Supporting Information

Asymmetric Allylation/RCM-Mediated Synthesis of Fluorinated Benzo-fused Bicyclic Homoallylic Amines as Dihydronaphthalene Derivatives

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Laboratorio de Moléculas Orgánicas, Centro de Investigación Príncipe Felipe, E-46012 Valencia, Spain

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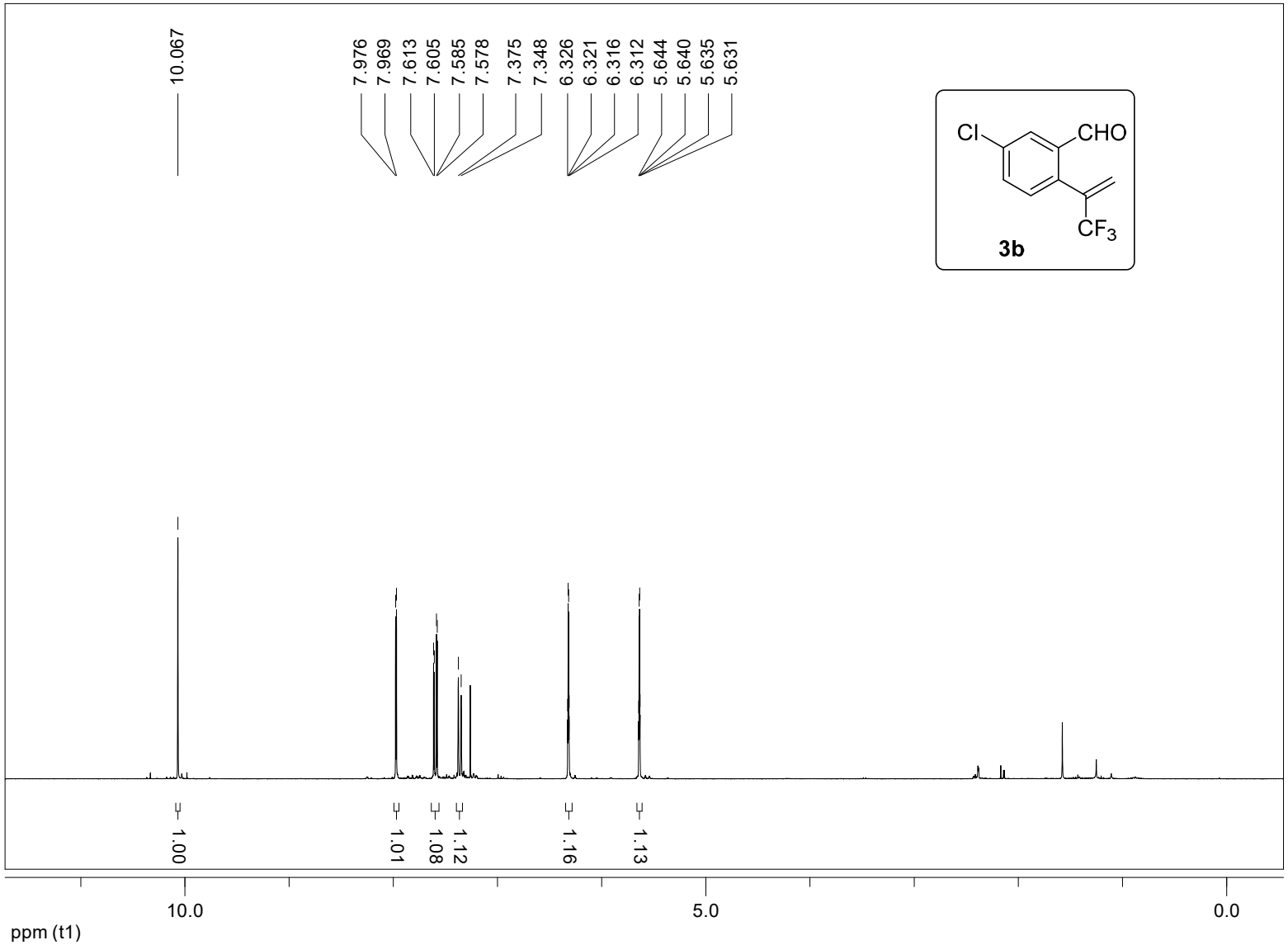
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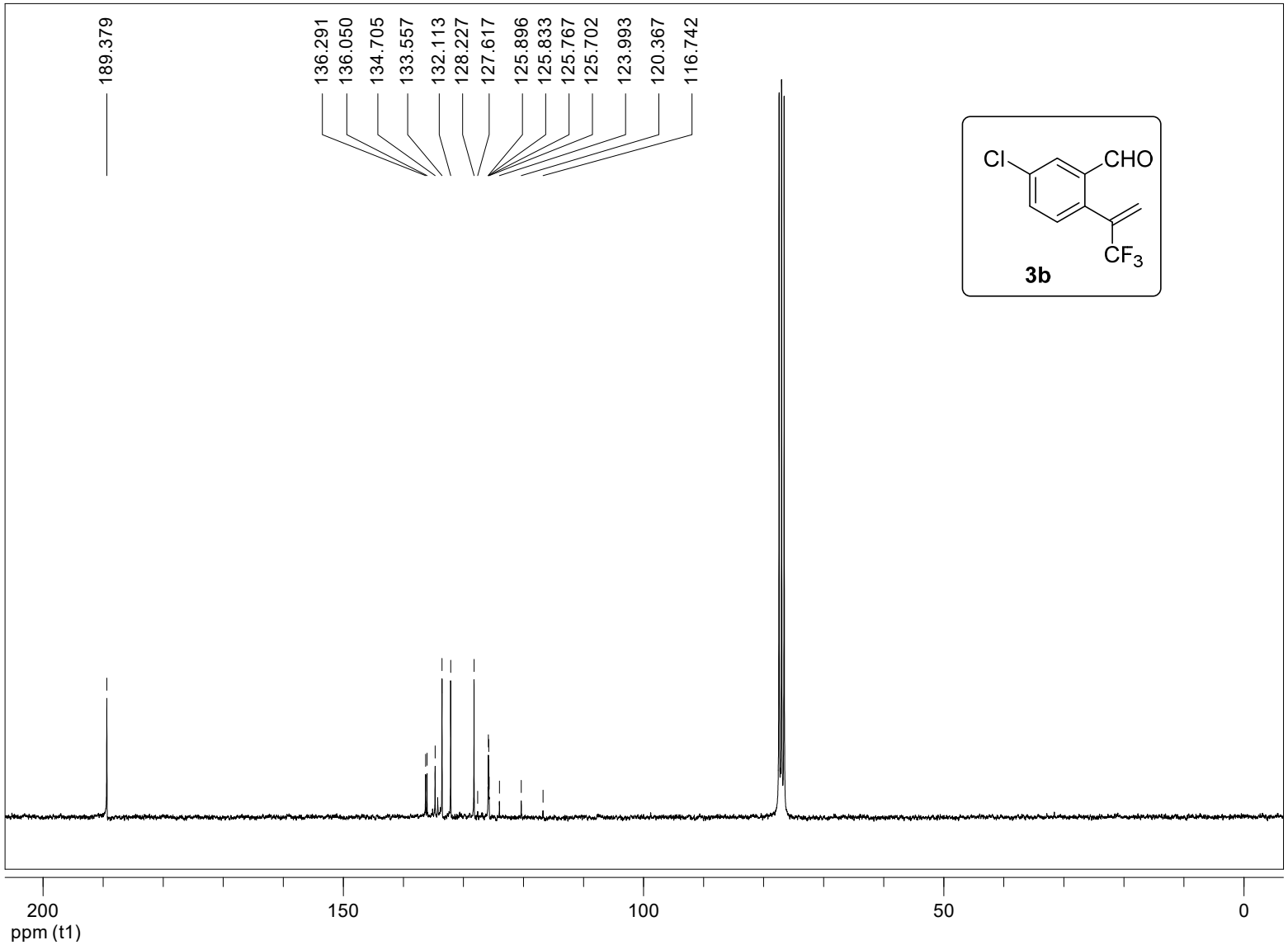
