Supporting Information for

Base-Promoted Tandem Ring-Opening/Ring-Closing of *N*-Alkynyl-2-oxazolidinones Enables Facile Synthesis 2-Oxazolines

Xingyuan Ye,[a] Peng Bao,[a] Yan Pan,[b] Han Xiao,[a] Qiuwen Li,[a] and Guangke He*[a]

[a] *Department of Applied Chemistry, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, P. R. China.*

[b] *School of Pharmaceutical, Nanjing Tech University, Nanjing 211816, P. R. China.*

*E-mail: hegk@njtech.edu.cn;

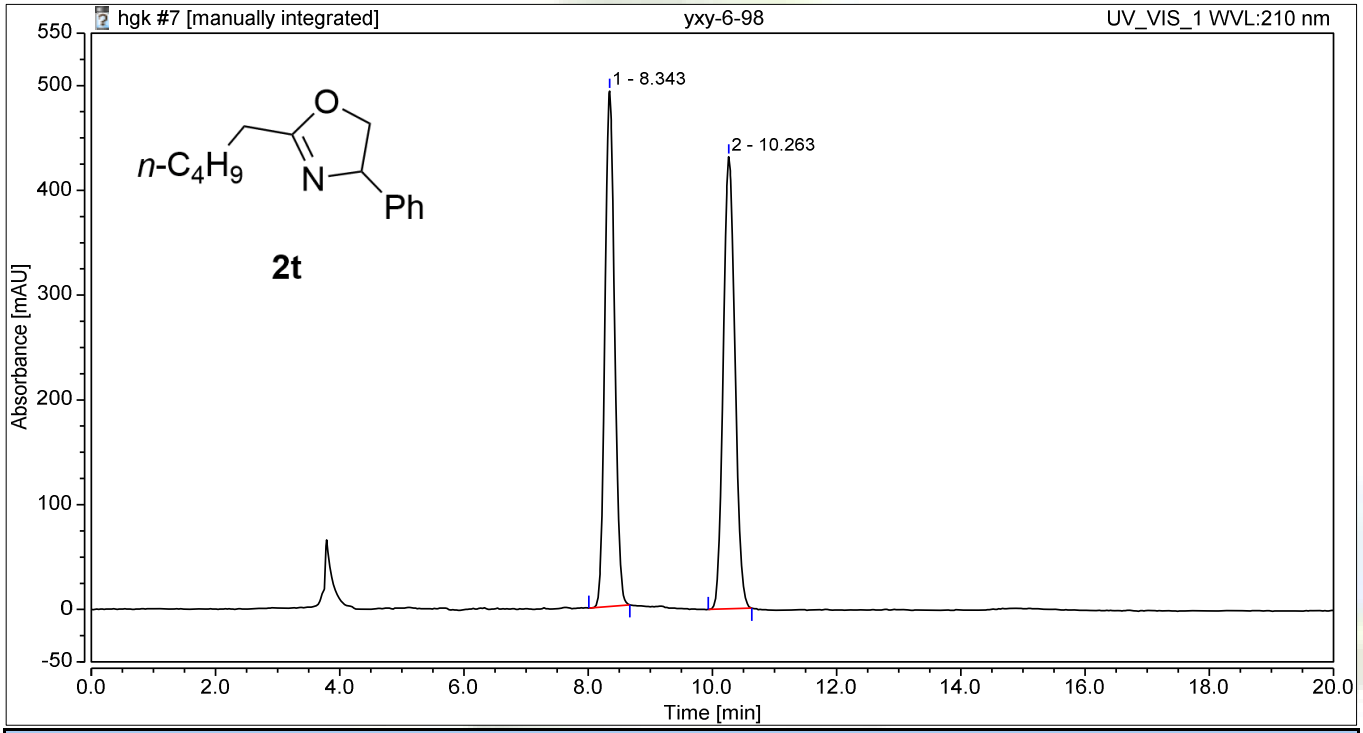
Spectra of Compounds 1w、2a~*d*$_2$-2a、3a、4e、5a

Chromatogram and Results

Injection Details

Injection Name:	**yxy-6-98**	*Run Time (min):*	**20.00**
Vial Number:	**RA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210**
Instrument Method:	**szm-25du-1ml-20min-97b-od-0.8**	*Bandwidth:*	**2**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**16/五月/24 15:46**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

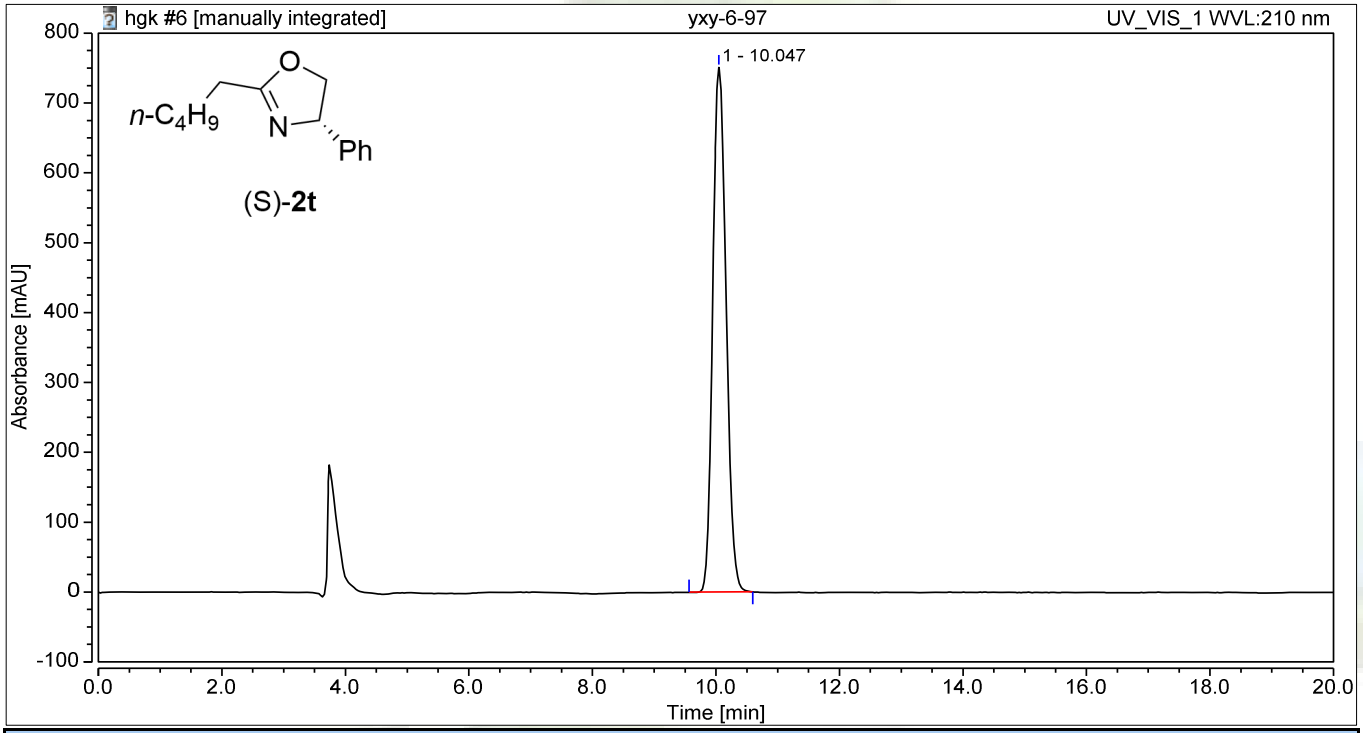
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.343	89.182	491.952	48.70	53.28	n.a.
2		10.263	93.939	431.420	51.30	46.72	n.a.
Total:			**183.120**	**923.372**	**100.00**	**100.00**	

Chromatogram and Results

Injection Details

Injection Name:	**yxy-6-97**	*Run Time (min):*	**20.00**
Vial Number:	**RA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210**
Instrument Method:	**szm-25du-1ml-20min-97b-od-0.8**	*Bandwidth:*	**2**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**16/五月/24 15:24**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

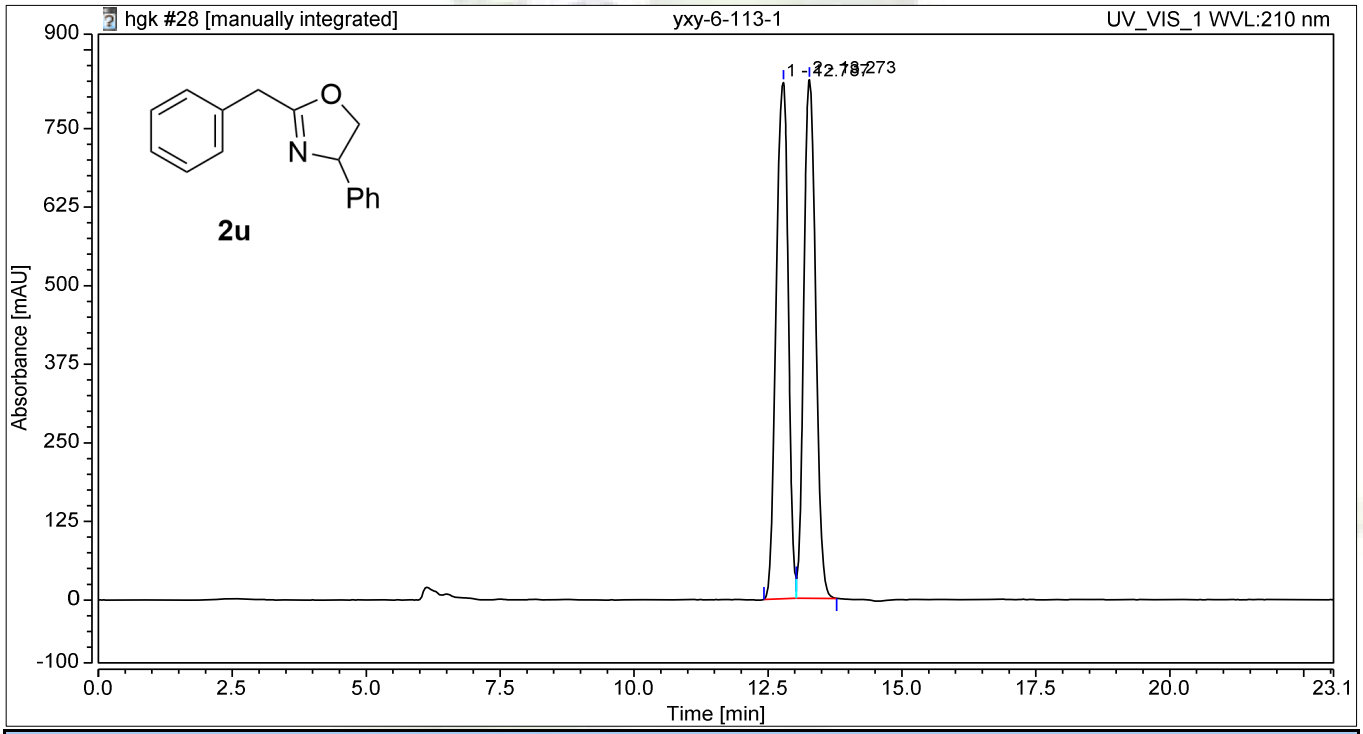
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.047	188.179	750.693	100.00	100.00	n.a.
Total:			**188.179**	**750.693**	**100.00**	**100.00**	

Chromatogram and Results

Injection Details

Injection Name:	**yxy-6-113-1**	*Run Time (min):*	**23.06**
Vial Number:	**RA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210**
Instrument Method:	**szm-25du-1ml-25min-80b-od-0.8**	*Bandwidth:*	**2**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**04/六月/24 12:41**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

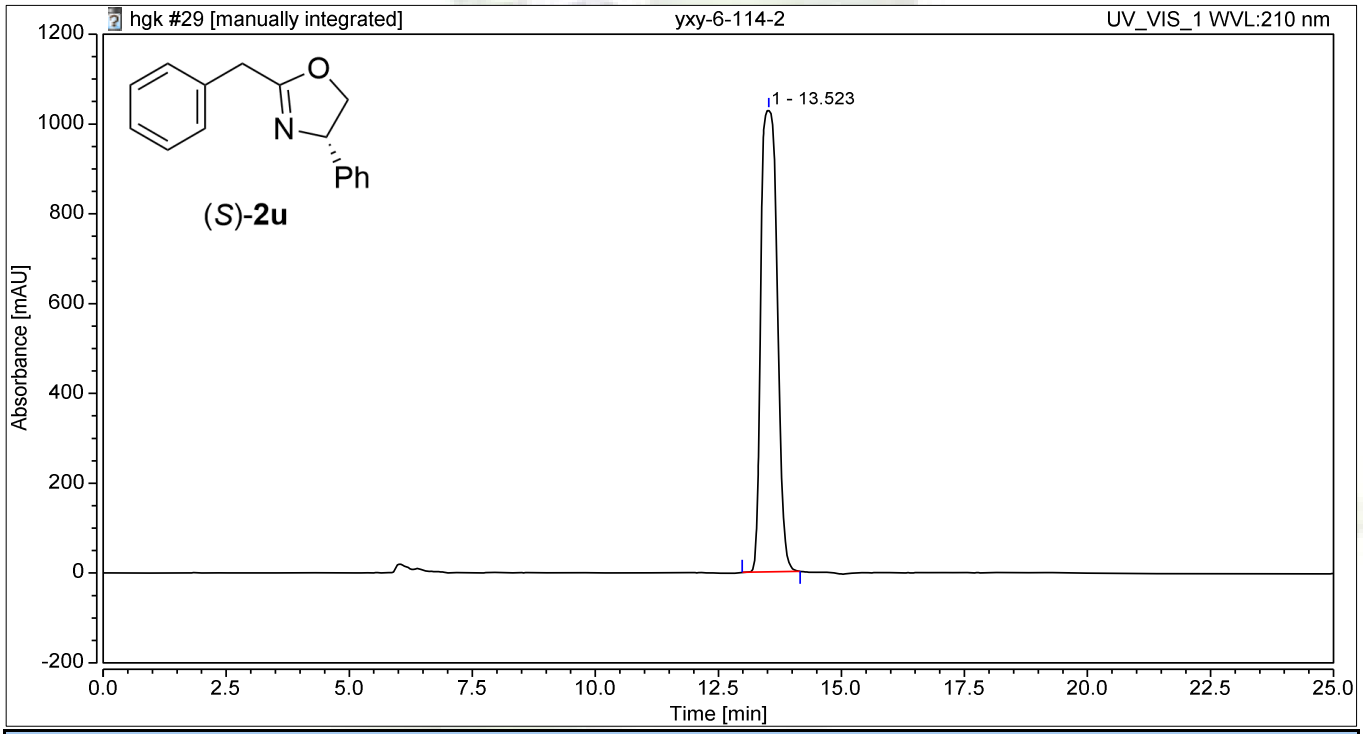
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12.787	215.525	821.353	50.32	49.89	n.a.
2		13.273	212.754	824.827	49.68	50.11	n.a.
Total:			**428.280**	**1646.180**	**100.00**	**100.00**	

Chromatogram and Results

Injection Details

Injection Name:	**yxy-6-114-2**	*Run Time (min):*	**25.00**
Vial Number:	**RA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210**
Instrument Method:	**szm-25du-1ml-25min-80b-od-0.8**	*Bandwidth:*	**2**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**04/六月/24 13:08**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

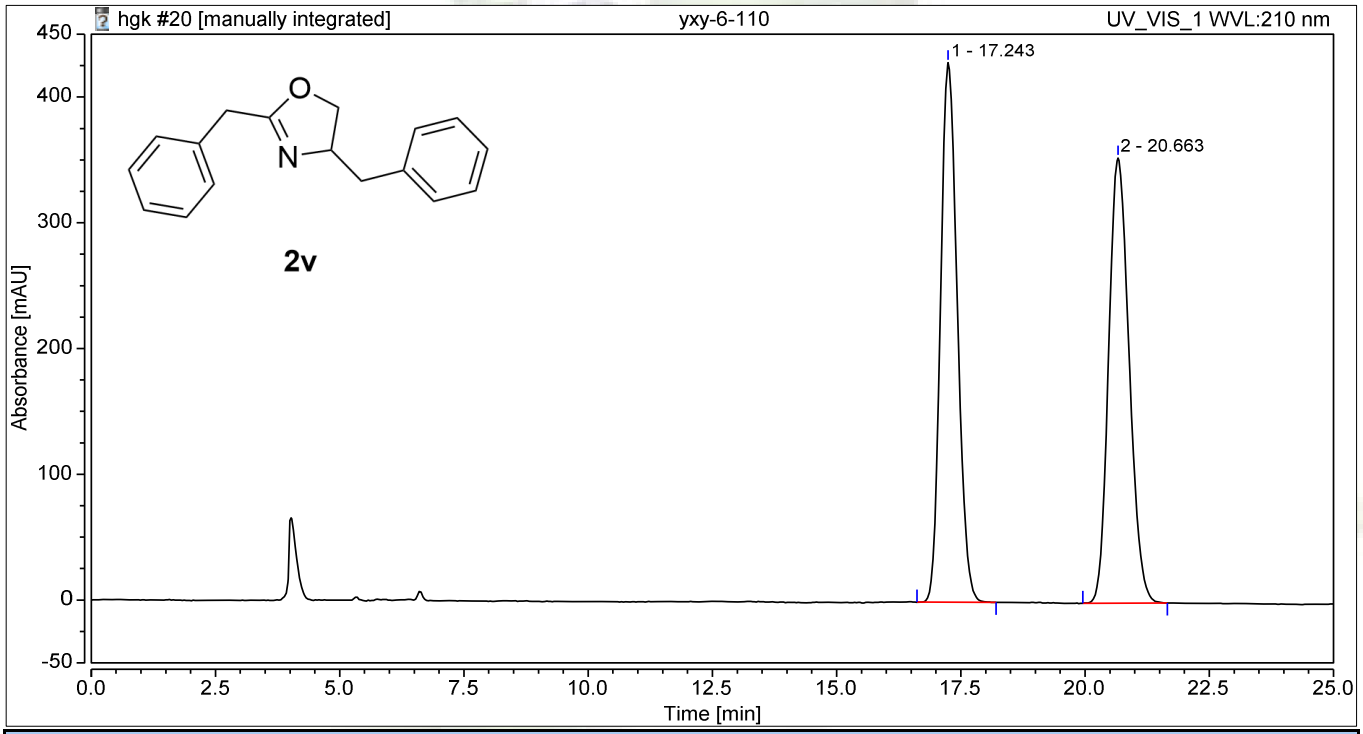
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.523	395.435	1027.758	100.00	100.00	n.a.
Total:			**395.435**	**1027.758**	**100.00**	**100.00**	

Chromatogram and Results

Injection Details

Injection Name:	**yxy-6-110**	*Run Time (min):*	**25.00**
Vial Number:	**RA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210**
Instrument Method:	**szm-25du-1ml-25min-97b-od-0.8**	*Bandwidth:*	**2**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**03/六月/24 16:00**	*Sample Weight:*	**1.0000**

Chromatogram



Integration Results

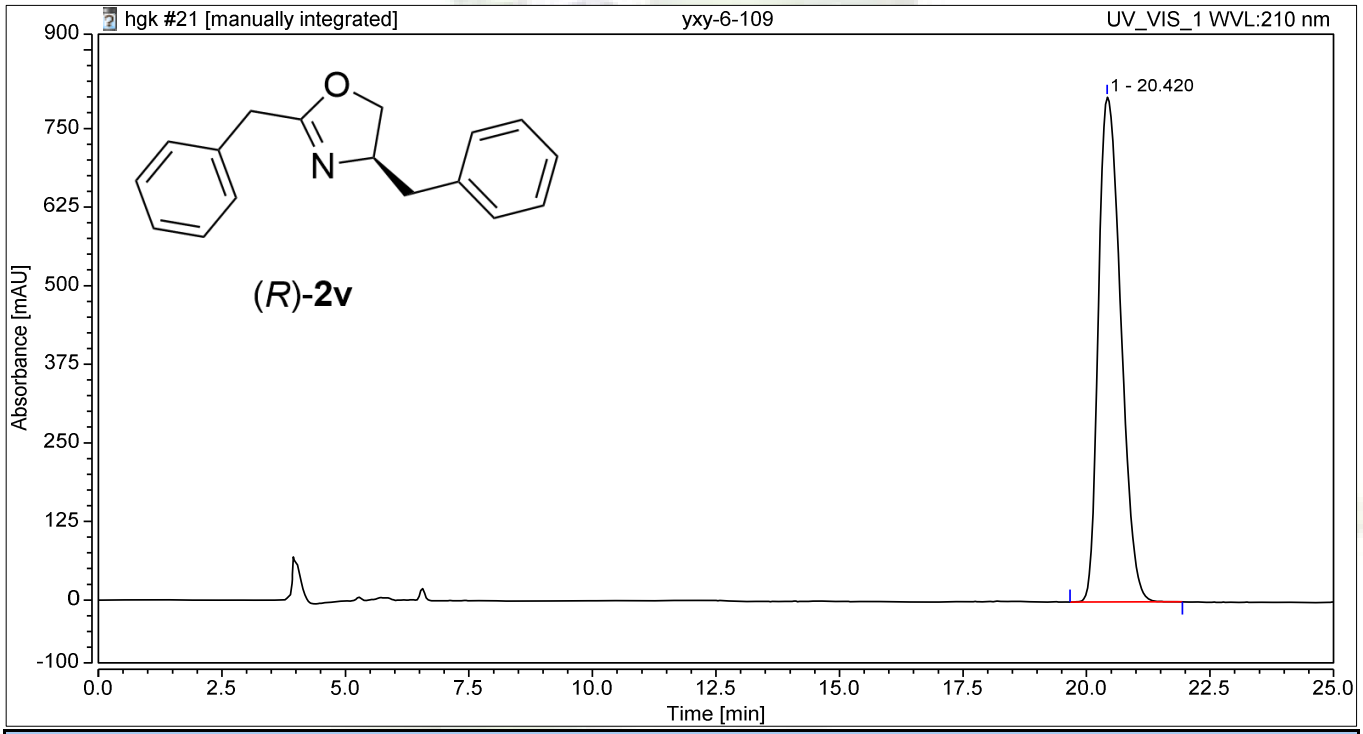
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.243	168.308	429.059	49.85	54.80	n.a.
2		20.663	169.337	353.946	50.15	45.20	n.a.
Total:			**337.645**	**783.005**	**100.00**	**100.00**	

Chromatogram and Results

Injection Details

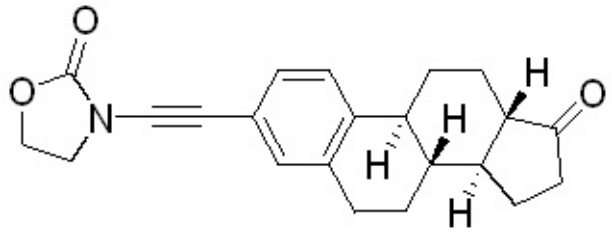
Injection Name:	**yxy-6-109**	*Run Time (min):*	**25.00**
Vial Number:	**RA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210**
Instrument Method:	**szm-25du-1ml-25min-97b-od-0.8**	*Bandwidth:*	**2**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**03/六月/24 16:26**	*Sample Weight:*	**1.0000**

Chromatogram

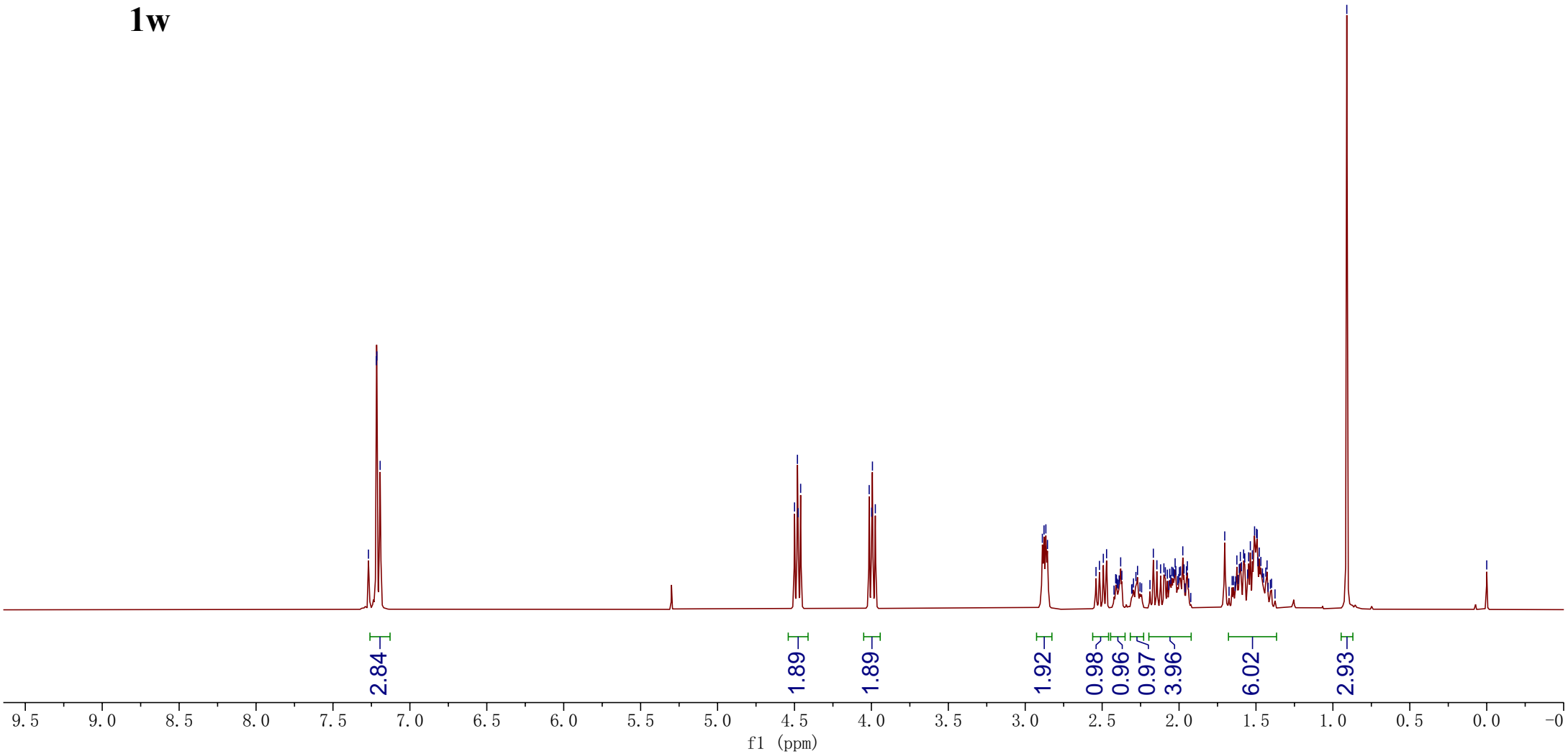


Integration Results

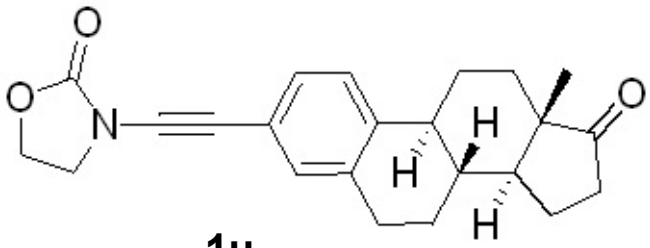
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		20.420	424.250	802.895	100.00	100.00	n.a.
Total:			**424.250**	**802.895**	**100.00**	**100.00**	



