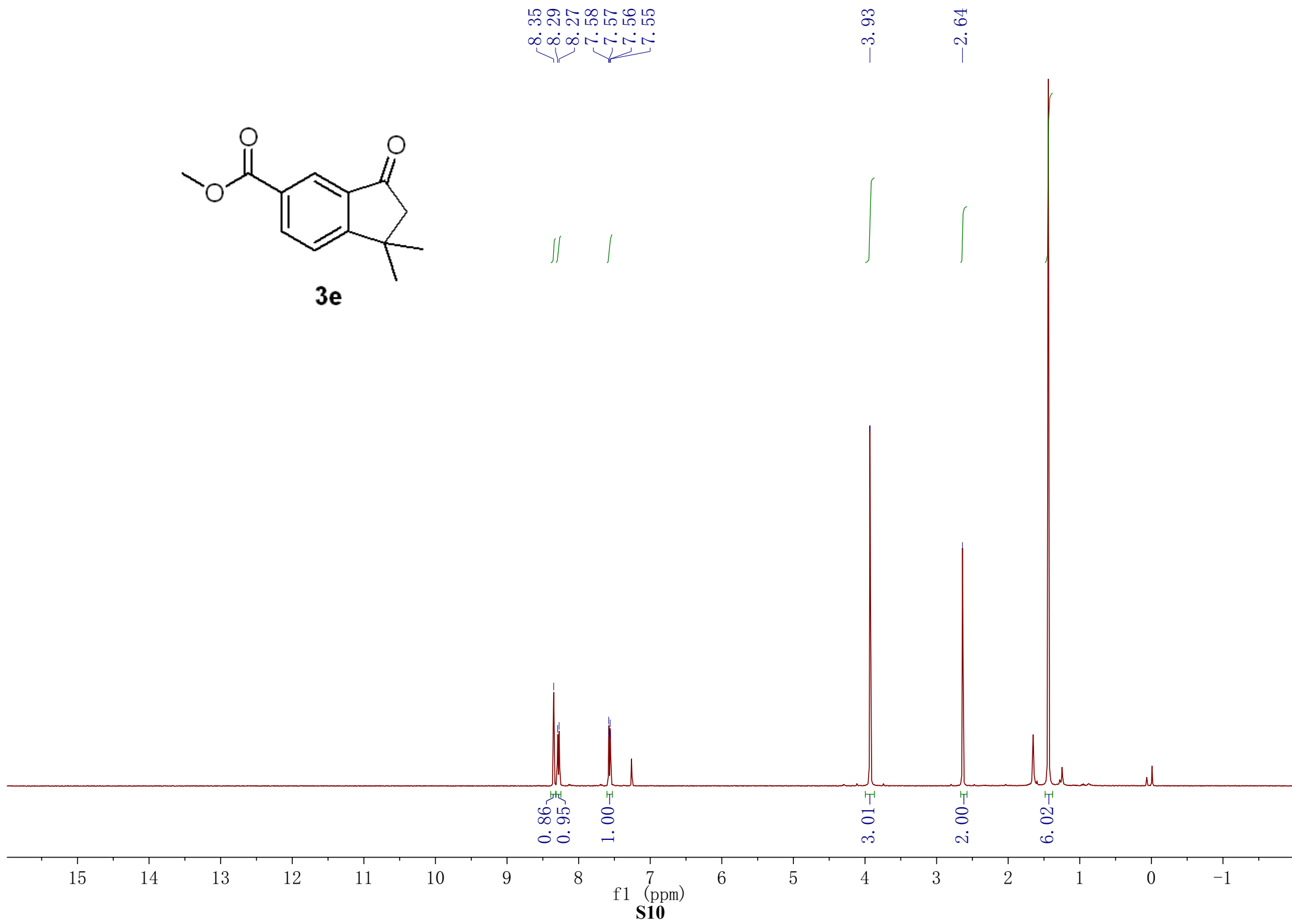
—37.9

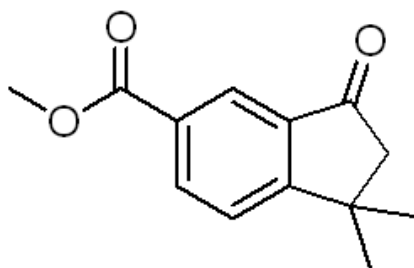
—30.0





3e





3e

—204.8

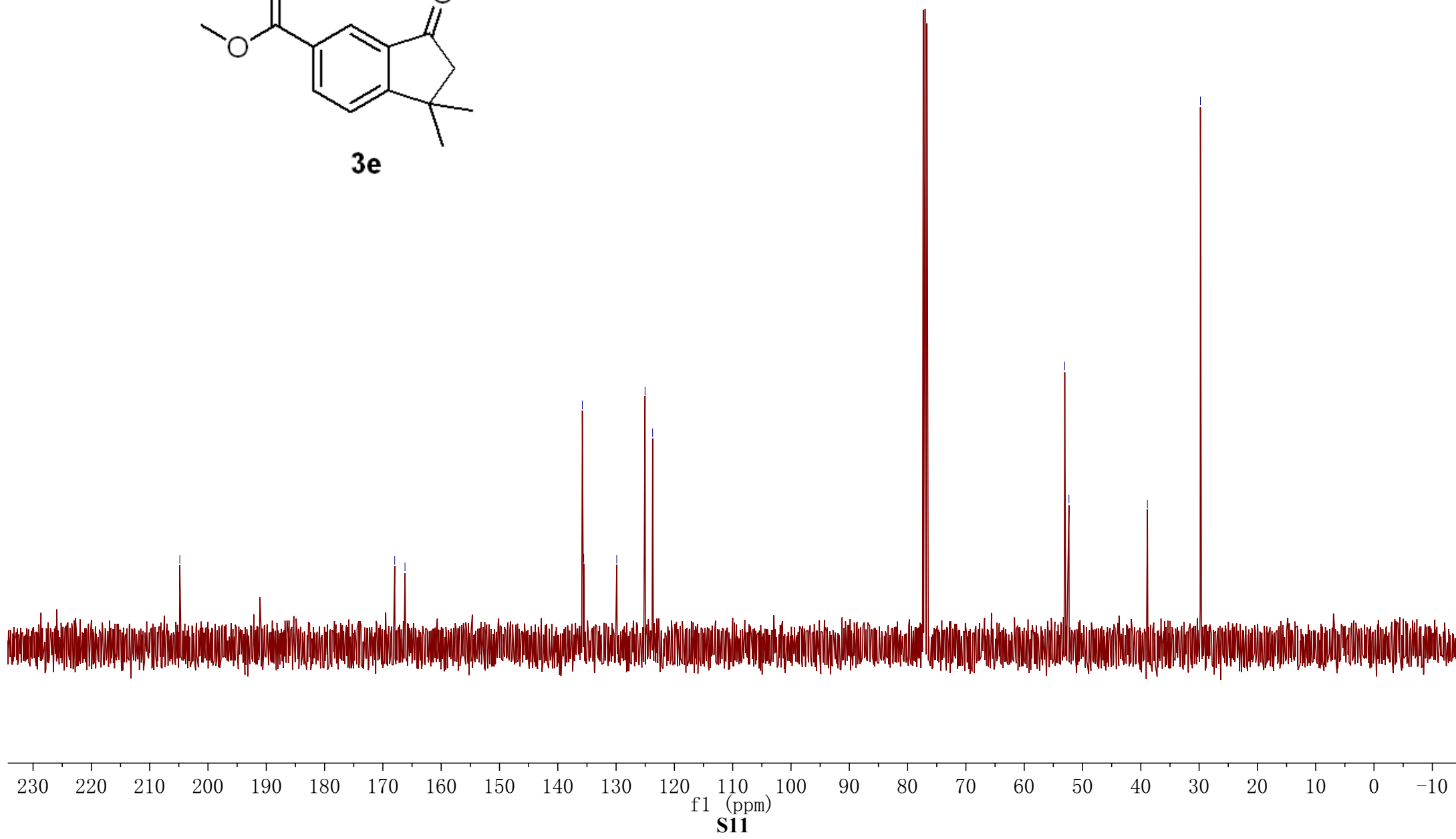
—168.0
—166.2

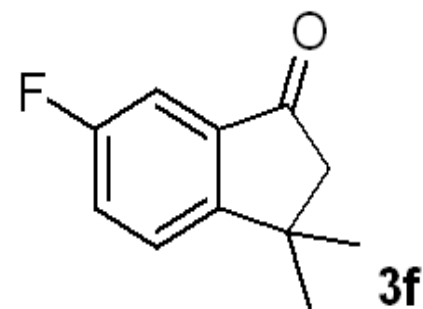
—135.8
—135.5
—129.9
—125.0
—123.7

—53.0
—52.3

—38.9

—29.8





7.47
7.46
7.46
7.45
7.44
7.33
7.32
7.31
7.30
7.30
7.29
7.28

1.00
1.88

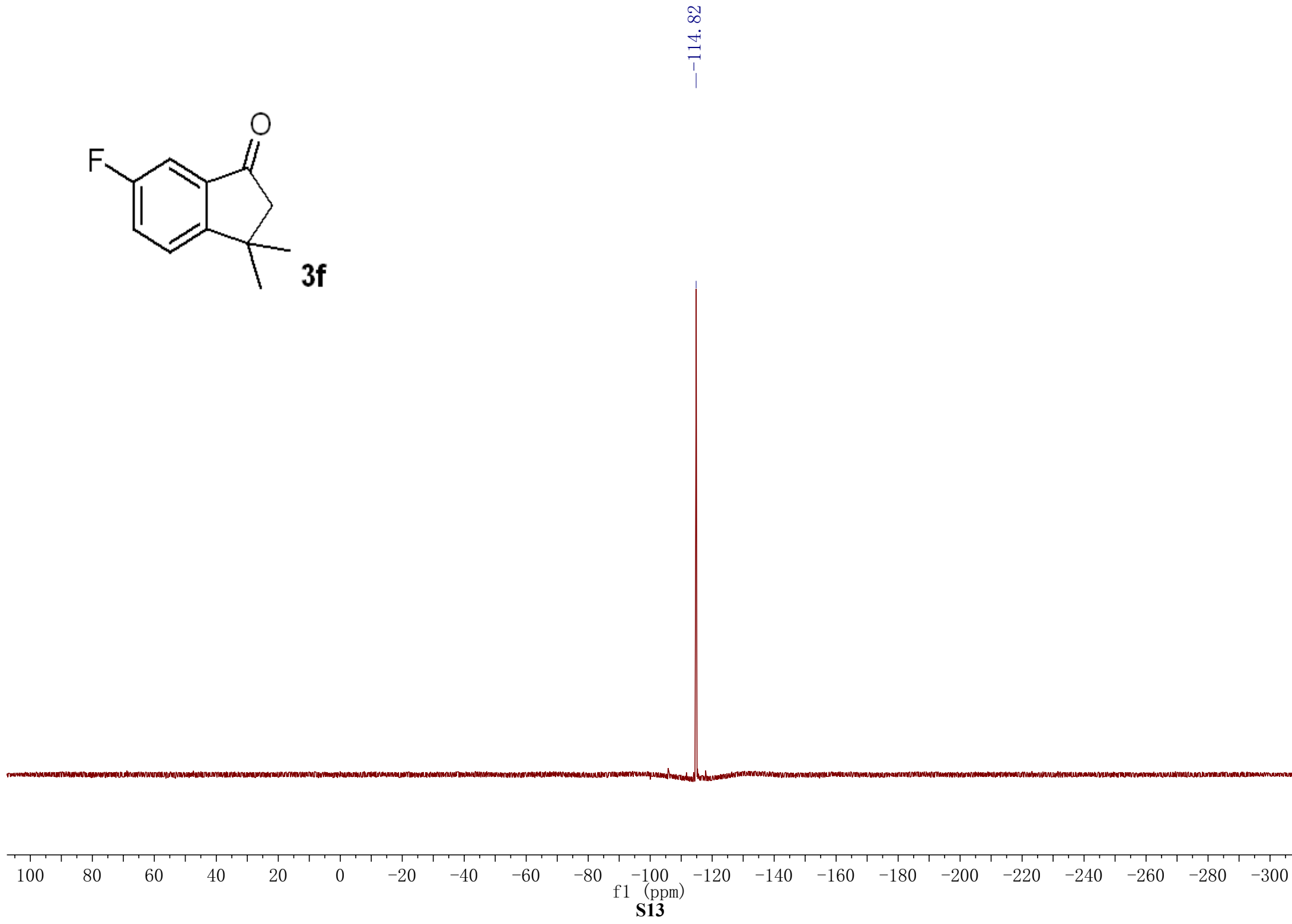
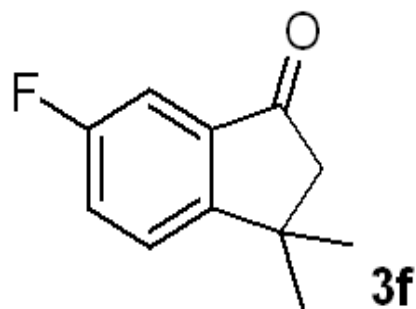
2.00

