Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

An asymmetric pericyclic cascade approach to 3-alkyl-3-aryloxindoles; generality, applications and mechanistic investigations

Spectra for Novel Compounds

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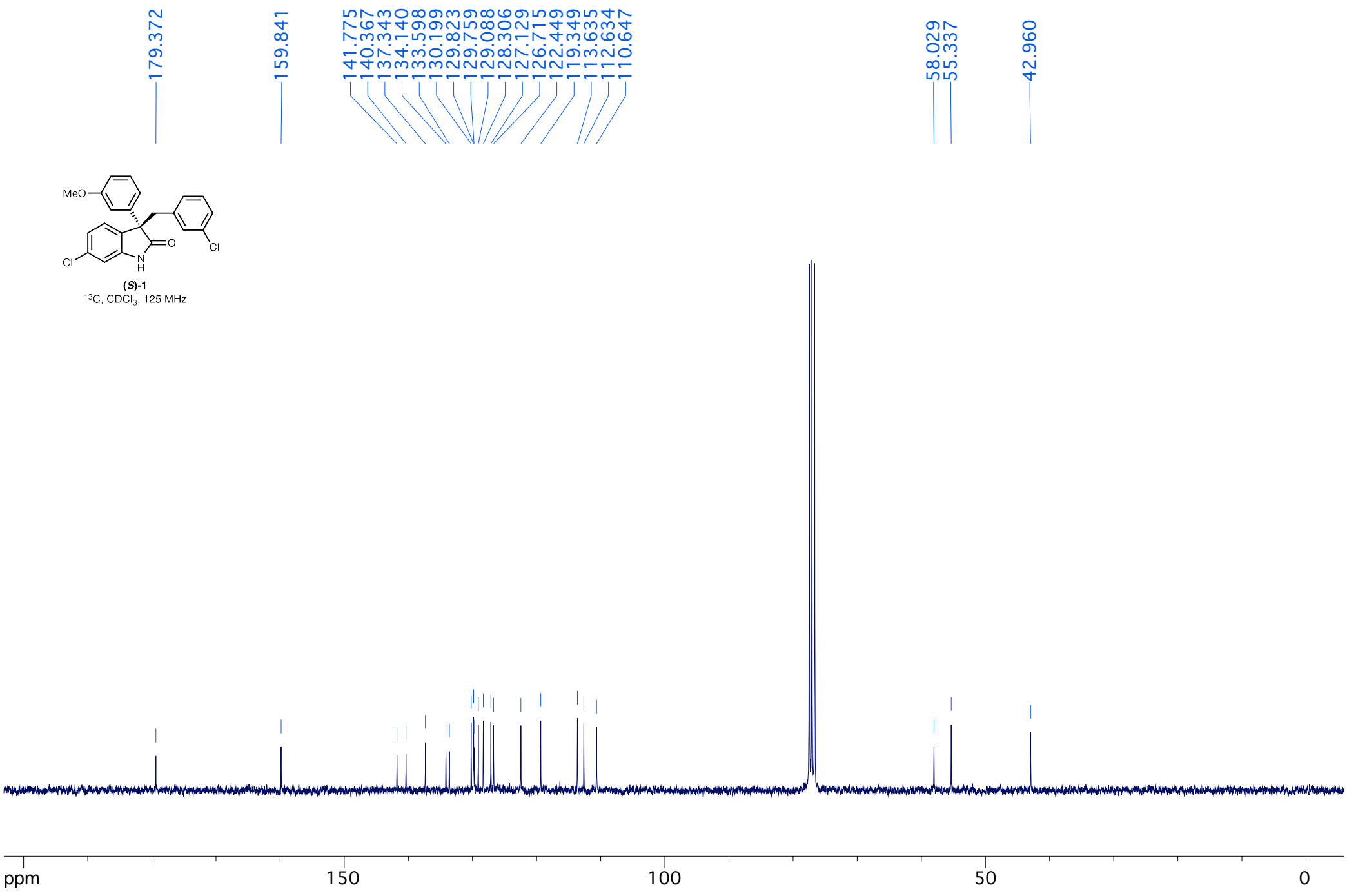
[b]*Department of Chemistry and Biochemistry, University of California, Los Angeles, 607 Charles E. Young Drive East, Los Angeles, CA 90095, USA.*

[c]*Department of Chemical Engineering, Yeditepe University, Istanbul, 34755, Turkey.*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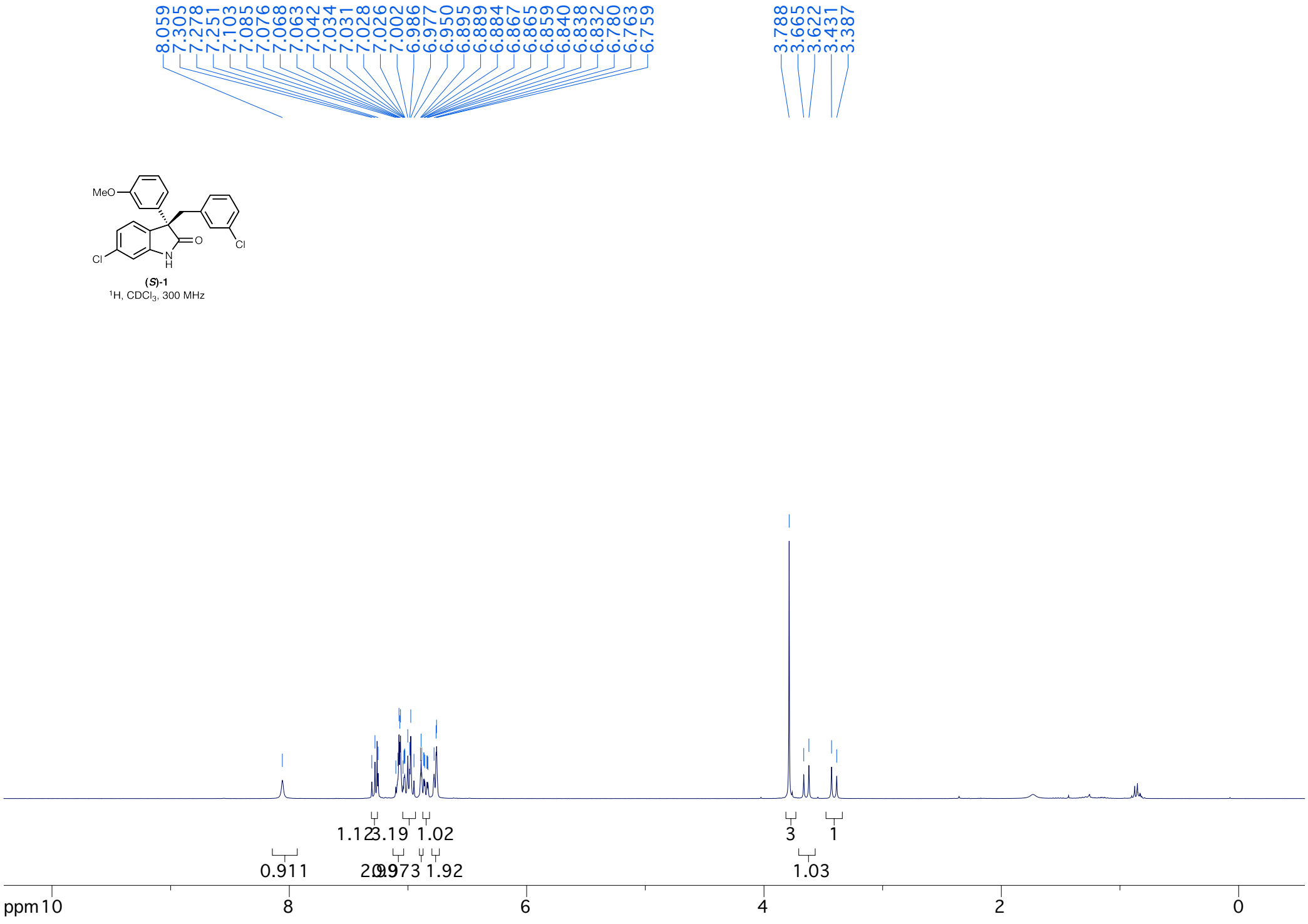
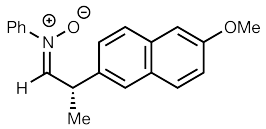
159.841
141.775
140.367
137.343
134.140
133.598
130.199
129.823
129.759
129.088
128.306
127.129
126.715
122.449
119.349
113.635
112.634
110.647
58.029
55.337
42.960
MeO
Cl
O
N
H
Cl
(S)-1
13C, CDCl3, 125 MHz
ppm
150
100
50
0


8.059
7.305
7.278
7.251
7.103
7.085
7.076
7.068
7.063
7.042
7.034
7.031
7.028
7.026
7.002
6.986
6.977
6.950
6.895
6.889
6.884
6.867
6.865
6.859
6.840
6.838
6.832
6.780
6.763
6.759
3.788
3.665
3.622
3.431
3.387
MeO
Cl
O
N
H
Cl
(S)-1
1H, CDCl3, 300 MHz
1.12
3.19
1.02
3
1
0.911
1.92
1.03
ppm
10
8
6
4
2
0

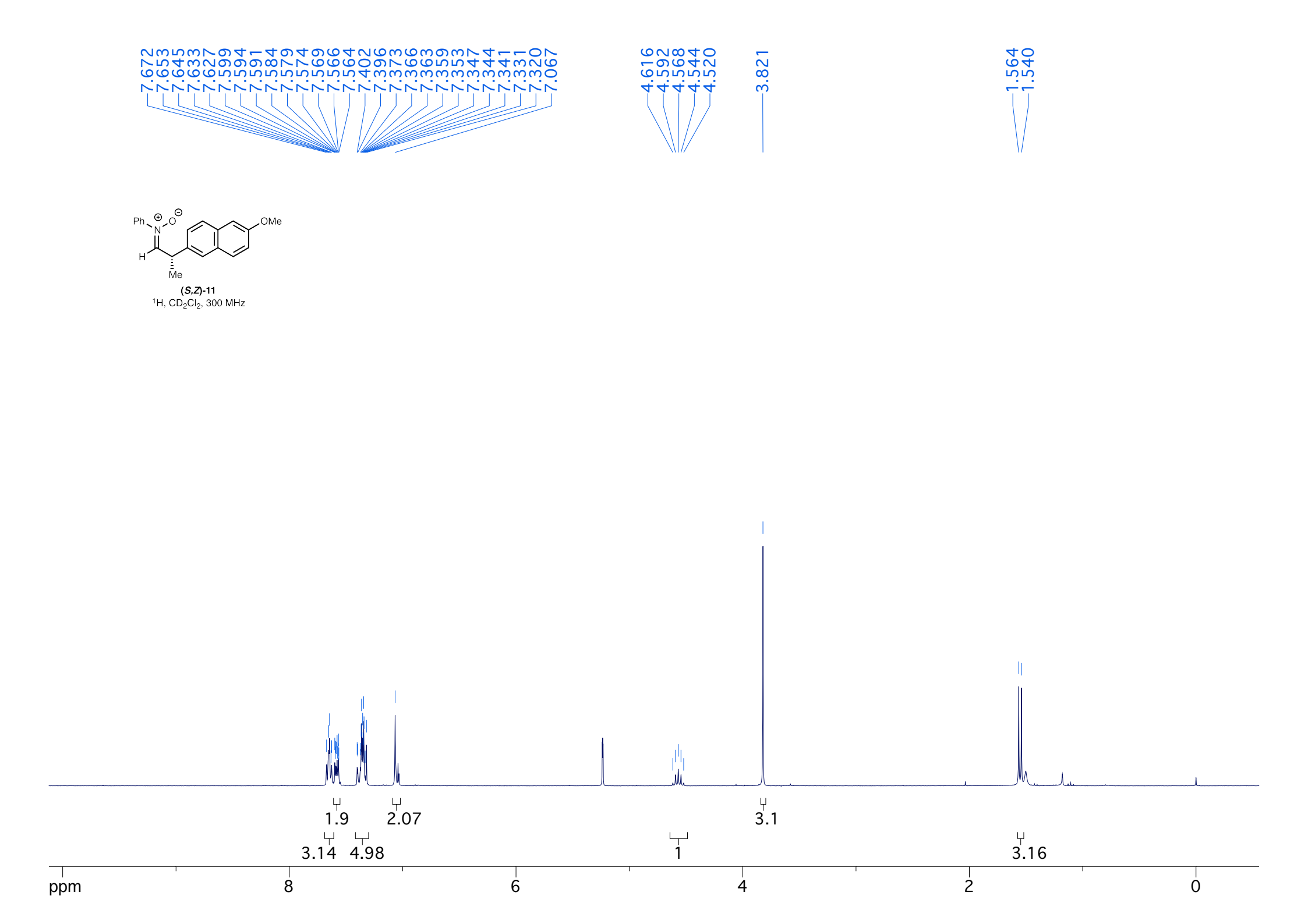


(*S,Z*)-11

^{13}C, CD_2Cl_2, 75 MHz

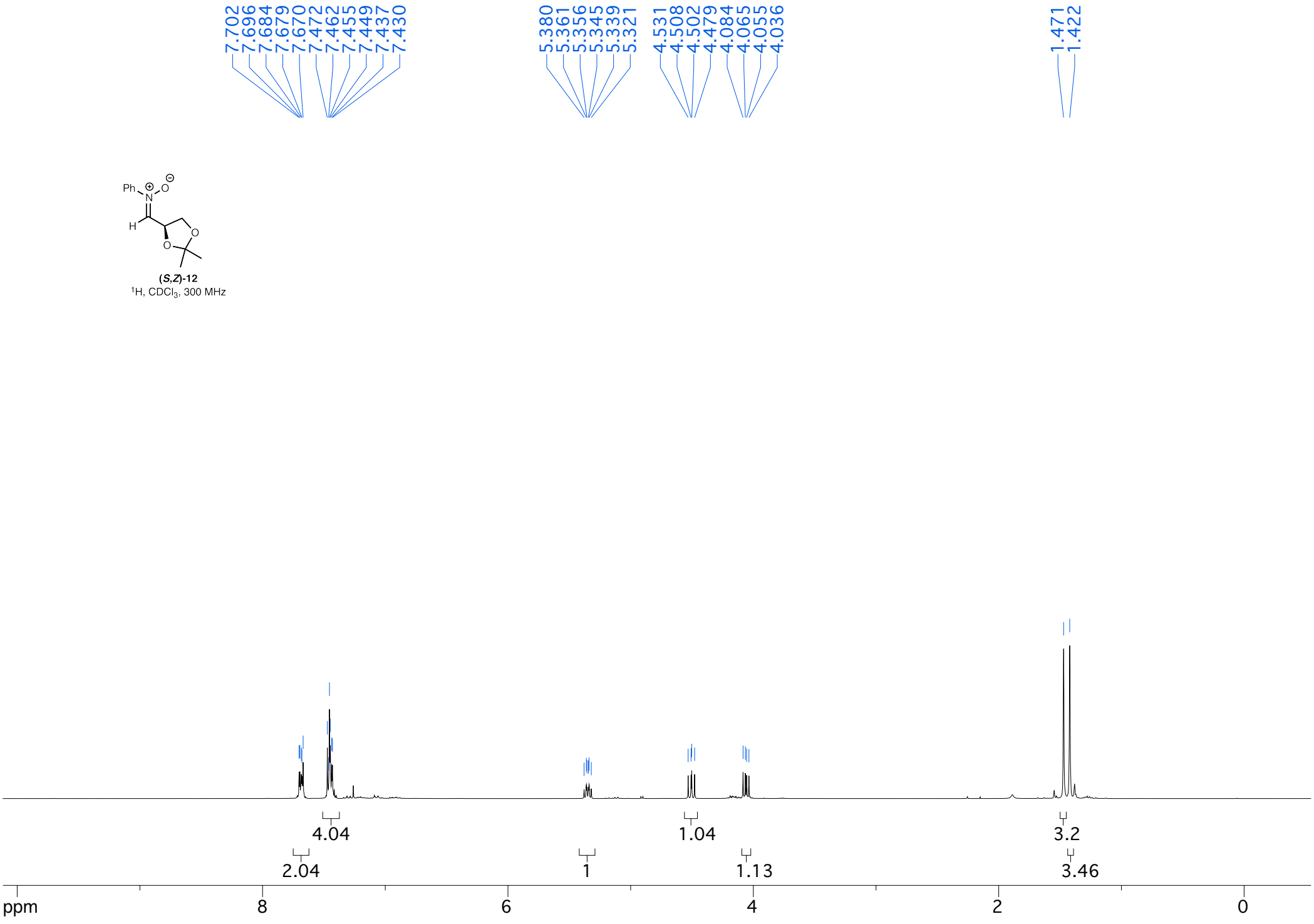
158.420
156.651
147.678
142.398
138.264
130.623
129.884
129.745
127.989
127.267
126.195
122.370
119.703
118.403
106.316
56.054
37.968
18.555

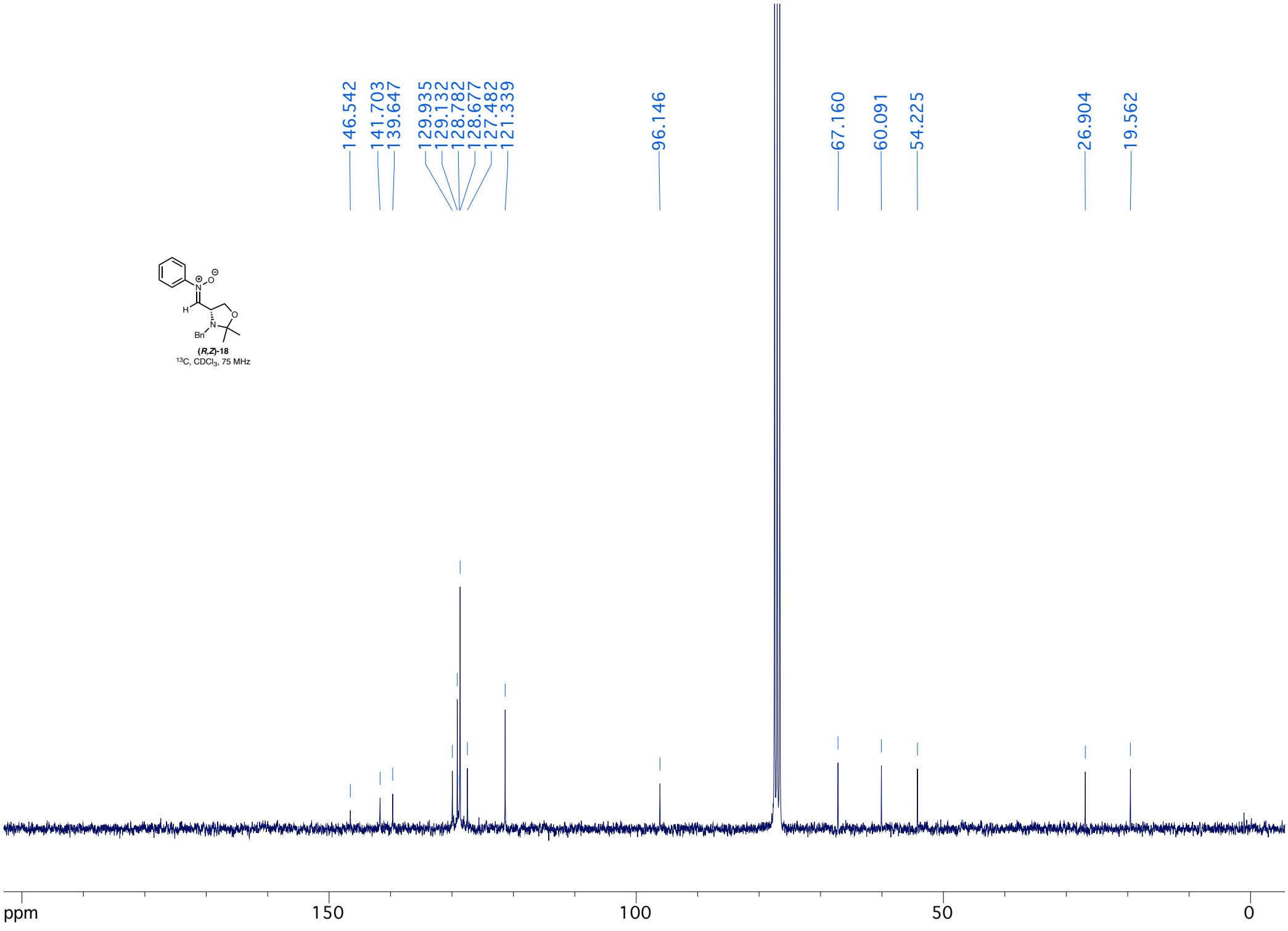
ppm 150 100 50 0

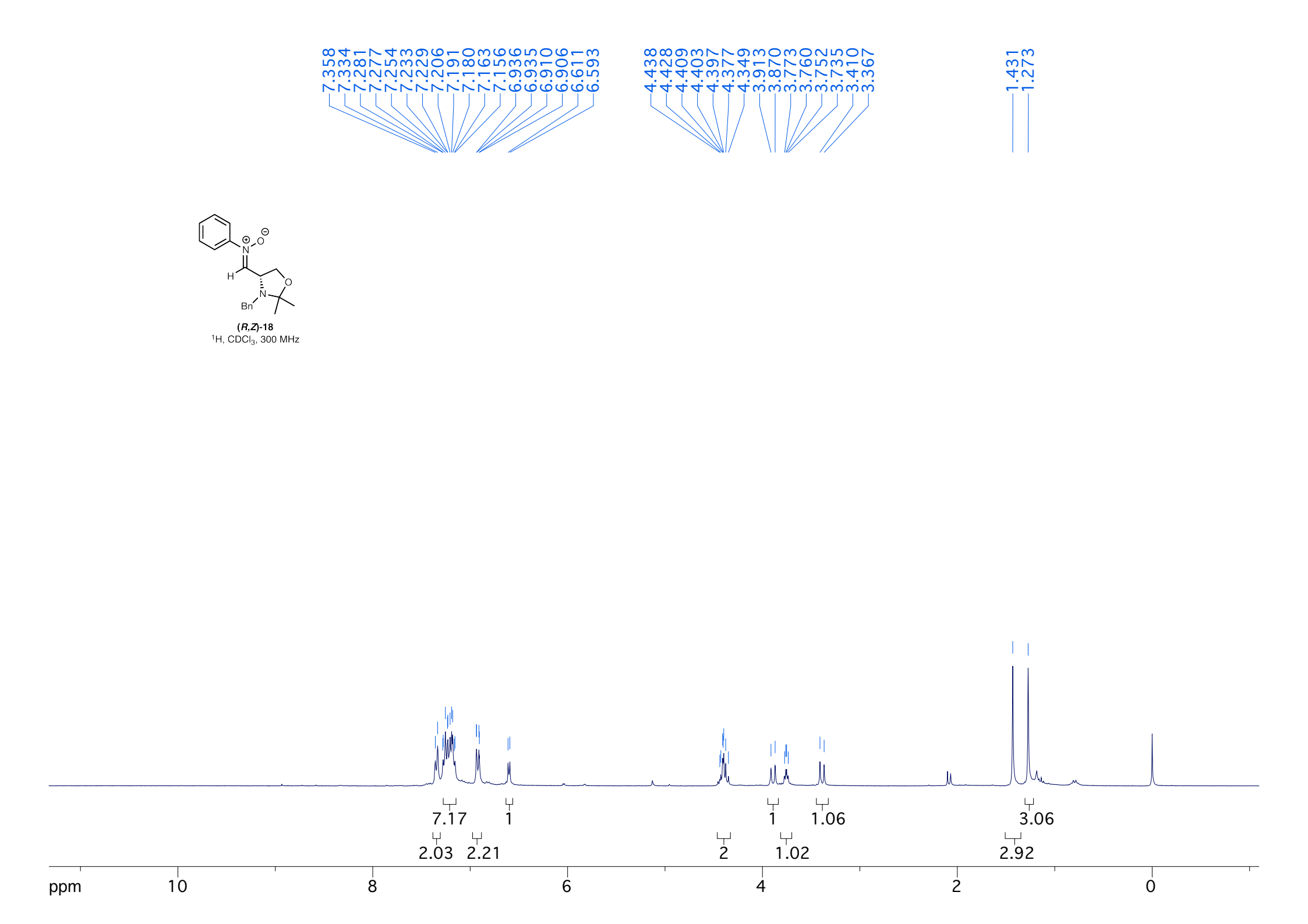


(*S,Z*)-11

^{1}H, CD_2Cl_2, 300 MHz


7.702
7.696
7.684
7.679
7.670
7.472
7.462
7.455
7.449
7.437
7.430
5.380
5.361
5.356
5.345
5.339
5.321
4.531
4.508
4.502
4.479
4.084
4.065
4.055
4.036
1.471
1.422
Ph
N
O
H
O
O
(S,Z)-12
1H, CDCl3, 300 MHz
4.04
1.04
3.2
2.04
1
1.13
3.46
ppm
8
6
4
2
0