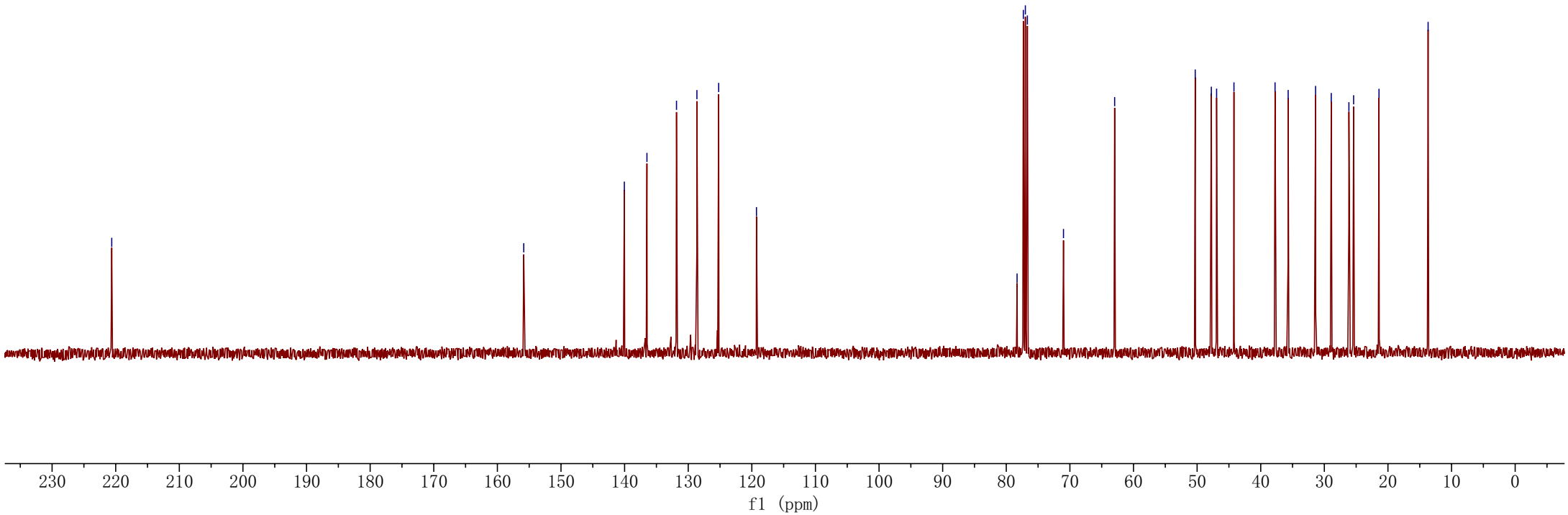
1w

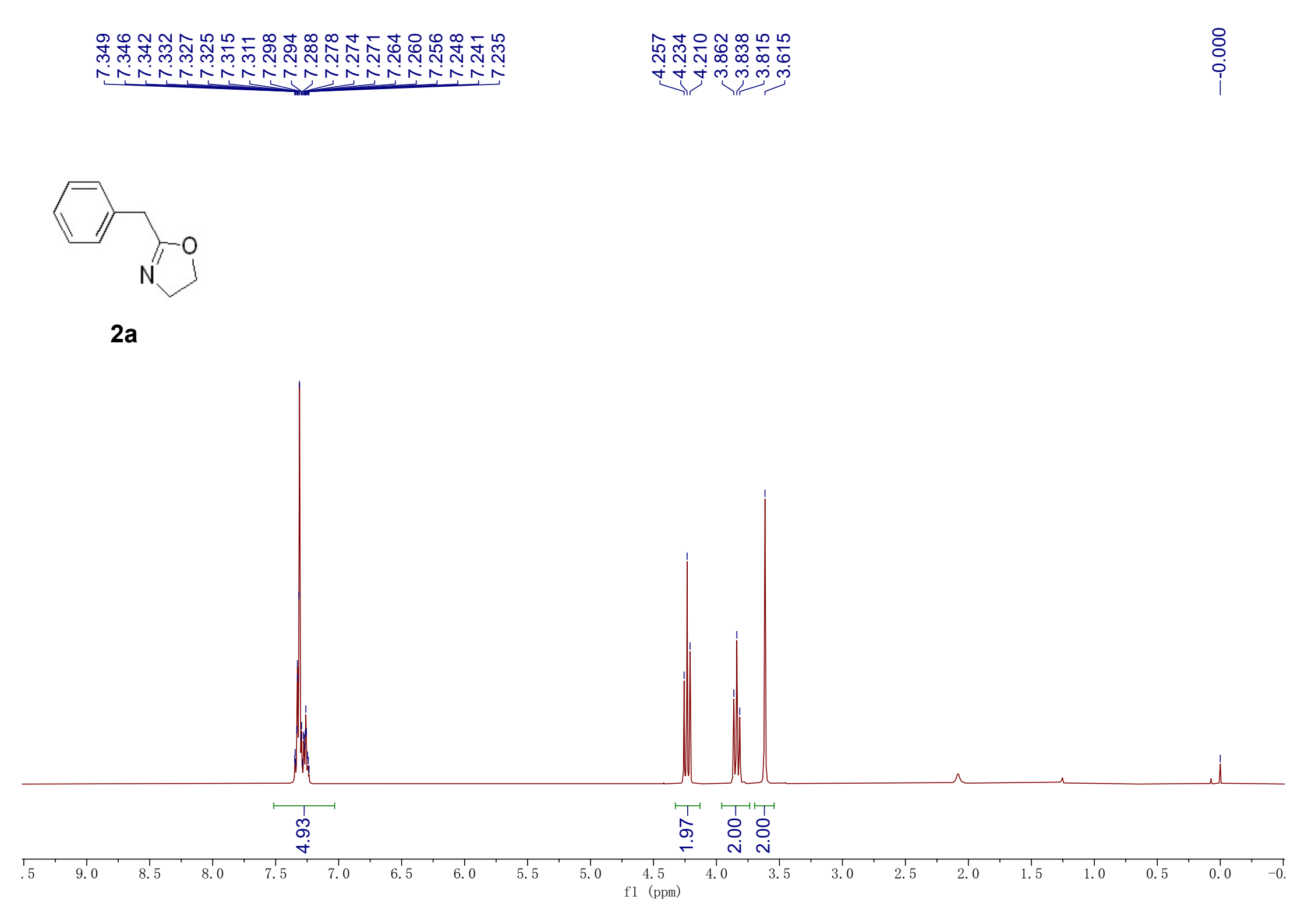


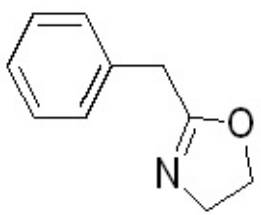
220.62
155.85
140.04
136.49
131.84
128.63
125.21
119.27
78.30
77.32
77.00
76.68
71.01
62.96
50.30
47.76
46.94
44.21
37.75
35.69
31.38
28.91
26.14
25.40
21.41
13.69



1u

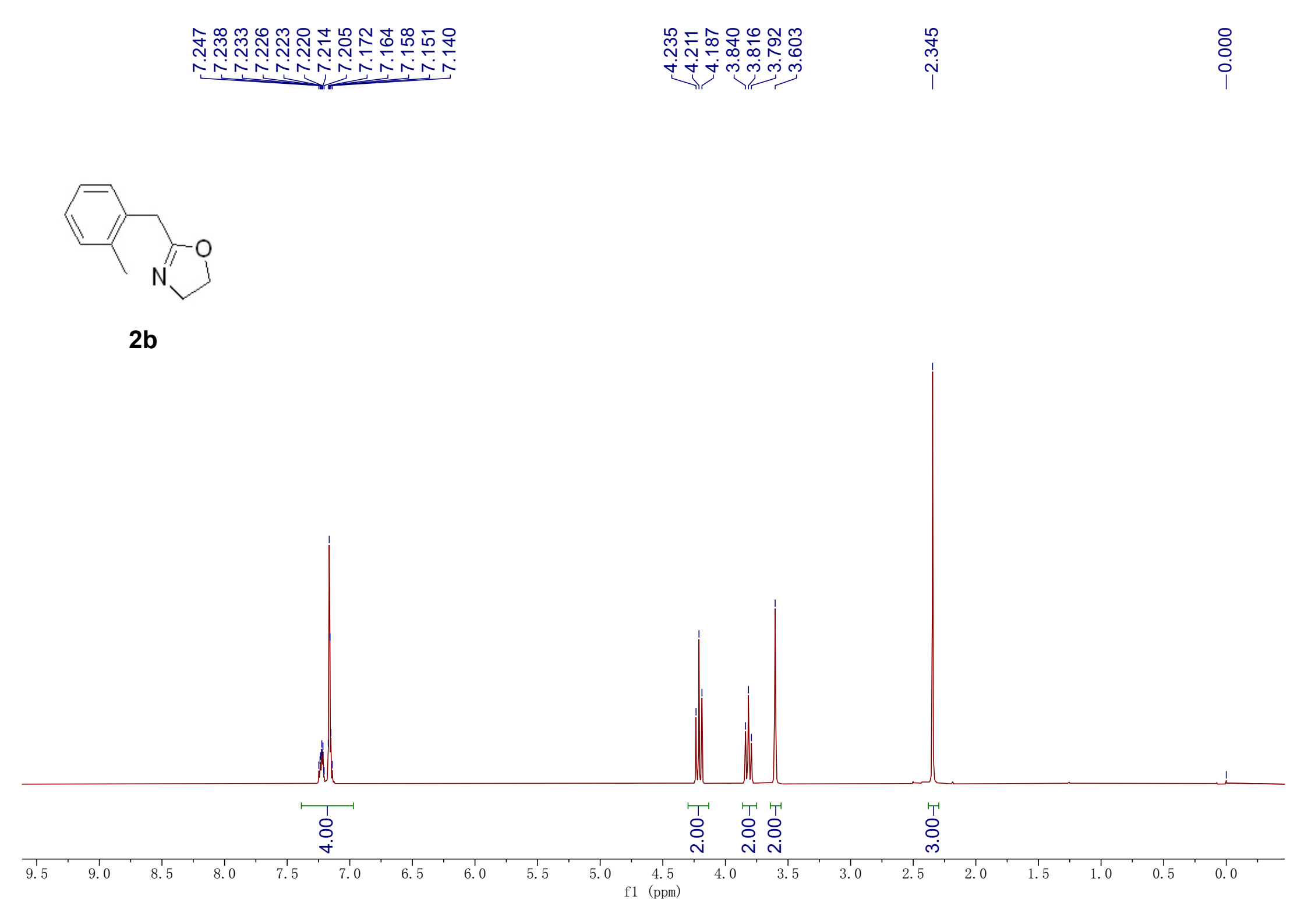


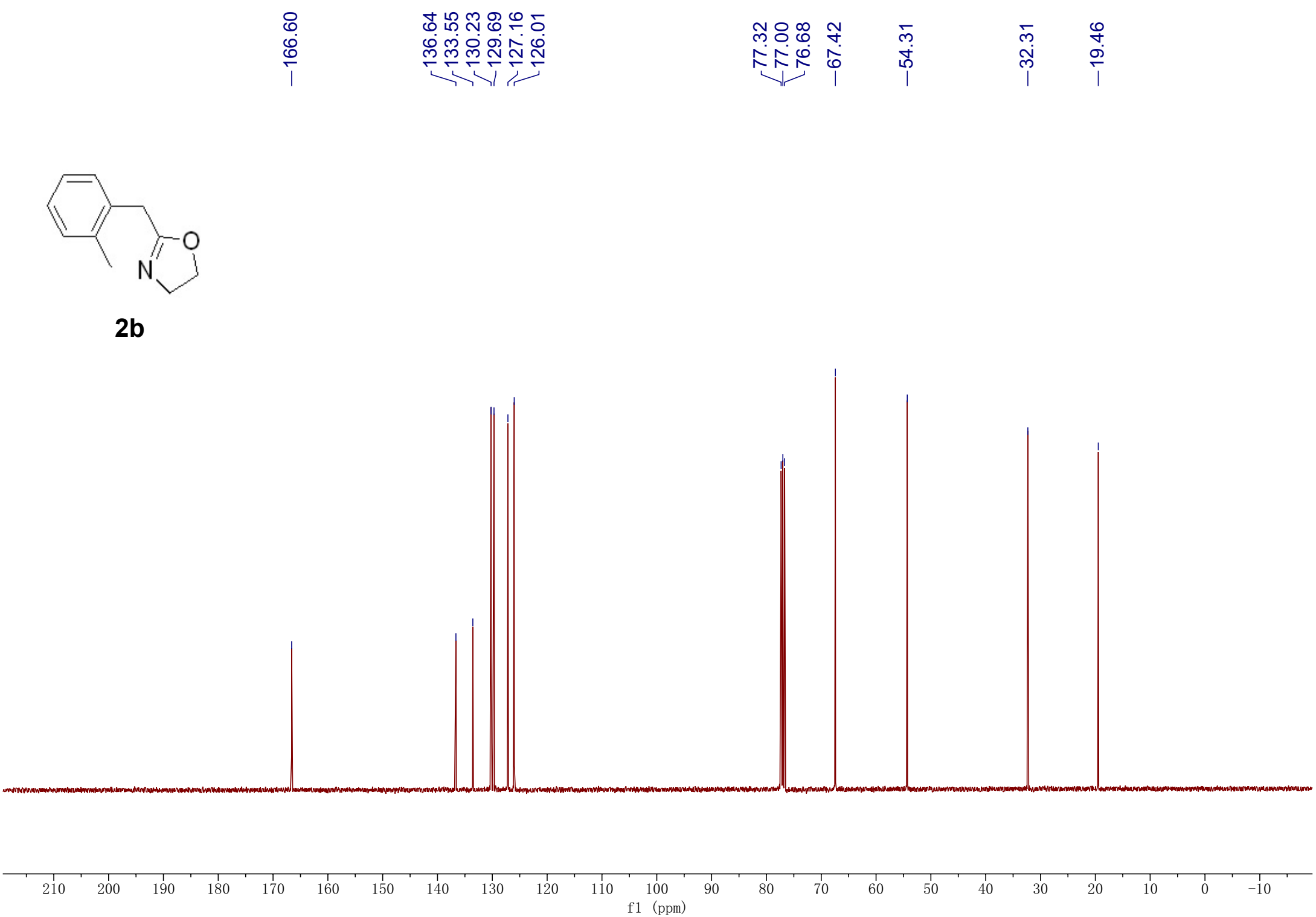

7.349
7.346
7.342
7.332
7.327
7.325
7.315
7.311
7.298
7.294
7.288
7.278
7.274
7.271
7.264
7.260
7.256
7.248
7.241
7.235
4.257
4.234
4.210
3.862
3.838
3.815
3.615
-0.000
O
N
2a
4.93
1.97
2.00
2.00
f1 (ppm)

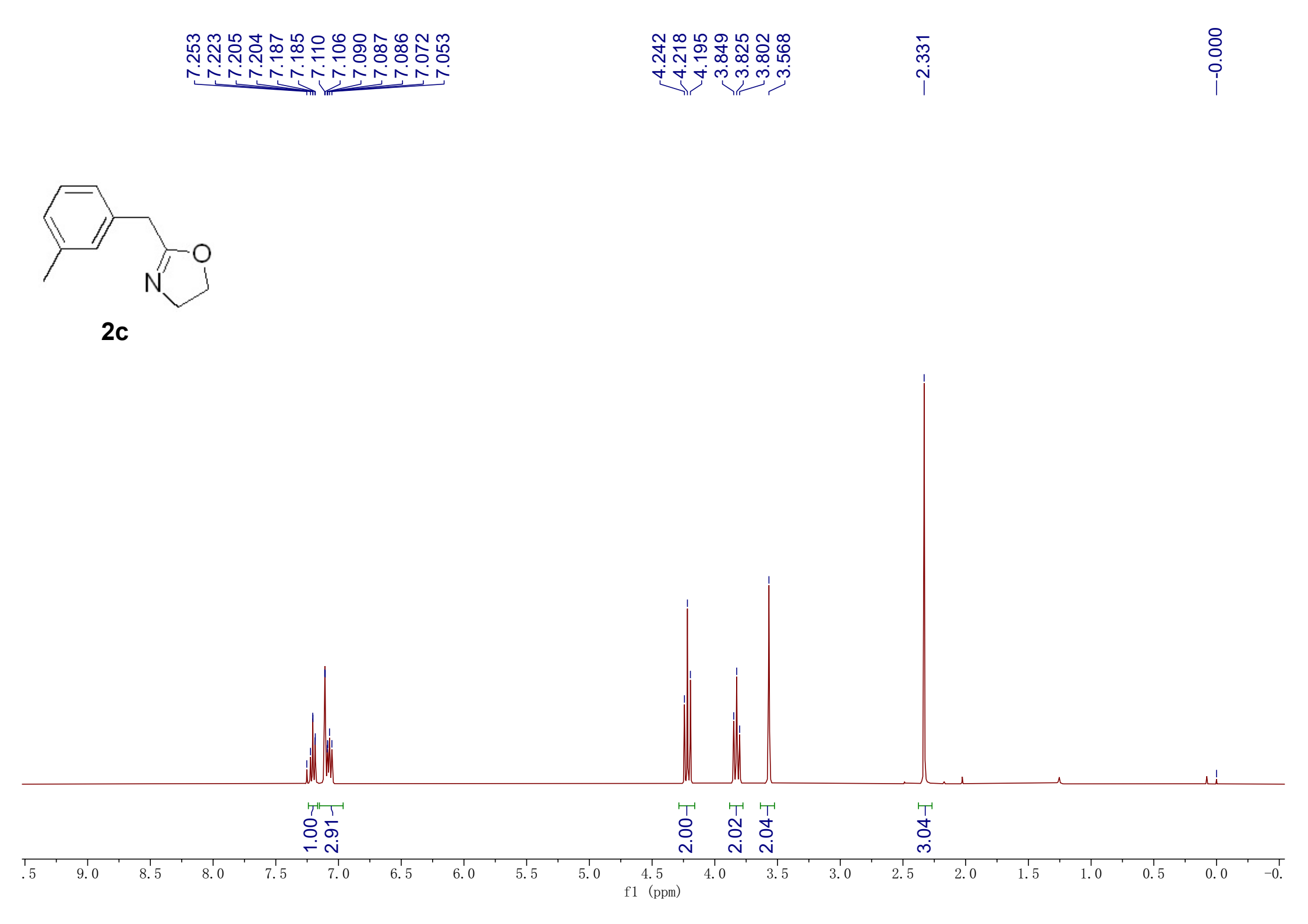

O
N

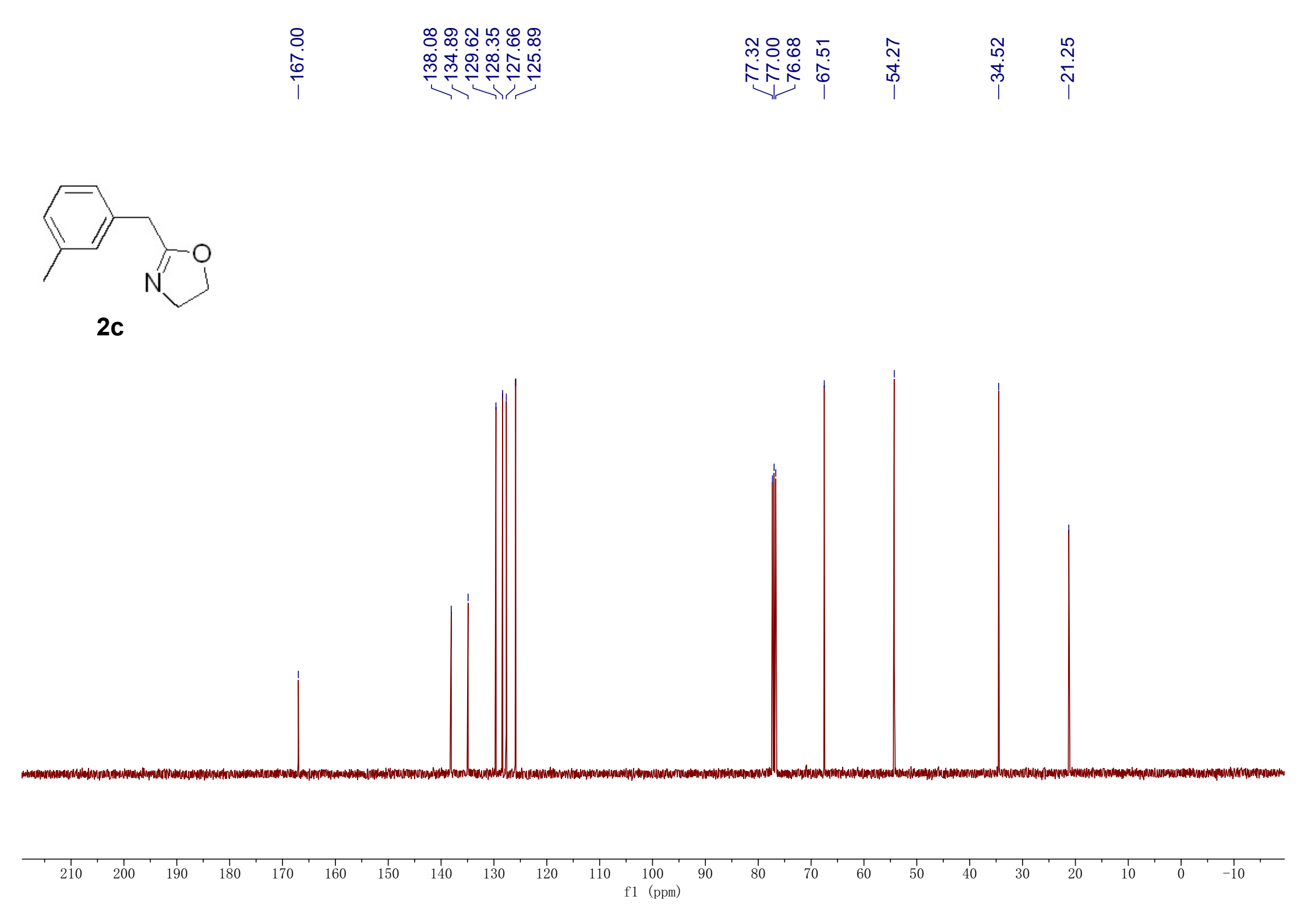
2a

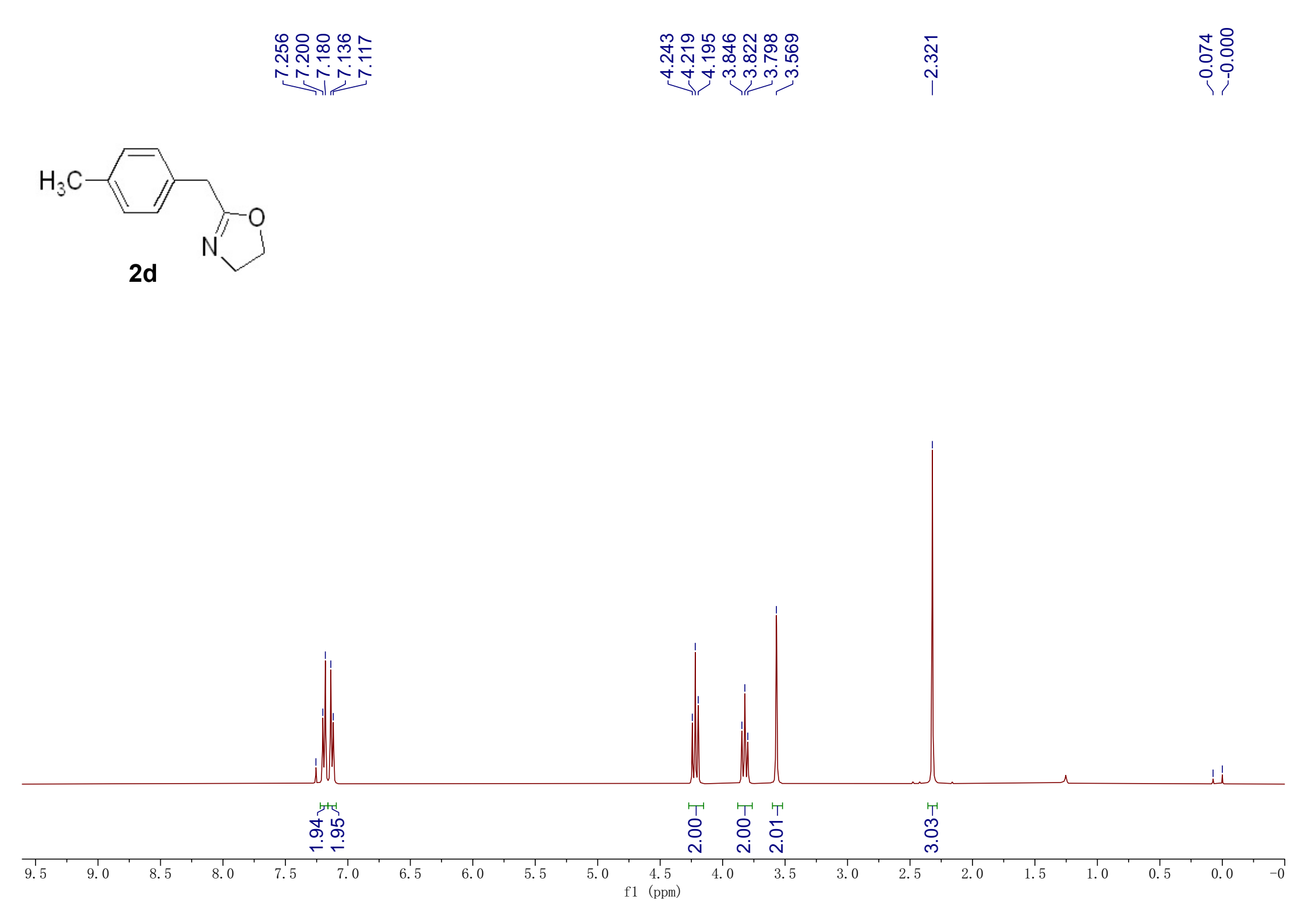
166.82
135.10
128.90
128.48
126.89
77.32
77.00
76.68
67.52
54.38
34.64
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

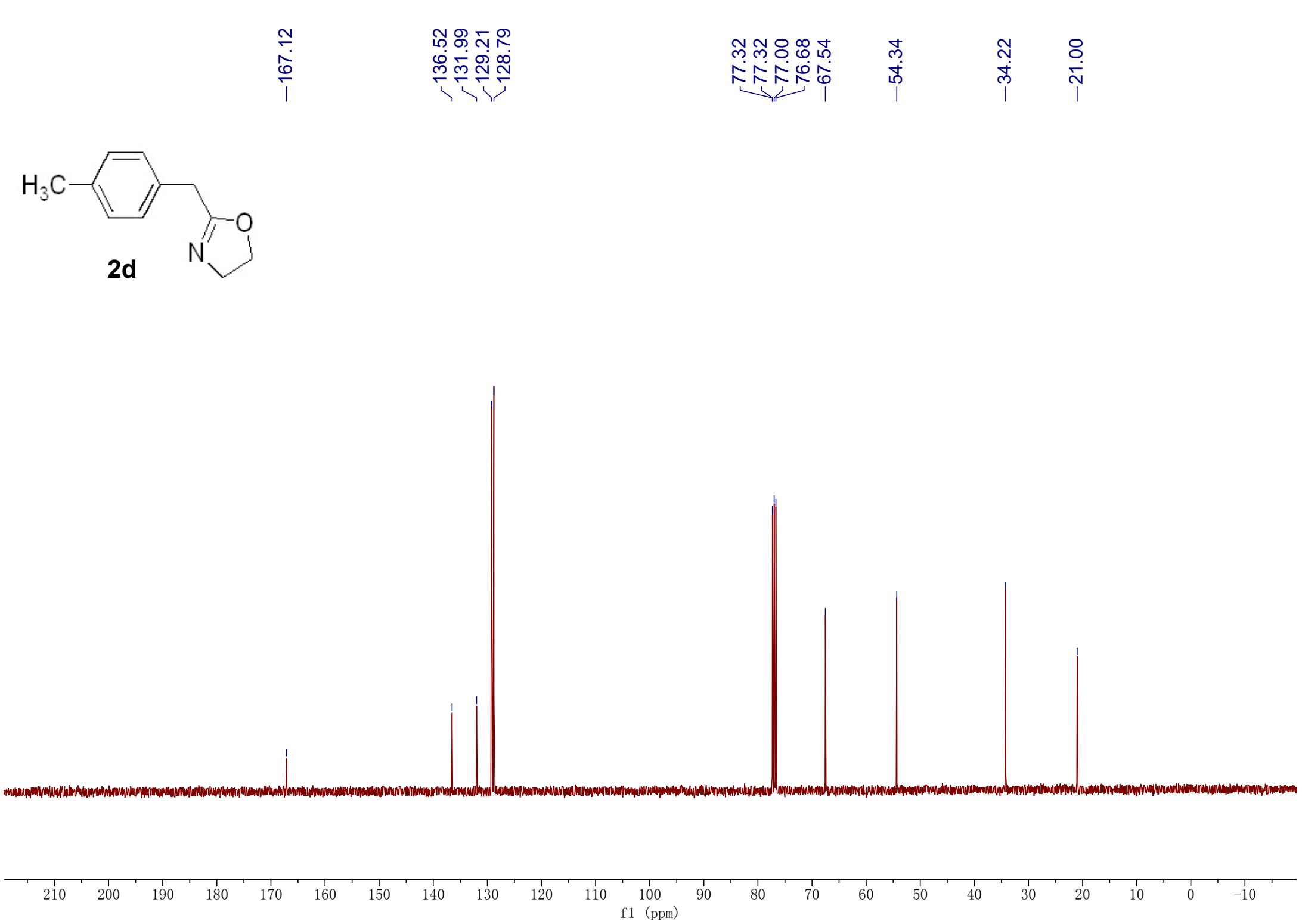

7.247
7.238
7.233
7.226
7.223
7.220
7.214
7.205
7.172
7.164
7.158
7.151
7.140
4.235
4.211
4.187
3.840
3.816
3.792
3.603
2.345
0.000
O
N
2b
4.00
2.00
2.00
2.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