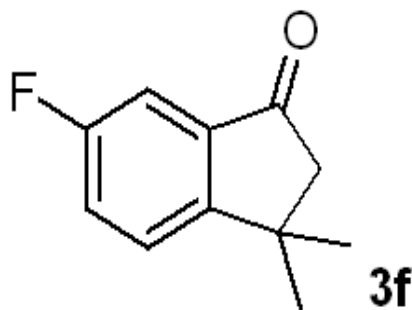
6.16

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

S12





204.6
204.5

163.5
161.0
159.3
159.3

137.1
137.0

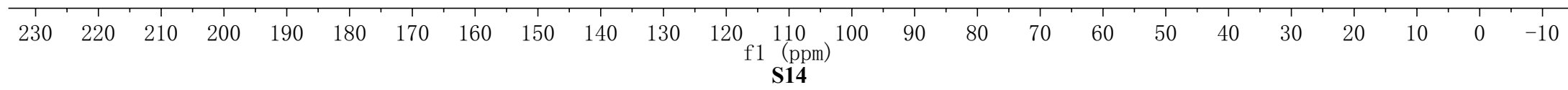
125.2
125.1
122.6
122.4

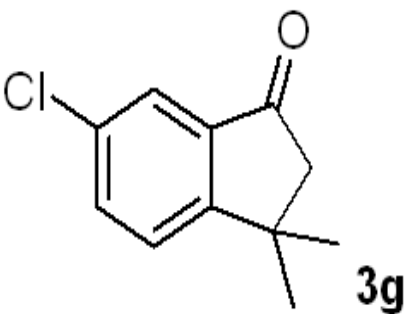
109.0
108.8

53.3

38.2

30.0



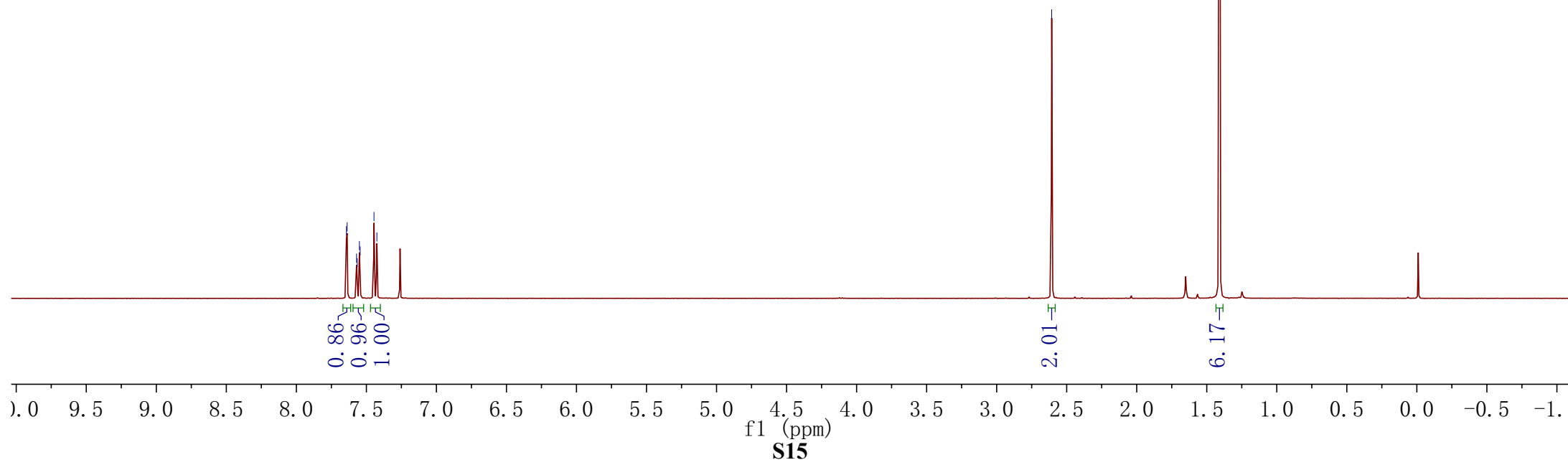


7.64
7.64
7.57
7.57
7.55
7.54
7.45
7.43

|||

2.61

1.41



—204.4

—161.9

∠136.8

∠134.9

∠133.8

∠124.9

∠123.1

∠77.6

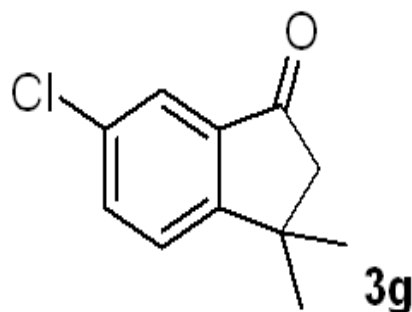
∠76.7

∠76.4

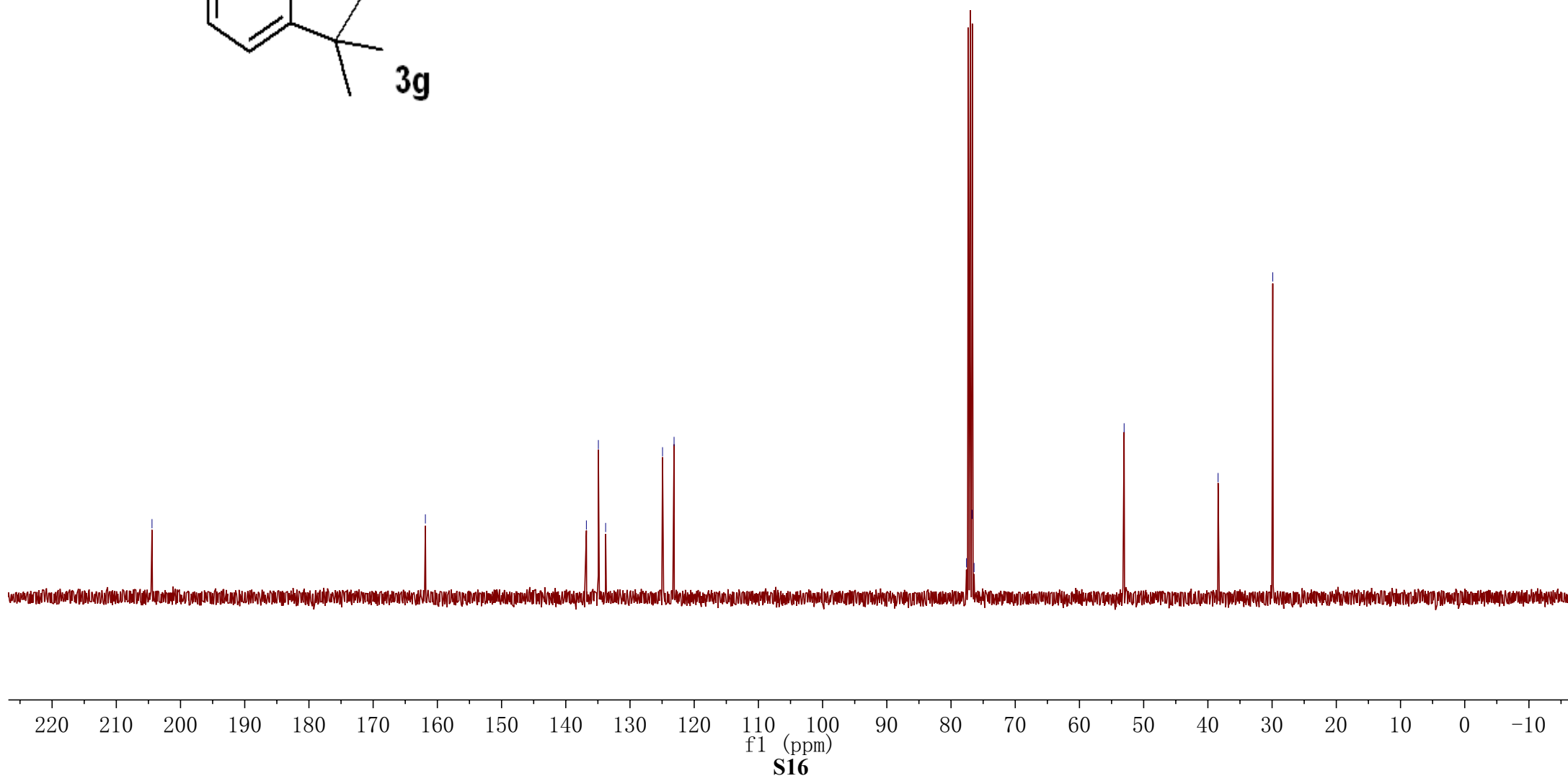
—53.0

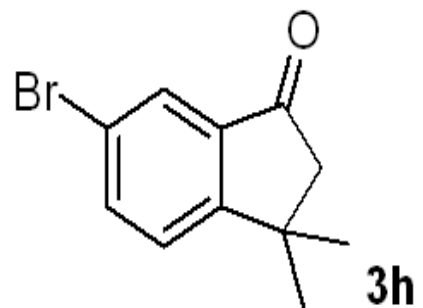
—38.4

—29.9



3g





7.81
7.80
7.71
7.71
7.69
7.69
7.39
7.37

1.02
0.98
0.86

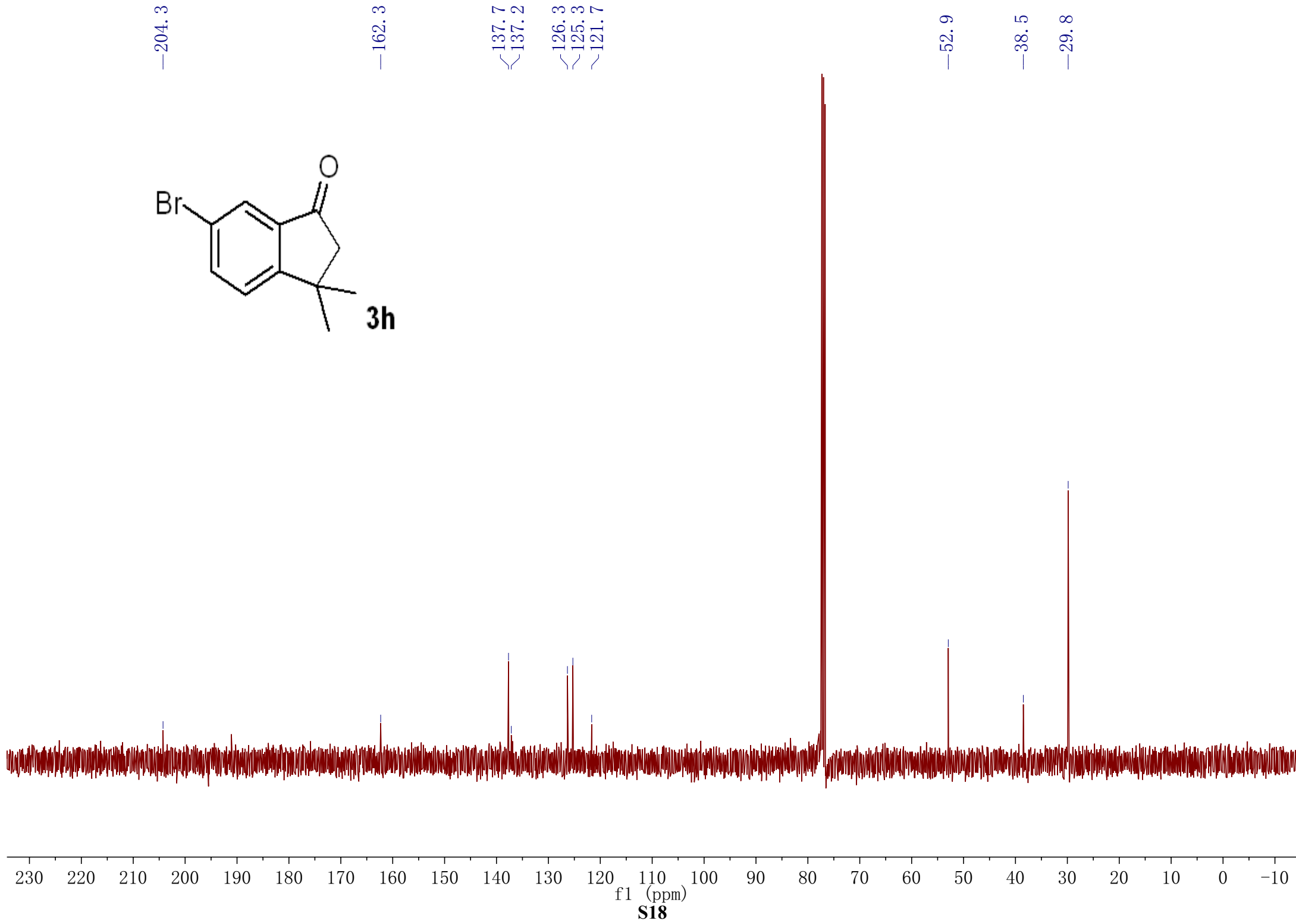
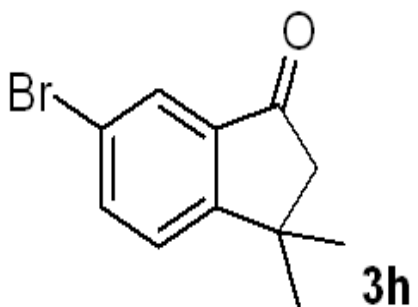
2.00

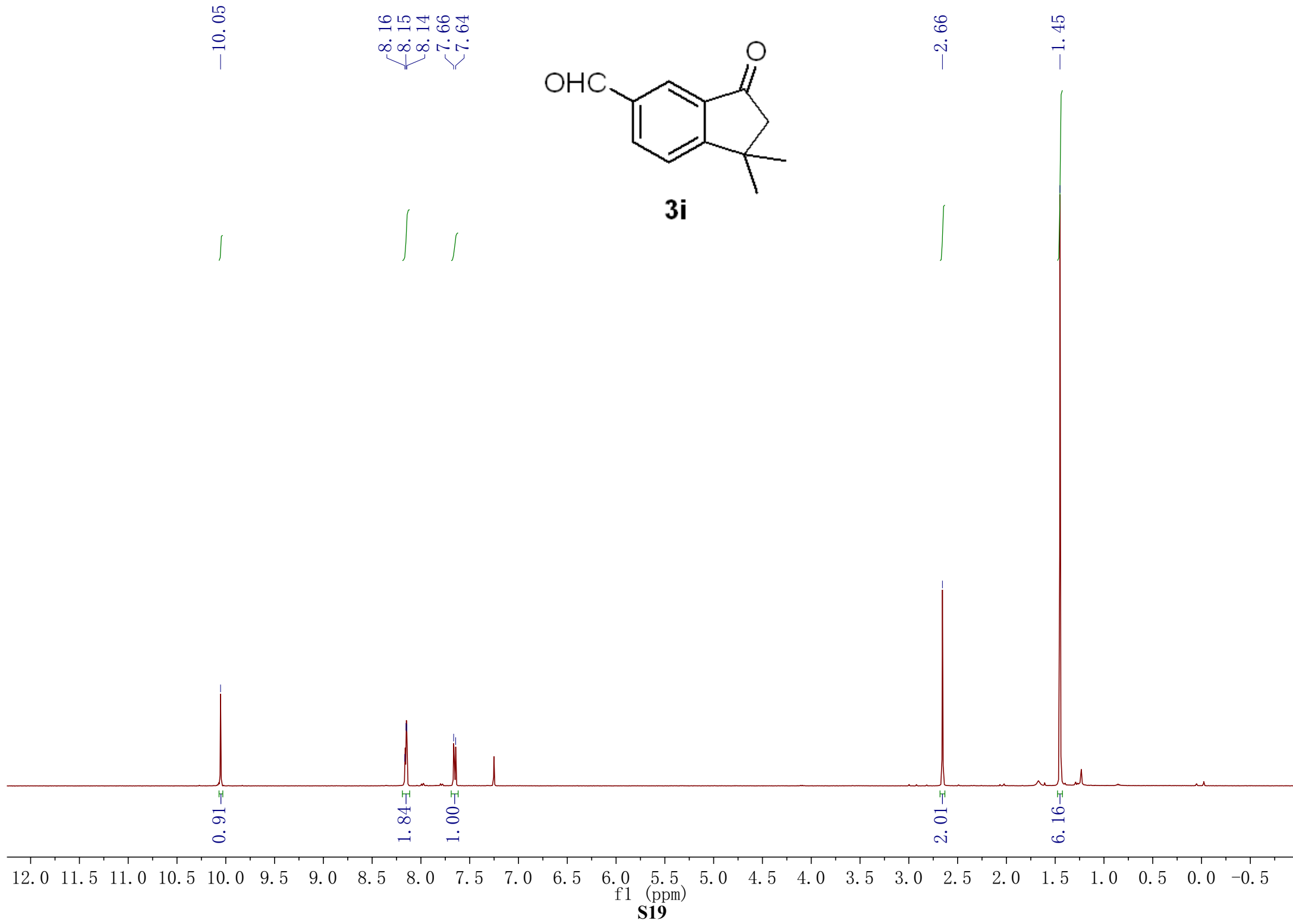
6.16

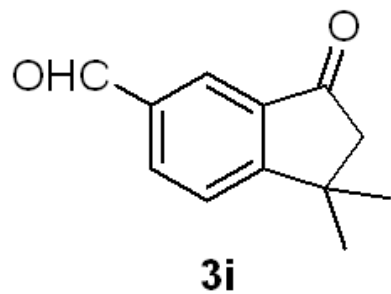
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)

