

Supporting Information

**Facile synthesis of α -alkoxyl amides via scandium-catalyzed oxidative reaction
between ynamides and alcohols**

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Ying-Wu Yin,* and Long-Wu Ye*

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Chemical Biology of Fujian Province, College of Chemistry and Chemical
Engineering, Xiamen University, Xiamen 361005, China

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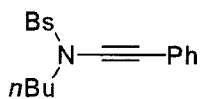
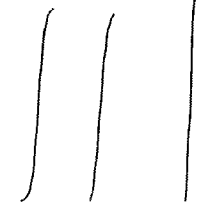
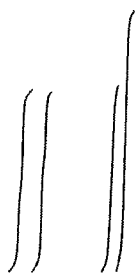
General Information. Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1, 2-dichloroethane (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

^1H NMR spectra and ^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform- d_3 . For ^1H NMR spectra, chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. For ^{13}C NMR spectra, chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

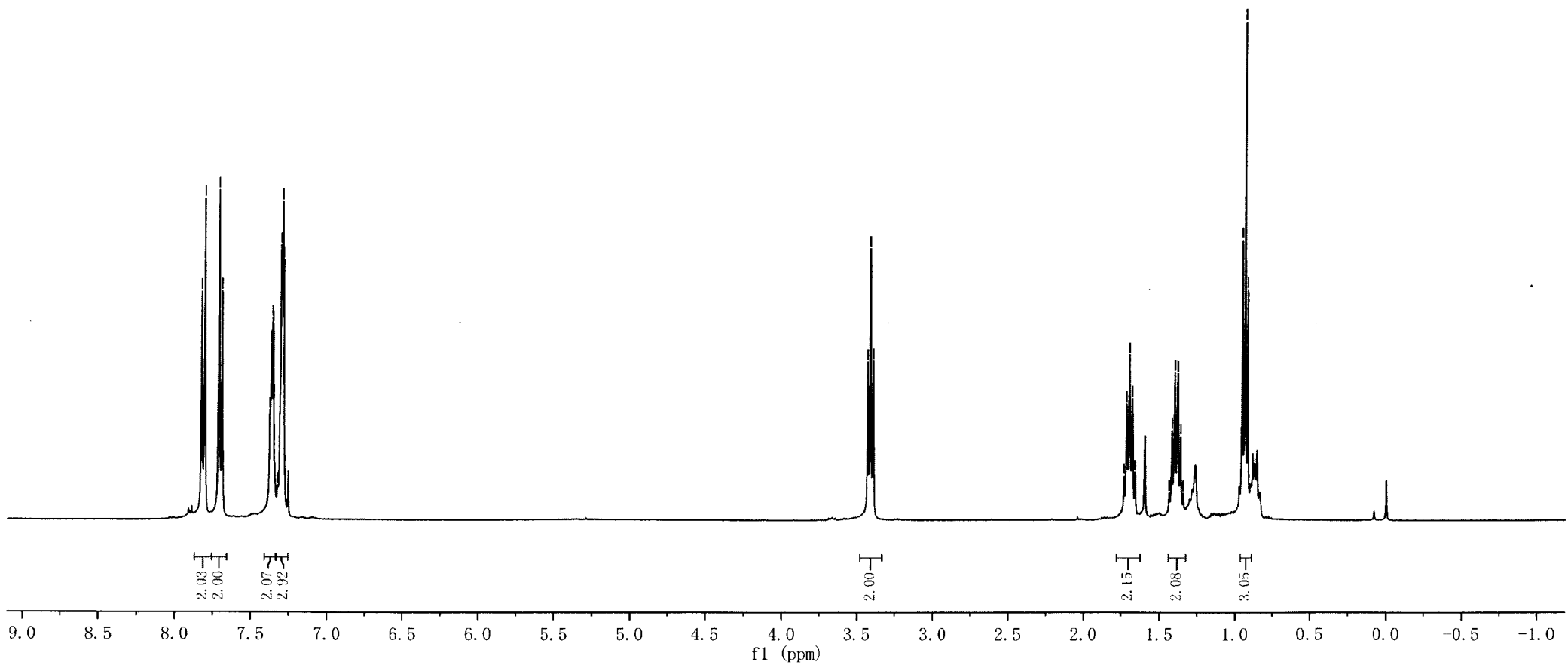
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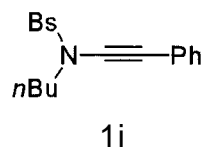
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1.732
1.714
1.695
1.677
1.658
1.417
1.399
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0.916



1i





136.47
132.42
131.40
129.01
128.74
128.29
127.95
122.54

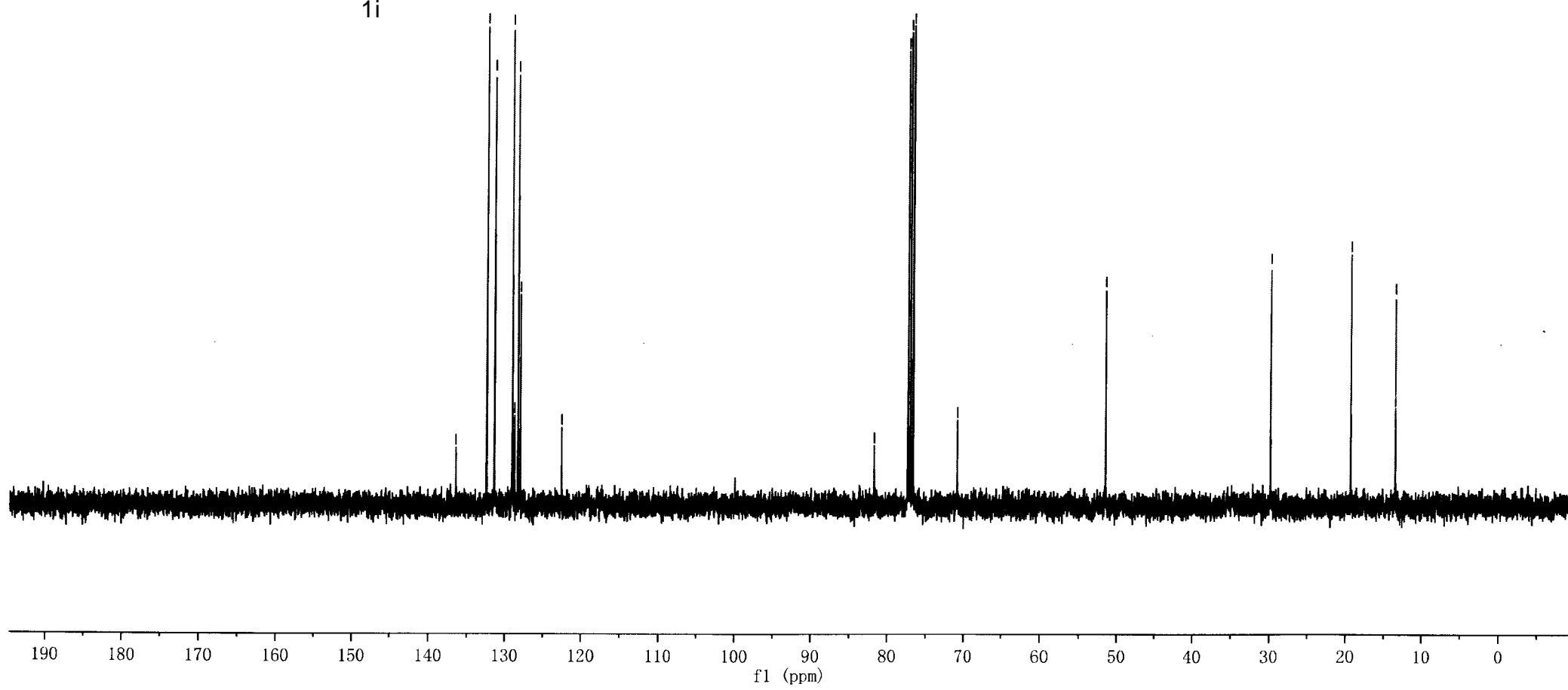
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29.90

19.42

13.53

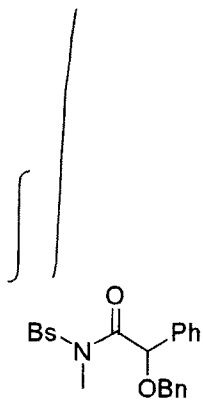


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7.269

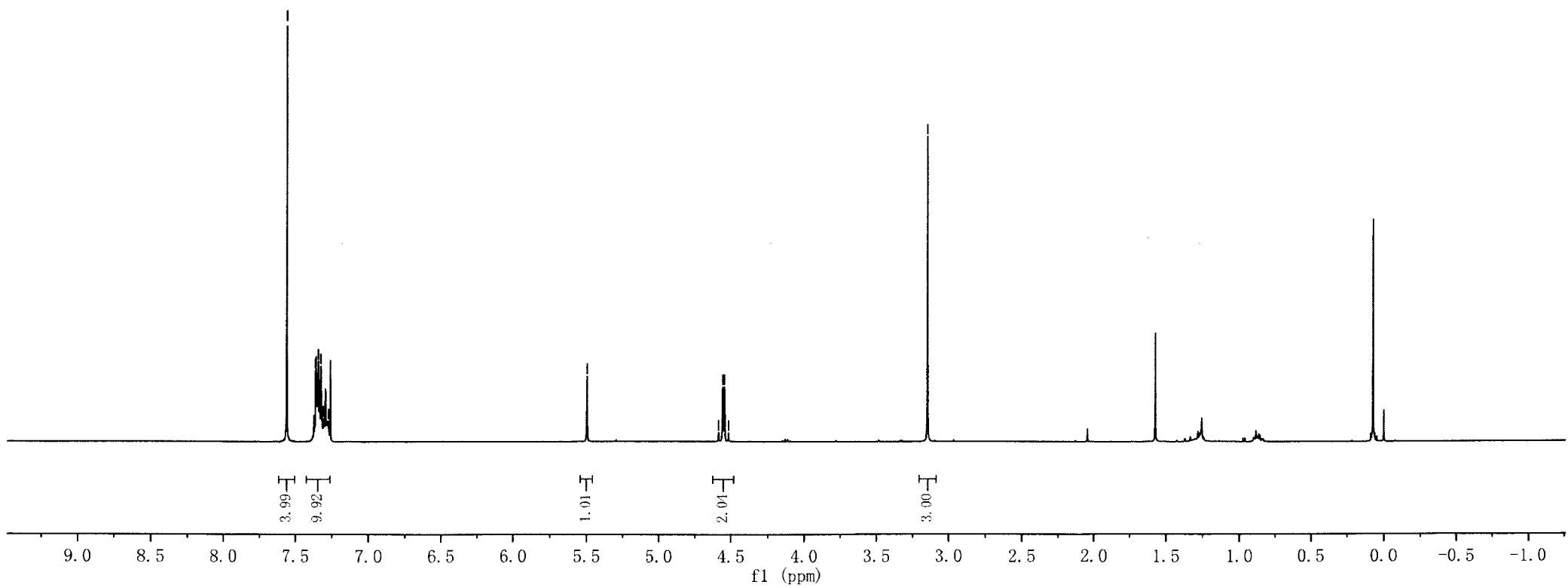
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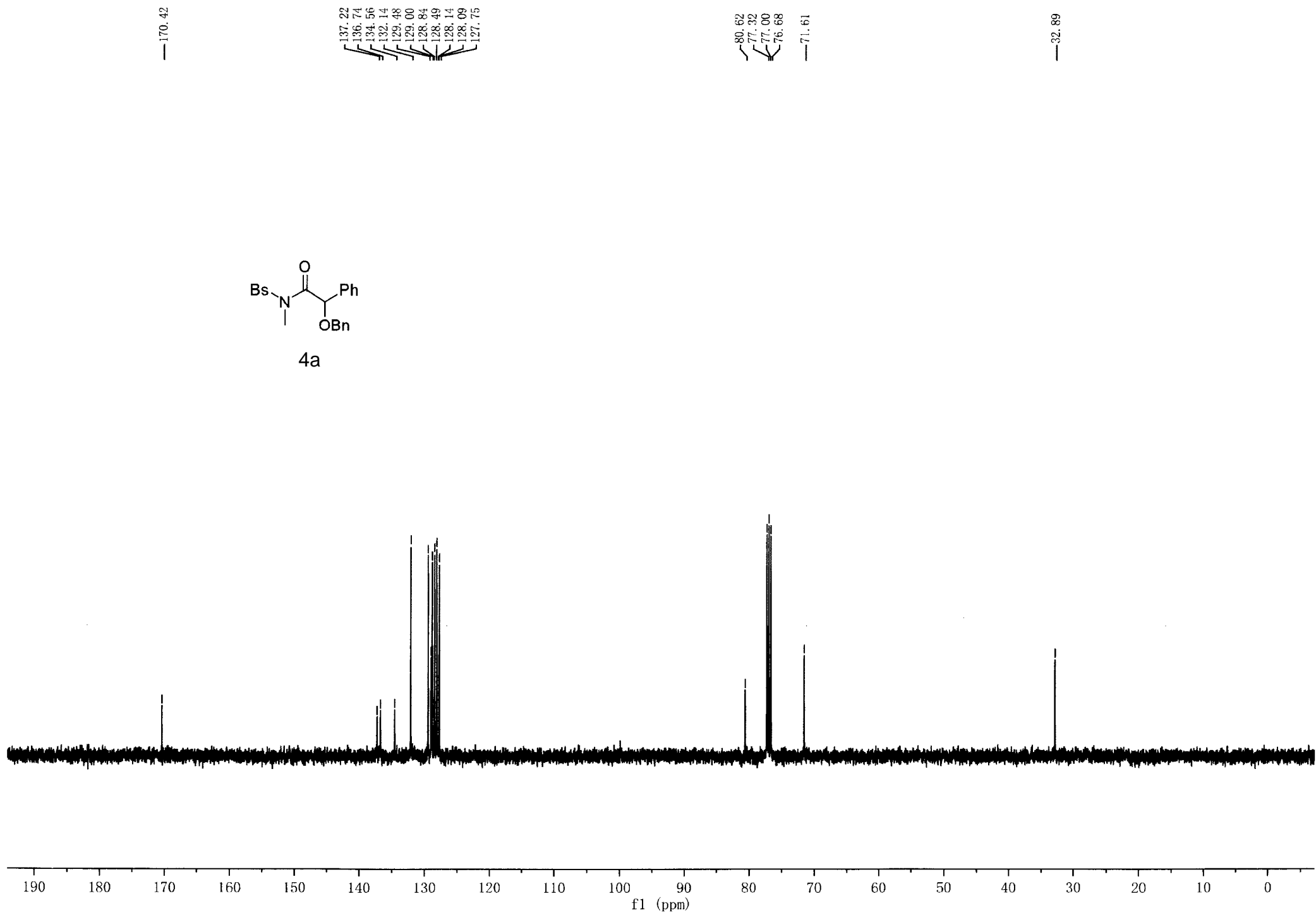
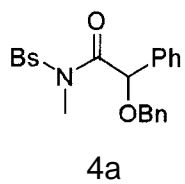
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4.545
4.516

3.146

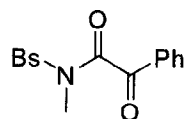


4a





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7.923
7.894
7.872
7.767
7.745
7.678
7.659
7.641
7.558
7.539
7.520



4aa

3.261

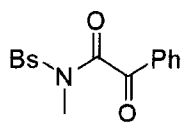


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1.91
2.00
1.03
1.95

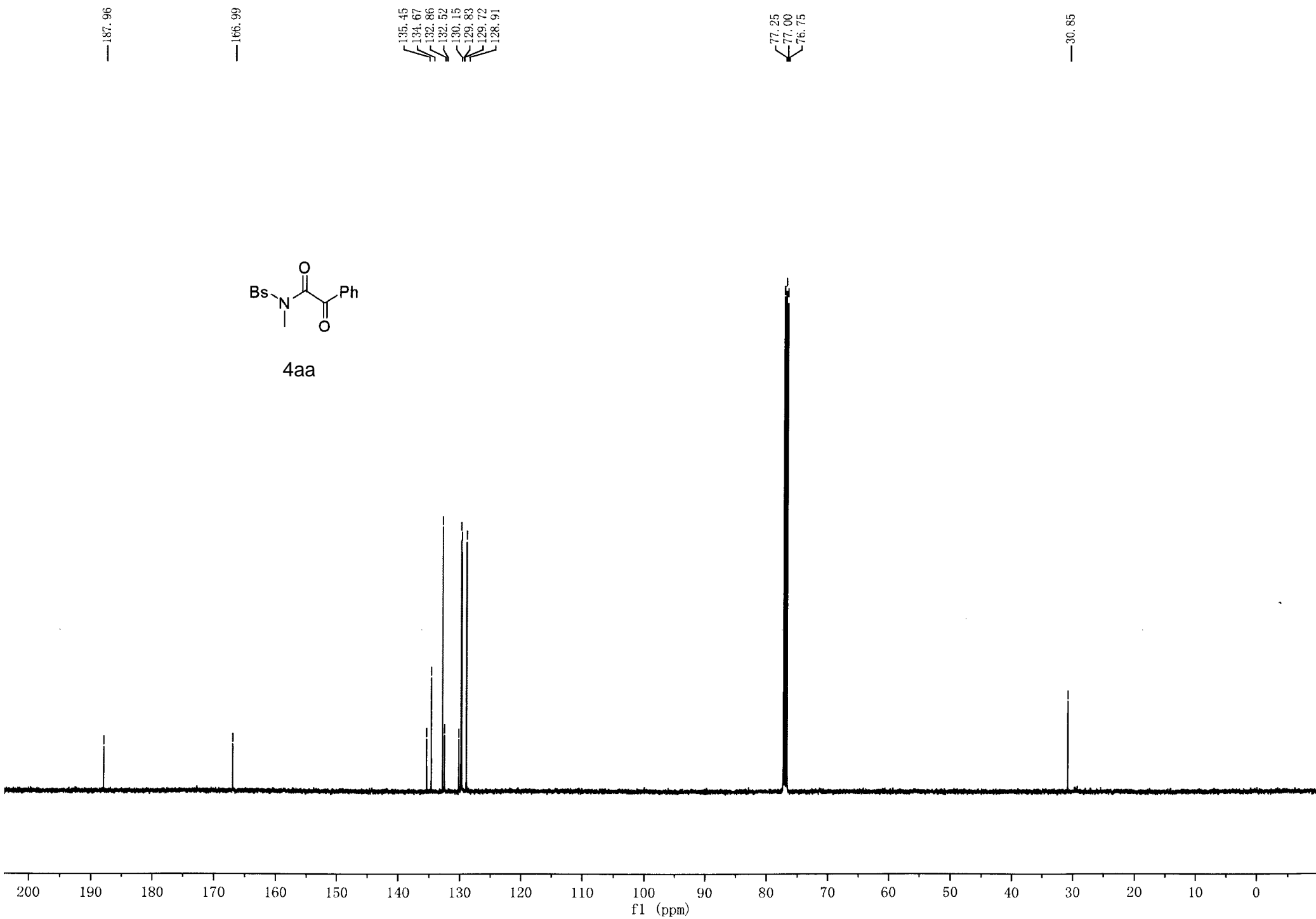
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f1 (ppm)



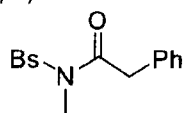
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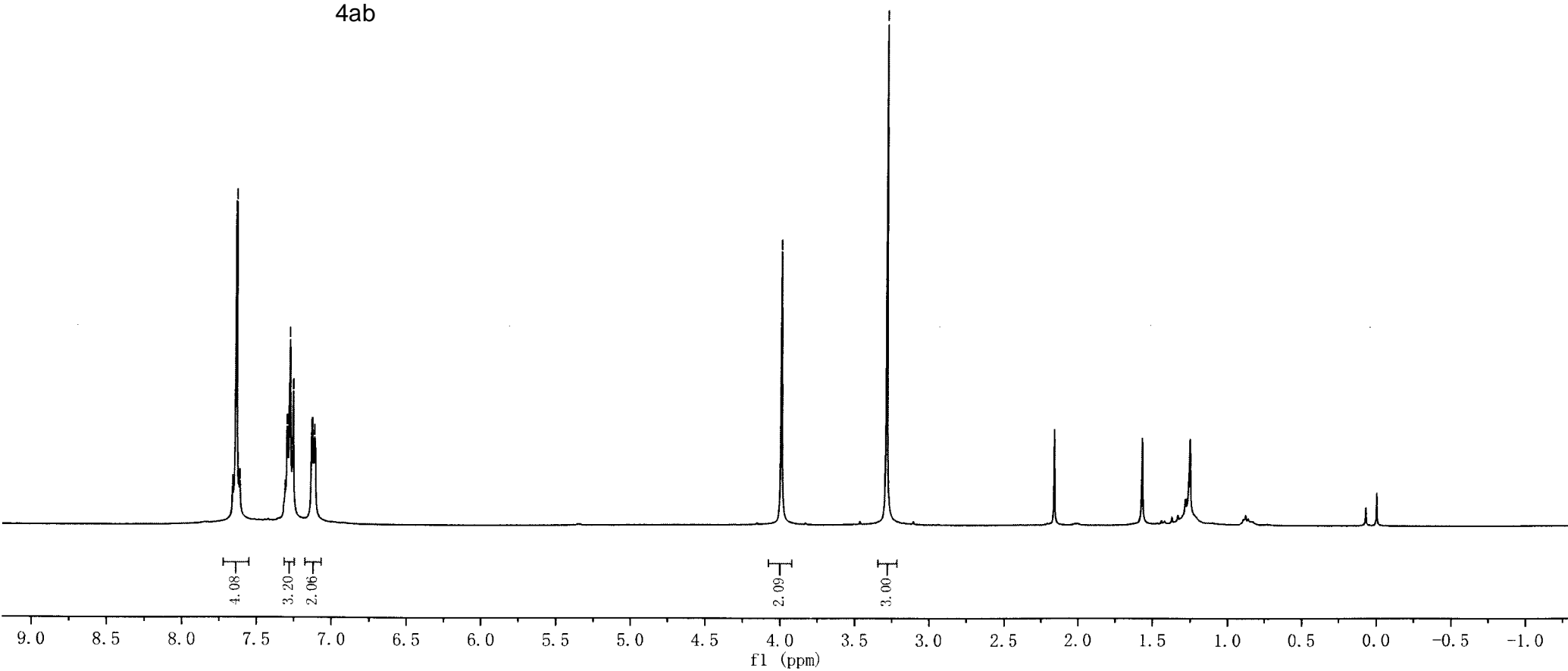
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7.128
7.113

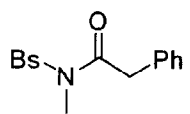
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3.288