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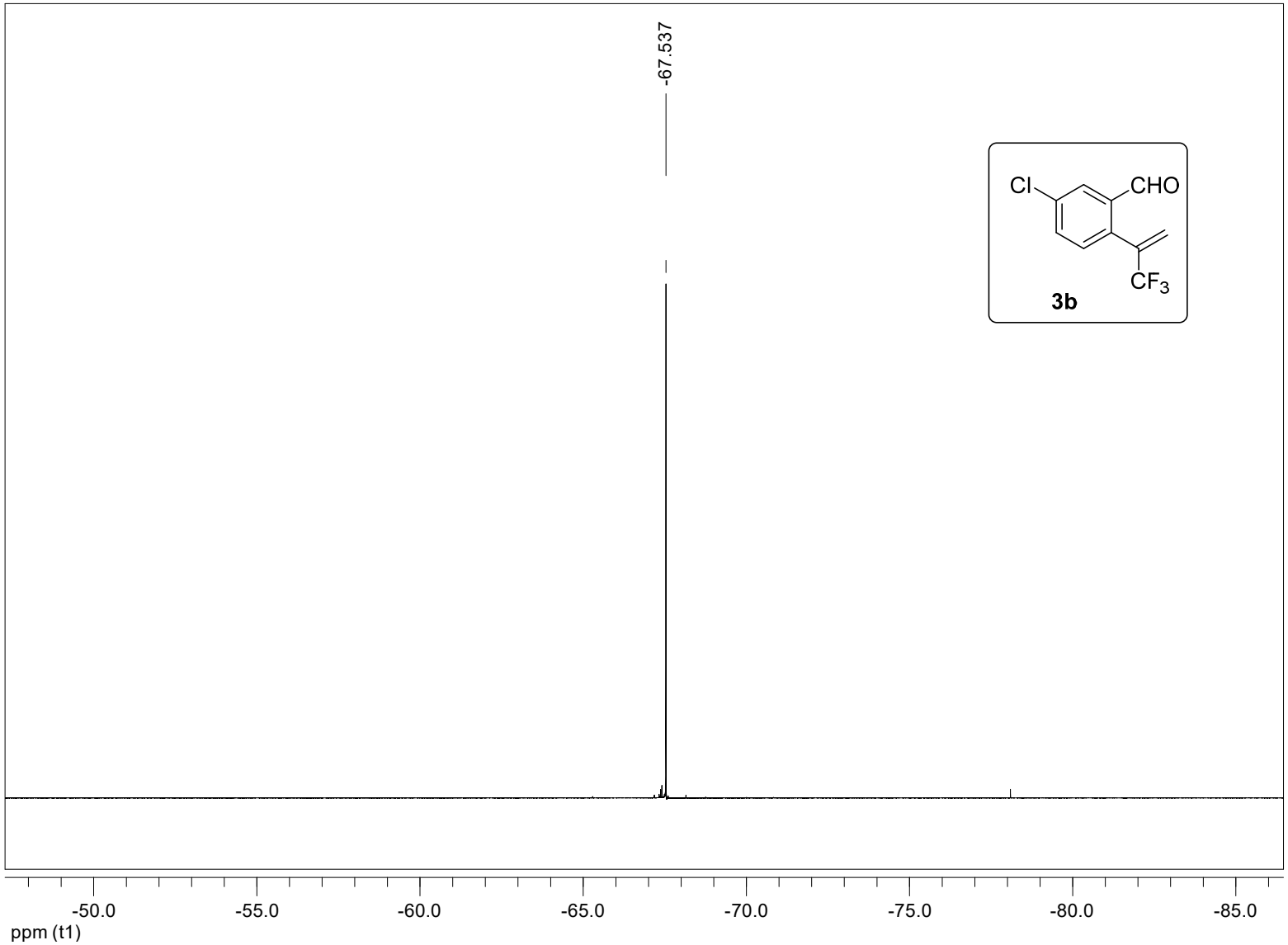
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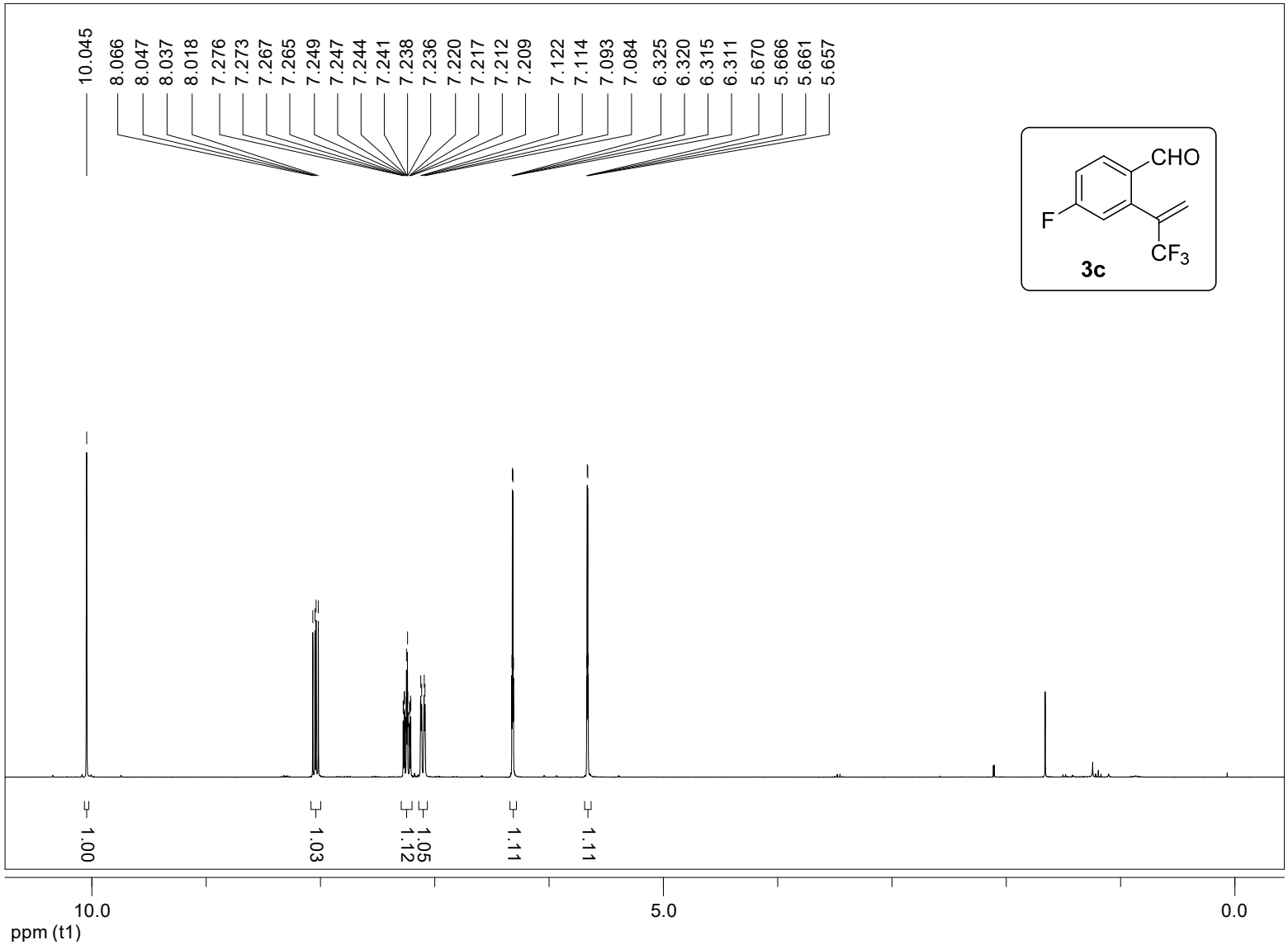
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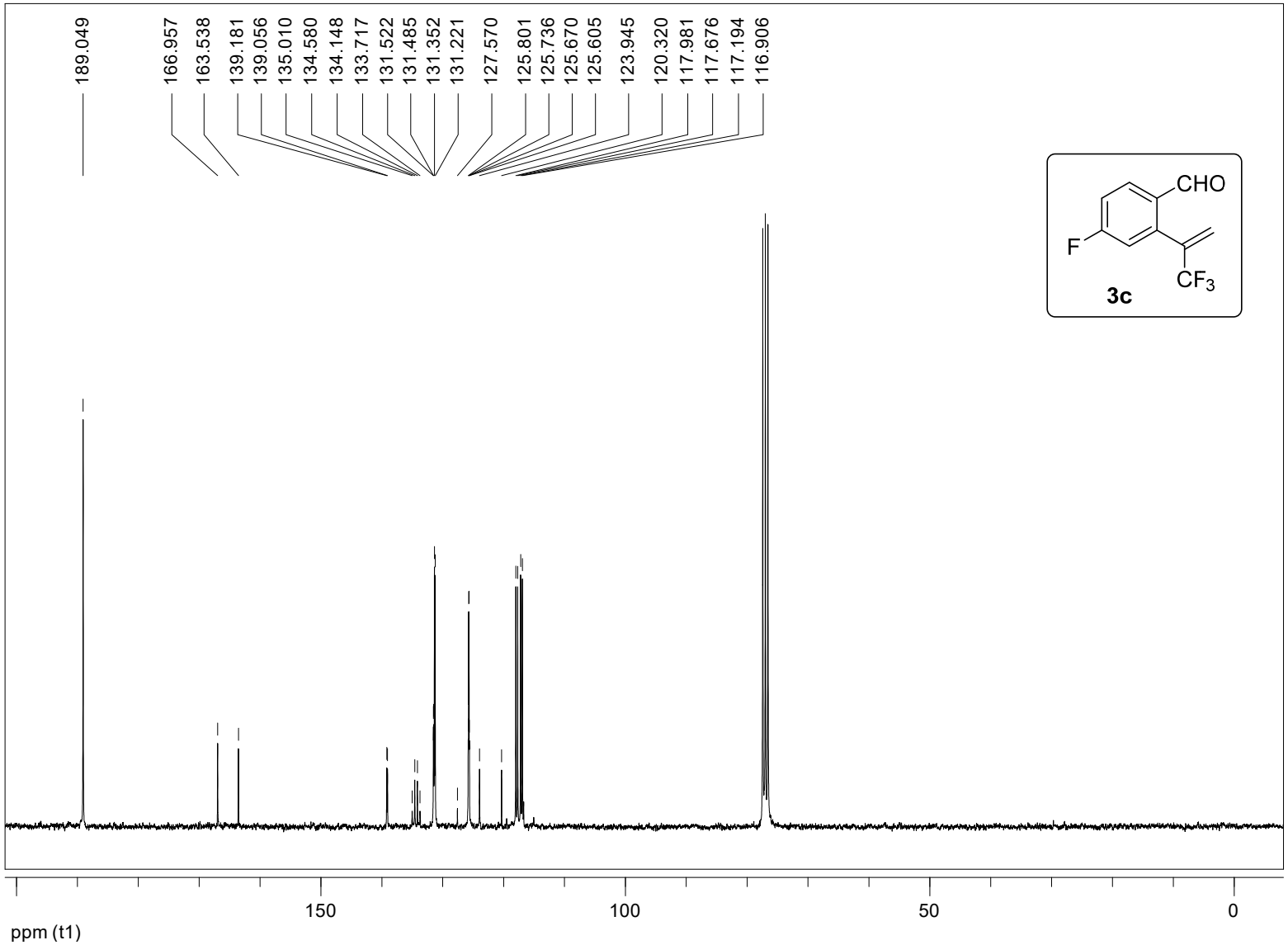
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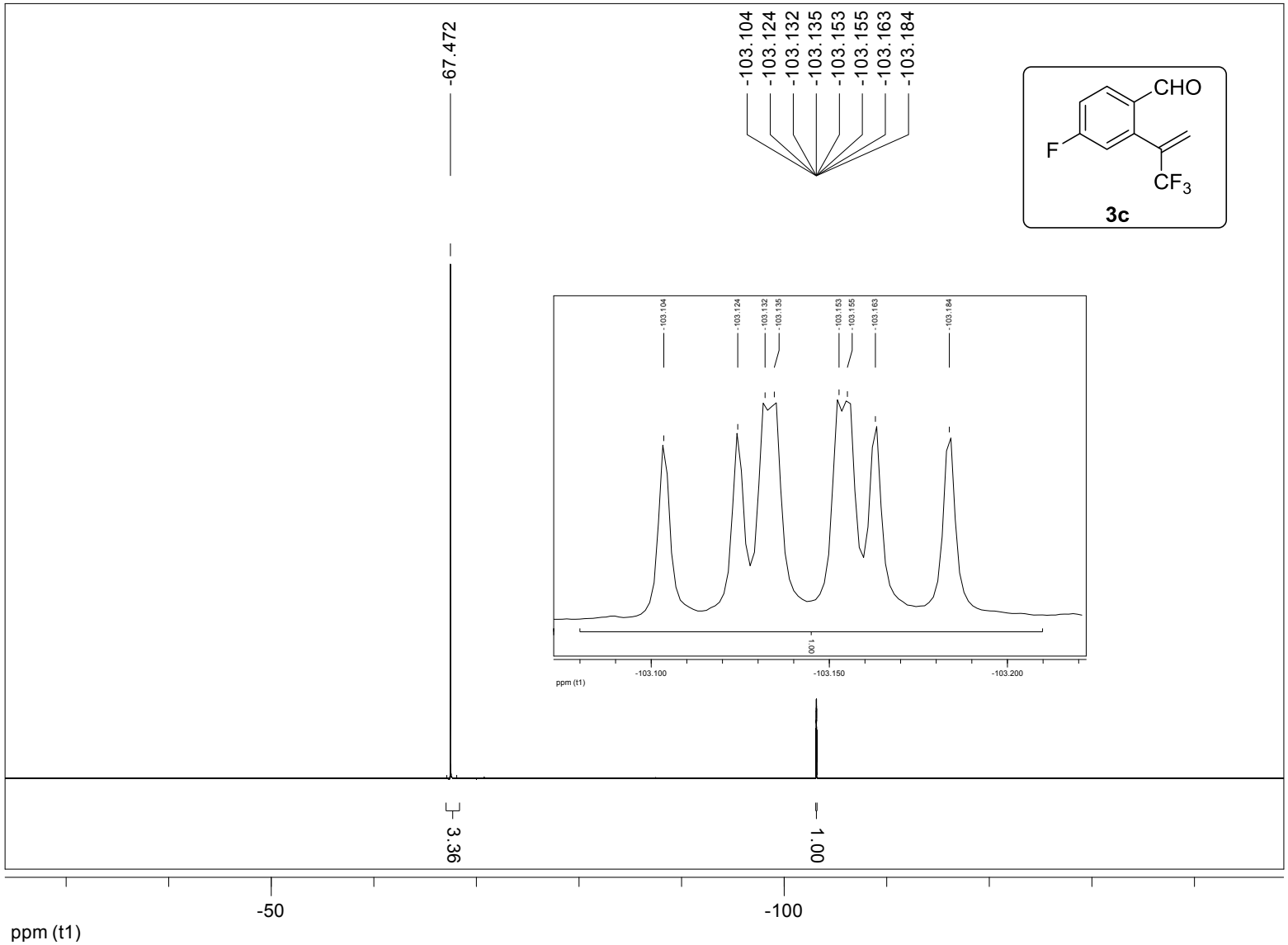
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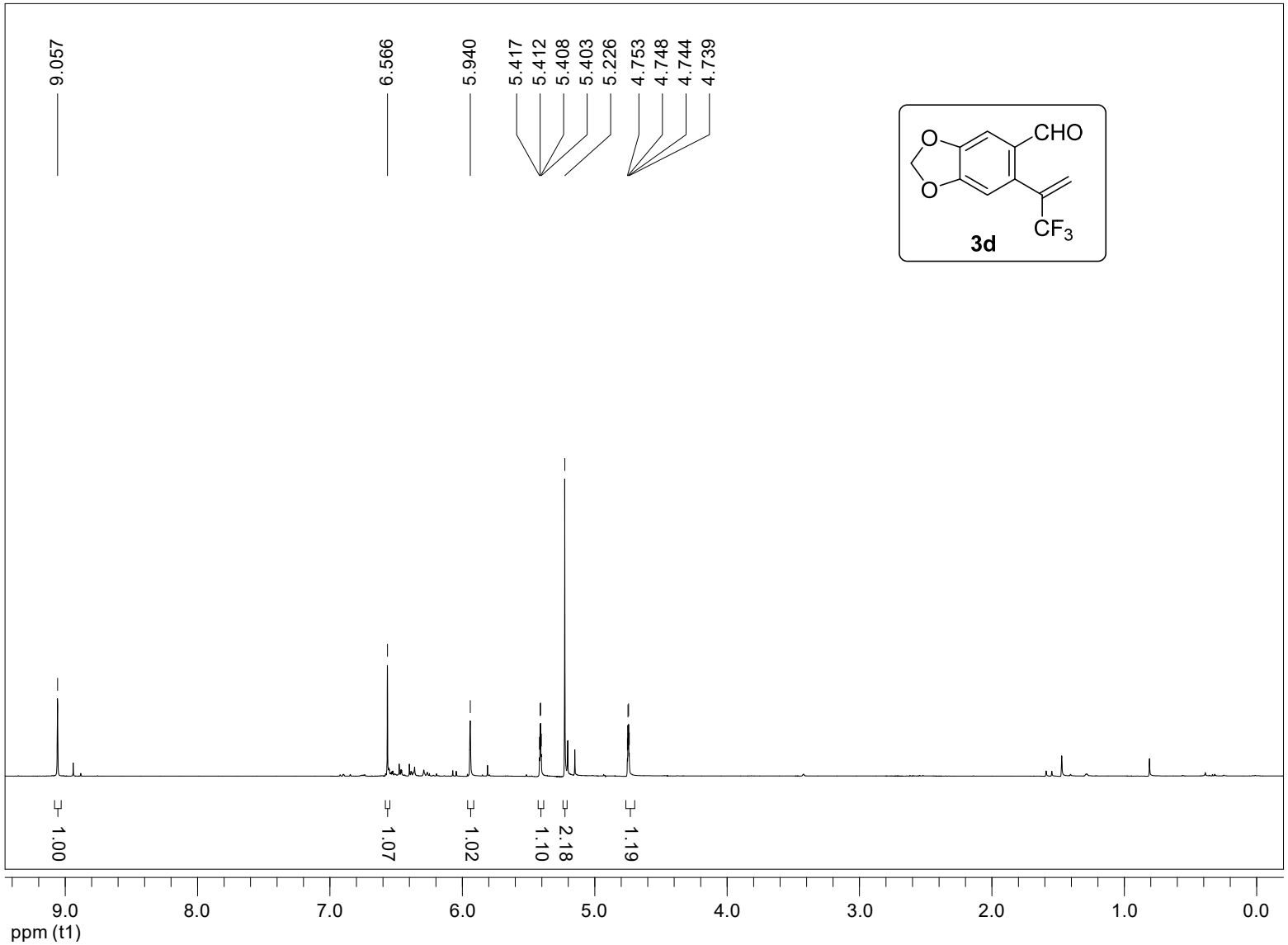