S17







—204.6

—191.1

—169.5

136.0

136.0

134.4

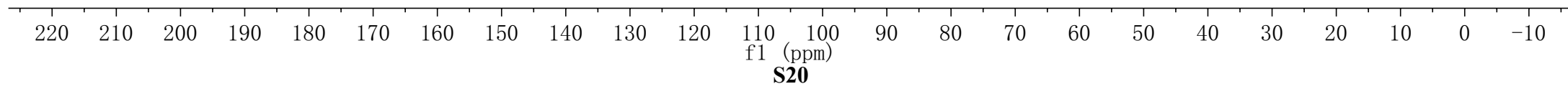
126.2

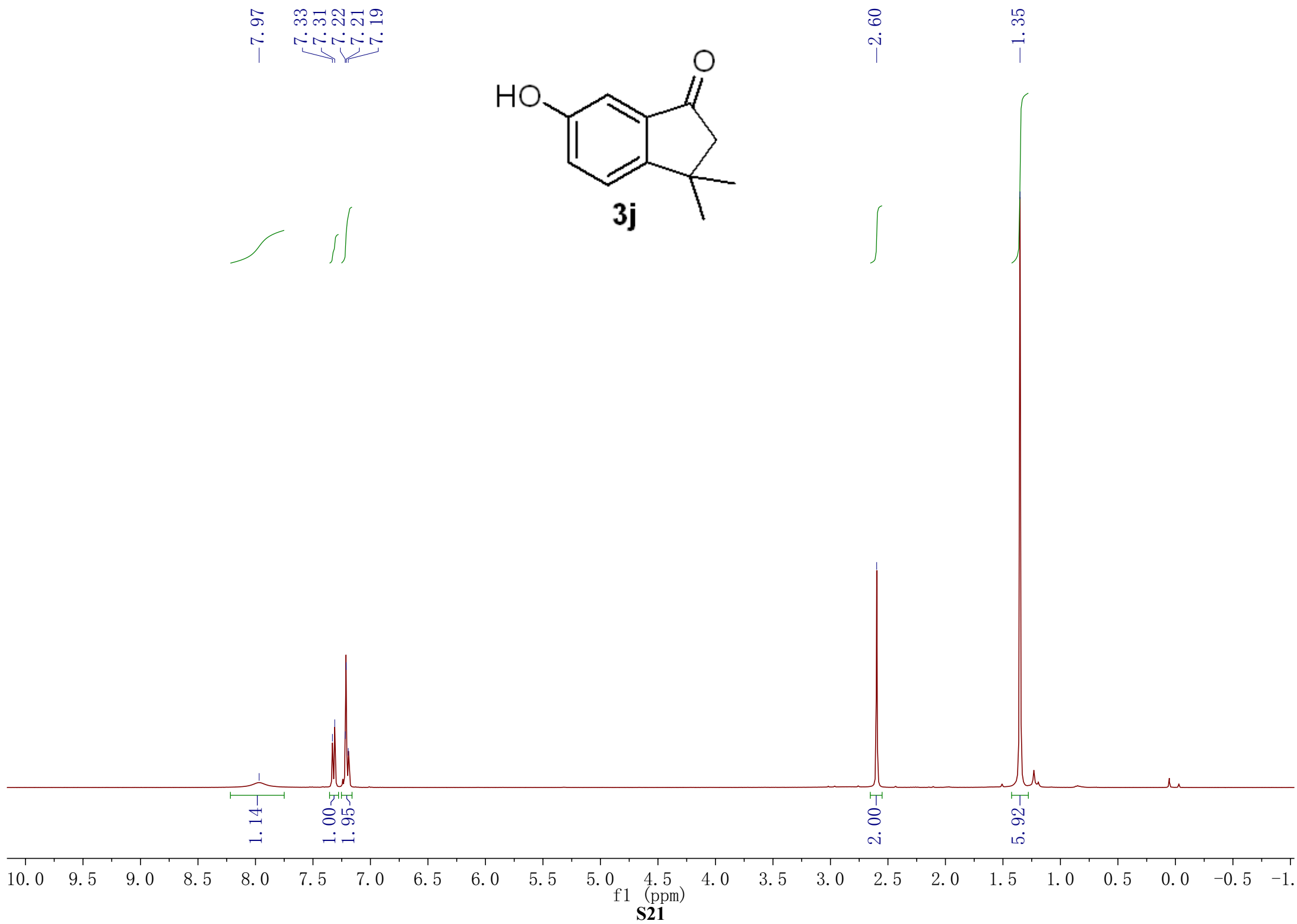
124.5

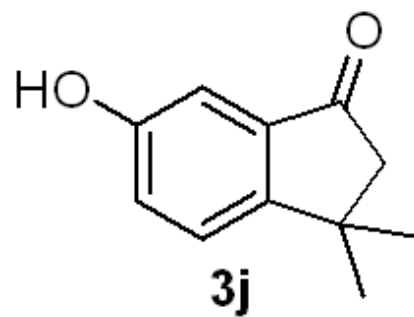
—52.9

—39.1

—29.7







—207.9

156.7
156.3

—136.2

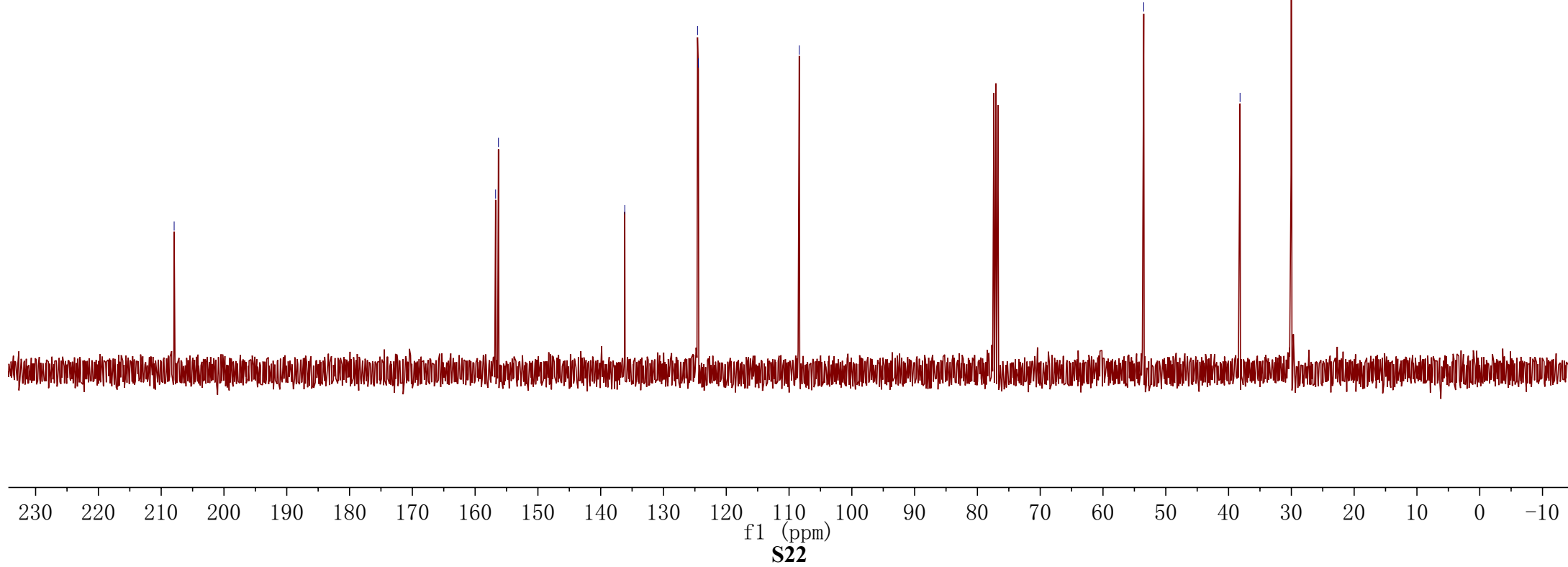
124.6
124.4

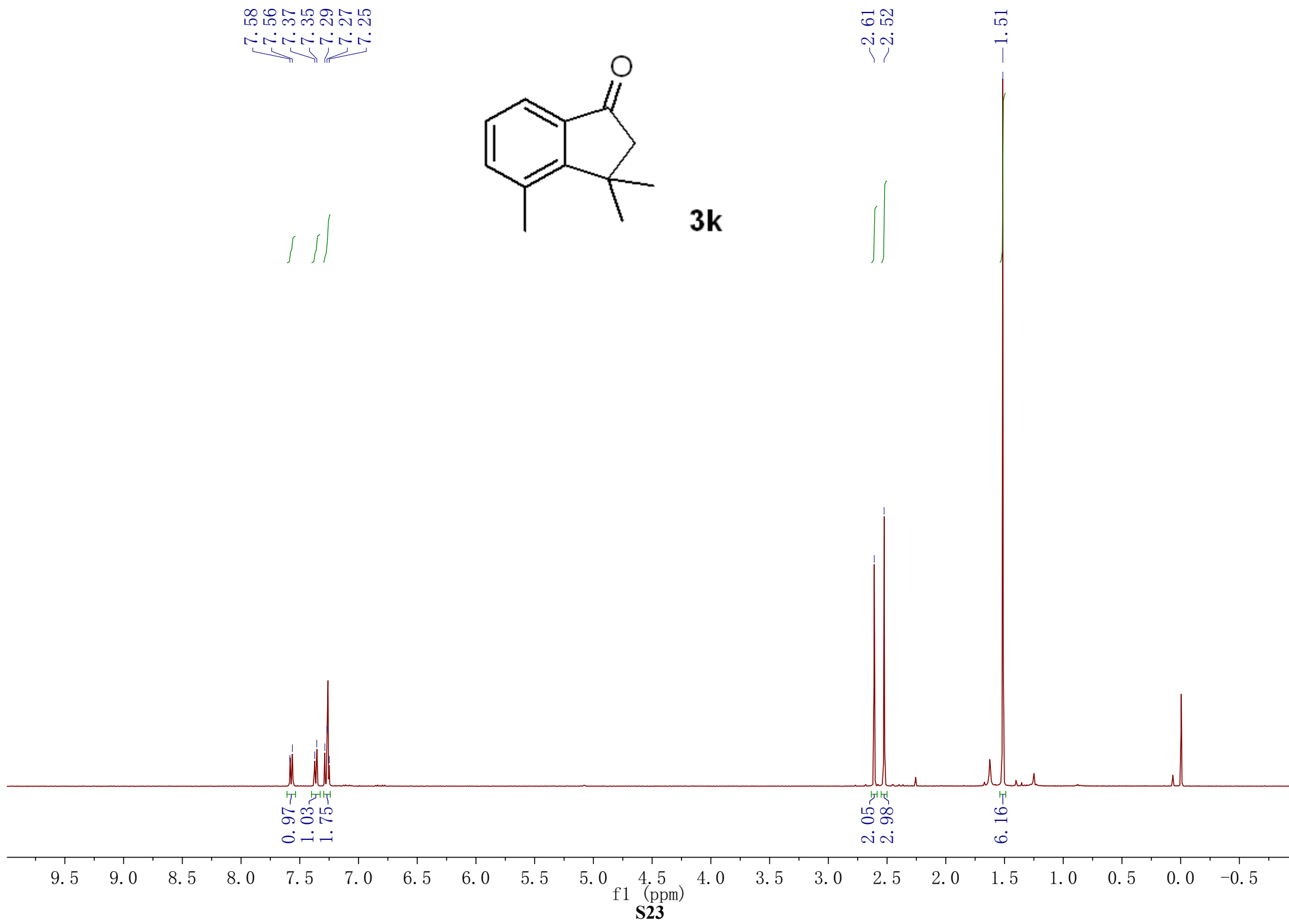
—108.4

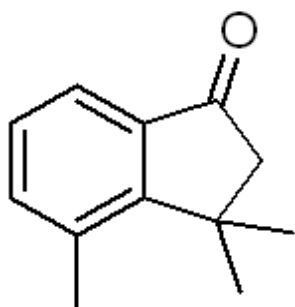
—53.5

—38.2

—30.0







3k

—206.3

—159.9

—137.7

—136.3

—135.4

—127.7

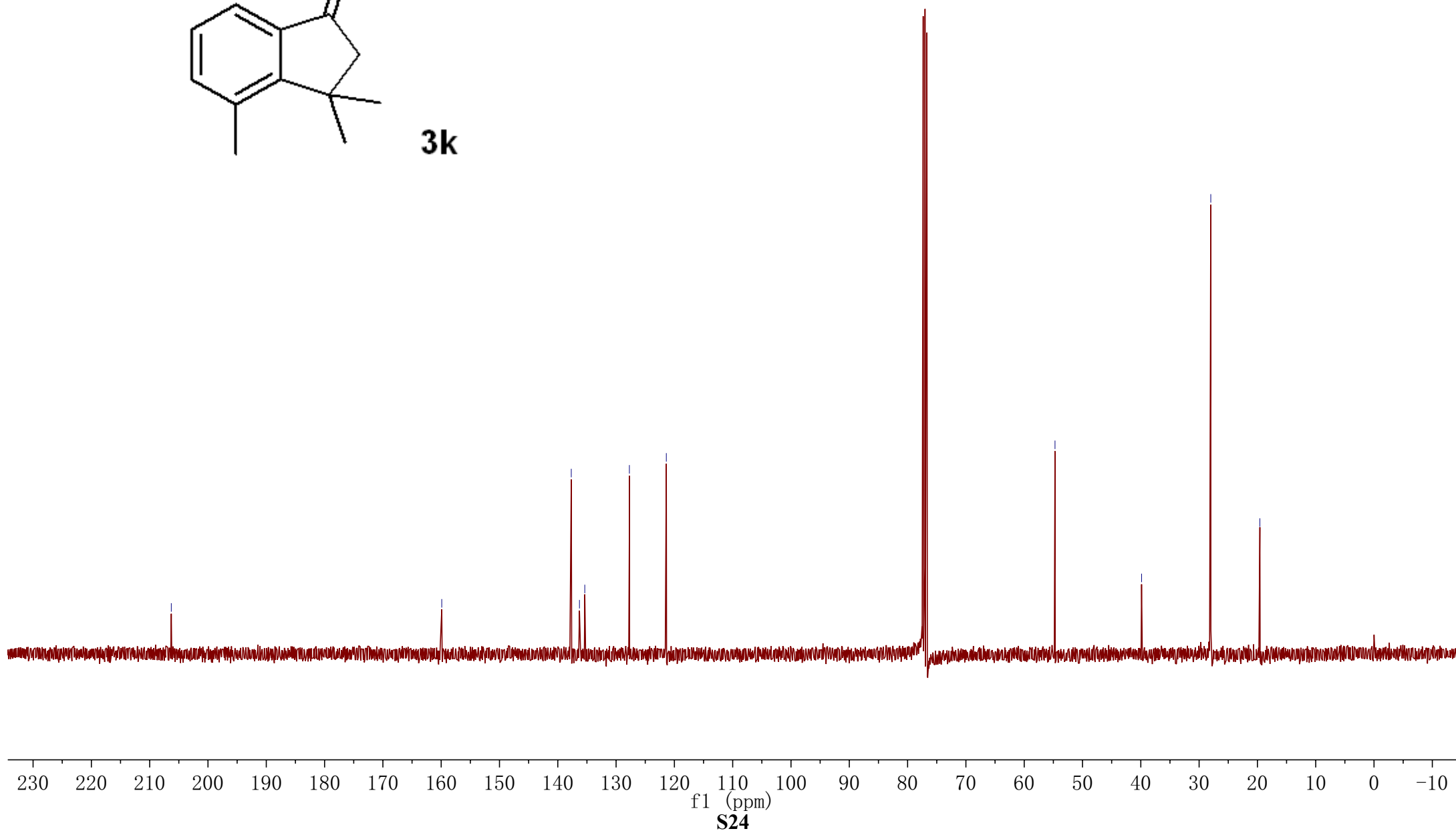
—121.4

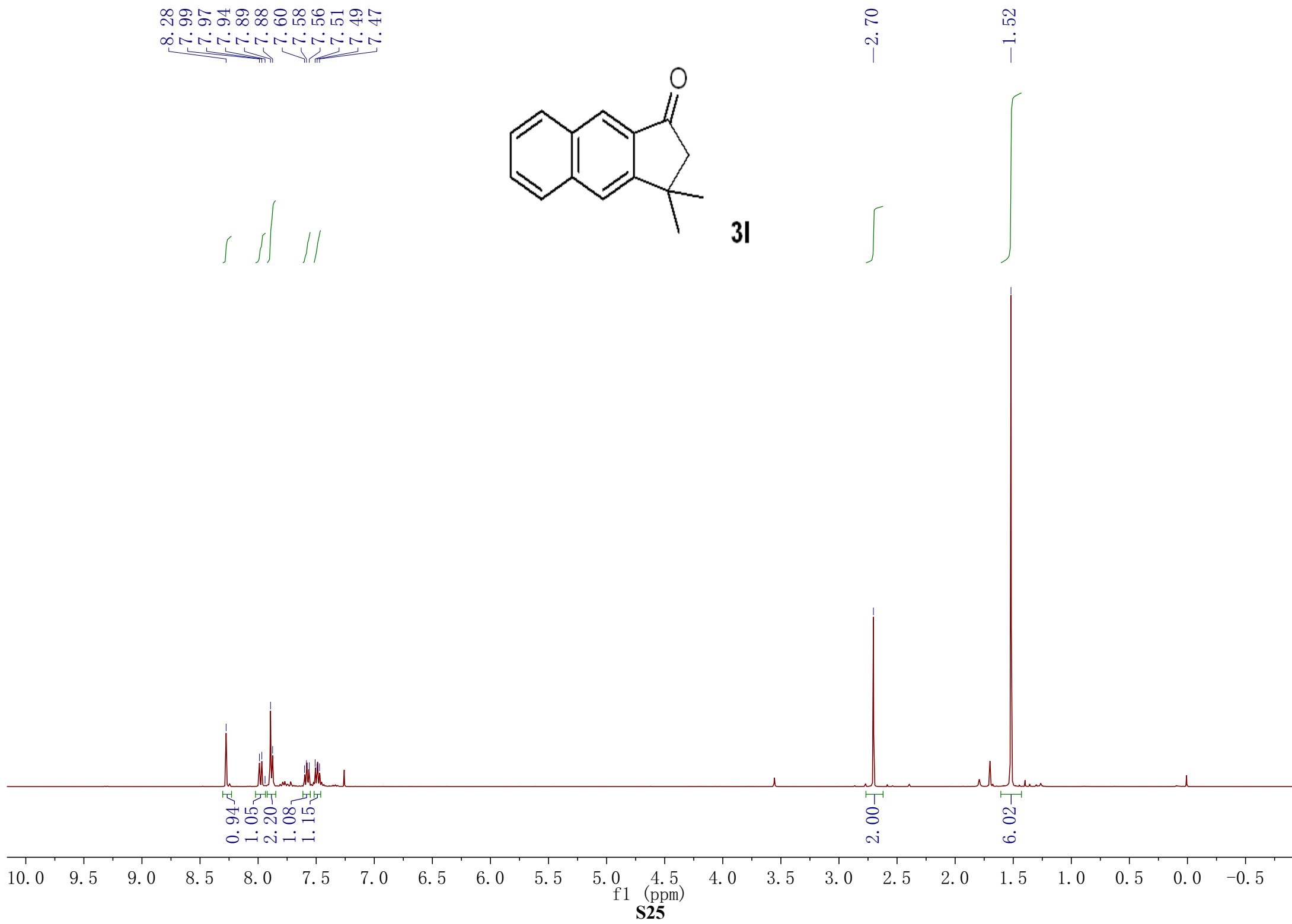
—54.7

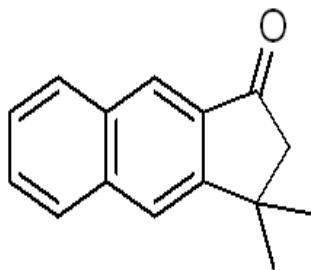
—39.9

—28.0

—19.6







3l

—206.3

—157.2

137.4

133.5

132.4

130.4

128.5

128.0

126.1

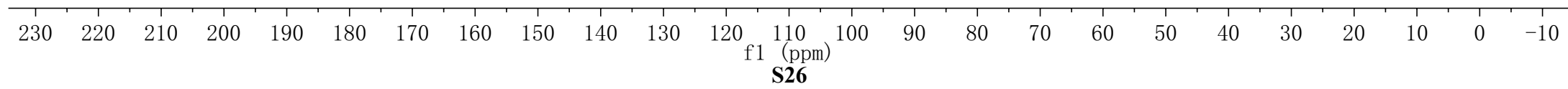
124.2

121.9

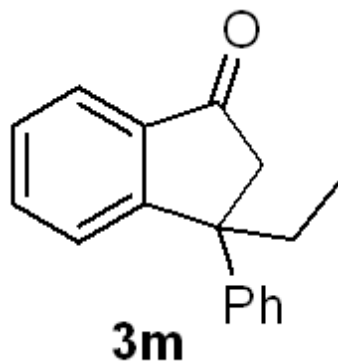
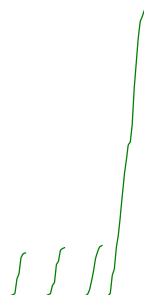
—53.7

—38.4

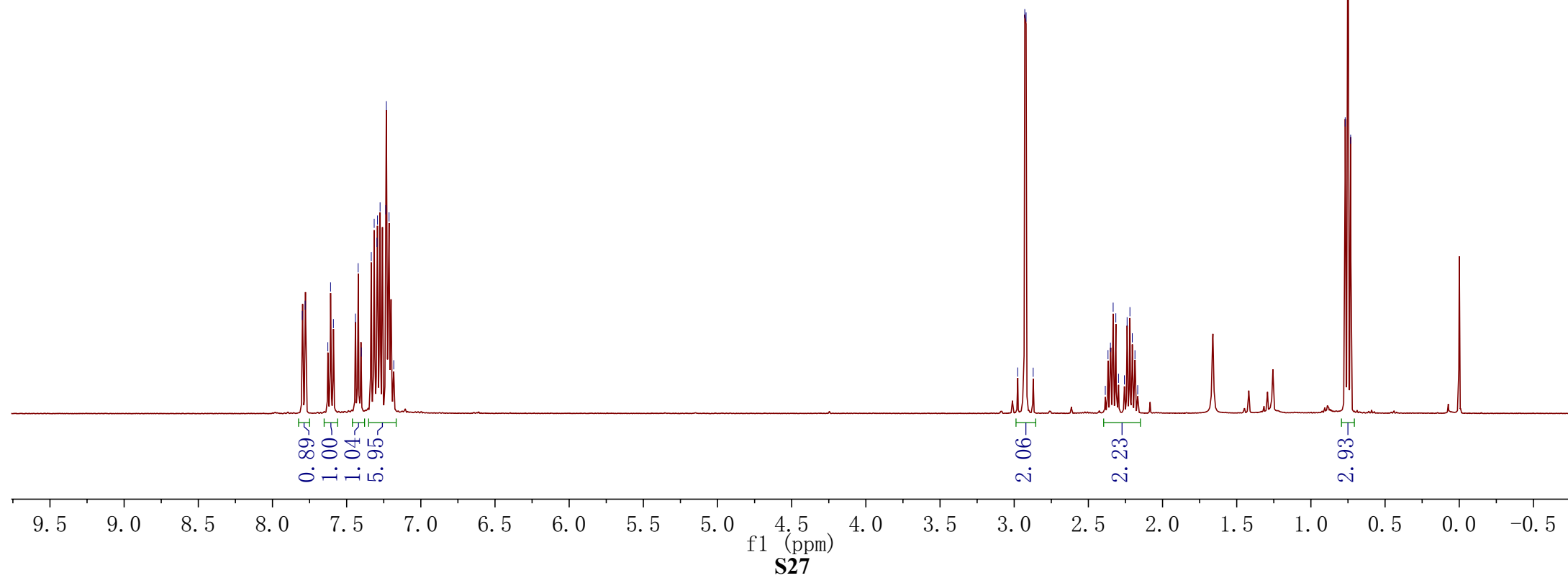
—30.7

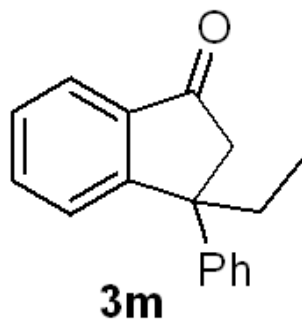


7.80
7.78
7.63
7.61
7.59
7.44
7.42
7.40
7.33
7.31
7.30
7.29
7.27
7.24
7.23
7.21
7.18



2.98
2.93
2.92
2.87
2.39
2.37
2.35
2.33
2.31
2.30
2.26
2.24
2.22
2.20
2.19
2.17
0.77
0.75
0.73