4ab





4ab

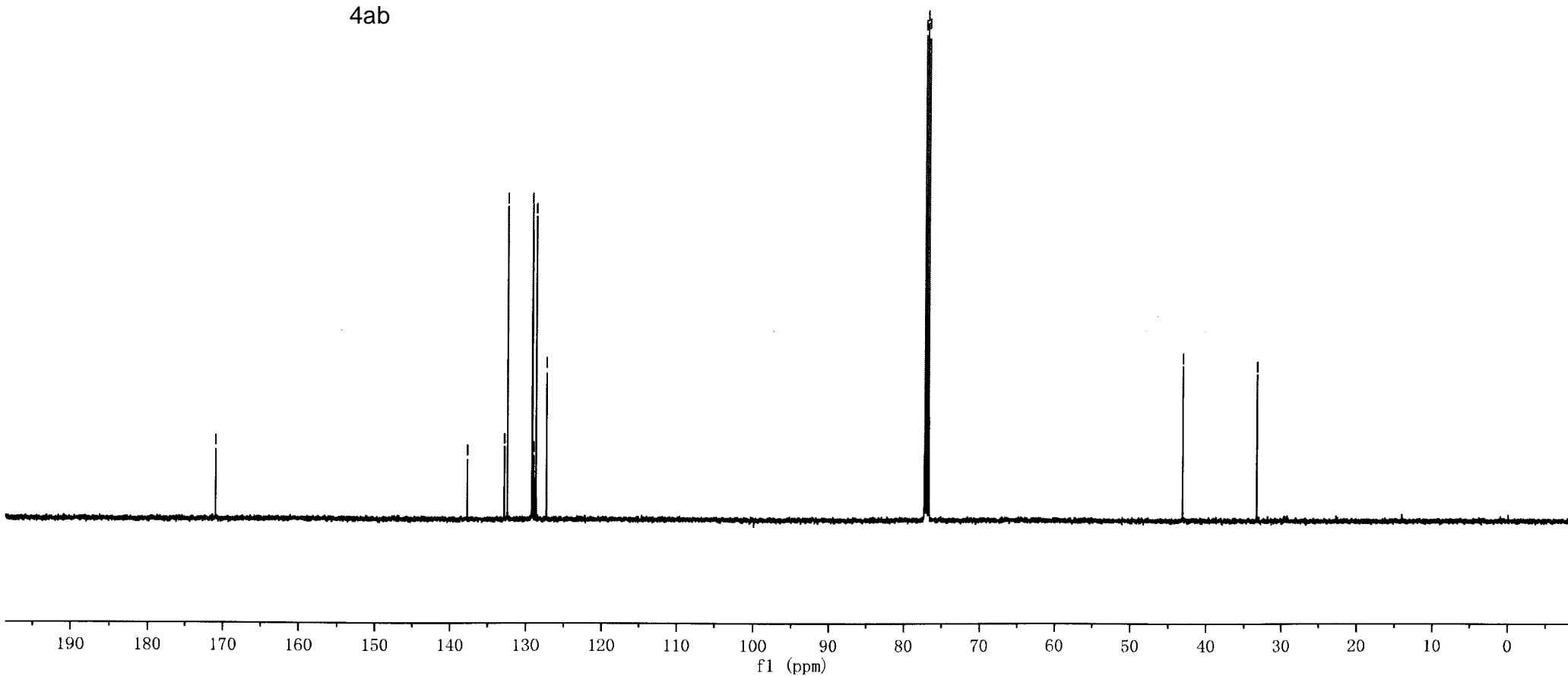
— 170.99

— 137.74
— 132.86
— 132.42
— 129.21
— 129.18
— 129.02
— 128.72
— 127.34

— 77.25
— 77.00
— 76.75

— 43.12

— 33.35

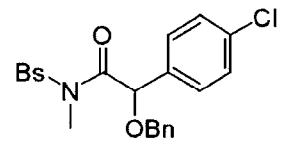


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7.279
7.274
7.255

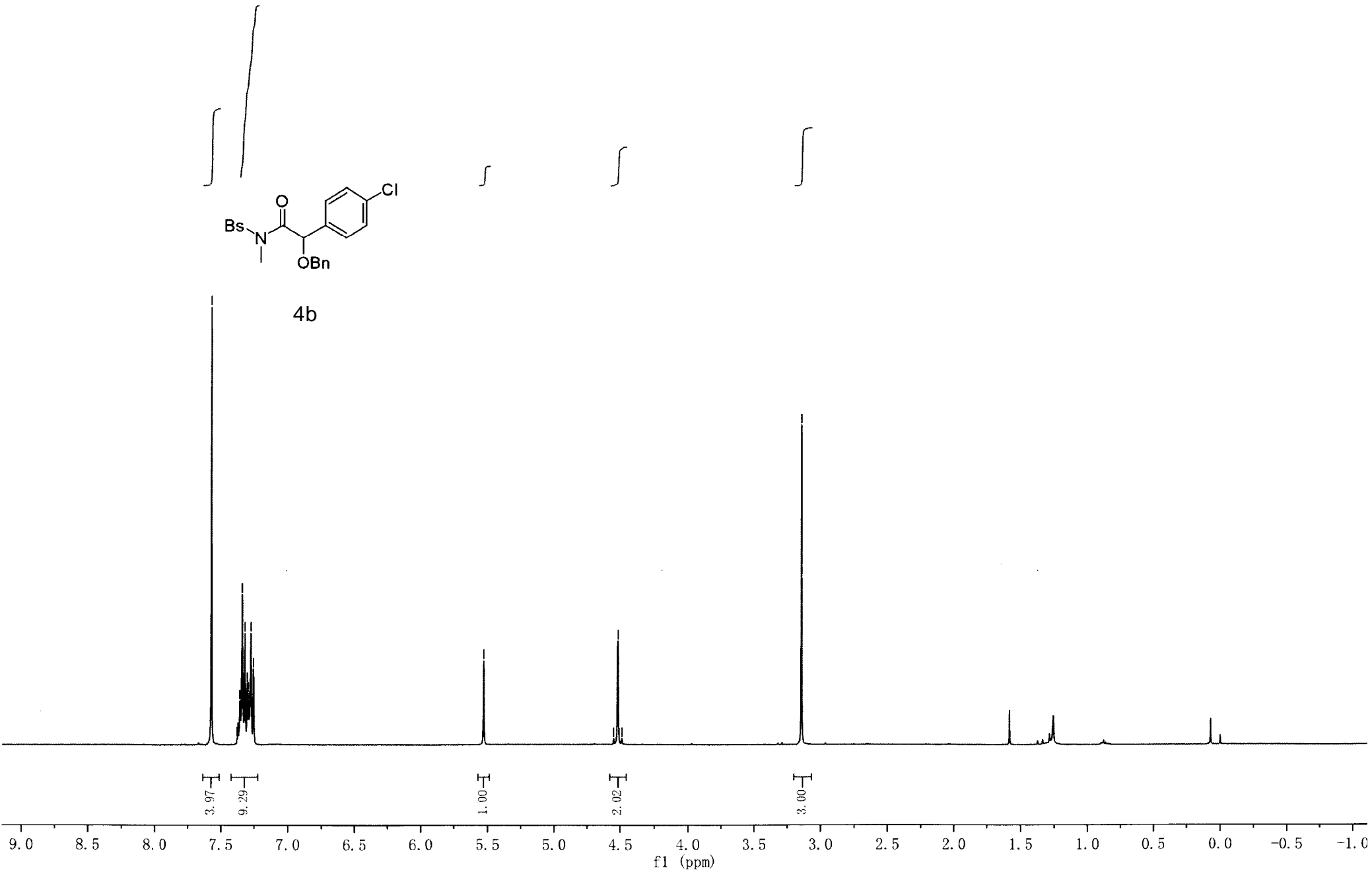
5.529

4.549
4.517
4.487

3.144



4b



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f1 (ppm)

3.97

9.29

1.00

2.02

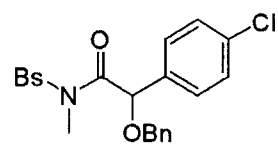
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—170.18

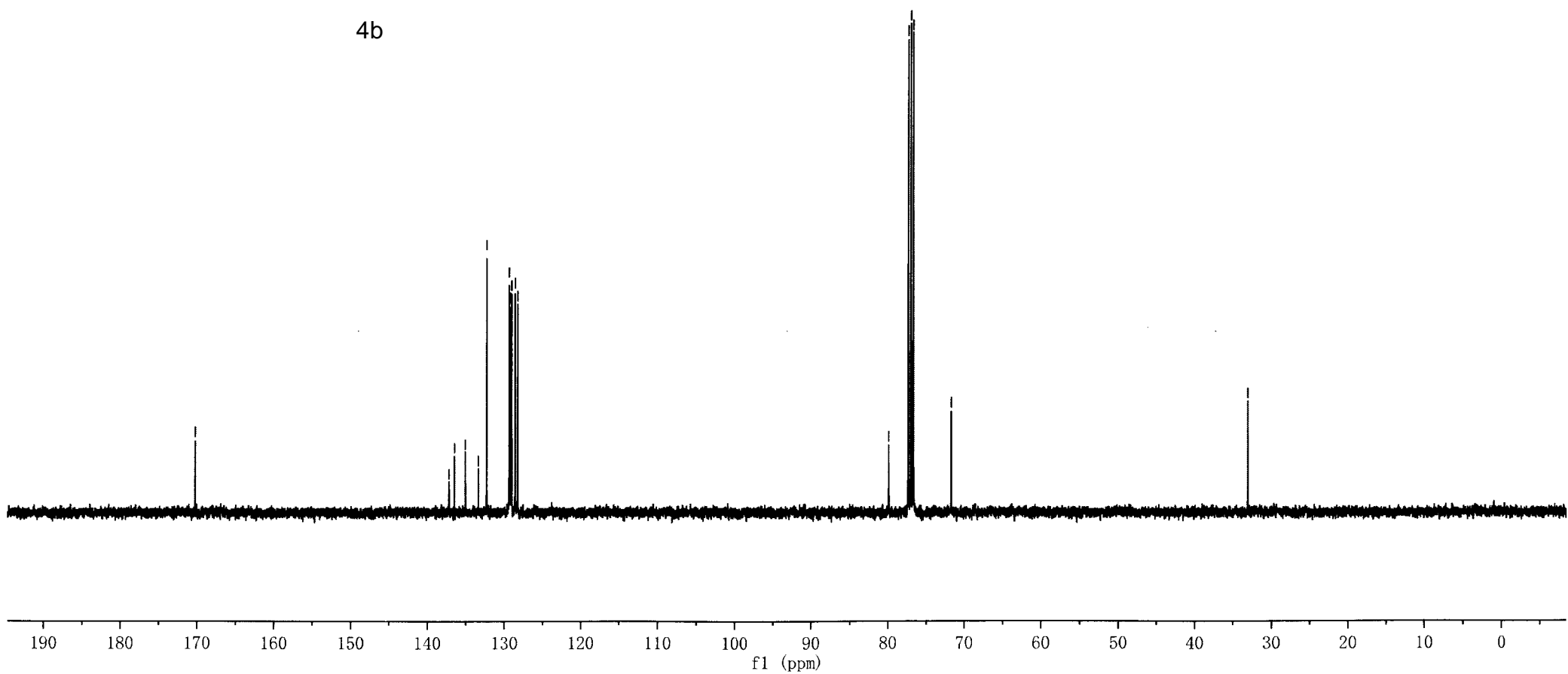
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77.32
77.00
76.68
71.72

—33.02



4b

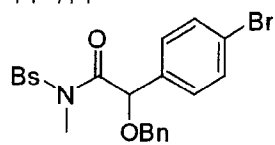


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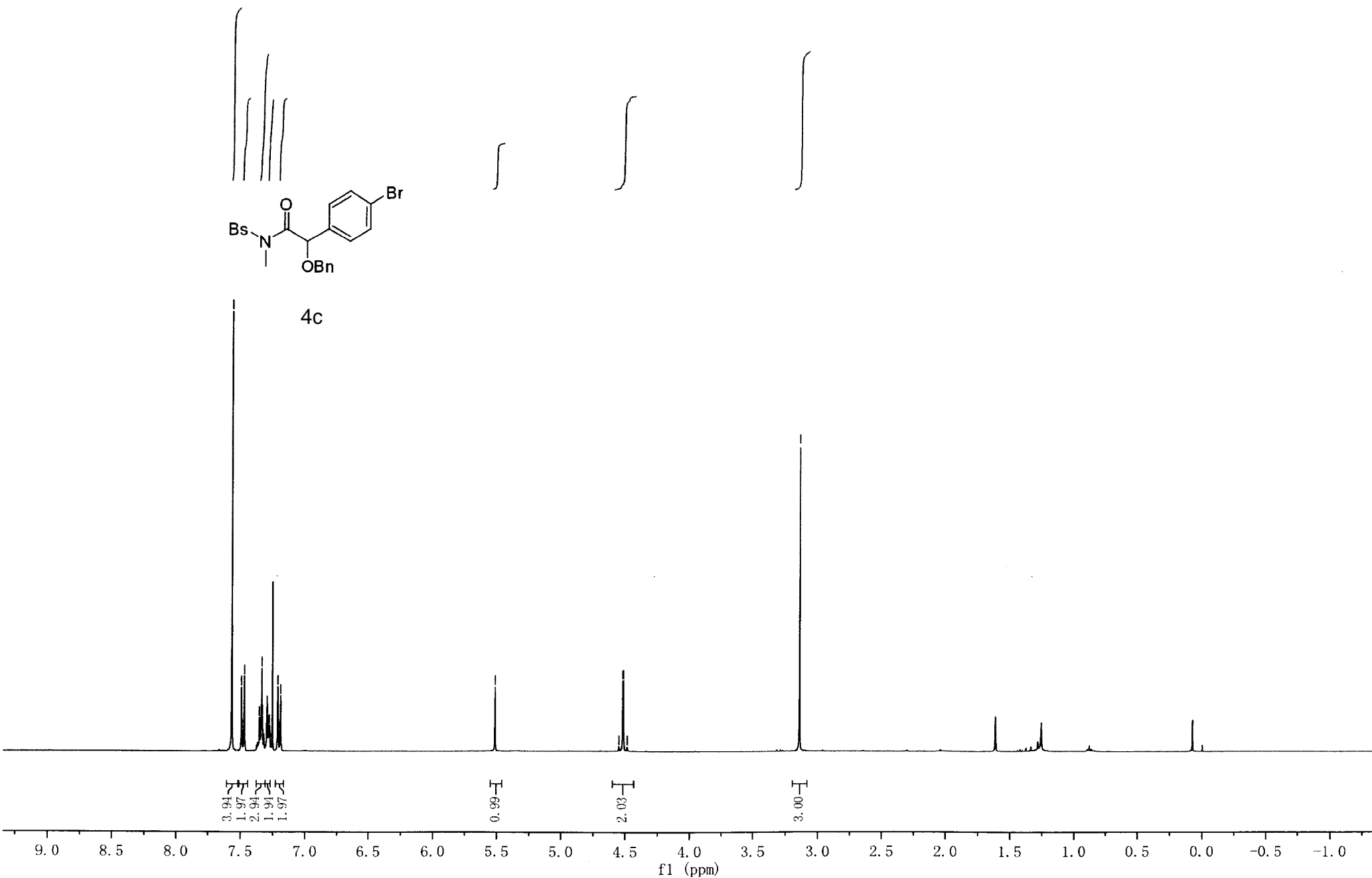
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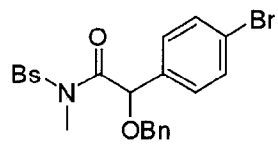
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3.143



4c





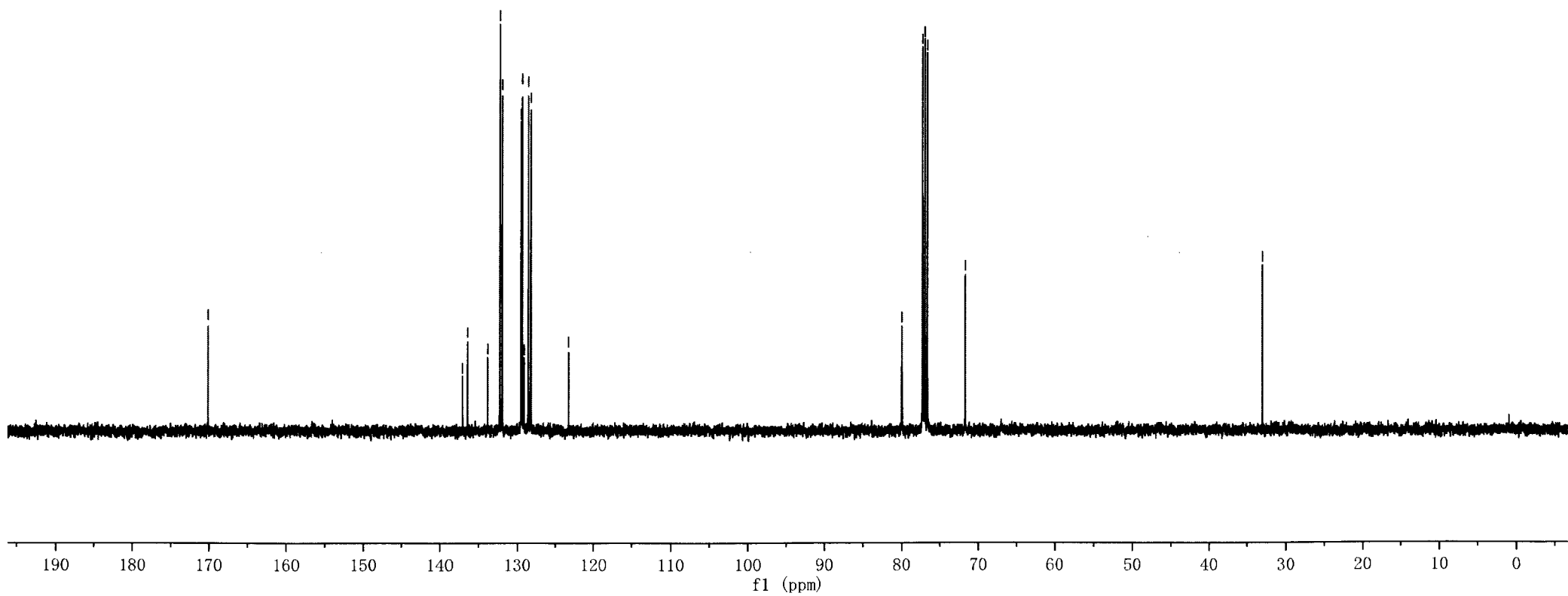
4c

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132.29
131.97
129.48
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129.13
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123.25

79.99
77.32
77.00
76.68
71.73

33.02



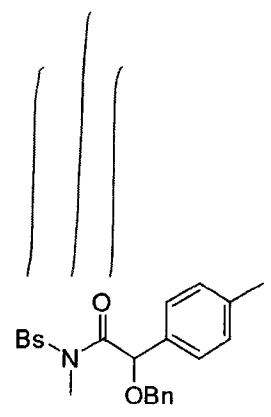
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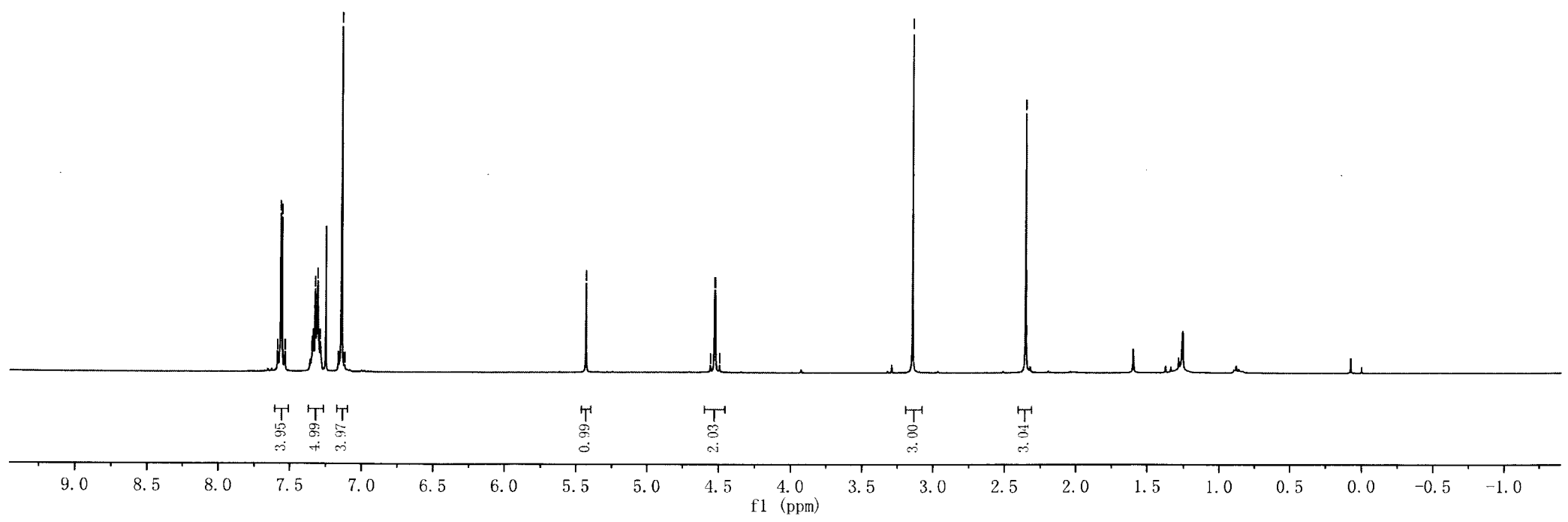
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4.491

3.145

2.353



4d



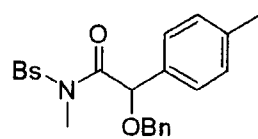
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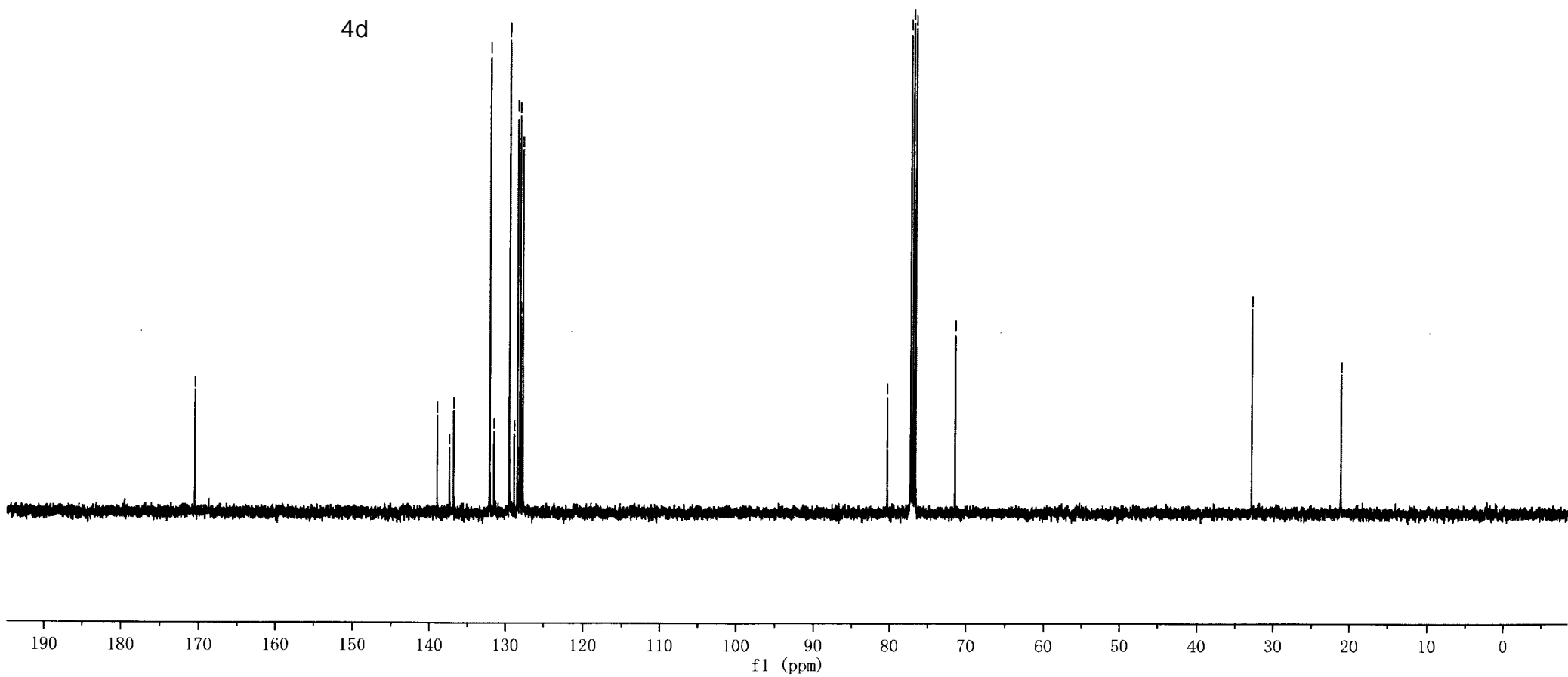
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32.91