146.542
141.703
139.647
129.935
129.132
128.782
128.677
127.482
121.339
96.146
67.160
60.091
54.225
26.904
19.562
(R,Z)-18
13C, CDCl3, 75 MHz
ppm
150
100
50
0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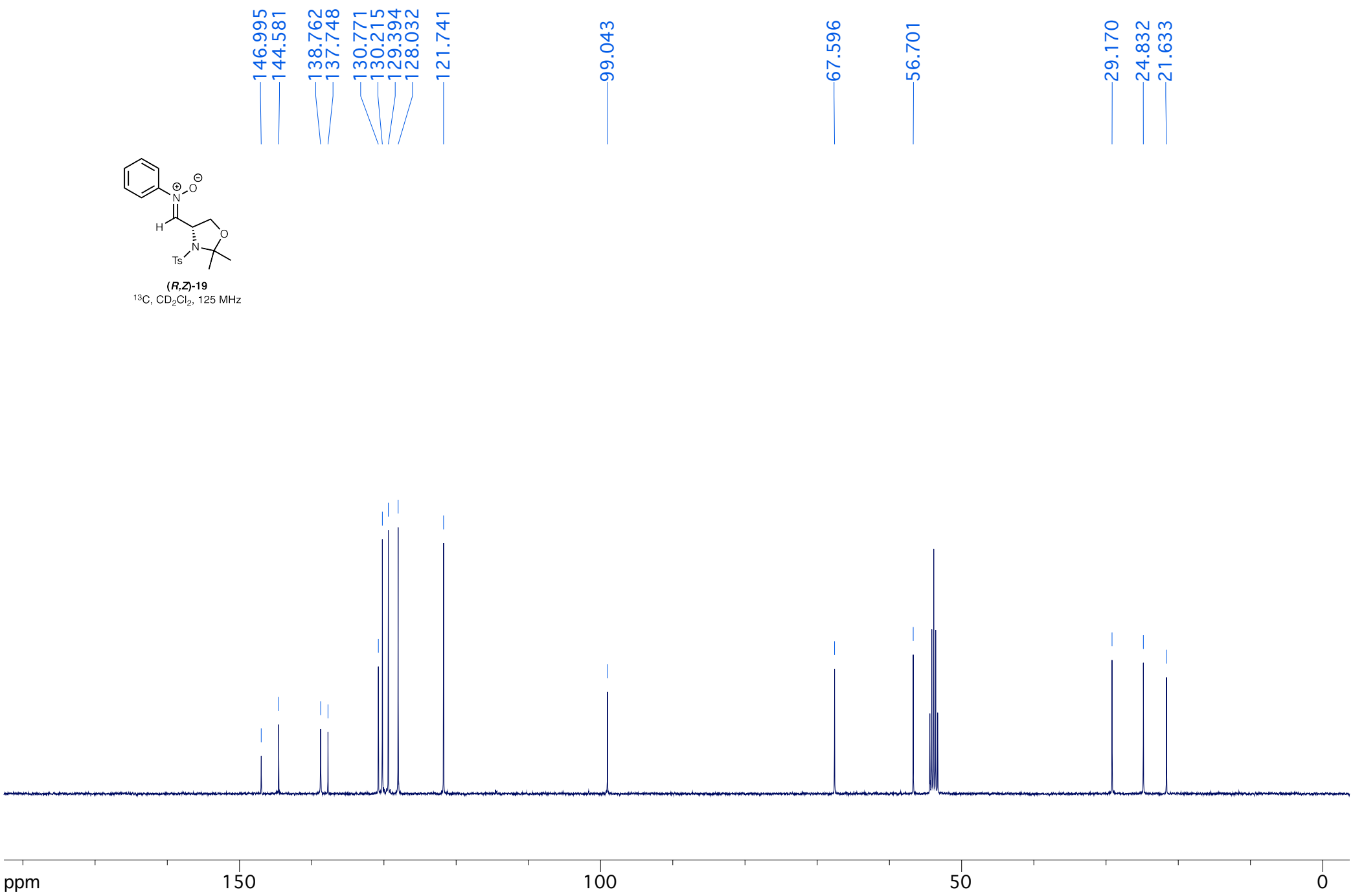
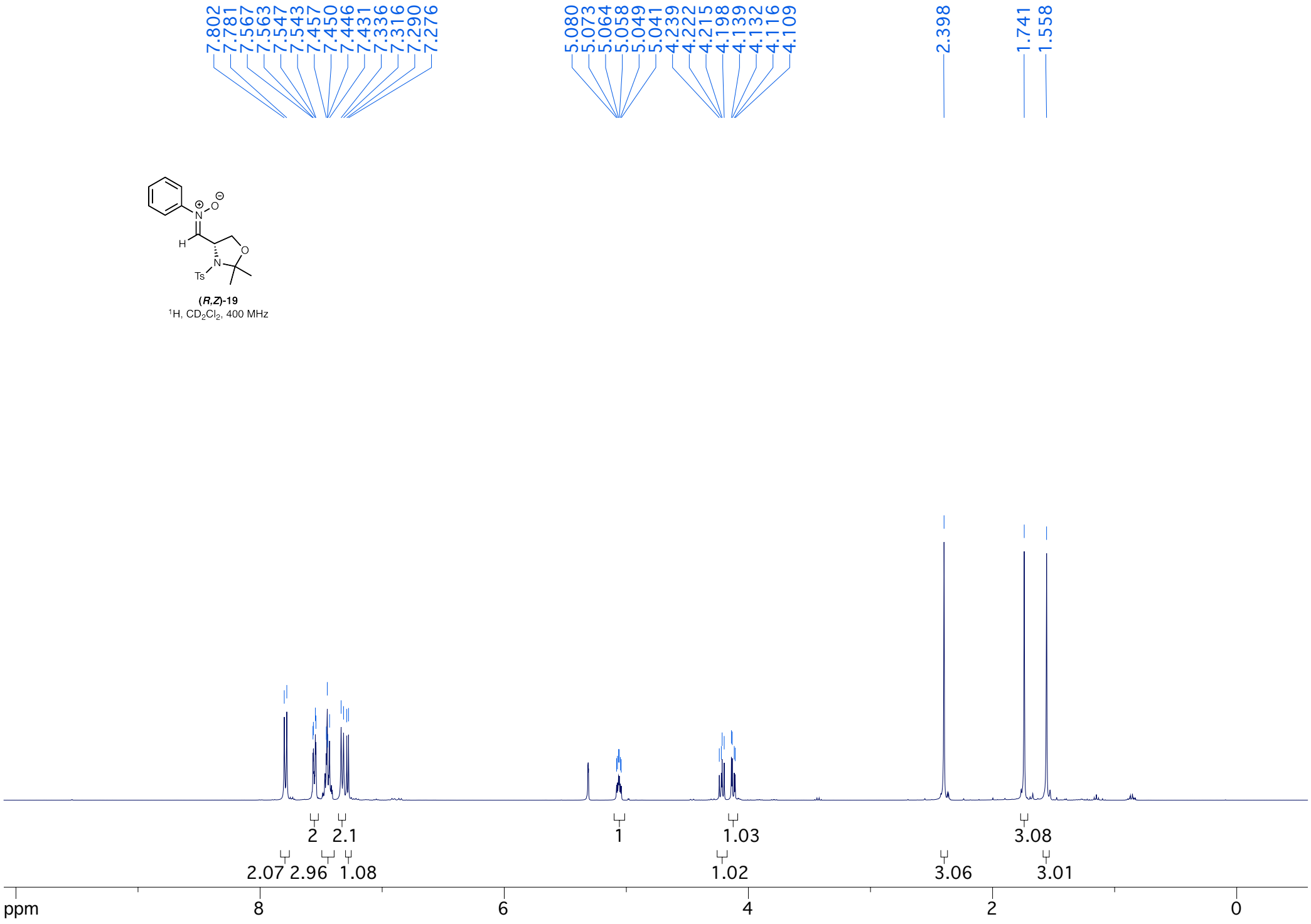
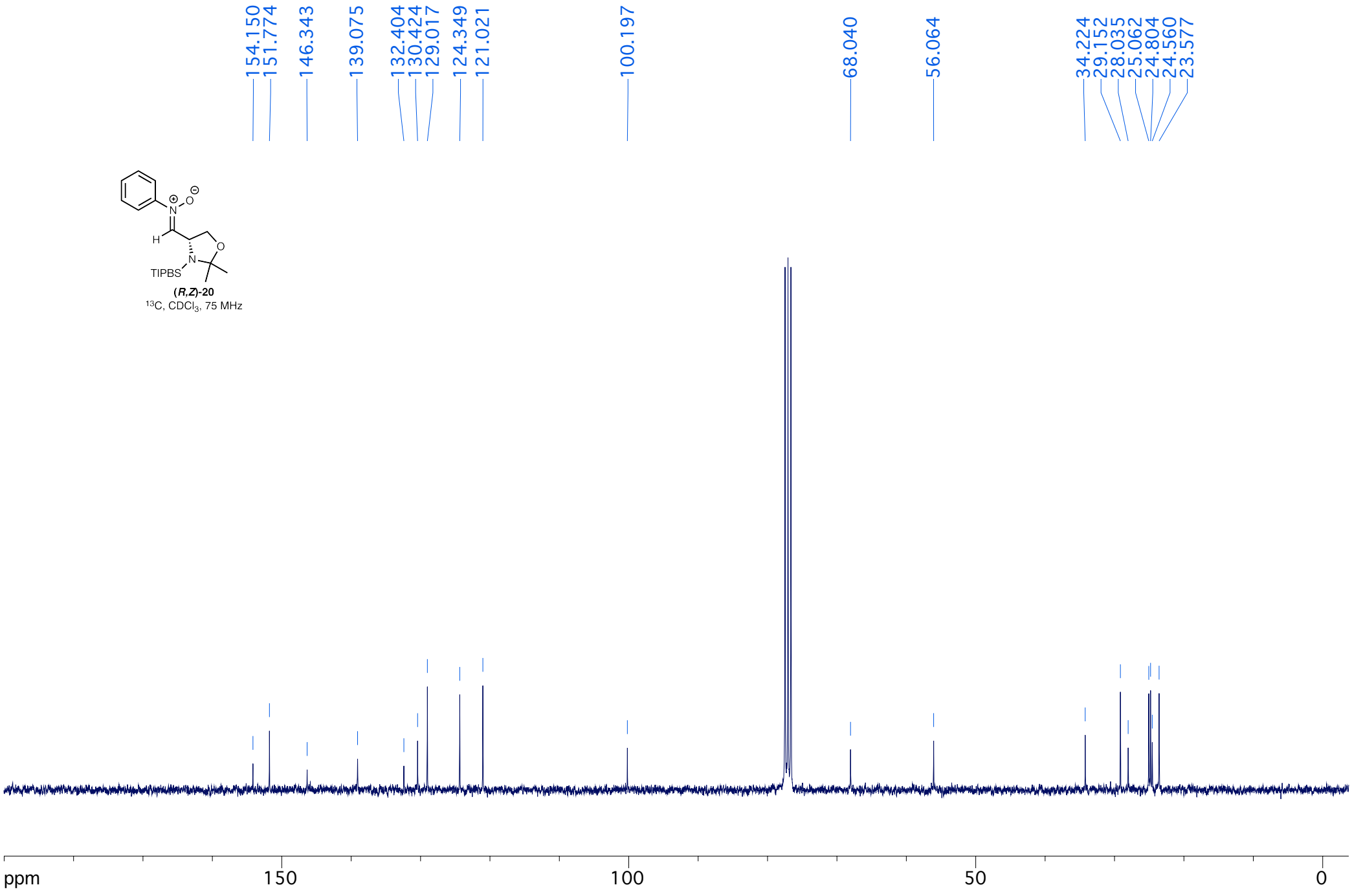
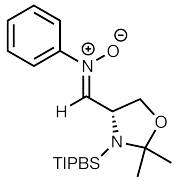
7.334
7.281
7.277
7.254
7.233
7.229
7.206
7.191
7.180
7.163
7.156
6.936
6.935
6.910
6.906
6.611
6.593
4.438
4.428
4.409
4.403
4.397
4.377
4.349
3.913
3.870
3.773
3.760
3.752
3.735
3.410
3.367
1.431
1.273
H
N
O
Bn
(R,Z)-18
1H, CDCl3, 300 MHz
7.17
1
1
1.06
3.06
2.03
2.21
2
1.02
2.92
ppm
10
8
6
4
2
0

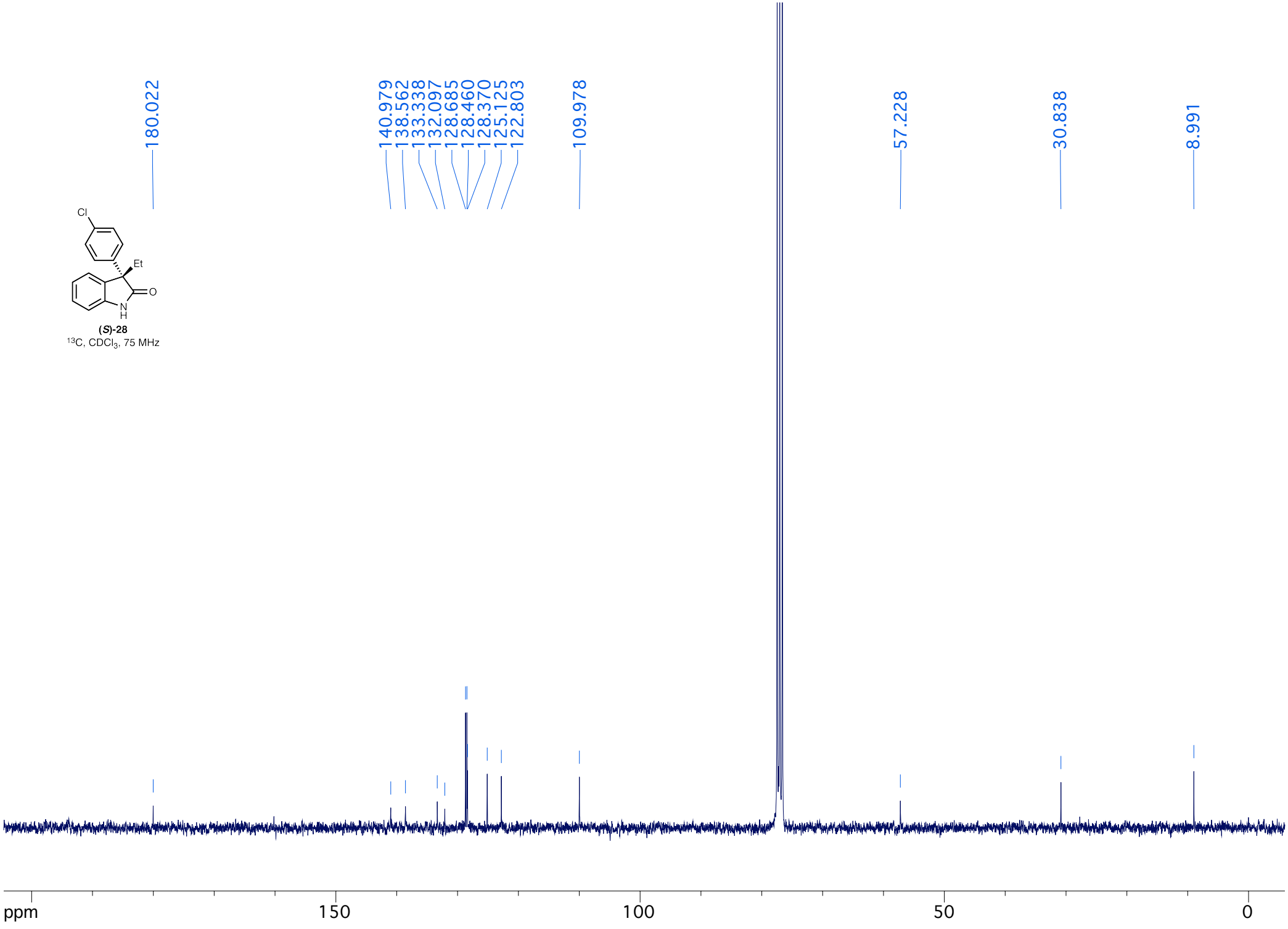

146.995
144.581
138.762
137.748
130.771
130.215
129.394
128.032
121.741
99.043
67.596
56.701
29.170
24.832
21.633
H
N
O
O
N
Ts
(R,Z)-19
13C, CD2Cl2, 125 MHz
ppm
150
100
50
0

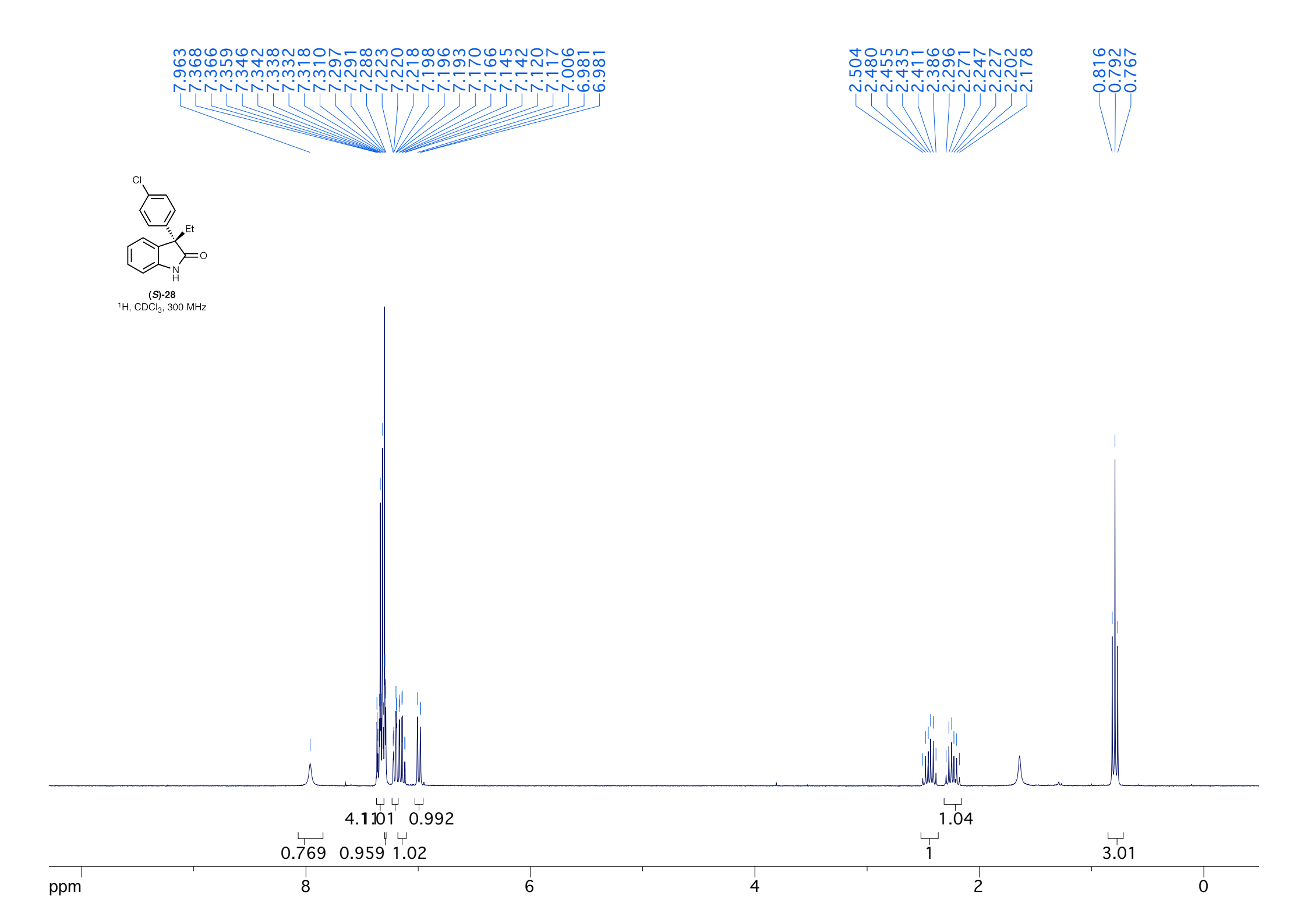

7.802
7.781
7.567
7.563
7.547
7.543
7.457
7.450
7.446
7.431
7.336
7.316
7.290
7.276
5.080
5.073
5.064
5.058
5.049
5.041
4.239
4.222
4.215
4.198
4.139
4.132
4.116
4.109
2.398
1.741
1.558
H
N
O
N
O
Ts
(R,Z)-19
1H, CD2Cl2, 400 MHz
2
2.1
1
1.03
3.08
2.07
2.96
1.08
1.02
3.06
3.01
ppm
8
6
4
2
0