—205.9

—160.4

—146.8

136.9

134.9

128.5

127.8

126.5

126.4

126.2

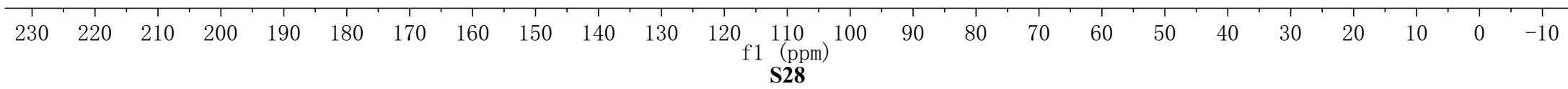
123.3

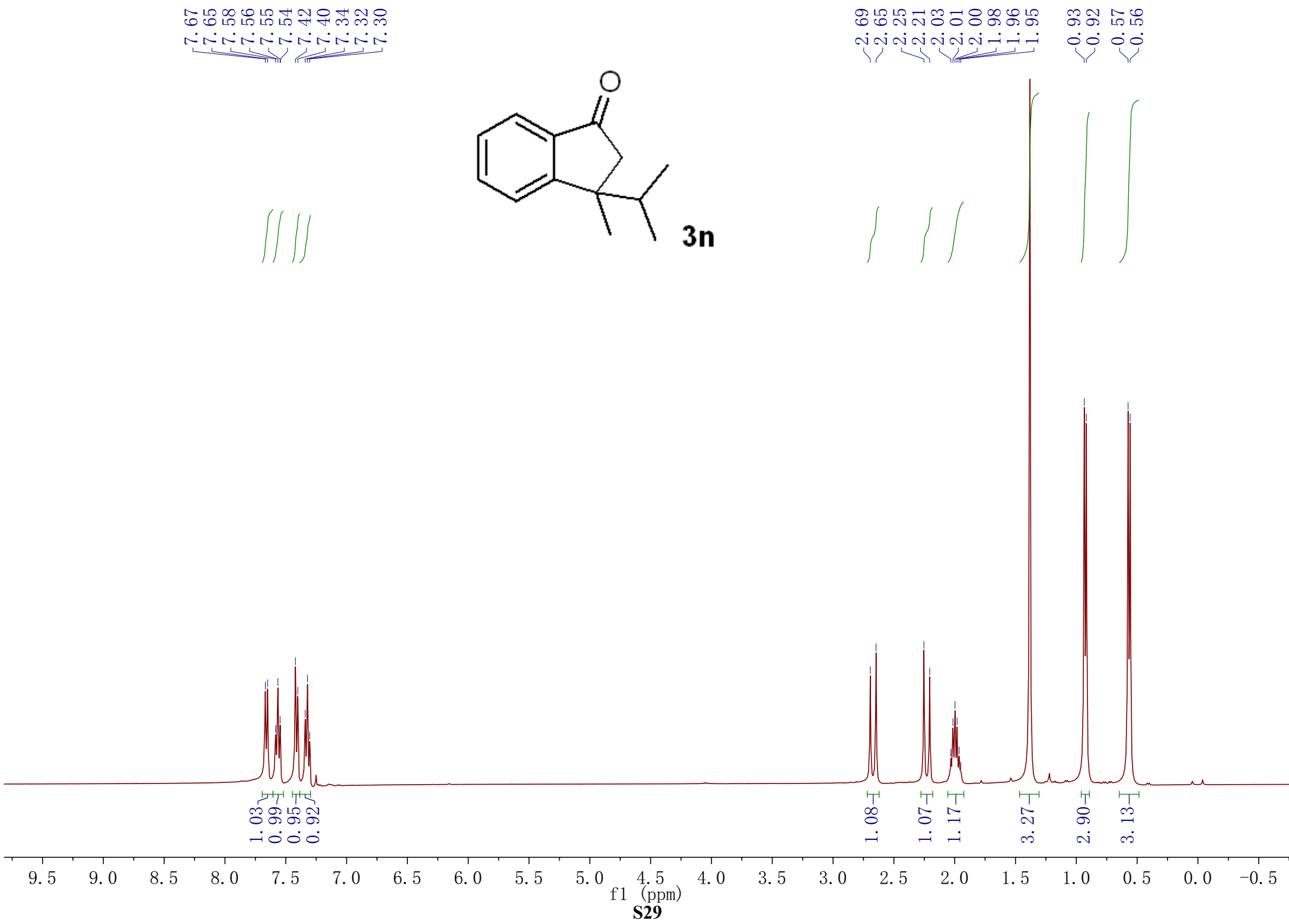
~52.4

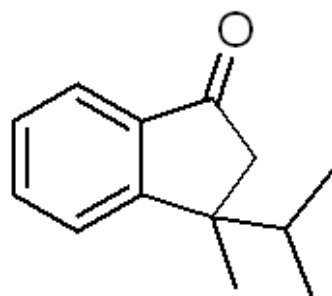
~50.3

—32.5

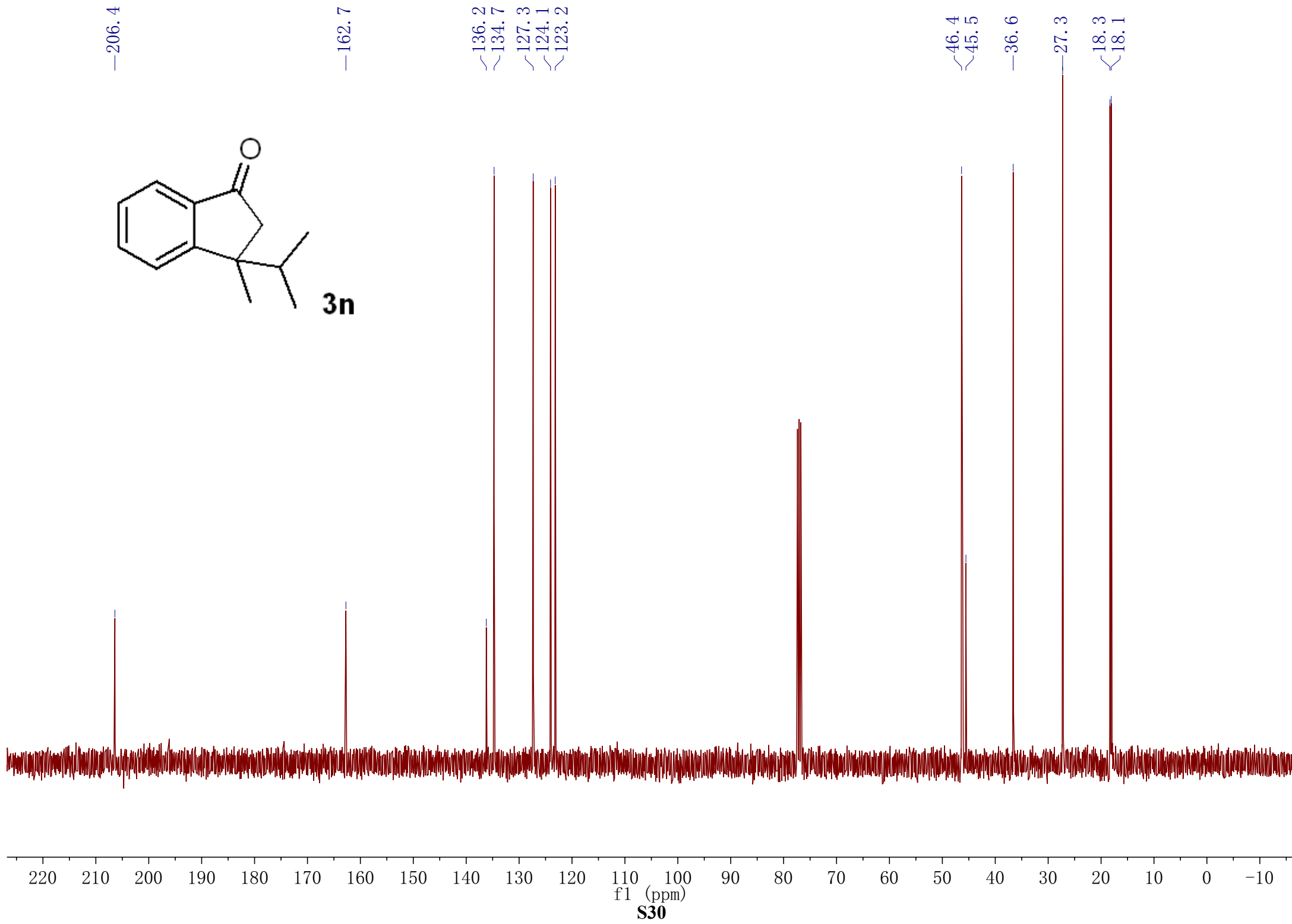
—9.3





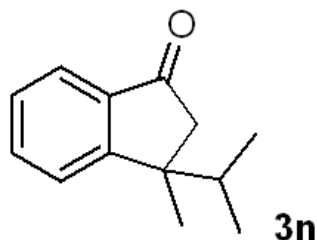


3n

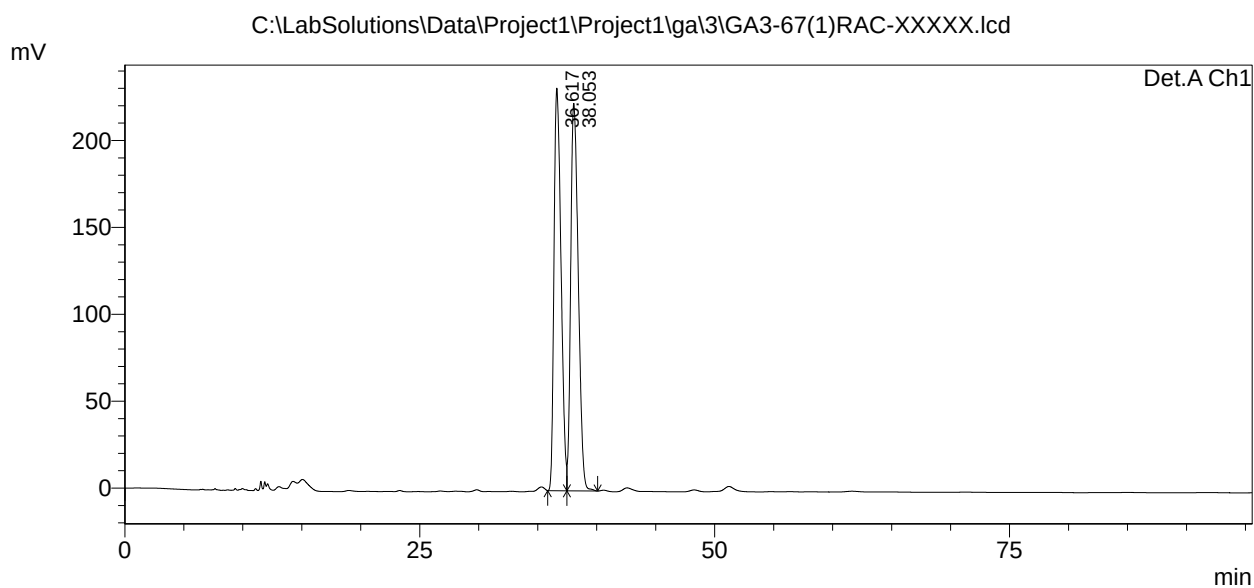


==== Shimadzu LCsolution Analysis Report =====

Acquired by : Admin
 Sample Name : GA3-67(1)RAC-XXXXX
 method : IC, 99.4/0.6, 0.5, 214
 Injection Volume : 2.5 μ L
 Data File Name : GA3-67(1)RAC-XXXXX.lcd
 Method File Name : 222.lcm
 Report File Name : 1.lcr
 Data Acquired : 2014-4-15 11:49:48
 Data Processed : 2016-9-21 12:10:52



<Chromatogram>



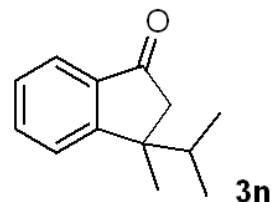
PeakTable

Detector A Ch1 254nm

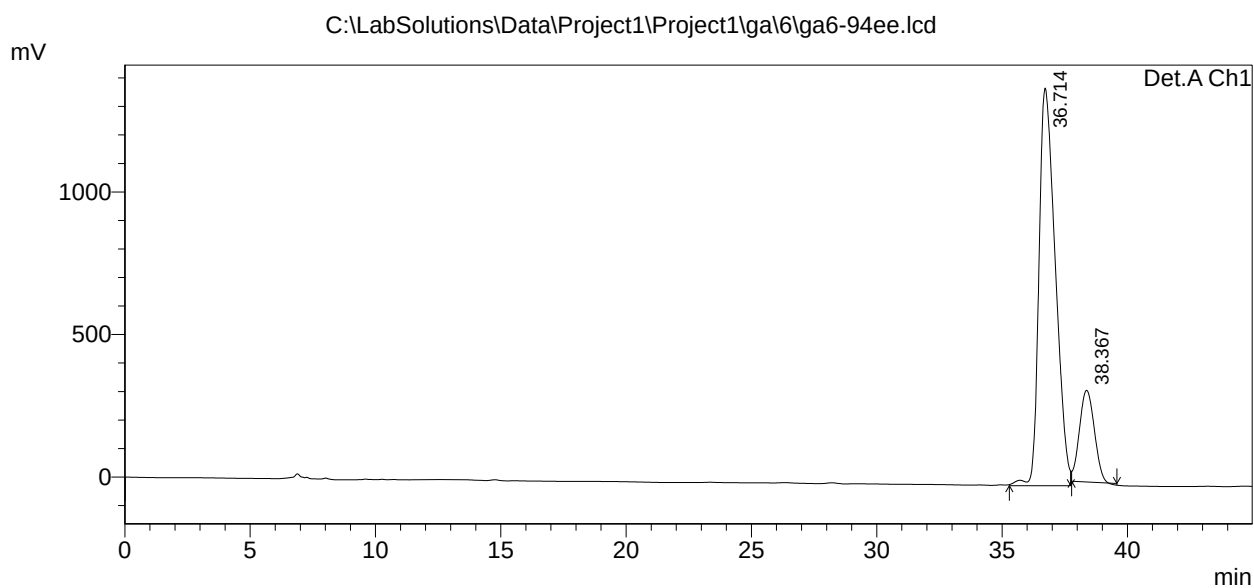
Peak#	Ret. Time	Area	Height	Area %
1	36.617	9594130	231610	49.075
2	38.053	9955905	222905	50.925
Total		19550035	454515	100.000

==== Shimadzu LcSolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\ga6\ga6-94ee.lcd
 Acquired by : Admin
 Sample Name : ga6-94ee
 Sample ID : IC, 99.4/0.6, 0.5, 214
 Vial # :
 Injection Volume : 1 uL
 Data File Name : ga6-94ee.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2015-3-13 10:13:02
 Data Processed : 2016-10-14 22:16:33