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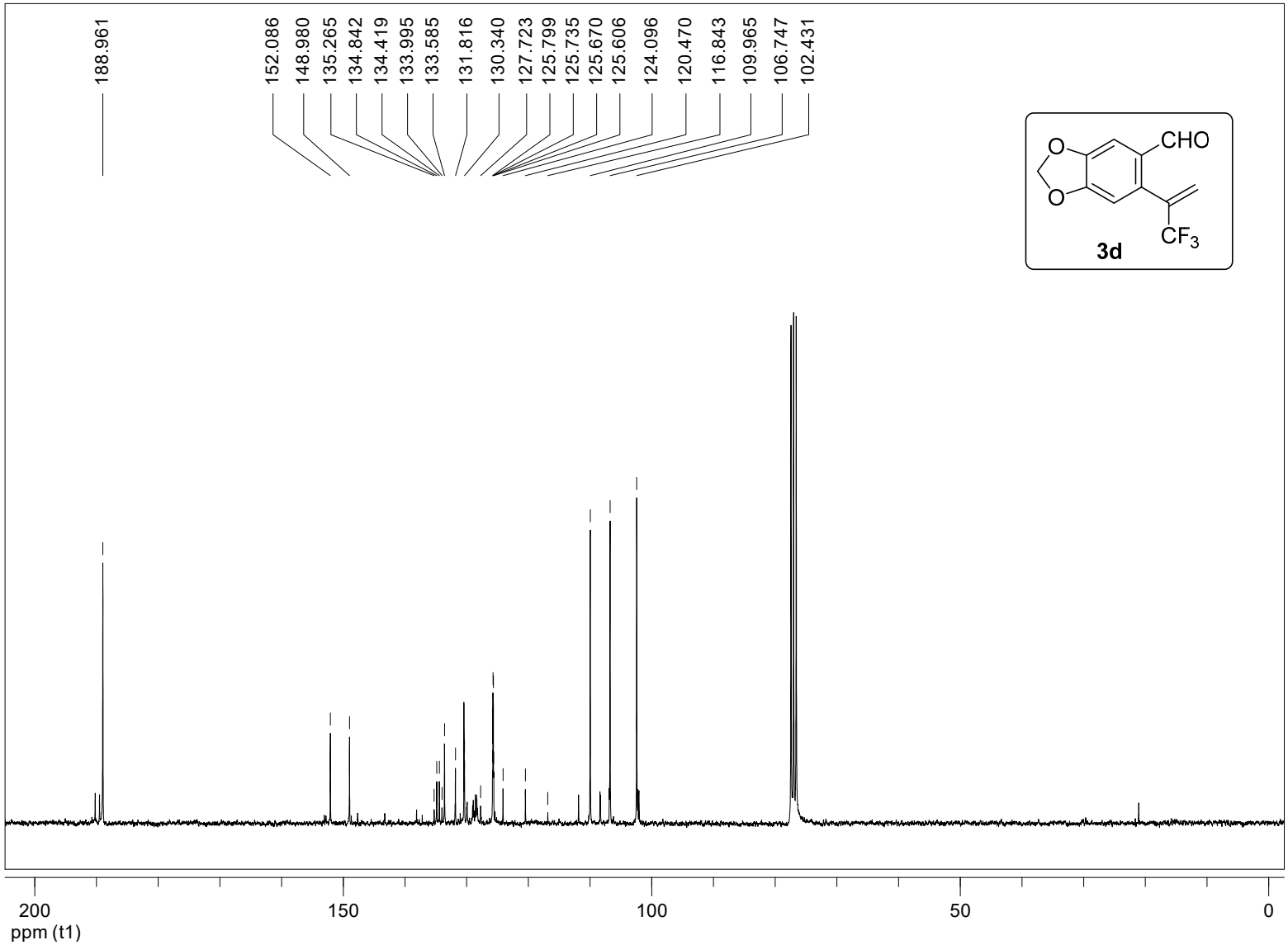
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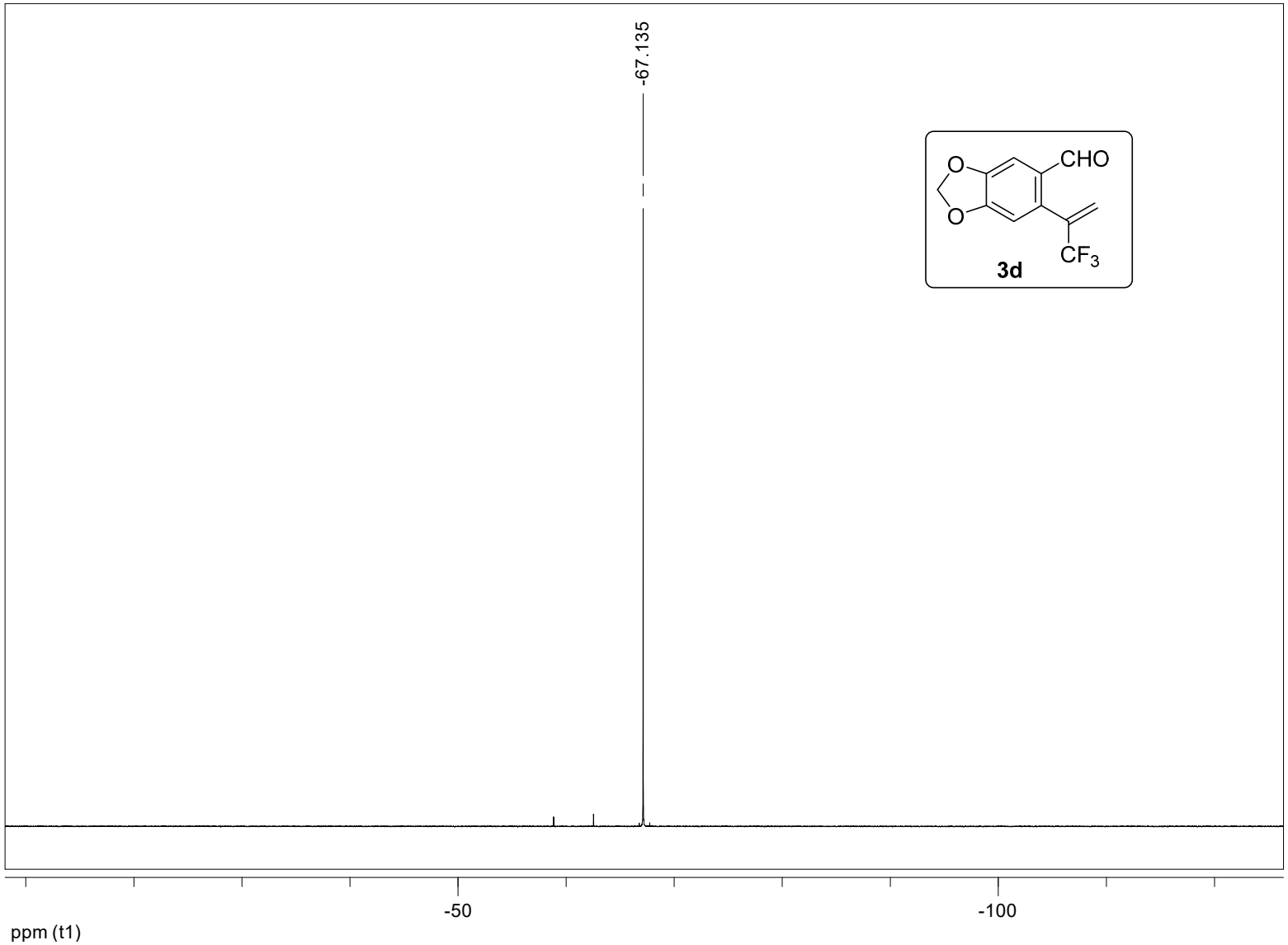
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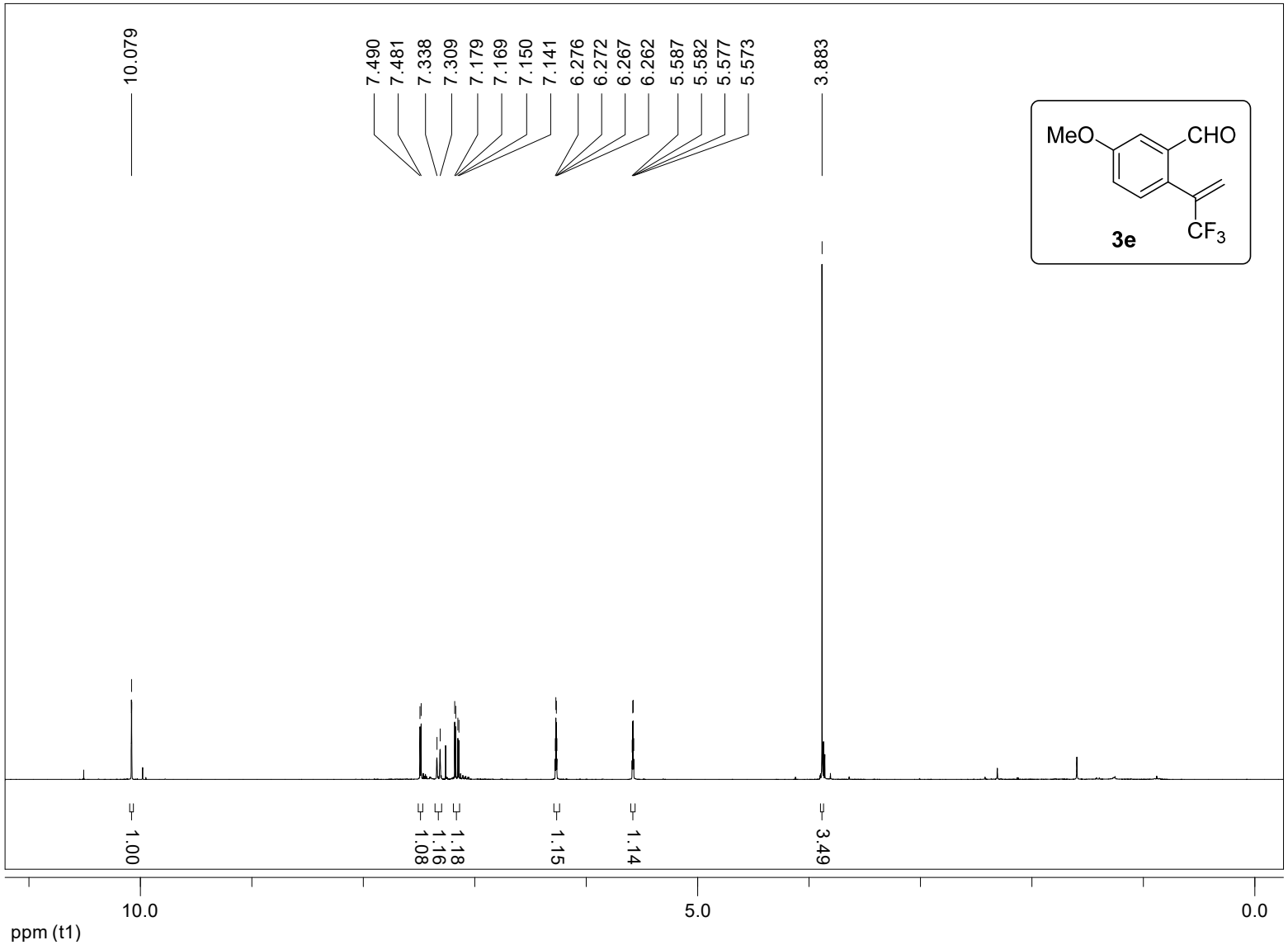
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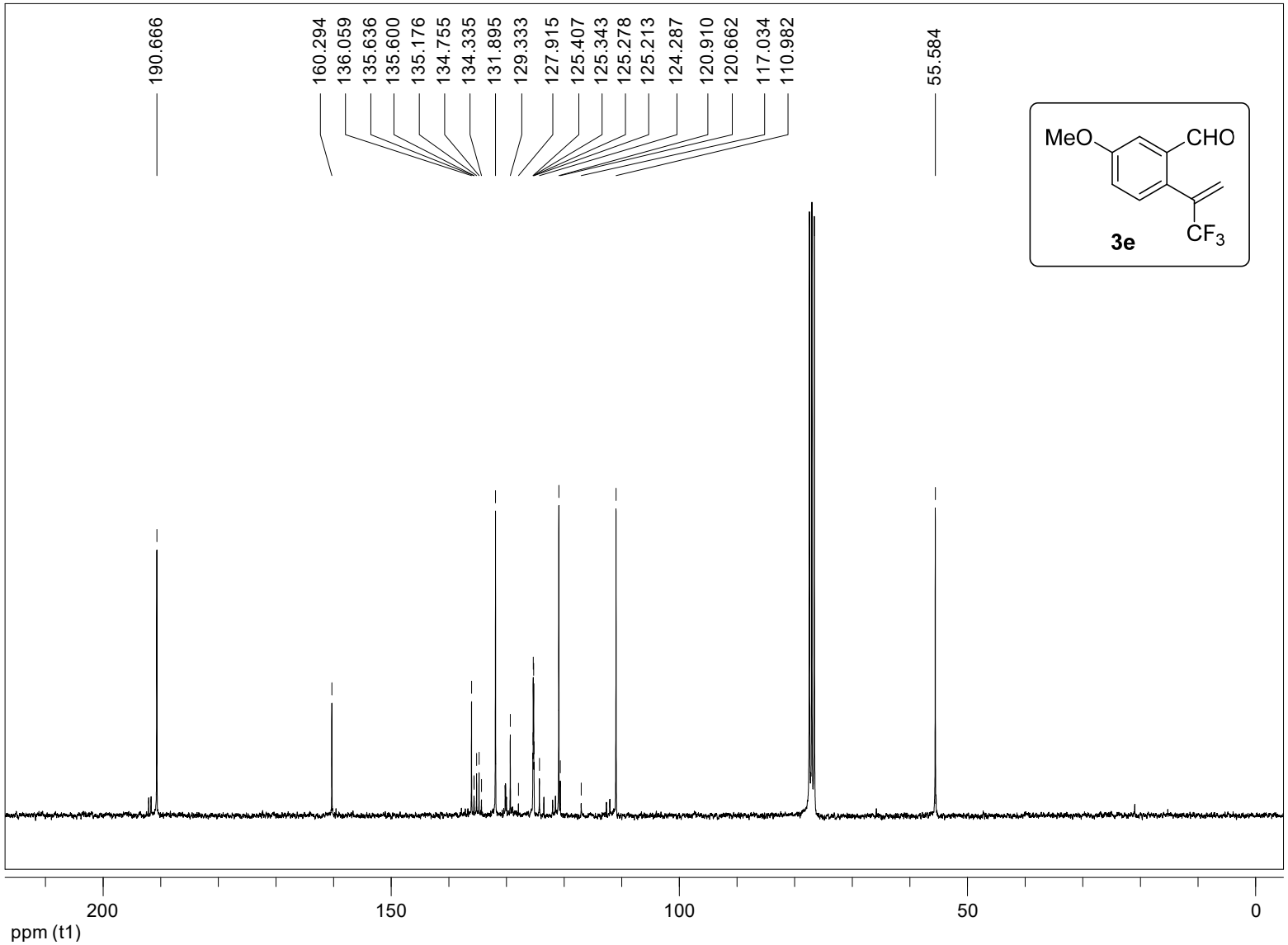
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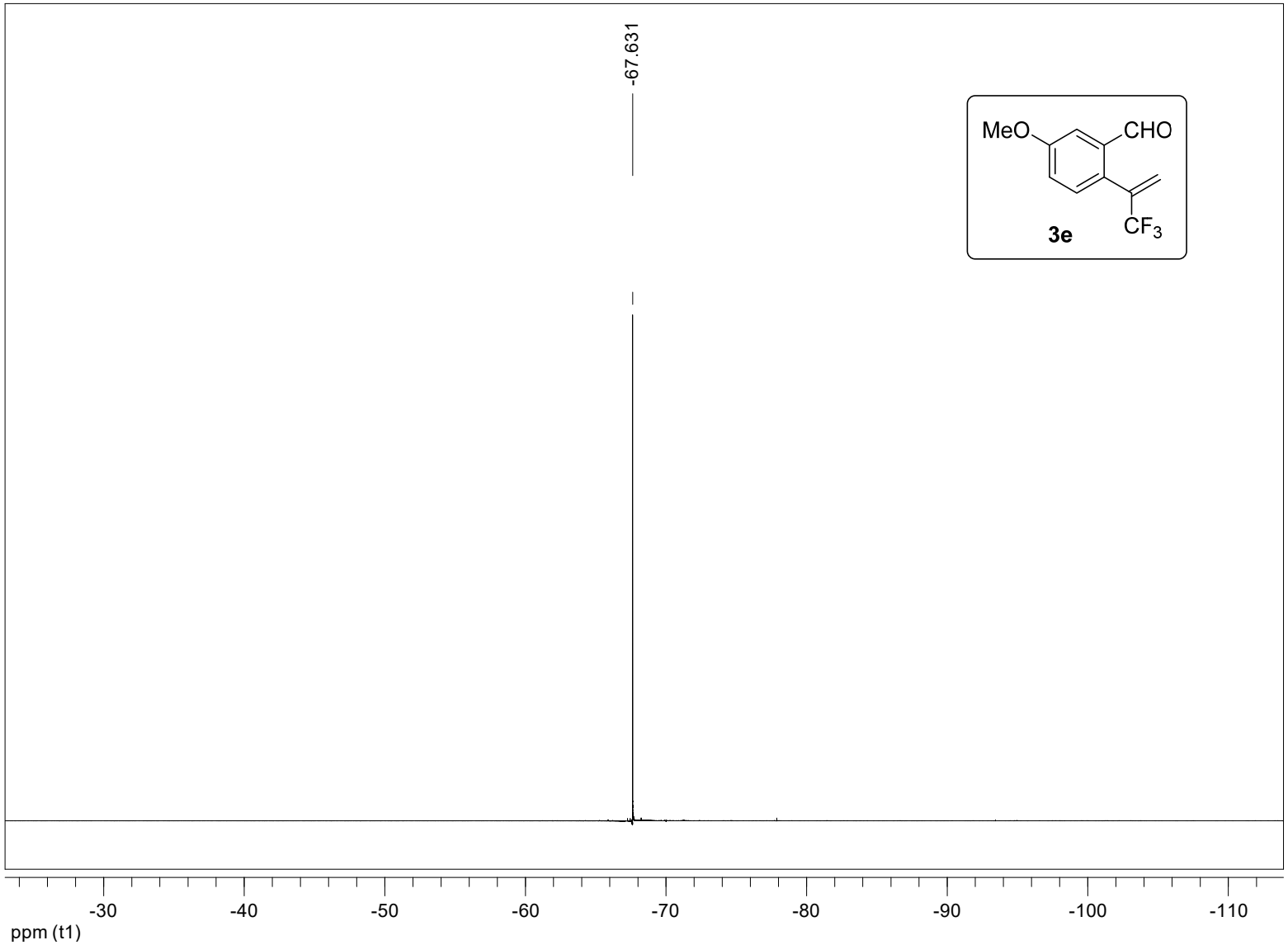