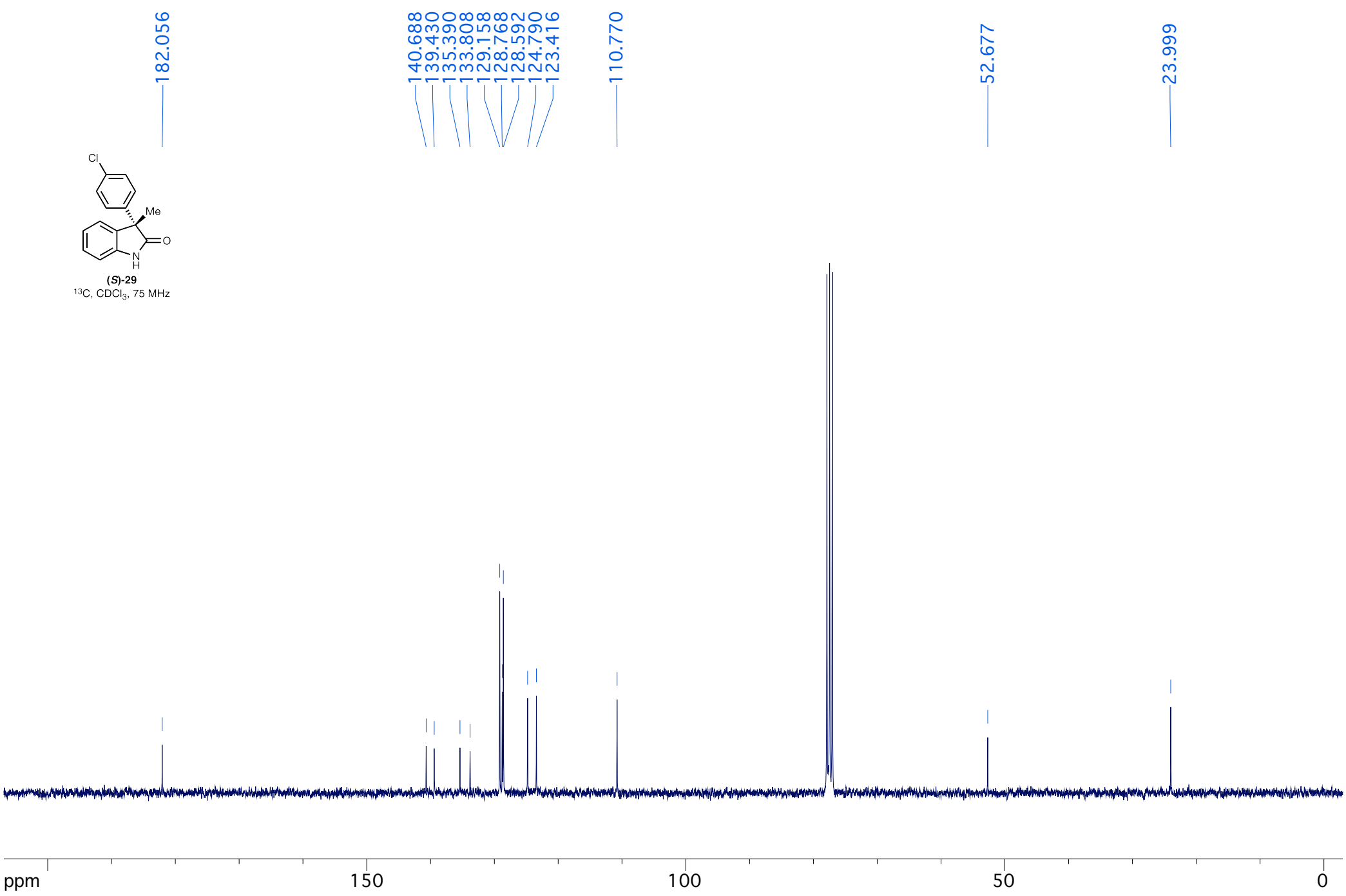

154.150
151.774
146.343
139.075
132.404
130.424
129.017
124.349
121.021
100.197
68.040
56.064
34.224
29.152
28.035
25.062
24.804
24.560
23.577
TIPBS
(R,Z)-20
13C, CDCl3, 75 MHz
ppm
150
100
50
0

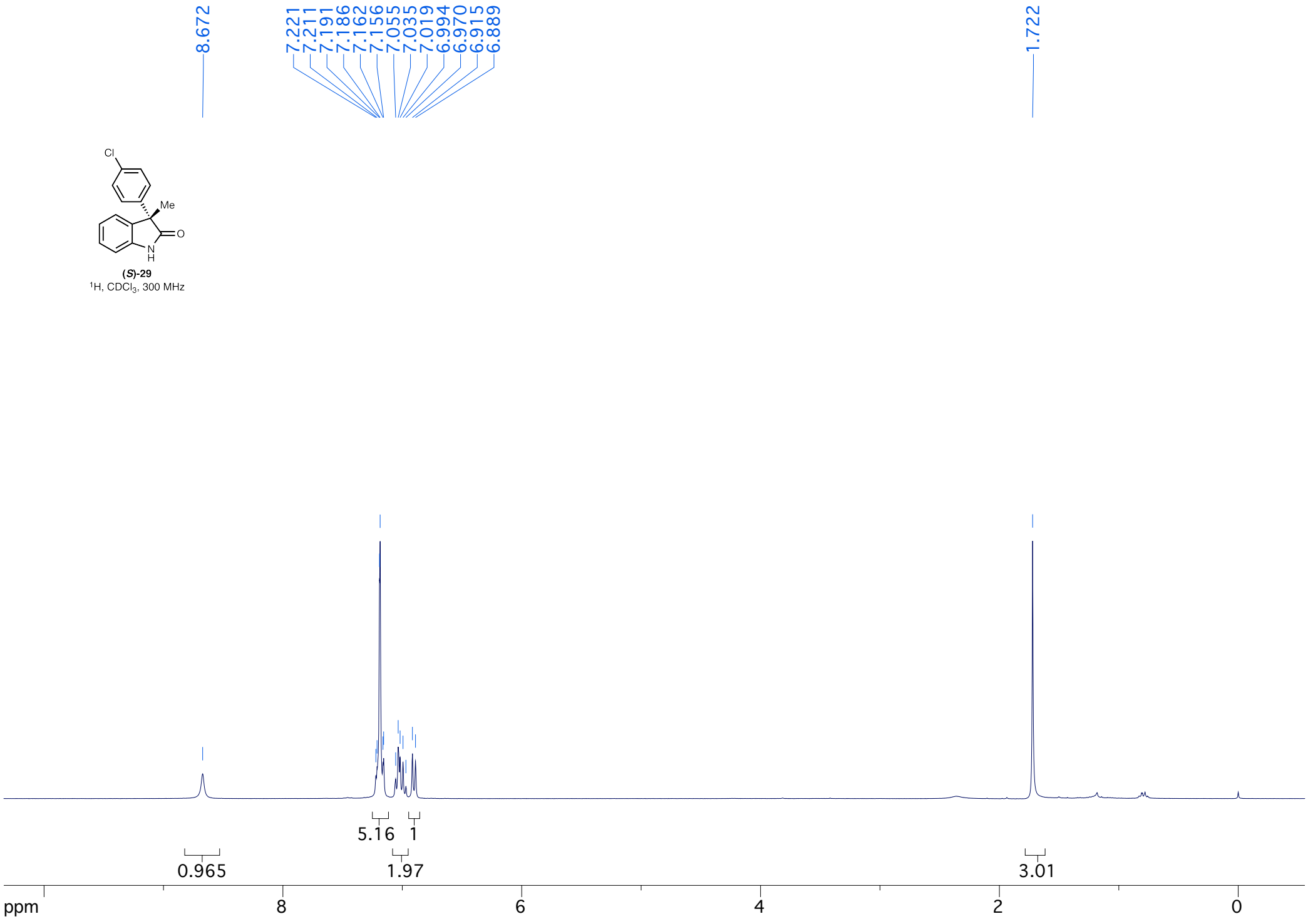


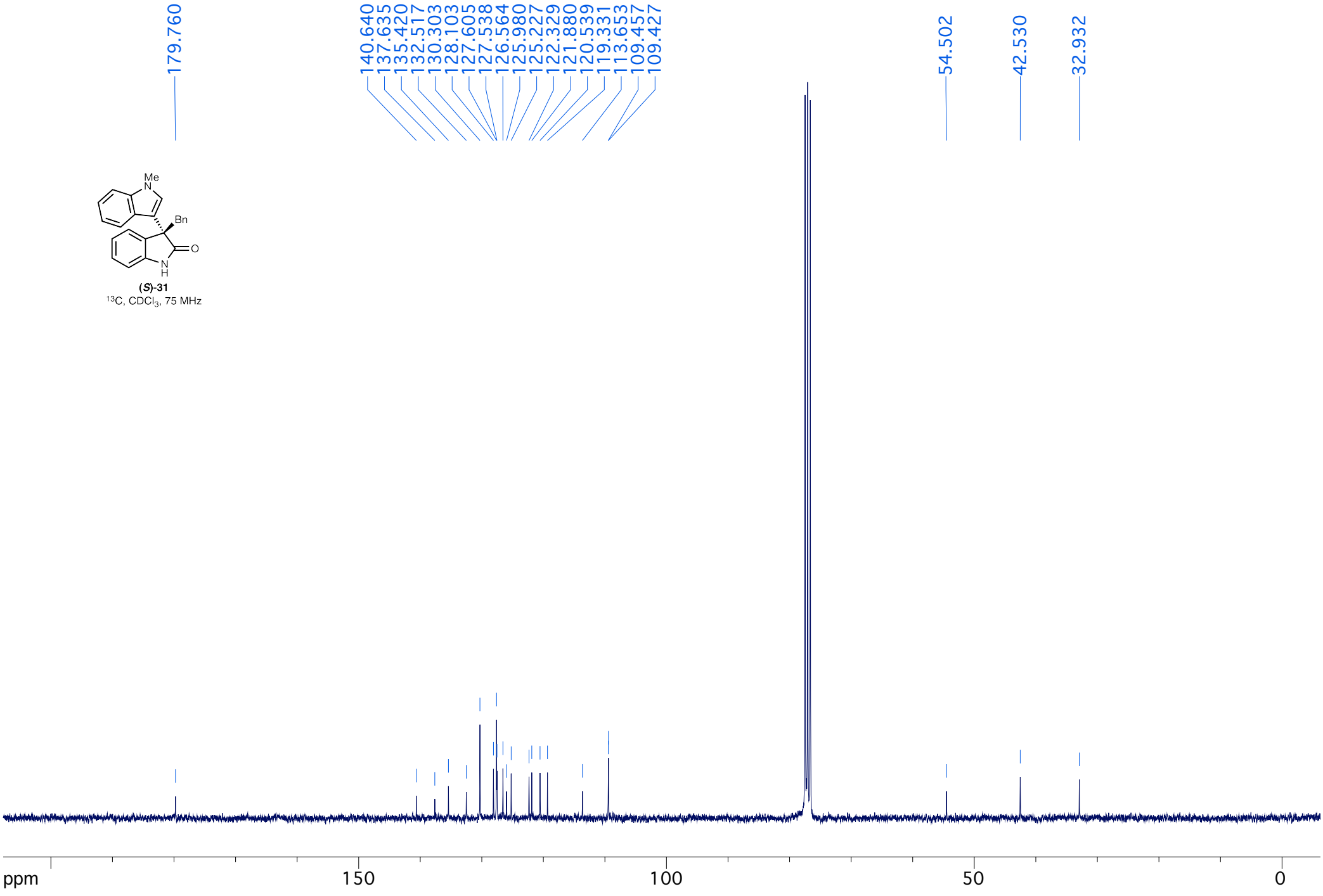
(*R,Z*)-20
^{1}H, $CDCl_3$, 300 MHz

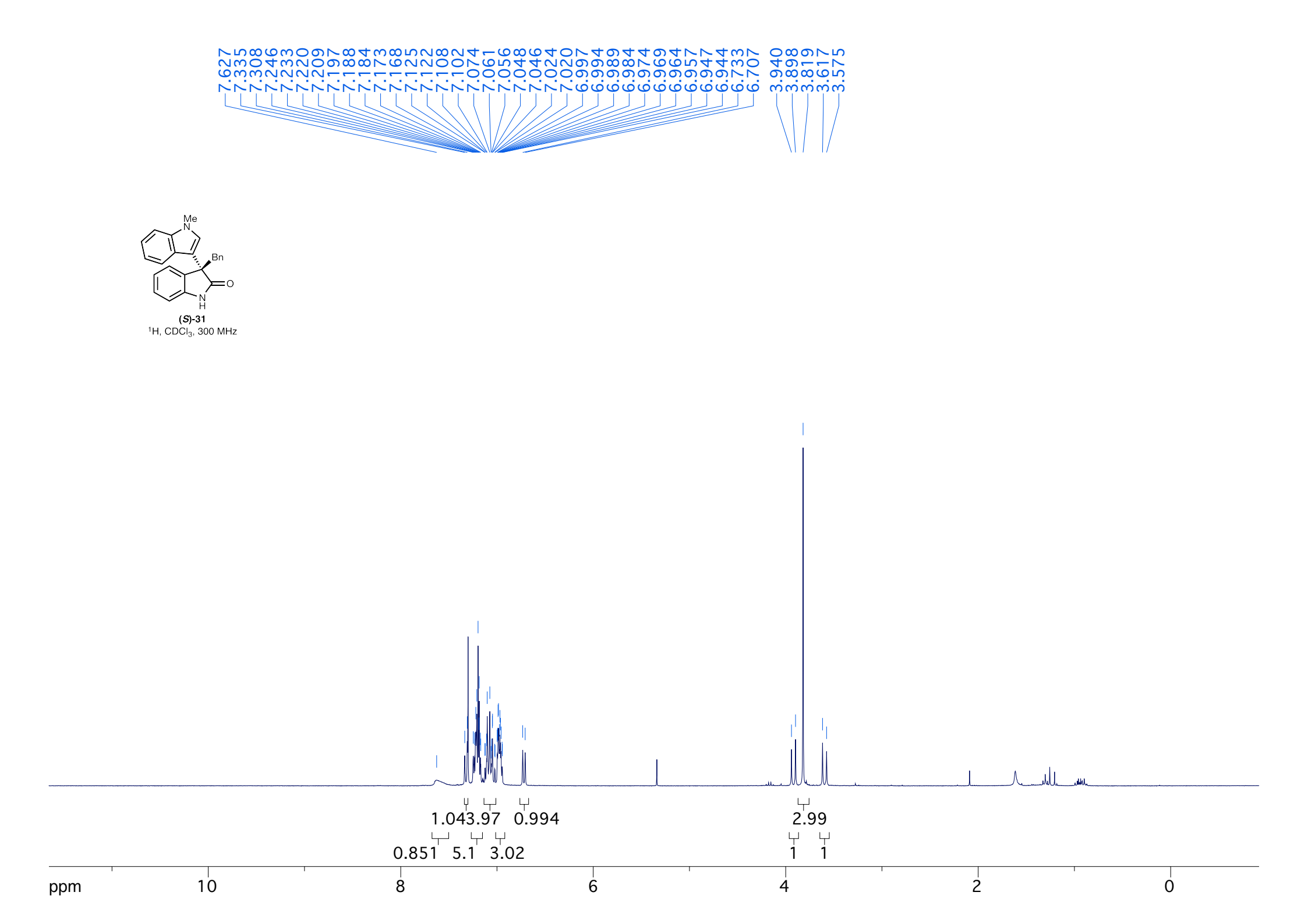

180.022
140.979
138.562
133.338
132.097
128.685
128.460
128.370
125.125
122.803
109.978
57.228
30.838
8.991
Cl
Et
O
N
H
(S)-28
13C, CDCl3, 75 MHz
ppm
150
100
50
0

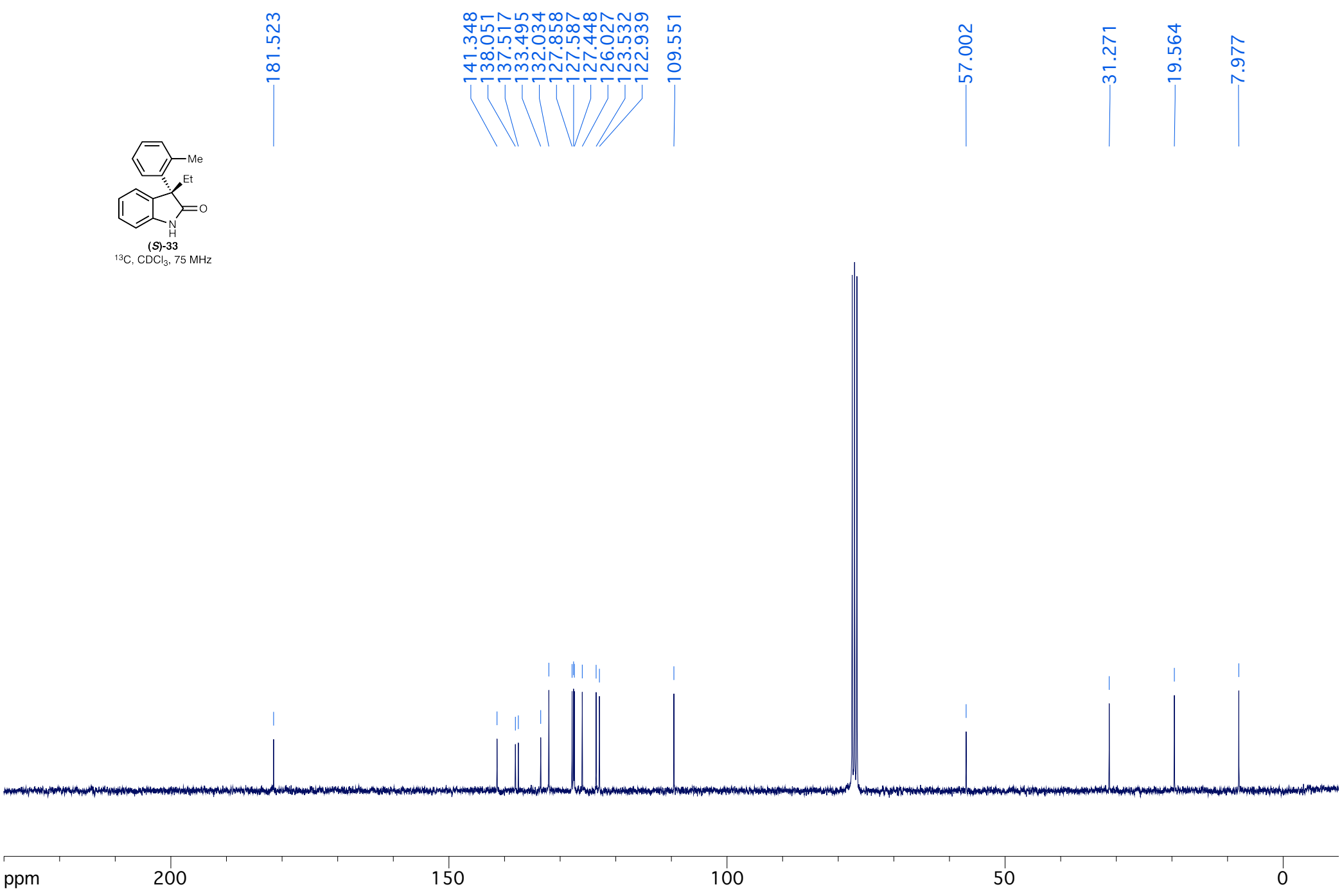

7.963
7.368
7.366
7.359
7.346
7.342
7.338
7.332
7.318
7.310
7.297
7.291
7.288
7.223
7.220
7.218
7.198
7.196
7.193
7.170
7.166
7.145
7.142
7.120
7.117
7.006
6.981
6.981
2.504
2.480
2.455
2.435
2.411
2.386
2.296
2.271
2.247
2.227
2.202
2.178
0.816
0.792
0.767
Cl
Et
O
N
H
(S)-28
1H, CDCl3, 300 MHz
4.11
1.01
0.992
1.04
0.769
0.959
1.02
1
3.01
ppm
8
6
4
2
0

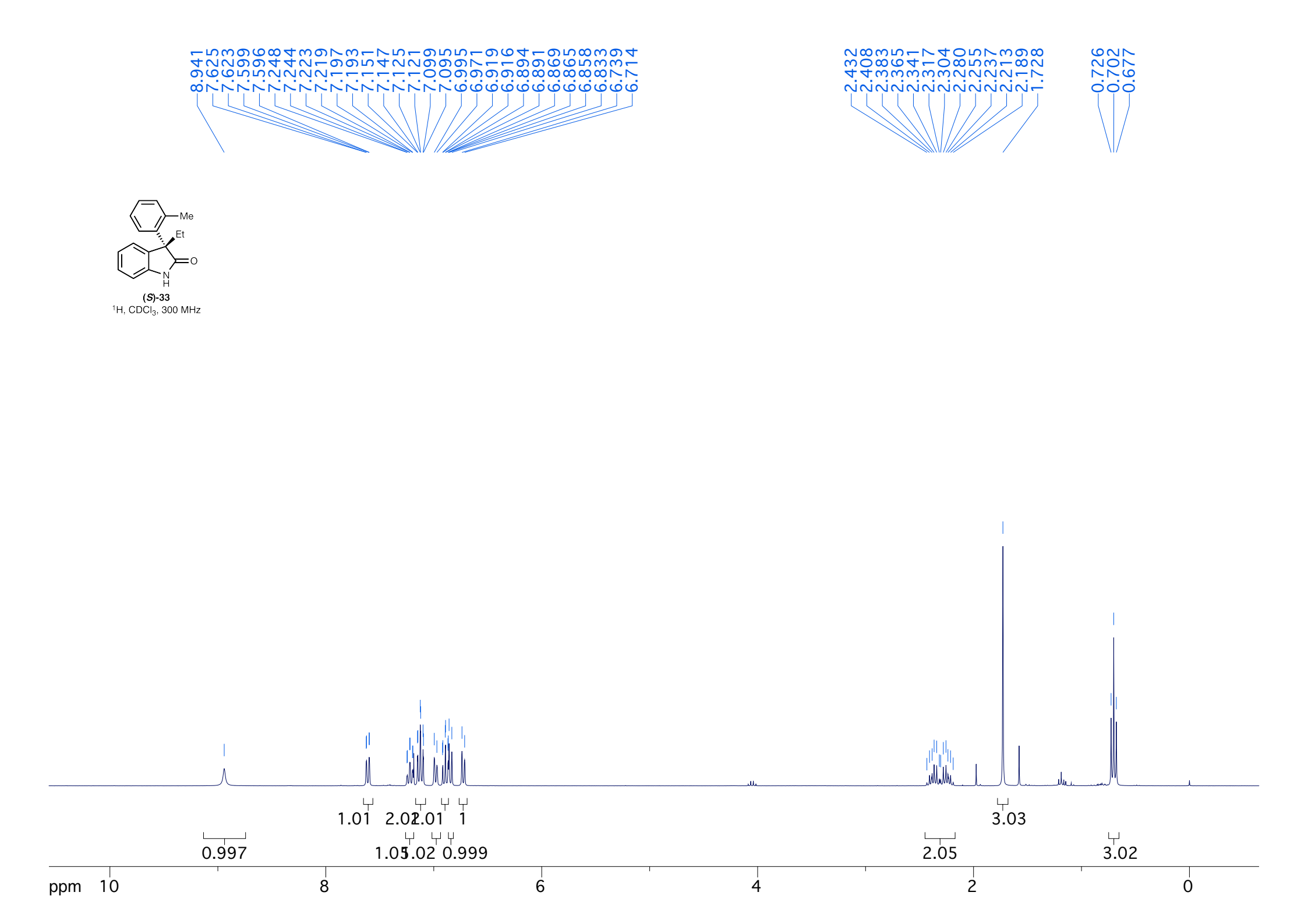

182.056
140.688
139.430
135.390
133.808
129.158
128.768
128.592
124.790
123.416
110.770
52.677
23.999
Cl
Me
O
N
H
(S)-29
13C, CDCl3, 75 MHz
ppm
150
100
50
0