21.17



4d



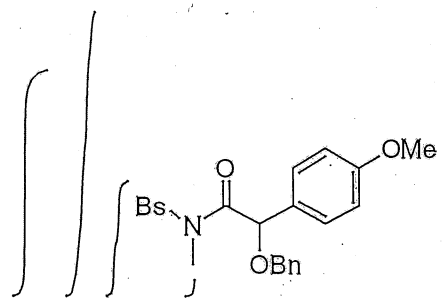
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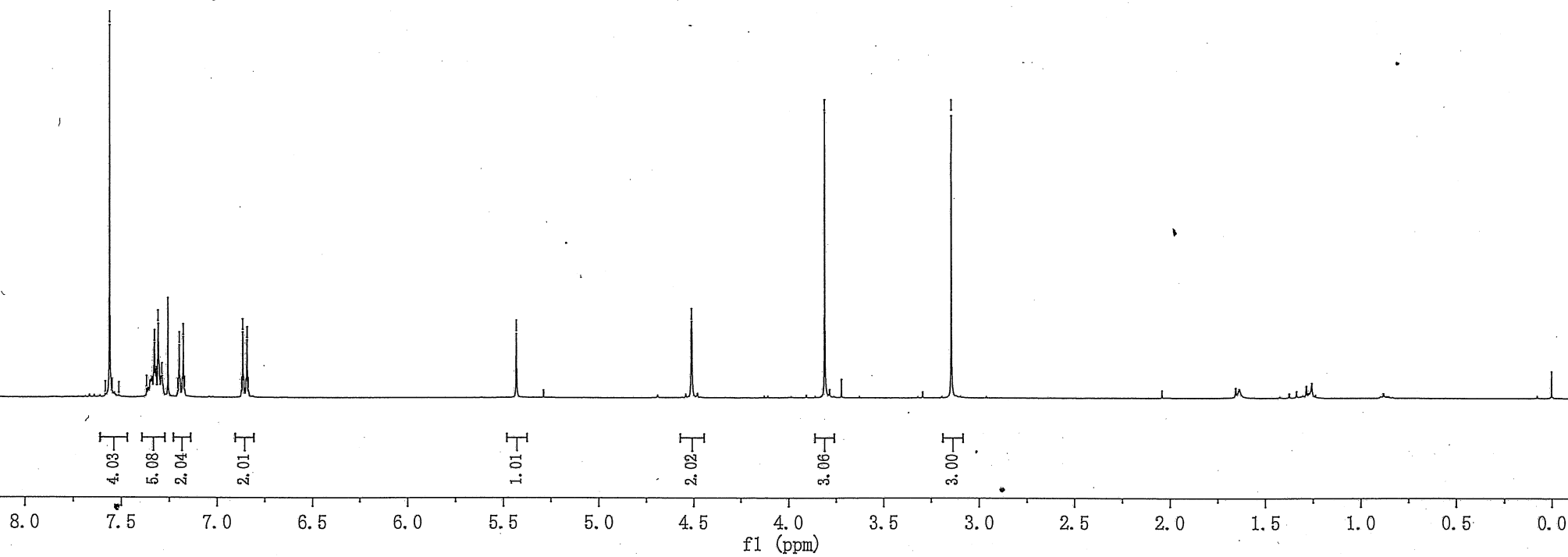
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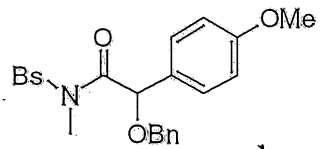
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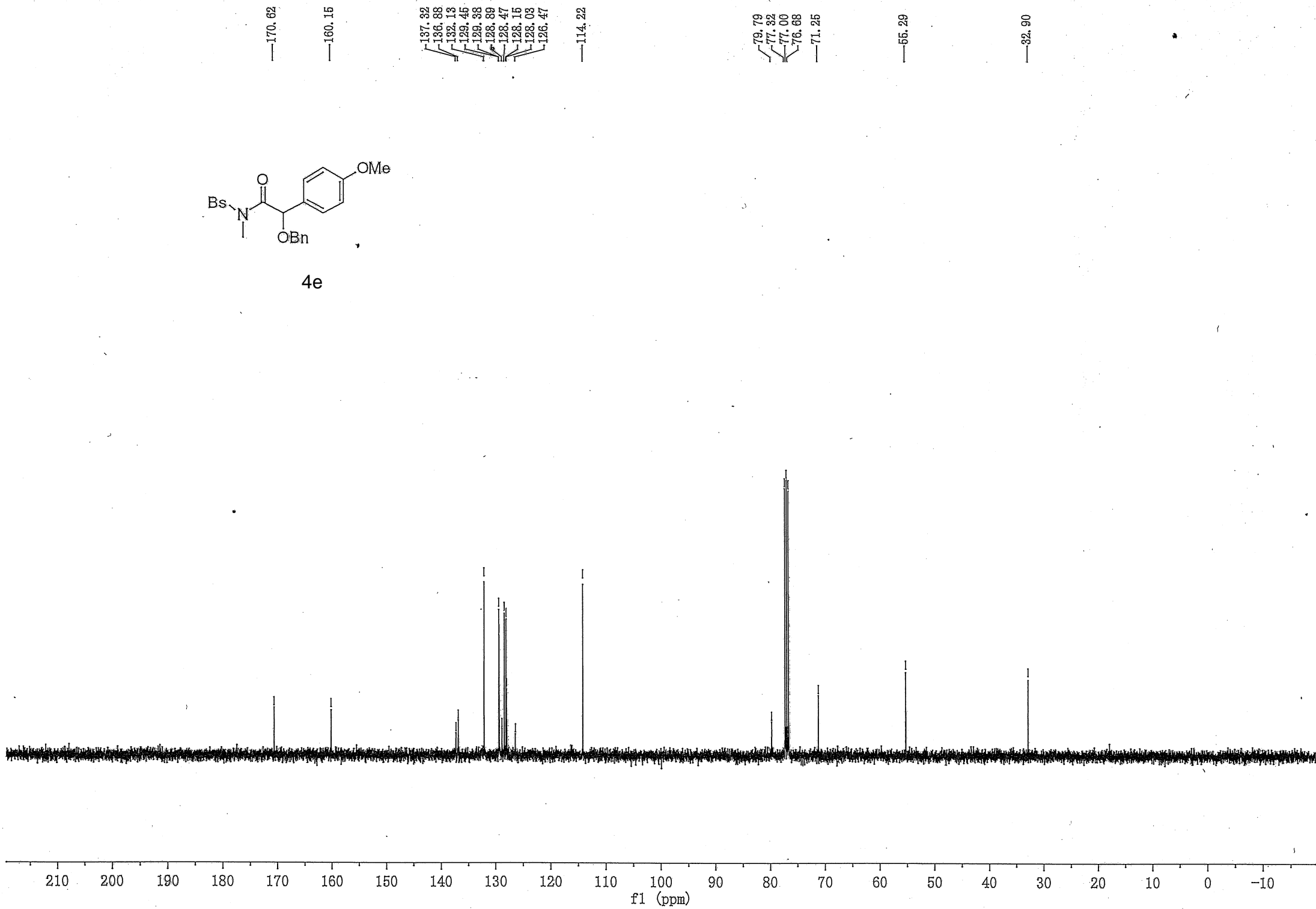


4e





4e

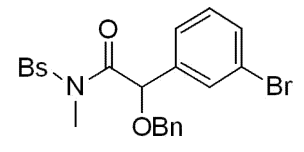


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7.292
7.256
7.248
7.235
7.216
7.196

5.497

4.578
4.549
4.538
4.509

3.159



4f

4.01
1.03
6.01
1.98

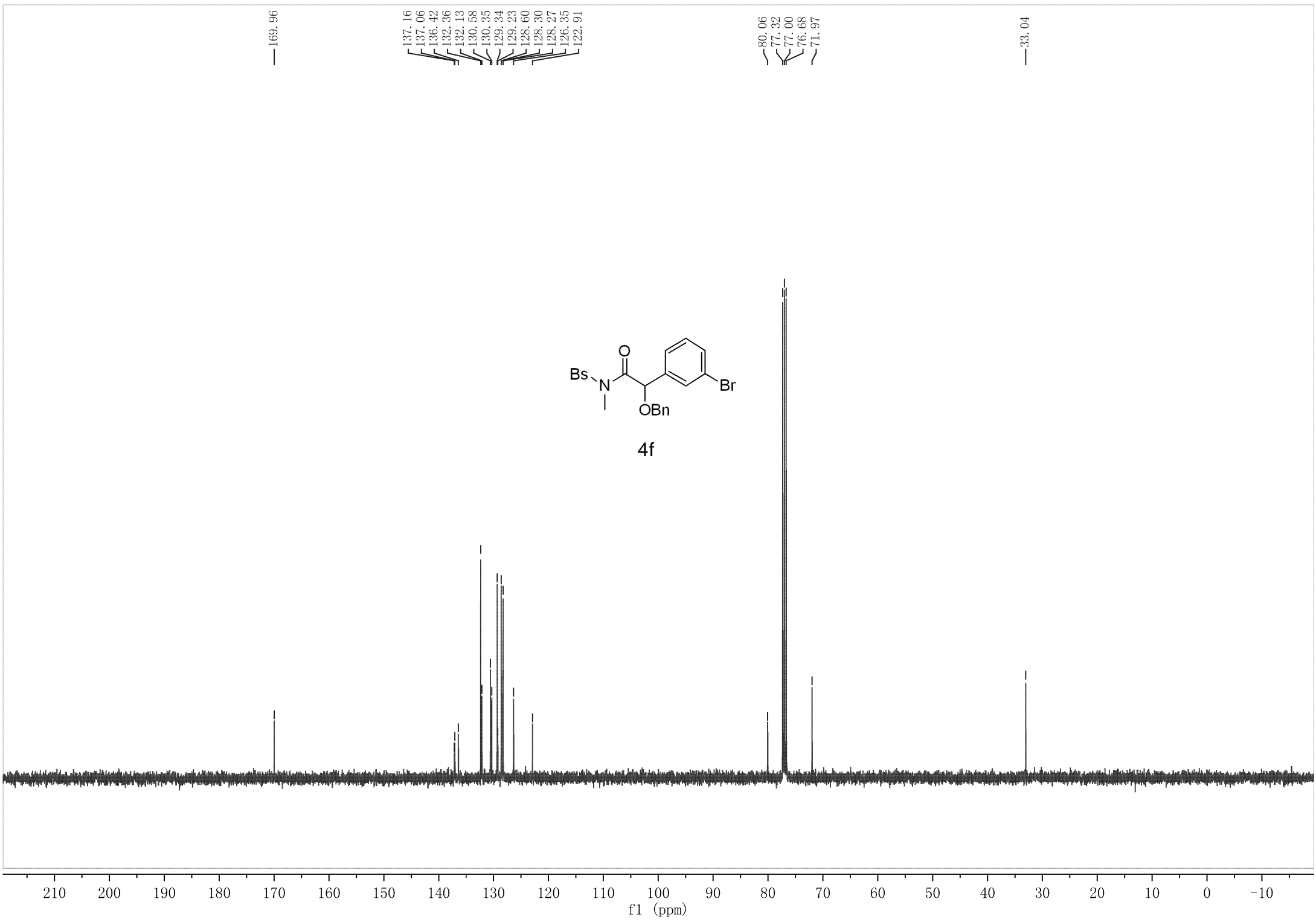
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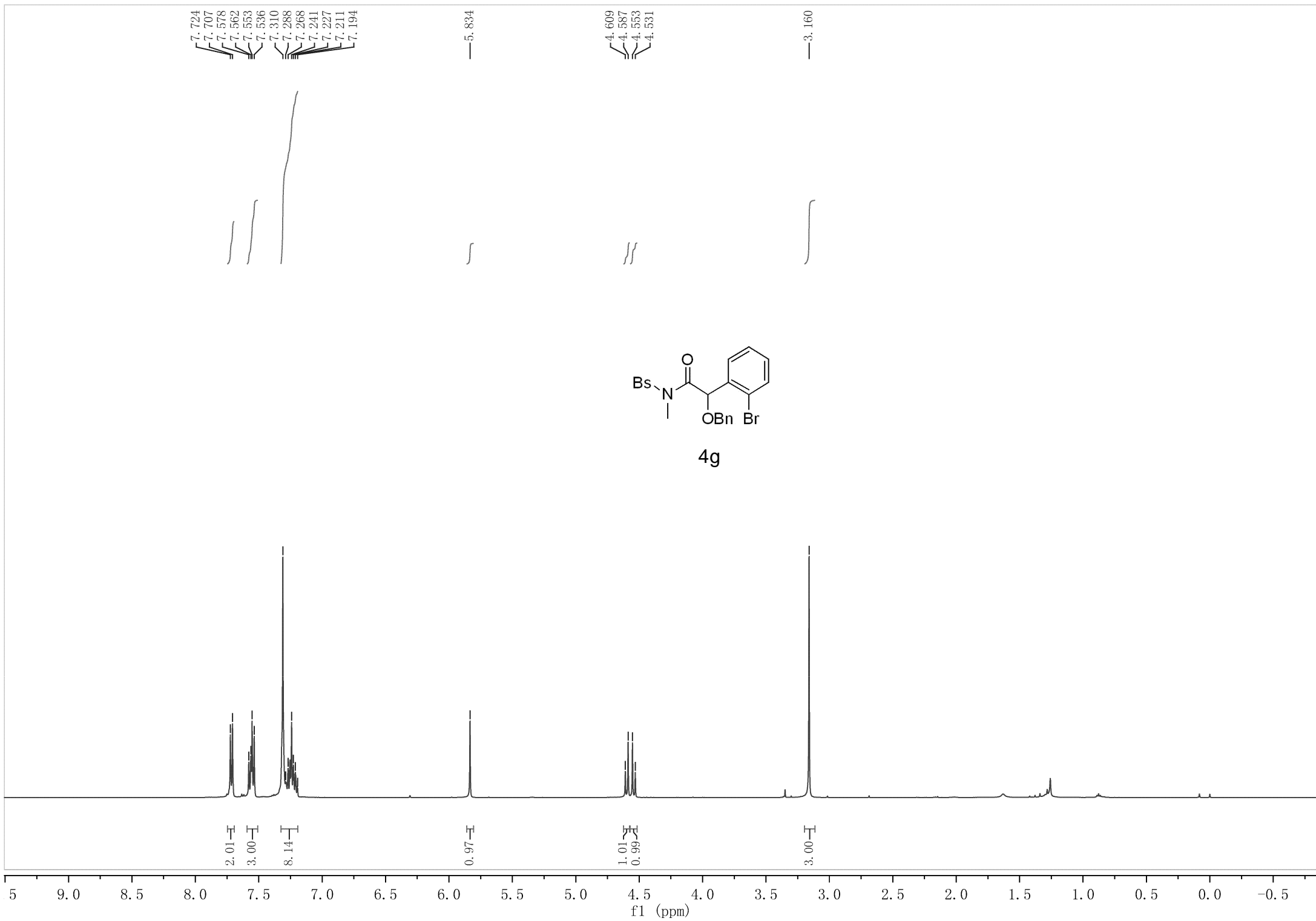
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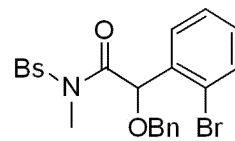
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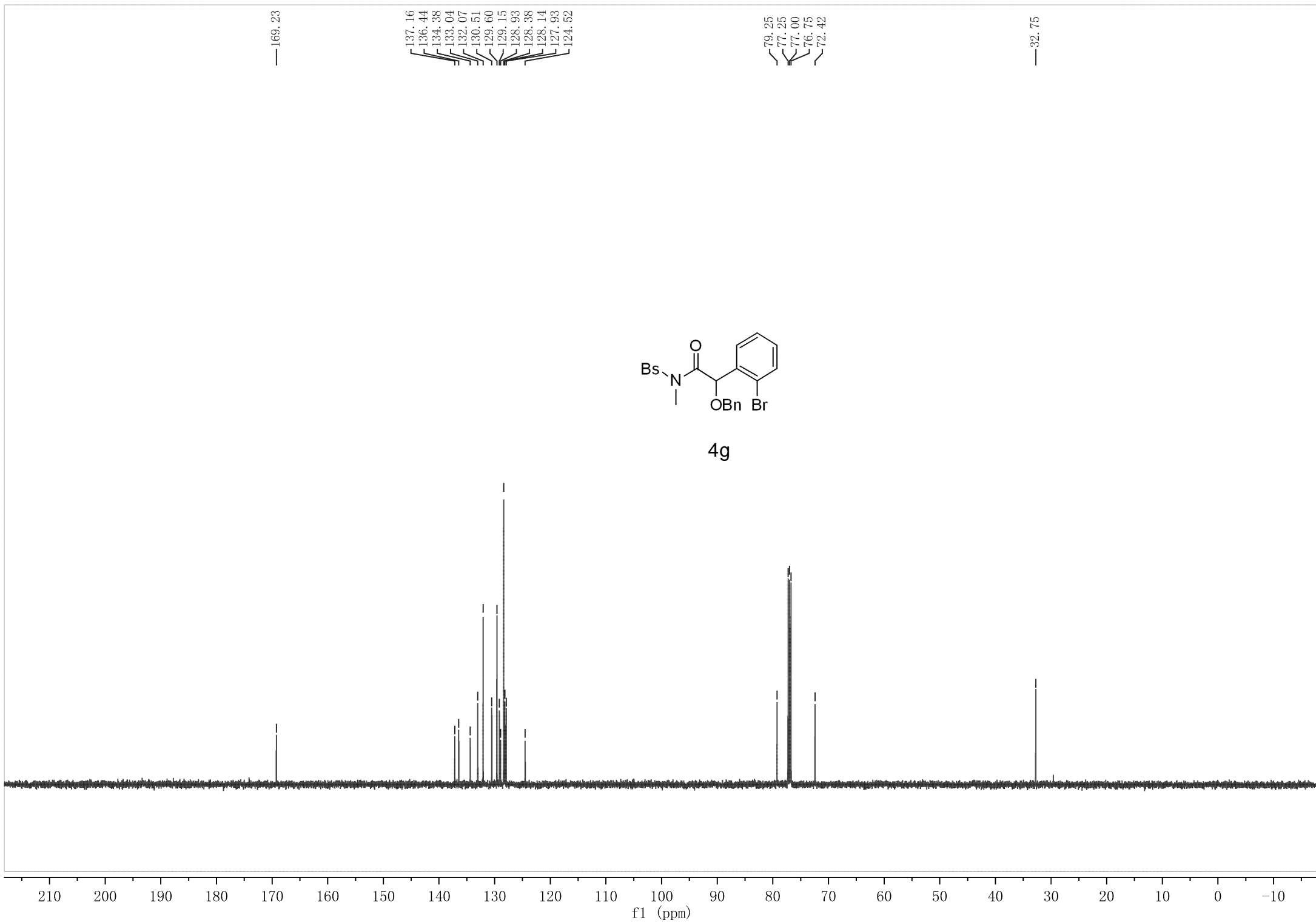
f1 (ppm)







4g

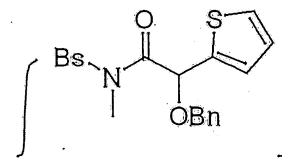


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6.966

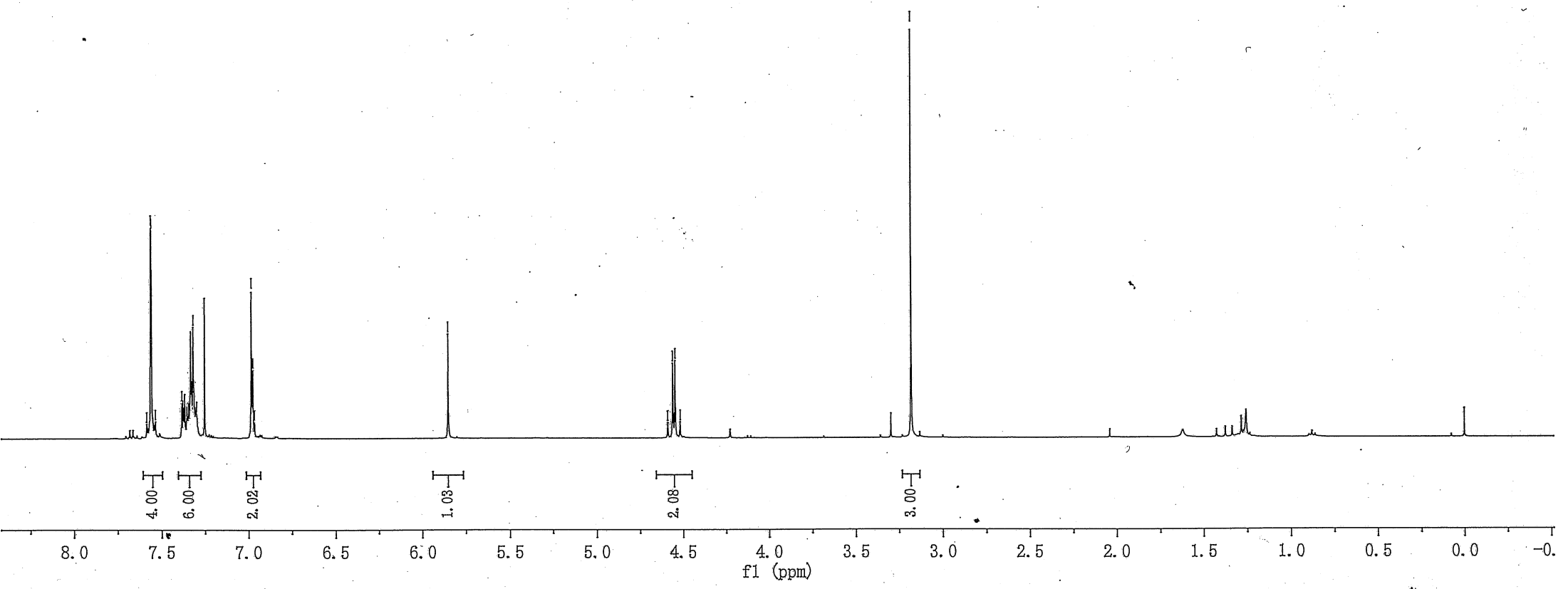
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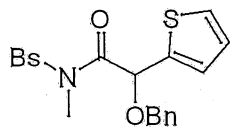
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4.547
4.518

3.181



4h





4h

169.60

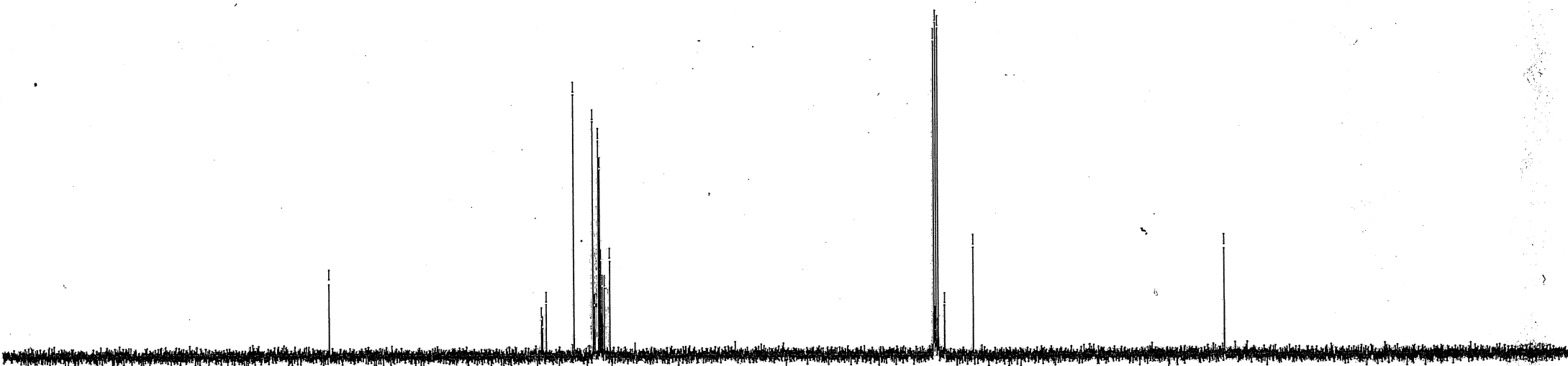
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77.32
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75.70
71.28

33.07

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)



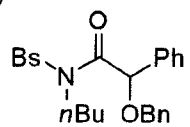
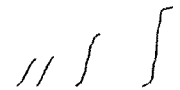
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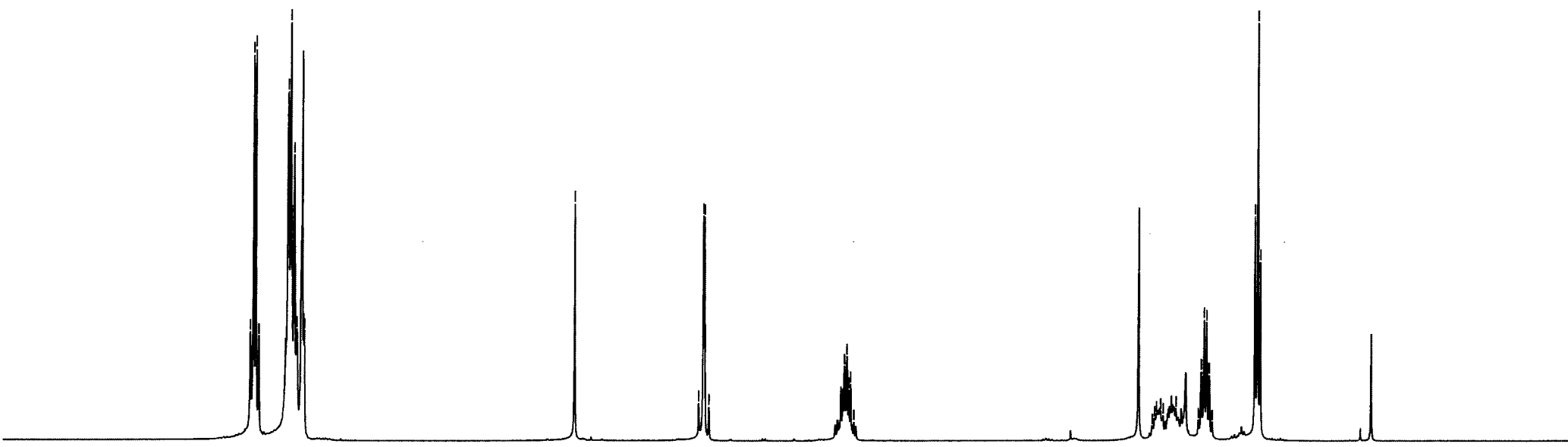
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4.494

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3.537
3.514

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1.425
1.409
1.352
1.321
1.171
1.153
1.134
1.116
1.097
1.078
0.793
0.774
0.756



4i



4.06
10.39

1.01

2.01

2.06

1.05
1.13
2.00
3.00

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 -1.0

f1 (ppm)

—170.21

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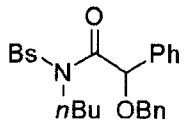
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—46.44