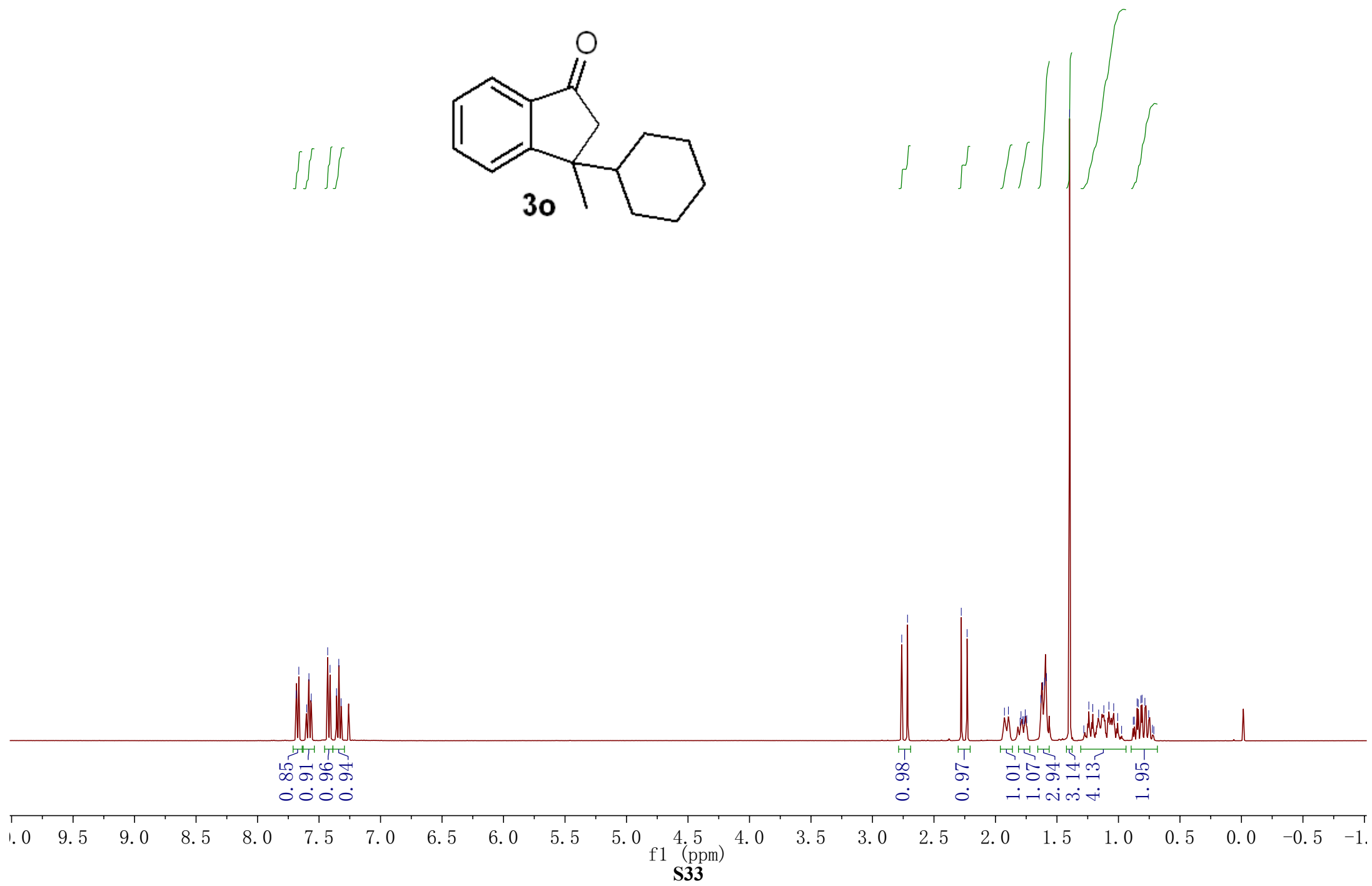
<Chromatogram>

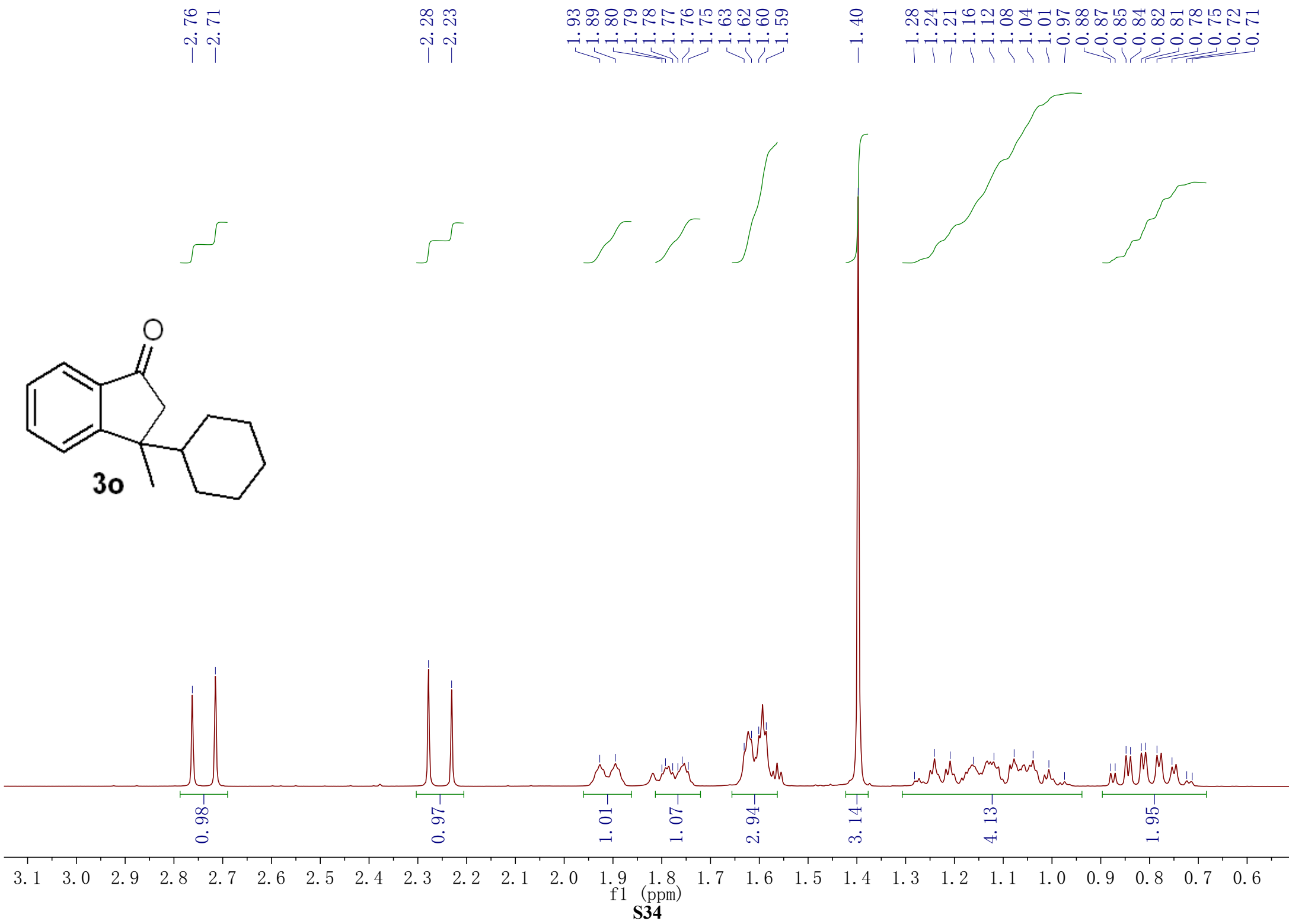


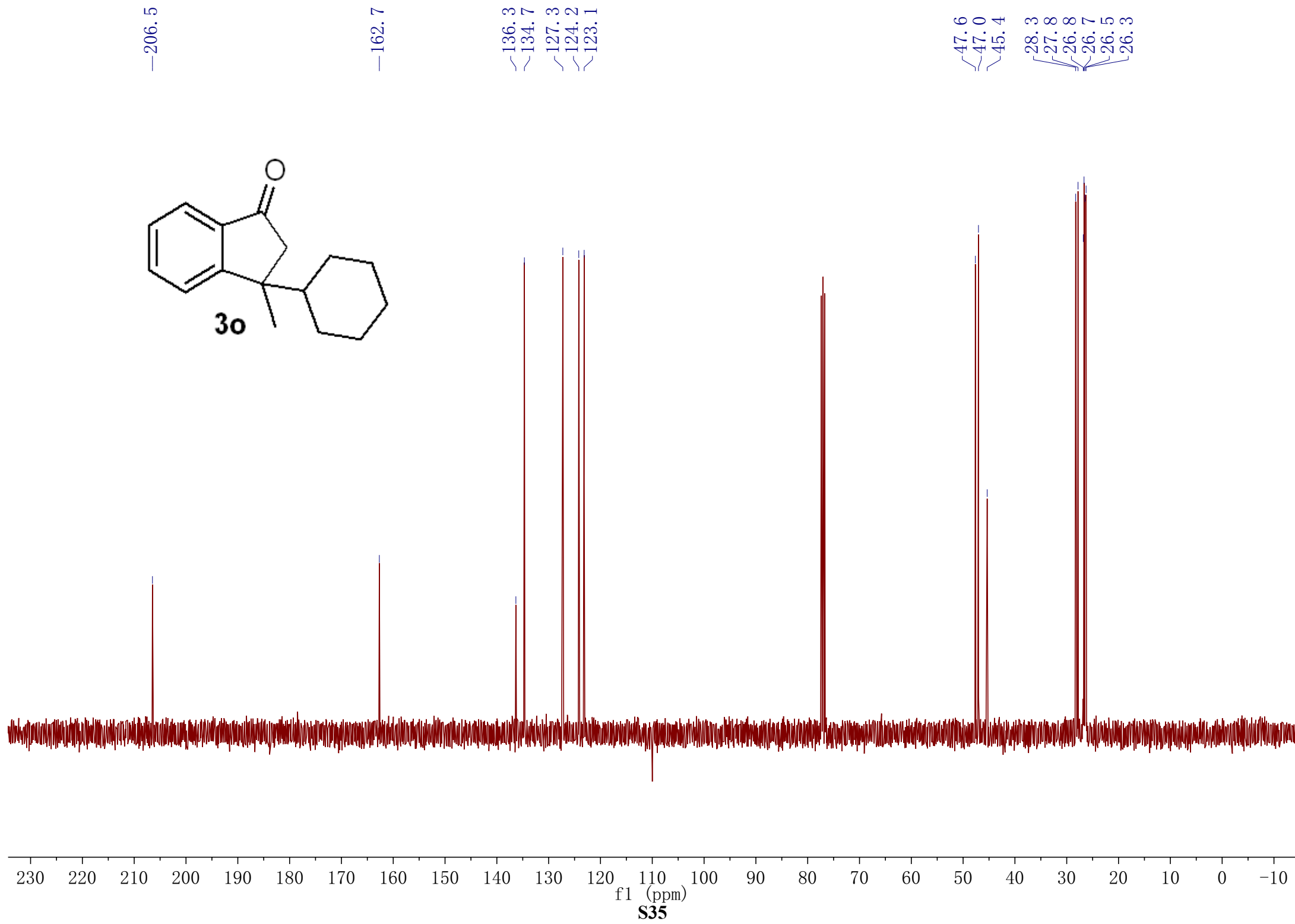
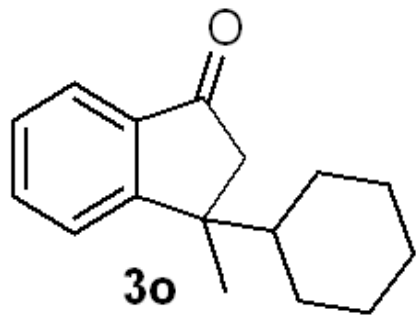
PeakTable

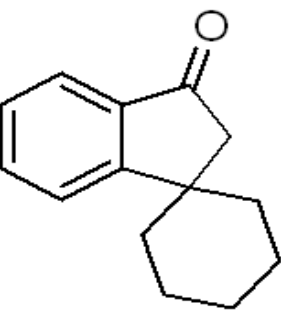
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	36.714	63325354	1394613	82.713	81.265
2	38.367	13234903	321519	17.287	18.735
Total		76560257	1716133	100.000	100.000

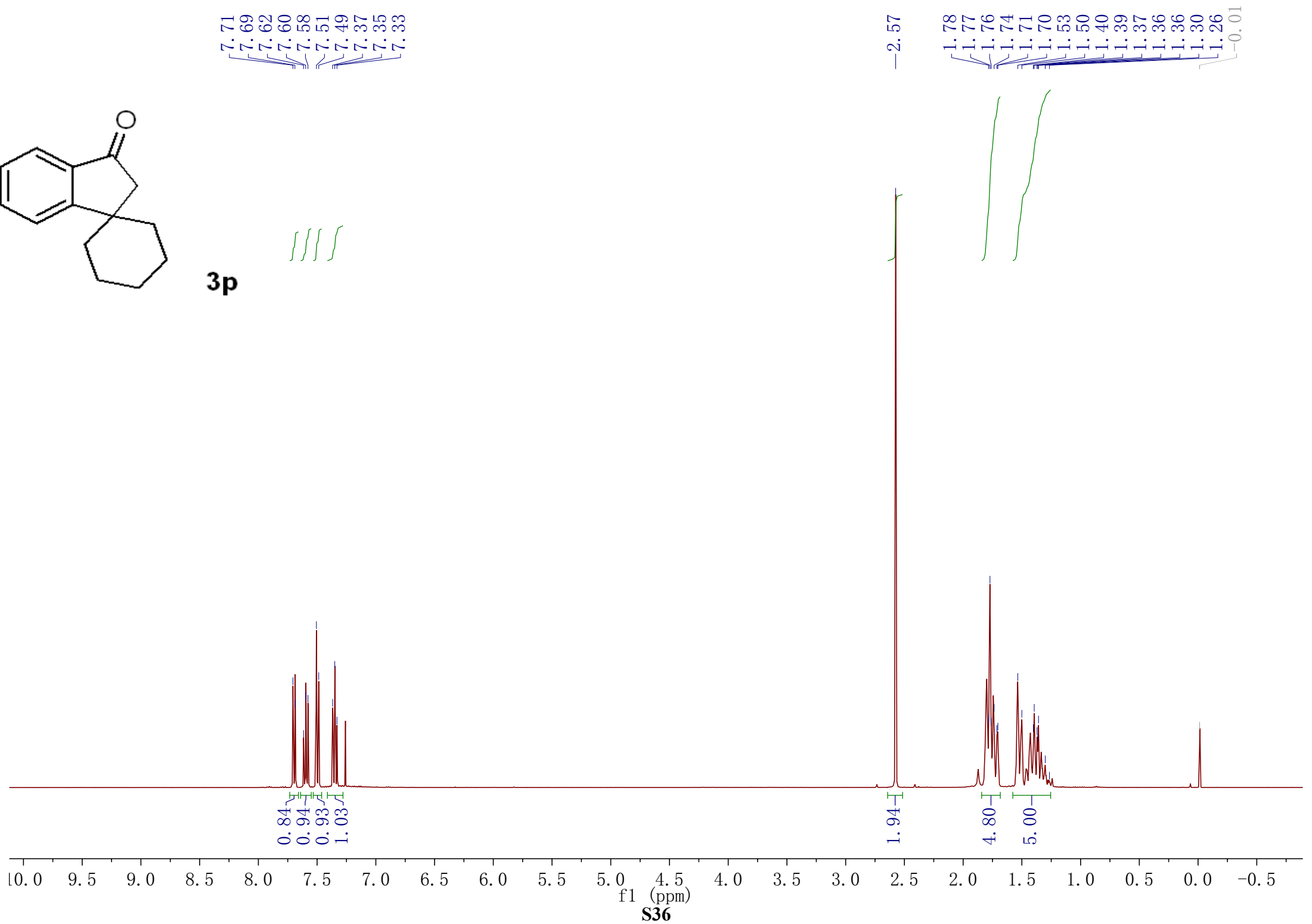


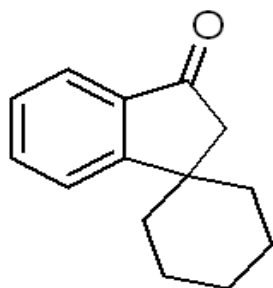






3p





3p

—206.2

—164.2

~135.5

~134.8

~127.5

~124.0

~123.4

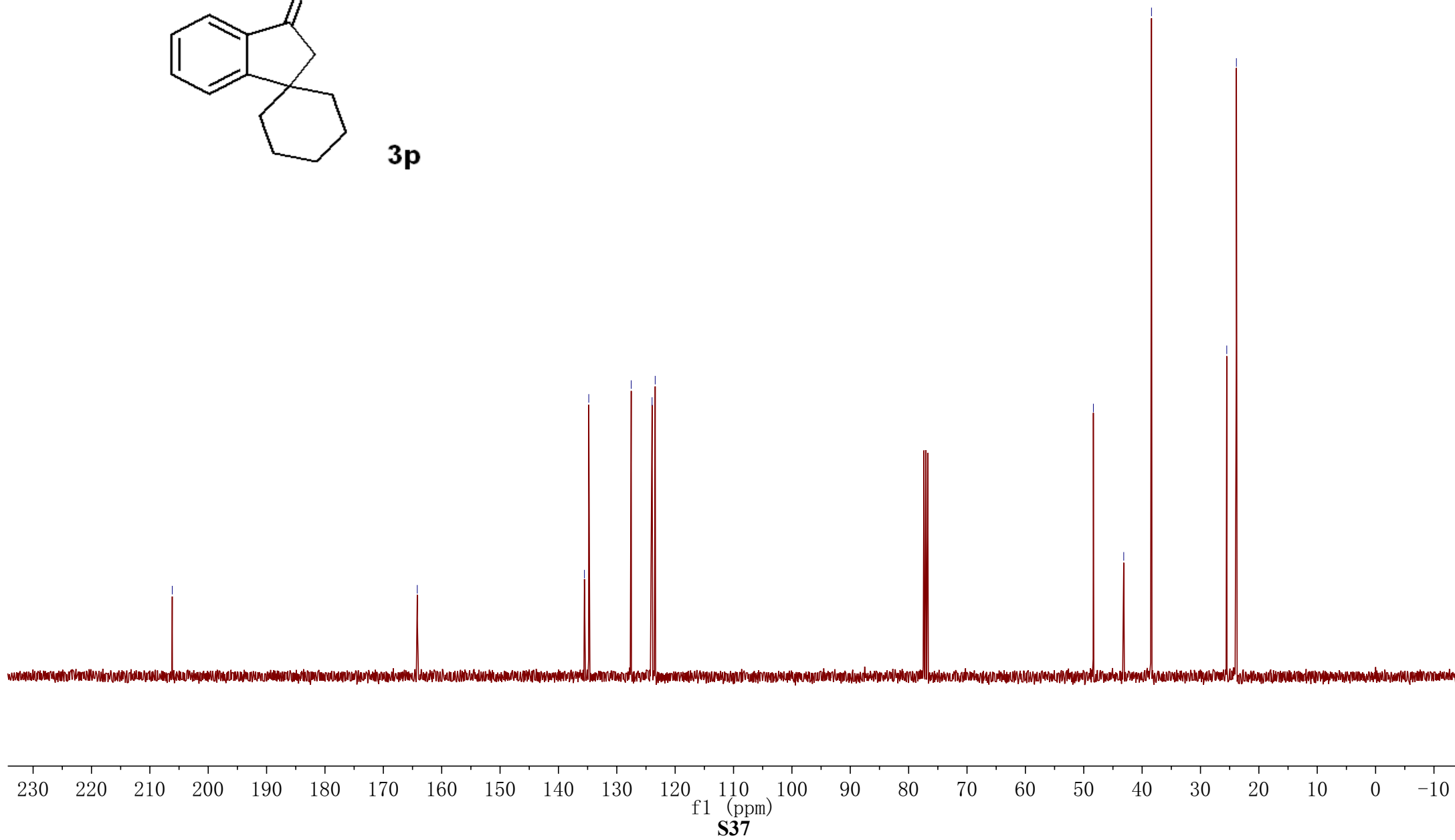
~48.4

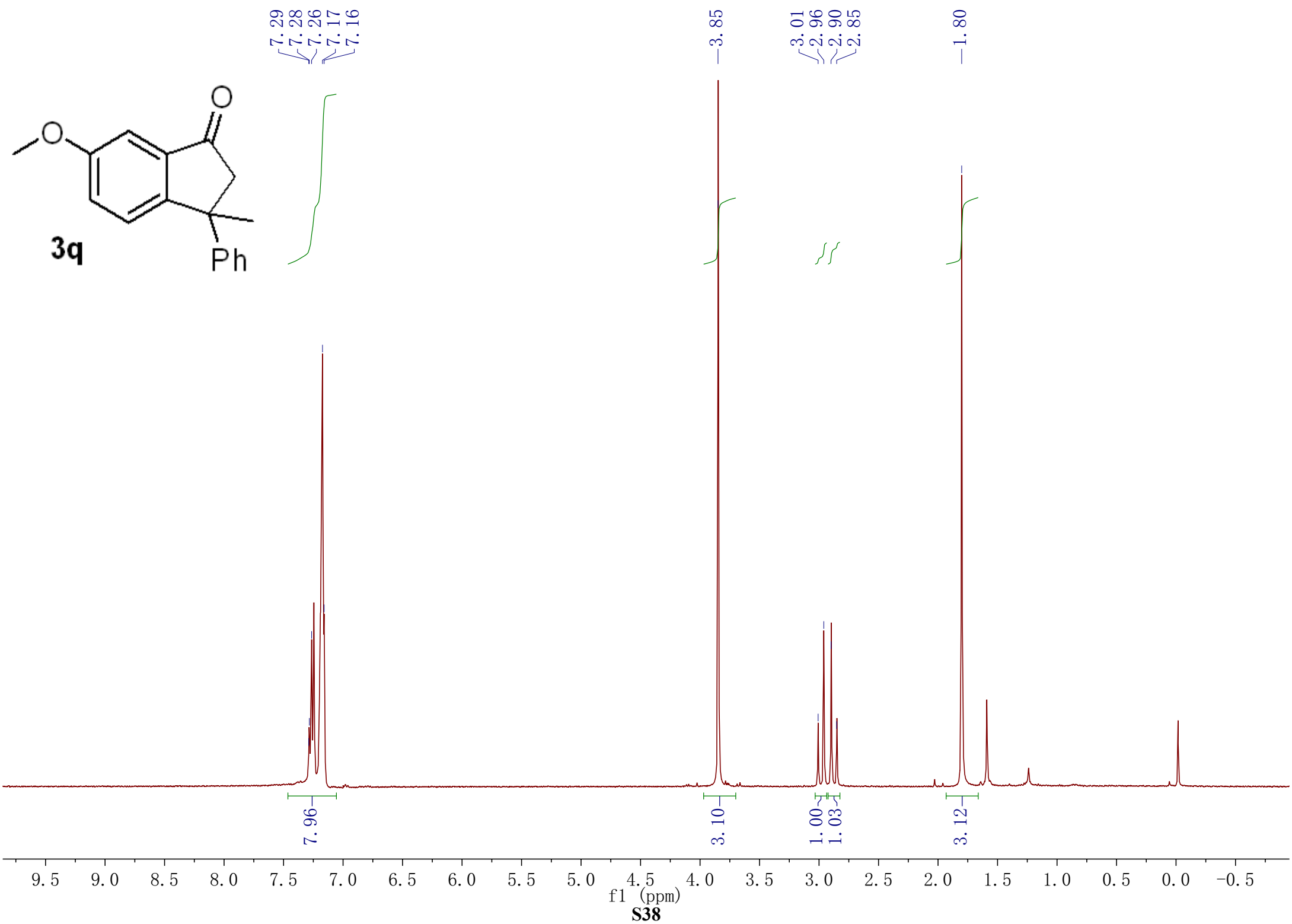
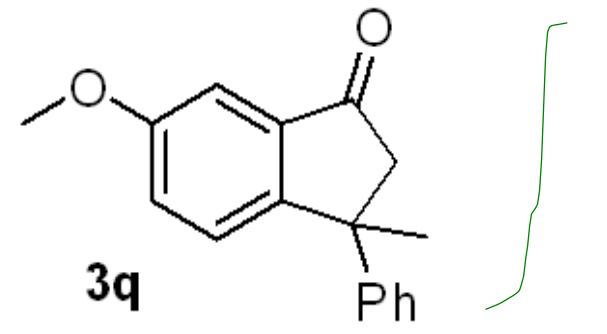
~43.1