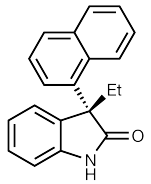

8.672
7.221
7.211
7.191
7.186
7.162
7.156
7.055
7.035
7.019
6.994
6.970
6.915
6.889
1.722
Cl
Me
O
N
H
(S)-29
1H, CDCl3, 300 MHz
5.16
1
0.965
1.97
3.01
ppm
8
6
4
2
0


179.760
140.640
137.635
135.420
132.517
130.303
128.103
127.605
127.538
126.564
125.980
125.227
122.329
121.880
120.539
119.331
113.653
109.457
109.427
54.502
42.530
32.932
Me
N
Bn
O
N
H
(S)-31
13C, CDCl3, 75 MHz
ppm
150
100
50
0


7.627
7.335
7.308
7.246
7.233
7.220
7.209
7.197
7.188
7.184
7.173
7.168
7.125
7.122
7.108
7.102
7.074
7.061
7.056
7.048
7.046
7.024
7.020
6.997
6.994
6.989
6.984
6.974
6.969
6.964
6.957
6.947
6.944
6.733
6.707
3.940
3.898
3.819
3.617
3.575
Me
N
Bn
O
N
H
(S)-31
1H, CDCl3, 300 MHz
1.043.97 0.994
2.99
0.851 5.1 3.02
1 1
ppm
10
8
6
4
2
0


181.523
141.348
138.051
137.517
133.495
132.034
127.858
127.587
127.448
126.027
123.532
122.939
109.551
57.002
31.271
19.564
7.977
Me
Et
O
N
H
(S)-33
13C, CDCl3, 75 MHz
ppm
200
150
100
50
0


8.941
7.625
7.623
7.599
7.596
7.248
7.244
7.223
7.219
7.197
7.193
7.151
7.147
7.125
7.121
7.099
7.095
6.995
6.971
6.919
6.916
6.894
6.891
6.869
6.865
6.858
6.833
6.739
6.714
2.432
2.408
2.383
2.365
2.341
2.317
2.304
2.280
2.255
2.237
2.213
2.189
1.728
0.726
0.702
0.677
Me
Et
O
N
H
(S)-33
1H, CDCl3, 300 MHz
1.01
2.02
2.01
1
3.03
0.997
1.05
1.02
0.999
2.05
3.02
ppm
10
8
6
4
2
0

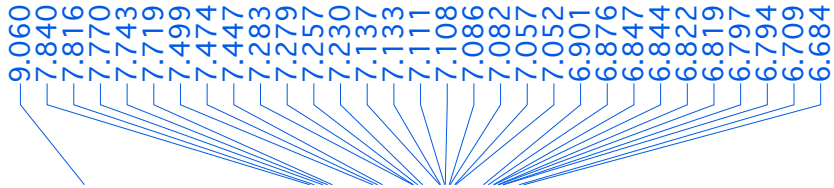


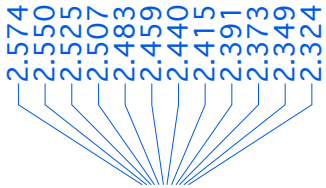
(*S*)-35

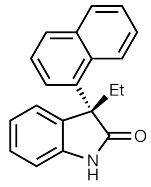
^{13}C, $CDCl_3$, 75 MHz

182.074
140.539
135.300
135.167
134.551
131.792
129.181
127.957
126.370
126.160
125.343
125.117
123.633
123.532
123.075
110.129
57.004
32.068
8.052

ppm 150 100 50 0

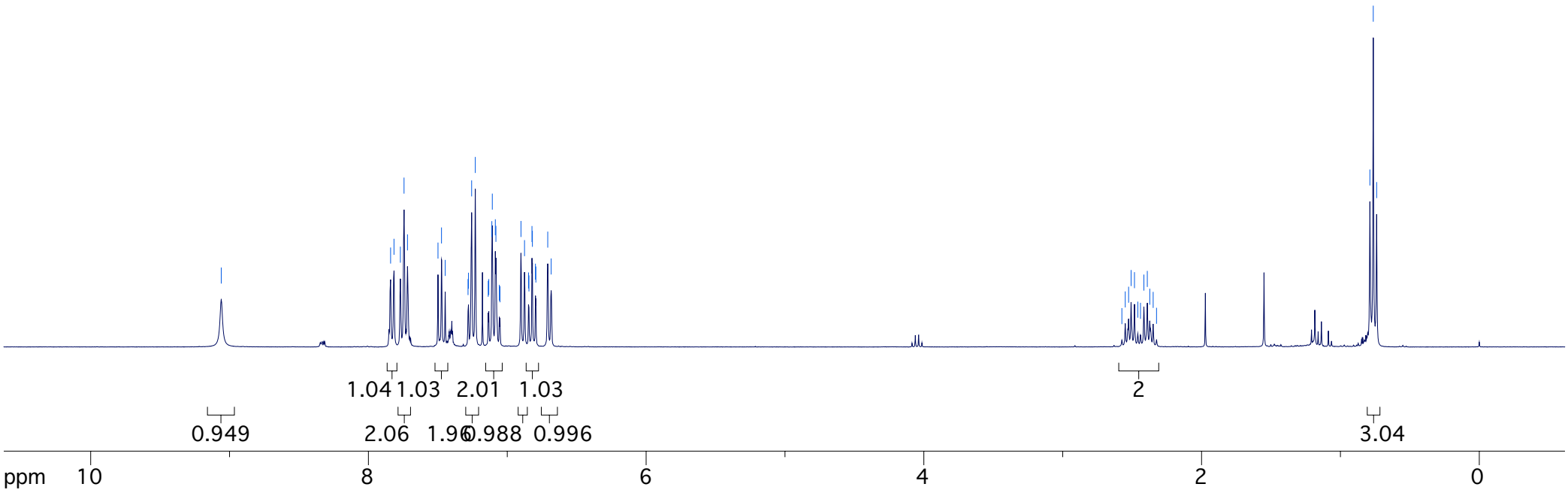


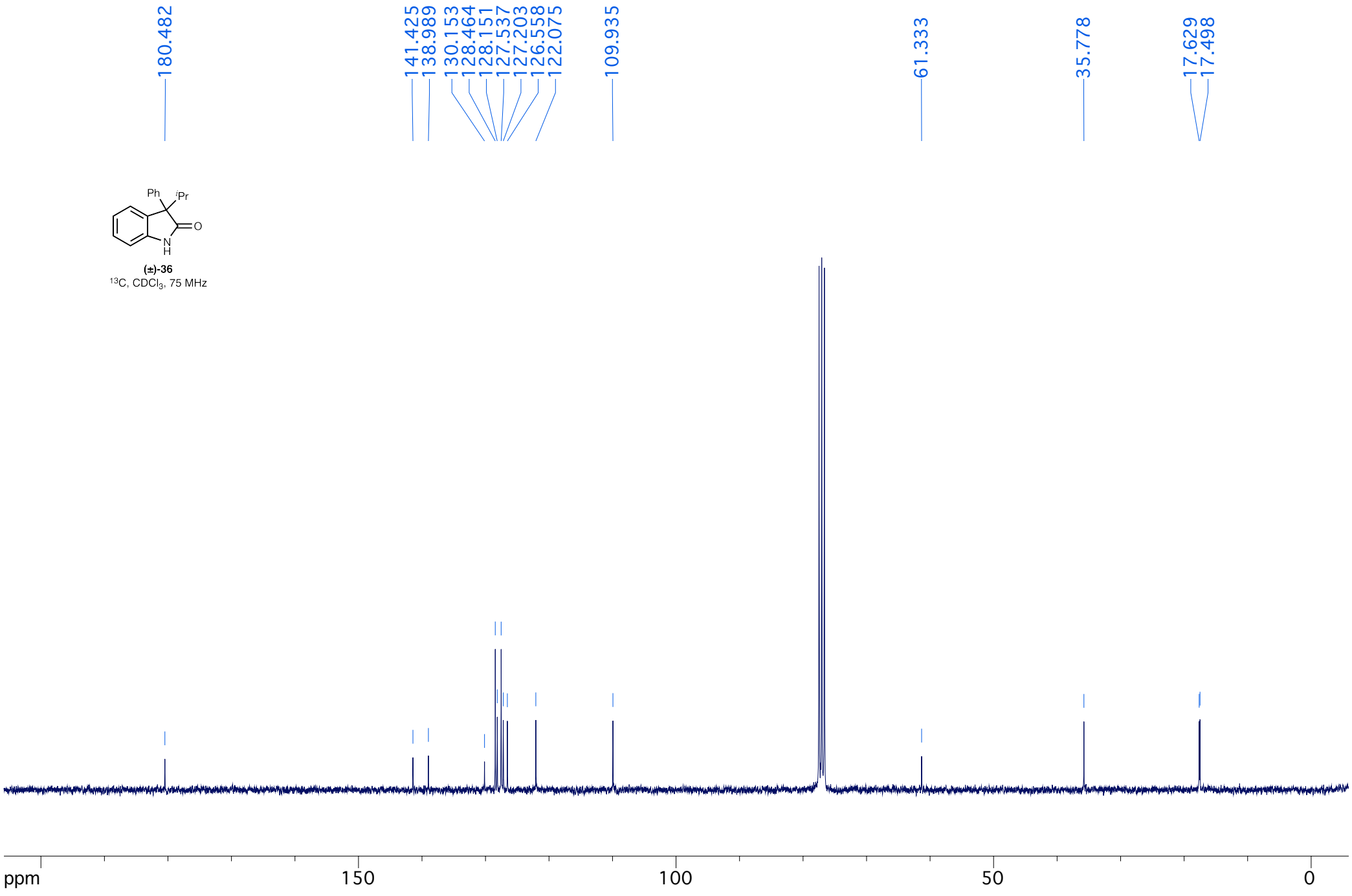


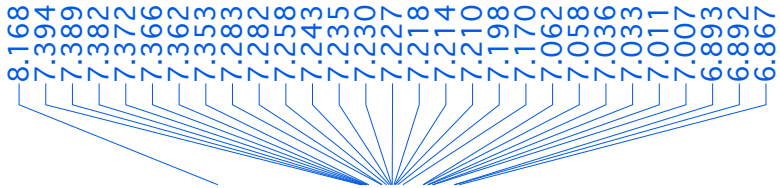


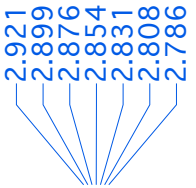
(*S*)-35

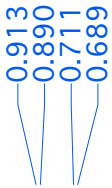
^{1}H, $CDCl_3$, 300 MHz

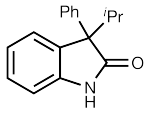



180.482
141.425
138.989
130.153
128.464
128.151
127.537
127.203
126.558
122.075
109.935
61.333
35.778
17.629
17.498
Ph
iPr
O
N
H
(±)-36
13C, CDCl3, 75 MHz
ppm
150
100
50
0

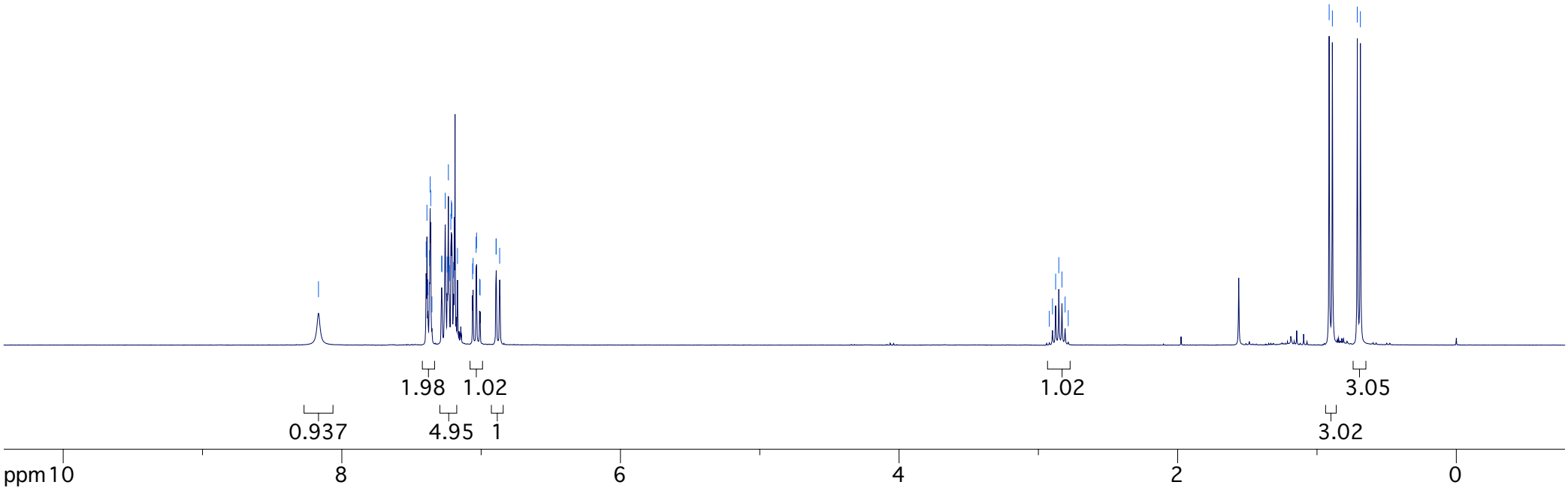


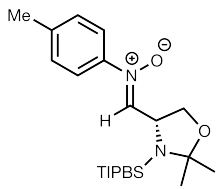






(±)-36
^{1}H, $CDCl_3$, 300 MHz

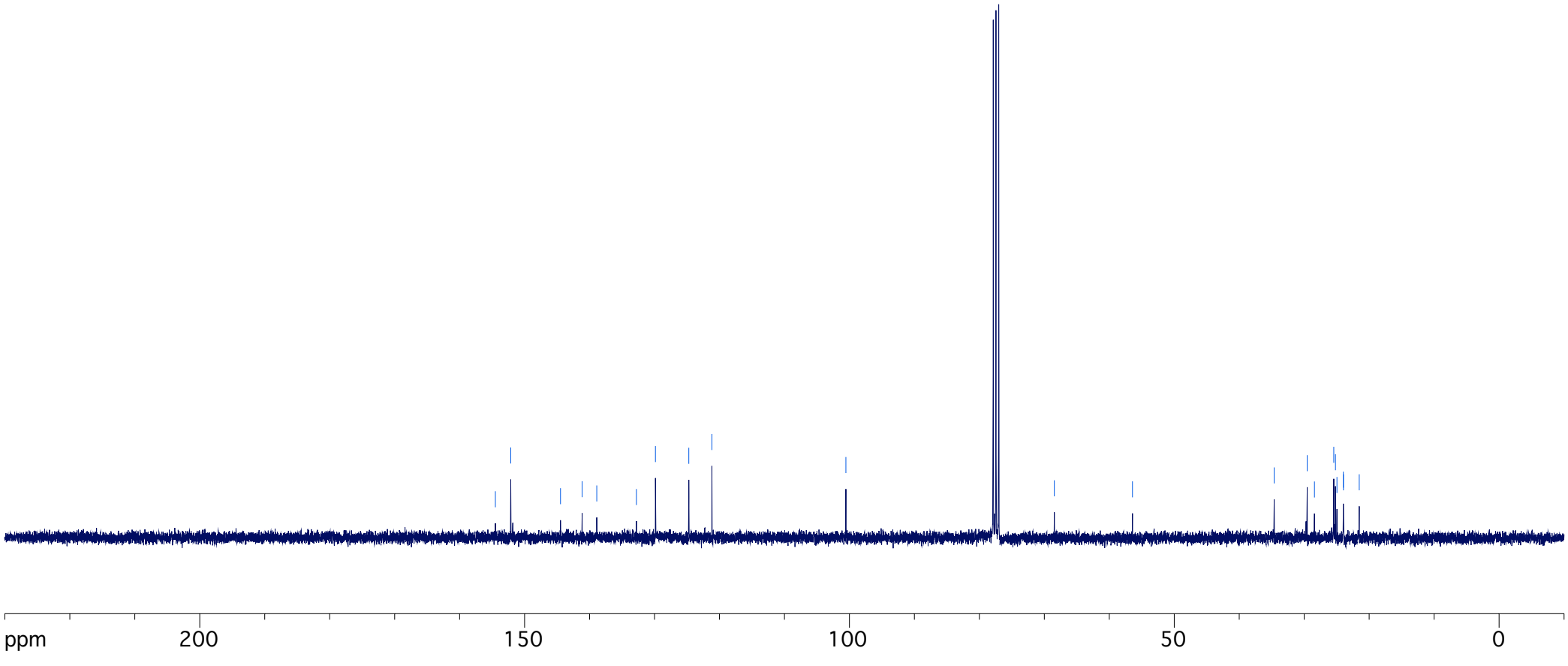


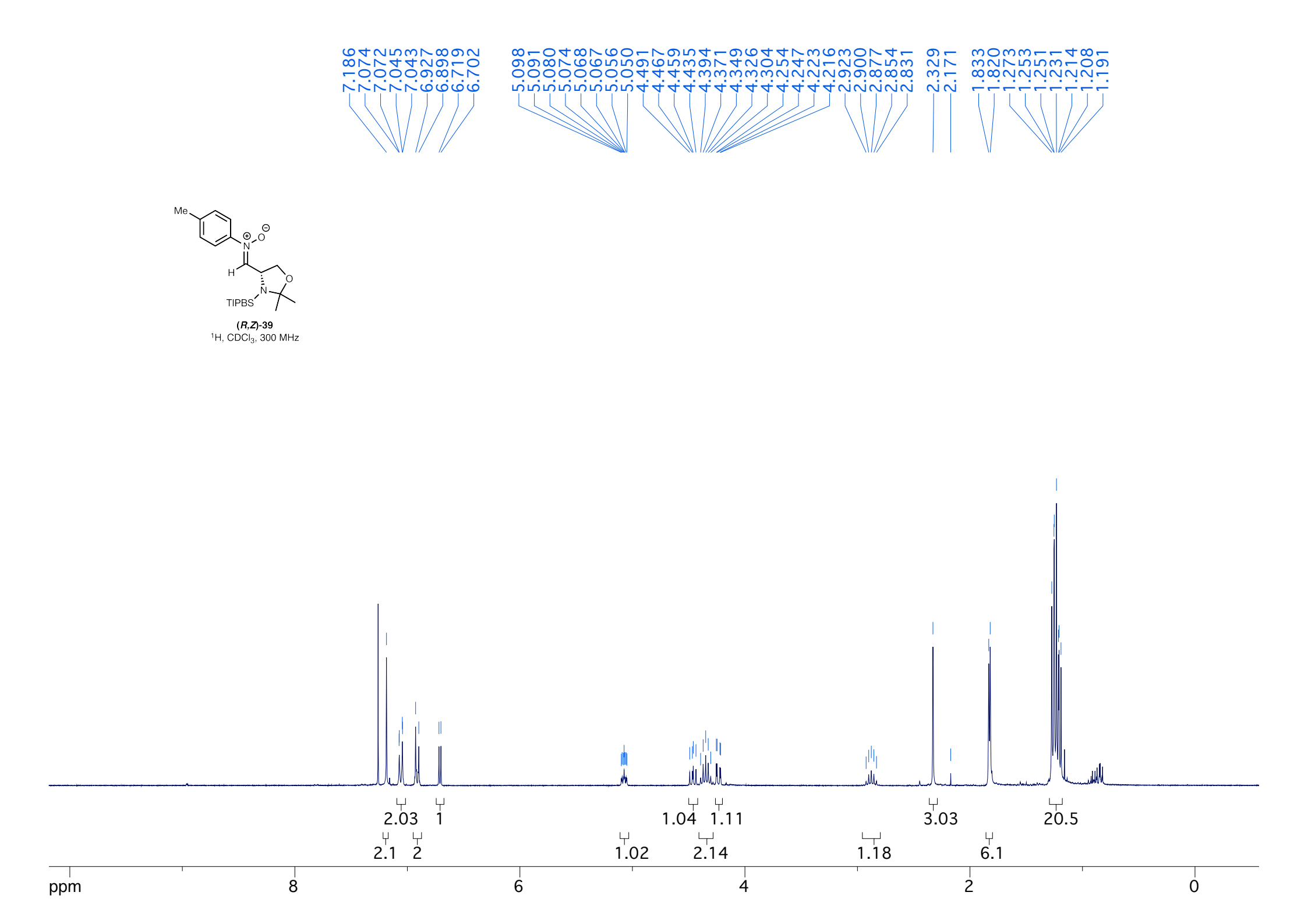


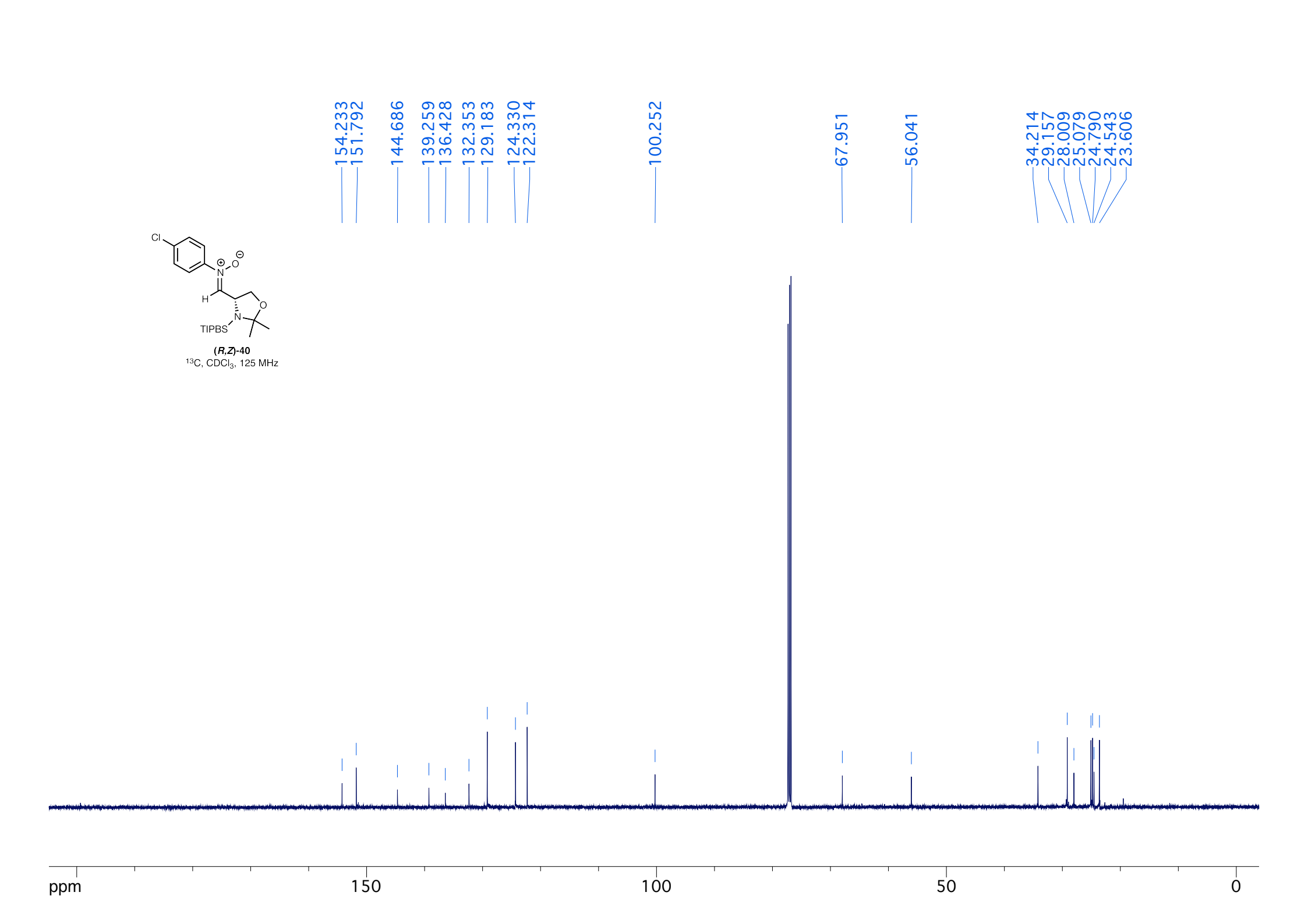
(*R*,*Z*)-39

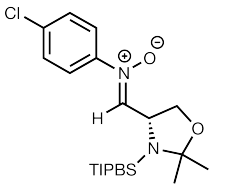
^{13}C, $CDCl_3$, 75 MHz

154.498
152.129
144.472
141.140
138.889
132.788
129.860
124.722
121.168
100.544
68.460
56.433
34.618
29.537
28.421
25.446
25.186
24.957
23.977
23.960
21.528