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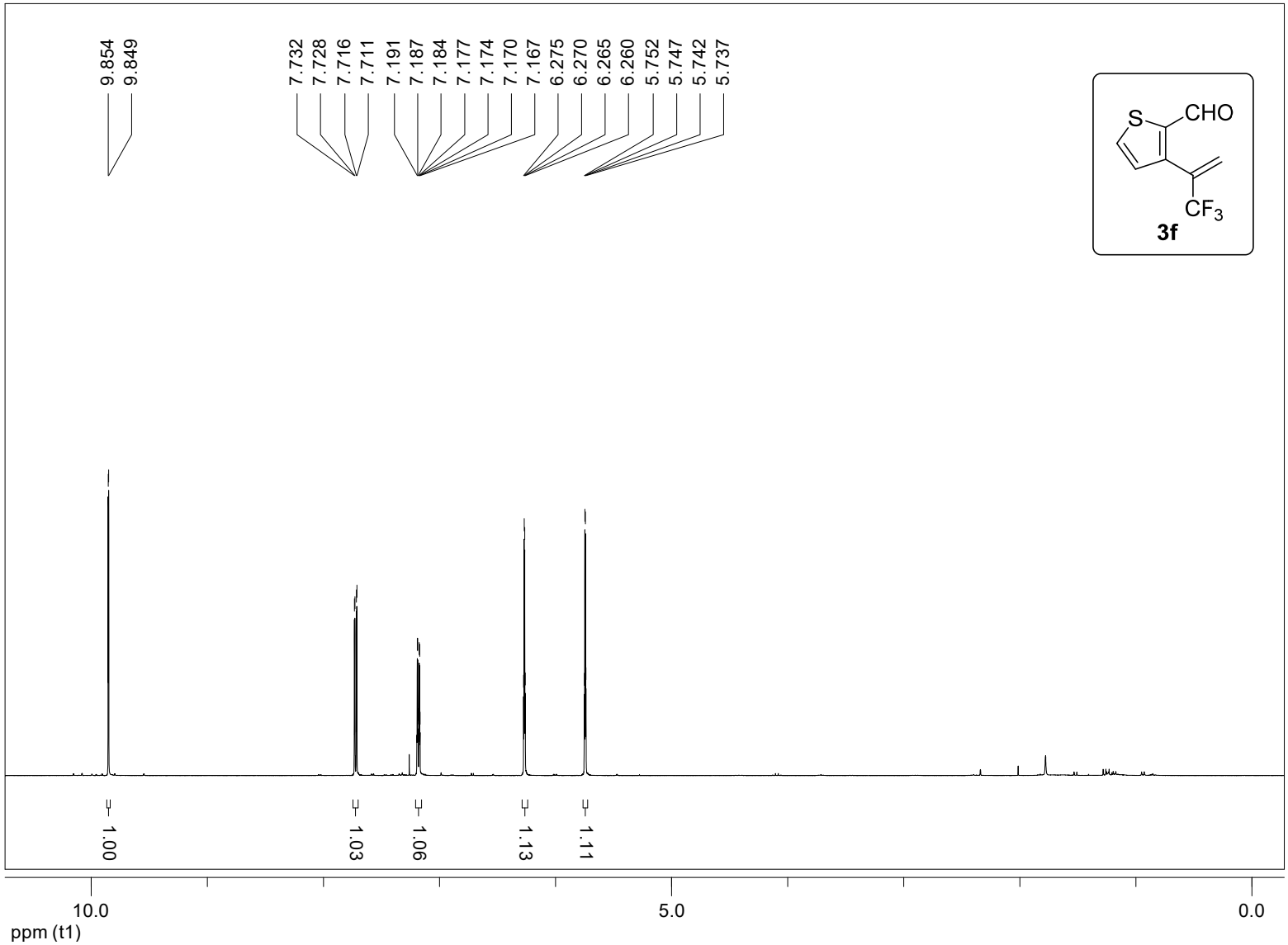
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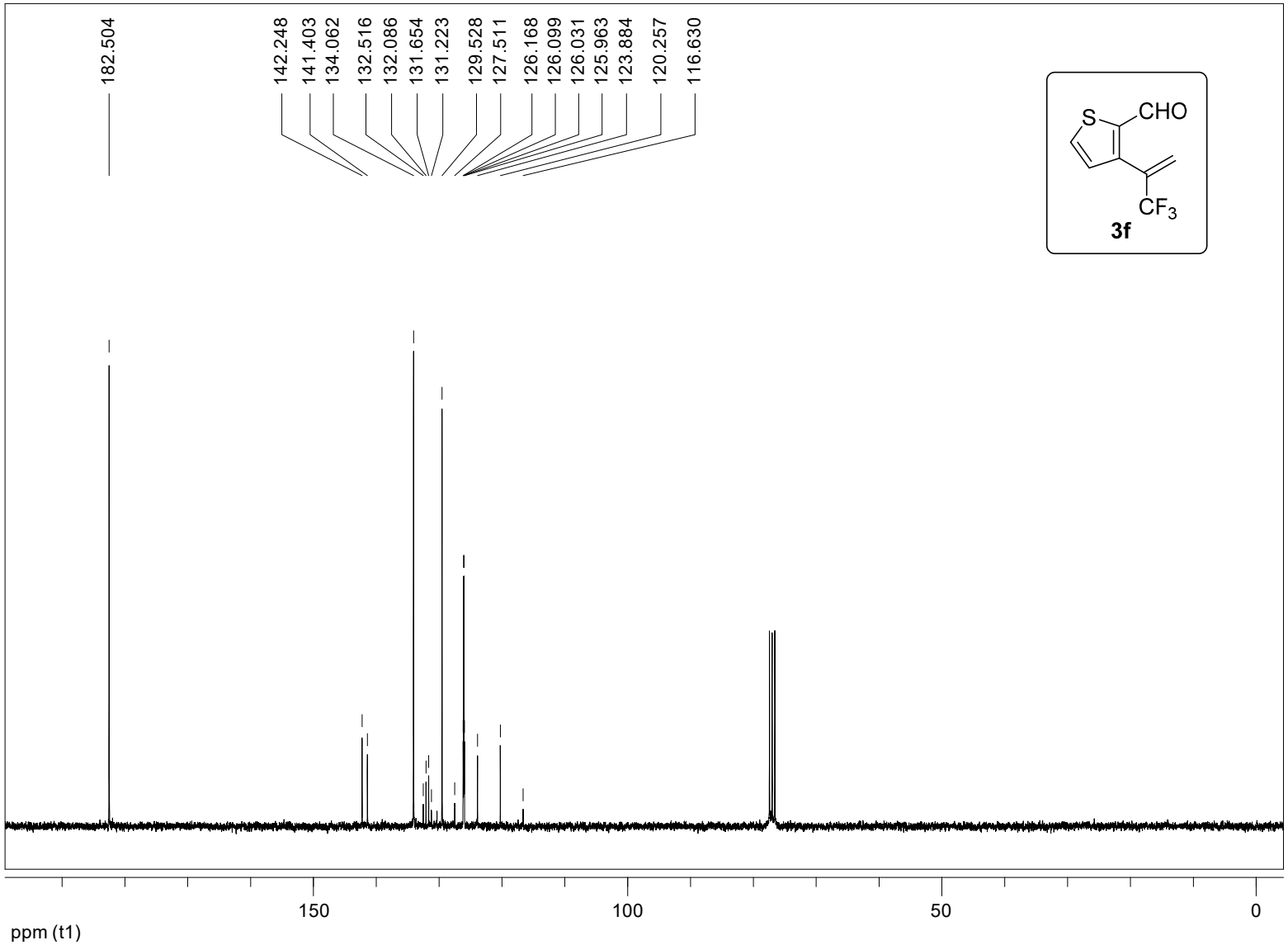
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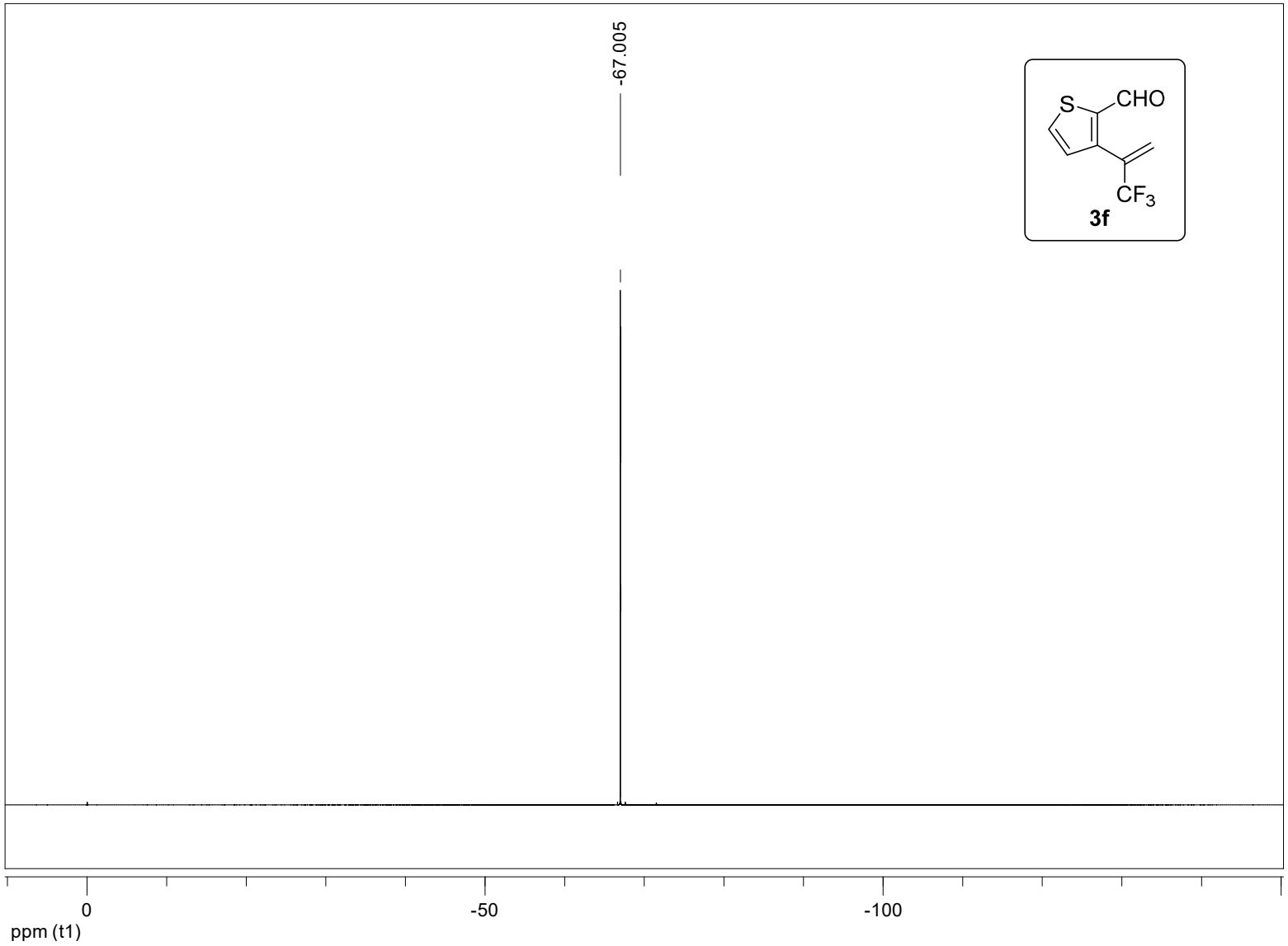
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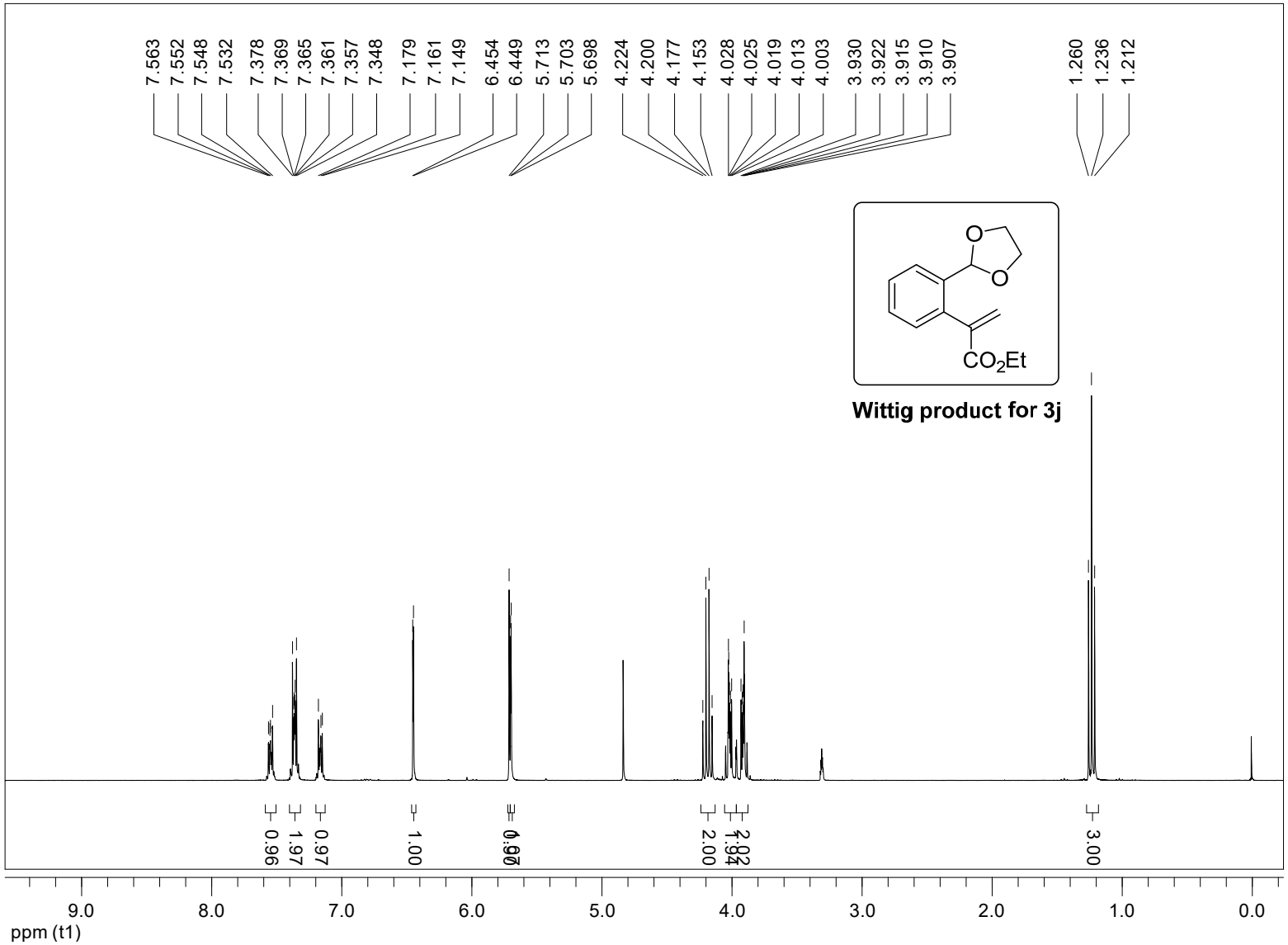
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3.915
3.910
3.907
1.260
1.236
1.212
O
O
CO2Et
Wittig product for 3j