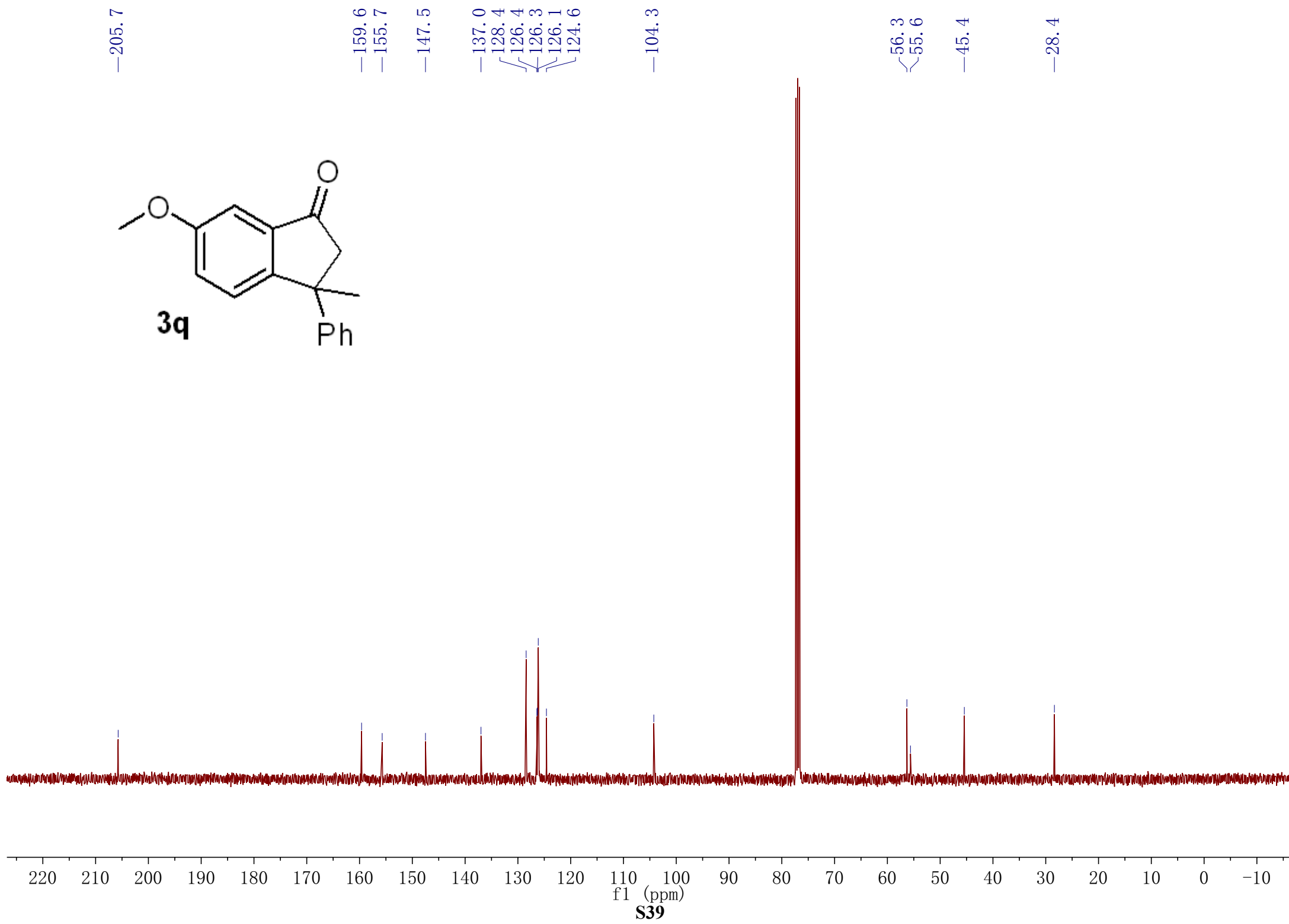
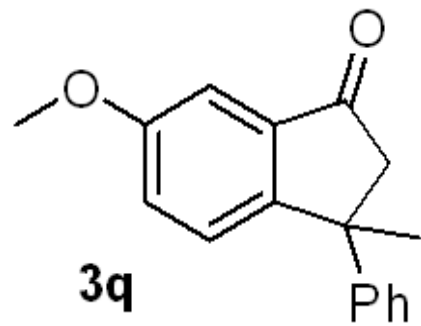
~38.4

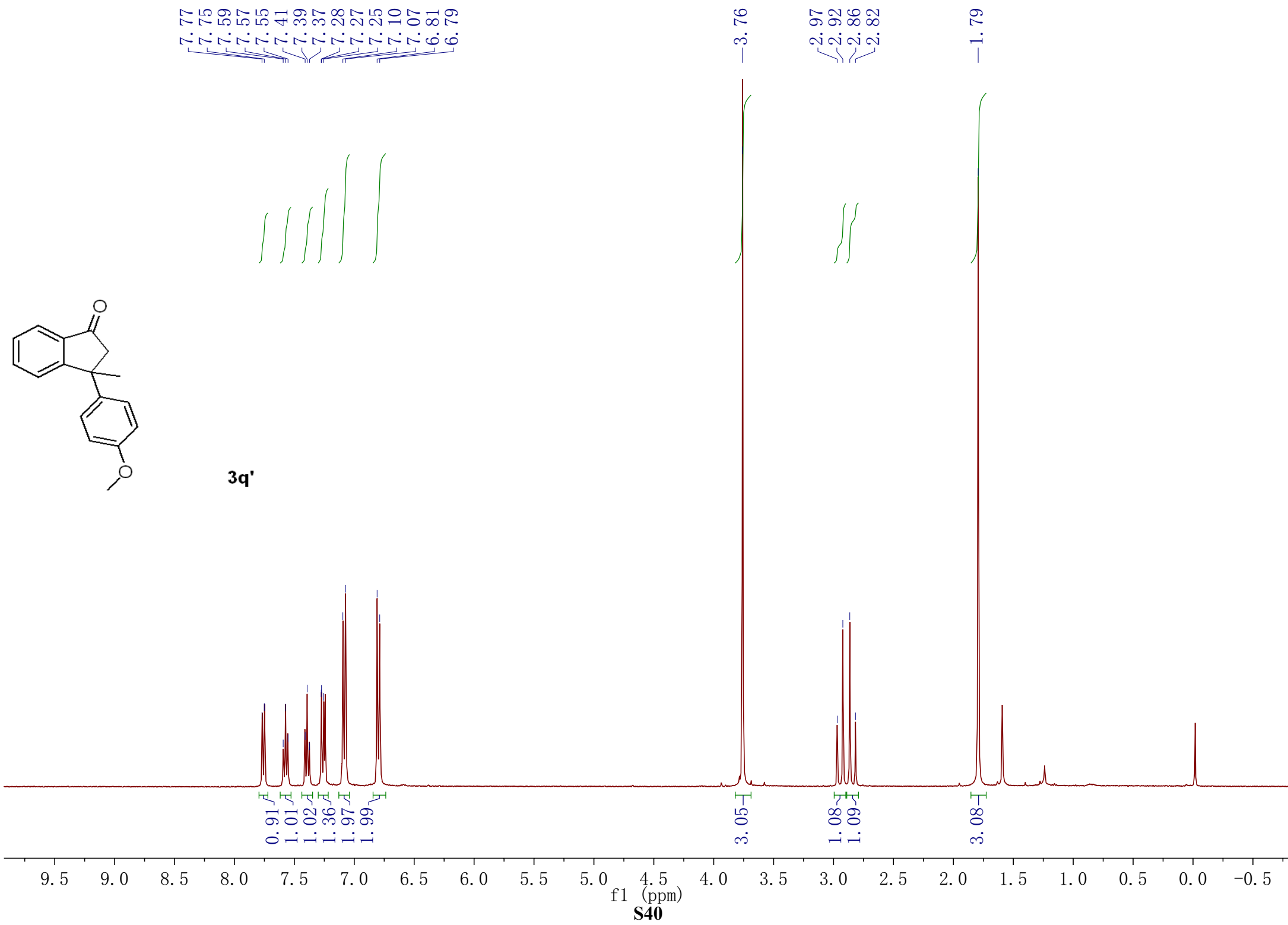
~25.5

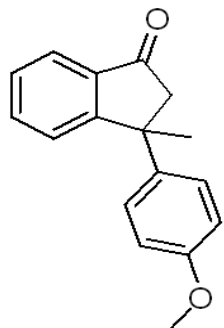
~23.8



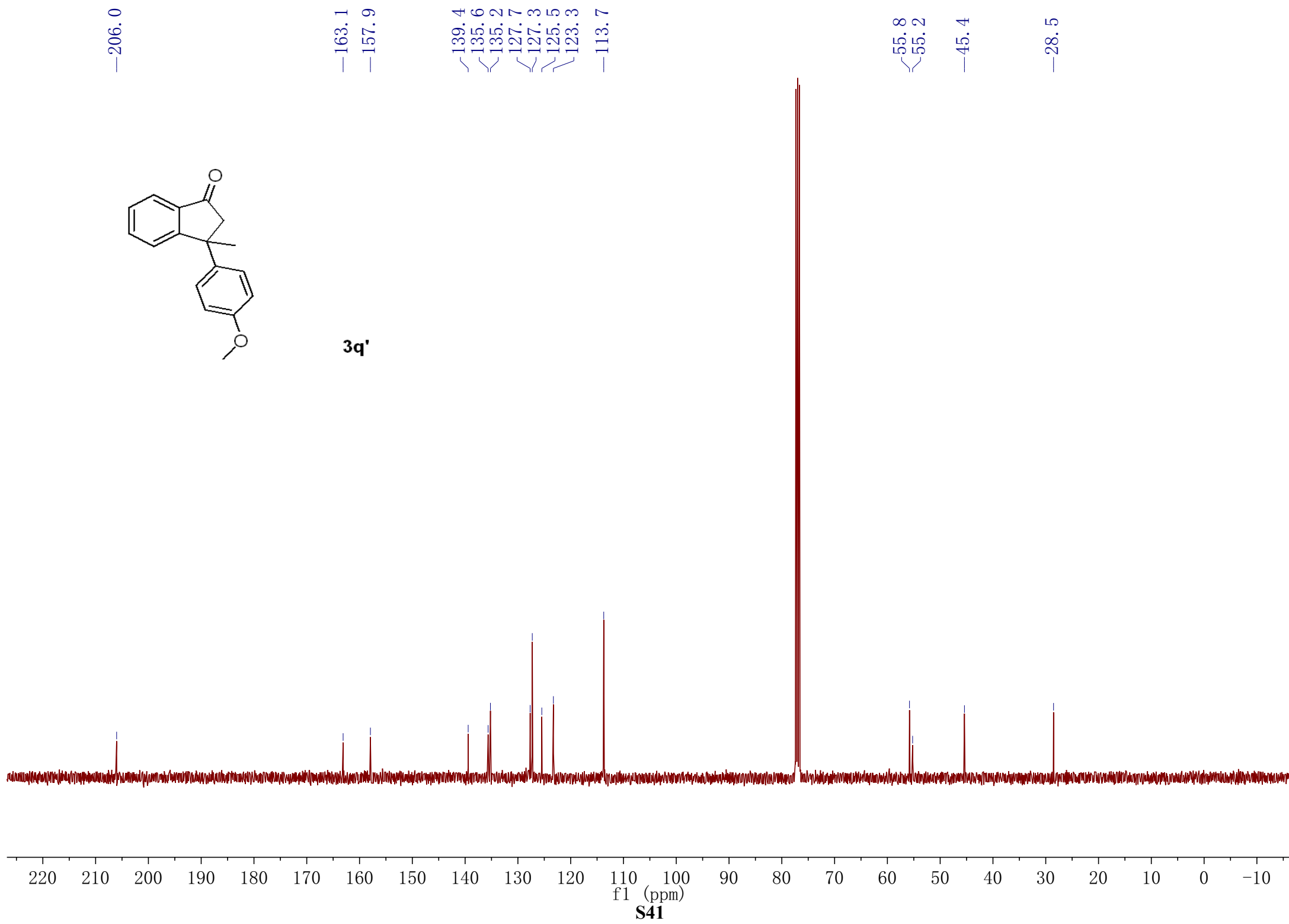






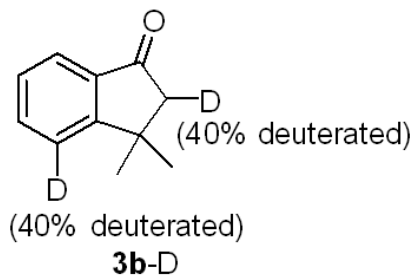


3q'



7.69
7.67
7.62
7.60
7.59
7.57
7.49
7.47
7.36
7.35
7.33

// // // //



-2.57

-1.40

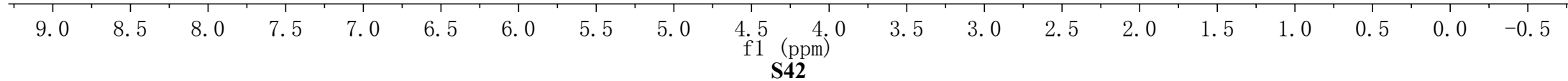
]

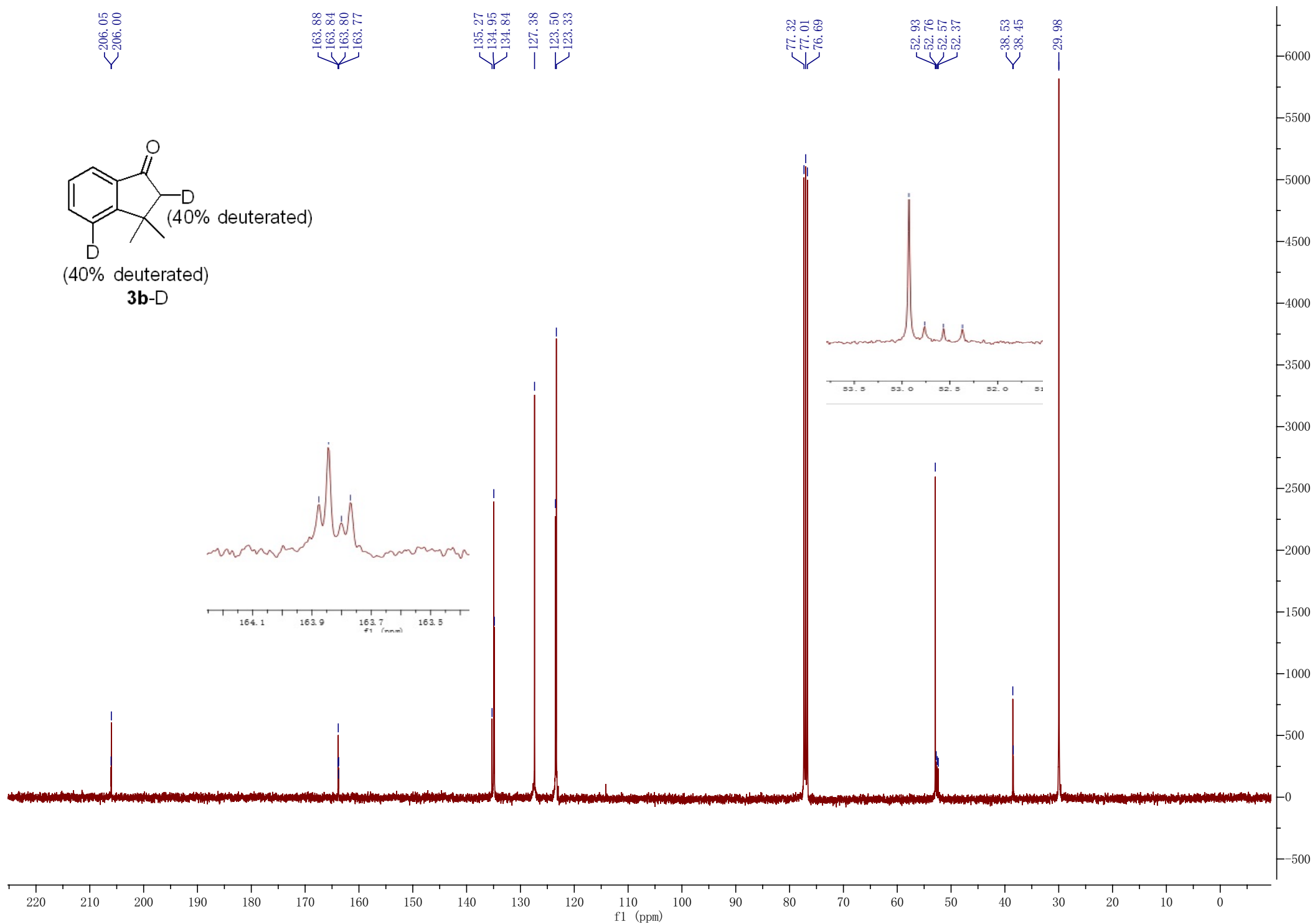
]