7.186
7.074
7.072
7.045
7.043
6.927
6.898
6.719
6.702
5.098
5.091
5.080
5.074
5.068
5.067
5.056
5.050
4.491
4.467
4.459
4.435
4.394
4.371
4.349
4.326
4.304
4.254
4.247
4.223
4.216
2.923
2.900
2.877
2.854
2.831
2.329
2.171
1.833
1.820
1.273
1.253
1.251
1.231
1.214
1.208
1.191
Me
N
O
H
O
N
TIPBS
(R,Z)-39
1H, CDCl3, 300 MHz
2.03
1
1.04
1.11
3.03
20.5
2.1
2
1.02
2.14
1.18
6.1
ppm
8
6
4
2
0


154.233
151.792
144.686
139.259
136.428
132.353
129.183
124.330
122.314
100.252
67.951
56.041
34.214
29.157
28.009
25.079
24.790
24.543
23.606
Cl
N
O
H
O
N
TIPBS
(R,Z)-40
13C, CDCl3, 125 MHz
ppm
150
100
50
0



(*R*,*Z*)-40

^{1}H, $CDCl_3$, 500 MHz

7.296 7.280 7.219 7.037 7.019 6.760 6.749

5.110 5.099 5.088 4.510 4.495 4.493 4.491 4.476 4.403 4.390 4.376 4.363 4.349 4.259 4.256 4.240 4.237

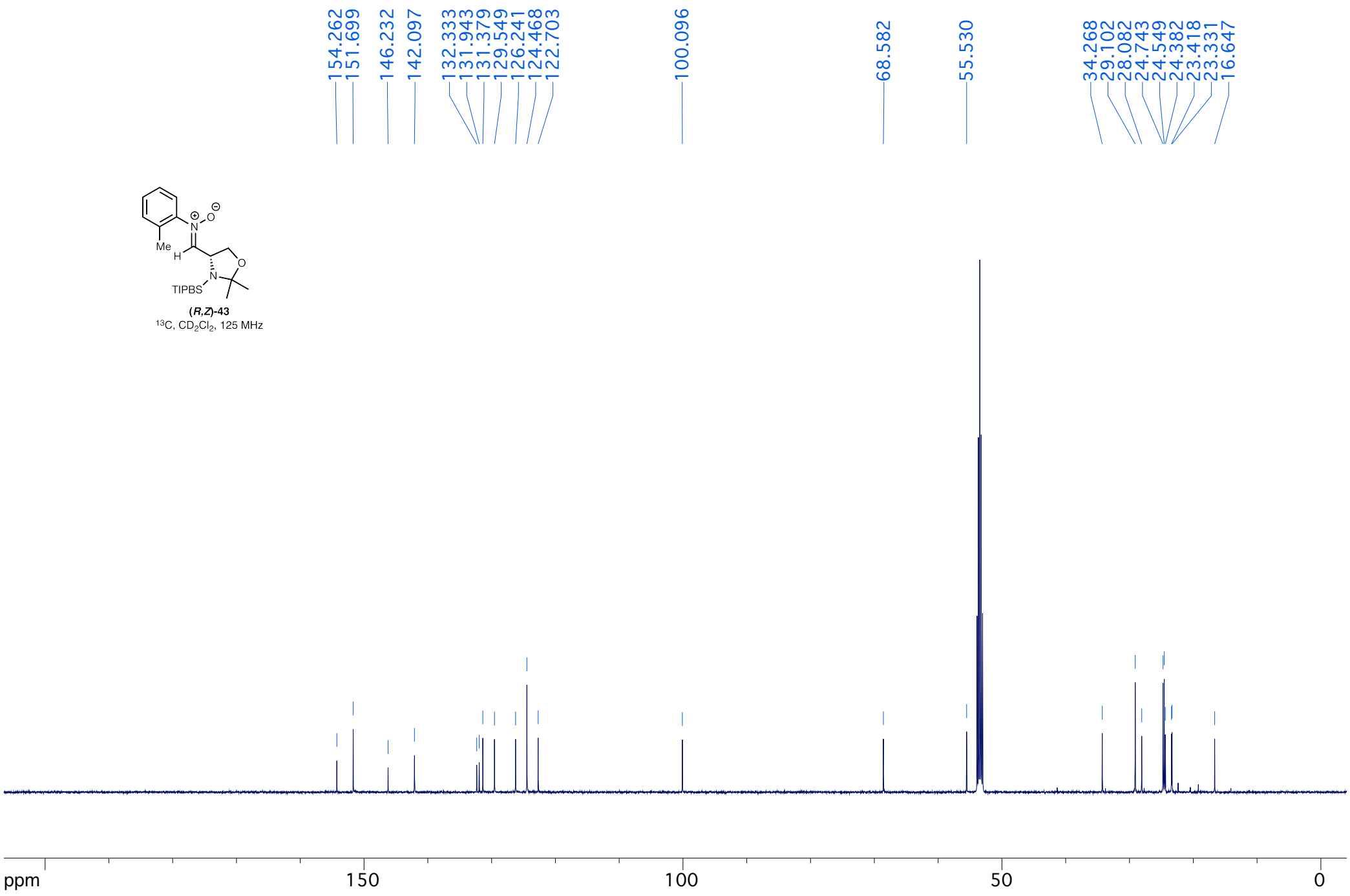
2.941 2.927 2.913 2.900 2.886

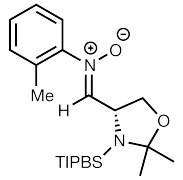
1.869 1.851 1.300 1.287 1.280 1.266 1.261 1.246 1.230

2.08 1 1.04 1.12 6.11

2.24 2.05 1.02 2.06 1.15 19.5

ppm 9 8 7 6 5 4 3 2 1 0


154.262
151.699
146.232
142.097
132.333
131.943
131.379
129.549
126.241
124.468
122.703
100.096
68.582
55.530
34.268
29.102
28.082
24.743
24.549
24.382
23.418
23.331
16.647
Me
H
N
O
O
N
TIPBS
(R,Z)-43
13C, CD2Cl2, 125 MHz
ppm
150
100
50
0



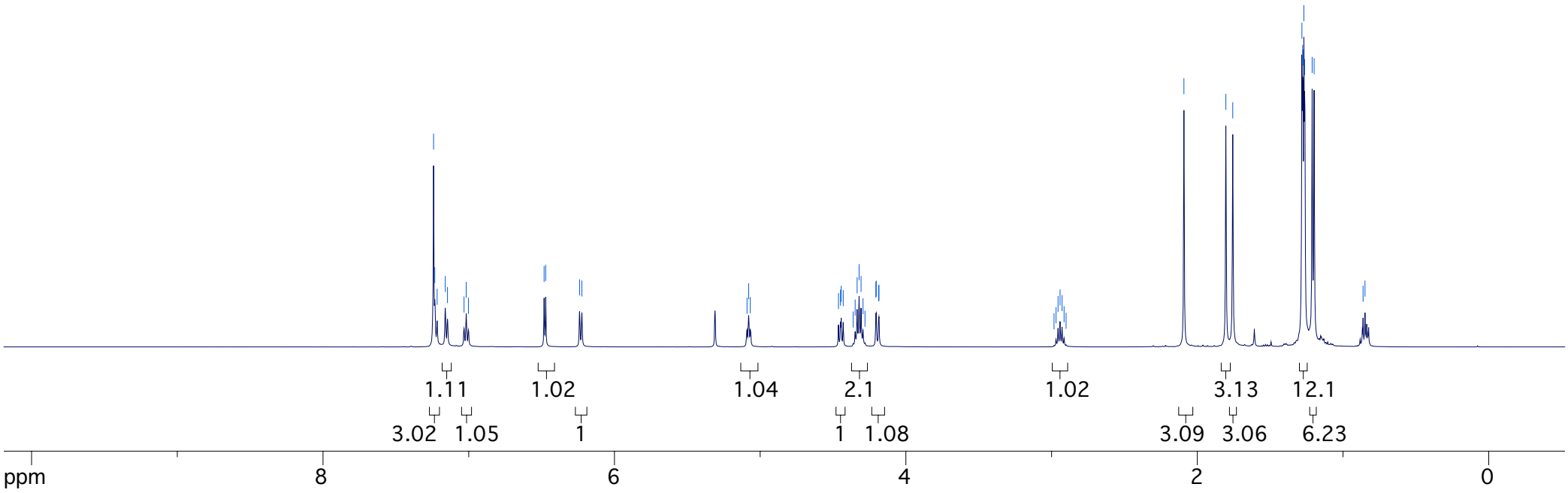
(*R*,*Z*)-43

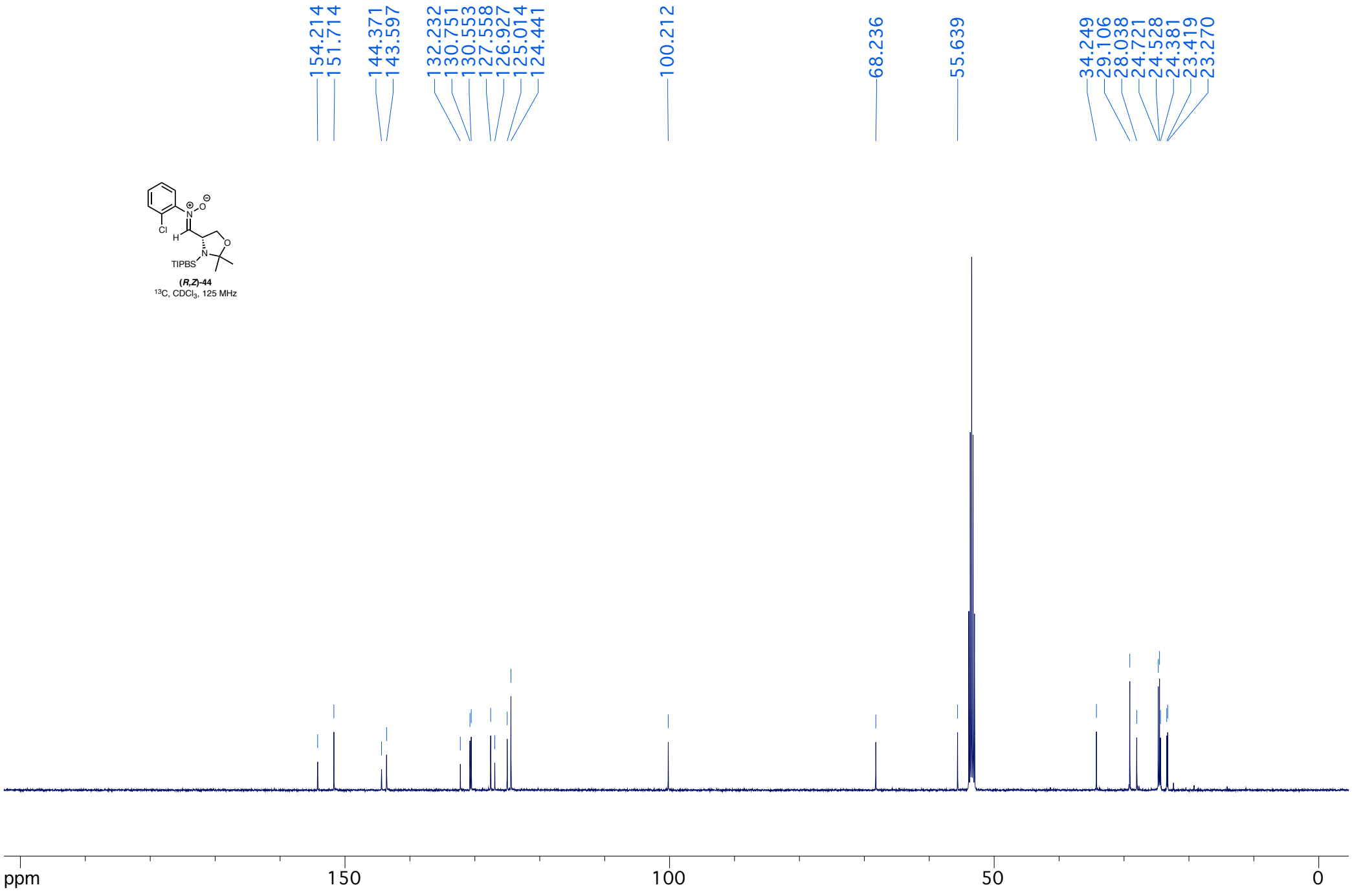
^{1}H, CD_2Cl_2, 500 MHz

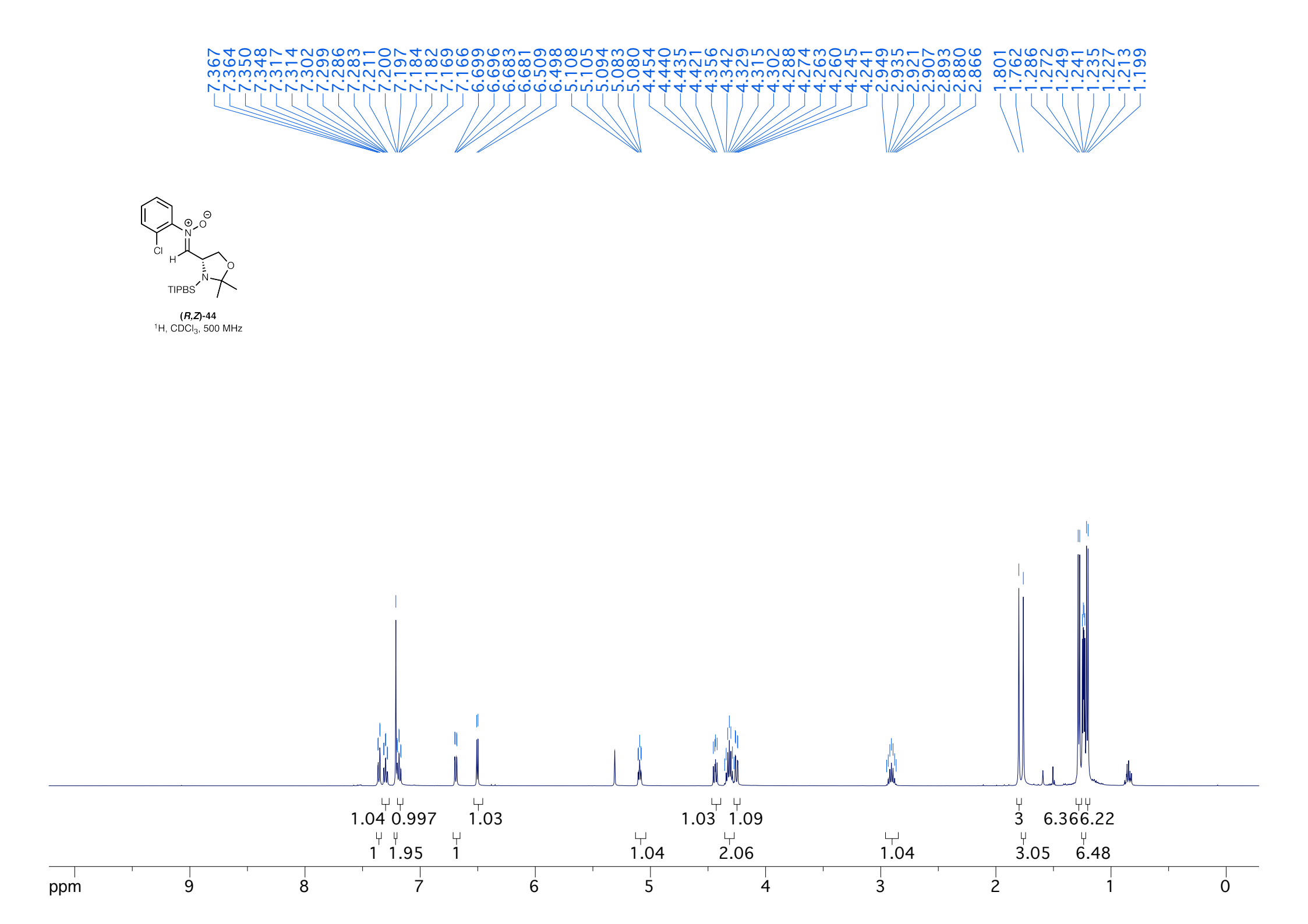
7.241 7.233 7.217 7.161 7.146 7.032 7.017 7.002 6.483 6.472 6.239 6.224

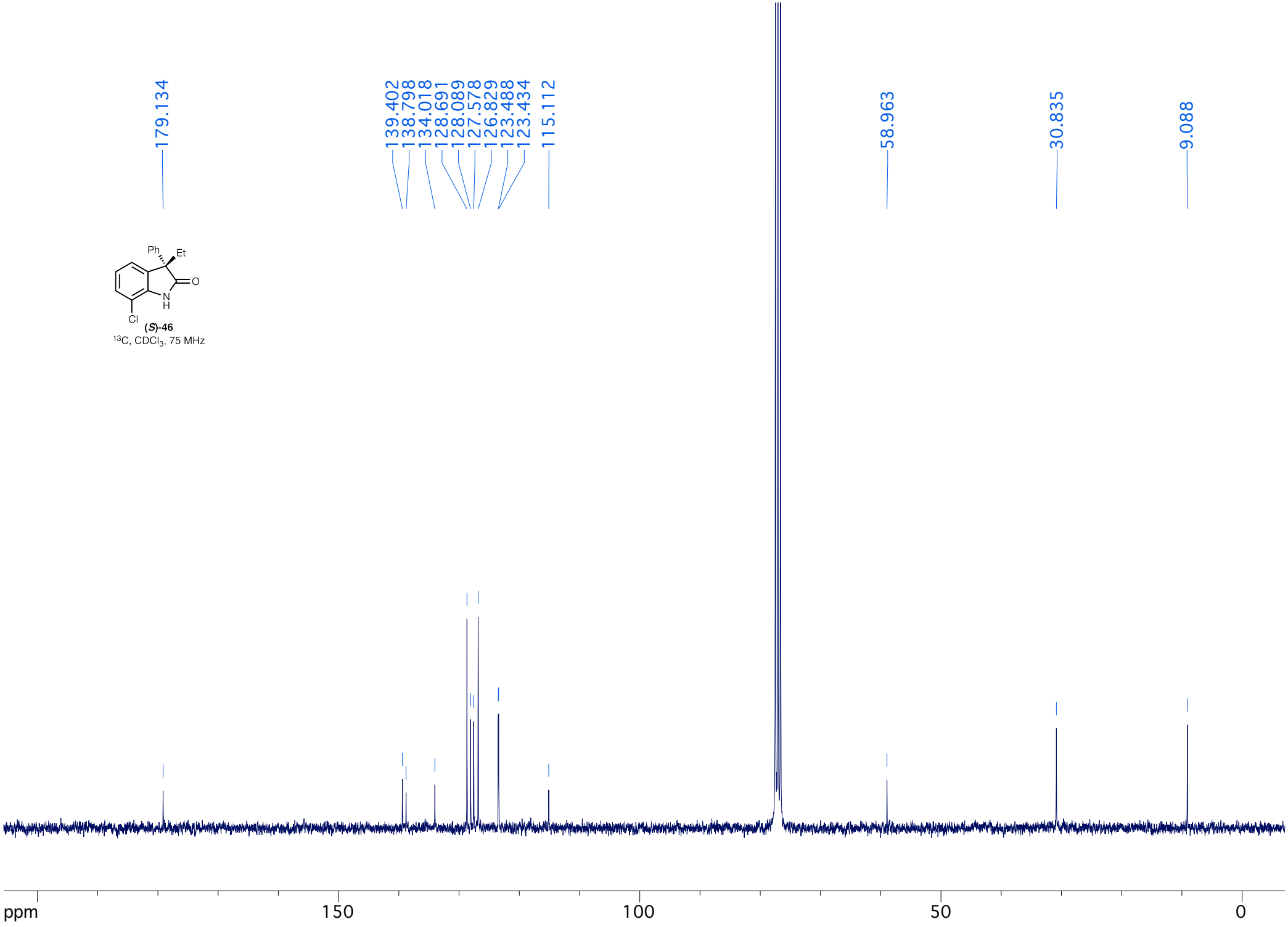
5.090 5.079 5.068 4.463 4.449 4.444 4.430 4.361 4.348 4.335 4.321 4.308 4.294 4.281 4.206 4.203 4.187 4.185 2.983 2.970 2.956 2.942 2.928 2.914 2.901