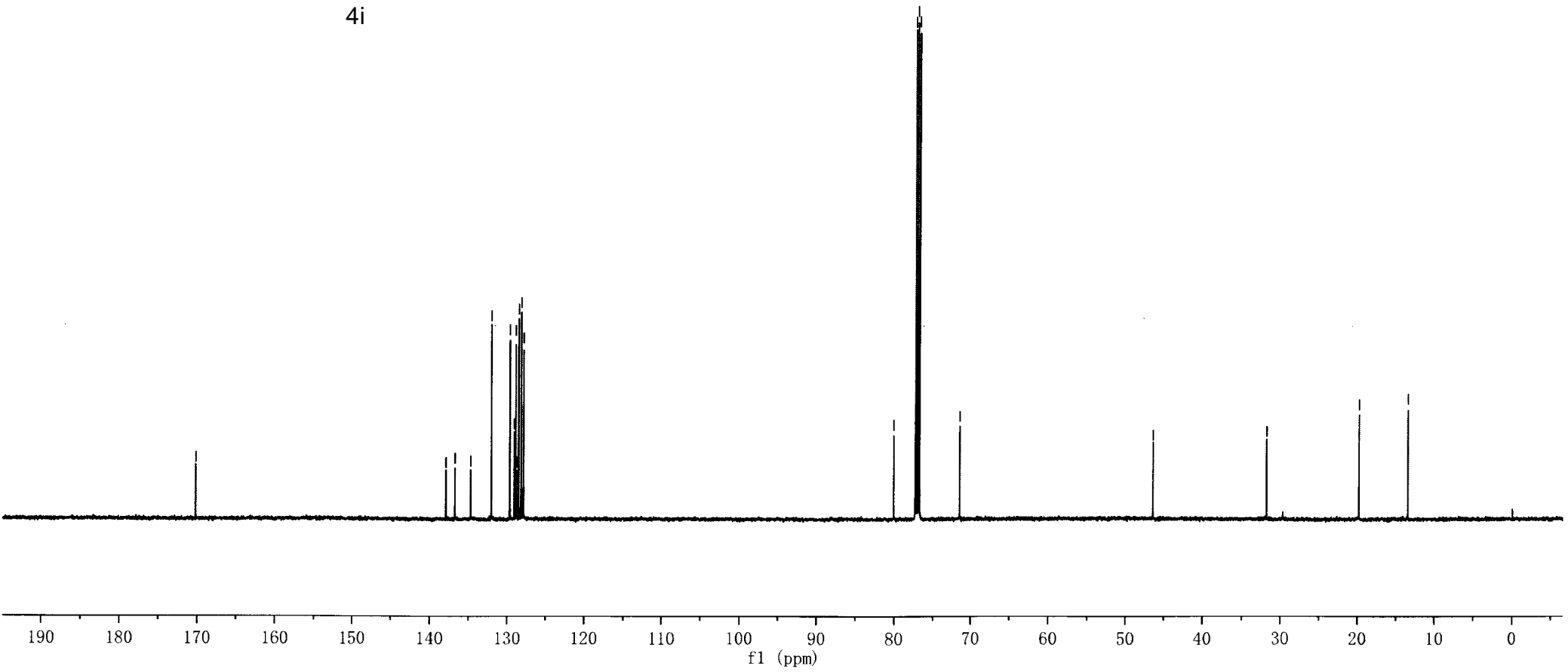
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—19.81

—13.44

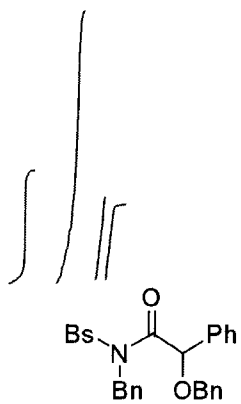


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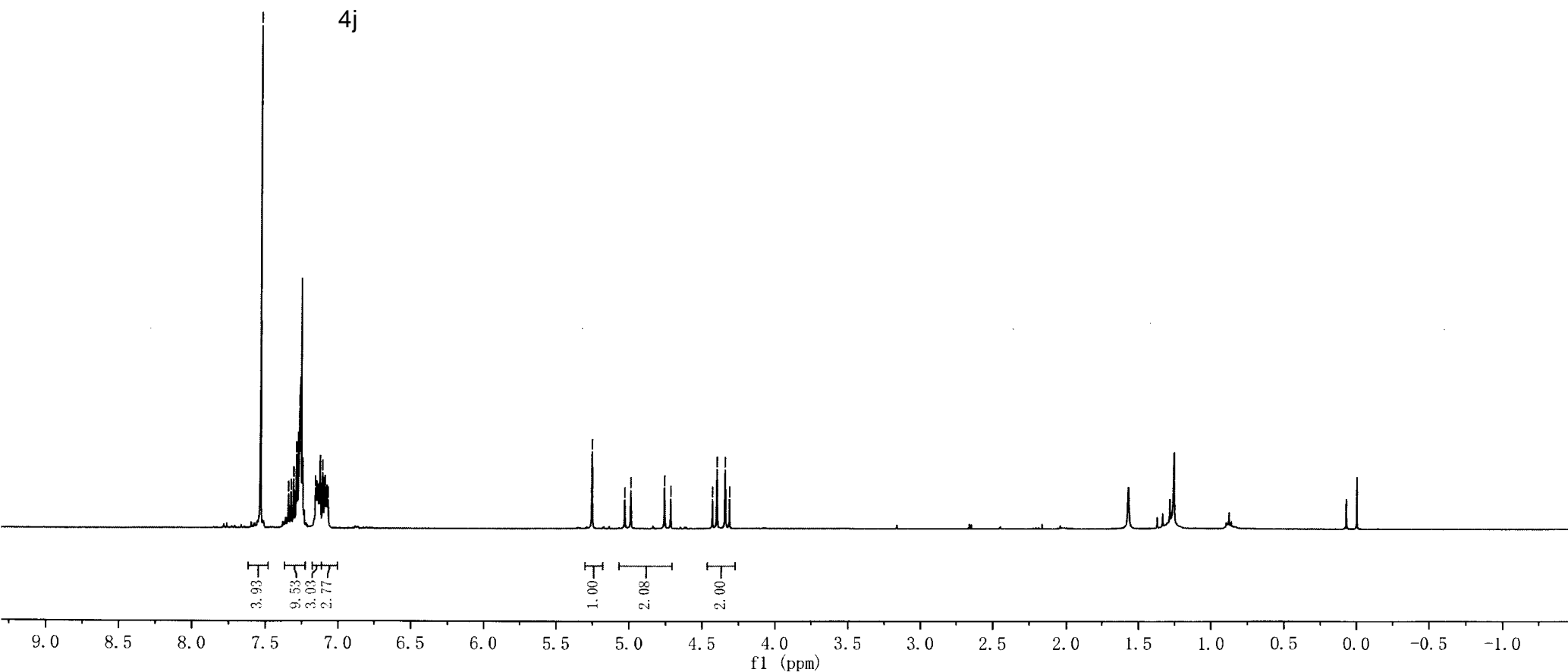


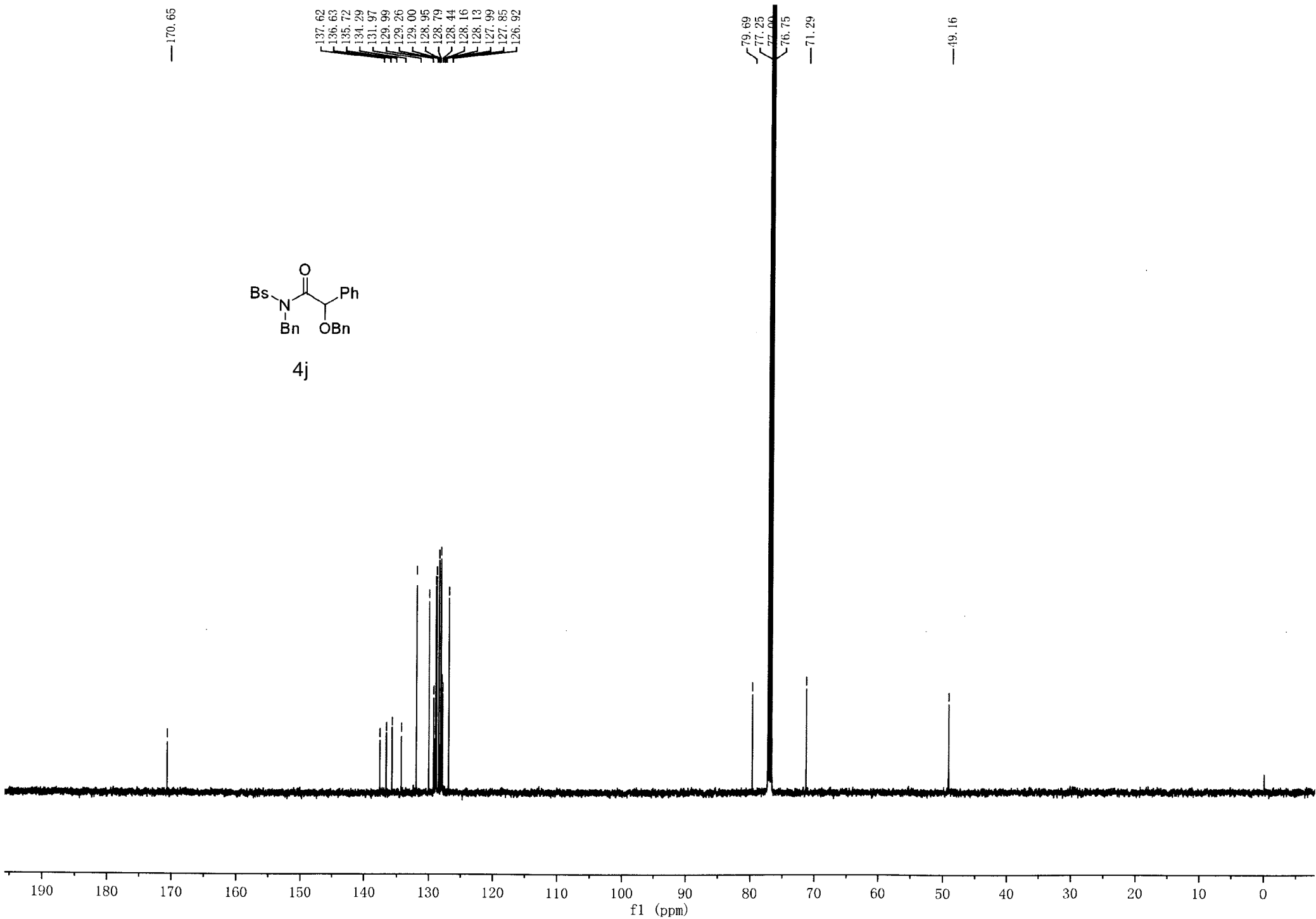
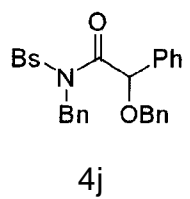
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7.094
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4.344
4.315



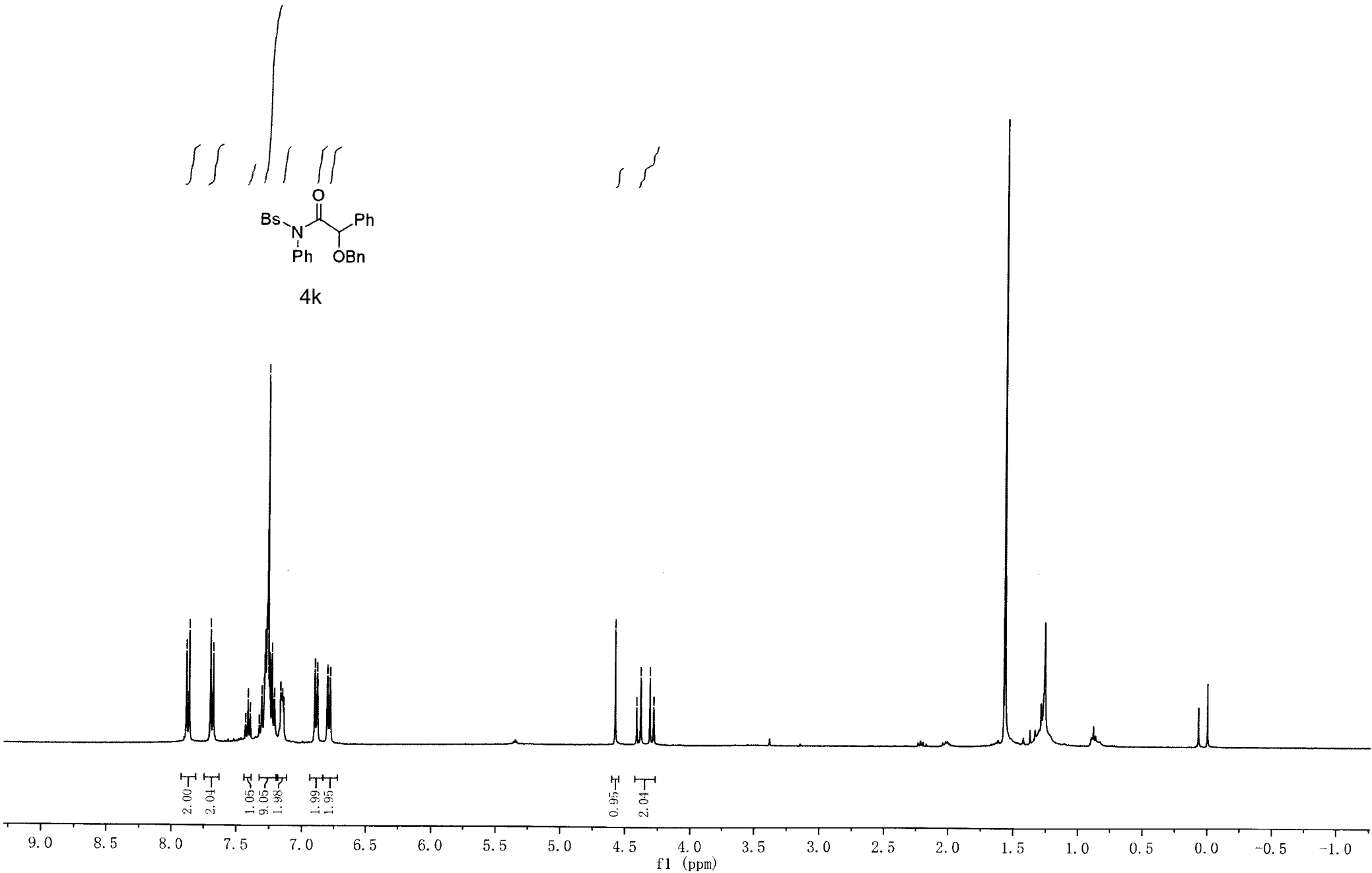
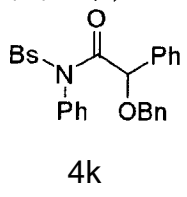
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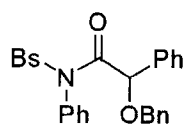




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6.801
6.783

4.575
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4.381
4.310
4.280





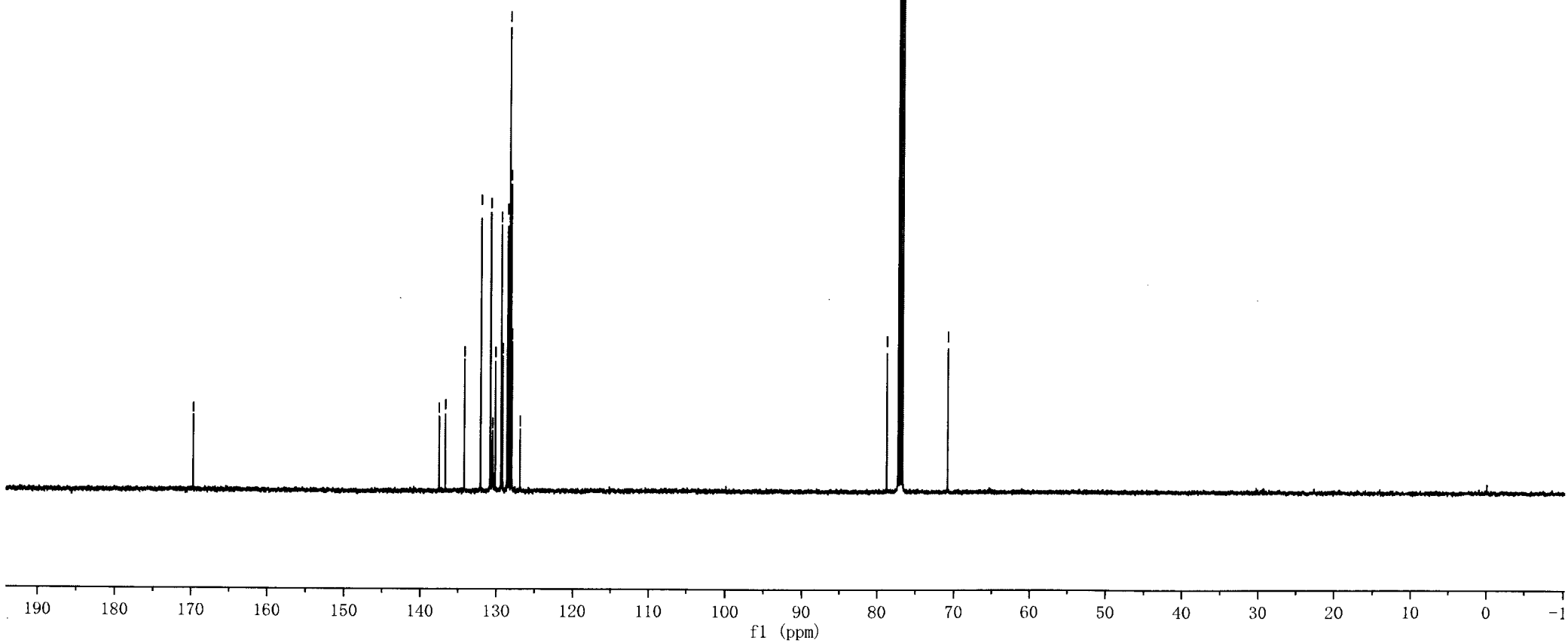
4k

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128.13
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126.94

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77.25
77.00
76.75

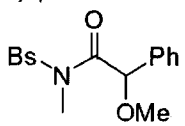
70.84



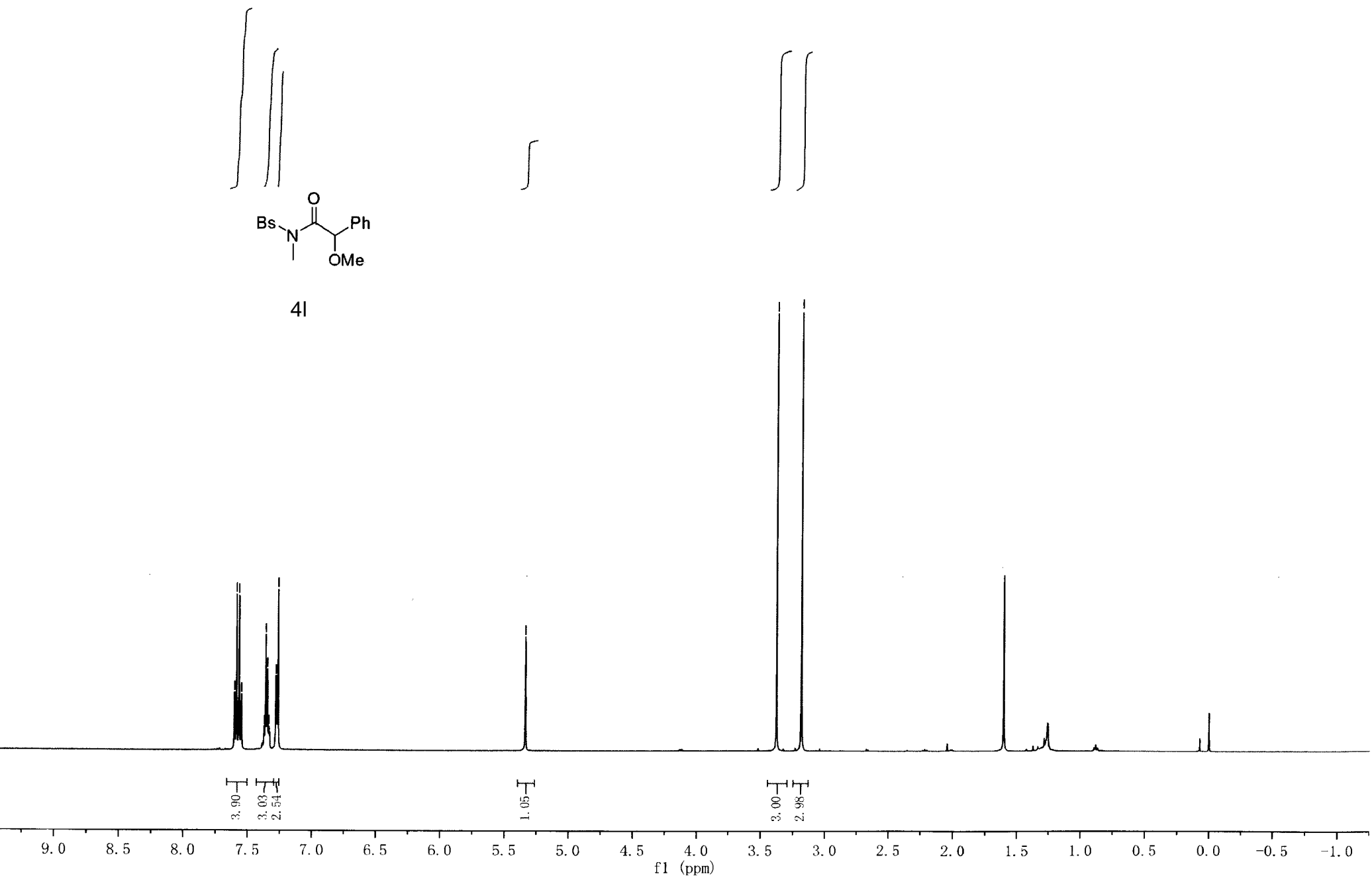
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7.278
7.264

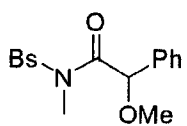
5.335

3.377
3.184



4l





4l

—170.46

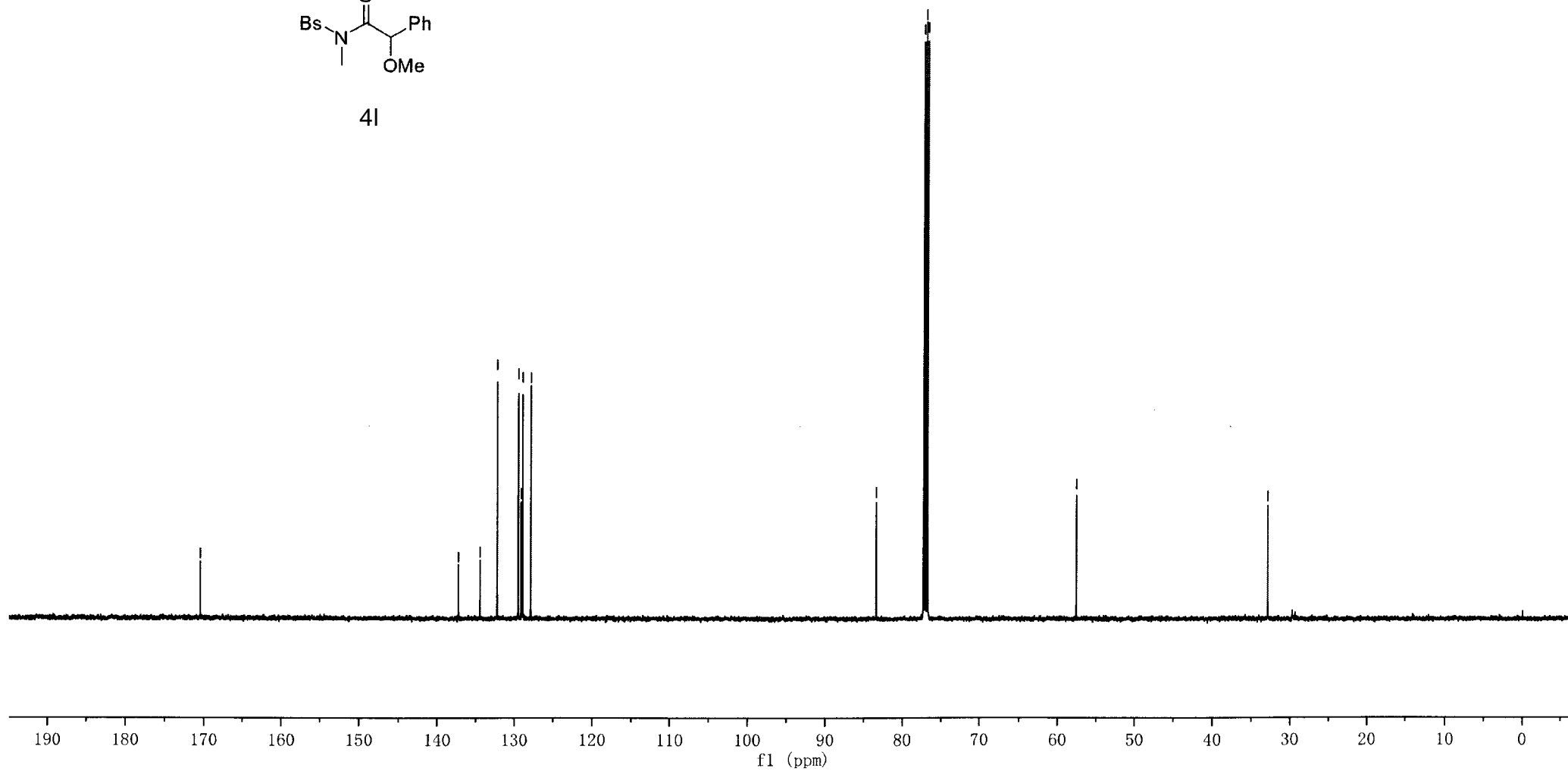
137.25
134.43
132.21
129.48
129.11
129.05
128.90
127.83