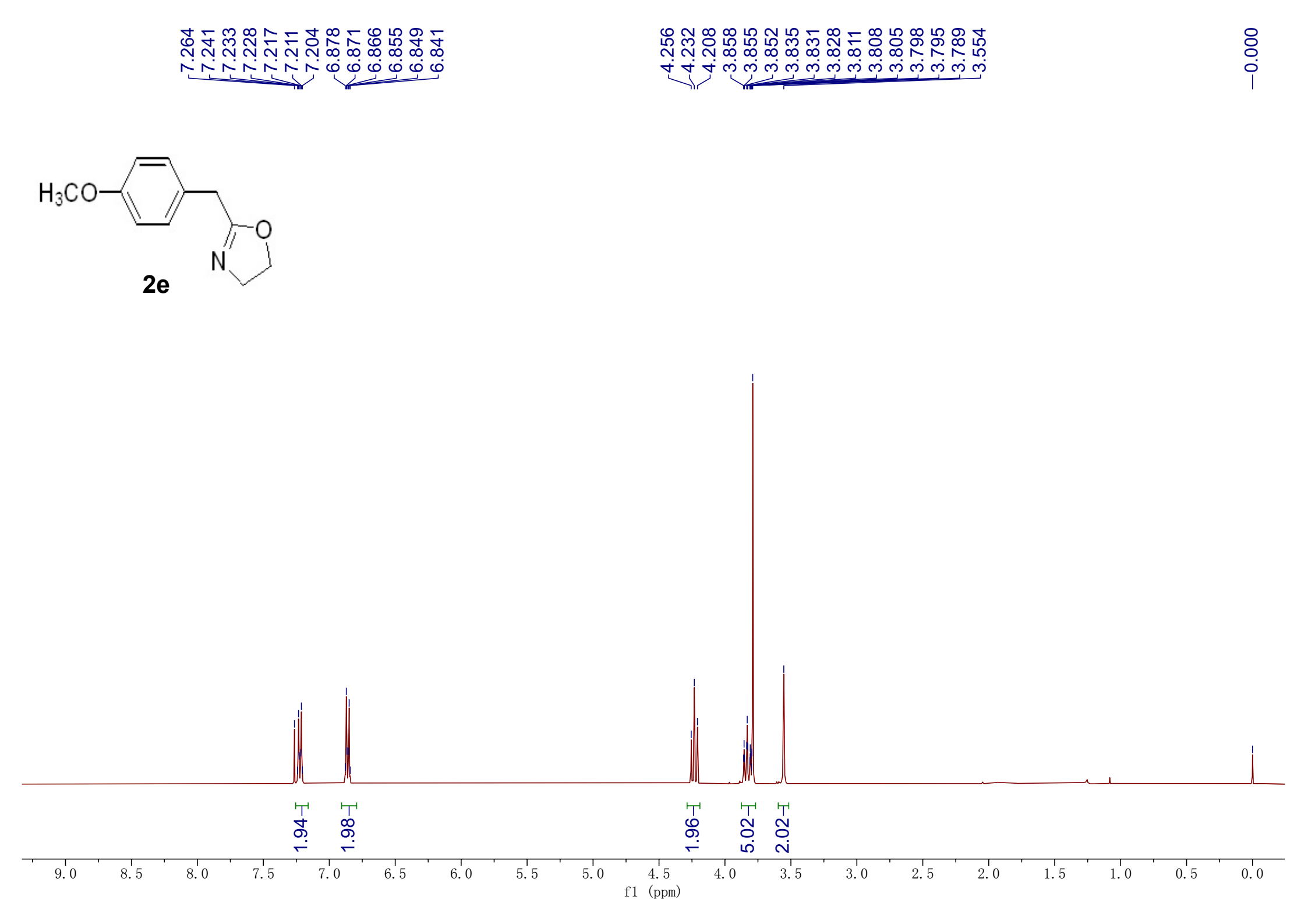

166.60
136.64
133.55
130.23
129.69
127.16
126.01
77.32
77.00
76.68
67.42
54.31
32.31
19.46
O
N
2b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

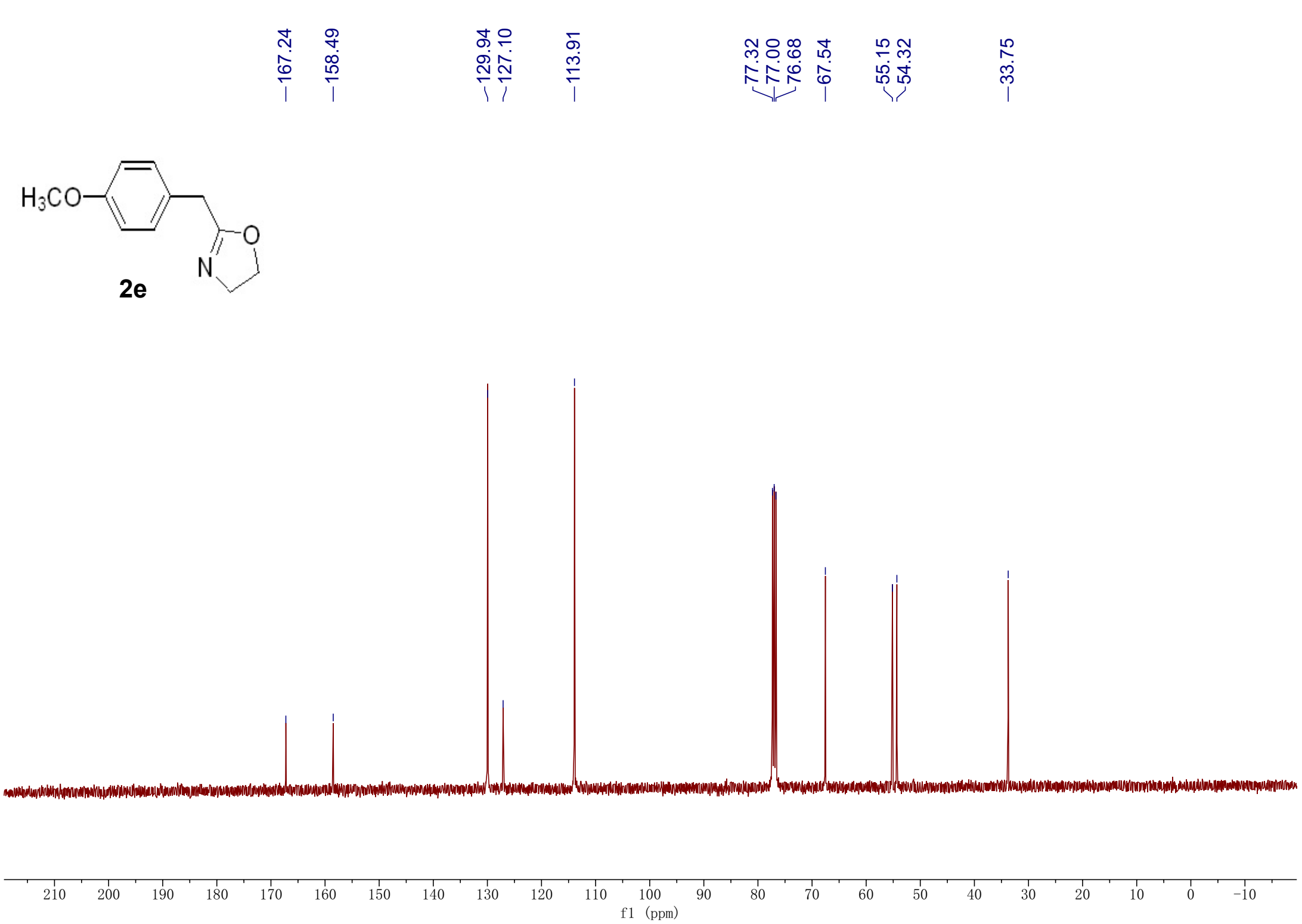

7.253
7.223
7.205
7.204
7.187
7.185
7.110
7.106
7.090
7.087
7.086
7.072
7.053
4.242
4.218
4.195
3.849
3.825
3.802
3.568
2.331
-0.000
O
N
2c
1.00
2.91
2.00
2.02
2.04
3.04
f1 (ppm)

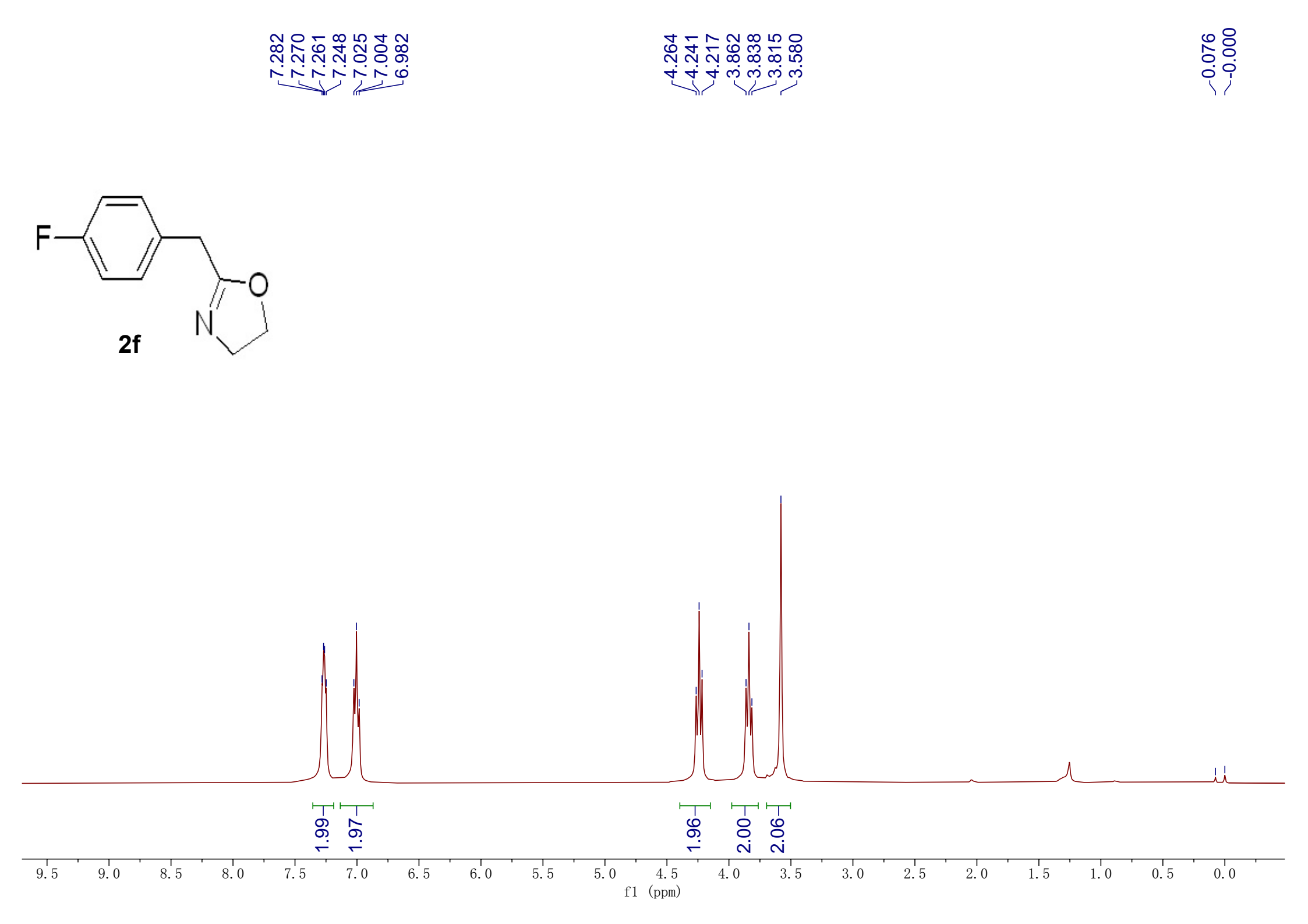

167.00
138.08
134.89
129.62
128.35
127.66
125.89
77.32
77.00
76.68
67.51
54.27
34.52
21.25
O
N
2c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

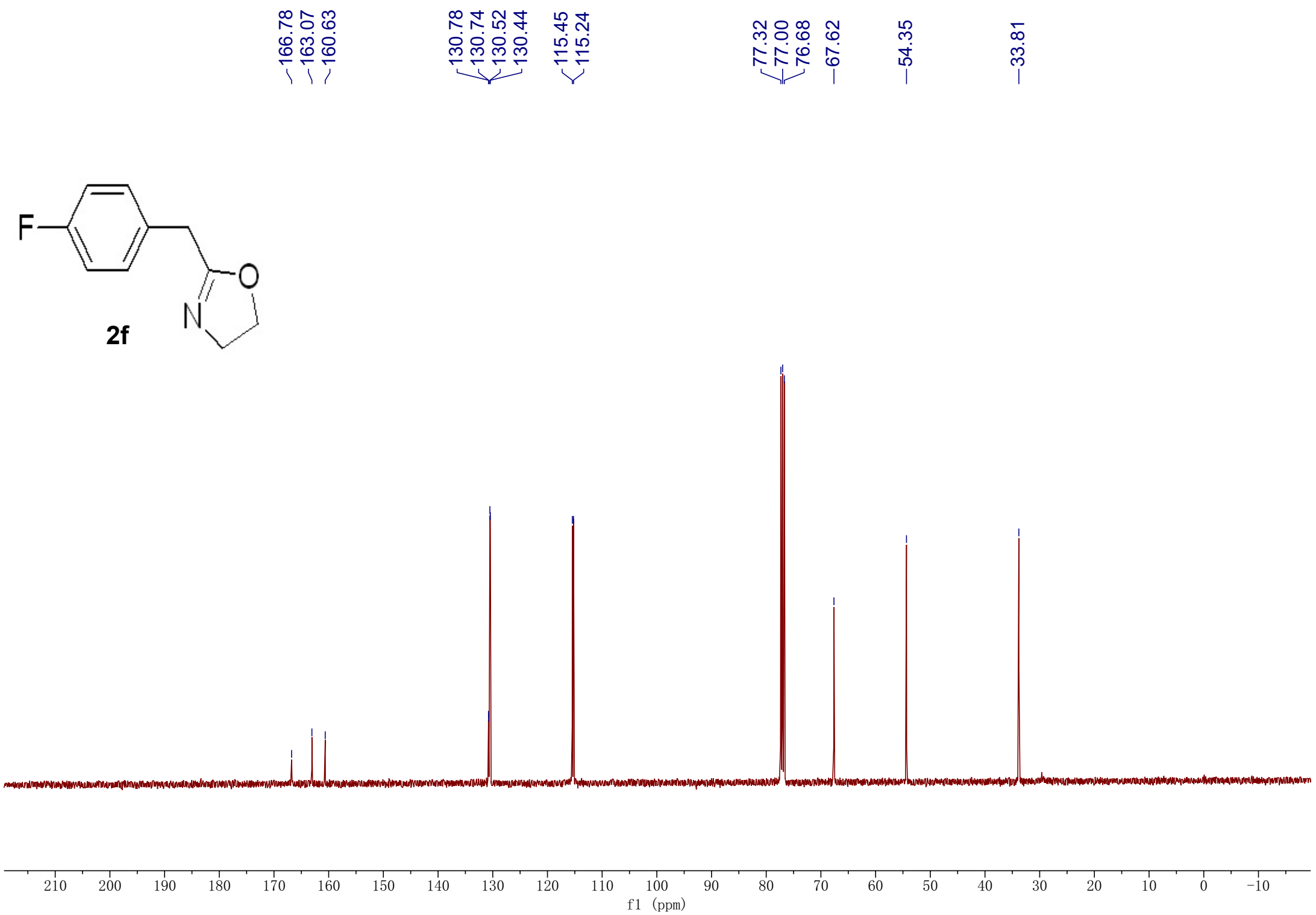

7.256
7.200
7.180
7.136
7.117
4.243
4.219
4.195
3.846
3.822
3.798
3.569
2.321
0.074
-0.000
H3C
O
N
2d
1.94
1.95
2.00
2.00
2.01
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

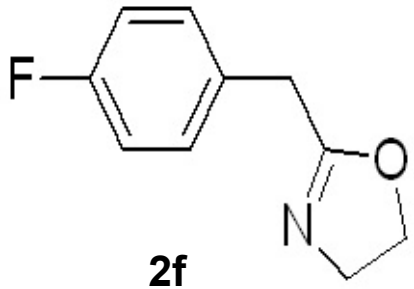

167.12
136.52
131.99
129.21
128.79
77.32
77.32
77.00
76.68
67.54
54.34
34.22
21.00
H3C
O
N
2d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.264
7.241
7.233
7.228
7.217
7.211
7.204
6.878
6.871
6.866
6.855
6.849
6.841
4.256
4.232
4.208
3.858
3.855
3.852
3.835
3.831
3.828
3.811
3.808
3.805
3.798
3.795
3.789
3.554
0.000
H3CO
O
N
2e
1.94
1.98
1.96
5.02
2.02
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
f1 (ppm)


167.24
158.49
129.94
127.10
113.91
77.32
77.00
76.68
67.54
55.15
54.32
33.75
H3CO
O
N
2e
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)

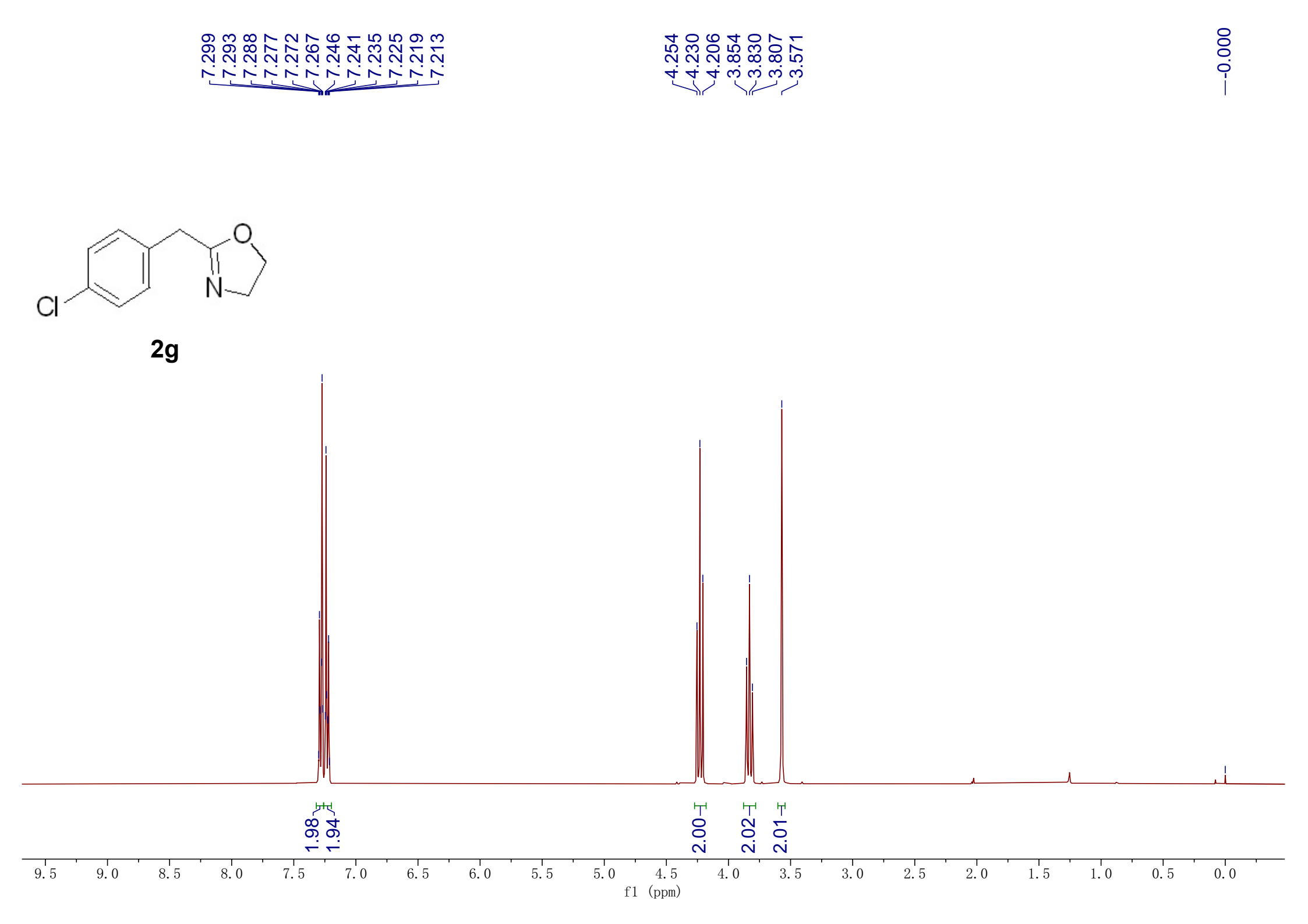

7.282
7.270
7.261
7.248
7.025
7.004
6.982
4.264
4.241
4.217
3.862
3.838
3.815
3.580
0.076
-0.000
F
O
N
2f
1.99
1.97
1.96
2.00
2.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

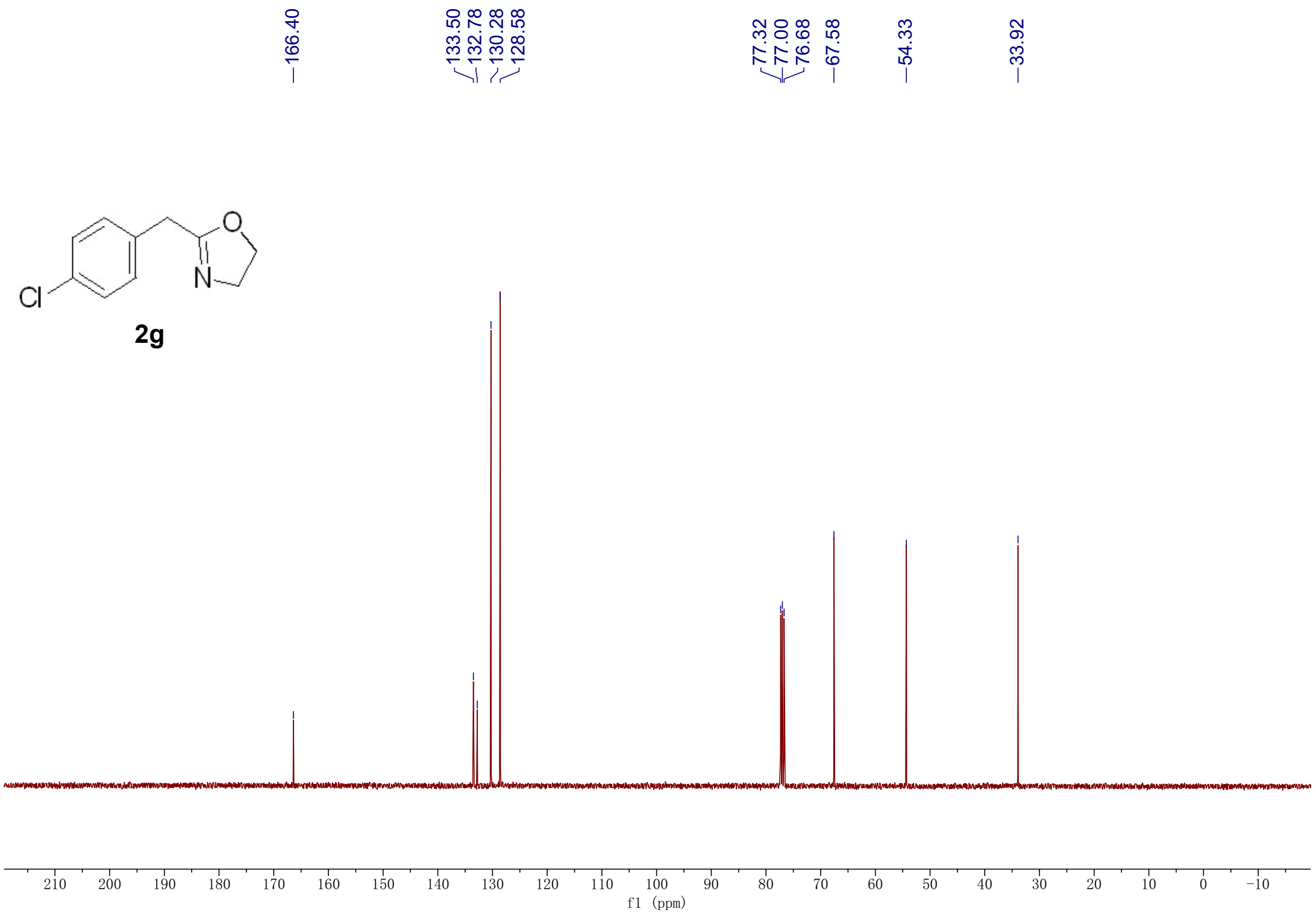

166.78
163.07
160.63
130.78
130.74
130.52
130.44
115.45
115.24
77.32
77.00
76.68
67.62
54.35
33.81
F
O
N
2f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

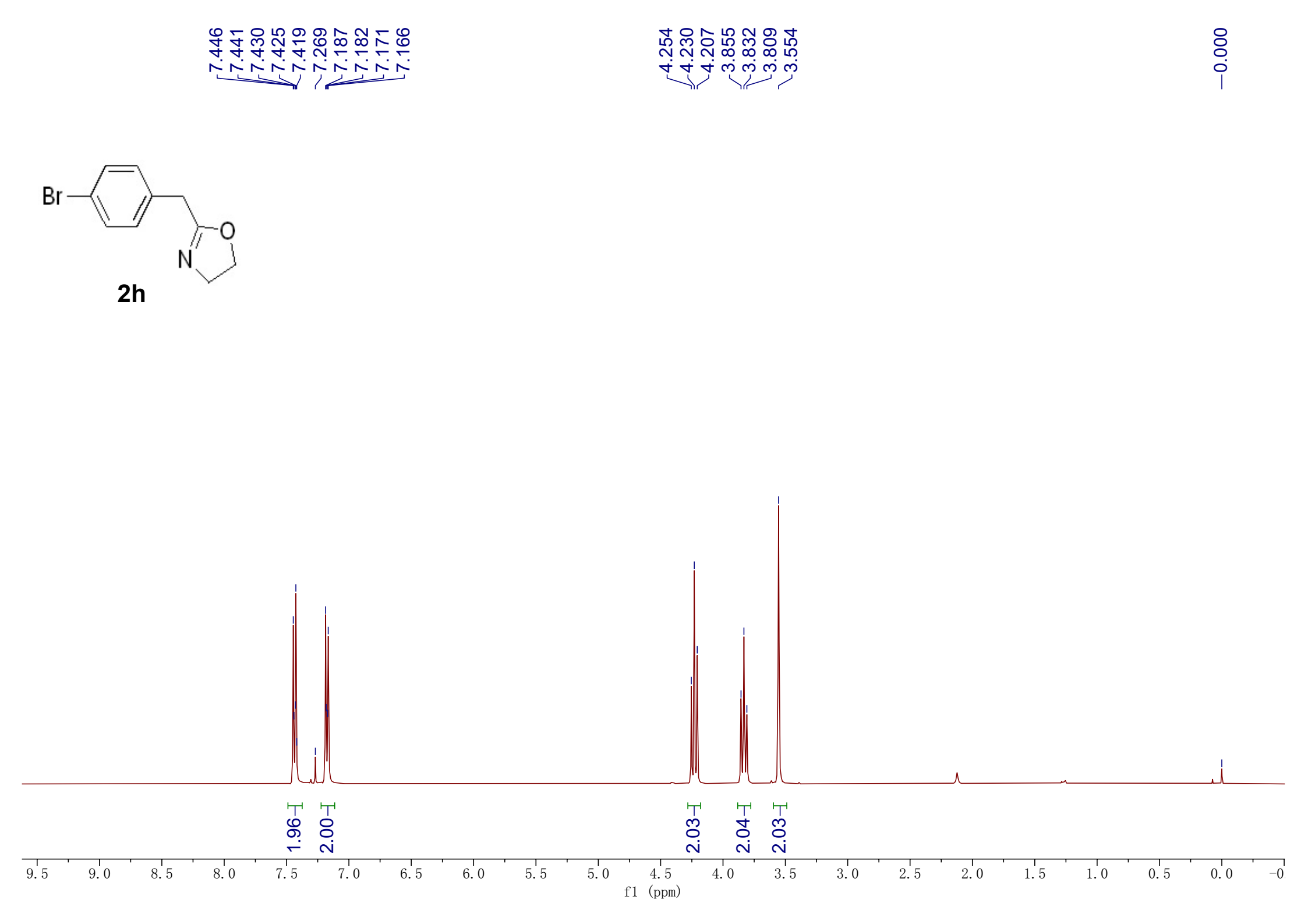

F
O
N

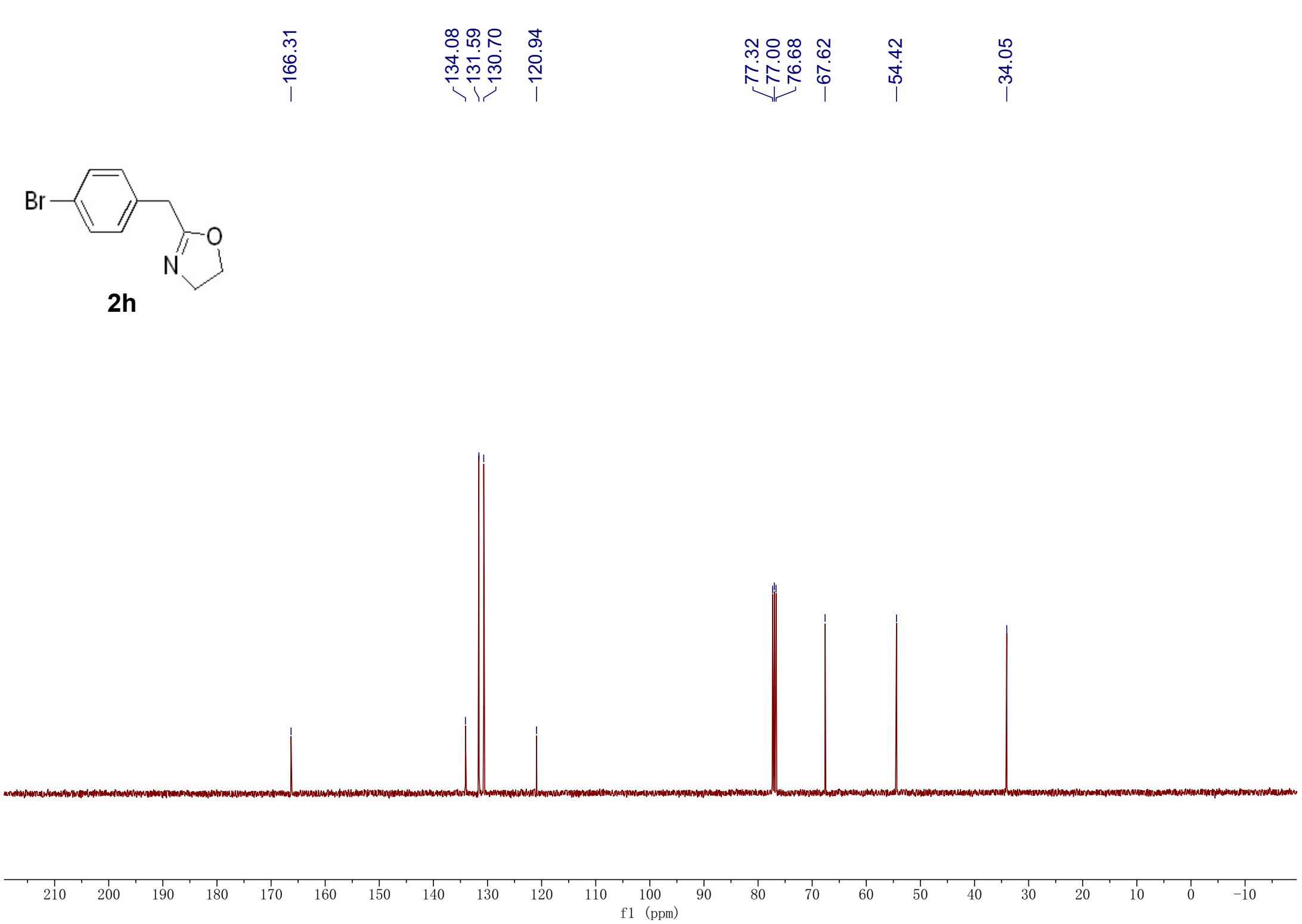
2f

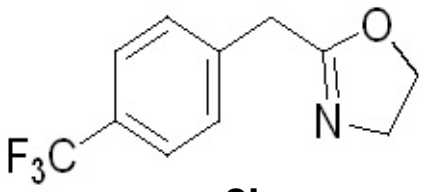
-115.9
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.299
7.293
7.288
7.277
7.272
7.267
7.246
7.241
7.235
7.225
7.219
7.213
4.254
4.230
4.206
3.854
3.830
3.807
3.571
0.000
Cl
O
N
2g
1.98
1.94
2.00
2.02
2.01
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
f1 (ppm)