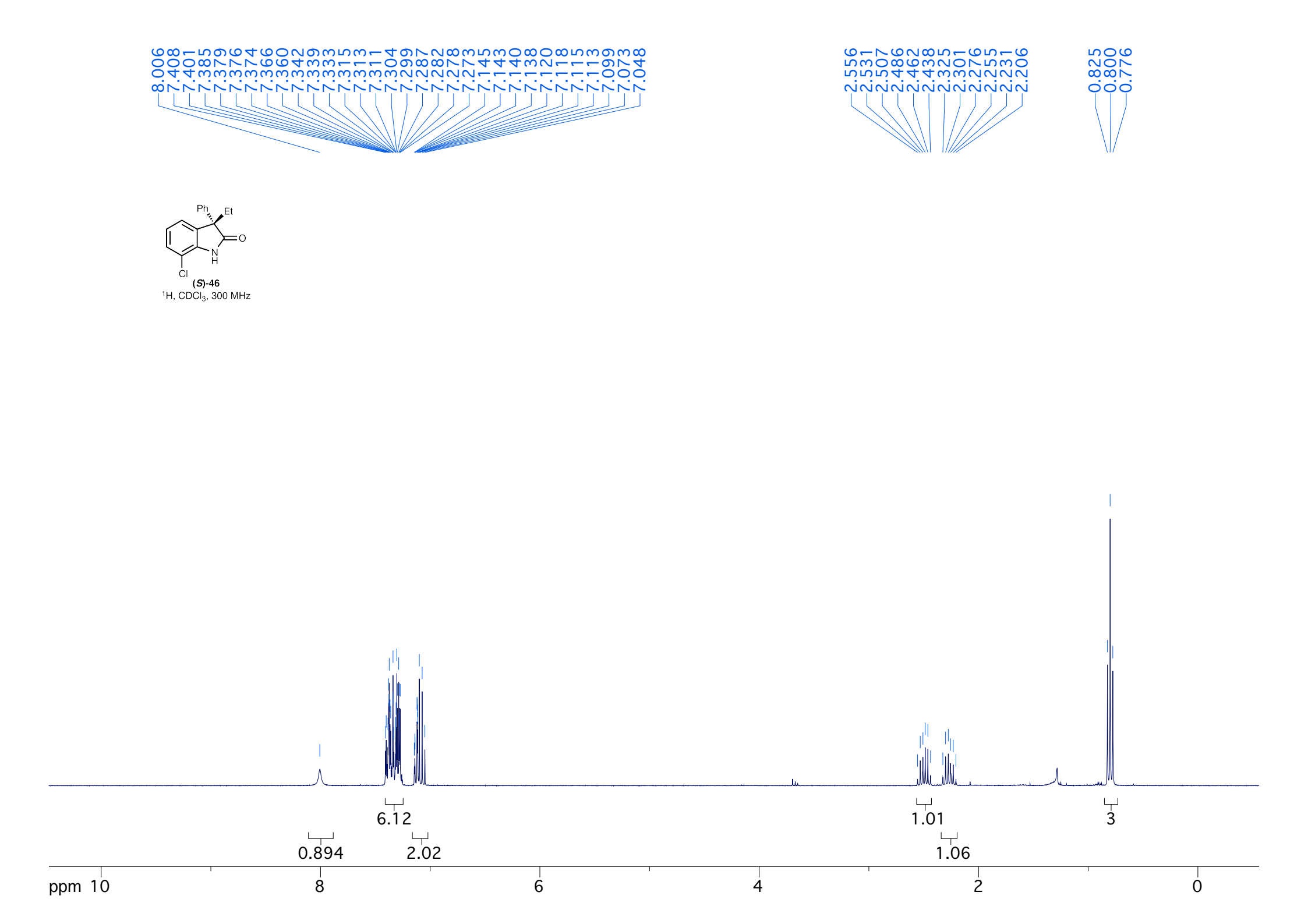
2.092 1.804 1.757 1.282 1.278 1.276 1.269 1.264 1.212 1.198 0.862 0.849

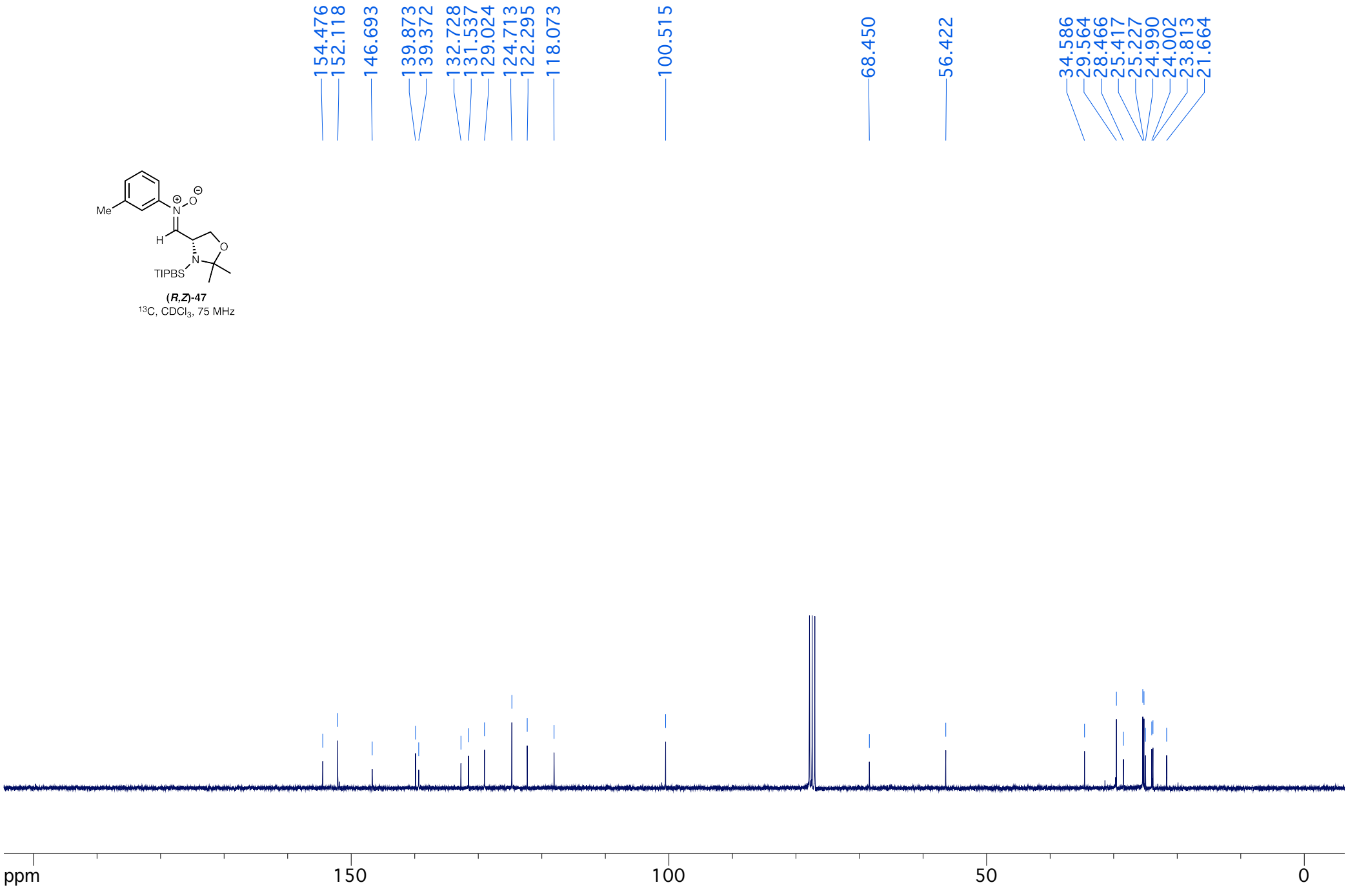



154.214
151.714
144.371
143.597
132.232
130.751
130.553
127.558
126.927
125.014
124.441
100.212
68.236
55.639
34.249
29.106
28.038
24.721
24.528
24.381
23.419
23.270
Cl
H
N
O
O
N
TIPBS
O
(R,Z)-44
13C, CDCl3, 125 MHz
ppm
150
100
50
0


7.367
7.364
7.350
7.348
7.317
7.314
7.302
7.299
7.286
7.283
7.211
7.200
7.197
7.184
7.182
7.169
7.166
6.699
6.696
6.683
6.681
6.509
6.498
5.108
5.105
5.094
5.083
5.080
4.454
4.440
4.435
4.421
4.356
4.342
4.329
4.315
4.302
4.288
4.274
4.263
4.260
4.245
4.241
2.949
2.935
2.921
2.907
2.893
2.880
2.866
1.801
1.762
1.286
1.272
1.249
1.241
1.235
1.227
1.213
1.199
Cl
H
N
O
O
N
TIPBS
(R,Z)-44
1H, CDCl3, 500 MHz
1.04
0.997
1.03
1.03
1.09
3
6.36
6.22
1
1.95
1
1.04
2.06
1.04
3.05
6.48
ppm
9
8
7
6
5
4
3
2
1
0

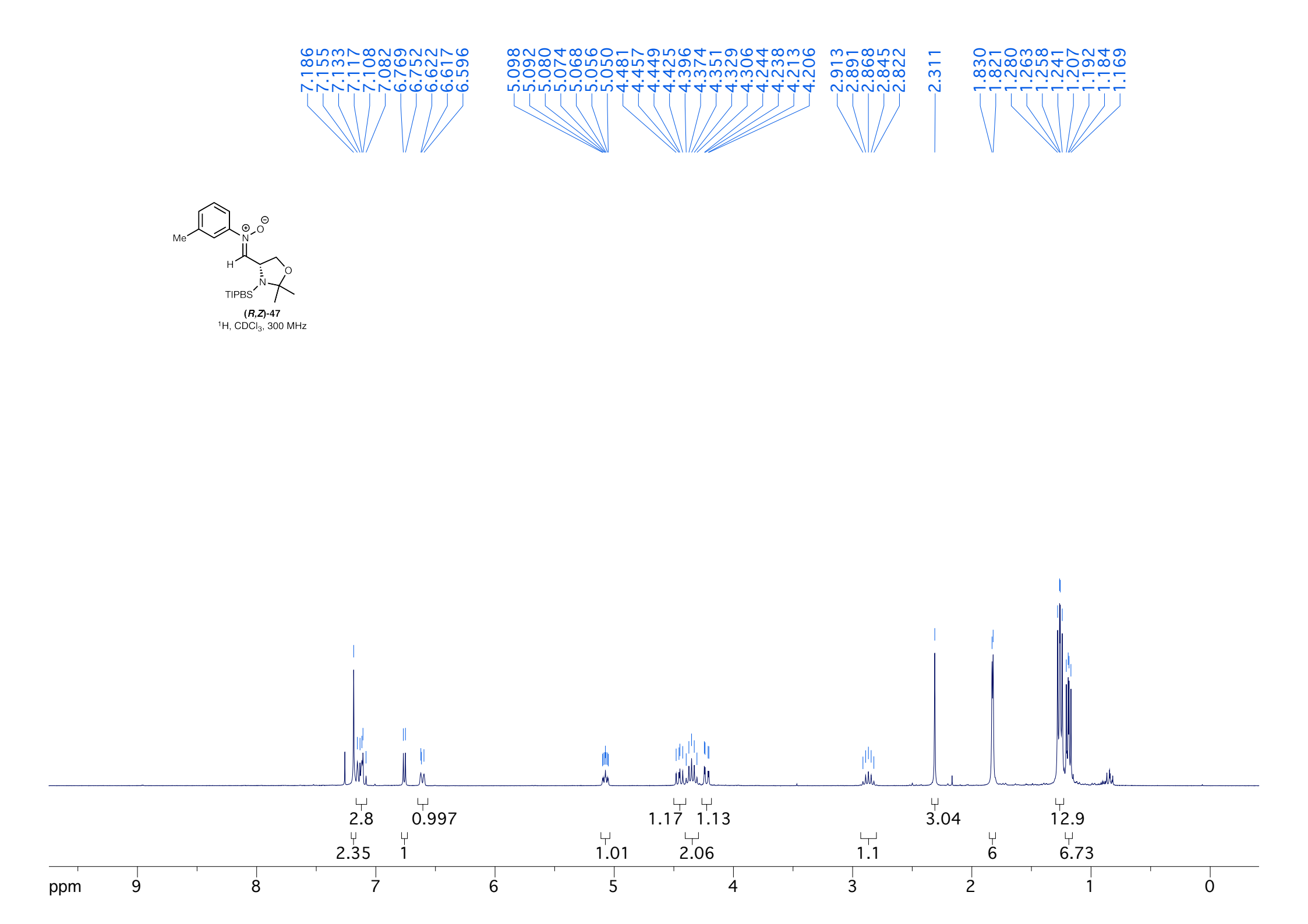

179.134
139.402
138.798
134.018
128.691
128.089
127.578
126.829
123.488
123.434
115.112
58.963
30.835
9.088
Ph
Et
O
N
H
Cl
(S)-46
13C, CDCl3, 75 MHz
ppm
150
100
50
0

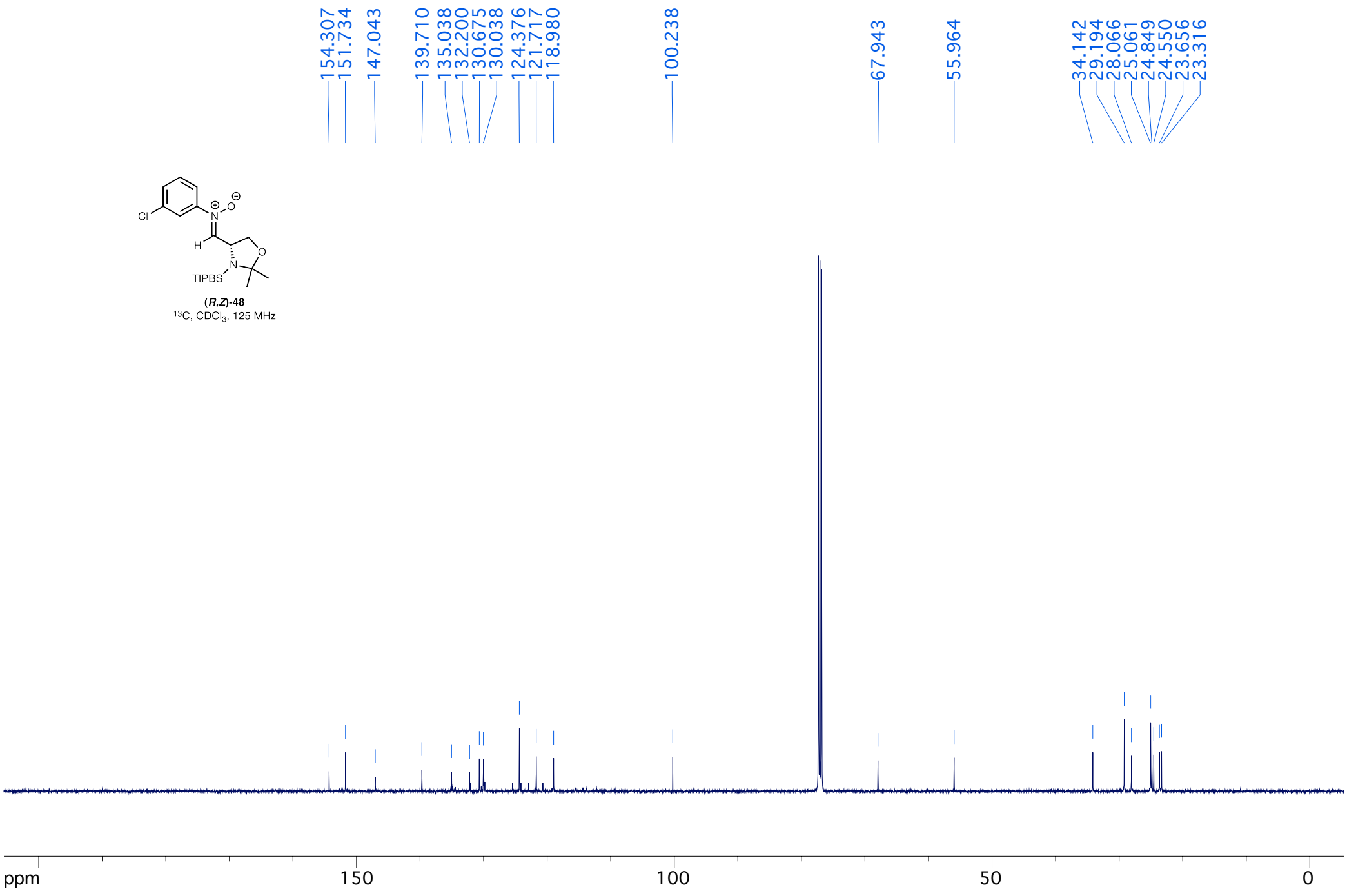

8.006
7.408
7.401
7.385
7.379
7.376
7.374
7.366
7.360
7.342
7.339
7.333
7.315
7.313
7.311
7.304
7.299
7.287
7.282
7.278
7.273
7.145
7.143
7.140
7.138
7.120
7.118
7.115
7.113
7.099
7.073
7.048
2.556
2.531
2.507
2.486
2.462
2.438
2.325
2.301
2.276
2.255
2.231
2.206
0.825
0.800
0.776
Ph
Et
O
N
H
Cl
(S)-46
1H, CDCl3, 300 MHz
6.12
1.01
3
0.894
2.02
1.06
ppm 10
8
6
4
2
0