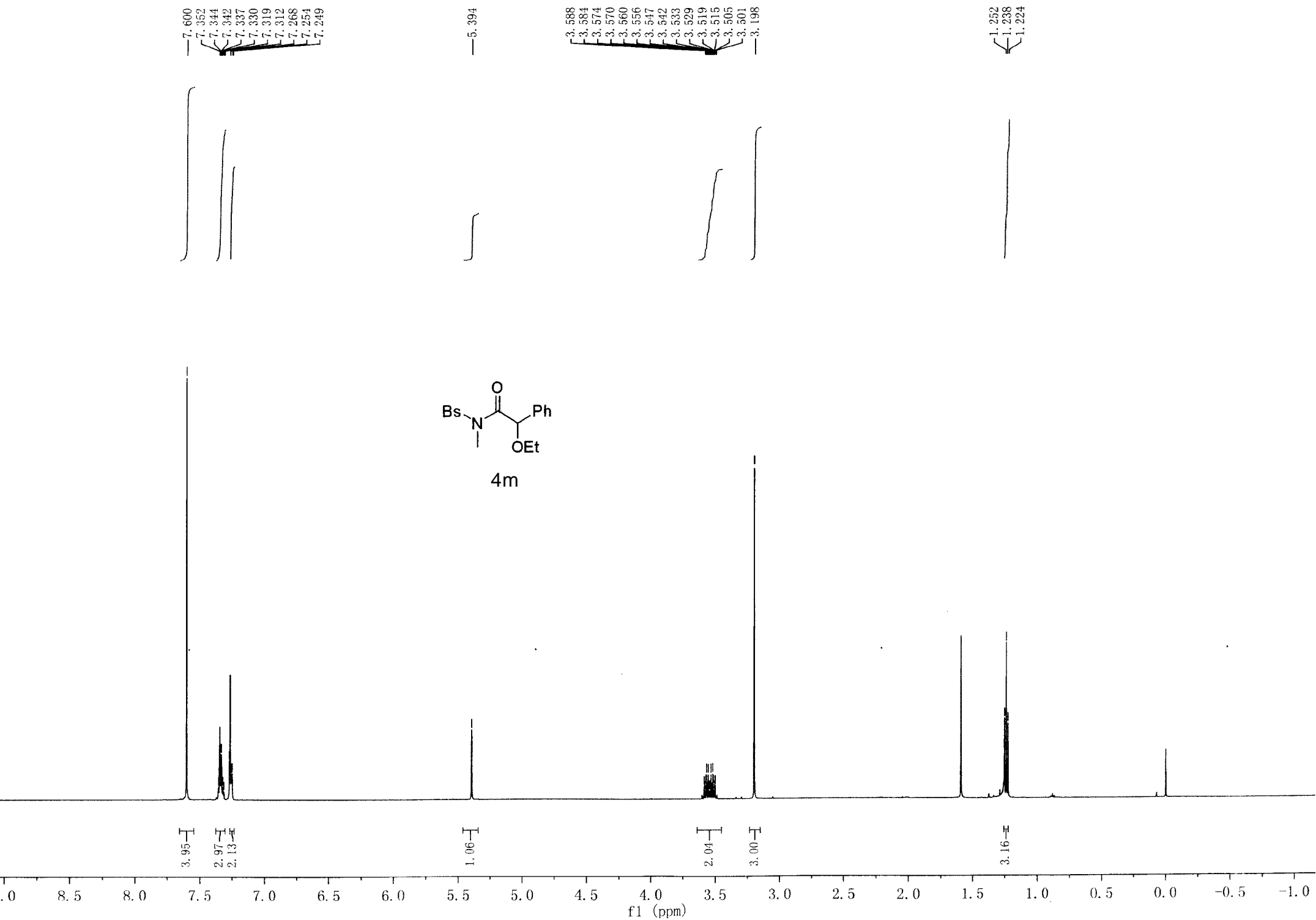
—83.40

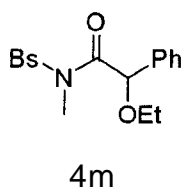
77.25
77.00
76.75

—57.58

—32.88







170.81

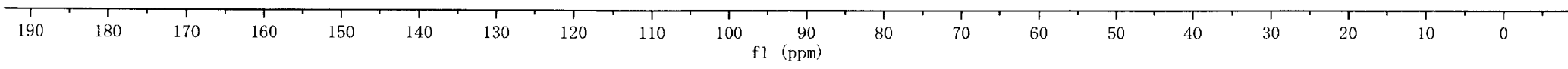
137.34
134.85
132.17
129.56
128.99
128.89
128.84
127.45

82.15
77.25
77.00
76.75

65.84

32.88

15.11

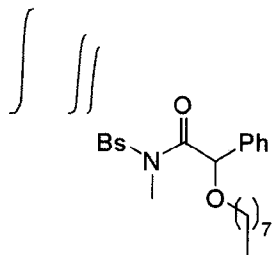


7.636
7.613
7.609
7.587
7.332
7.320
7.260
7.247

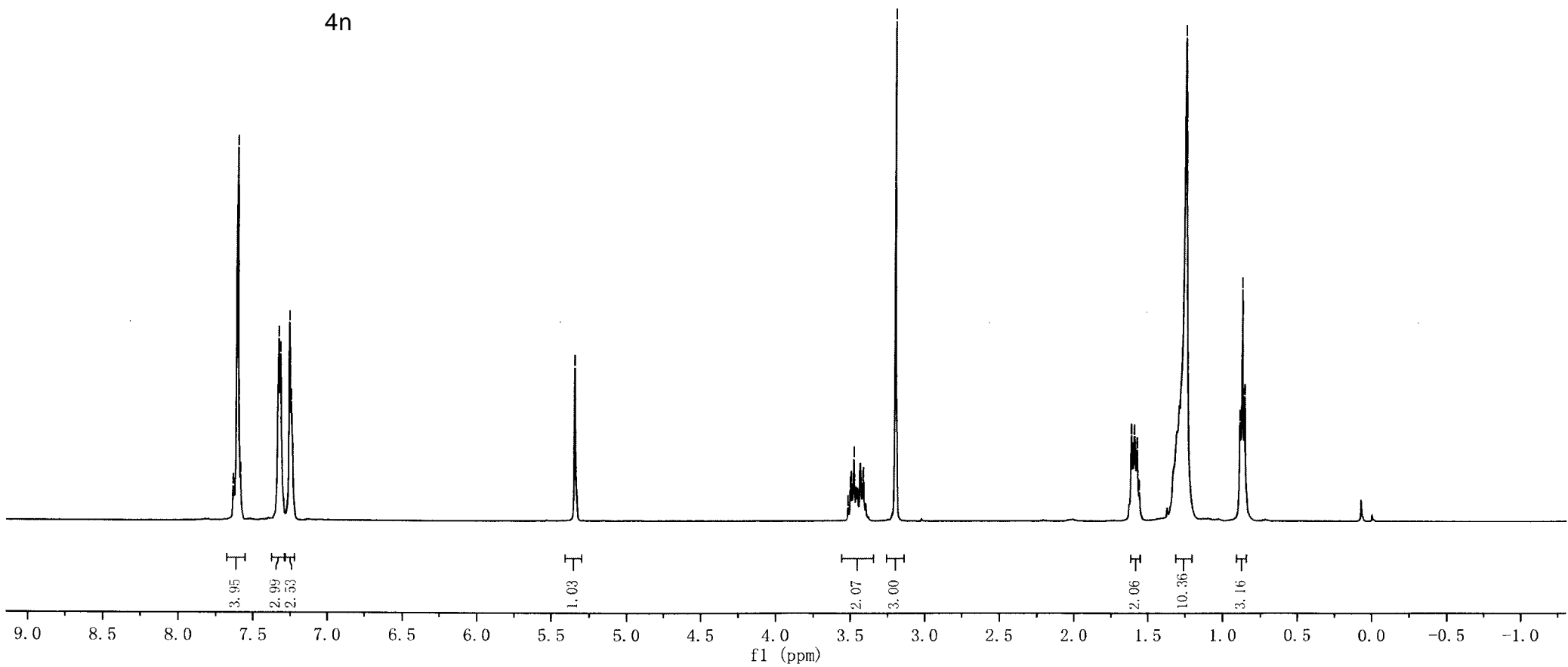
5.348

3.517
3.500
3.495
3.479
3.419
3.414
3.203
3.189

1.615
1.595
1.578
1.561
1.255
0.892
0.877
0.859



4n



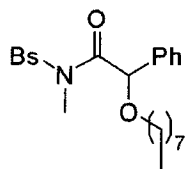
—170.83

137.48
134.96
132.13
129.56
128.93
128.76
127.19

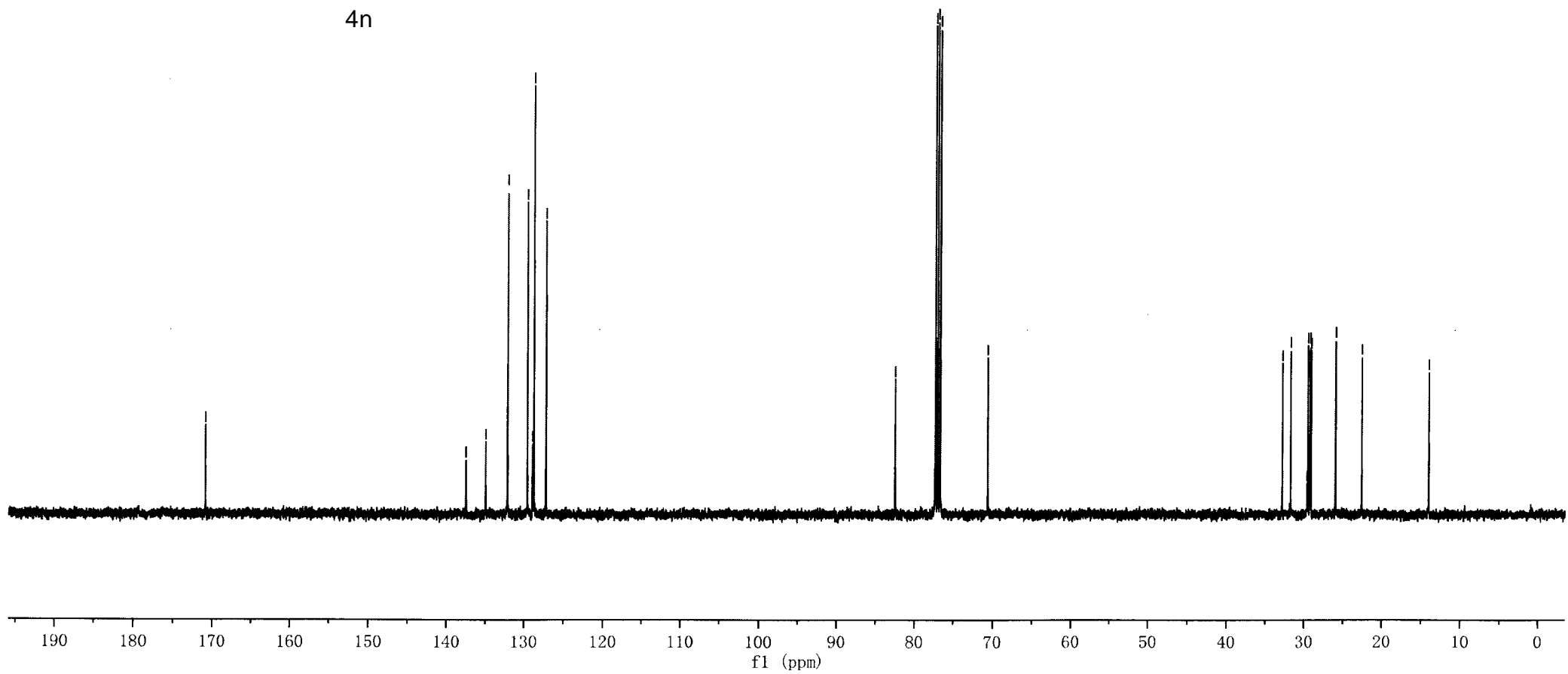
—82.52
77.32
77.00
76.68
—70.59

32.84
31.75
29.65
29.56
29.27
29.15
25.99
22.59

—14.04



4n

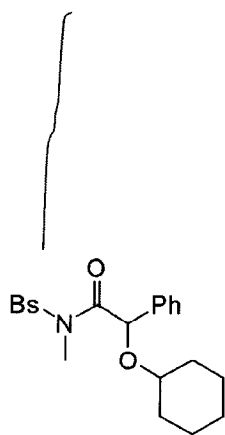


7.658
7.640
7.620
7.603
7.355
7.350
7.319
7.315
7.308
7.306
7.289
7.264
7.243
7.239
7.232
7.225

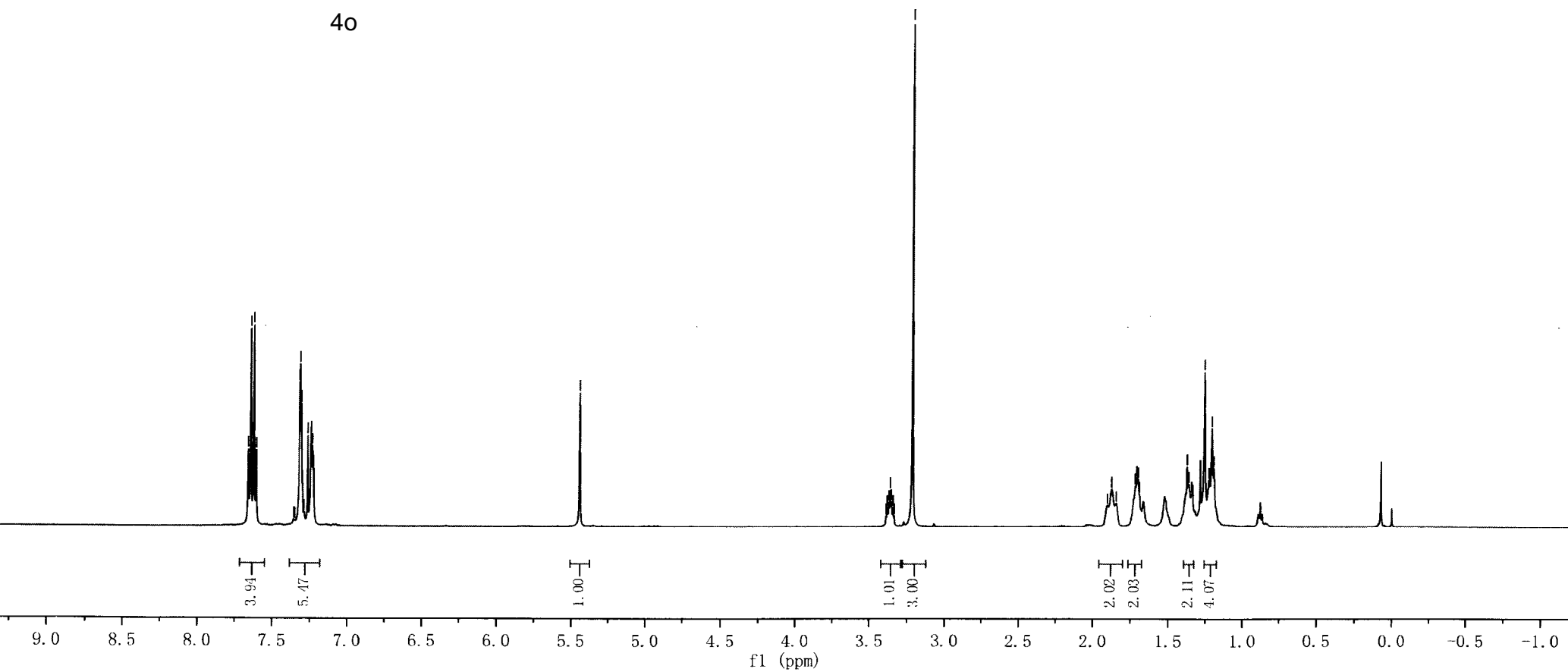
5.443

3.387
3.380
3.369
3.361
3.353
3.342
3.335
3.215

1.903
1.875
1.845
1.719
1.710
1.701
1.692
1.375
1.364
1.345
1.257
1.222
1.208
1.193