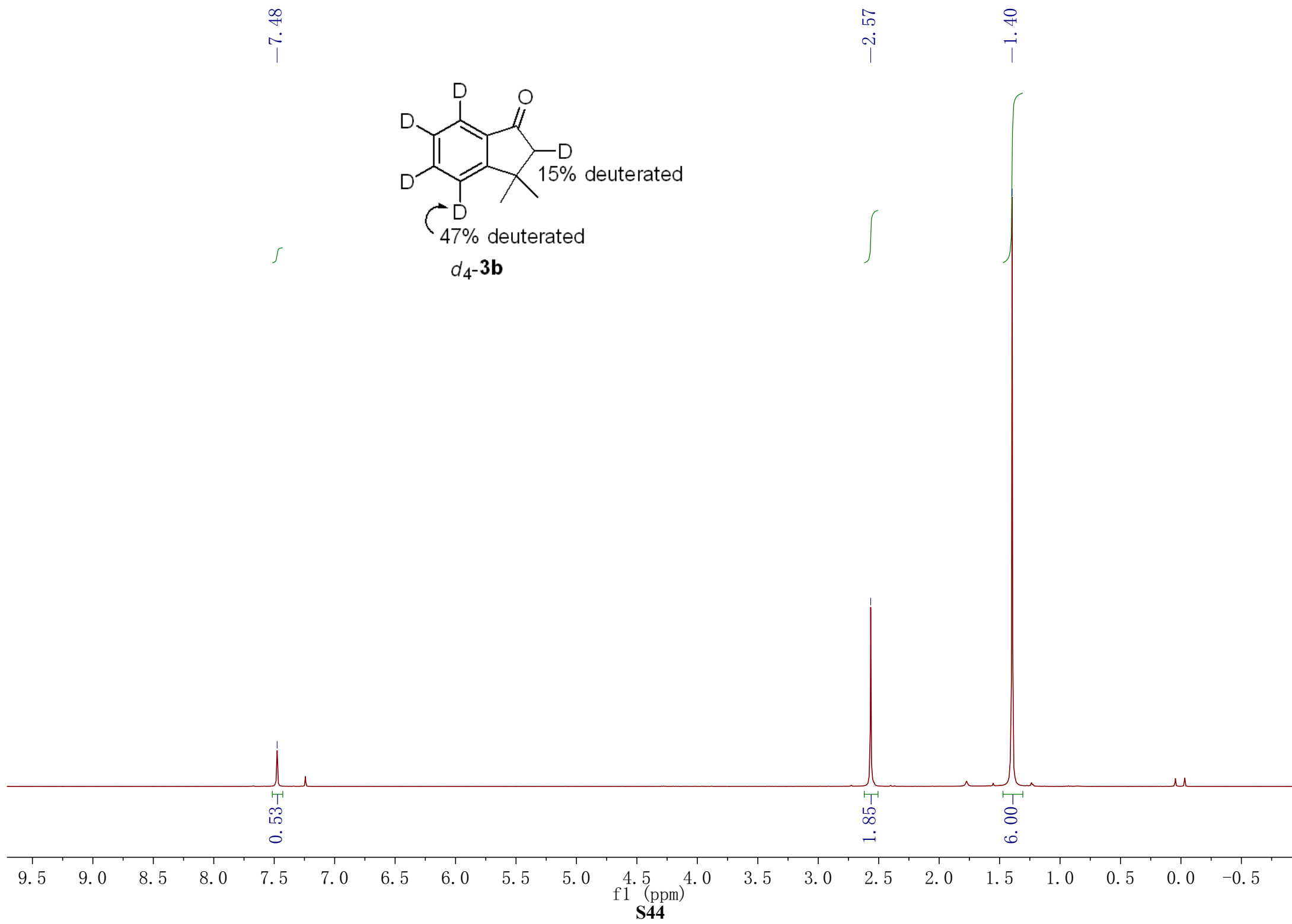
0.94
0.98
0.60
0.95

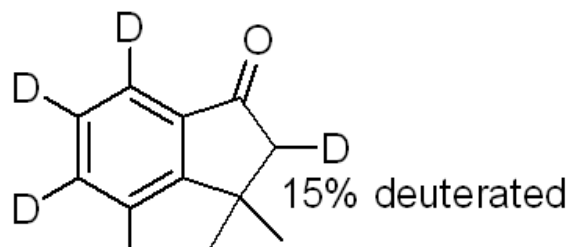
1.60

6.00









—205.9

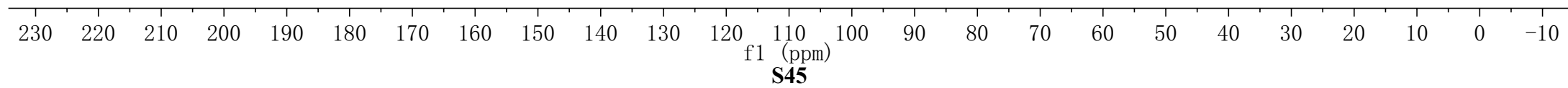
163.8
163.7

135.2
134.8
134.5
134.3
127.1
126.9
126.6
123.4
123.1
122.9
122.6

—52.9

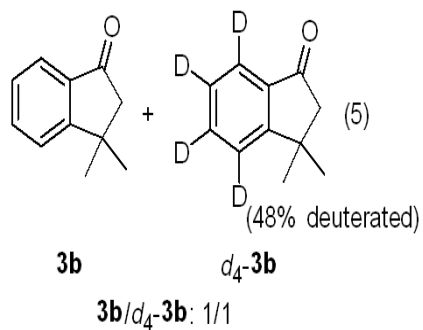
—38.5

30.0



7.68
7.66
7.61
7.59
7.57
7.49
7.49
7.48
7.47
7.47
7.36
7.34
7.32

// //



-2.57

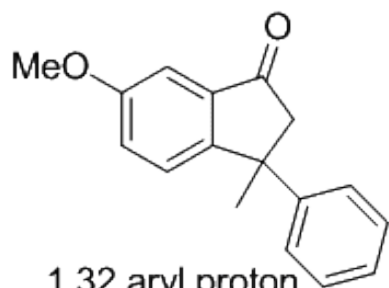
-1.40

0.50
0.50
0.76
0.50

1.97

6.00

f1 (ppm)
S46



1.32 aryl proton
deuterated

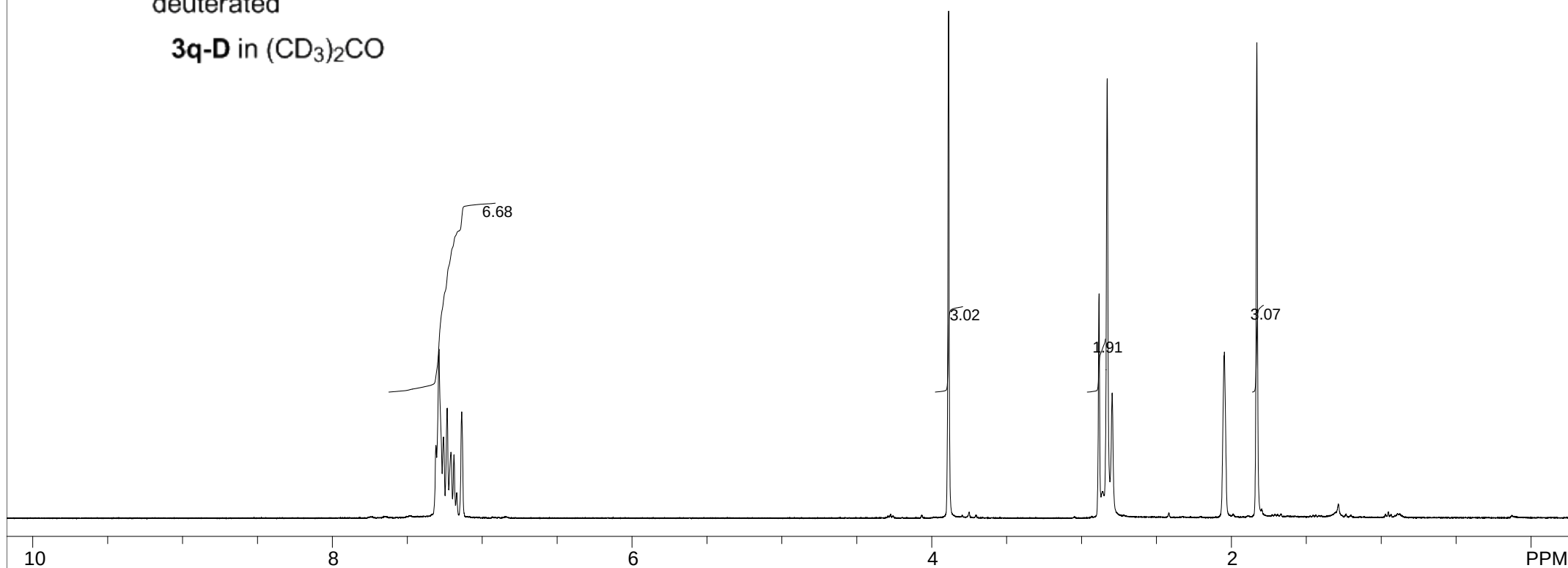
3q-D in (CD₃)₂CO

7.308
7.289
7.258
7.233
7.209
7.189
7.137

3.888

2.884
2.829
2.796

2.050
2.047
1.831



Std proton;blank line

USER: -- DATE: Jul 5 2017

F1: 400.032 F2: 100.597

SW1: 7225

OF1: 727.1

PTS1d: 32768

EX: s2pul

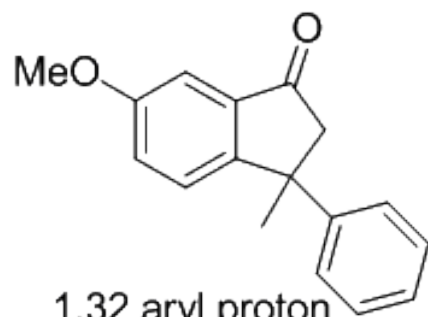
PW: 10.4 usec

PD: 1.0 sec

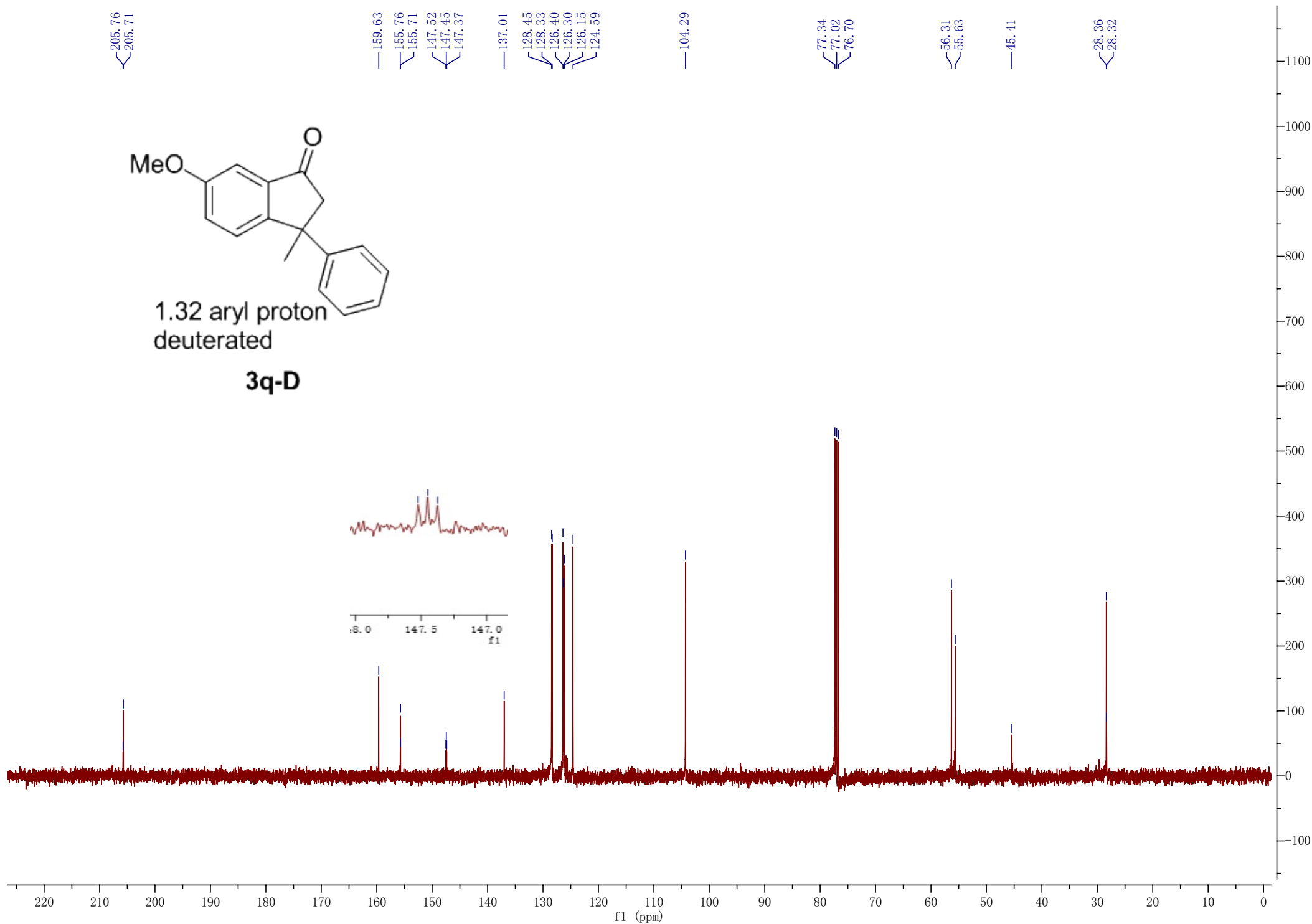
NA: 16

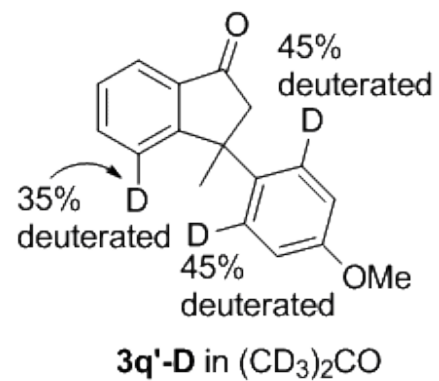
LB: 0.0

Nuts - \$lxy-5-92-1-1111.fid



3q-D



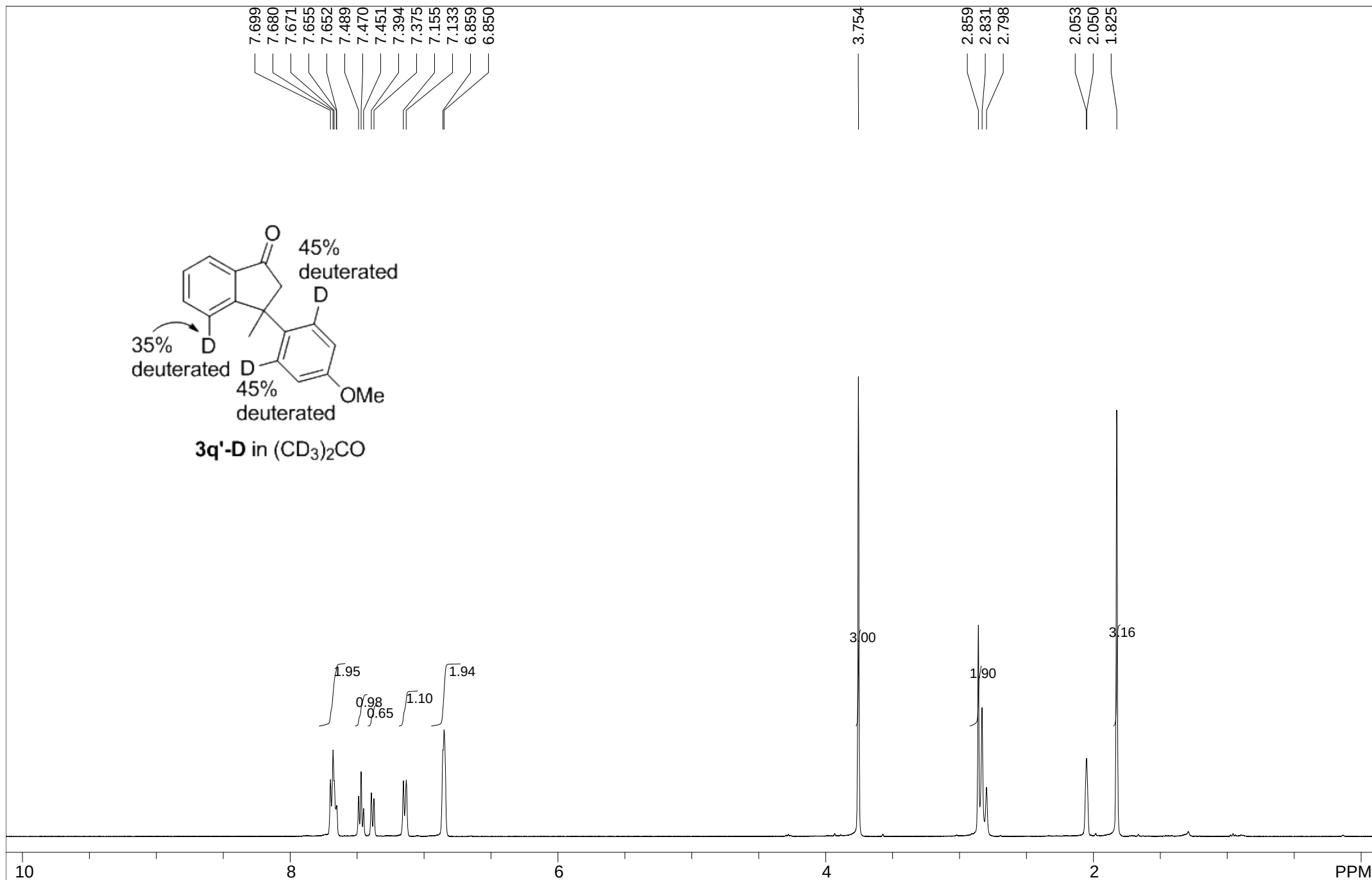


7.699
 7.680
 7.671
 7.655
 7.652
 7.489
 7.470
 7.451
 7.394
 7.375
 7.155
 7.133
 6.859
 6.850