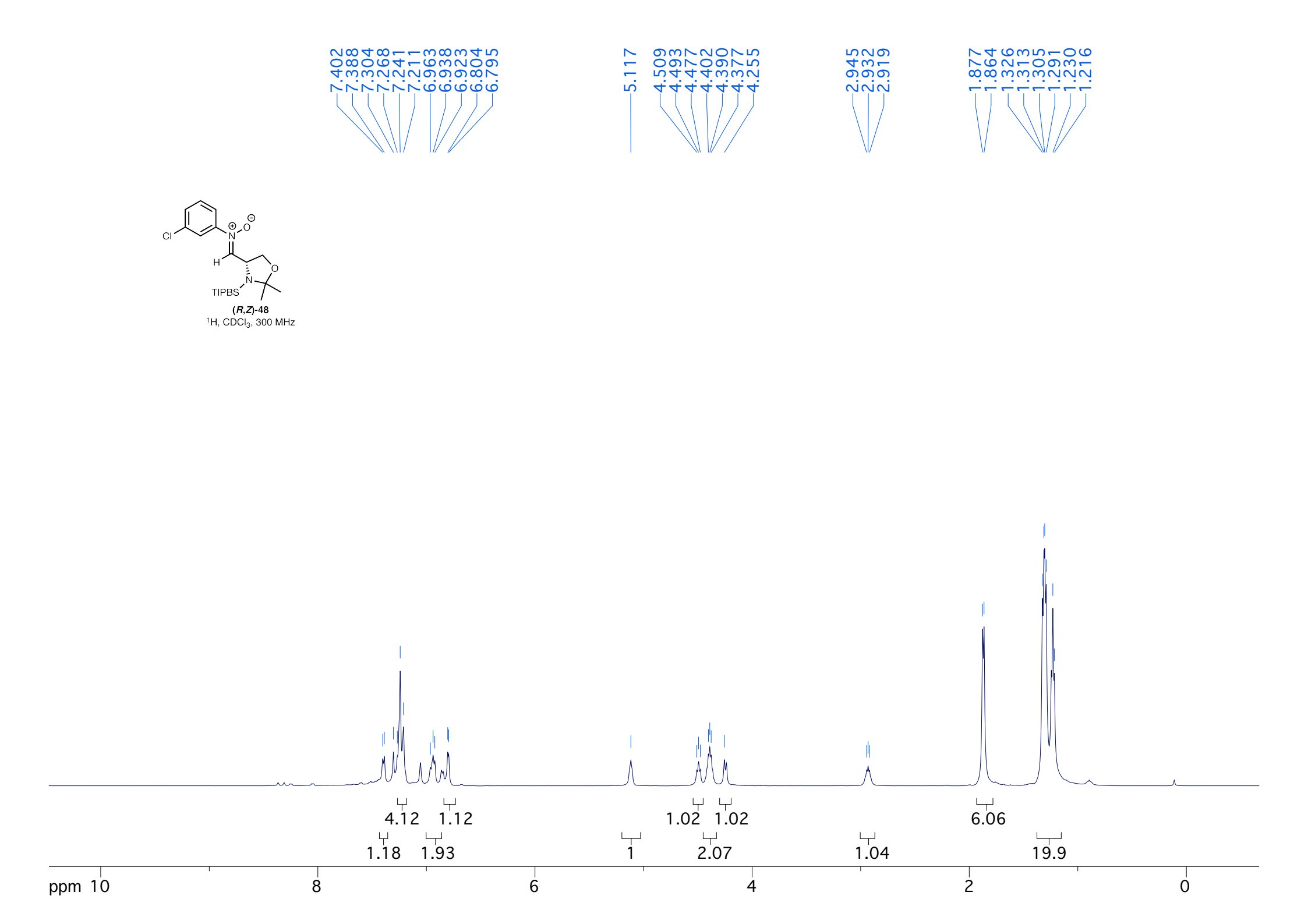


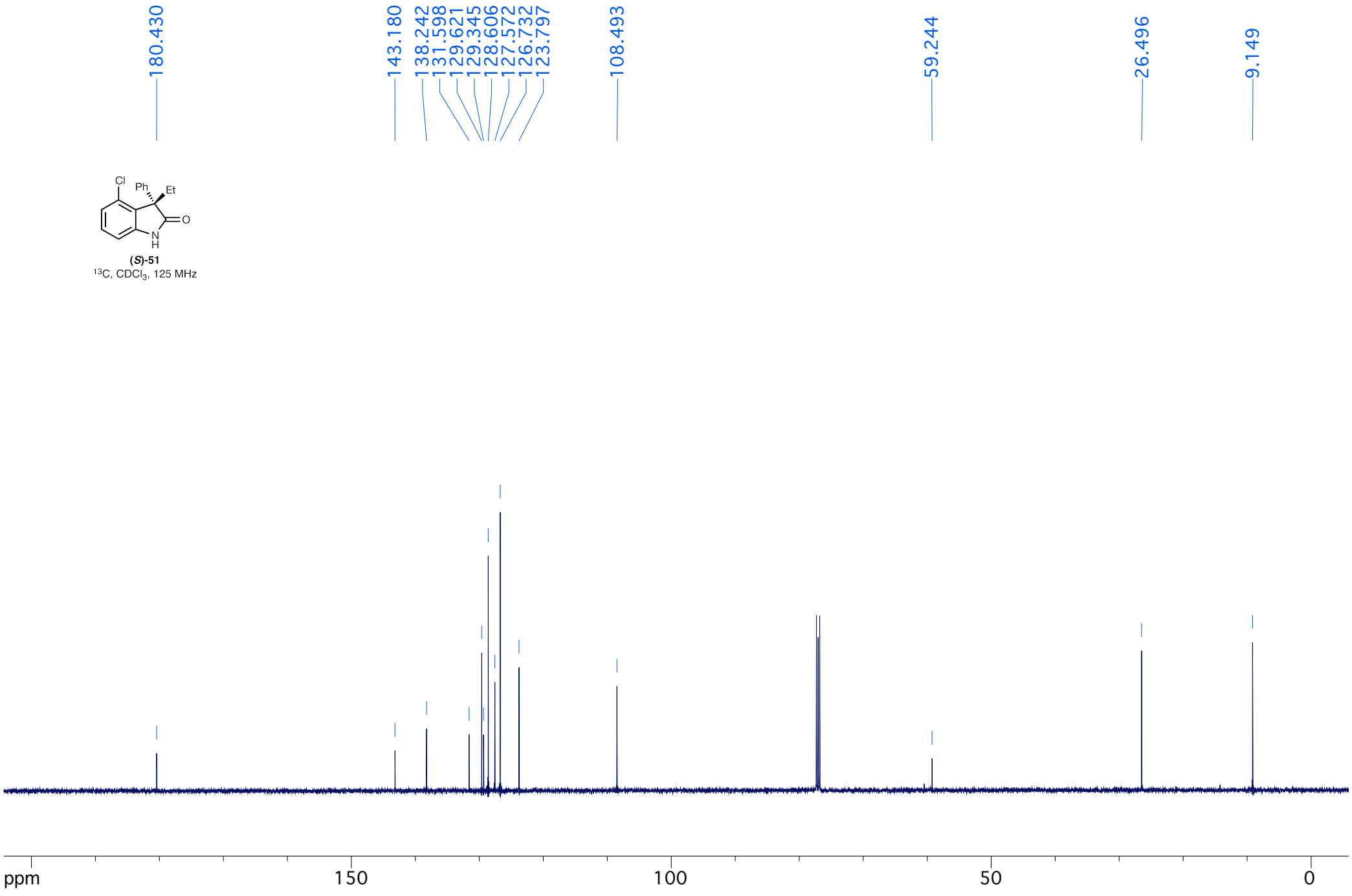
(*R,Z*)-47

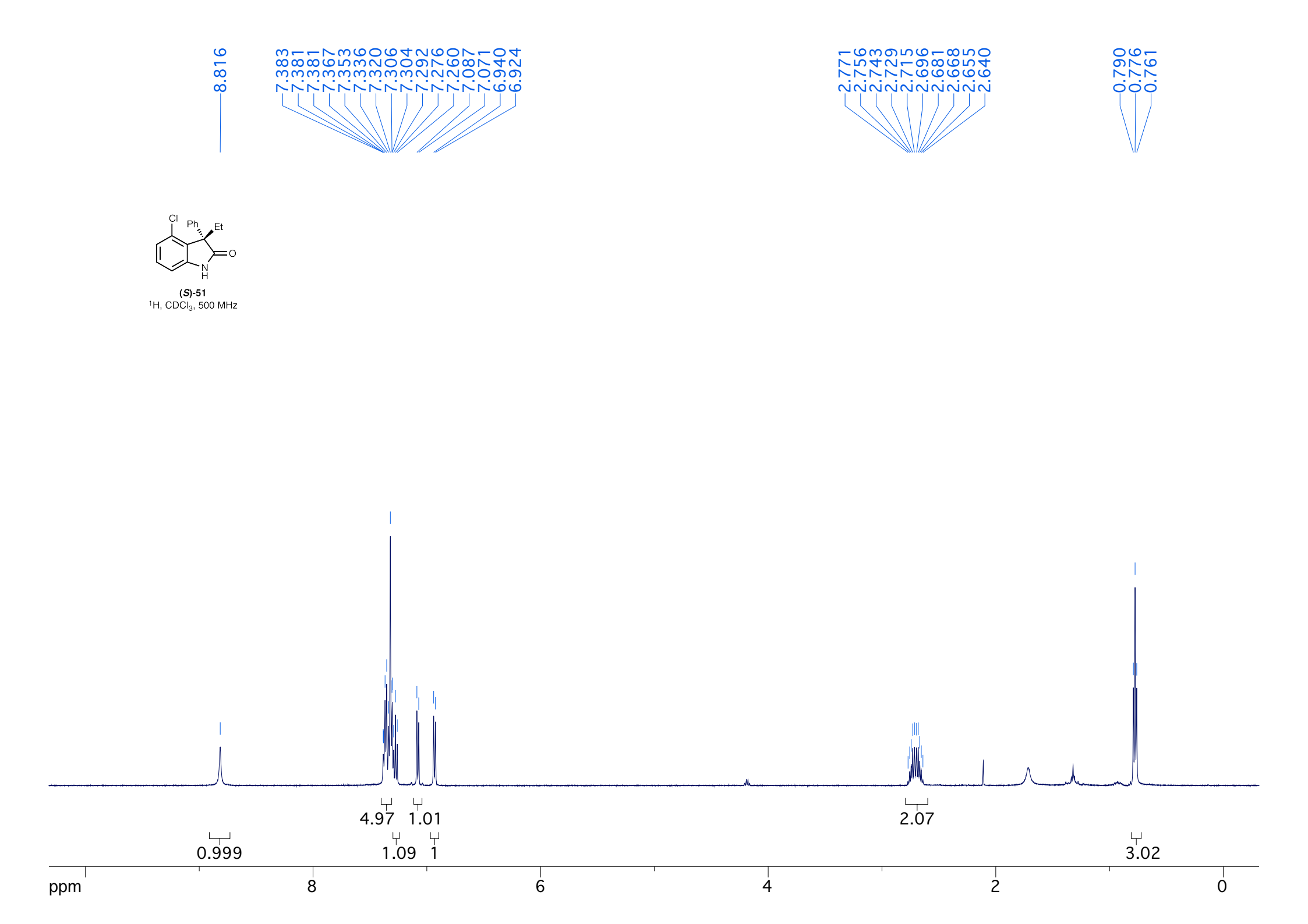
^{13}C, $CDCl_3$, 75 MHz

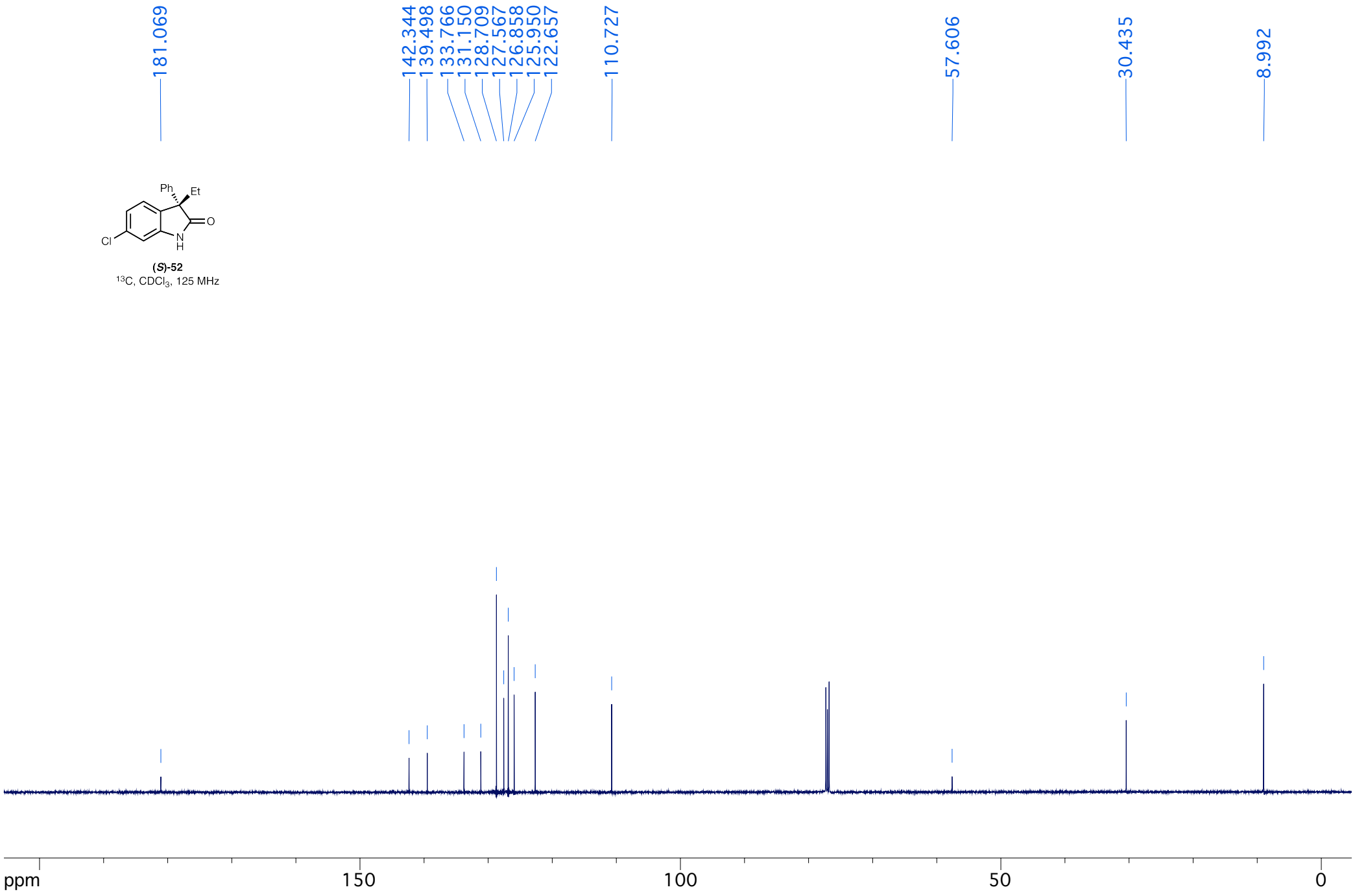

7.186
7.155
7.133
7.117
7.108
7.082
6.769
6.752
6.622
6.617
6.596
5.098
5.092
5.080
5.074
5.068
5.056
5.050
4.481
4.457
4.449
4.425
4.396
4.374
4.351
4.329
4.306
4.244
4.238
4.213
4.206
2.913
2.891
2.868
2.845
2.822
2.311
1.830
1.821
1.280
1.263
1.258
1.241
1.207
1.192
1.184
1.169
Me
N
O
H
O
N
TIPBS
(R,Z)-47
1H, CDCl3, 300 MHz
2.8
0.997
1.17
1.13
3.04
12.9
2.35
1
1.01
2.06
1.1
6
6.73
ppm
9
8
7
6
5
4
3
2
1
0

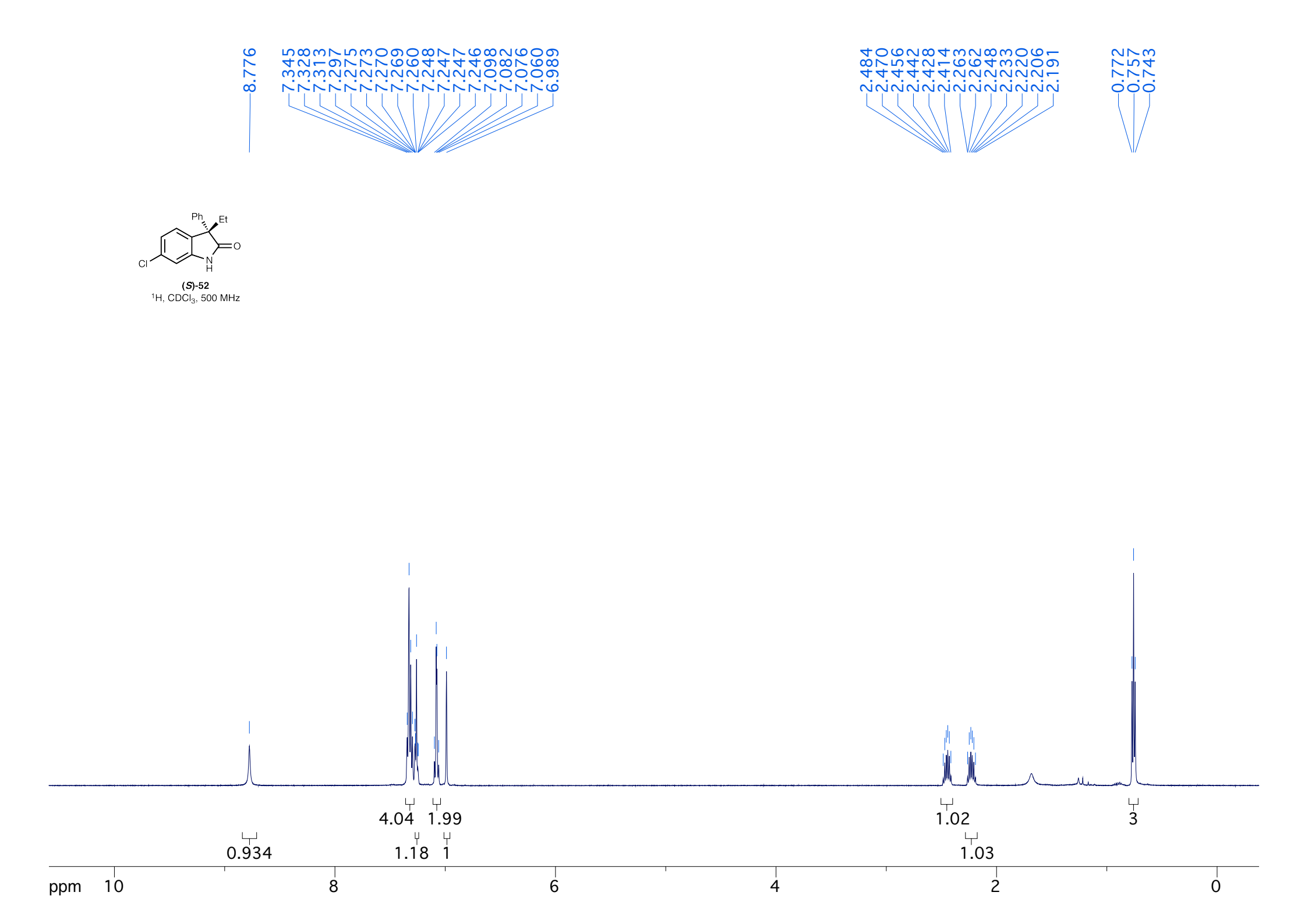

154.307
151.734
147.043
139.710
135.038
132.200
130.675
130.038
124.376
121.717
118.980
100.238
67.943
55.964
34.142
29.194
28.066
25.061
24.849
24.550
23.656
23.316
Cl
N
O
H
O
N
TIPBS
(R,Z)-48
13C, CDCl3, 125 MHz
ppm
150
100
50
0

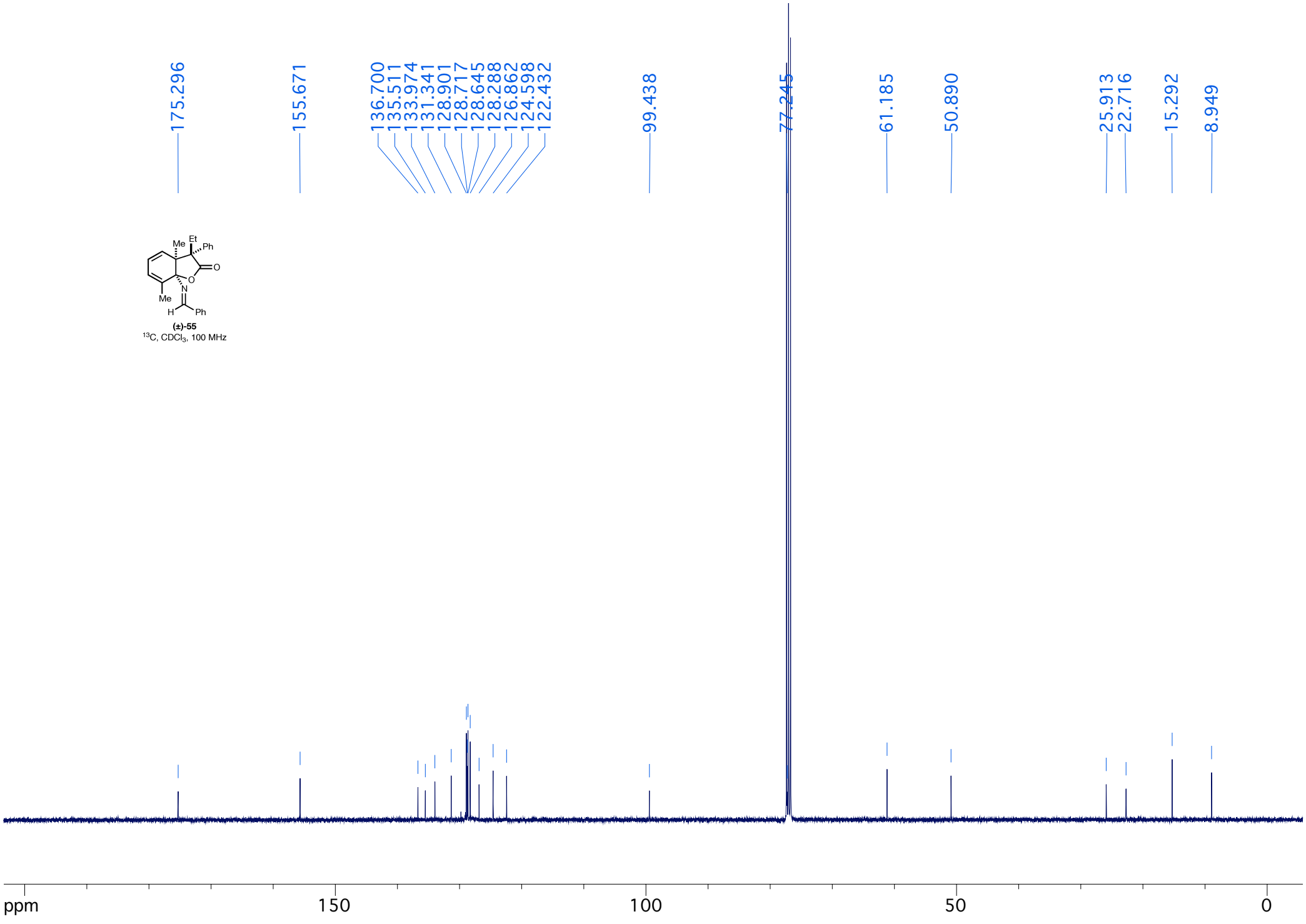

7.402
7.388
7.304
7.268
7.241
7.211
6.963
6.938
6.923
6.804
6.795
5.117
4.509
4.493
4.477
4.402
4.390
4.377
4.255
2.945
2.932
2.919
1.877
1.864
1.326
1.313
1.305
1.291
1.230
1.216
Cl
N
O
H
O
N
TIPBS
(R,Z)-48
1H, CDCl3, 300 MHz
4.12
1.12
1.02
1.02
6.06
1.18
1.93
1
2.07
1.04
19.9
ppm 10
8
6
4
2
0

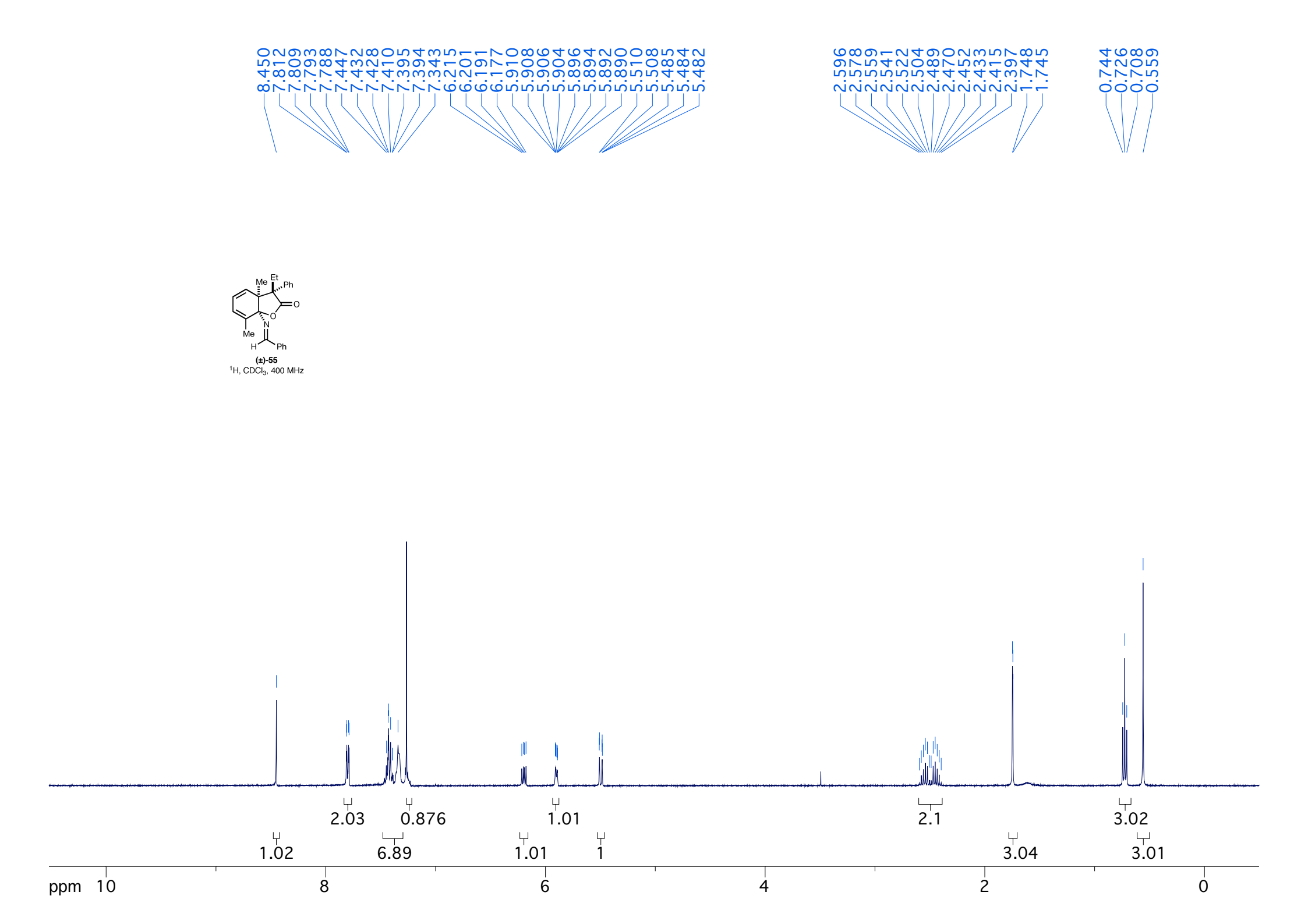

180.430
143.180
138.242
131.598
129.621
129.345
128.606
127.572
126.732
123.797
108.493
59.244
26.496
9.149
Cl
Ph
Et
O
N
H
(S)-51
13C, CDCl3, 125 MHz
ppm
150
100
50
0