4o



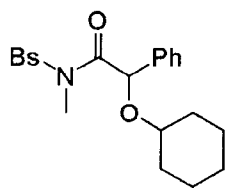
— 171.51

137.31
135.39
132.01
129.67
128.91
128.75
128.50
126.46

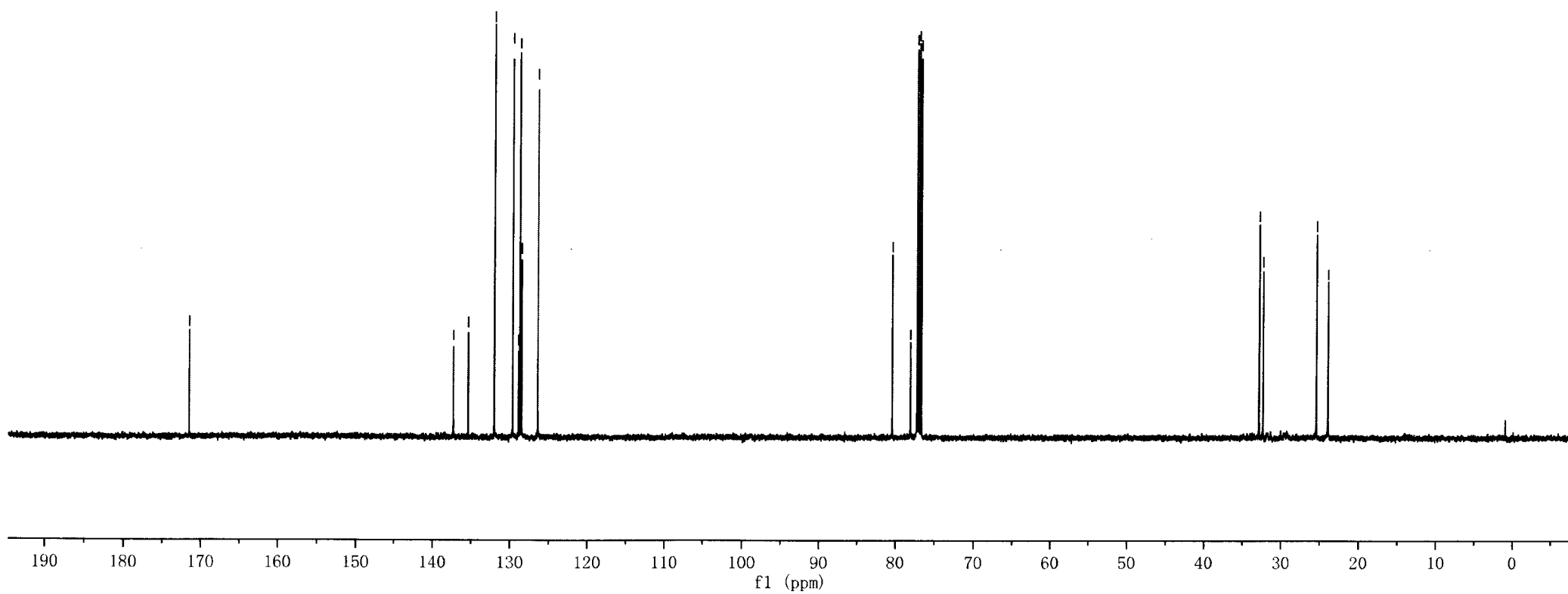
80.45
78.08
77.25
77.00
76.75

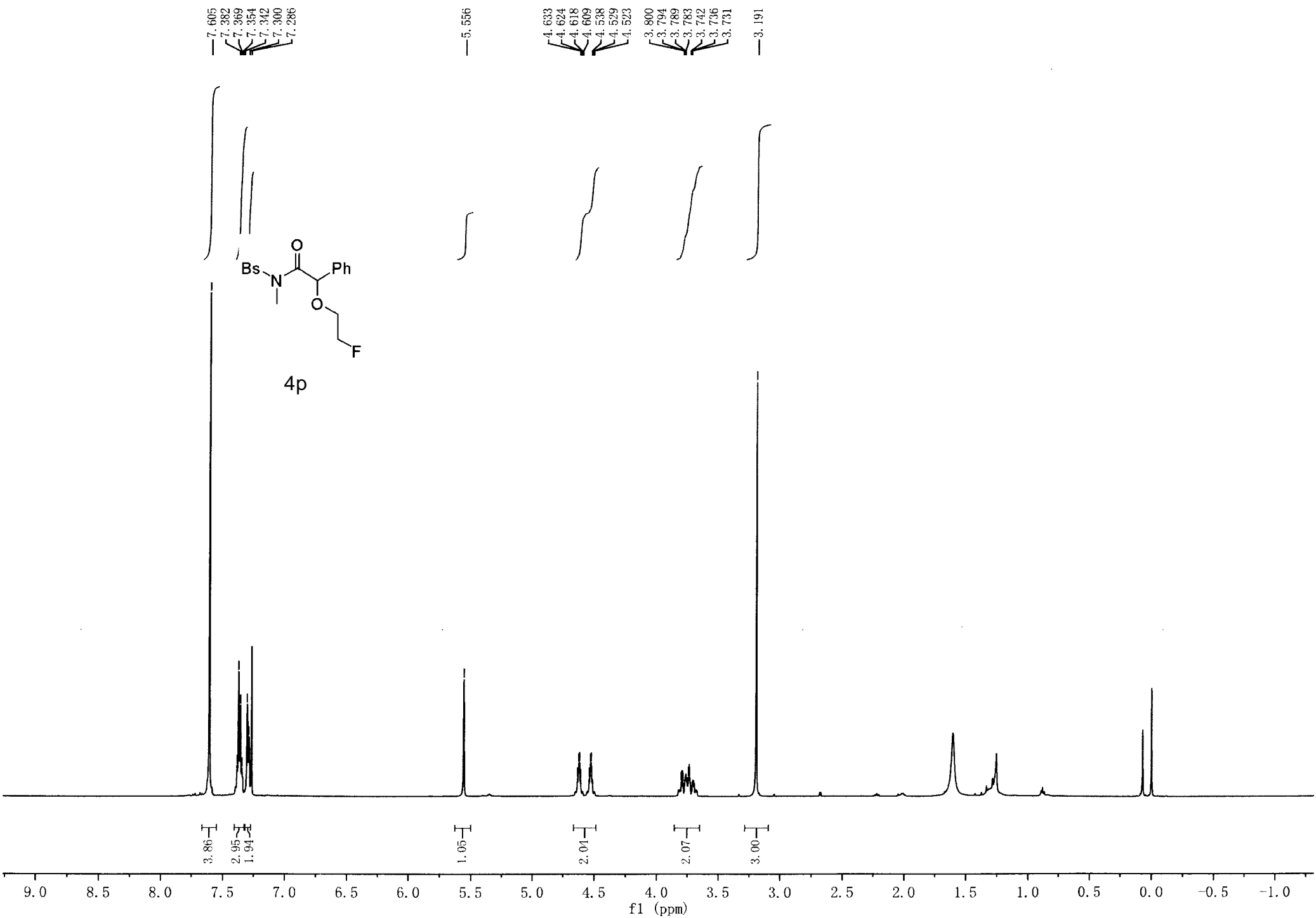
32.92
32.41

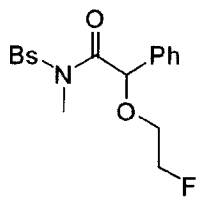
25.46
23.92



40







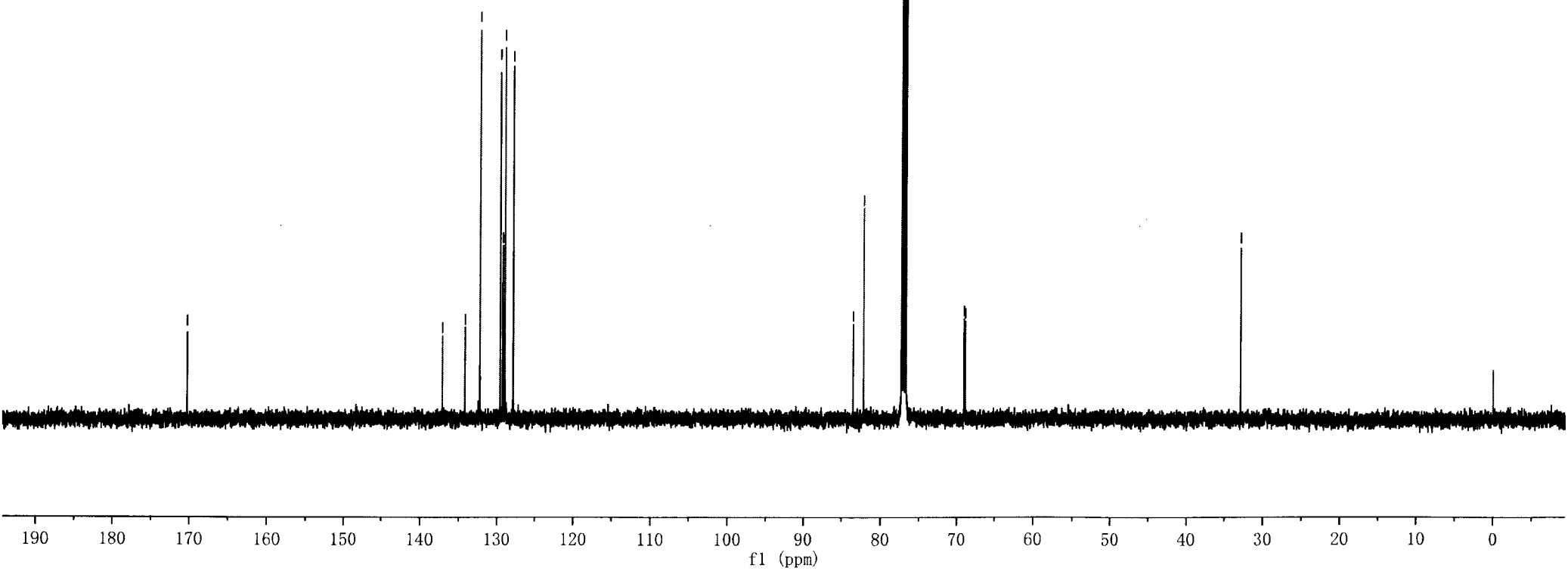
4p

170.26

137.13
134.22
132.23
129.57
129.22
129.11
128.96
127.85

83.55
82.20
77.25
77.00
76.75
69.06
68.90

32.89



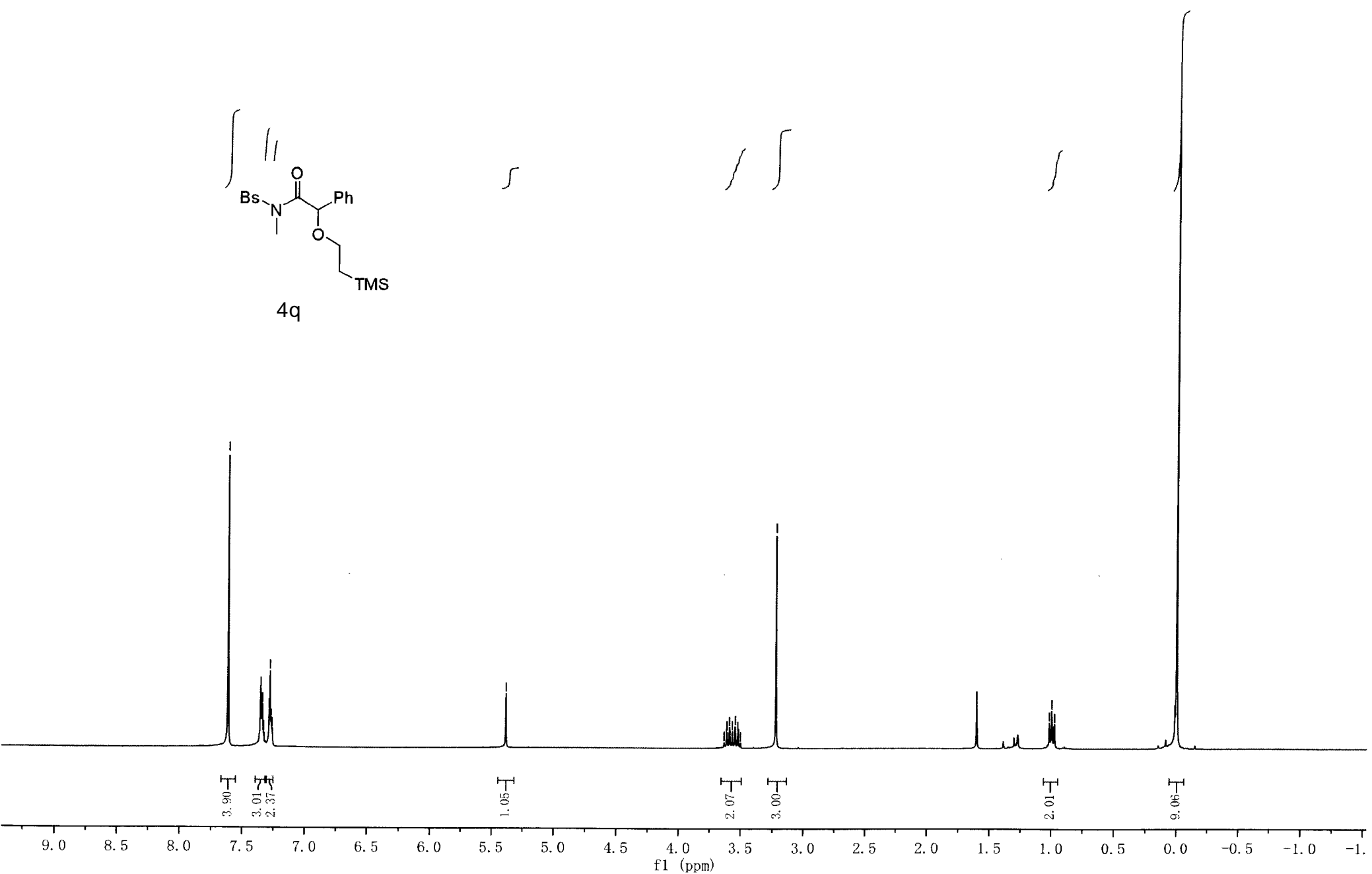
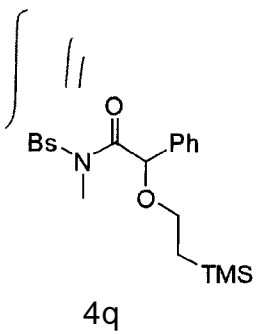
7.614
7.355
7.350
7.342
7.338
7.328
7.283
7.277
7.270
7.260

5.385

3.632
3.614
3.609
3.590
3.566
3.544
3.524
3.519
3.501
3.221

1.017
0.997
0.976

0.000



3.90
3.01
2.37

1.05

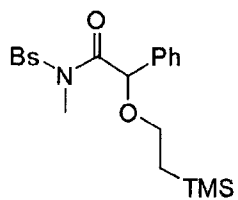
2.07
3.00

2.01

9.06

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 -1.0 -1.5

f1 (ppm)



4q

—170.90

137.35
134.92
132.14
129.56
128.97
128.81
128.78
127.28

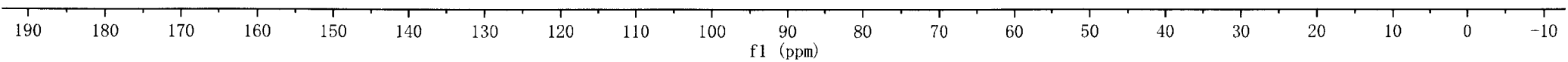
82.04
77.25
77.00
76.75

—67.91

—32.88

—18.28

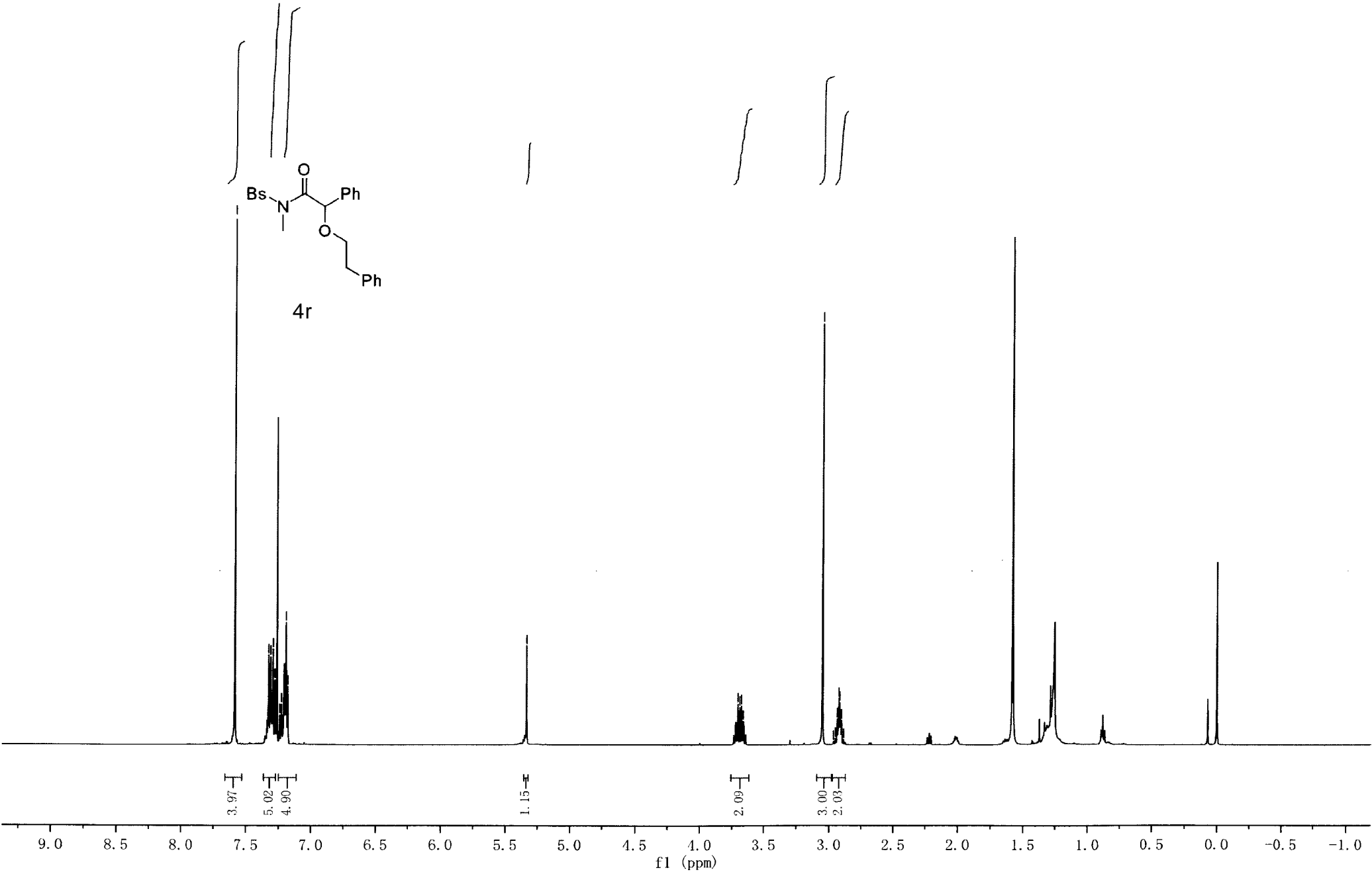
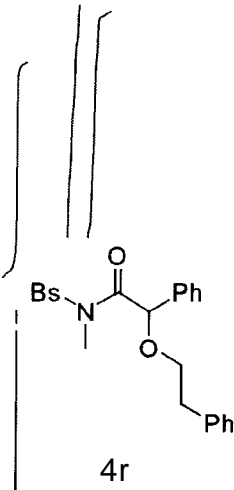
—1.46

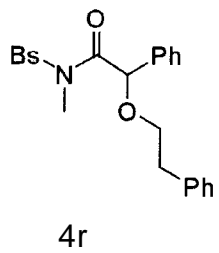


7.584
7.325
7.309
7.292
7.277
7.240
7.225
7.207
7.205
7.192
7.178

5.334

3.702
3.687
3.673
3.659
3.049
2.965
2.951
2.937
2.929
2.923
2.915
2.909
2.902
2.888



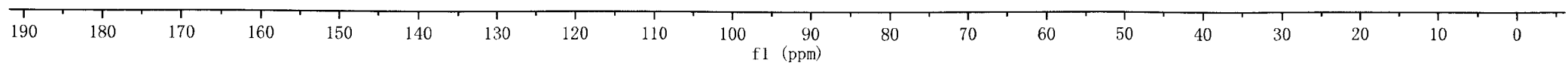


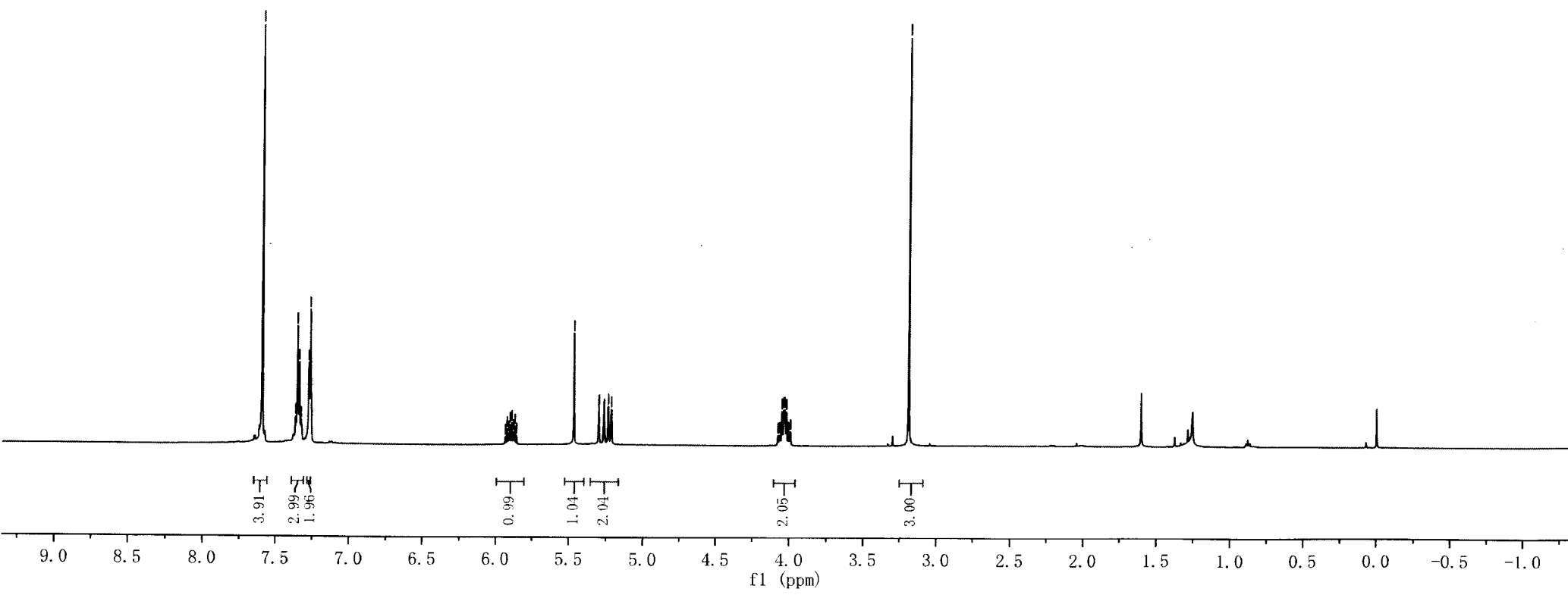
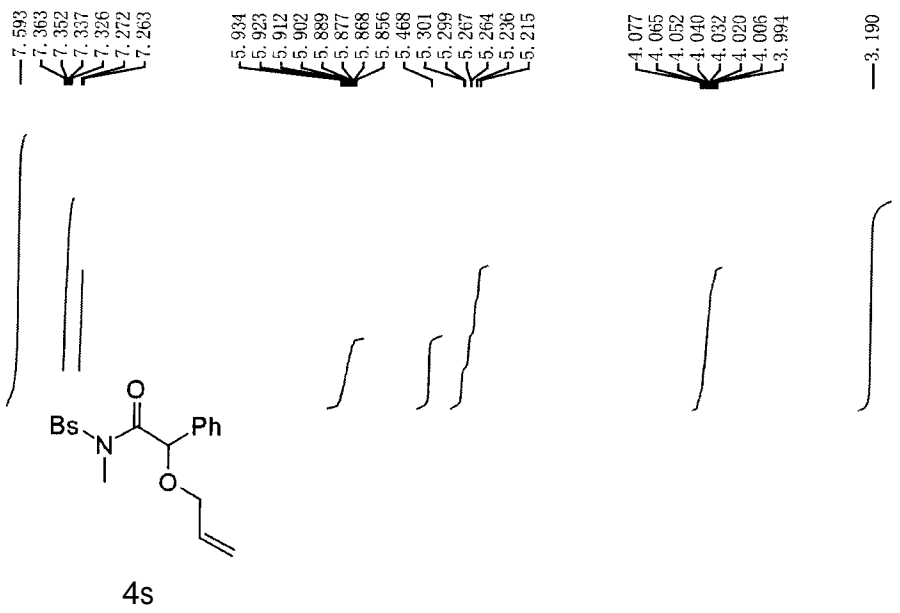
—170.60

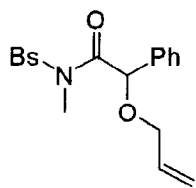
138.36
137.36
134.56
132.14
129.57
128.99
128.93
128.87
128.82
128.42
127.20
126.43

—82.61
77.25
77.00
76.75
—71.23

—36.20
—32.70







4s

170.52

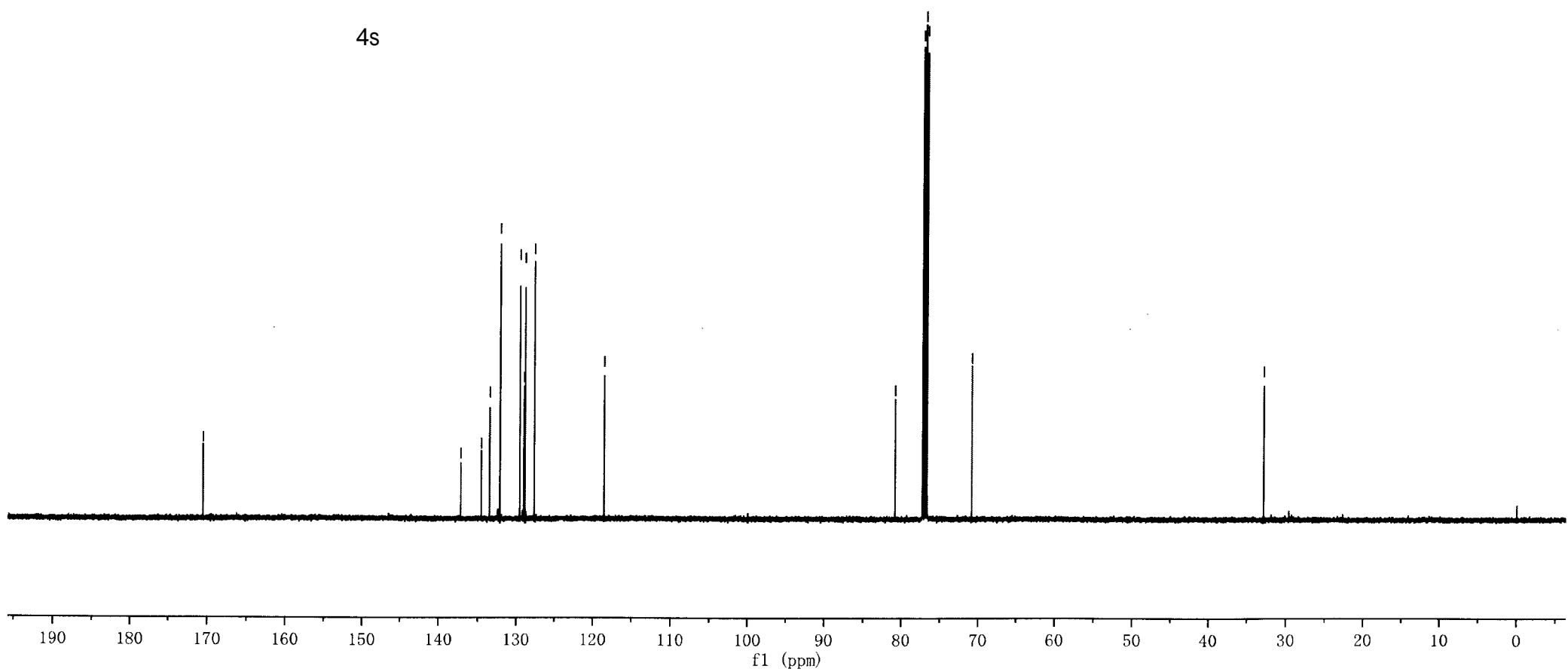
137.20
134.52
133.48
132.16
129.57
129.02
129.01
128.88
127.69

118.53

80.85
77.25
77.00
76.75

70.81

32.89



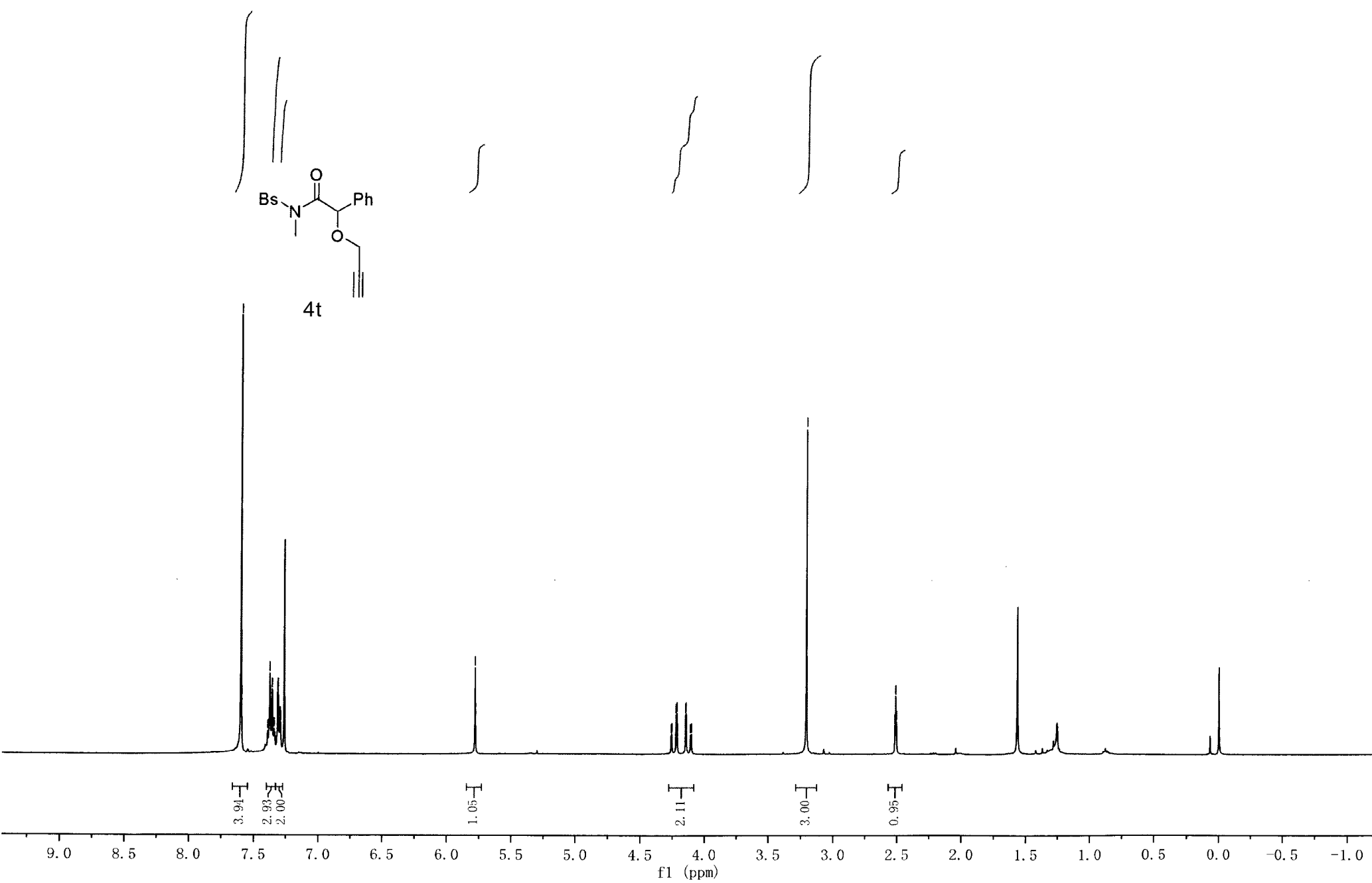
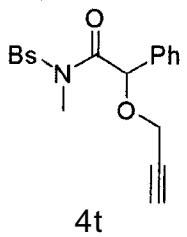
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7.391
7.380
7.376
7.371
7.356
7.342
7.314
7.311
7.295
7.291