3.754

2.859
 2.831
 2.798

2.053
 2.050
 1.825



Std proton;blank line

USER: -- DATE: Jul 5 2017

F1: 400.032

F2: 100.597

SW1: 7225

OF1: 727.7

PTS1d: 32768

EX: s2pul

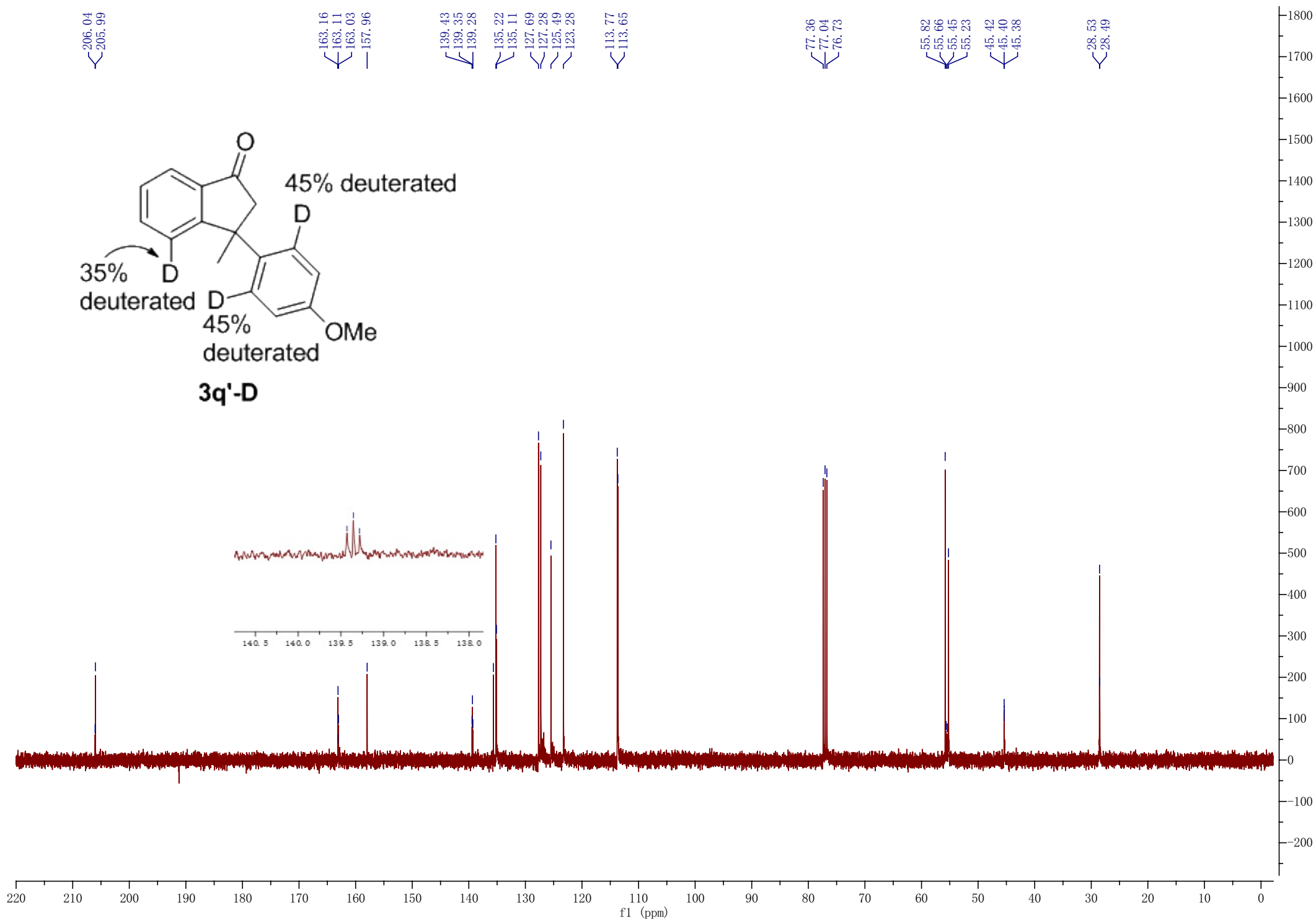
PW: 10.4 usec

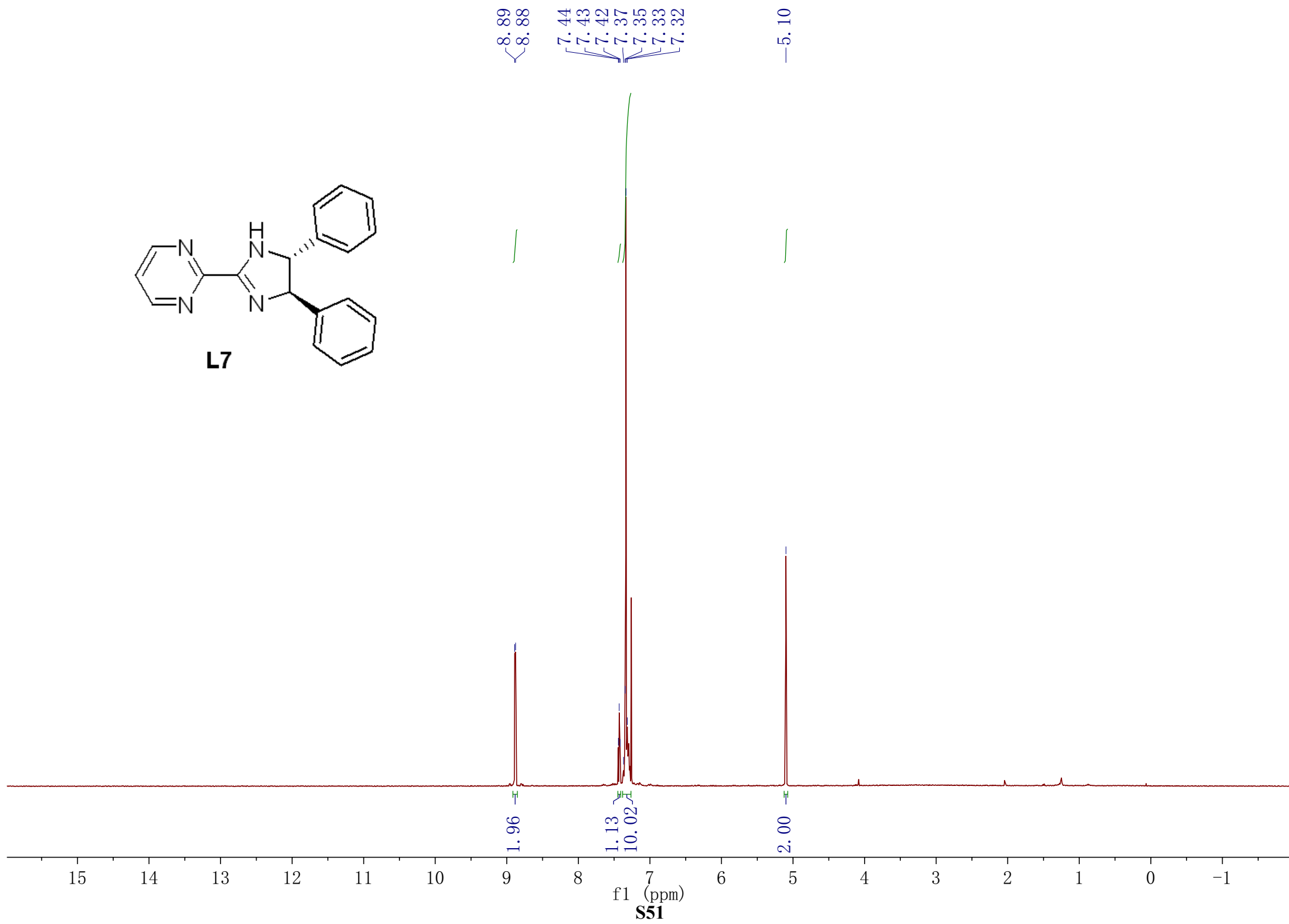
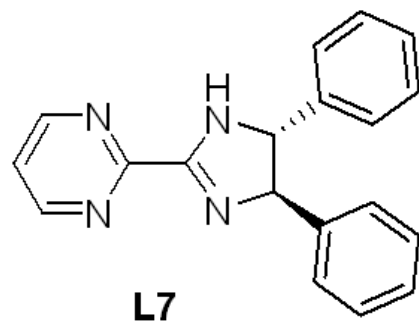
PD: 1.0 sec

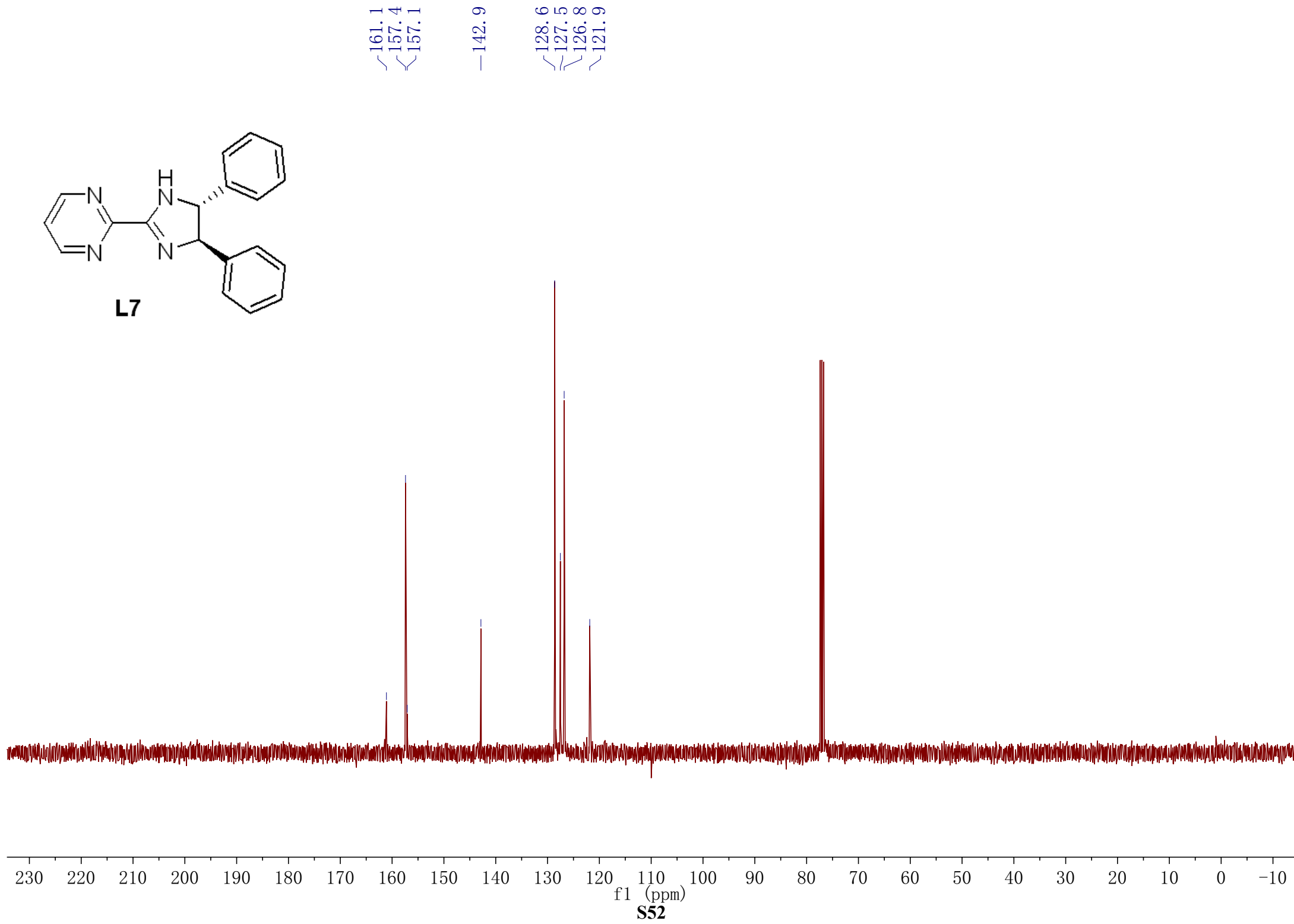
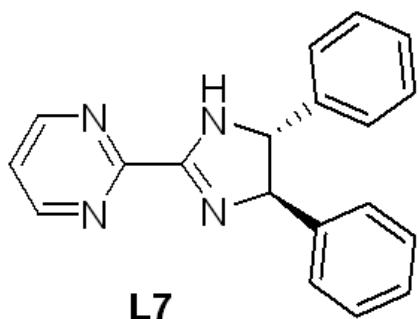
NA: 16

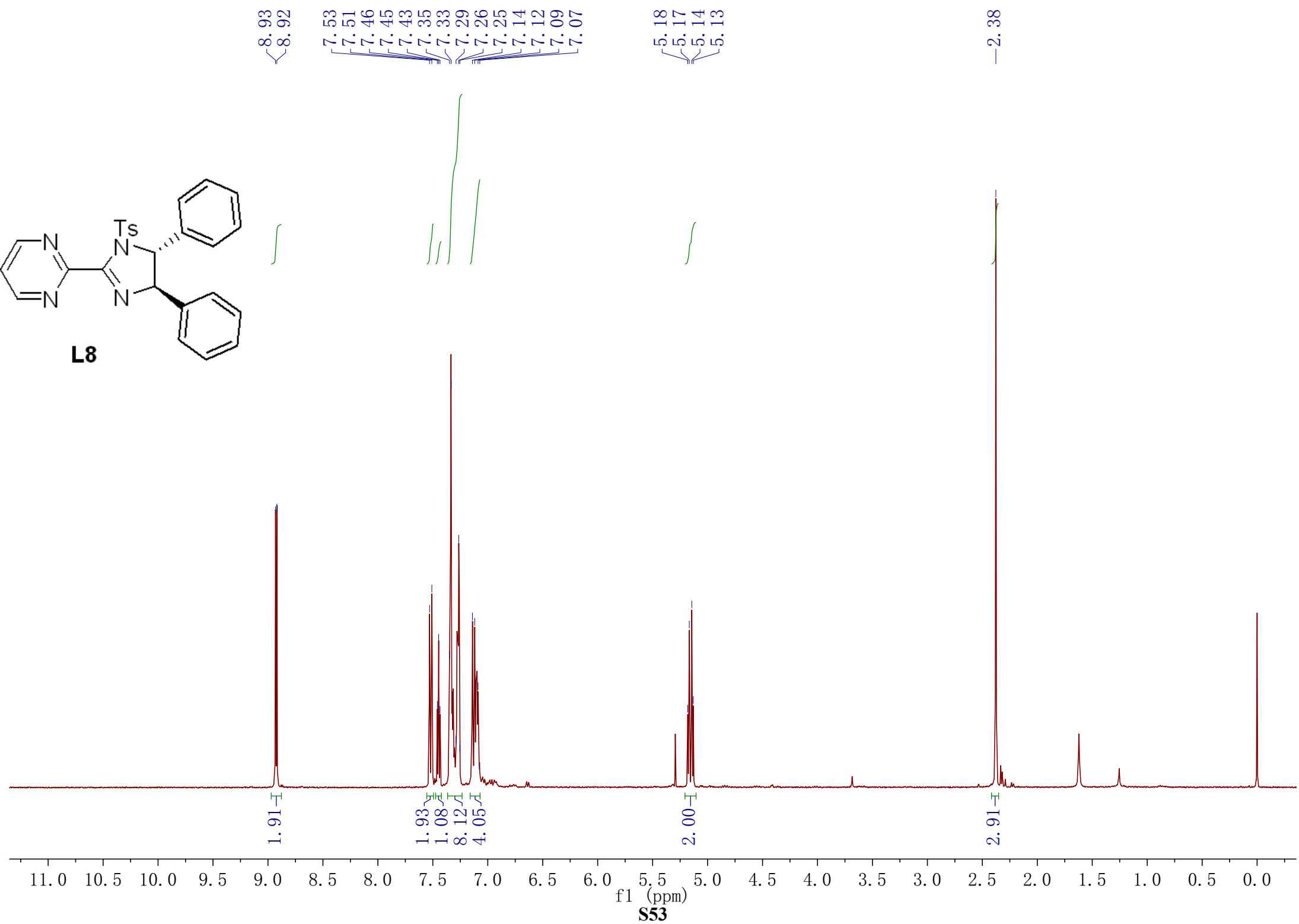
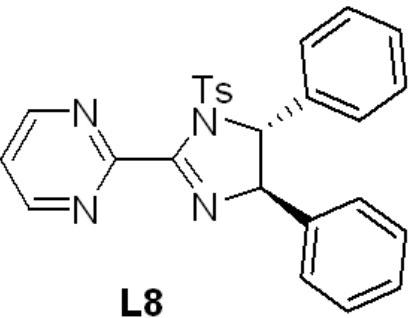
LB: 0.0

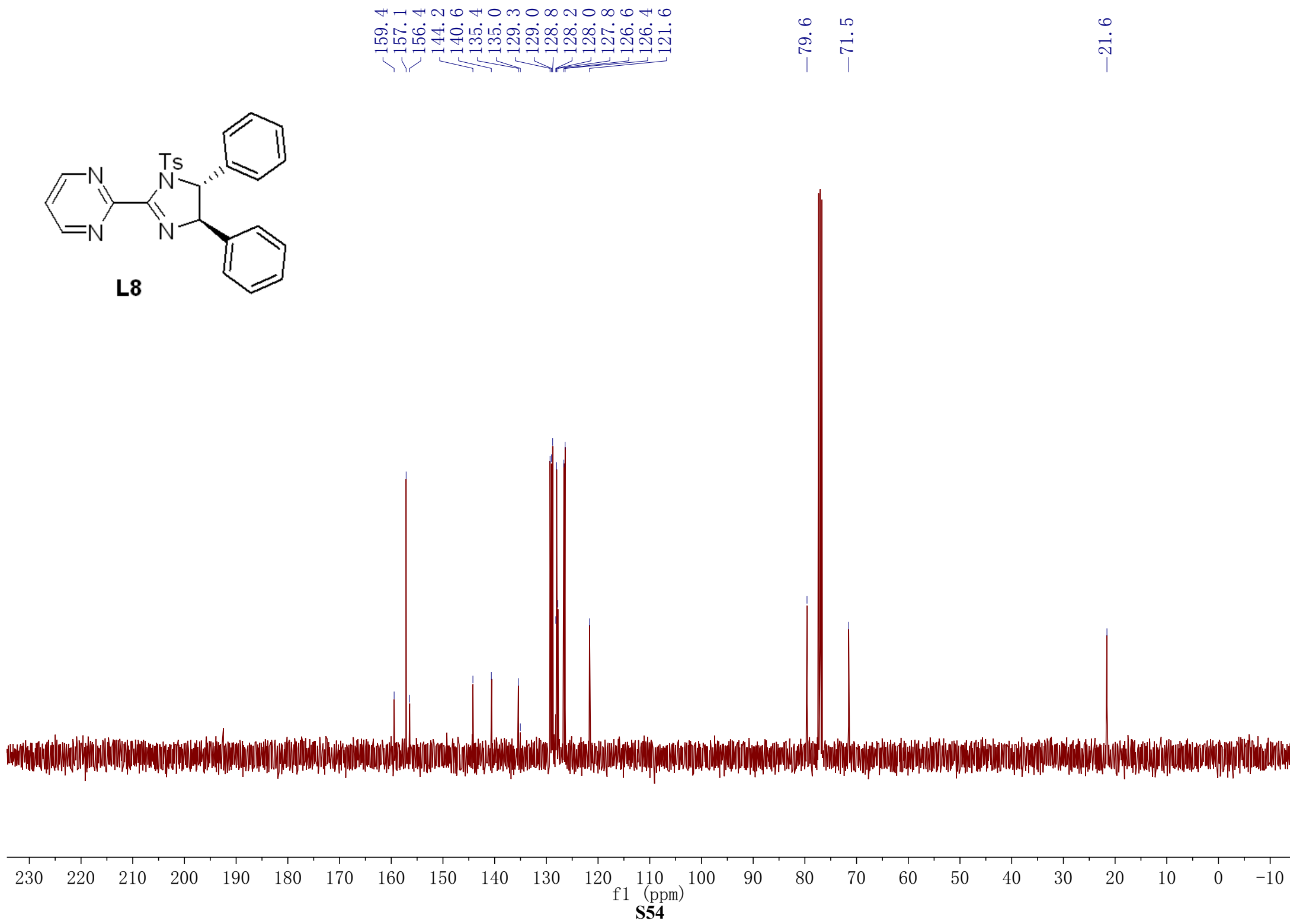
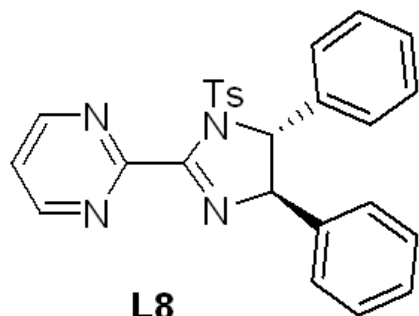
Nuts - \$lxy-5-92-1-2222.fid



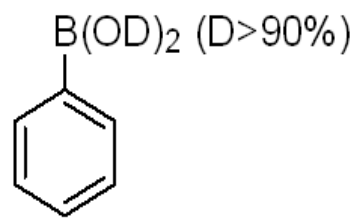




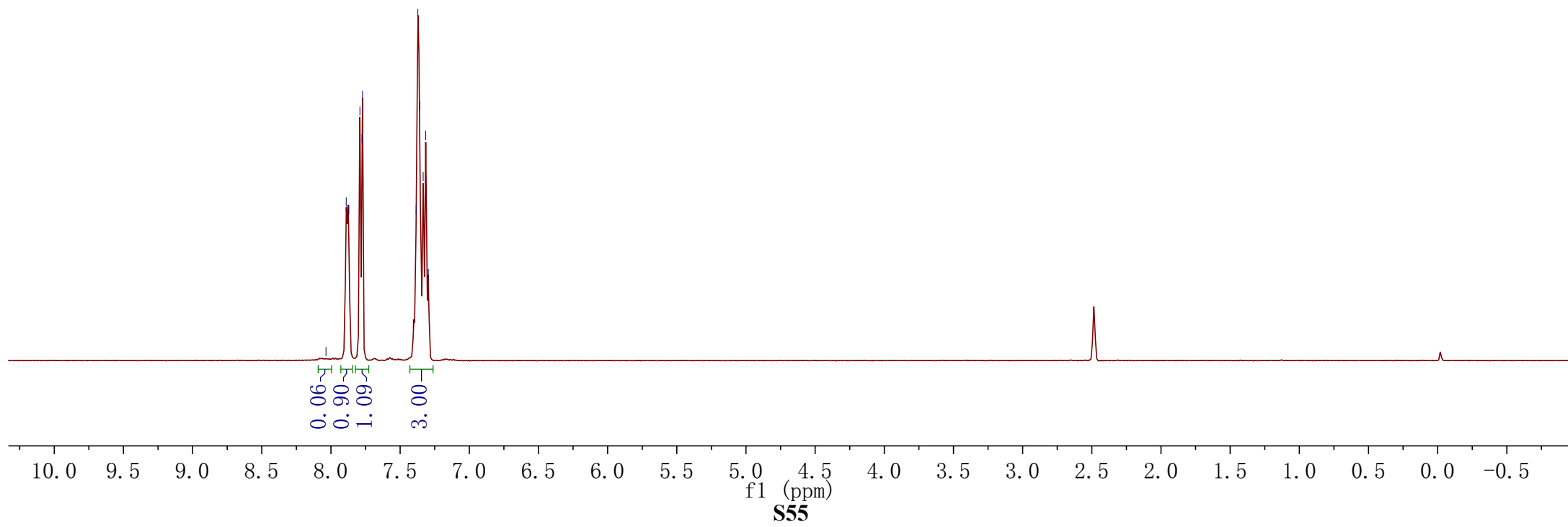


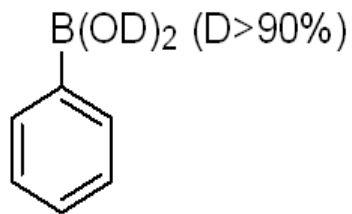


8.04
7.89
7.87
7.79
7.78
7.77
7.40
7.38
7.37
7.36
7.33
7.31
7.30



with 30%mol (PhBO)₃





with 30%mol (PhBO)₃