166.40
133.50
132.78
130.28
128.58
77.32
77.00
76.68
67.58
54.33
33.92
Cl
O
N
2g
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)

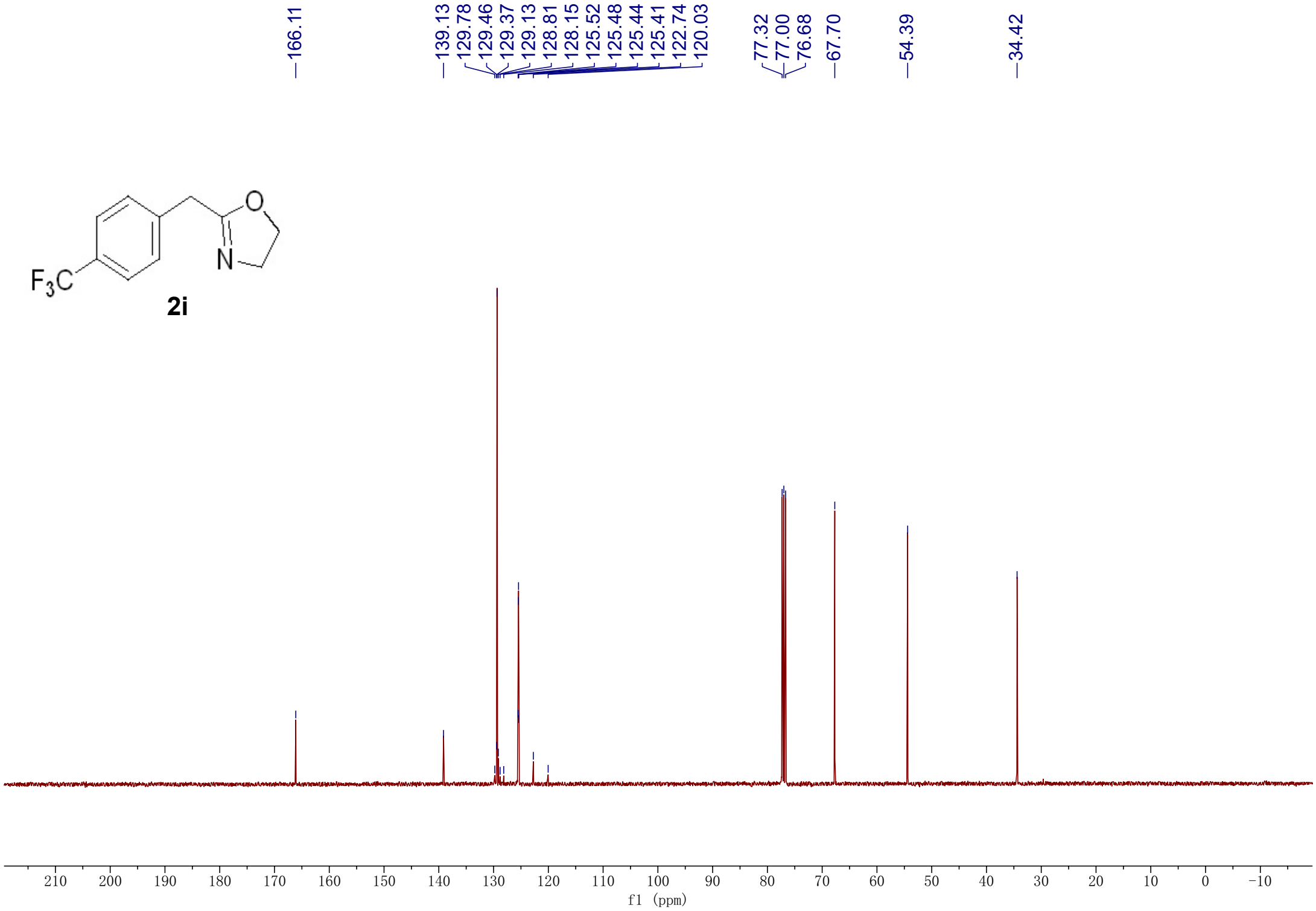

7.446
7.441
7.430
7.425
7.419
7.269
7.187
7.182
7.171
7.166
4.254
4.230
4.207
3.855
3.832
3.809
3.554
0.000
Br
O
N
2h
1.96
2.00
2.03
2.04
2.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

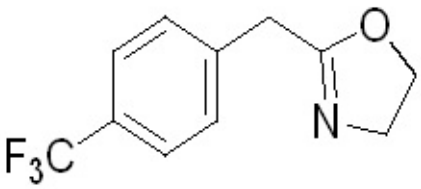

166.31
134.08
131.59
130.70
120.94
77.32
77.00
76.68
67.62
54.42
34.05
Br
O
N
2h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
F3C

2i

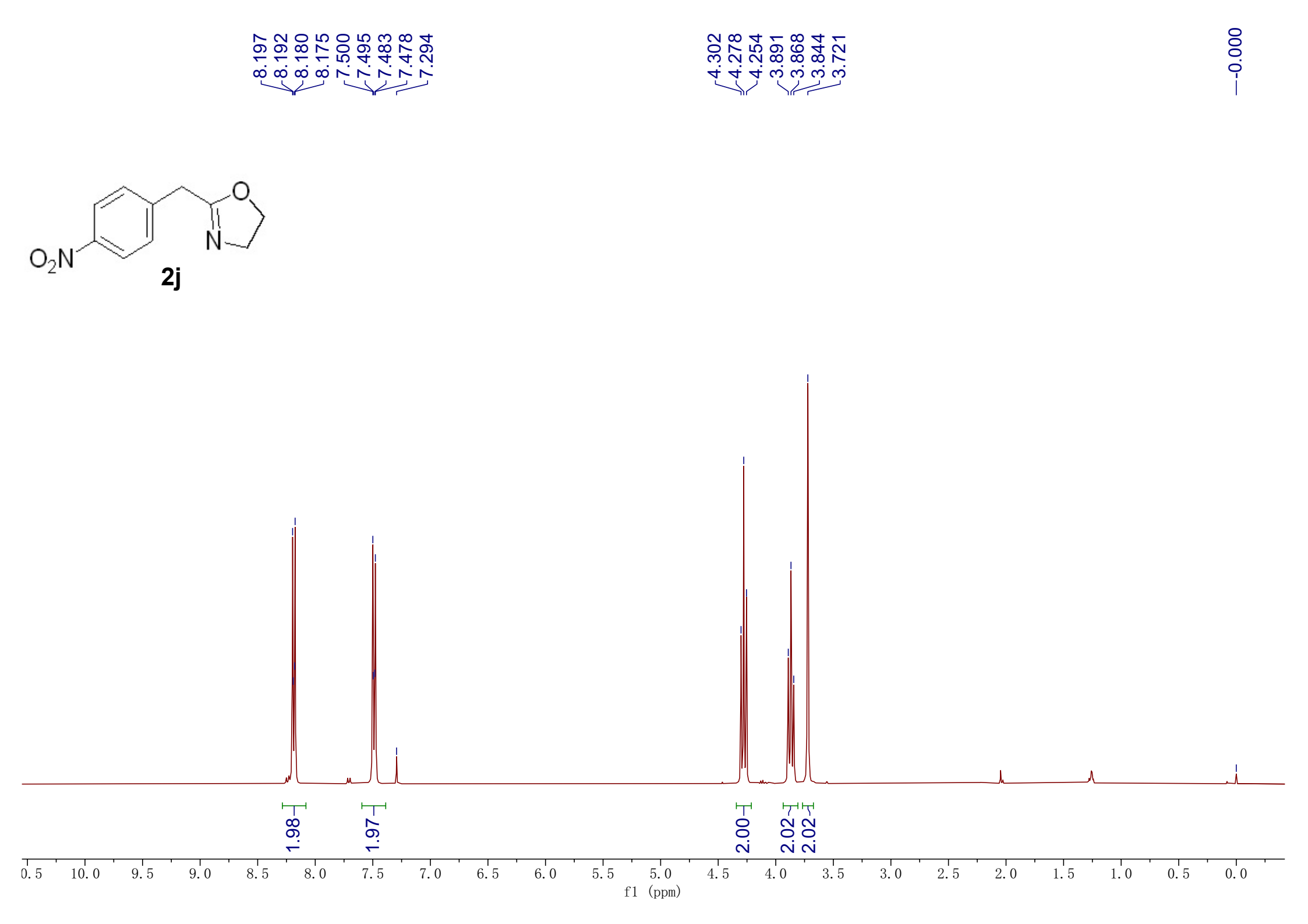
7.591
7.571
7.436
7.416
7.272
4.279
4.255
4.231
3.876
3.853
3.829
3.667
0.000
2.00
1.95
2.00
2.01
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

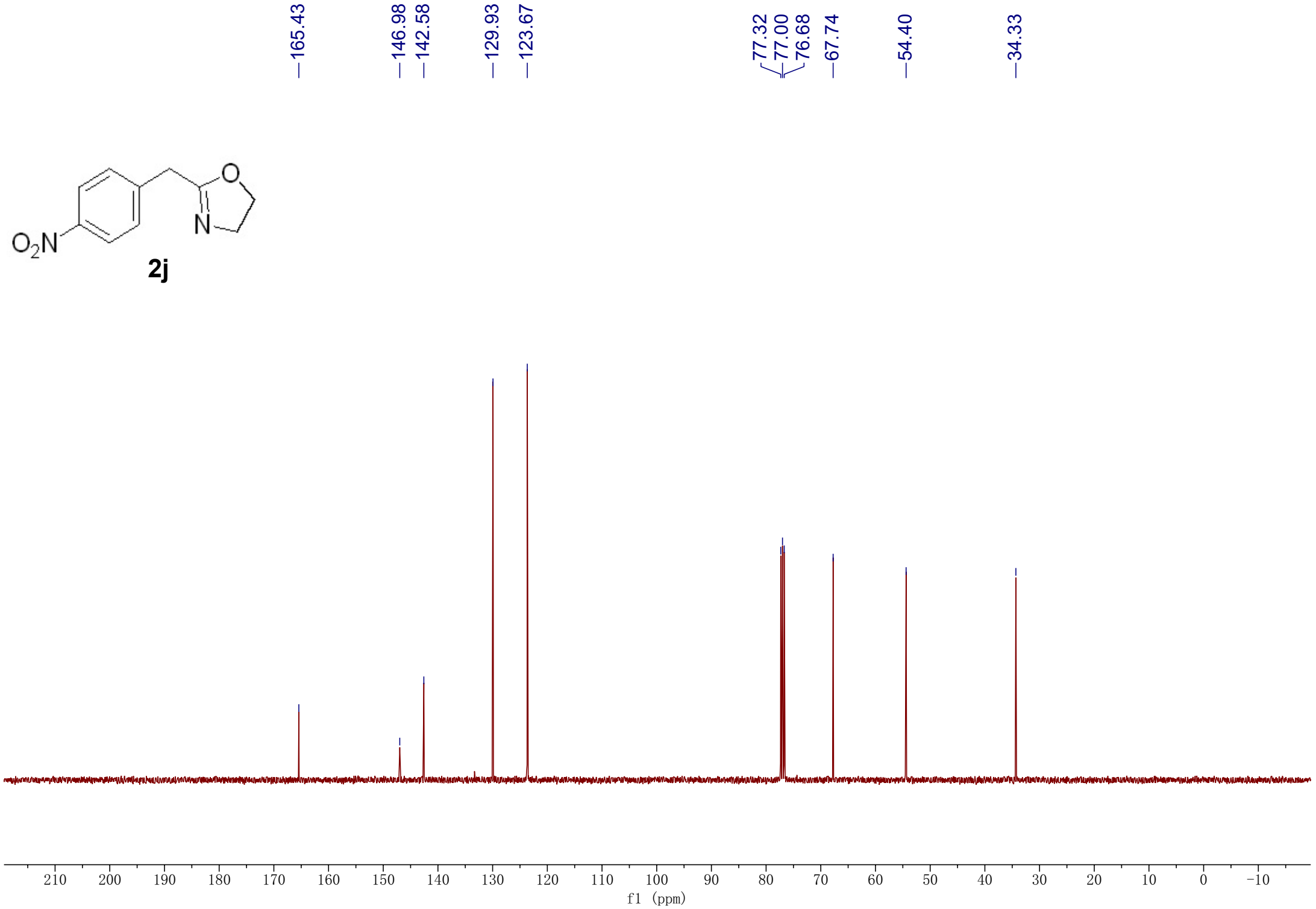

166.11
139.13
129.78
129.46
129.37
129.13
128.81
128.15
125.52
125.48
125.44
125.41
122.74
120.03
77.32
77.00
76.68
67.70
54.39
34.42
O
N
F3C
2i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

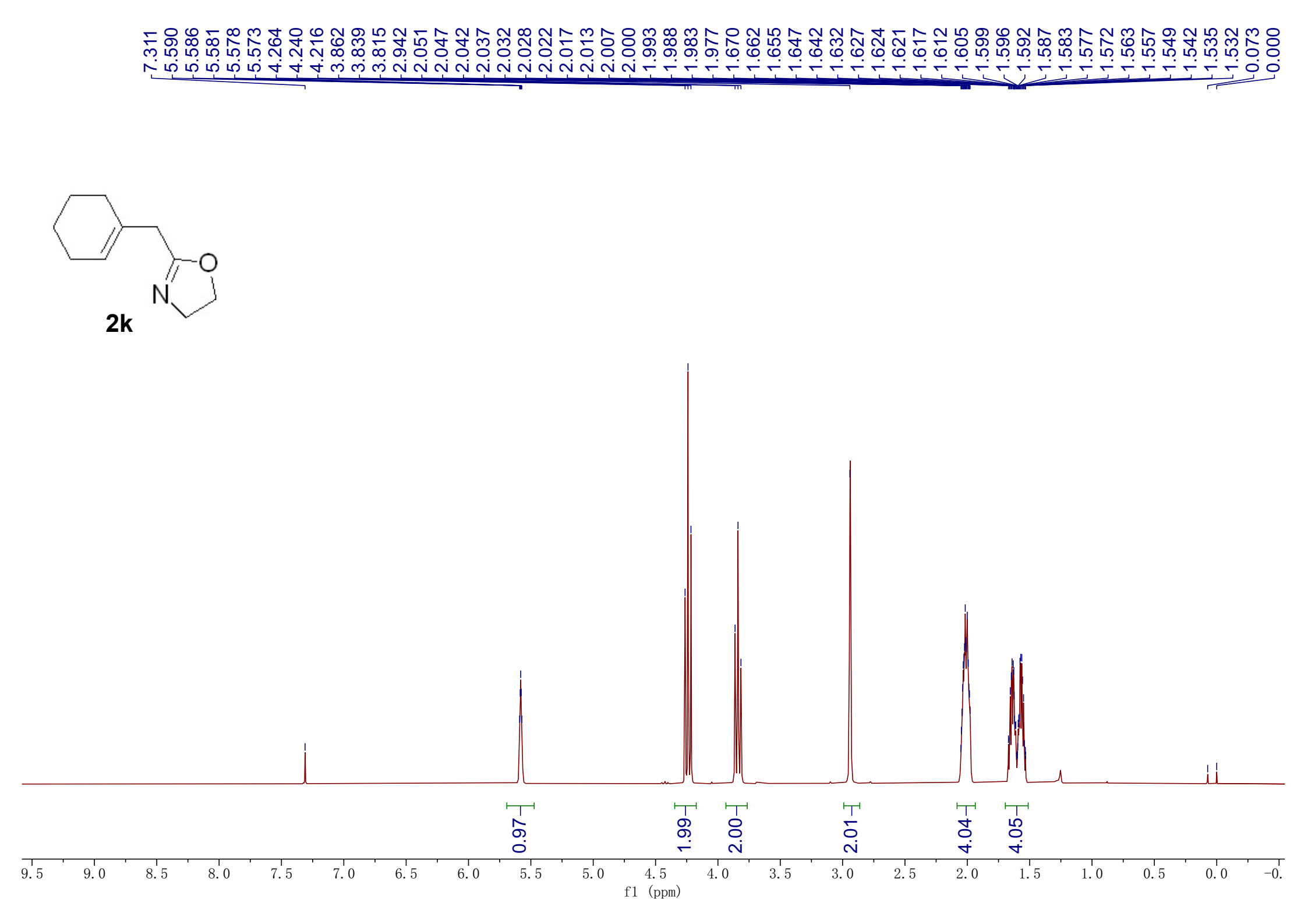

O
N
F3C

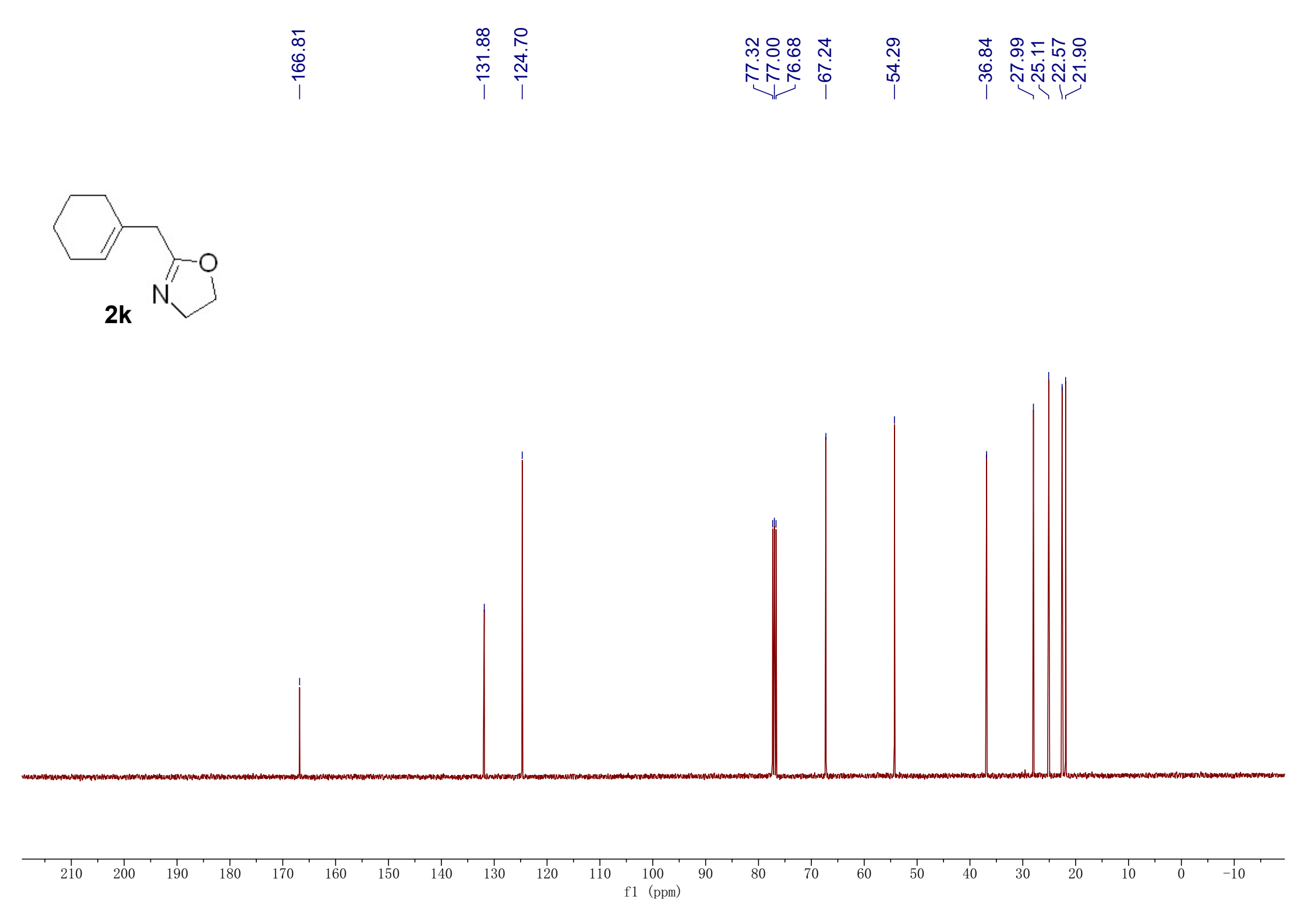
2i

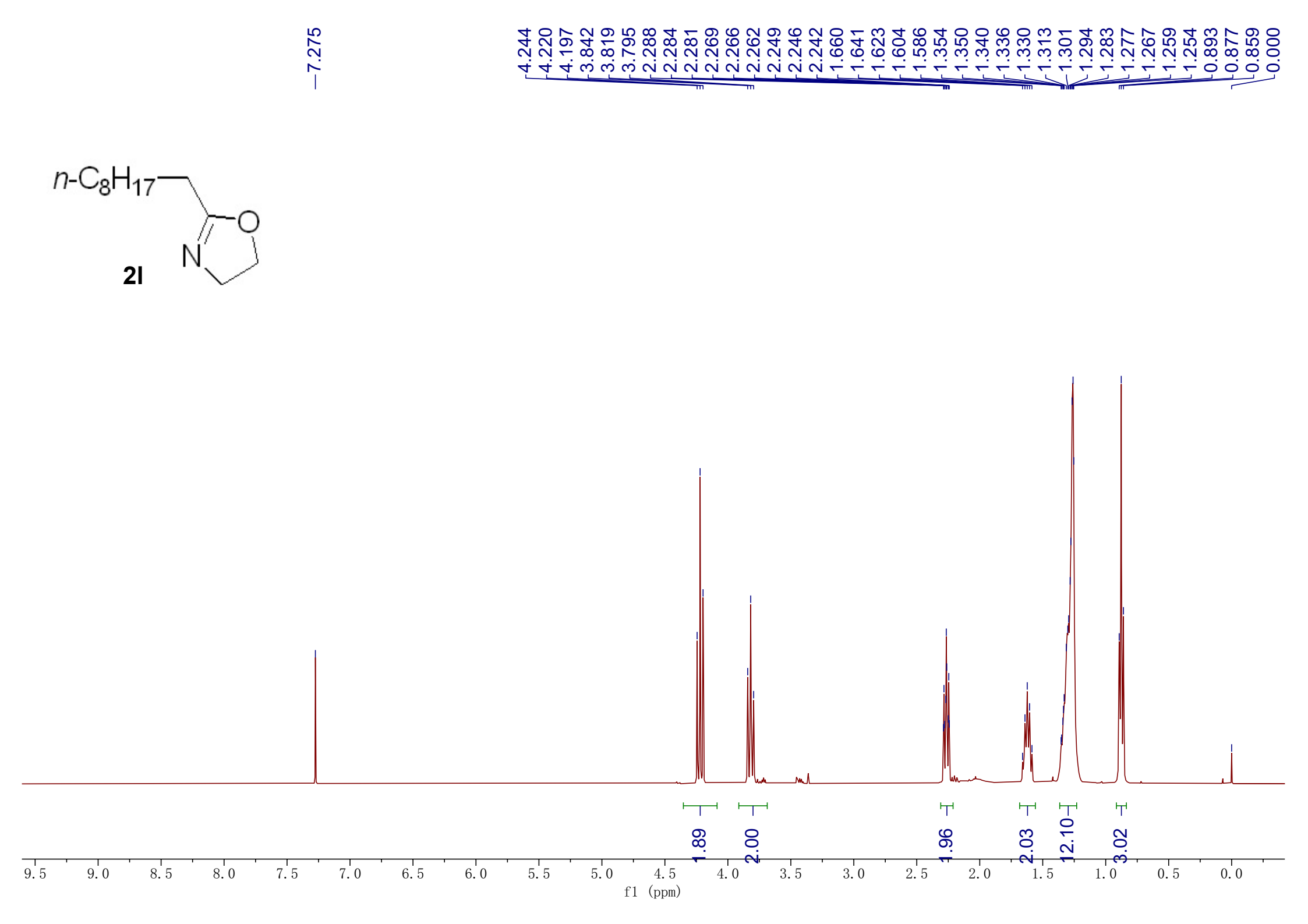
-62.5
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

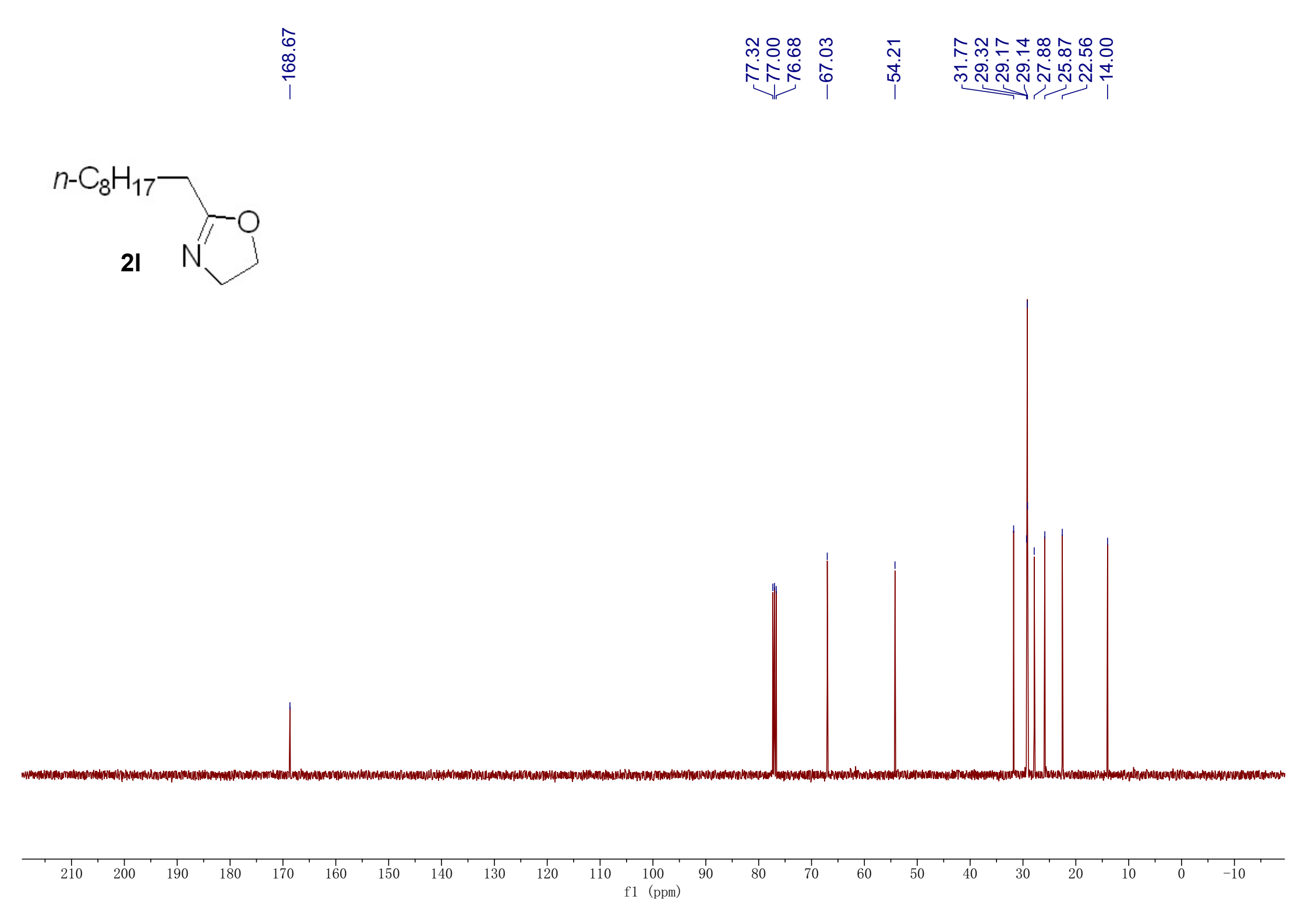

8.197
8.192
8.180
8.175
7.500
7.495
7.483
7.478
7.294
4.302
4.278
4.254
3.891
3.868
3.844
3.721
-0.000
O
N
O_2N
2j
1.98
1.97
2.00
2.02
2.02
f1 (ppm)