0.96
1.97
0.97
1.00
0.97
0.90
2.00
2.02
1.94
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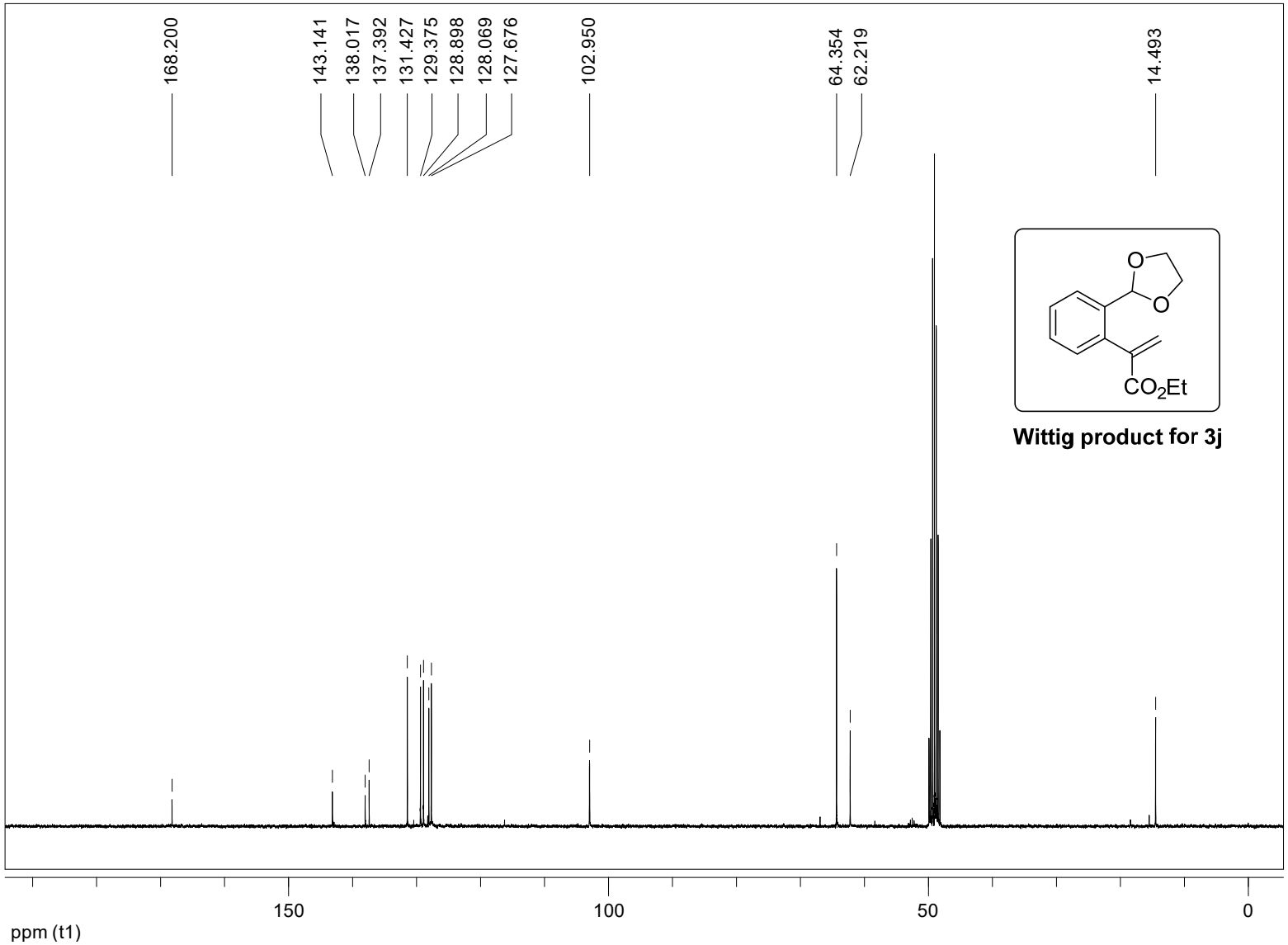
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CO2Et
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50
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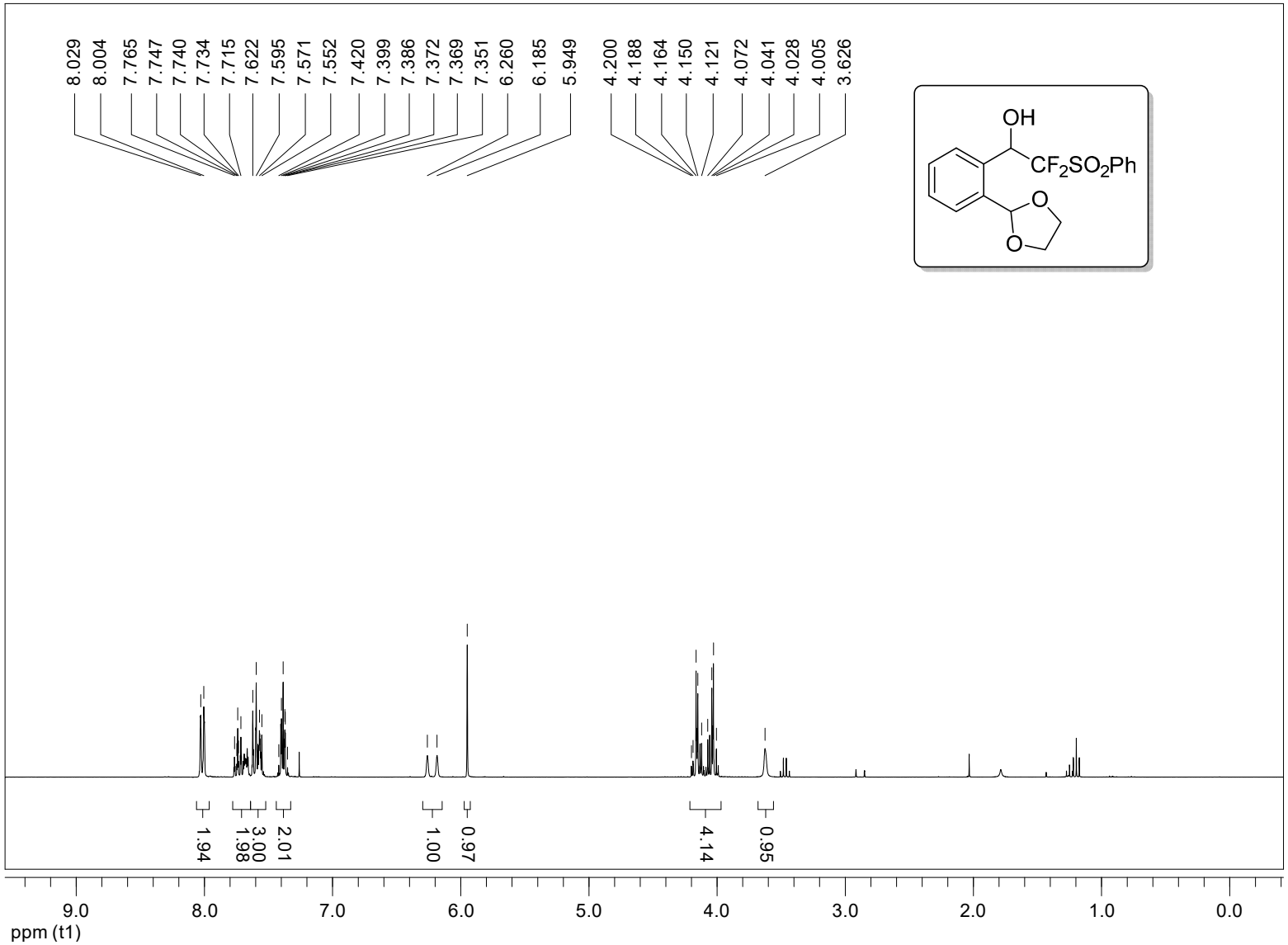
ppm (t1)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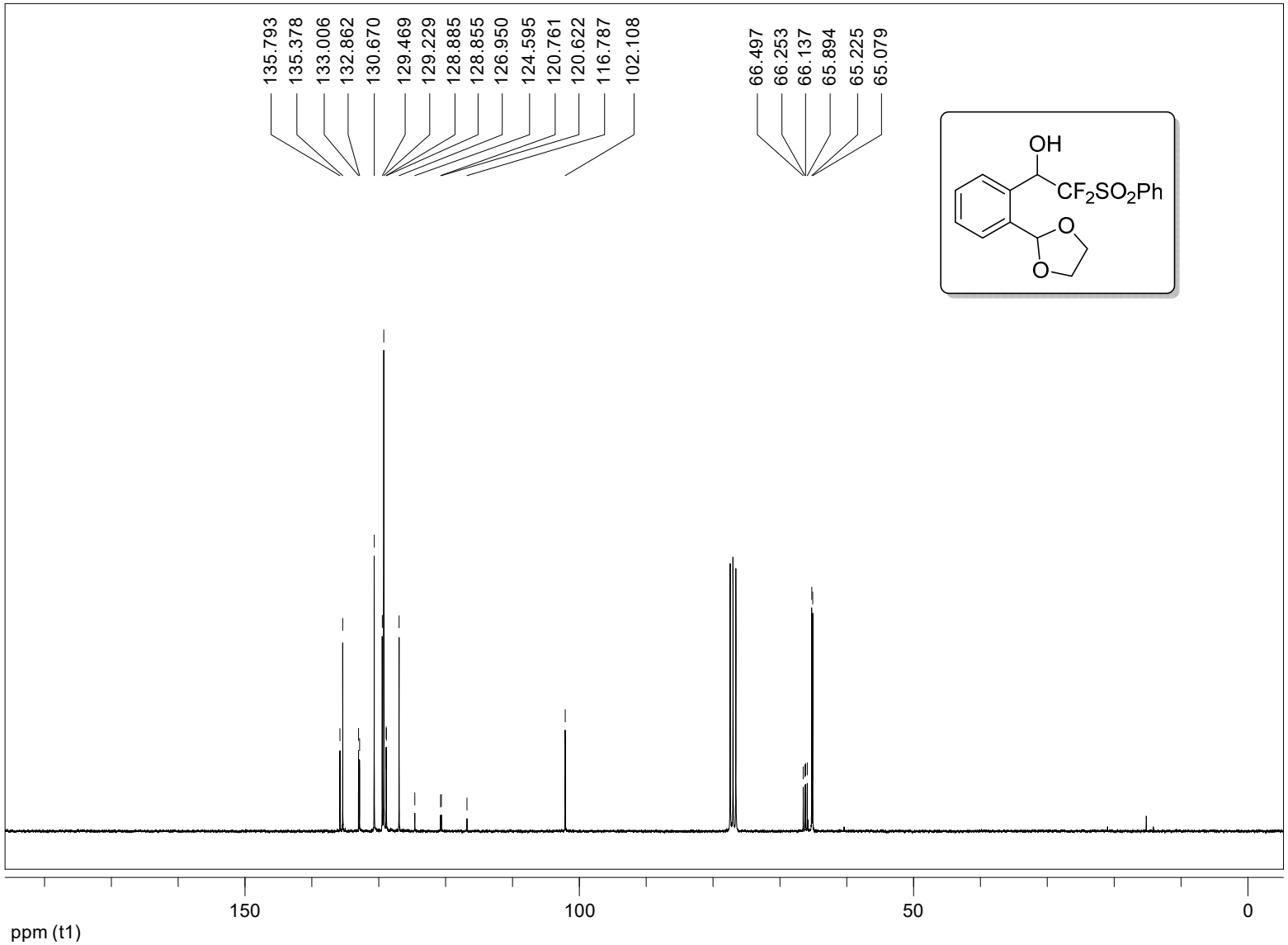