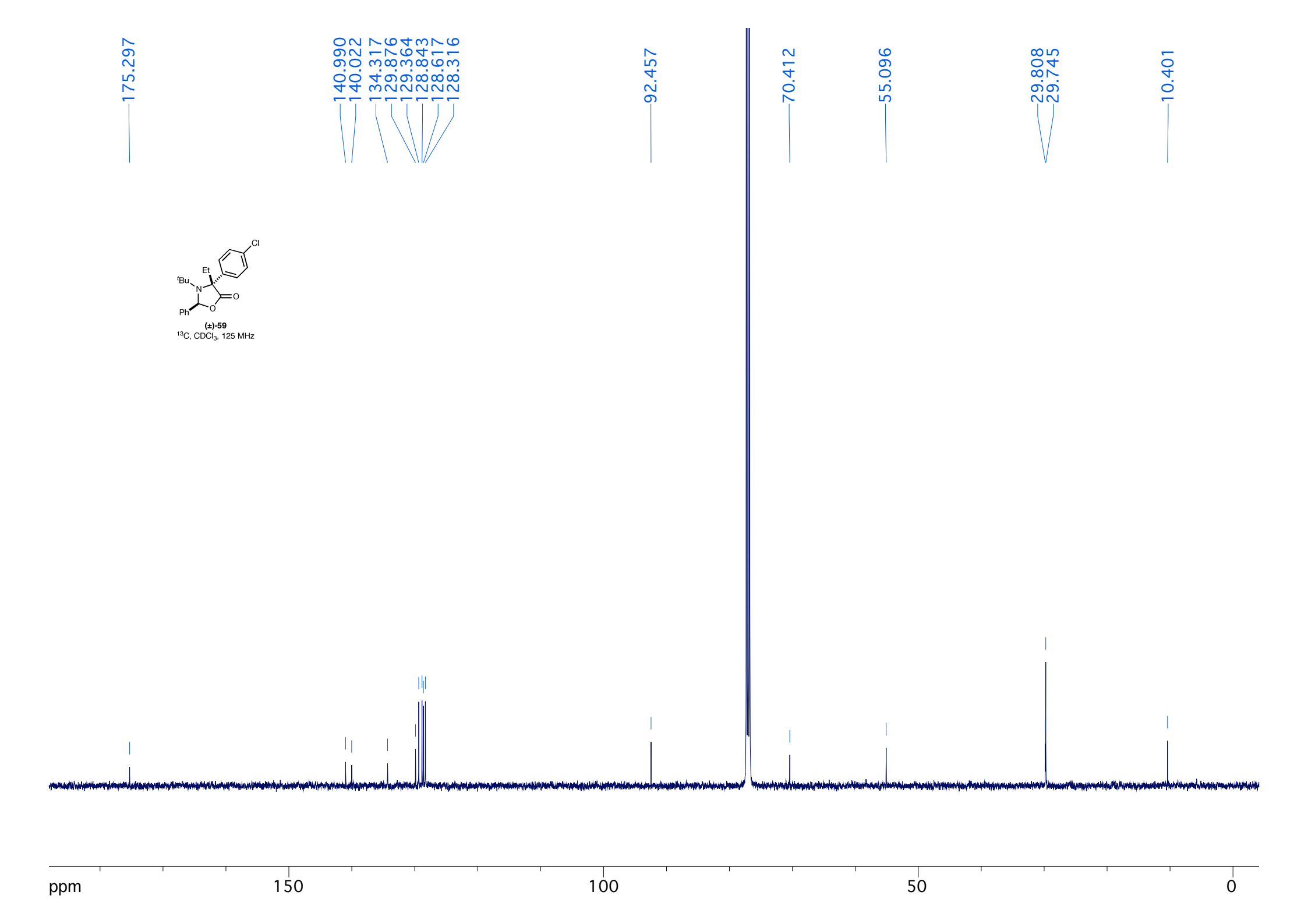

8.816
7.383
7.381
7.381
7.367
7.353
7.336
7.320
7.306
7.304
7.292
7.276
7.260
7.087
7.071
6.940
6.924
2.771
2.756
2.743
2.729
2.715
2.696
2.681
2.668
2.655
2.640
0.790
0.776
0.761
Cl
Ph
Et
O
N
H
(S)-51
1H, CDCl3, 500 MHz
4.97
1.01
2.07
0.999
1.09
1
3.02
ppm
8
6
4
2
0

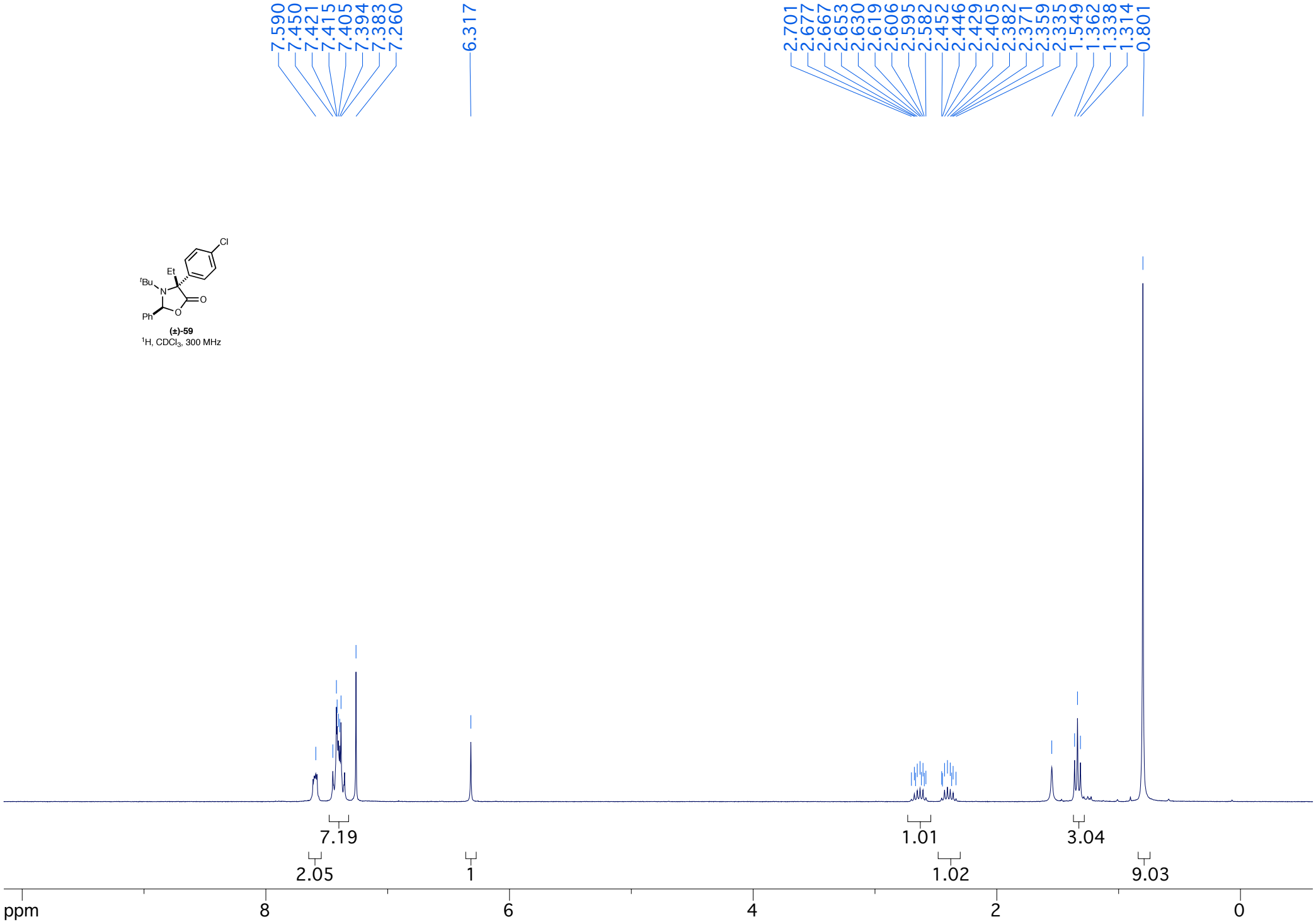

181.069
142.344
139.498
133.766
131.150
128.709
127.567
126.858
125.950
122.657
110.727
57.606
30.435
8.992
Ph
Et
O
Cl
N
H
(S)-52
13C, CDCl3, 125 MHz
ppm
150
100
50
0

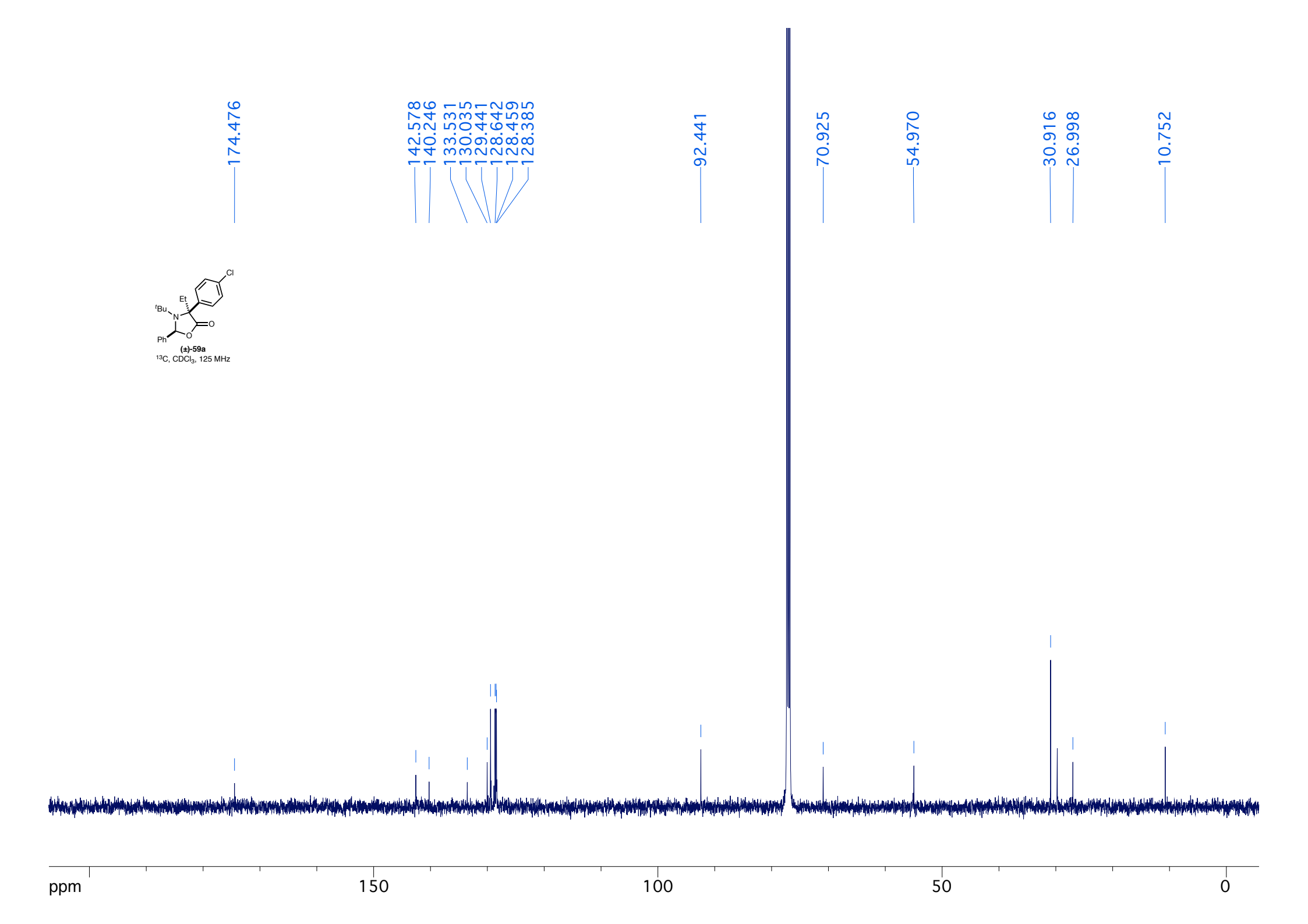

8.776
7.345
7.328
7.313
7.297
7.275
7.273
7.270
7.269
7.260
7.248
7.247
7.247
7.246
7.098
7.082
7.076
7.060
6.989
2.484
2.470
2.456
2.442
2.428
2.414
2.263
2.262
2.248
2.233
2.220
2.206
2.191
0.772
0.757
0.743
Ph
Et
O
Cl
N
H
(S)-52
1H, CDCl3, 500 MHz
0.934
4.04
1.99
1.18
1
1.02
1.03
3
ppm
10
8
6
4
2
0

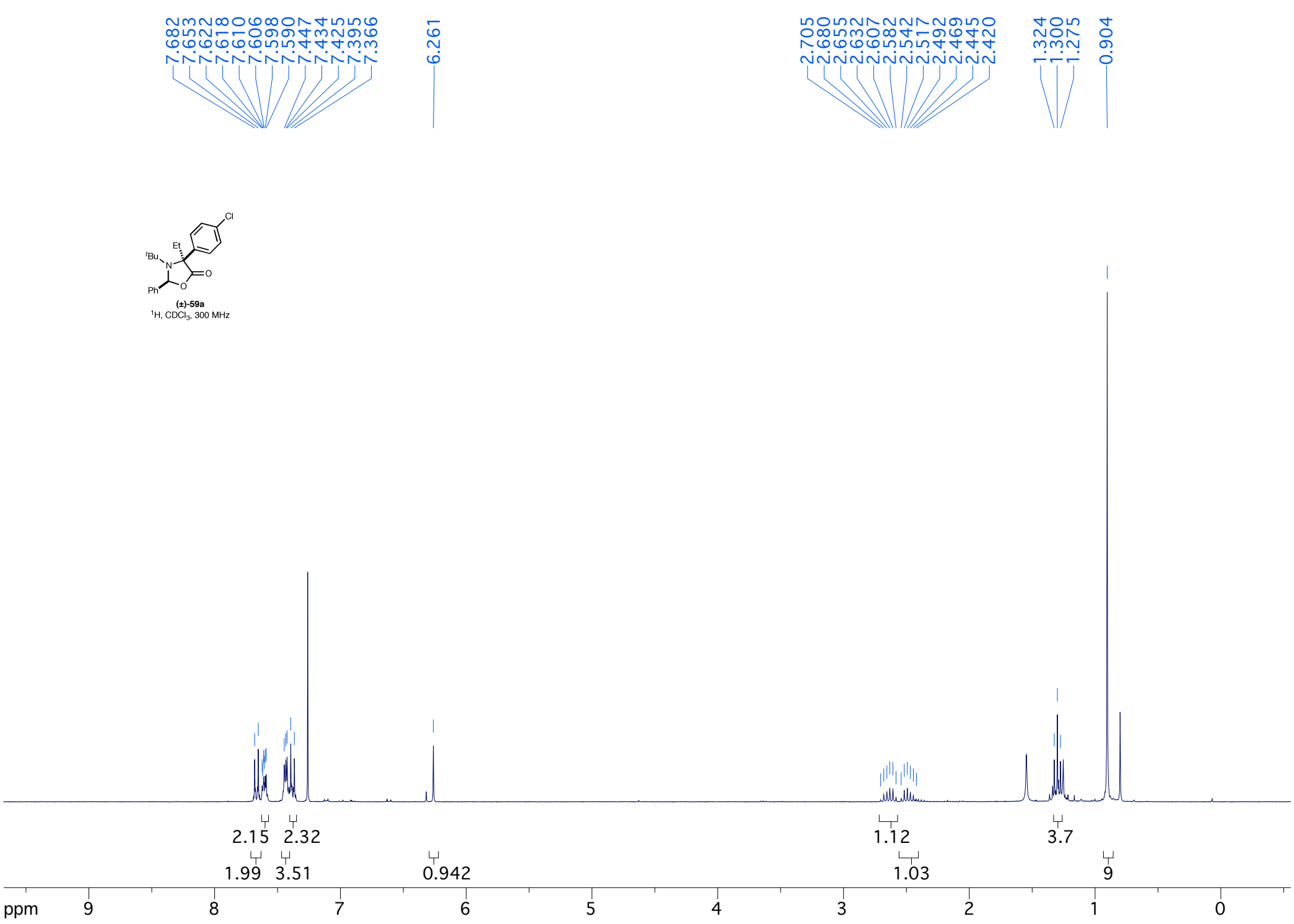

175.296
155.671
136.700
135.511
133.974
131.341
128.901
128.717
128.645
128.288
126.862
124.598
122.432
99.438
77.245
61.185
50.890
25.913
22.716
15.292
8.949
Me
Et
Ph
O
O
N
Me
H
Ph
(±)-55
13C, CDCl3, 100 MHz
ppm
150
100
50
0

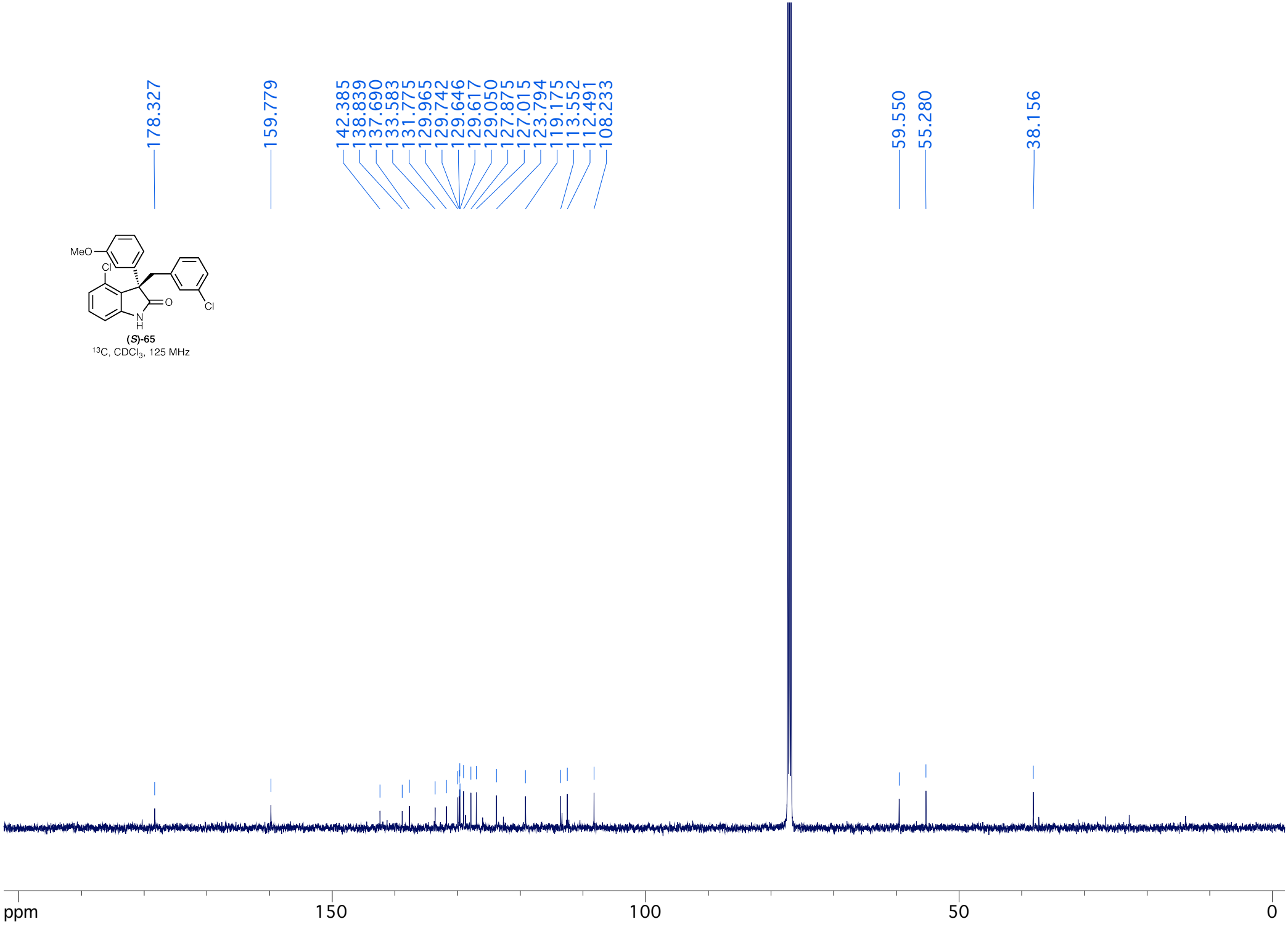

8.450
7.812
7.809
7.793
7.788
7.447
7.432
7.428
7.410
7.395
7.394
7.343
6.215
6.201
6.191
6.177
5.910
5.908
5.906
5.904
5.896
5.894
5.892
5.890
5.510
5.508
5.485
5.484
5.482
2.596
2.578
2.559
2.541
2.522
2.504
2.489
2.470
2.452
2.433
2.415
2.397
1.748
1.745
0.744
0.726
0.708
0.559
Me
Et
Ph
O
O
N
Me
H
Ph
(±)-55
^{1}H, $CDCl_3$, 400 MHz
2.03
0.876
1.01
2.1
3.02
1.02
6.89
1.01
1
3.04
3.01
ppm
10
8
6
4
2
0

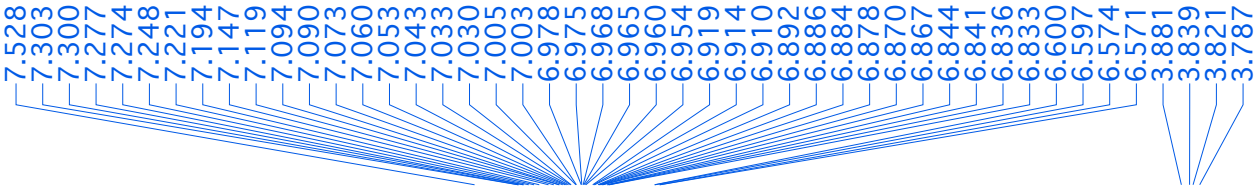

175.297
140.990
140.022
134.317
129.876
129.364
128.843
128.617
128.316
92.457
70.412
55.096
29.808
29.745
10.401
Cl
Et
tBu
N
O
O
Ph
(±)-59
13C, CDCl3, 125 MHz
ppm
150
100
50
0

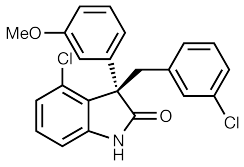

7.590
7.450
7.421
7.415
7.405
7.394
7.383
7.260
6.317
2.701
2.677
2.667
2.653
2.630
2.619
2.606
2.595
2.582
2.452
2.446
2.429
2.405
2.382
2.371
2.359
2.335
1.549
1.362
1.338
1.314
0.801
Cl
Et
tBu
N
O
O
Ph
(±)-59
1H, CDCl3, 300 MHz
7.19
1.01
3.04
2.05
1
1.02
9.03
ppm
8
6
4
2
0


174.476
142.578
140.246
133.531
130.035
129.441
128.642
128.459
128.385
92.441
70.925
54.970
30.916
26.998
10.752
Cl
Et
tBu
N
O
O
Ph
(±)-59a
13C, CDCl3, 125 MHz
ppm
150
100
50
0


7.682
7.653
7.622
7.618
7.610
7.606
7.598
7.590
7.447
7.434
7.425
7.395
7.366
6.261
2.705
2.680
2.655
2.632
2.607
2.582
2.542
2.517
2.492
2.469
2.445
2.420
1.324
1.300
1.275
0.904
Cl
Et
tBu
N
O
O
Ph
(±)-59a
1H, CDCl3, 300 MHz
2.15
2.32
1.12
3.7
1.99
3.51
0.942
1.03
9
ppm
9
8
7
6
5
4
3
2
1
0


178.327
159.779
142.385
138.839
137.690
133.583
131.775
129.965
129.742
129.646
129.617
129.050
127.875
127.015
123.794
119.175
113.552
112.491
108.233
59.550
55.280
38.156
MeO
Cl
O
N
H
Cl
(S)-65
13C, CDCl3, 125 MHz
ppm
150
100
50
0





(*S*)-65

^{1}H, $CDCl_3$, 300 MHz