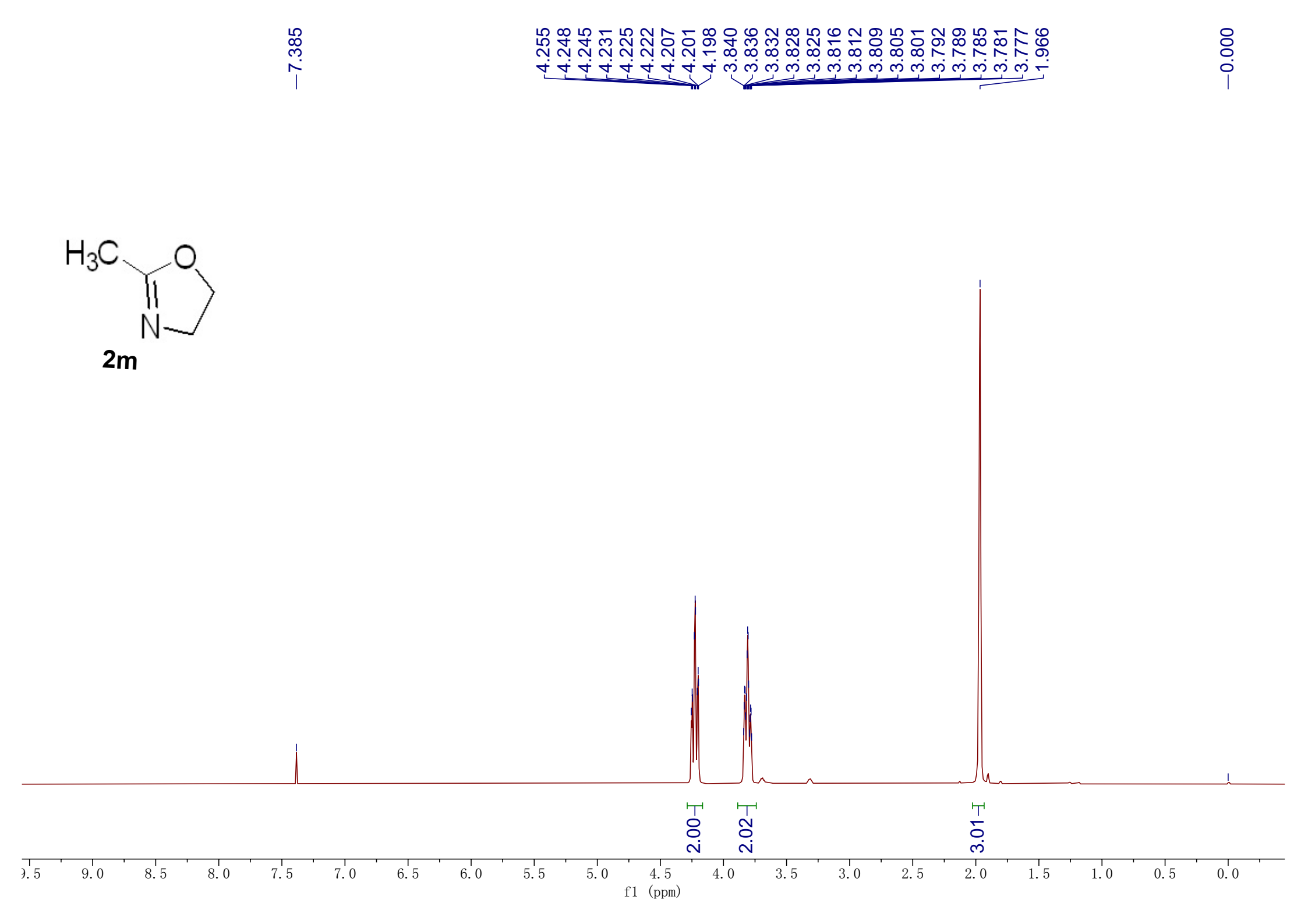

165.43
146.98
142.58
129.93
123.67
77.32
77.00
76.68
67.74
54.40
34.33
O
N
O2N
2j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

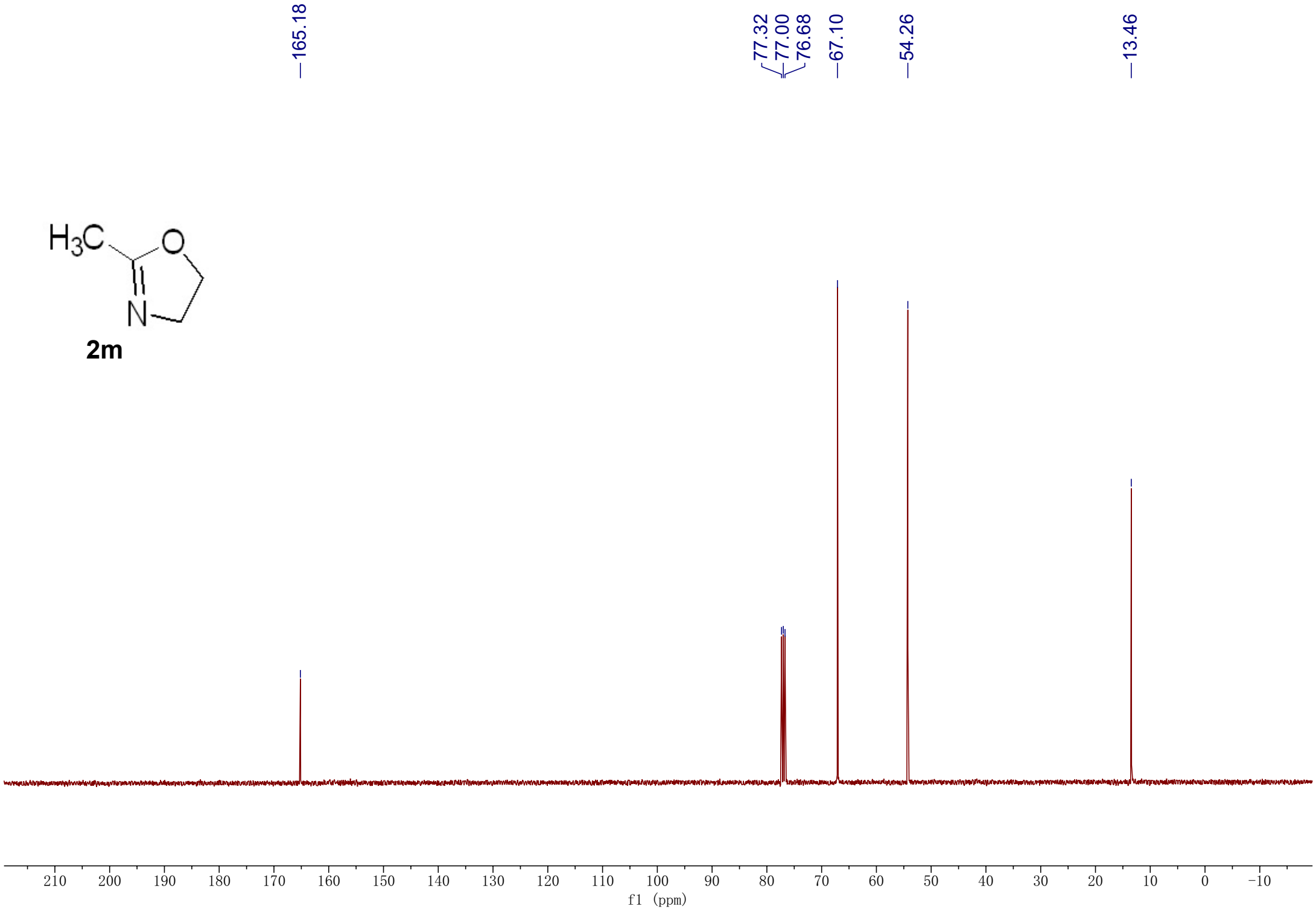

7.311
5.590
5.586
5.581
5.578
5.573
4.264
4.240
4.216
3.862
3.839
3.815
2.942
2.051
2.047
2.042
2.037
2.032
2.028
2.022
2.017
2.013
2.007
2.000
1.993
1.988
1.983
1.977
1.670
1.662
1.655
1.647
1.642
1.632
1.627
1.624
1.621
1.617
1.612
1.605
1.599
1.596
1.592
1.587
1.583
1.577
1.572
1.563
1.557
1.549
1.542
1.535
1.532
0.073
0.000
O
N
2k
0.97
1.99
2.00
2.01
4.04
4.05
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.
f1 (ppm)

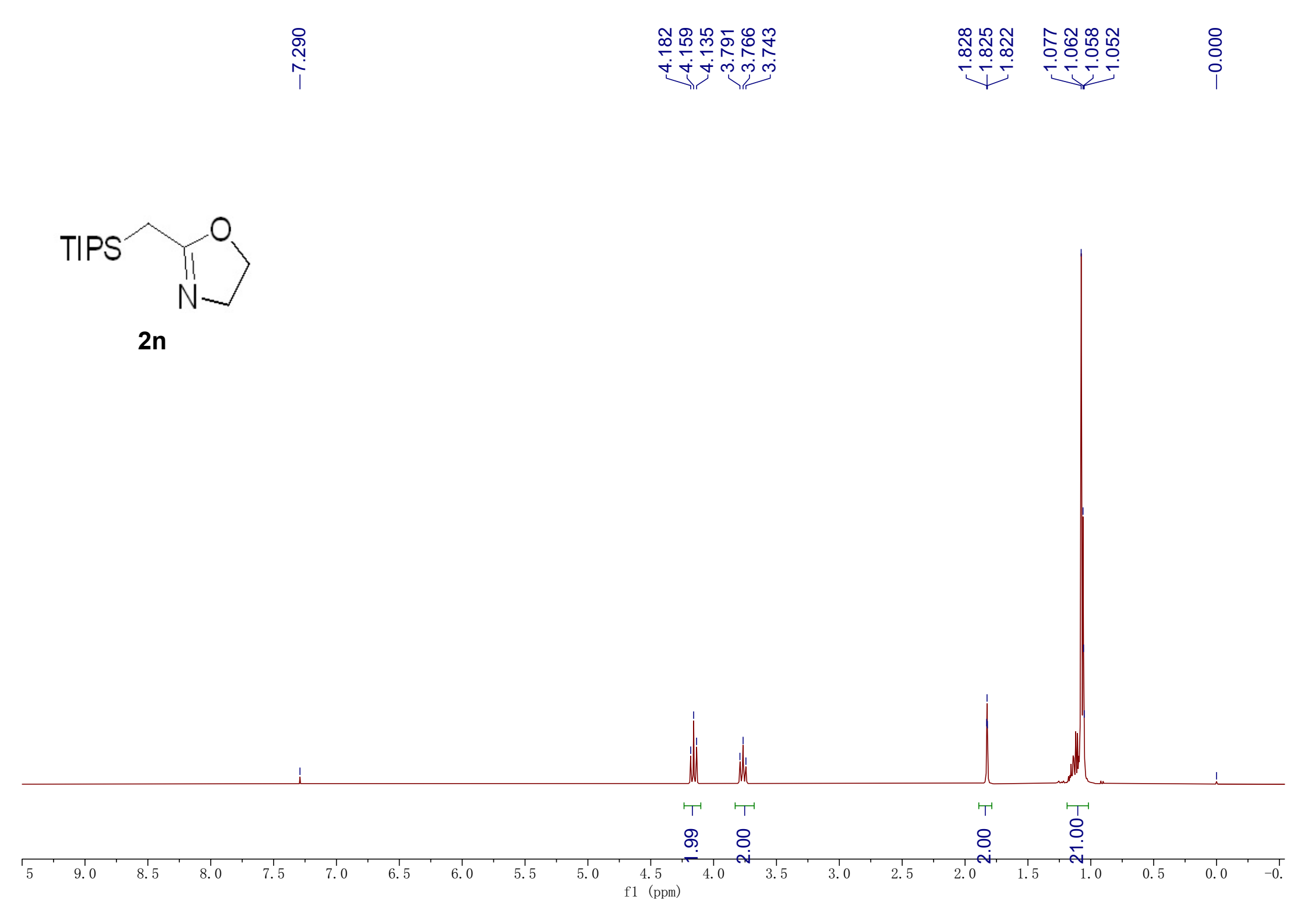

166.81
131.88
124.70
77.32
77.00
76.68
67.24
54.29
36.84
27.99
25.11
22.57
21.90
O
N
2k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

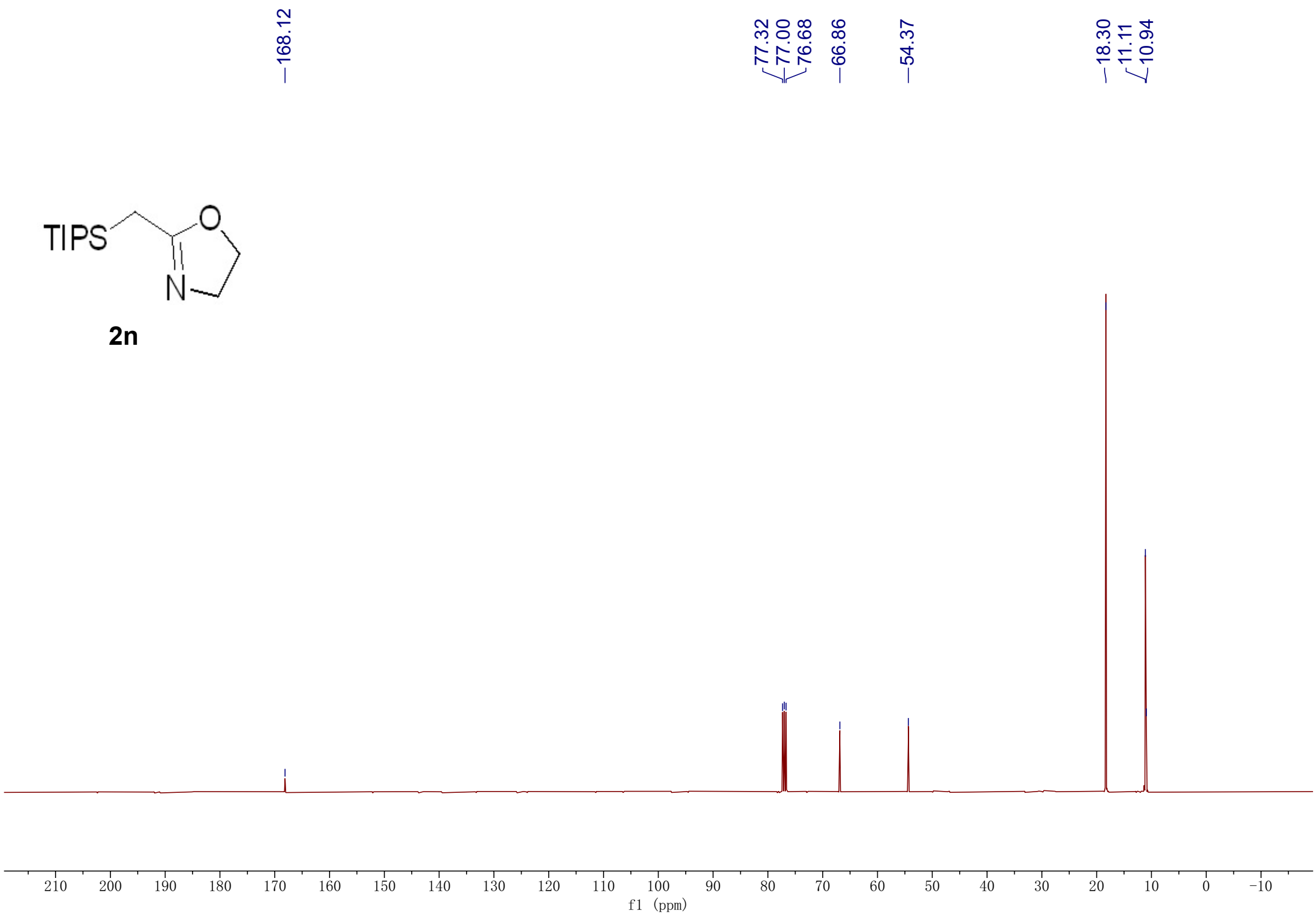

7.275
4.244
4.220
4.197
3.842
3.819
3.795
2.288
2.284
2.281
2.269
2.266
2.262
2.249
2.246
2.242
1.660
1.641
1.623
1.604
1.586
1.354
1.350
1.340
1.336
1.330
1.313
1.301
1.294
1.283
1.277
1.267
1.259
1.254
0.893
0.877
0.859
0.000
n-C8H17
O
N
2l
1.89
2.00
1.96
2.03
12.10
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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
f1 (ppm)

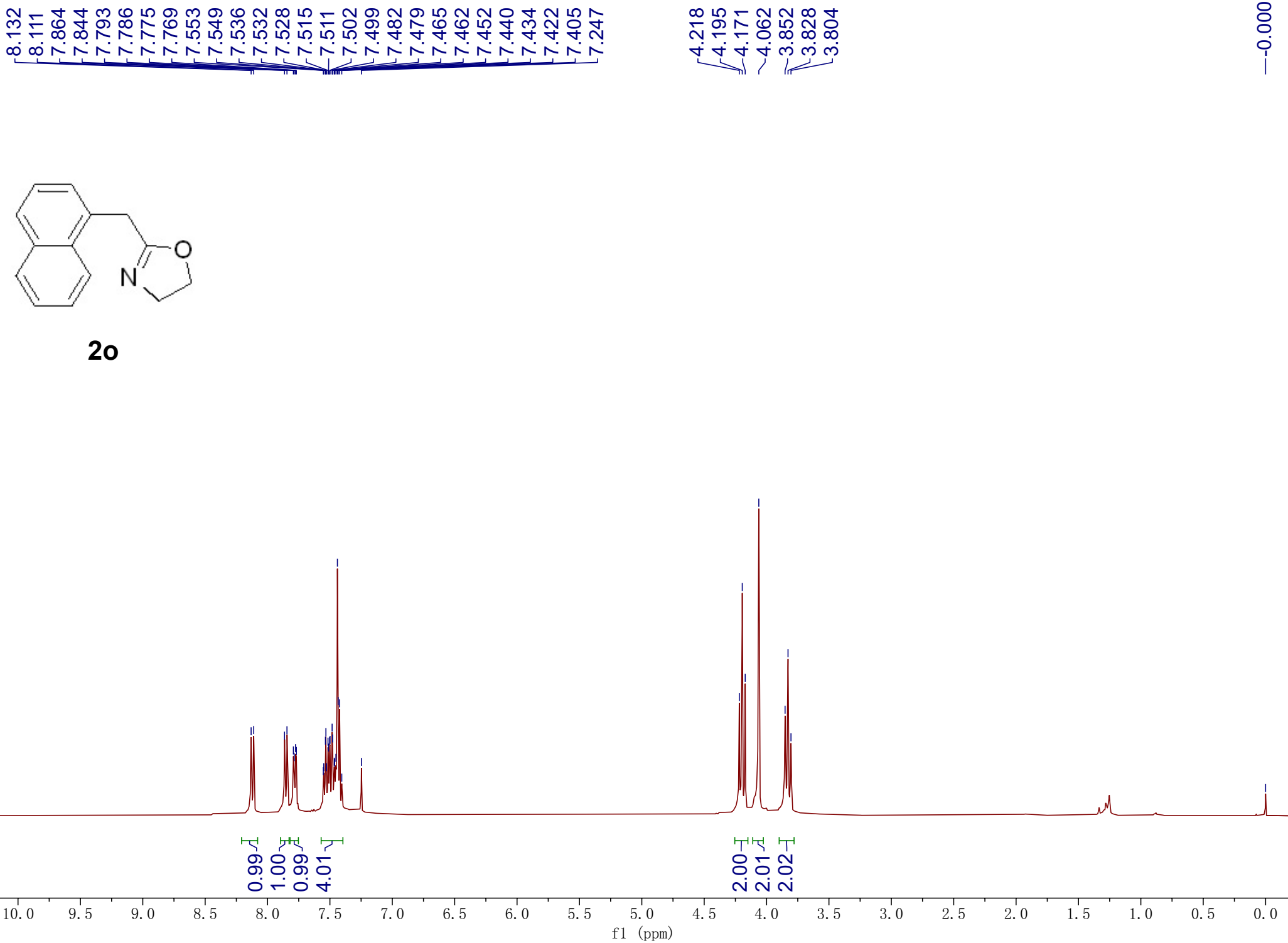

168.67
77.32
77.00
76.68
67.03
54.21
31.77
29.32
29.17
29.14
27.88
25.87
22.56
14.00
n-C8H17
O
N
2l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.385
4.255
4.248
4.245
4.231
4.225
4.222
4.207
4.201
4.198
3.840
3.836
3.832
3.828
3.825
3.816
3.812
3.809
3.805
3.801
3.792
3.789
3.785
3.781
3.777
1.966
0.000
H3C
O
N
2m
2.00
2.02
3.01
f1 (ppm)

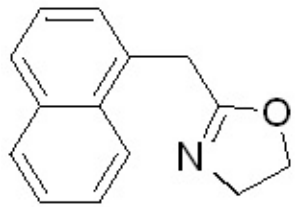

165.18
77.32
77.00
76.68
67.10
54.26
13.46
H3C
O
N
2m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.290
4.182
4.159
4.135
3.791
3.766
3.743
1.828
1.825
1.822
1.077
1.062
1.058
1.052
0.000
TIPS
O
N
2n
1.99
2.00
2.00
21.00
f1 (ppm)


168.12
77.32
77.00
76.68
66.86
54.37
18.30
11.11
10.94
TIPS
O
N
2n
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)

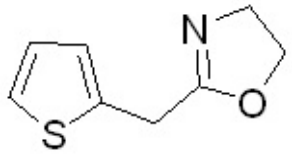

8.132
8.111
7.864
7.844
7.793
7.786
7.775
7.769
7.553
7.549
7.536
7.532
7.528
7.515
7.511
7.502
7.499
7.482
7.479
7.465
7.462
7.452
7.440
7.434
7.422
7.405
7.247
4.218
4.195
4.171
4.062
3.852
3.828
3.804
-0.000
O
N
0.99
1.00
0.99
4.01
2.00
2.01
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

2o


O
N

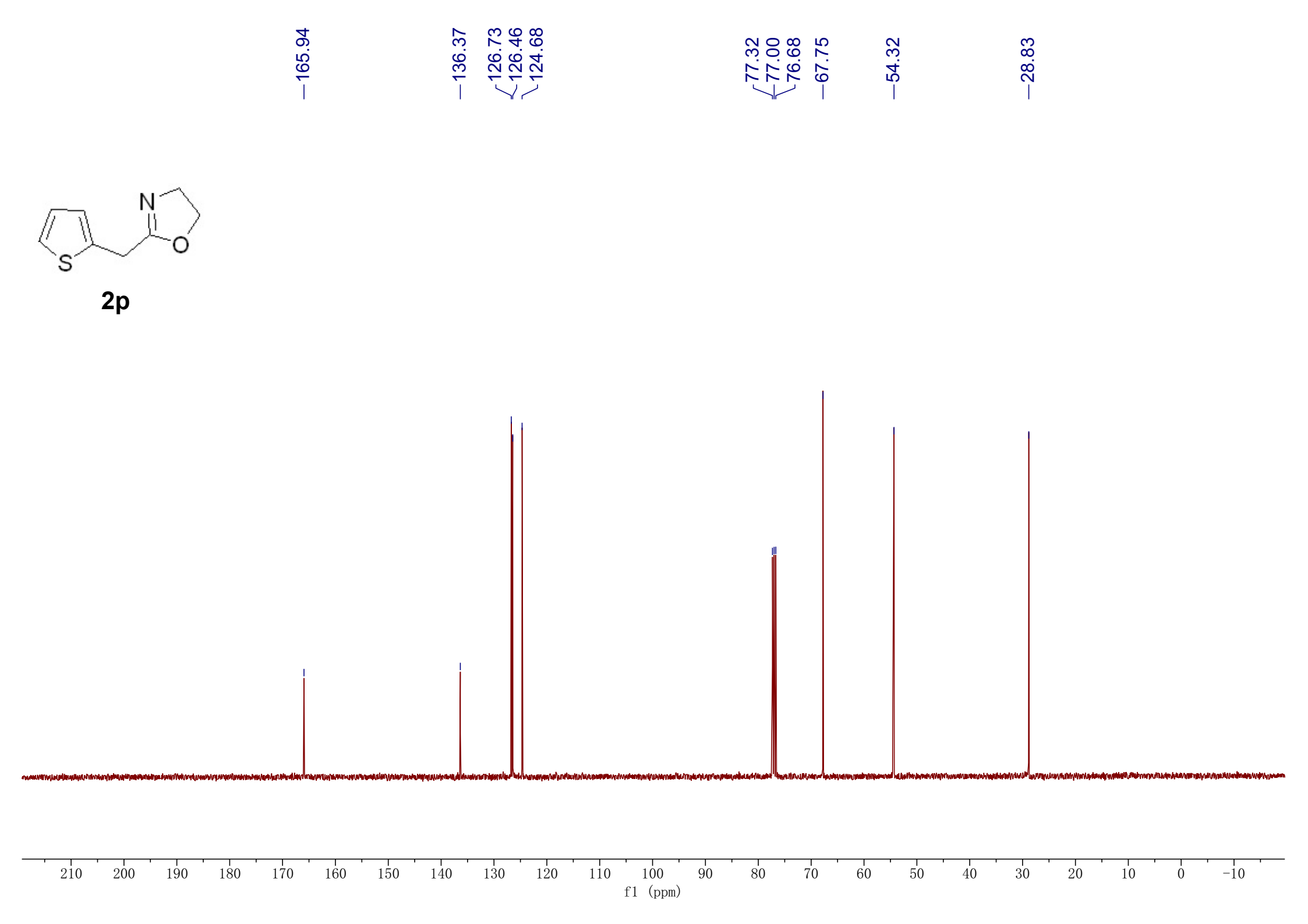
2o

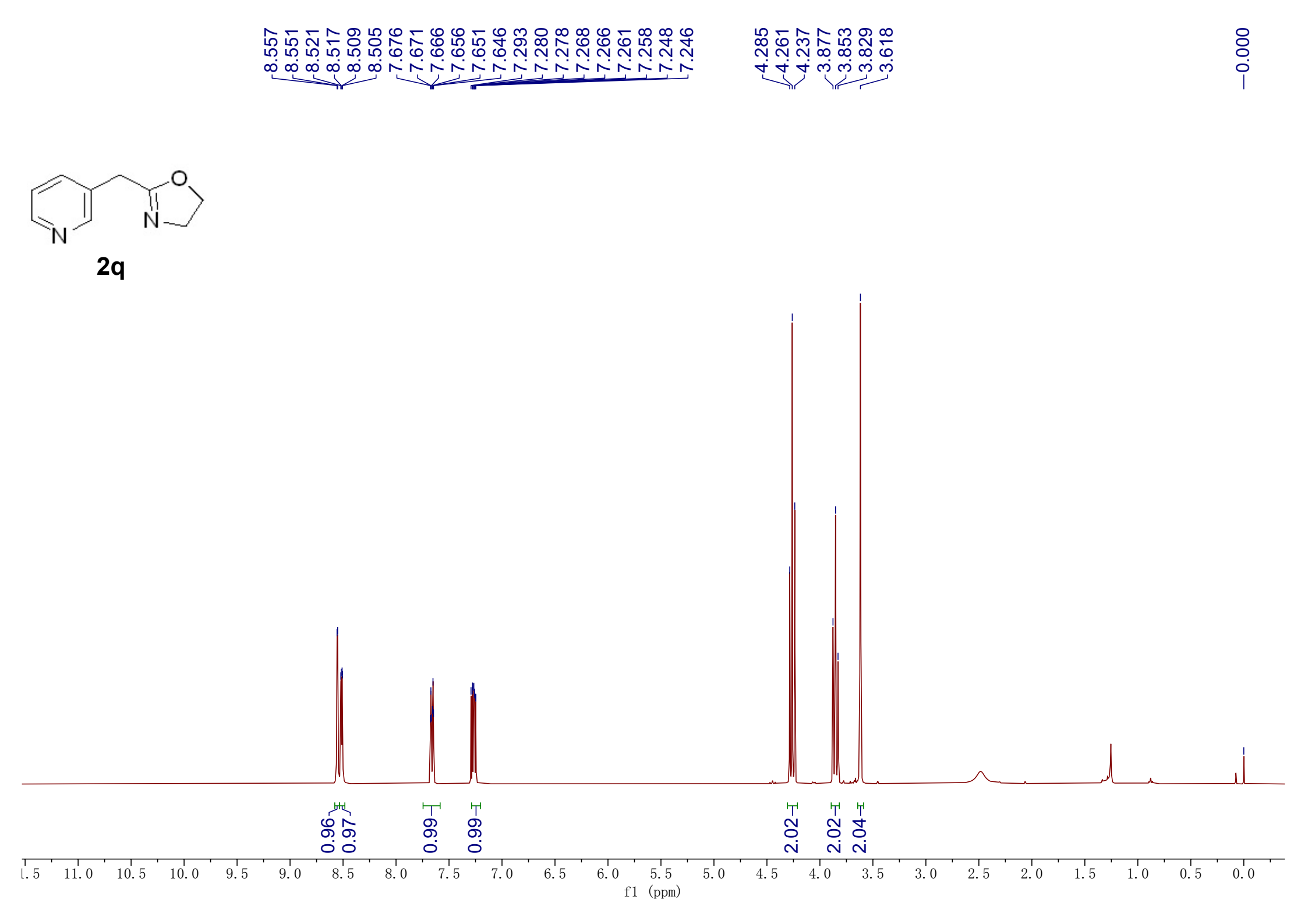
166.75
133.71
131.94
131.35
128.55
127.83
127.46
126.12
125.60
125.37
123.84
77.32
77.00
76.68
67.49
54.33
32.31
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