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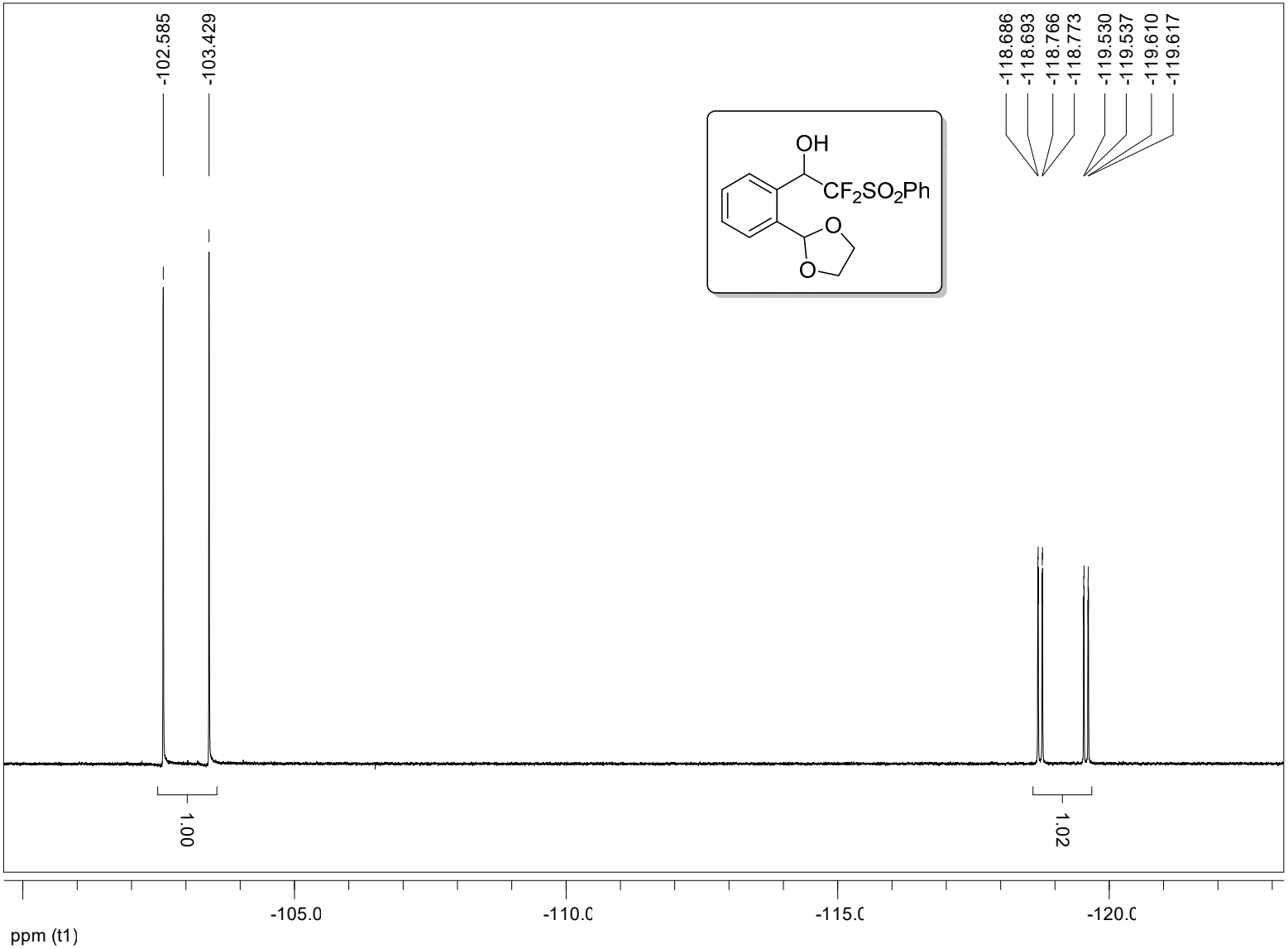
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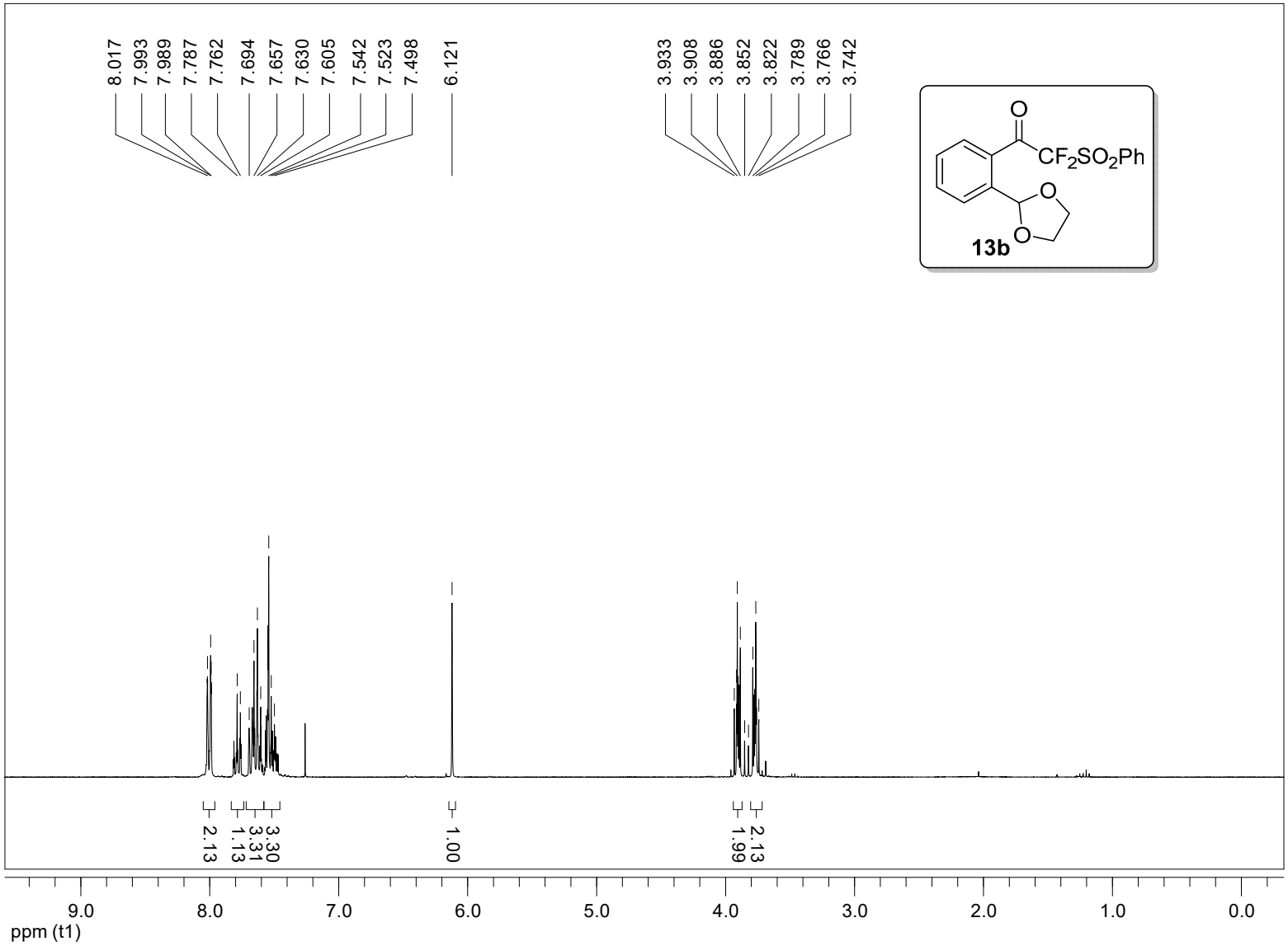
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3.933
3.908
3.886
3.852
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3.789
3.766
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O
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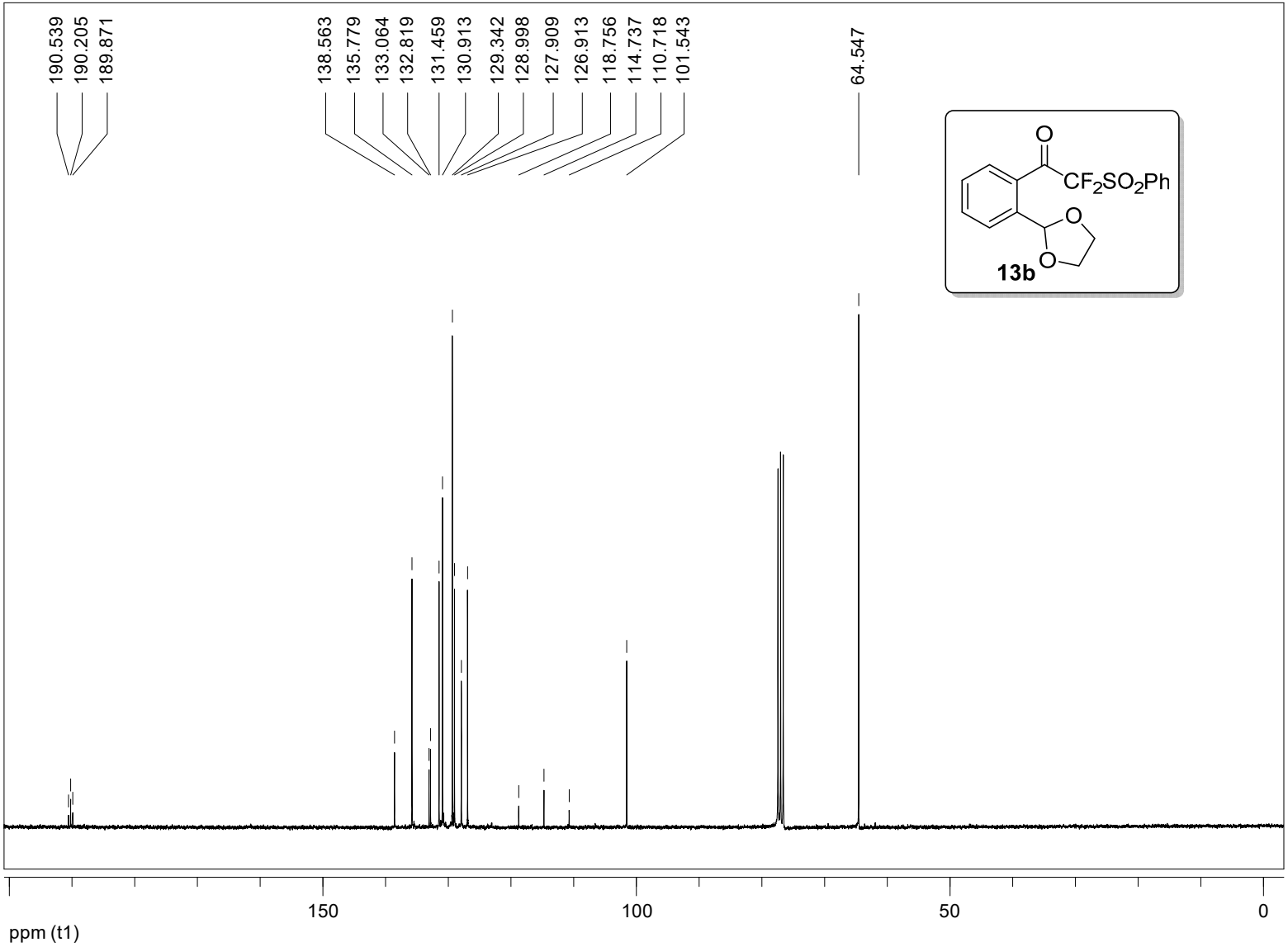