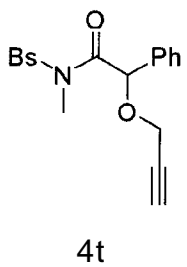
5.781

4.261
4.255
4.221
4.215
4.148
4.142
4.108
4.102

3.209

2.517
2.511
2.505





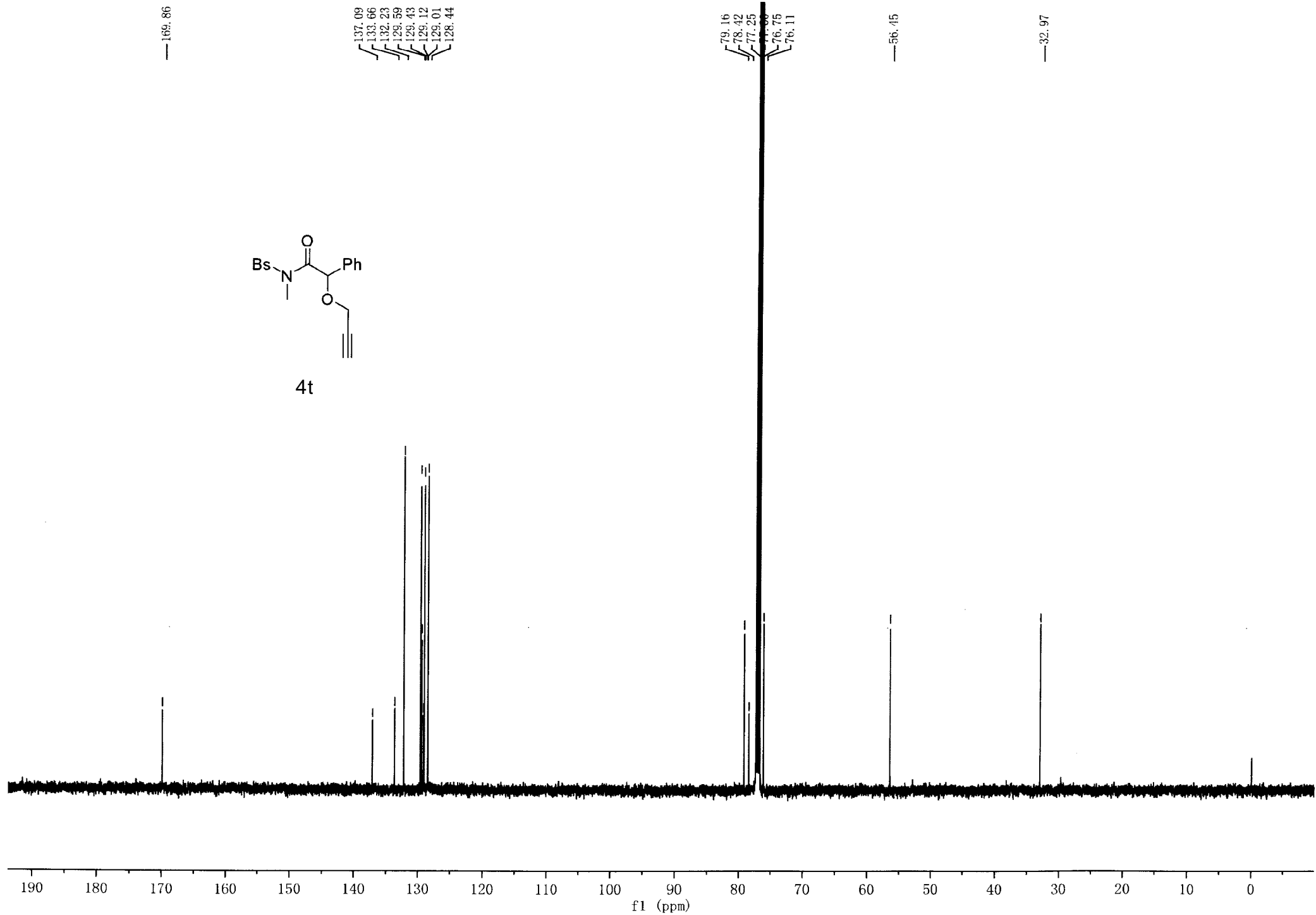
— 169.86

137.09
133.66
132.23
129.59
129.43
129.12
129.01
128.44

79.16
78.42
77.25
76.75
76.11

— 56.45

— 32.97



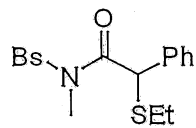
7.644
7.610
7.587
7.543
7.361
7.347
7.309
7.289

5.369

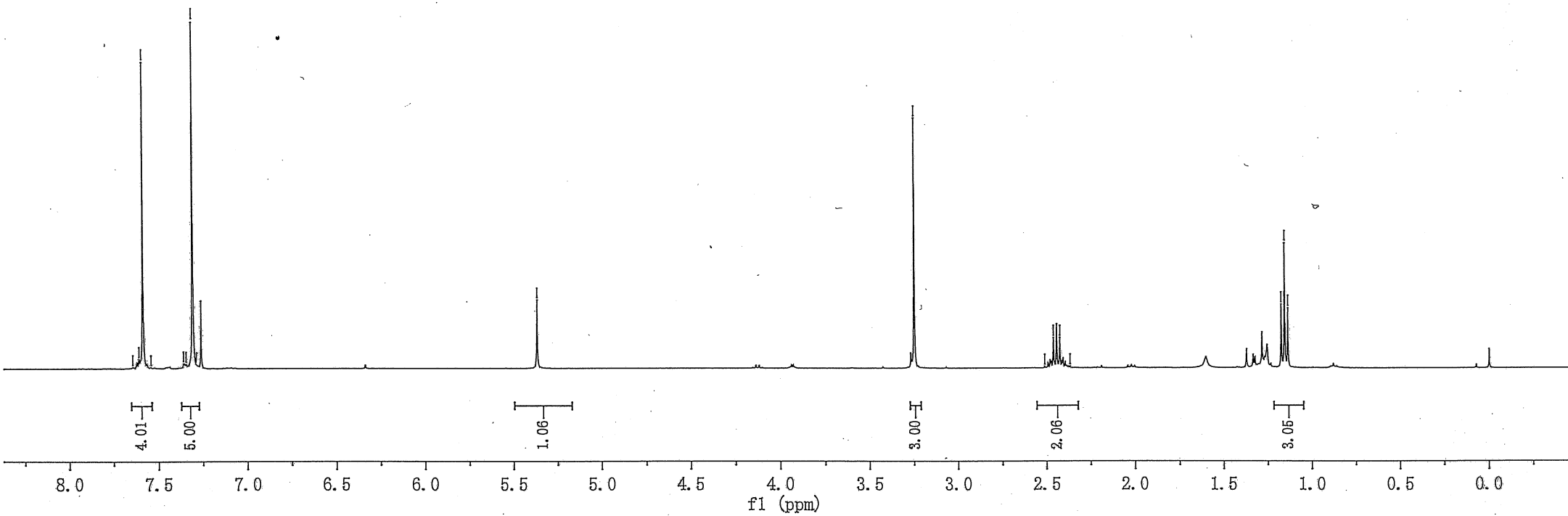
3.260

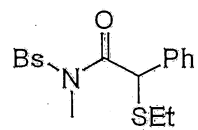
2.511
2.462
2.426
2.368

1.176
1.157
1.139



6a





6a

170.28

137.35
135.32
132.31
129.31
129.04
128.84
128.61
128.22

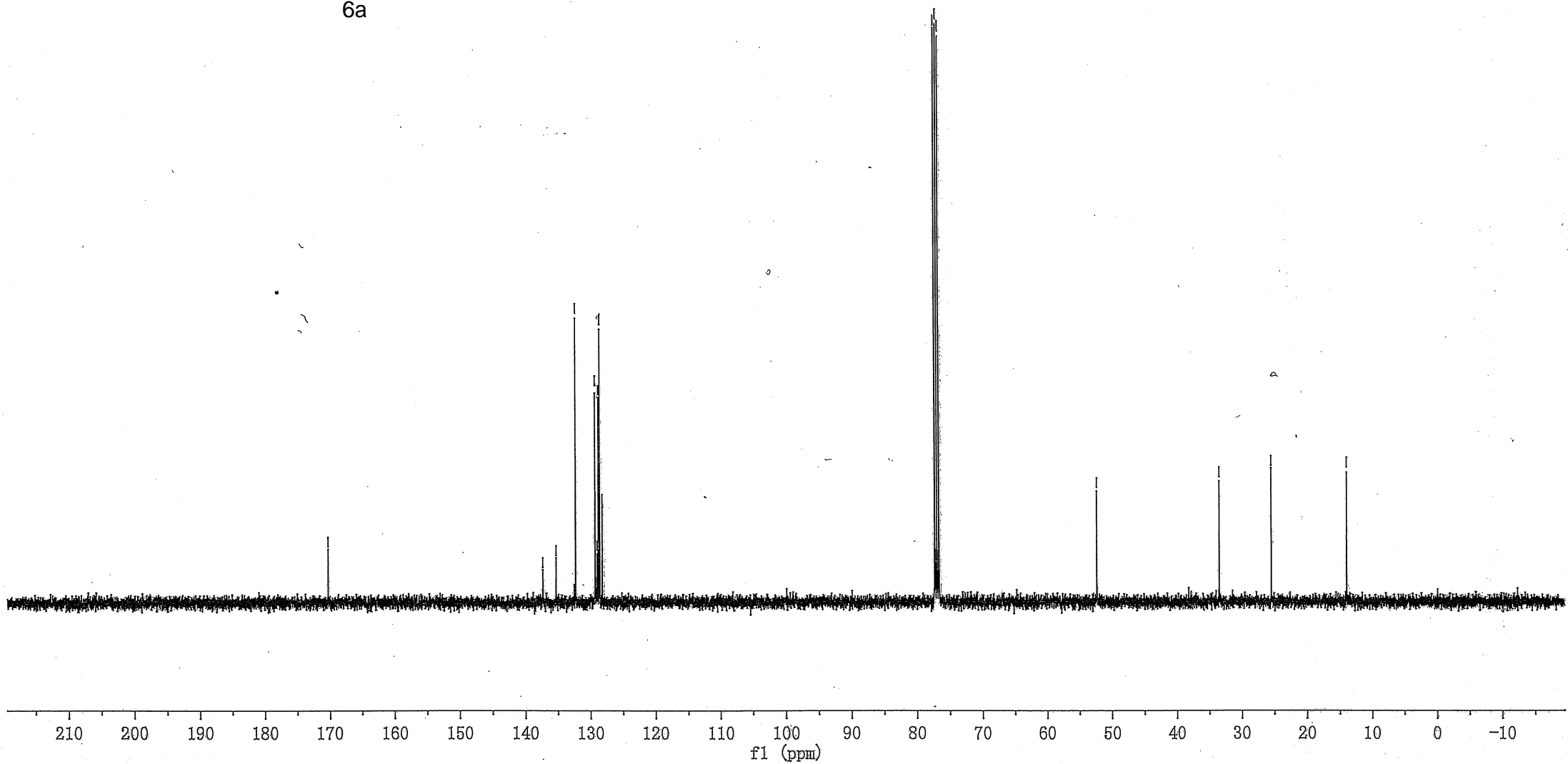
77.32
77.00
76.68

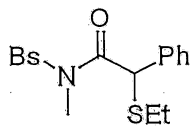
52.38

33.50

25.51

13.97





6a

132.31
129.32
128.84
128.62
128.22

52.38

38.50

25.51

18.97

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

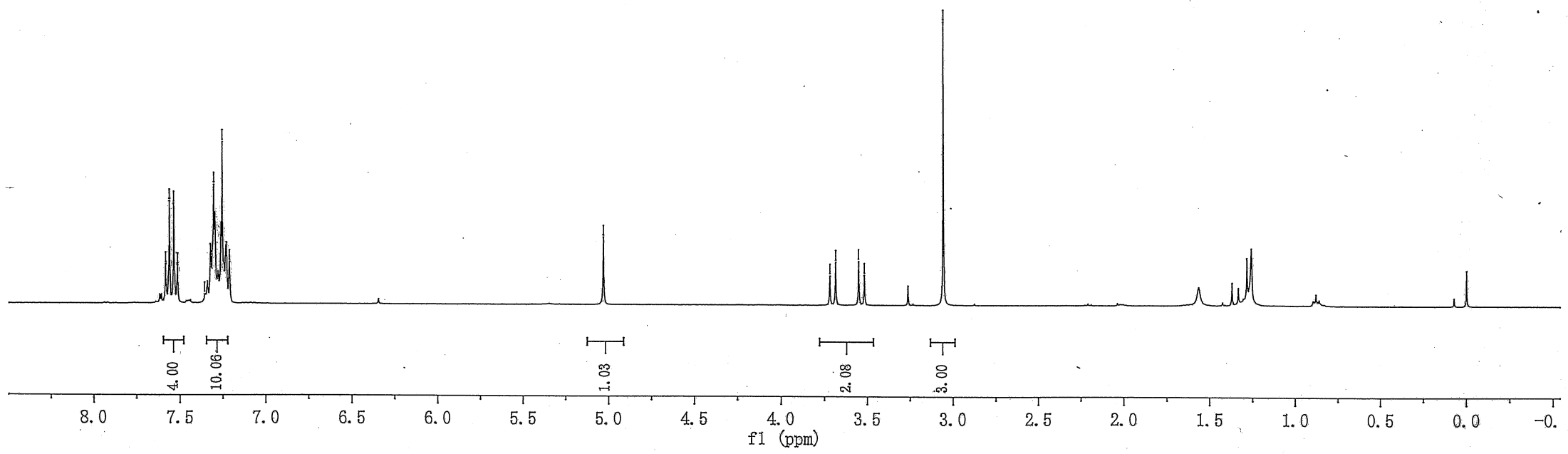
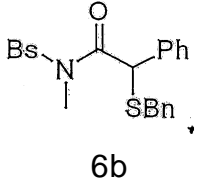
f1 (ppm)

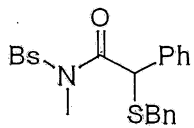
7.584
7.562
7.537
7.515
7.357
7.304
7.265
7.218

5.032

3.719
3.686
3.552
3.518

3.058





6b

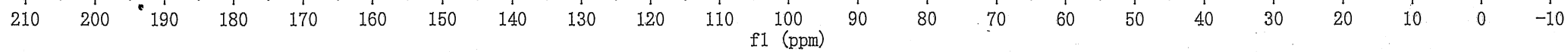
169.81

137.42
137.11
134.67
132.25
129.43
129.08
129.00
128.89
128.86
128.67
128.41
127.40

77.32
77.00
76.68

51.74

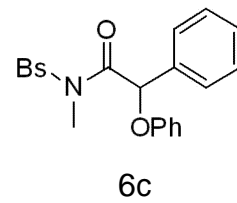
35.96
33.16



7.532
7.510
7.467
7.426
7.393
7.380
7.255
7.237
7.218
7.019
6.982
6.883
6.862

6.316

3.235



2.00
7.01
1.99

1.02
2.03

1.01

3.00

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

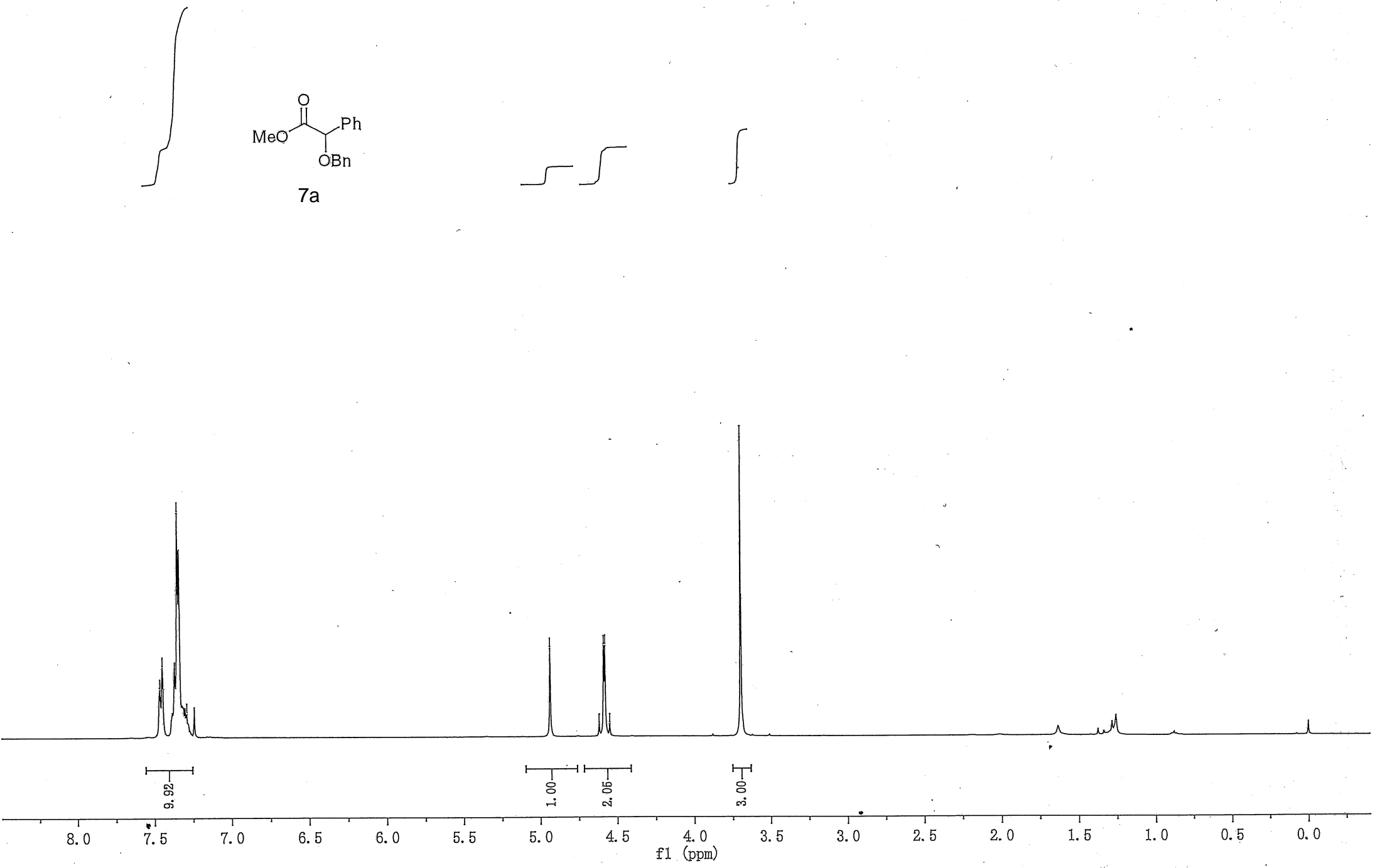
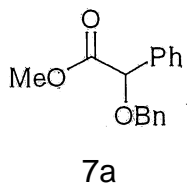
f1 (ppm)

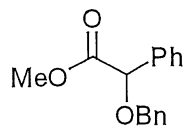
7.466
7.450
7.352
7.292

4.937

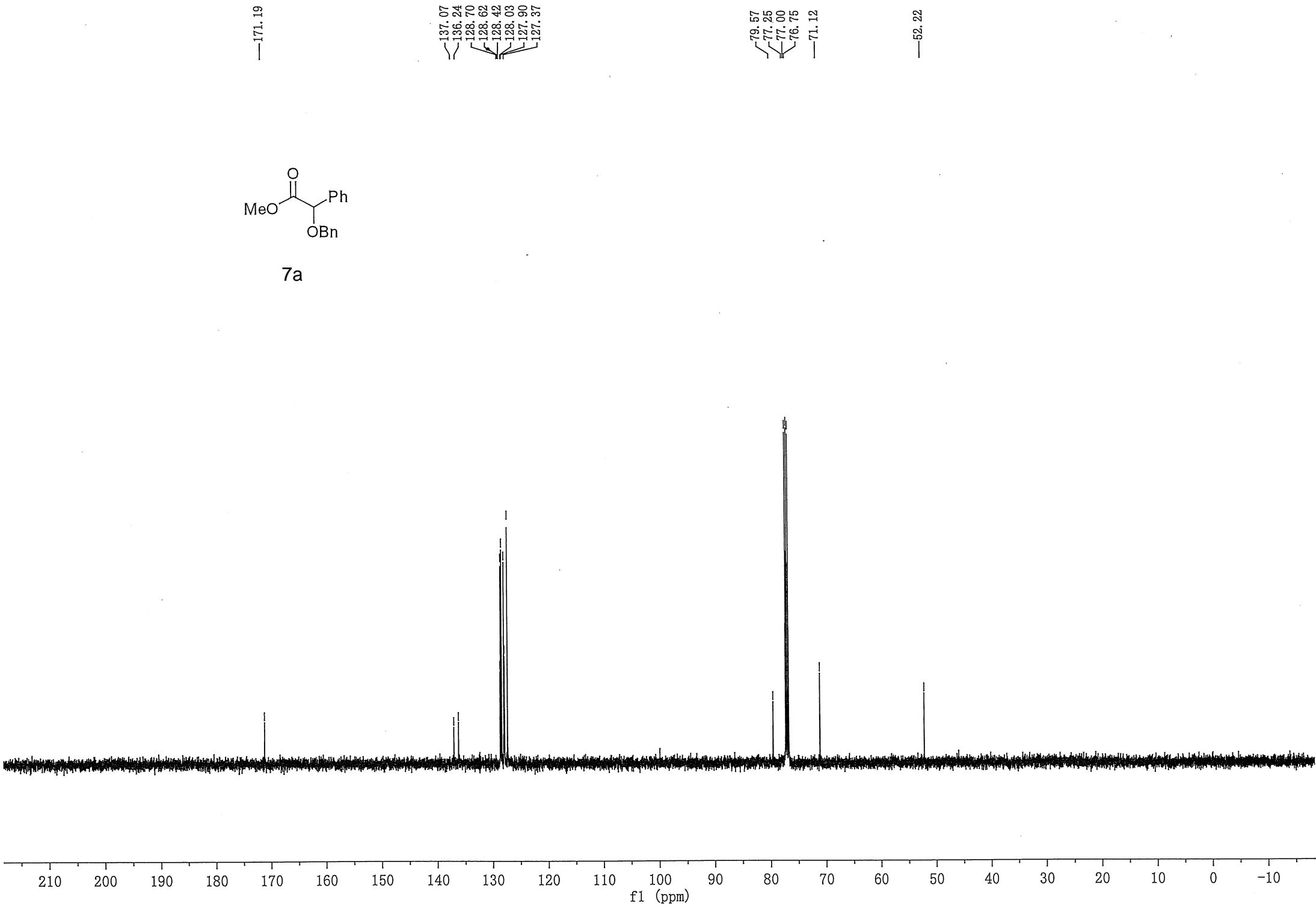
4.618
4.589
4.580
4.550

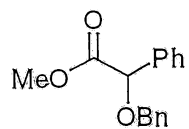
3.699





7a





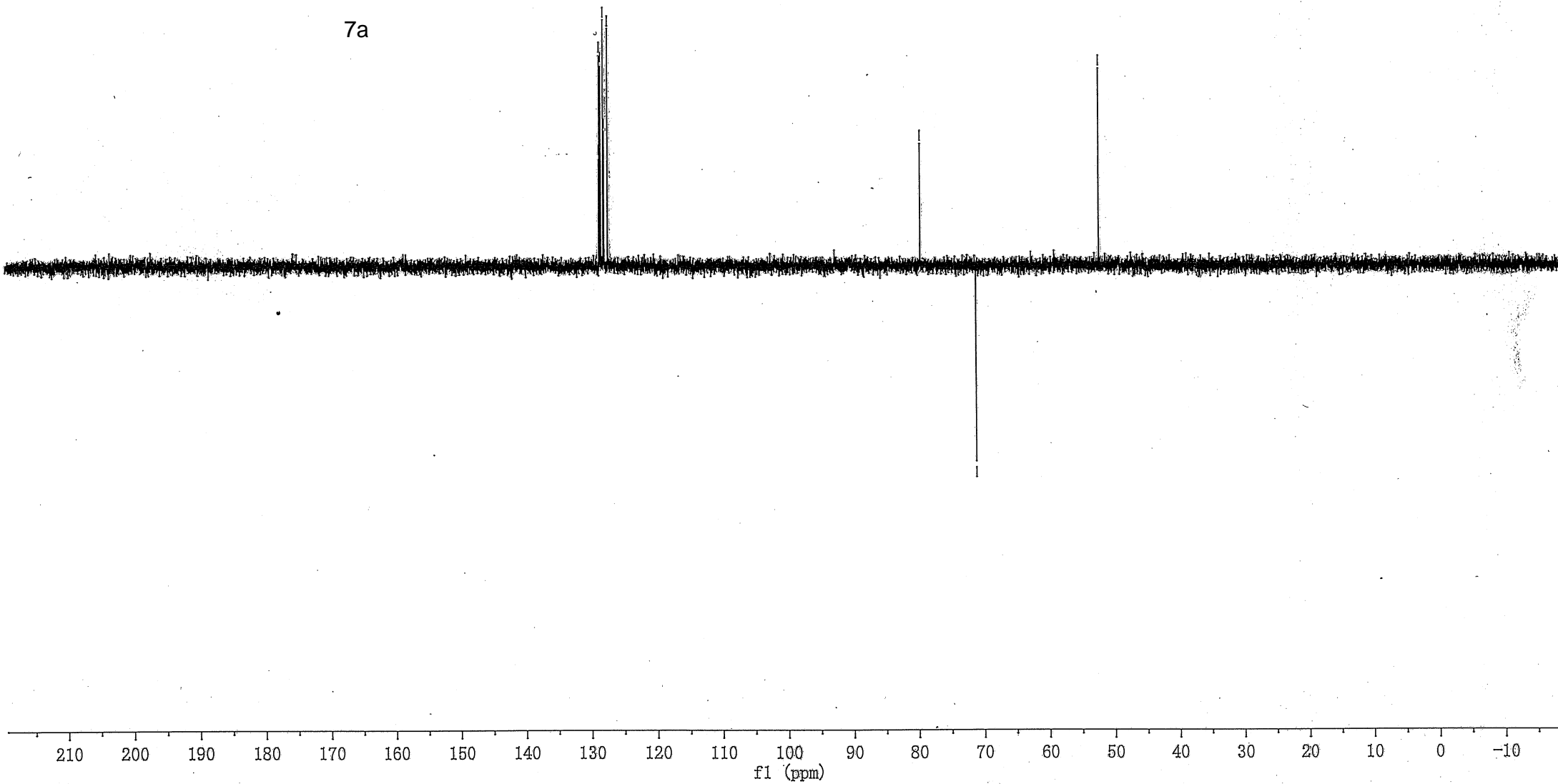
7a

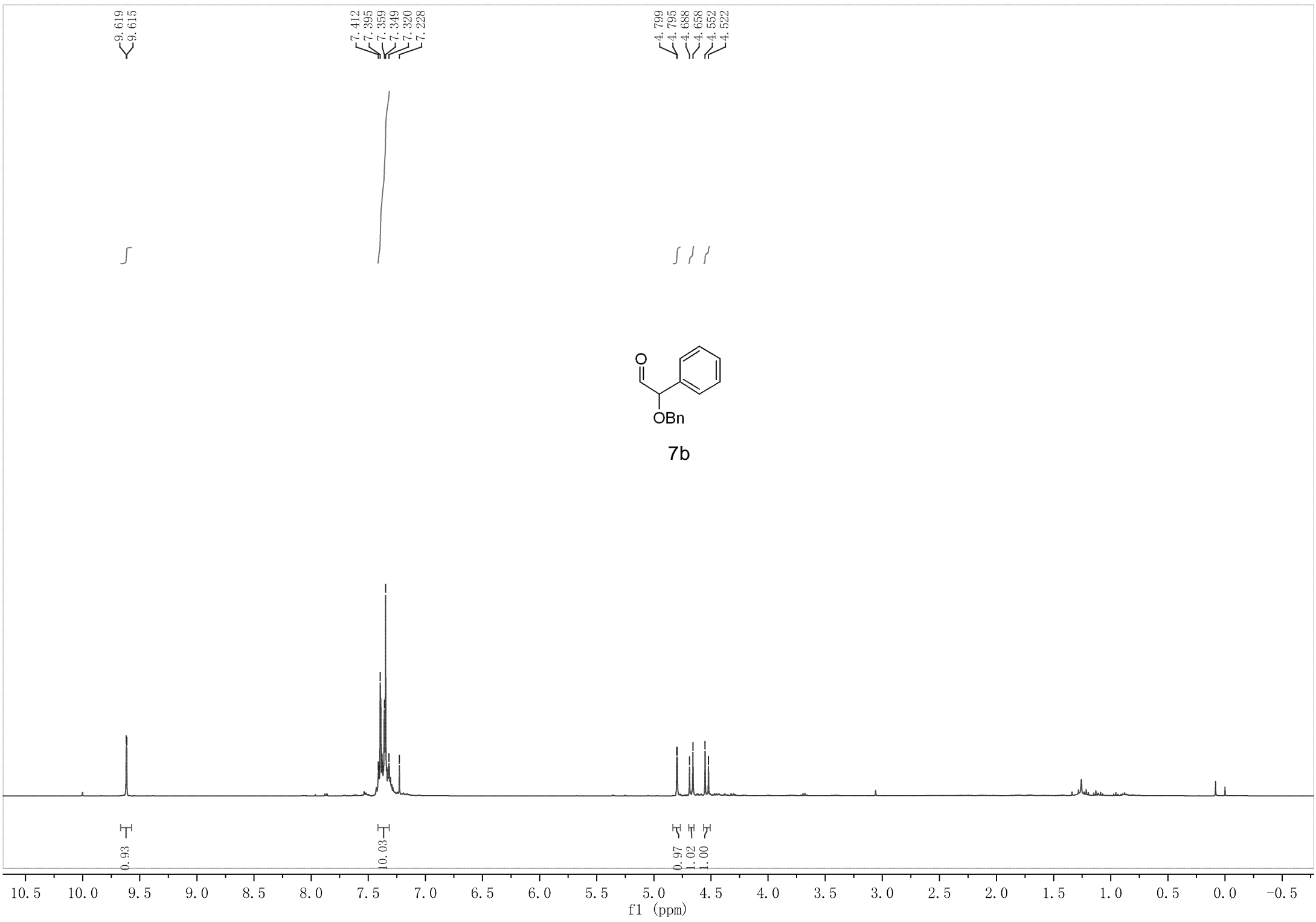
128.69
128.61
128.41
128.02
127.89
127.35