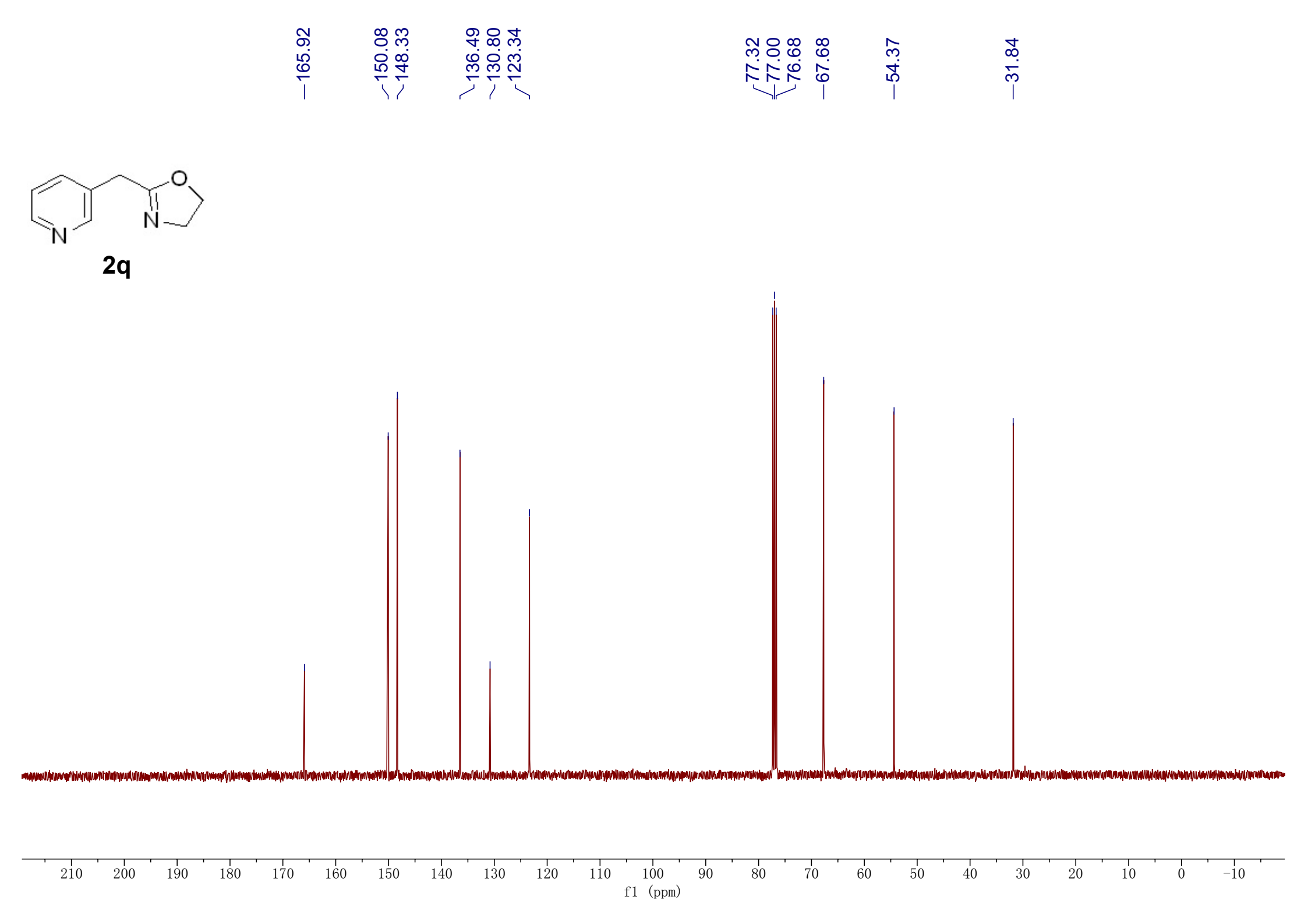

N
O
S

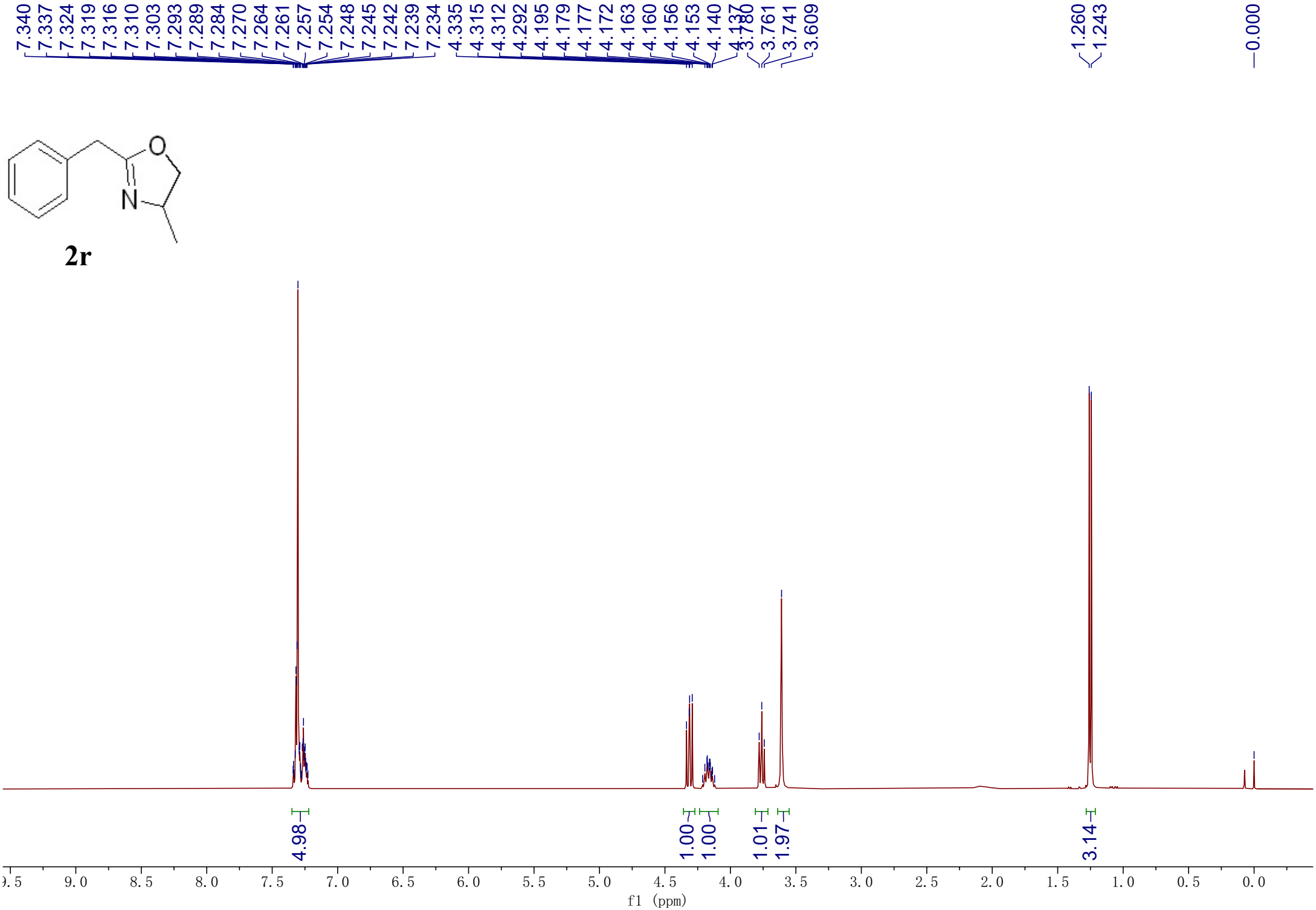
2p

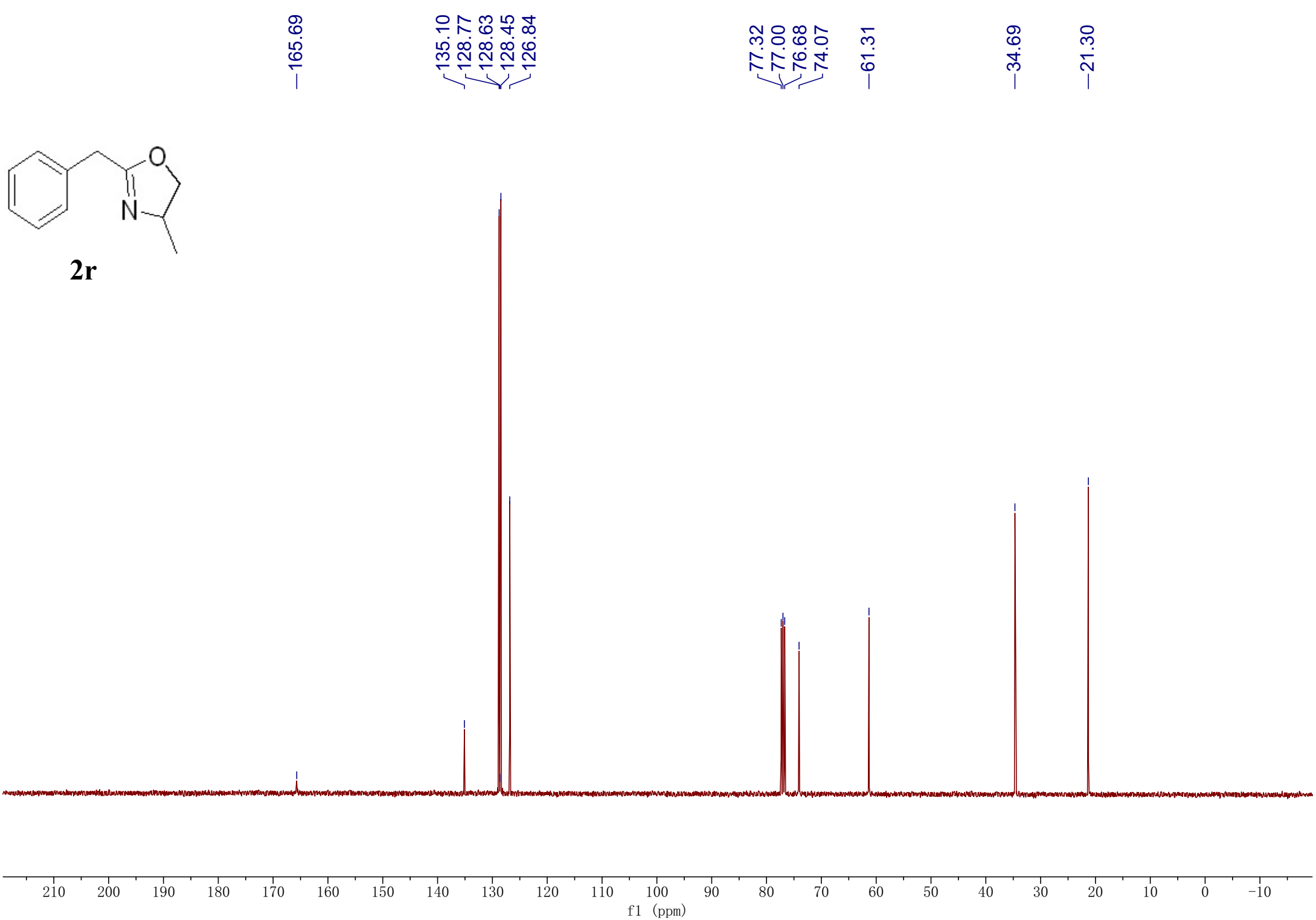
7.272
7.199
7.194
7.189
7.183
6.961
6.951
6.946
6.944
6.940
6.931
4.291
4.267
4.243
3.880
3.877
3.874
3.853
3.824
0.000
0.95
1.91
2.00
4.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

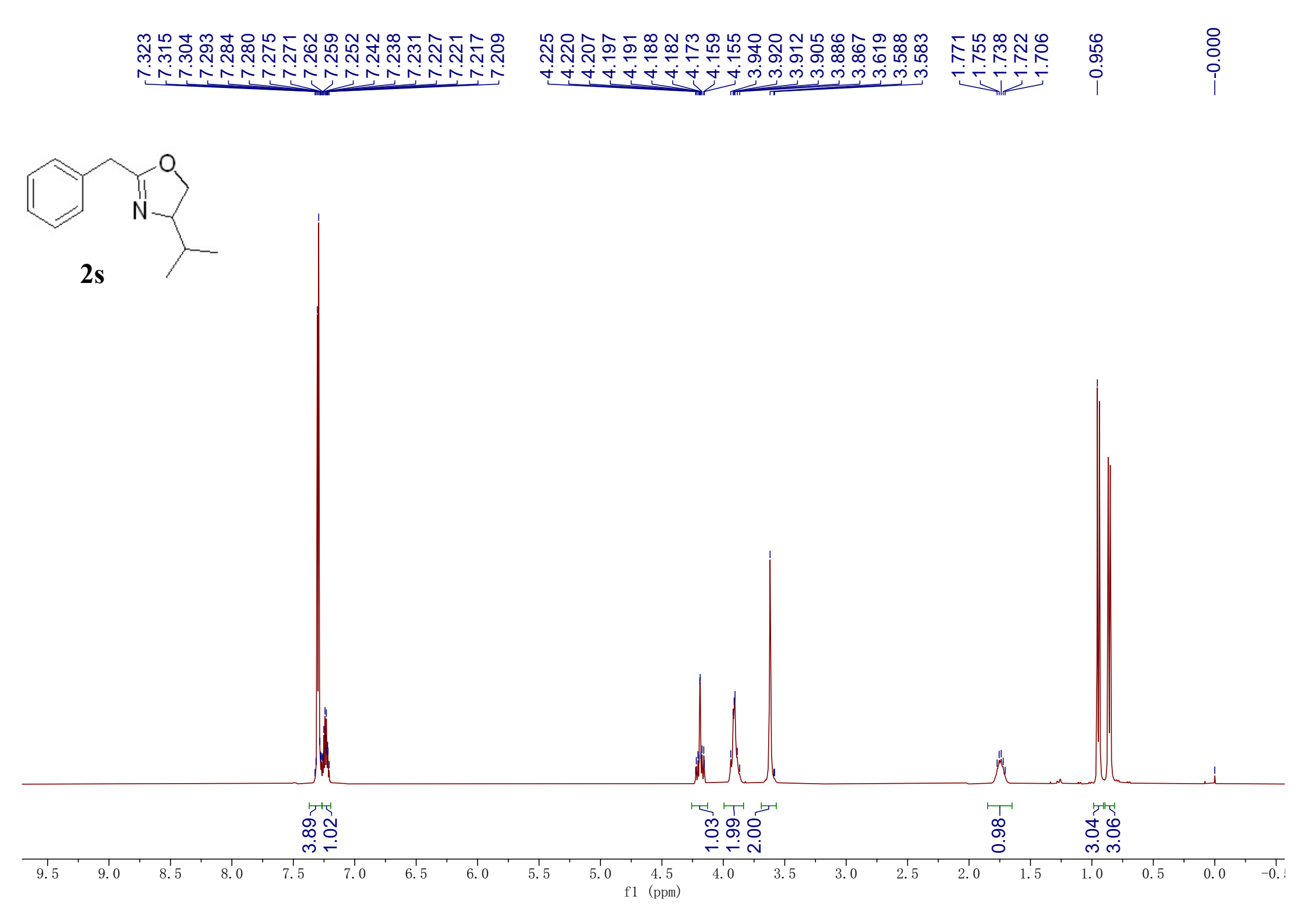

165.94
136.37
126.73
126.46
124.68
77.32
77.00
76.68
67.75
54.32
28.83
N
O
S
2p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

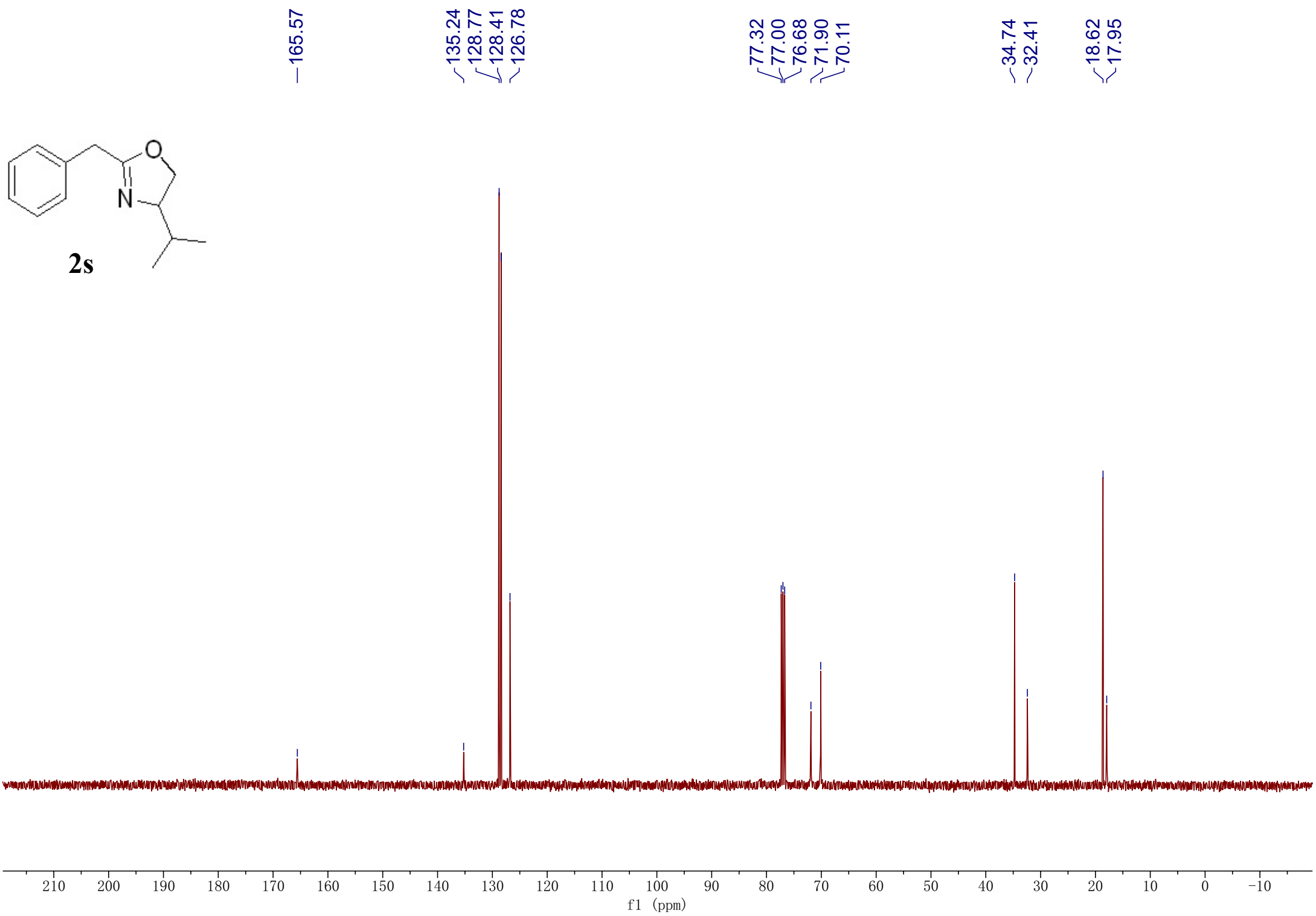

8.557
8.551
8.521
8.517
8.509
8.505
7.676
7.671
7.666
7.656
7.651
7.646
7.293
7.280
7.278
7.268
7.266
7.261
7.258
7.248
7.246
4.285
4.261
4.237
3.877
3.853
3.829
3.618
0.000
O
N
N
2q
0.96
0.97
0.99
0.99
2.02
2.02
2.04
f1 (ppm)

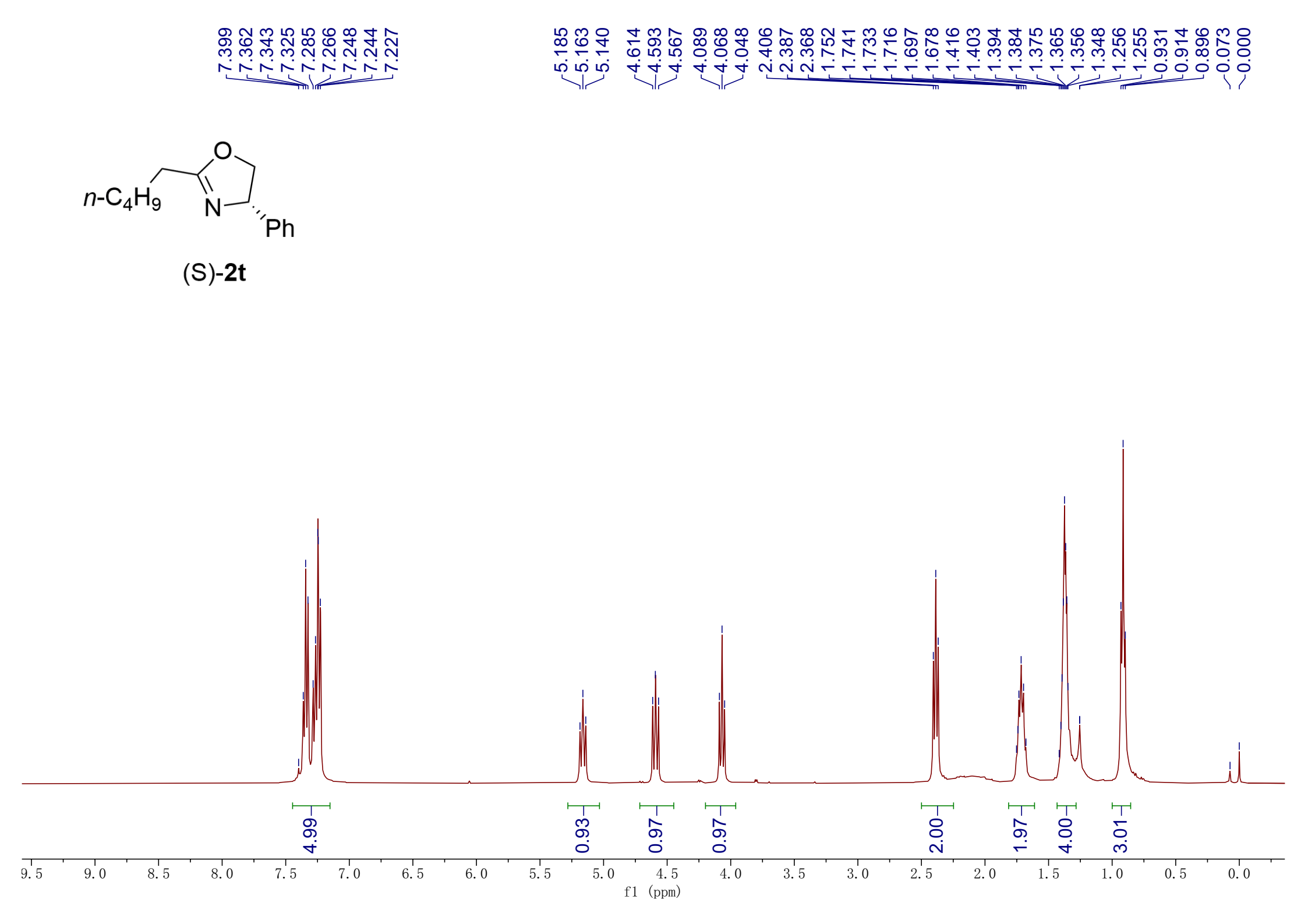

165.92
150.08
148.33
136.49
130.80
123.34
77.32
77.00
76.68
67.68
54.37
31.84
O
N
N
2q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

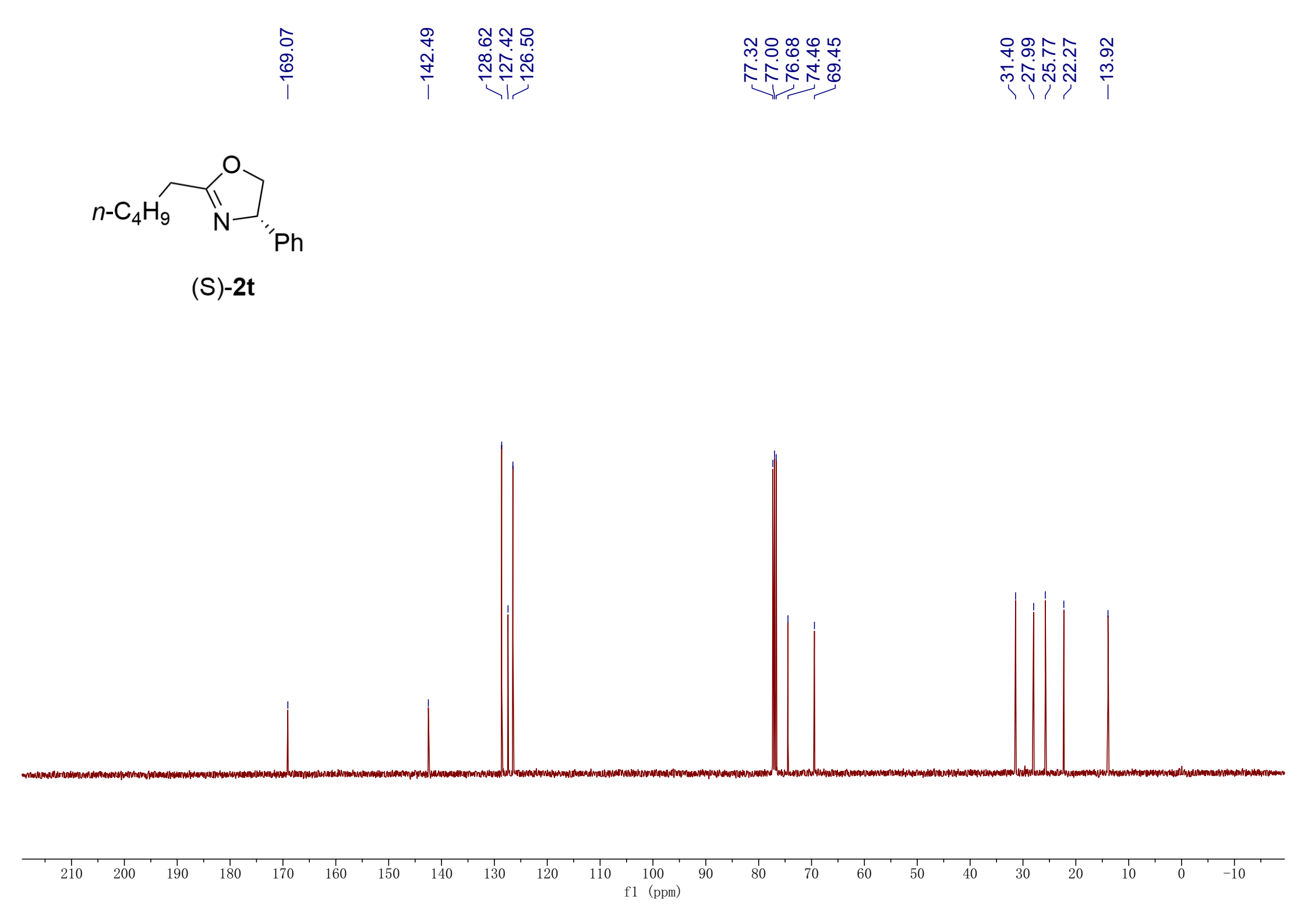

7.340
7.337
7.324
7.319
7.316
7.310
7.303
7.293
7.289
7.284
7.270
7.264
7.261
7.257
7.254
7.248
7.245
7.242
7.239
7.234
4.335
4.315
4.312
4.292
4.195
4.179
4.177
4.172
4.163
4.160
4.156
4.153
4.140
4.137
3.780
3.761
3.741
3.609
1.260
1.243
0.000
O
N
2r
4.98
1.00
1.00
1.01
1.97
3.14
f1 (ppm)

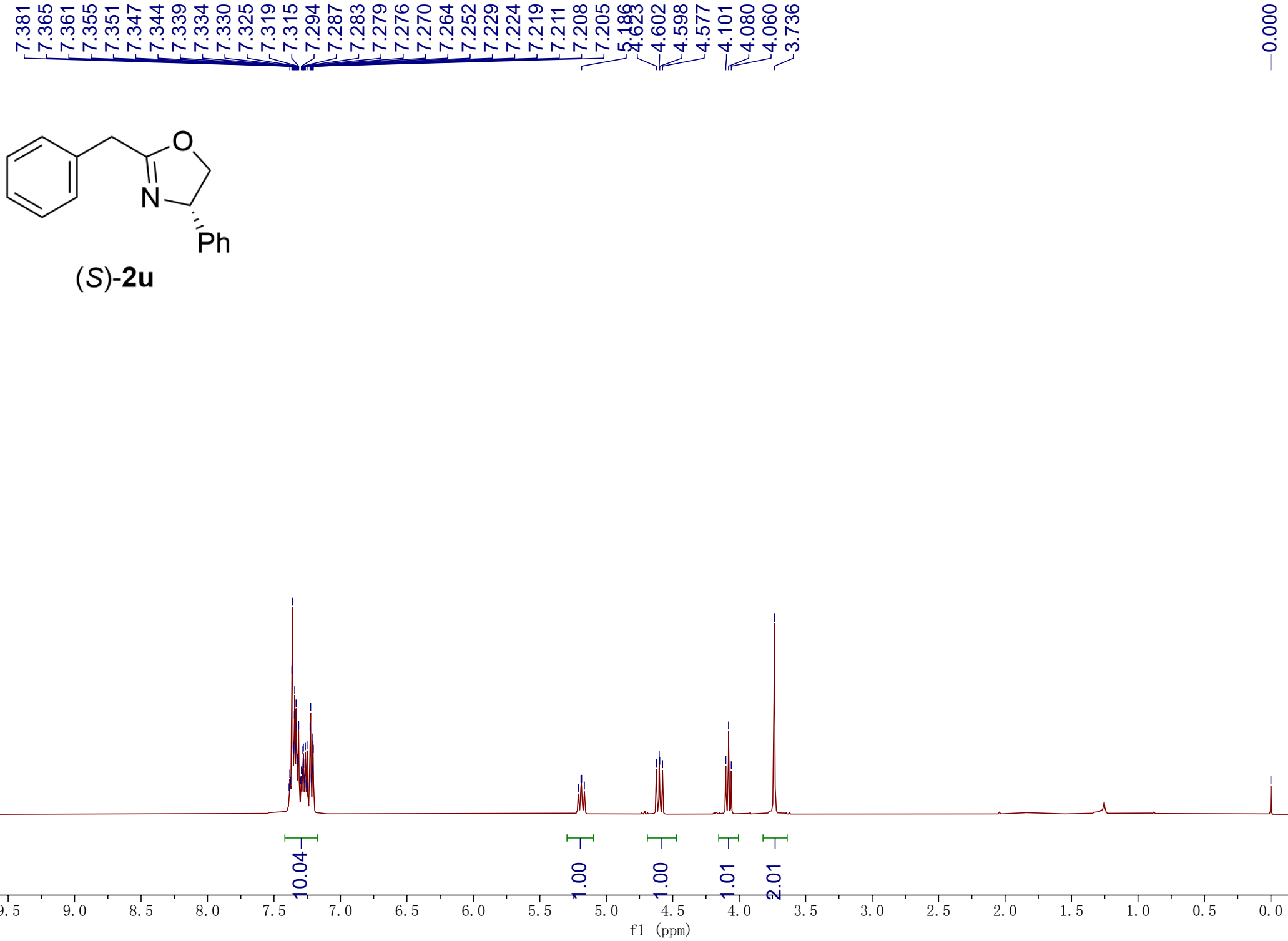

165.69
135.10
128.77
128.63
128.45
126.84
77.32
77.00
76.68
74.07
61.31
34.69
21.30
O
N
2r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