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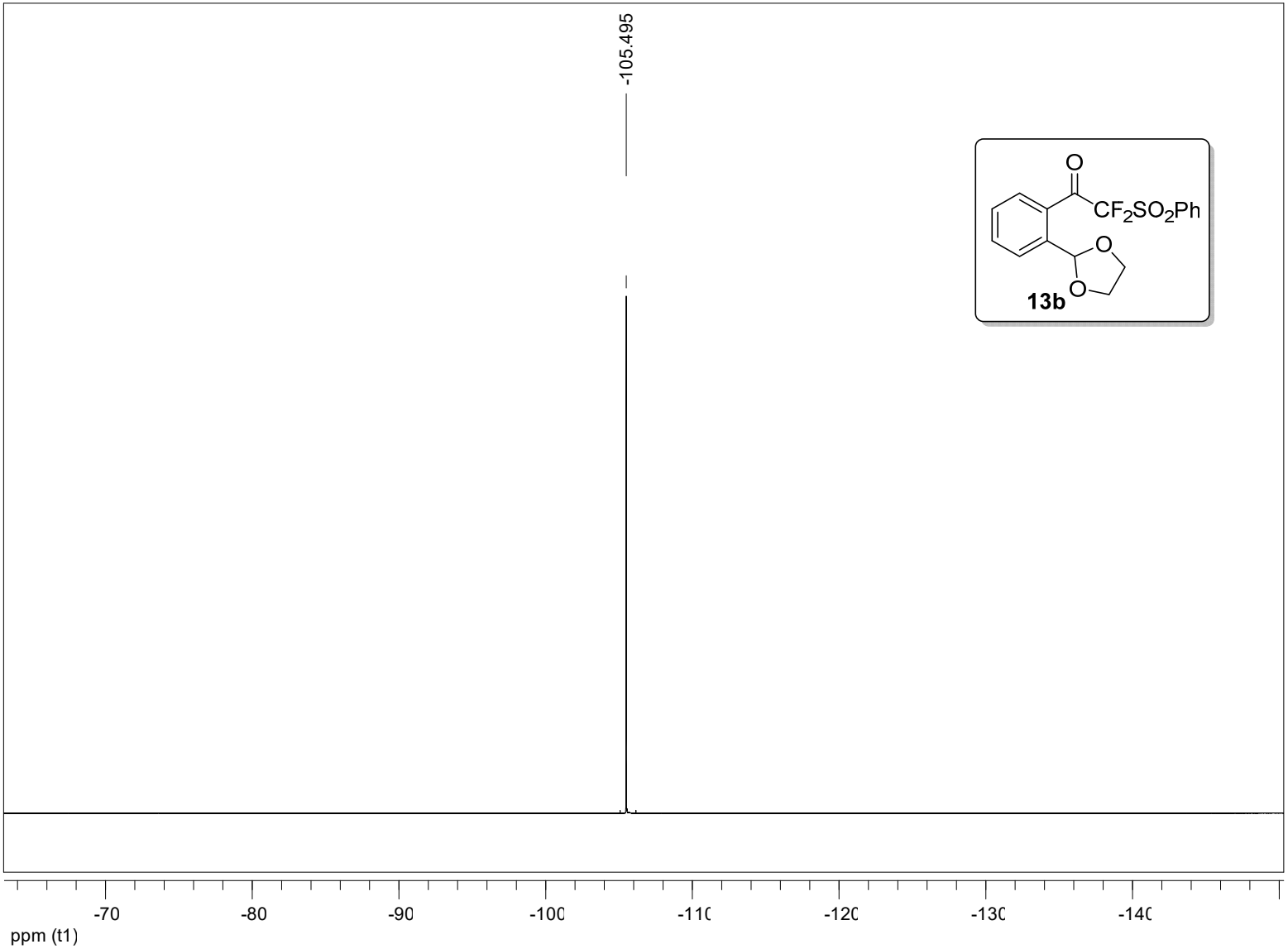
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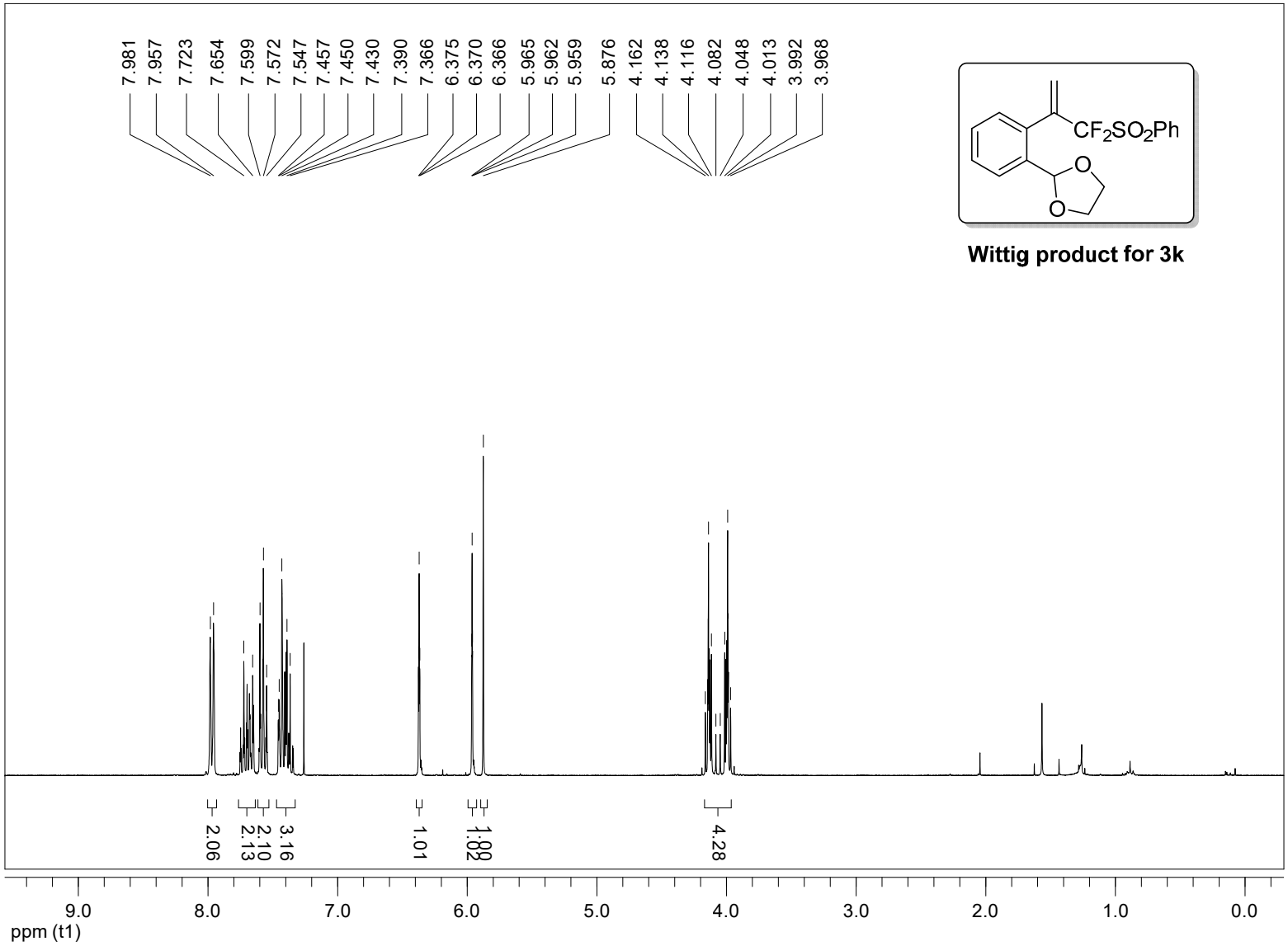
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7.547
7.457
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6.370
6.366
5.965
5.962
5.959
5.876
4.162
4.138
4.116
4.082
4.048
4.013
3.992
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CF2SO2Ph
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O