79.51

71.08

52.22

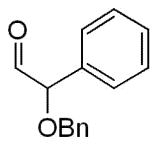




9.619
9.615

7.412
7.395
7.359
7.349
7.320
7.228

4.799
4.795
4.688
4.658
4.552
4.522



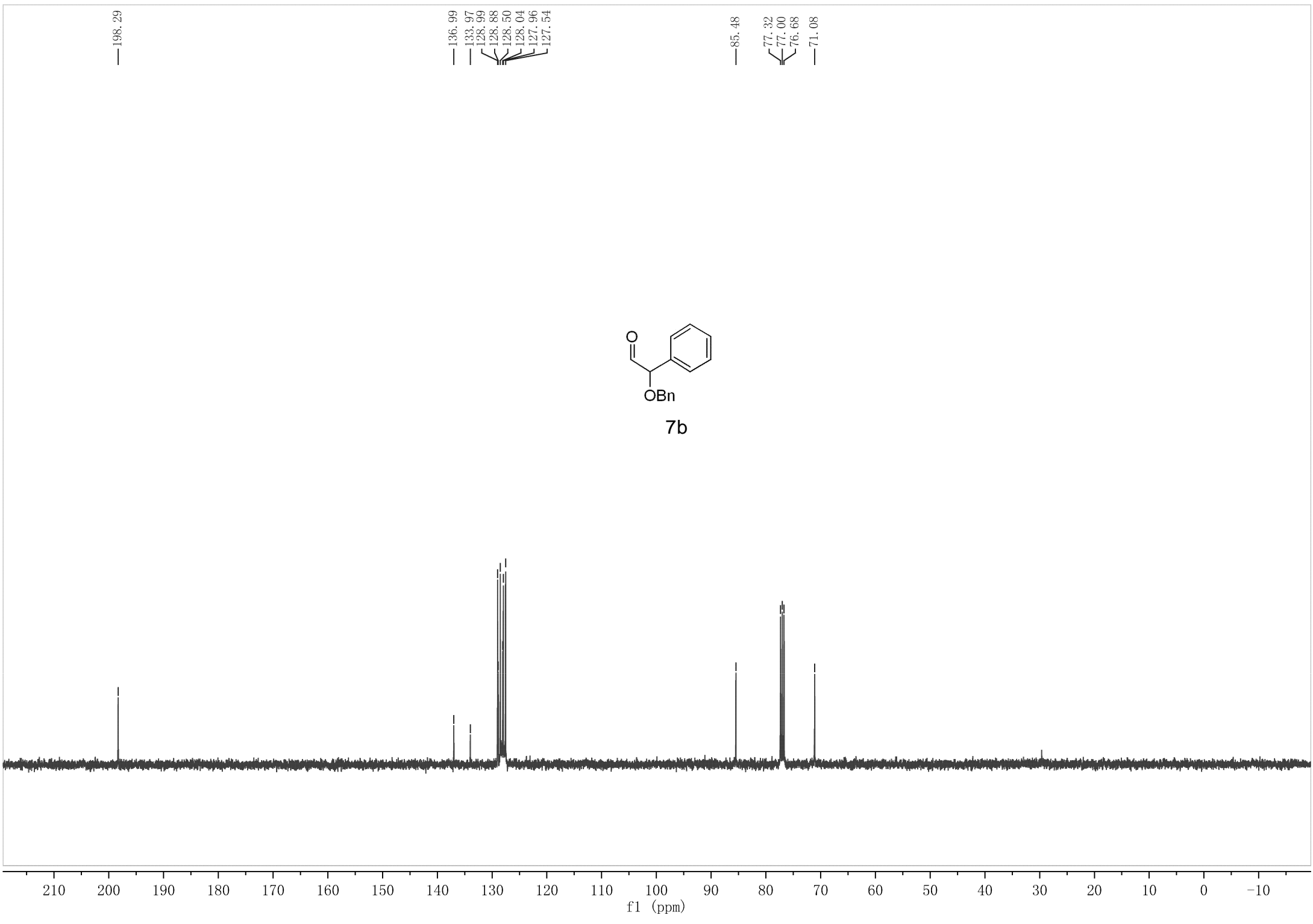
7b

0.93

10.03

0.97
1.02
1.00

10.5 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)

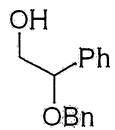


7.405
7.375
7.327
7.283

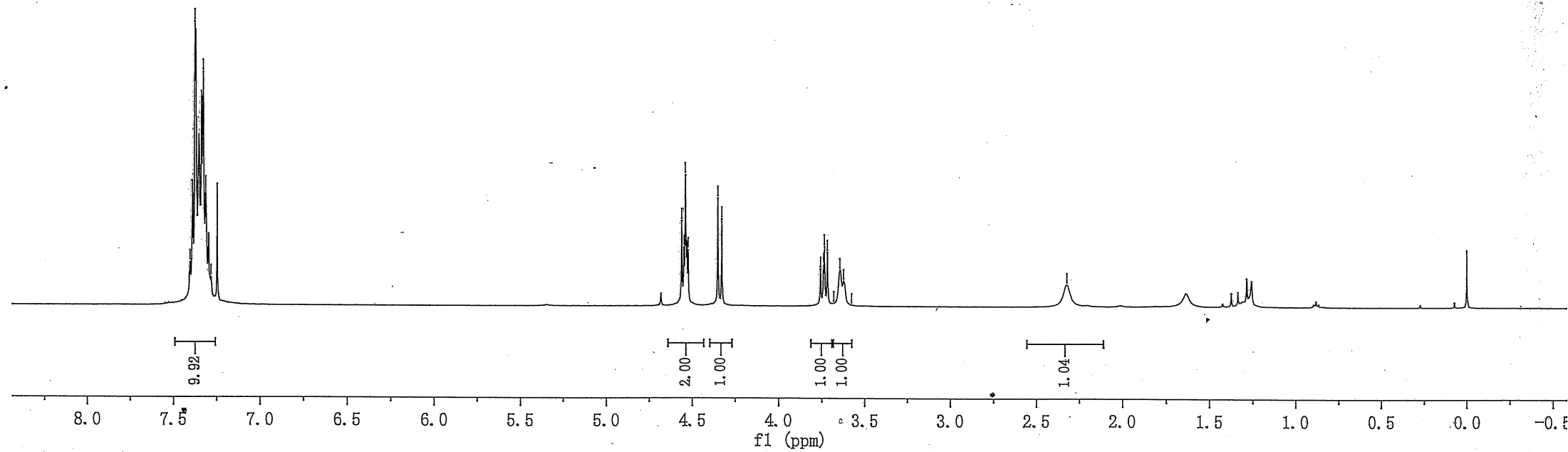
4.562
4.548
4.539
4.524
4.352
4.329

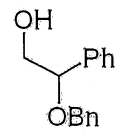
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3.741
3.735
3.717
3.681
3.644
3.623
3.577

2.323



7c

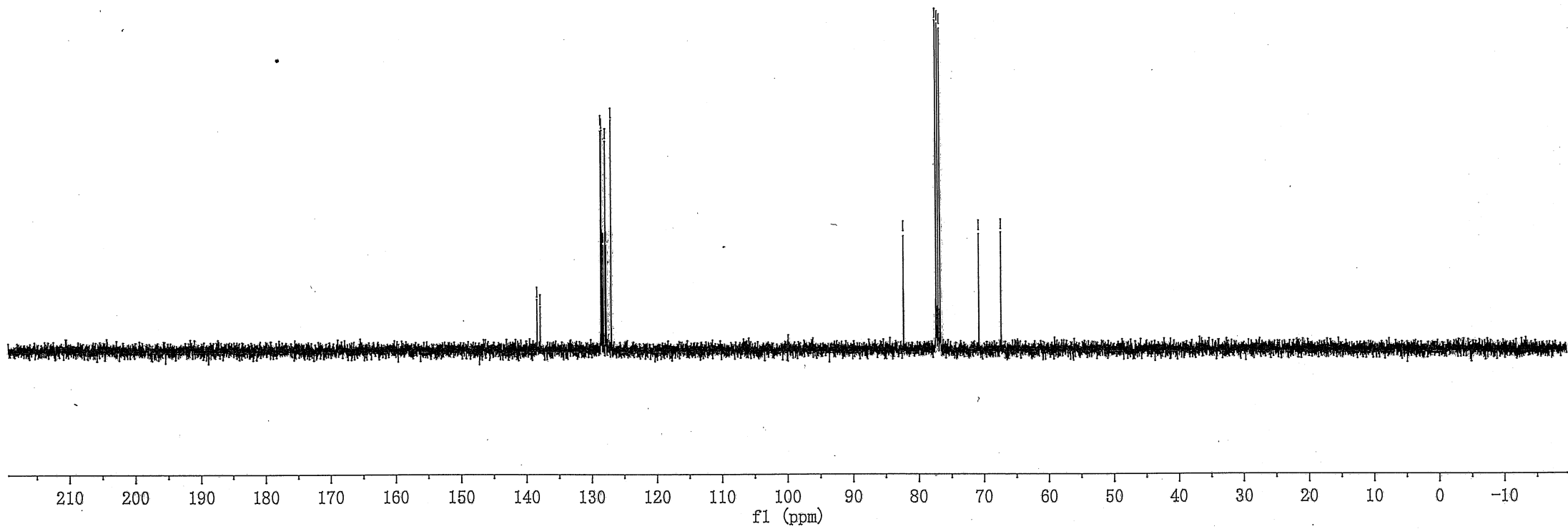


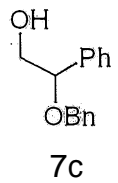


7c

138.88
137.90
128.60
128.44
128.21
127.89
127.78
126.99

82.28
77.32
77.00
76.68
70.74
67.35





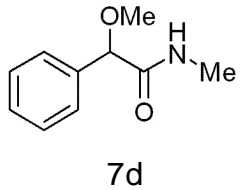
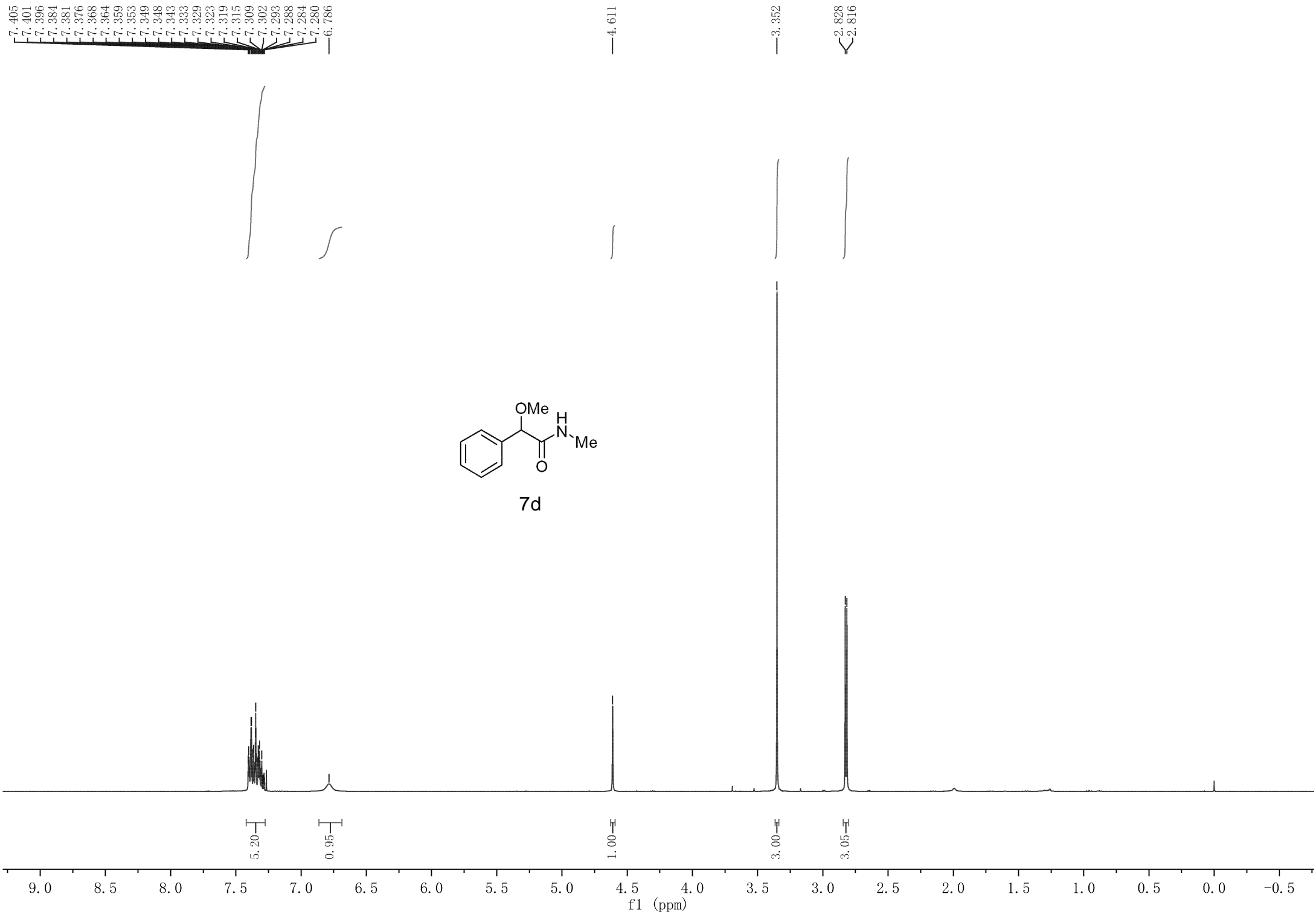
128.60
128.44
128.21
127.89
127.78
127.00

82.28

70.75

67.35

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.405
7.401
7.396
7.384
7.381
7.376
7.368
7.364
7.359
7.353
7.349
7.348
7.343
7.333
7.329
7.323
7.319
7.315
7.309
7.302
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7.288
7.284
7.280
6.786

4.611
3.352
2.828
2.816

5.20

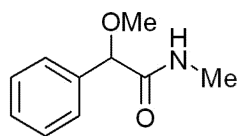
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1.00

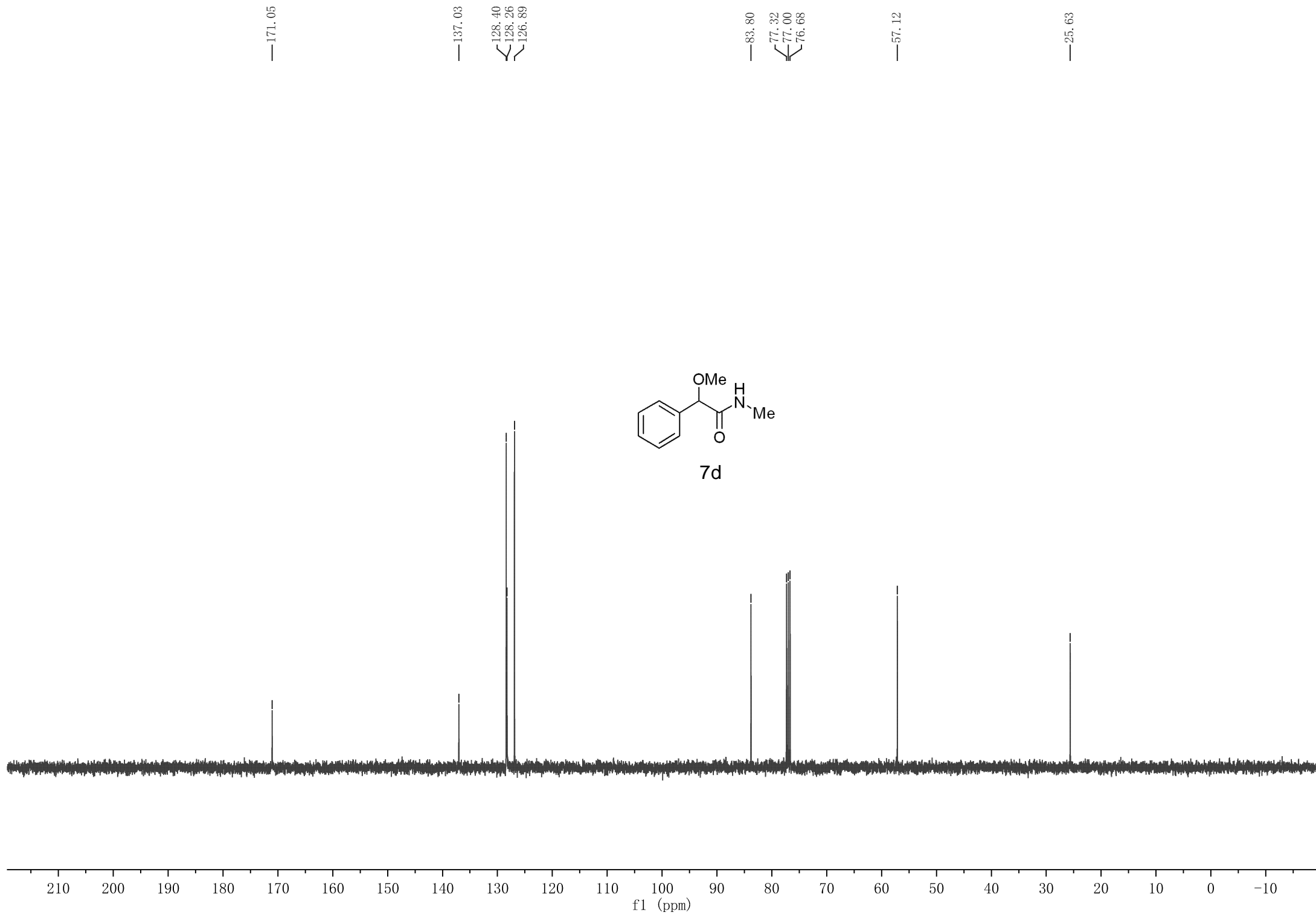
3.00

3.05

f1 (ppm)



7d



—9.582

—8.177

7.472

7.448

7.394

7.377

7.359

7.351

7.094

7.078

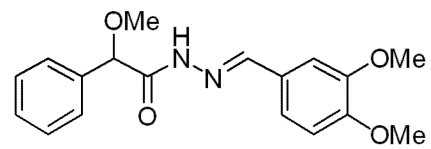
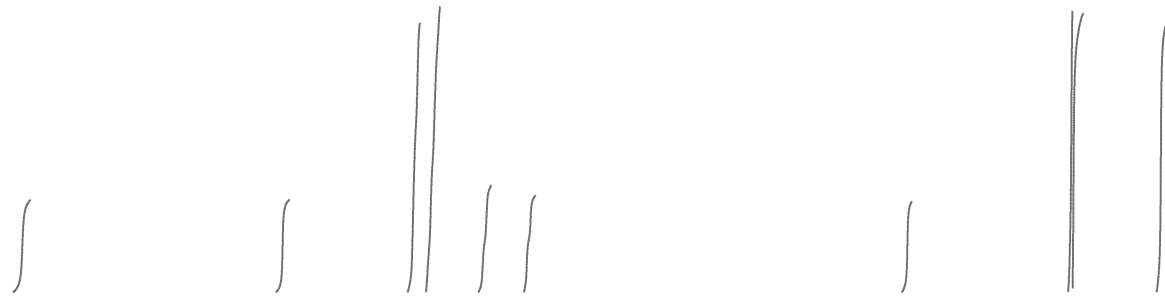
6.859

6.838

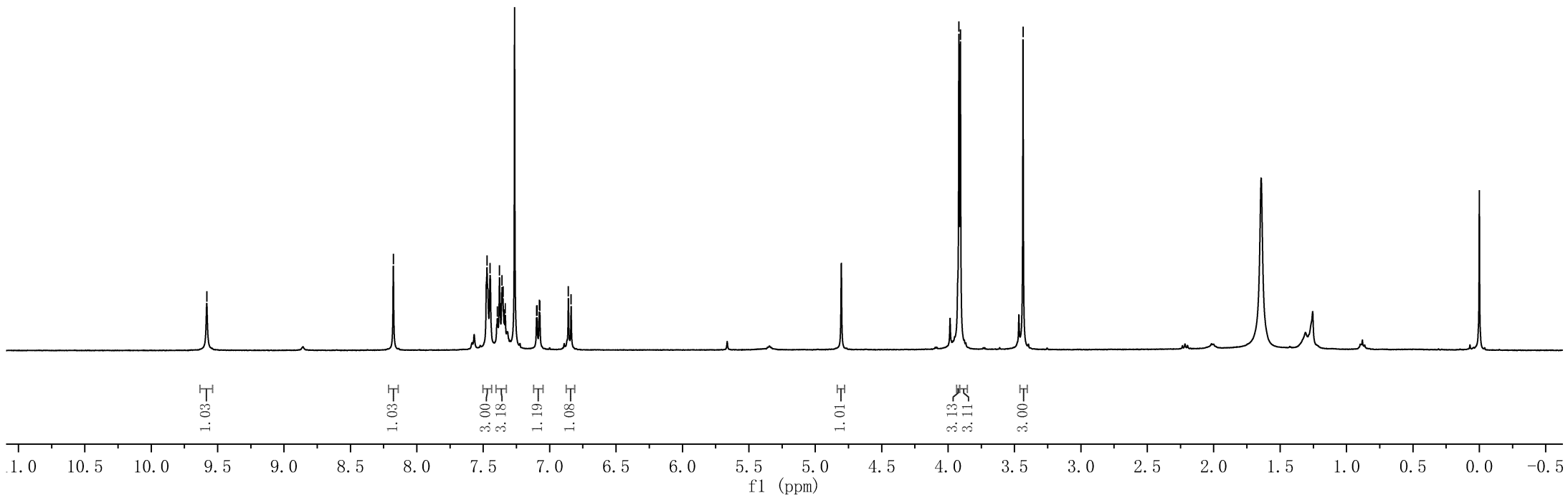
3.919

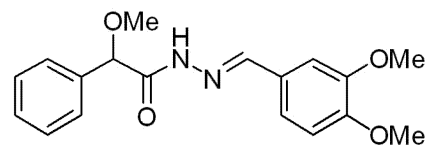
3.907

—3.436



7e





7e