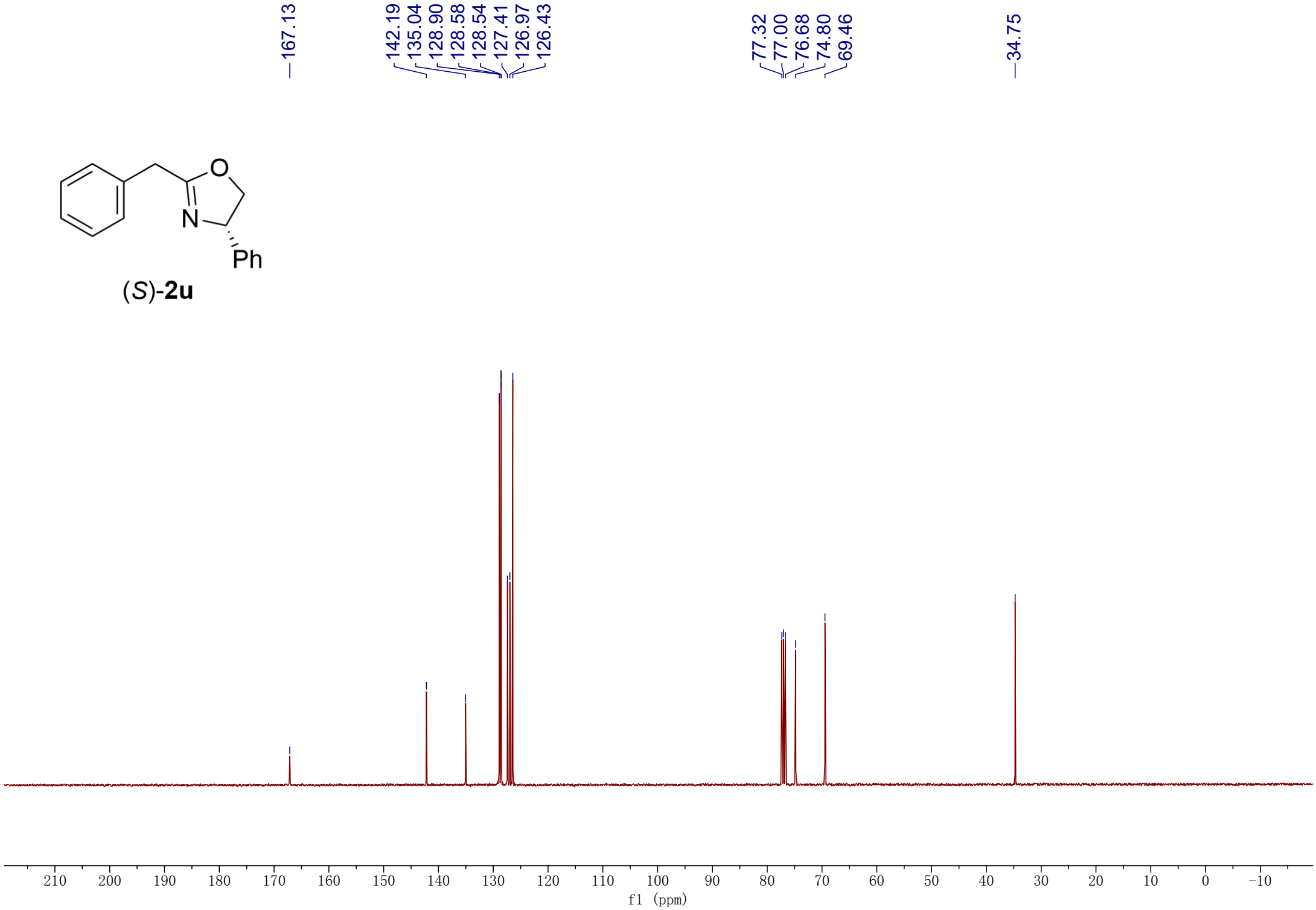

7.323
7.315
7.304
7.293
7.284
7.280
7.275
7.271
7.262
7.259
7.252
7.242
7.238
7.231
7.227
7.221
7.217
7.209
4.225
4.220
4.207
4.197
4.191
4.188
4.182
4.173
4.159
4.155
3.940
3.920
3.912
3.905
3.886
3.867
3.619
3.588
3.583
1.771
1.755
1.738
1.722
1.706
0.956
-0.000
O
N
2s
3.89
1.02
1.03
1.99
2.00
0.98
3.04
3.06
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
f1 (ppm)

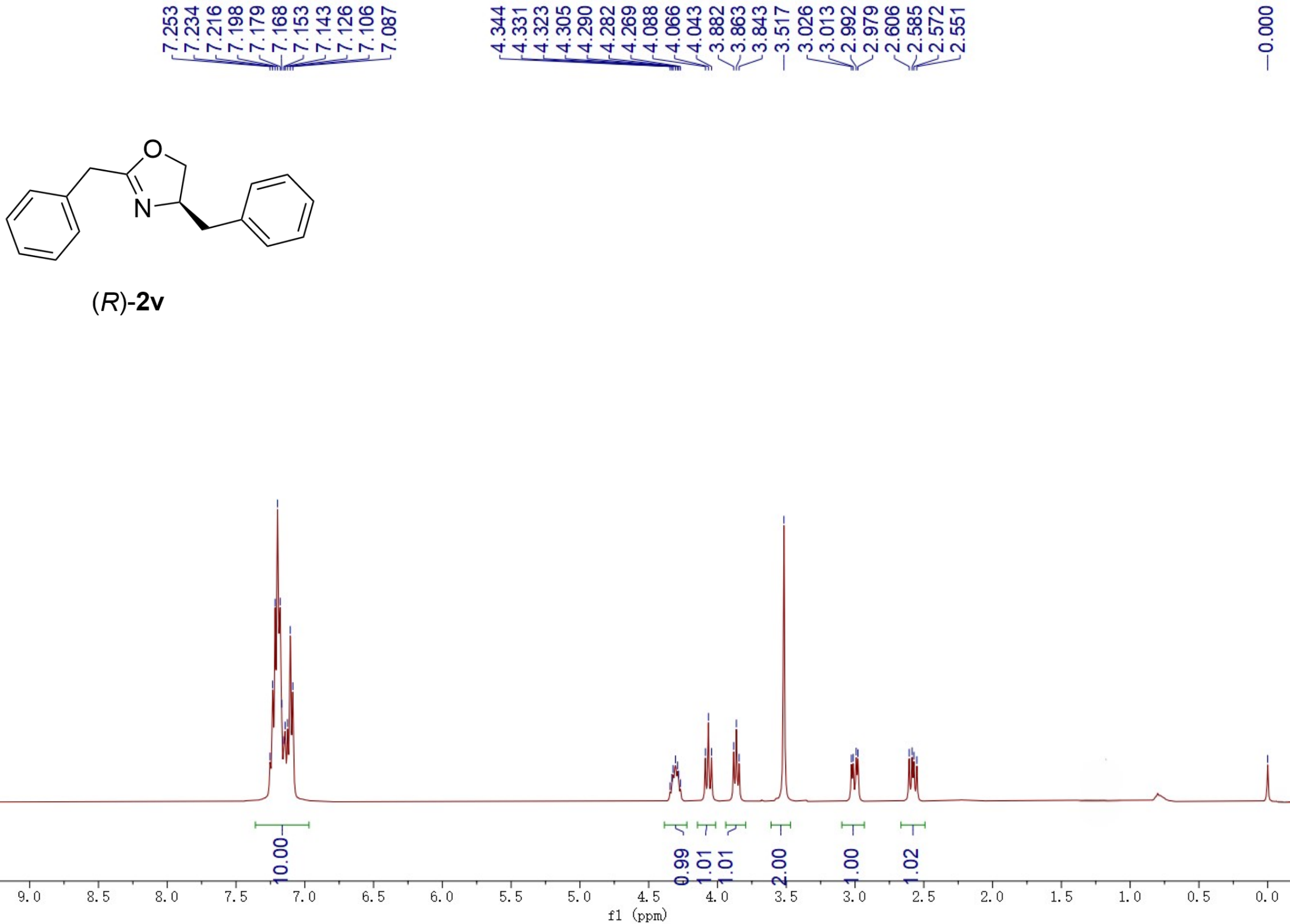

165.57
135.24
128.77
128.41
126.78
77.32
77.00
76.68
71.90
70.11
34.74
32.41
18.62
17.95
O
N
2s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.399
7.362
7.343
7.325
7.285
7.266
7.248
7.244
7.227
5.185
5.163
5.140
4.614
4.593
4.567
4.089
4.068
4.048
2.406
2.387
2.368
1.752
1.741
1.733
1.716
1.697
1.678
1.416
1.403
1.394
1.384
1.375
1.365
1.356
1.348
1.256
1.255
0.931
0.914
0.896
0.073
0.000
n-C4H9
O
N
Ph
(S)-2t
4.99
0.93
0.97
0.97
2.00
1.97
4.00
3.01
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
f1 (ppm)

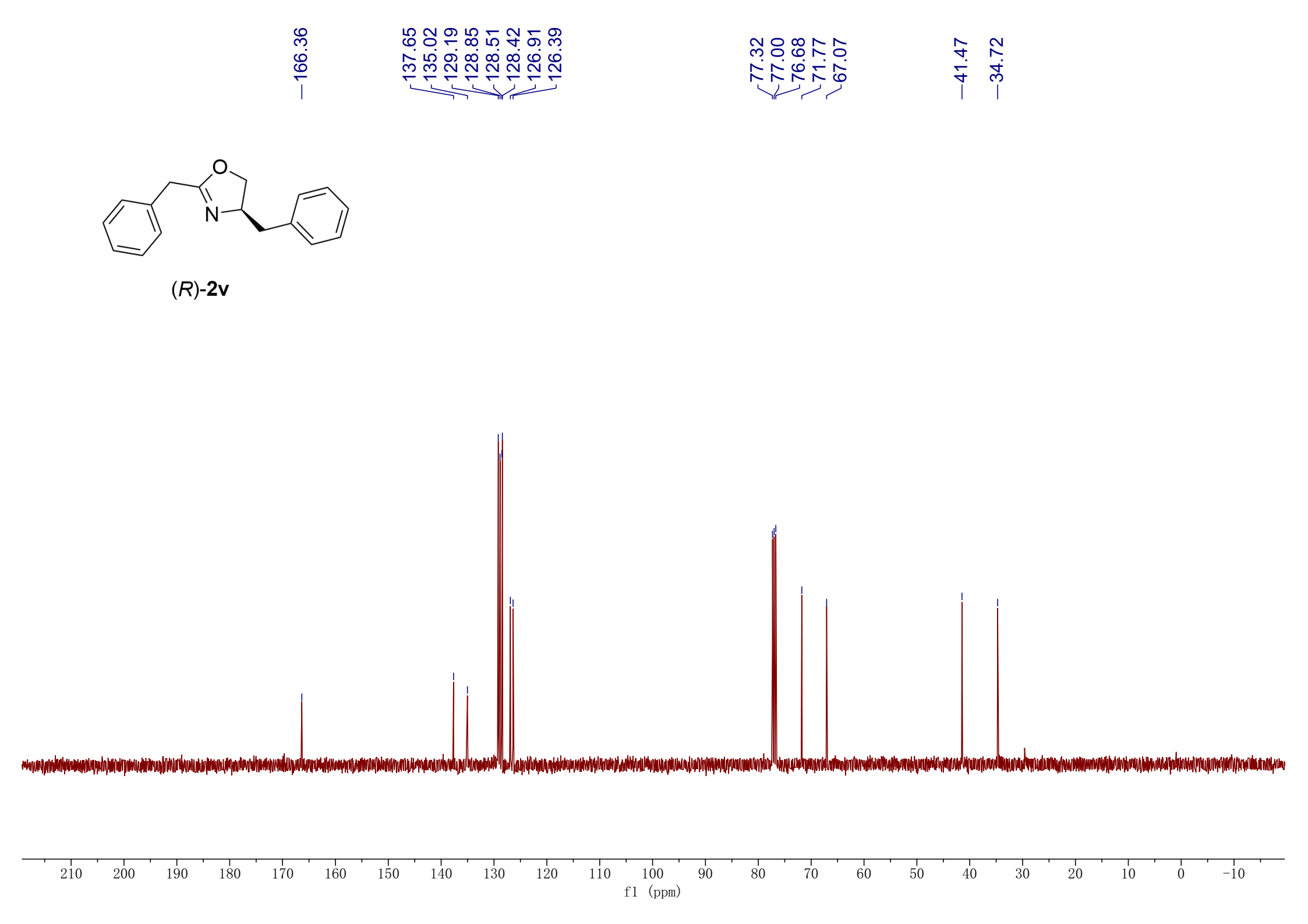

169.07
142.49
128.62
127.42
126.50
77.32
77.00
76.68
74.46
69.45
31.40
27.99
25.77
22.27
13.92
O
N
n-C4H9
Ph
(S)-2t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

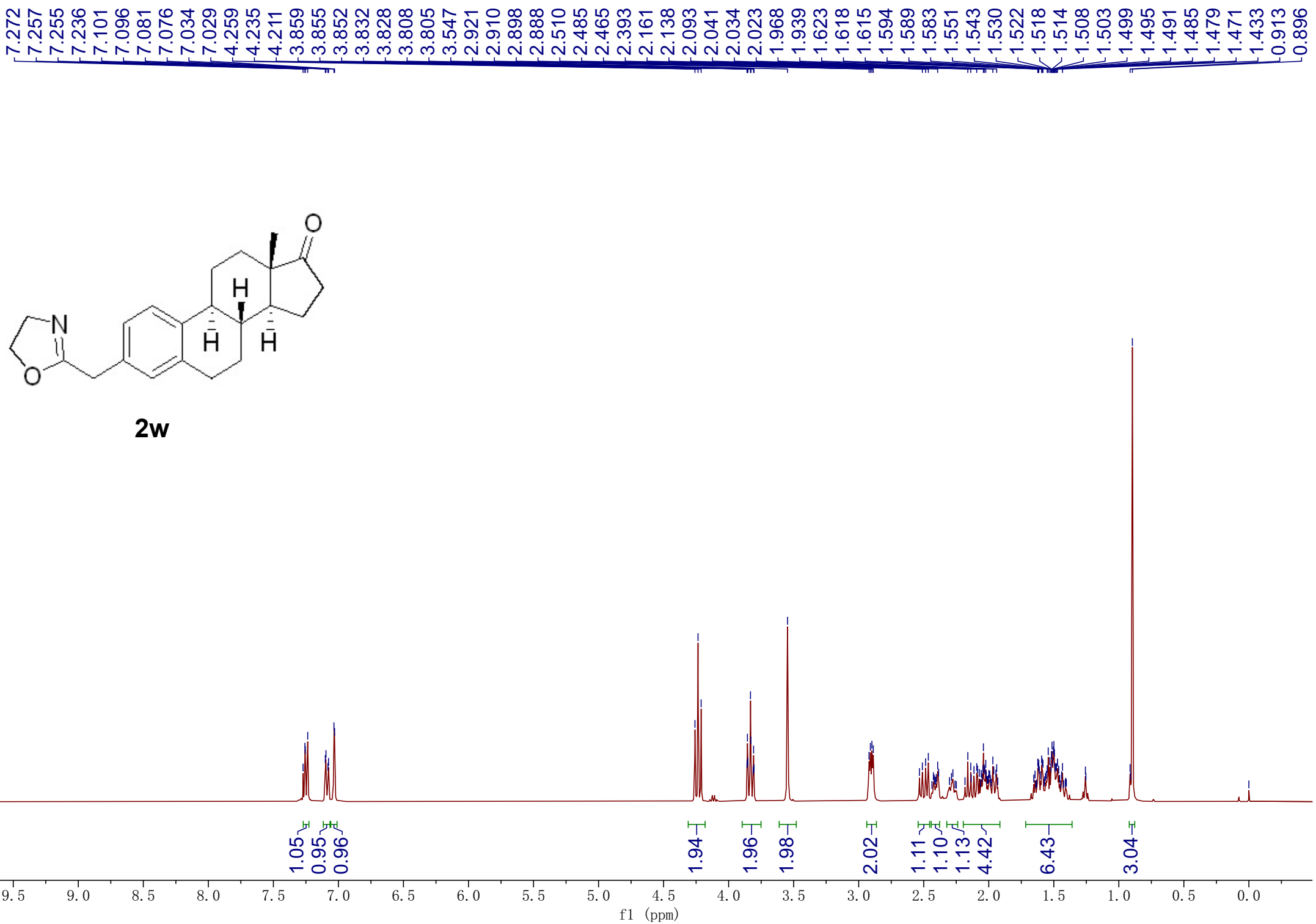

7.381
7.365
7.361
7.355
7.351
7.347
7.344
7.339
7.334
7.330
7.325
7.319
7.315
7.294
7.287
7.283
7.279
7.276
7.270
7.264
7.252
7.229
7.224
7.219
7.211
7.208
7.205
5.186
5.183
4.623
4.602
4.598
4.577
4.101
4.080
4.060
3.736
0.000
O
N
Ph
(S)-2u
10.04
1.00
1.00
1.01
2.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

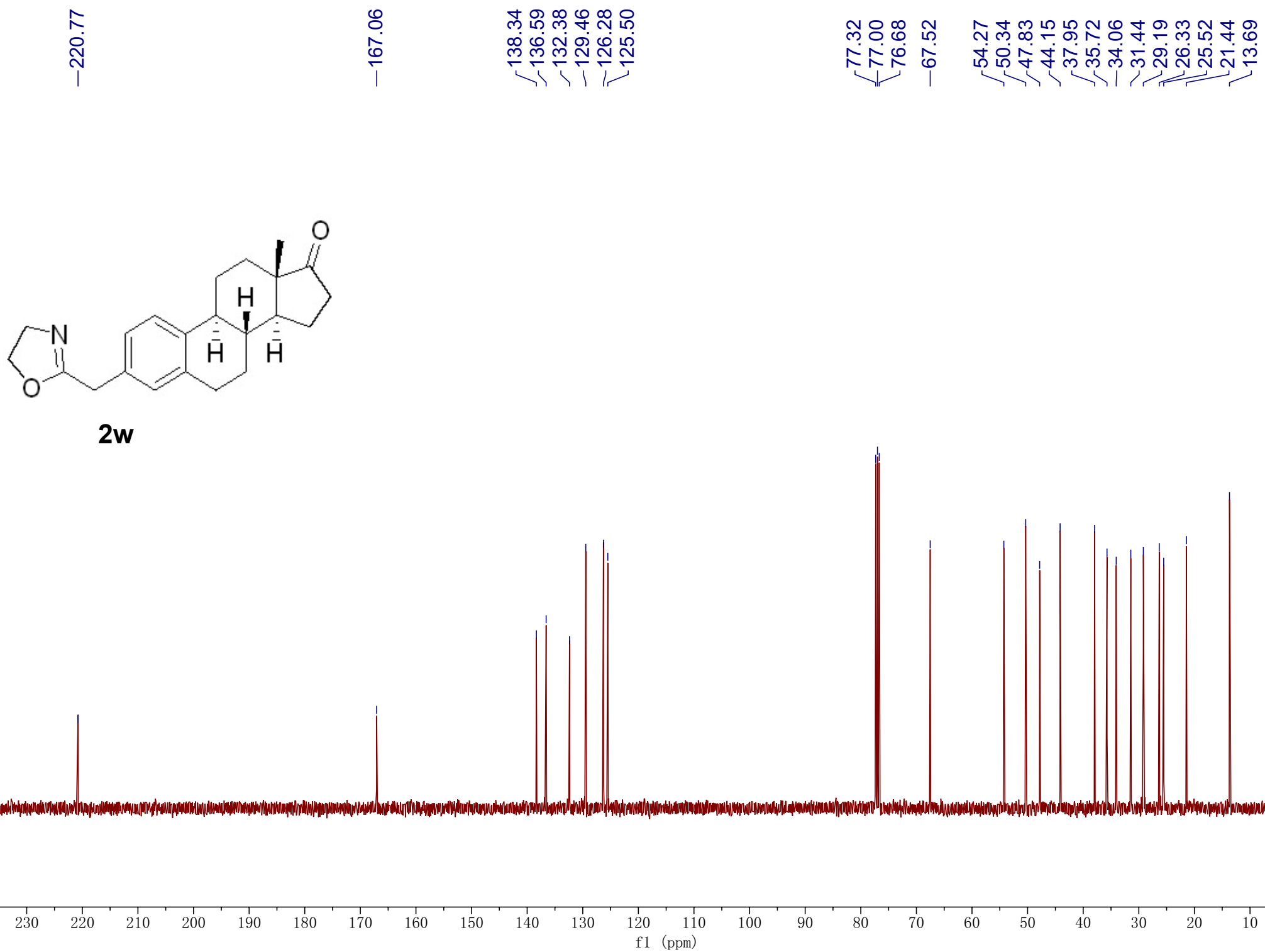

167.13
142.19
135.04
128.90
128.58
128.54
127.41
126.97
126.43
77.32
77.00
76.68
74.80
69.46
34.75
O
N
Ph
(S)-2u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

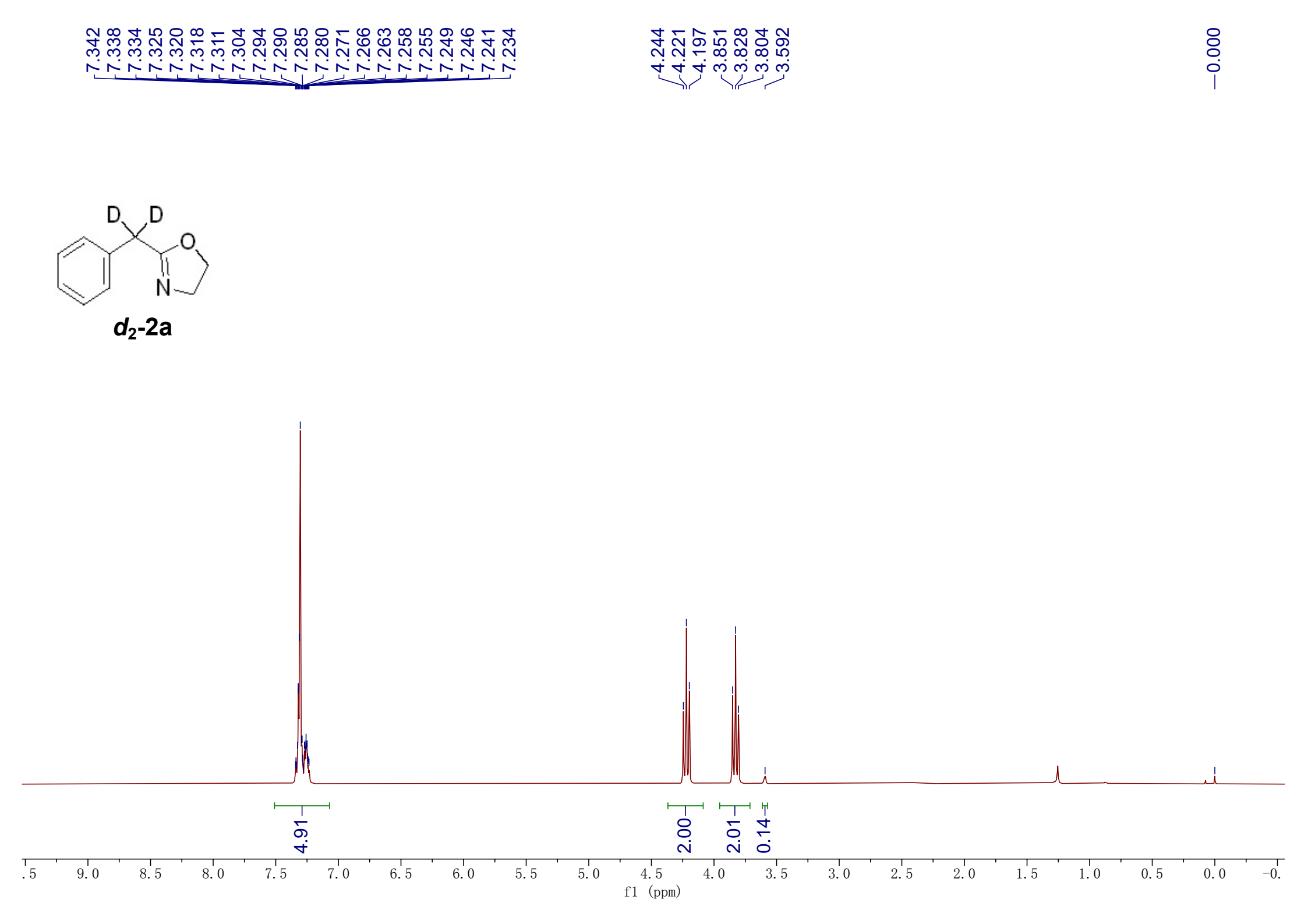

7.253
7.234
7.216
7.198
7.179
7.168
7.153
7.143
7.126
7.106
7.087
4.344
4.331
4.323
4.305
4.290
4.282
4.269
4.088
4.066
4.043
3.882
3.863
3.843
3.517
3.026
3.013
2.992
2.979
2.606
2.585
2.572
2.551
0.000
O
N
10.00
0.99
1.01
1.01
2.00
1.00
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

(*R*)-**2v**

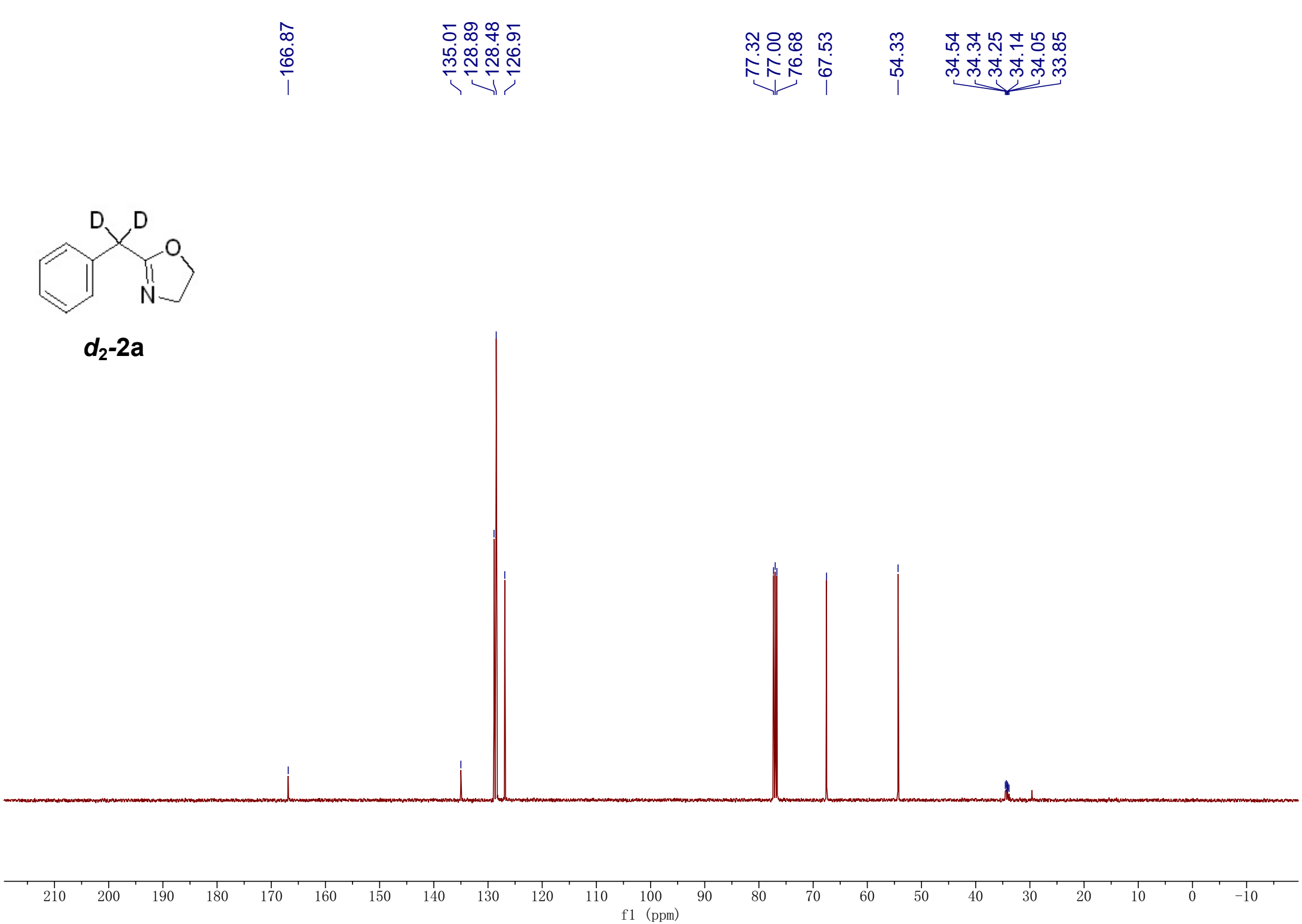

166.36
137.65
135.02
129.19
128.85
128.51
128.42
126.91
126.39
77.32
77.00
76.68
71.77
67.07
41.47
34.72
O
N
(R)-2v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.272
7.257
7.255
7.236
7.101
7.096
7.081
7.076
7.034
7.029
4.259
4.235
4.211
3.859
3.855
3.852
3.832
3.828
3.808
3.805
3.547
2.921
2.910
2.898
2.888
2.510
2.485
2.465
2.393
2.161
2.138
2.093
2.041
2.034
2.023
1.968
1.939
1.623
1.618
1.615
1.594
1.589
1.583
1.551
1.543
1.530
1.522
1.518
1.514
1.508
1.503
1.499
1.495
1.491
1.485
1.479
1.471
1.433
0.913
0.896
N
O
H
H
H
O
2w
1.05
0.95
0.96
1.94
1.96
1.98
2.02
1.11
1.10
1.13
4.42
6.43
3.04
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
f1 (ppm)

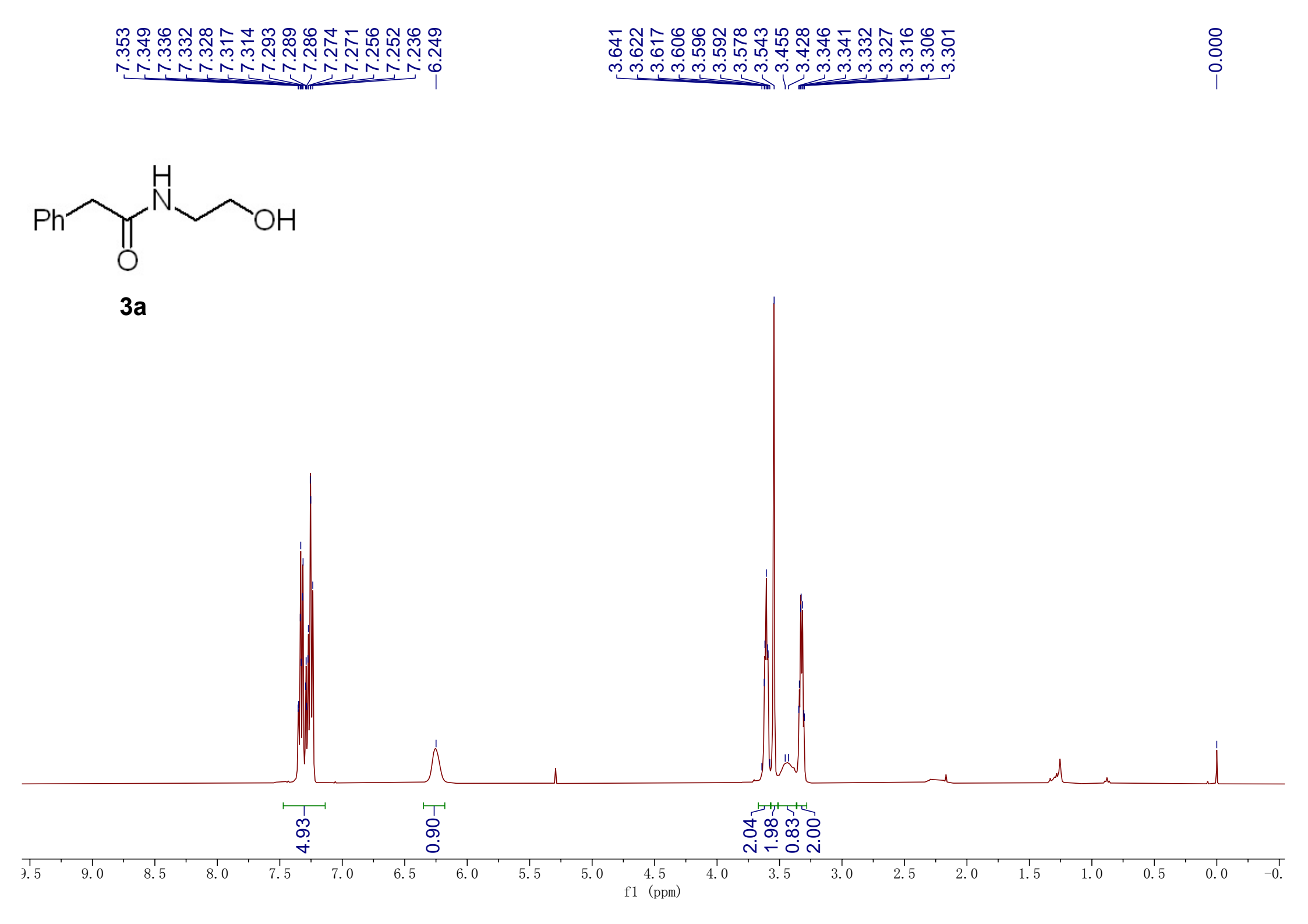

220.77
167.06
138.34
136.59
132.38
129.46
126.28
125.50
77.32
77.00
76.68
67.52
54.27
50.34
47.83
44.15
37.95
35.72
34.06
31.44
29.19
26.33
25.52
21.44
13.69
N
O
O
H
H
H
2w
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

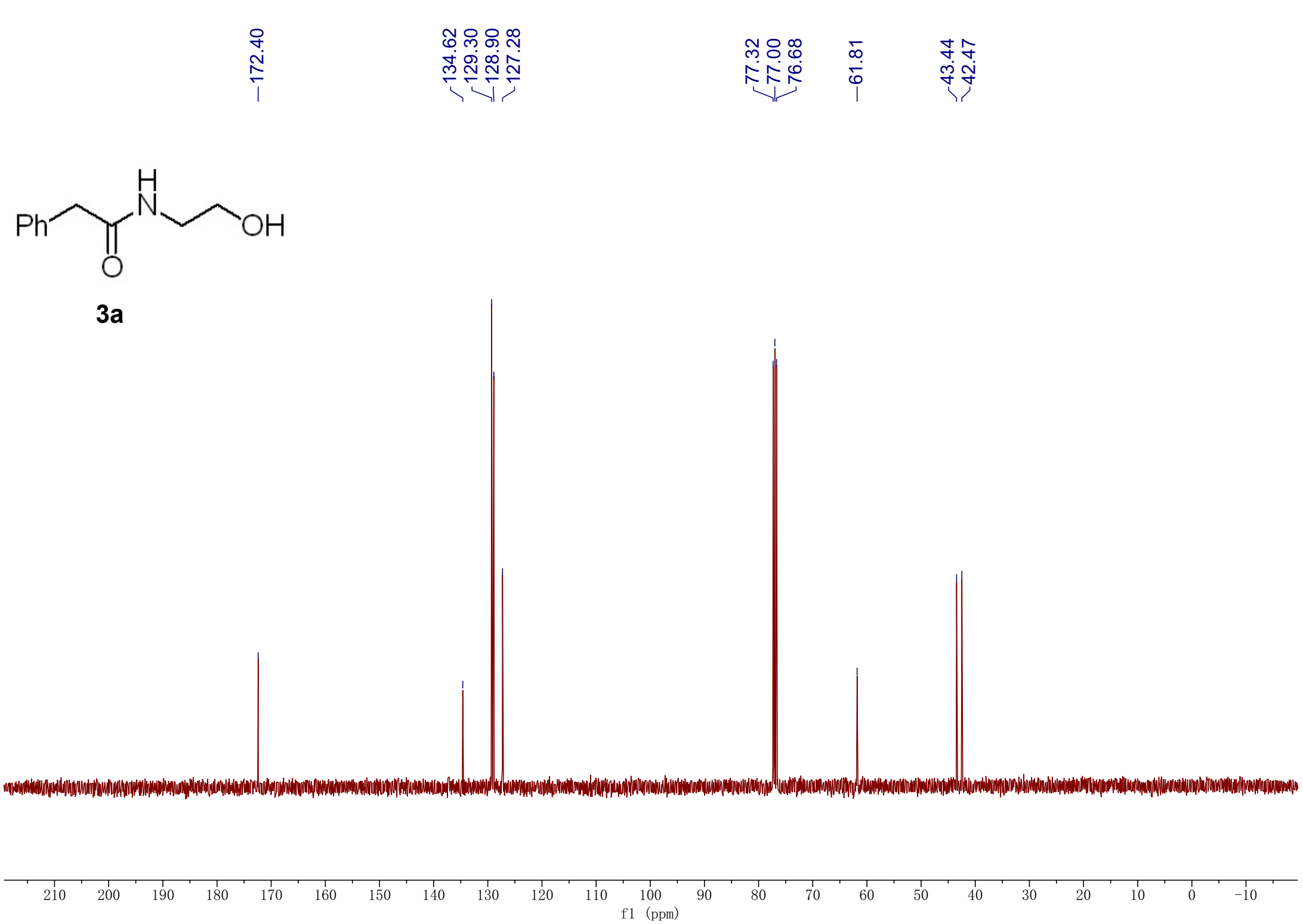

7.342
7.338
7.334
7.325
7.320
7.318
7.311
7.304
7.294
7.290
7.285
7.280
7.271
7.266
7.263
7.258
7.255
7.249
7.246
7.241
7.234
4.244
4.221
4.197
3.851
3.828
3.804
3.592
0.000
D
D
O
N
4.91
2.00
2.01
0.14
f1 (ppm)

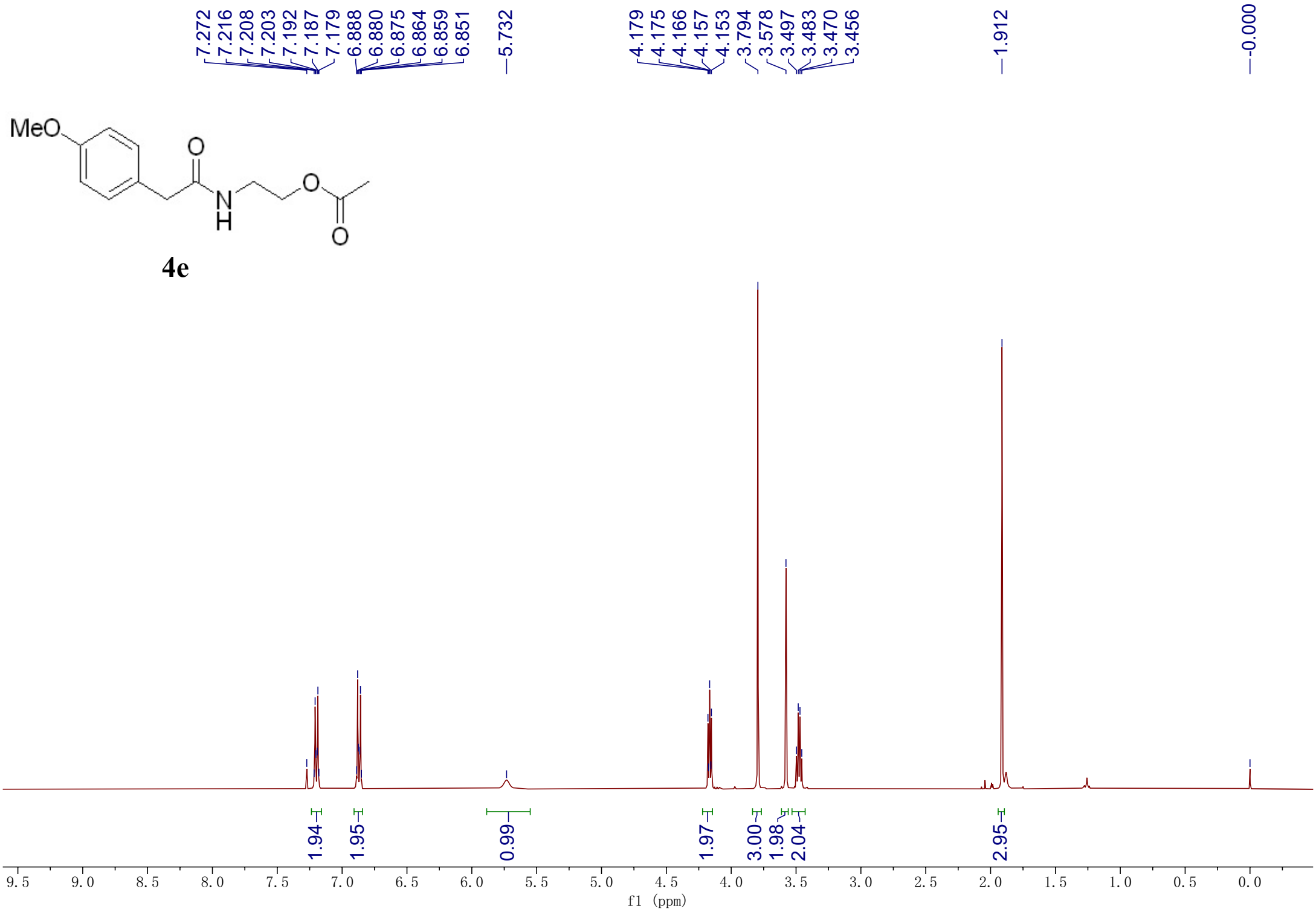
***d*$_2$-2a**

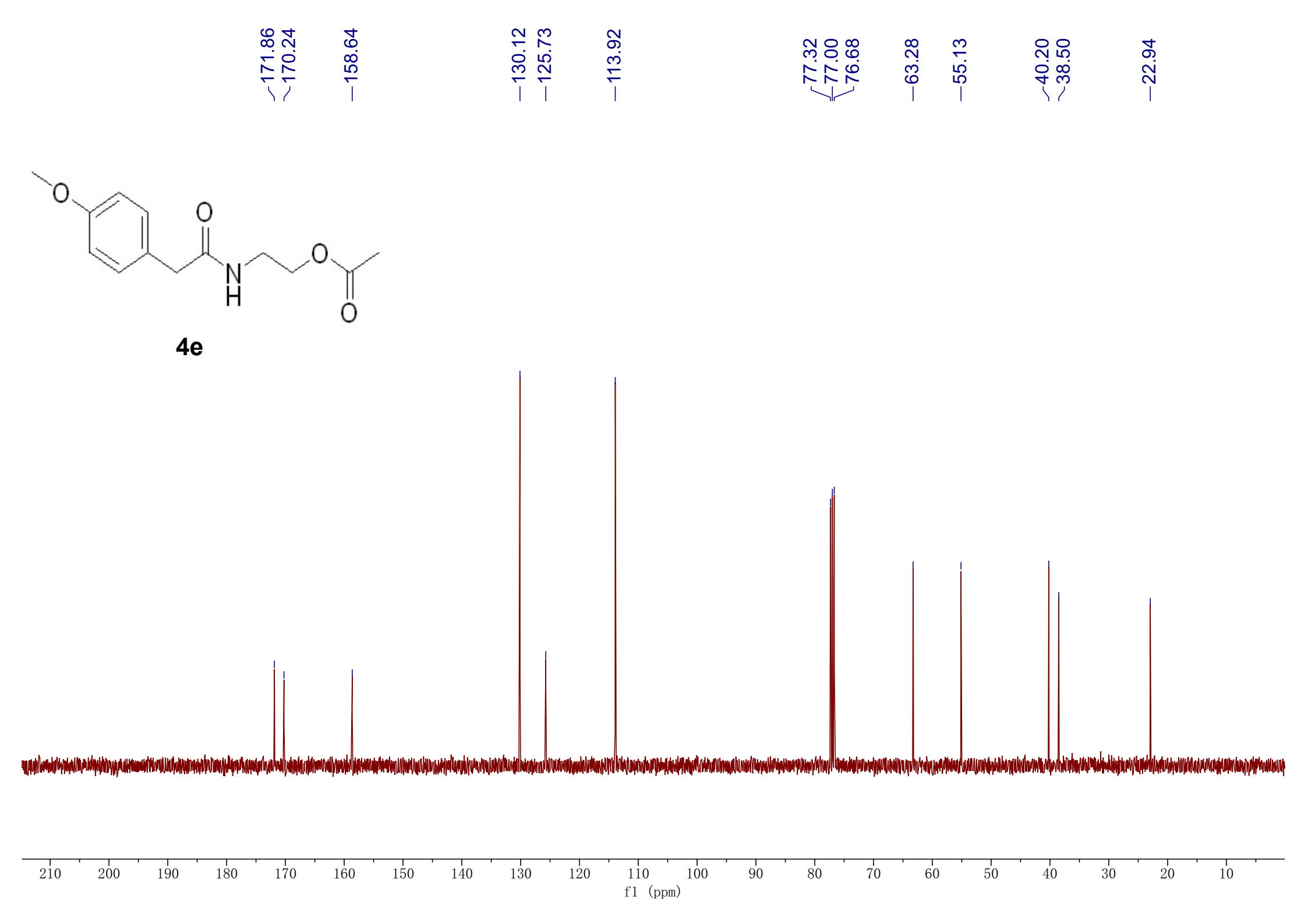

166.87
135.01
128.89
128.48
126.91
77.32
77.00
76.68
67.53
54.33
34.54
34.34
34.25
34.14
34.05
33.85
D
D
O
N
f1 (ppm)

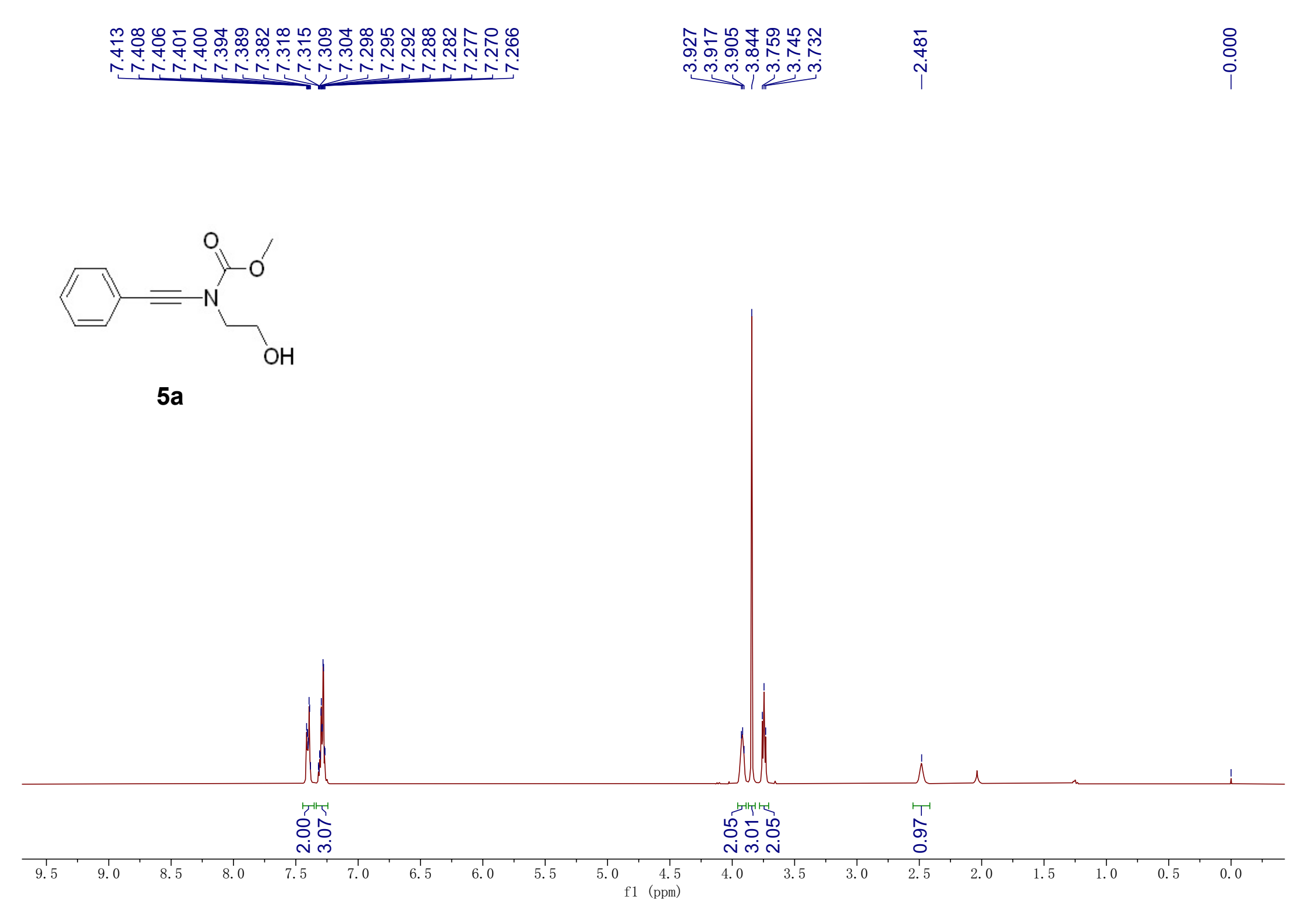
***d*$_2$-2a**

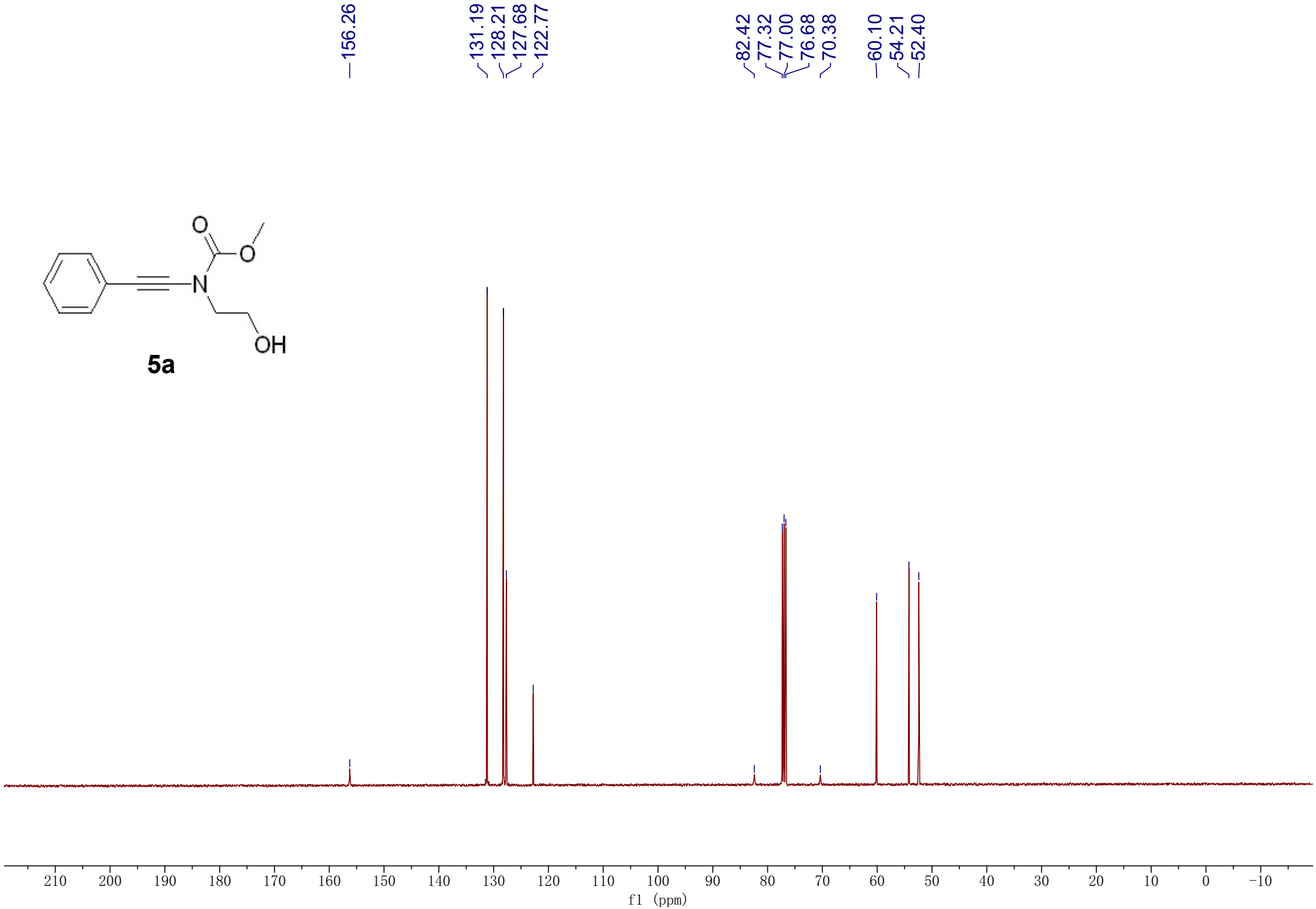

7.353
7.349
7.336
7.332
7.328
7.317
7.314
7.293
7.289
7.286
7.274
7.271
7.256
7.252
7.236
6.249
3.641
3.622
3.617
3.606
3.596
3.592
3.578
3.543
3.455
3.428
3.346
3.341
3.332
3.327
3.316
3.306
3.301
0.000
Ph
H
N
O
OH
3a
4.93
0.90
2.04
1.98
0.83
2.00
f1 (ppm)


172.40
134.62
129.30
128.90
127.28
77.32
77.00
76.68
61.81
43.44
42.47
Ph
H
N
O
OH
3a
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)


7.272
7.216
7.208
7.203
7.192
7.187
7.179
6.888
6.880
6.875
6.864
6.859
6.851
5.732
4.179
4.175
4.166
4.157
4.153
3.794
3.578
3.497
3.483
3.470
3.456
1.912
0.000
MeO
O
N
H
O
O
4e
1.94
1.95
0.99
1.97
3.00
1.98
2.04
2.95
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
f1 (ppm)


171.86
170.24
158.64
130.12
125.73
113.92
77.32
77.00
76.68
63.28
55.13
40.20
38.50
22.94
O
O
N
H
O
O
4e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.413
7.408
7.406
7.401
7.400
7.394
7.389
7.382
7.318
7.315
7.309
7.304
7.298
7.295
7.292
7.288
7.282
7.277
7.270
7.266
3.927
3.917
3.905
3.844
3.759
3.745
3.732
2.481
0.000
O
O
N
OH
5a
2.00
3.07
2.05
3.01
2.05
0.97
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
f1 (ppm)


156.26
131.19
128.21
127.68
122.77
82.42
77.32
77.00
76.68
70.38
60.10
54.21
52.40
O
O
N
OH
5a
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)

X-ray of 2j

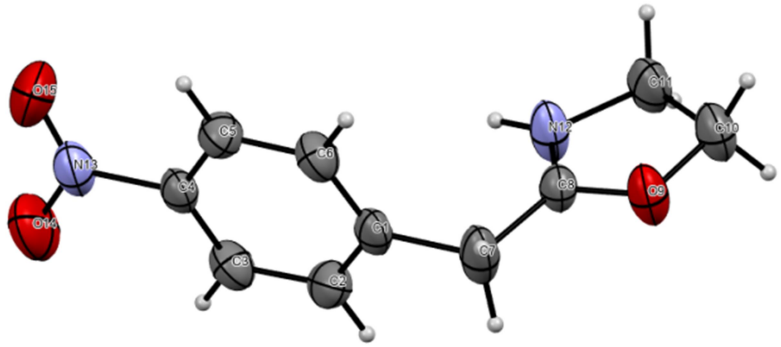


Figure S1. X-ray of Compound **2j**

Crystal data for **2j**: $C_{10}H_{11}N_2O_3$, M = 207.21, monoclinic, space group P 21/n, final R indices [$I > 2\sigma(I)$]: $R1$ = 0.0858, w$R2$ = 0.1900, R indices (all data): R_1 = 0.0592, wR_2 = 0.1734, a = 10.6496(14), b = 4.9316(6), c = 19.212(2) Å, β = 100.692(12) °, V = 991.5(2) Å 3 , T = 301 K (2), Z = 4, reflections collected/unique: 7026/2282 (R_{int} = 0.0277), number of observations [$I > 2\sigma(I)$]: 1499, parameters: 136. **CCDC 2321759** data for this paper contains the supplementary crystallographic.

CheckCIF/PLATON Report

Structure factors have been supplied for datablock(s) 1_auto

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1_auto

```
Bond precision:   C-C = 0.0031 A          Wavelength=0.71073

Cell:             a=10.6496(14)     b=4.9316(6)          c=19.212(2)
                  alpha=90          beta=100.692(12)     gamma=90
Temperature:      301 K

                 Calculated                Reported
Volume           991.5(2)                  991.5(2)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C10 H11 N2 O3             ?
Sum formula      C10 H11 N2 O3             C10 H11 N2 O3
Mr               207.21                    207.21
Dx,g cm-3        1.388                     1.388
Z                4                         4
Mu (mm-1)        0.104                     0.104
F000             436.0                     436.0
F000'            436.22
h,k,lmax                                   14,6,25
Nref                                       2282
Tmin,Tmax        0.986,0.988
Tmin'            0.986

Correction method= Not given

Data completeness=                  Theta(max)= 29.843

R(reflections)= 0.0592( 1499)                    wR2(reflections)=
                                                 0.1900( 2282)
S = 1.048                  Npar= 136
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C8 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C1       -C6       .       1.37 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H3       ..H12      .       2.06 Ang.
                                    3/2-x,-1/2+y,3/2-z  =      2_646 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N12      --H12      .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.425 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.408 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
             -10  0  8,  -5  5  9,  -4  5 10,  -4  5 11, -11  0 15,  -9  0 19,
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
            H12
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O9       .      105.9 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        540 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          3 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 29/11/2023; check.def file version of 14/09/2023

Datablock 1_auto - ellipsoid plot