Wittig product for 3k
2.06
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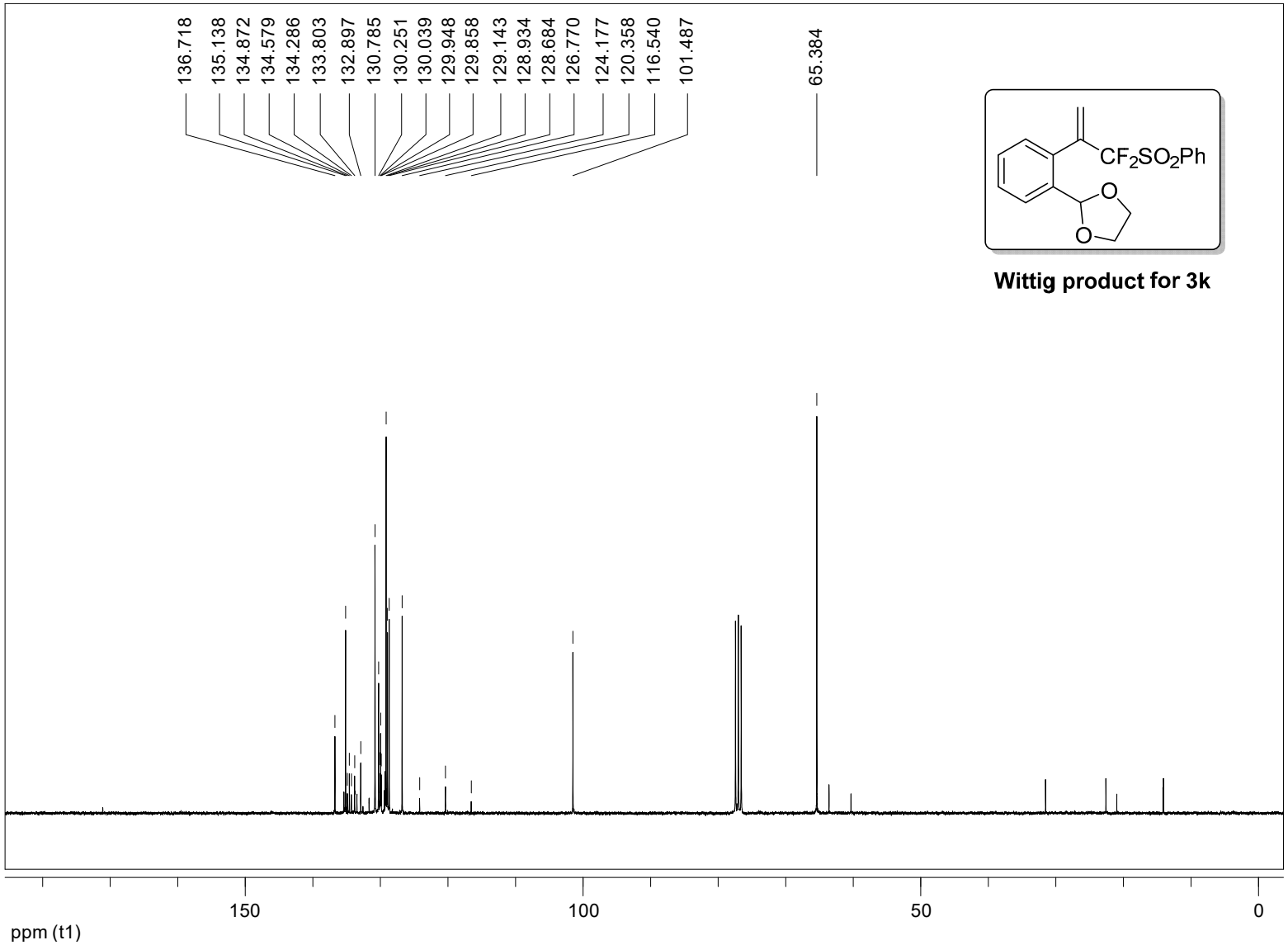
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124.177
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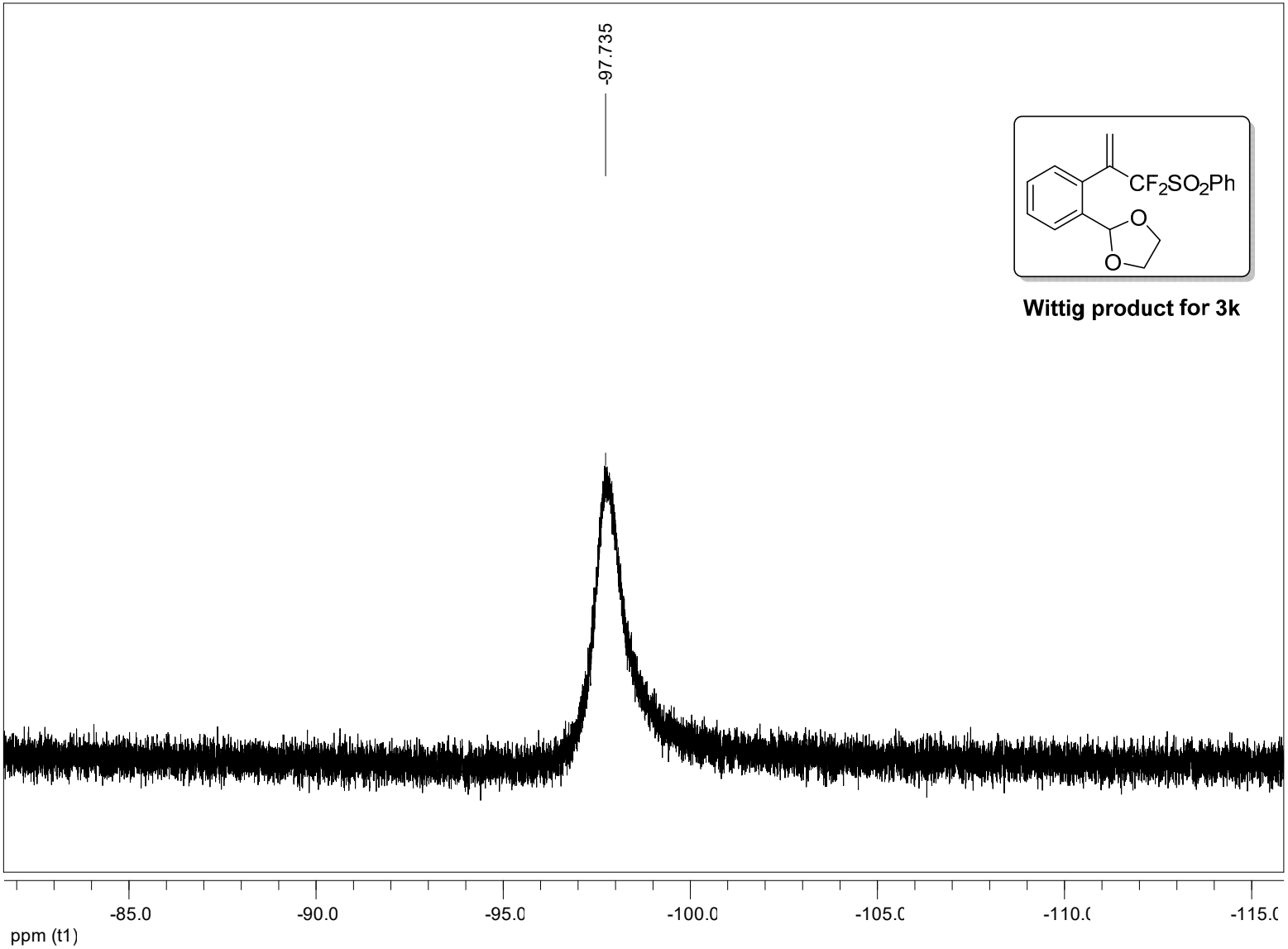
0
ppm (t1)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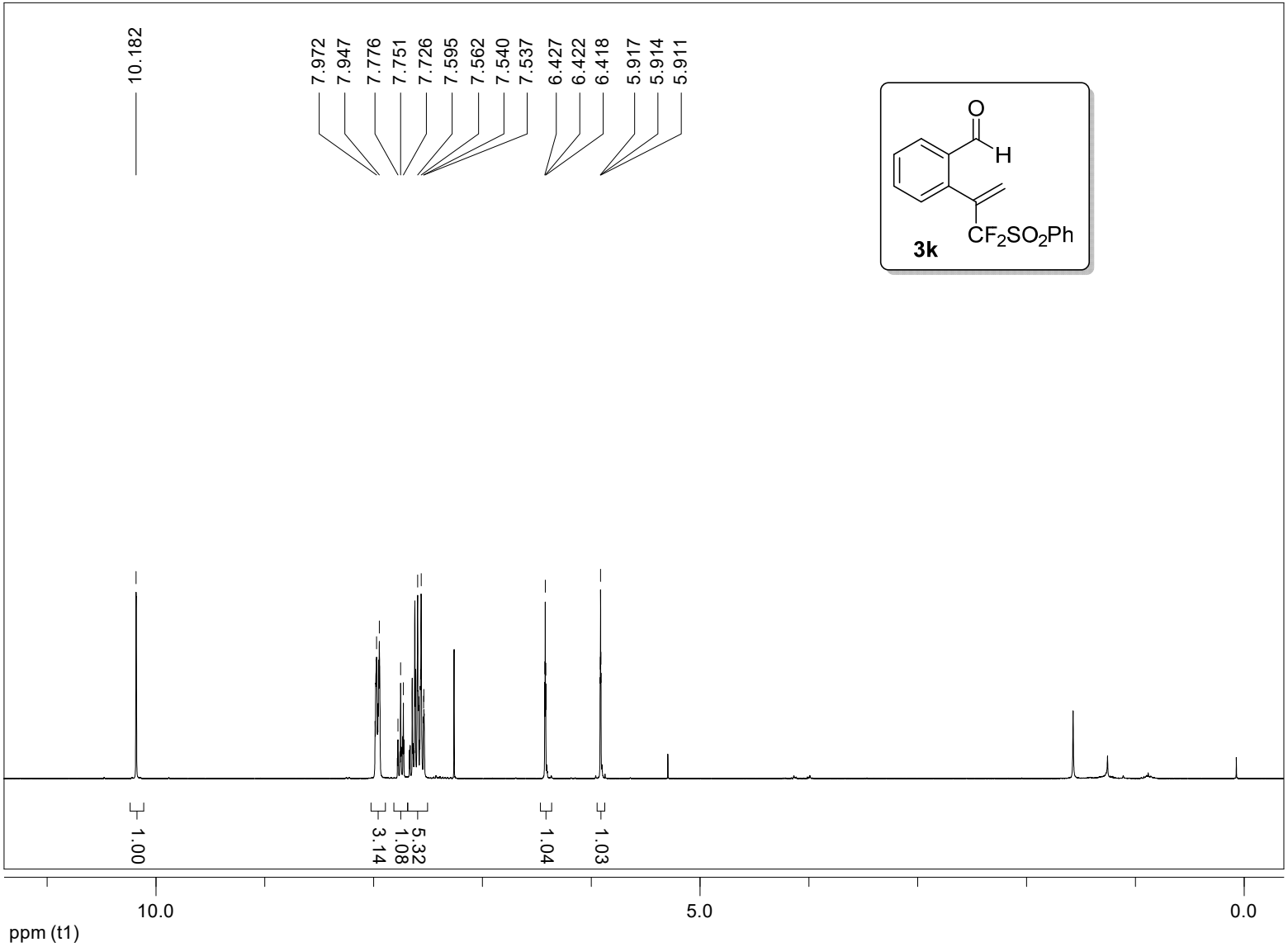
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O
H
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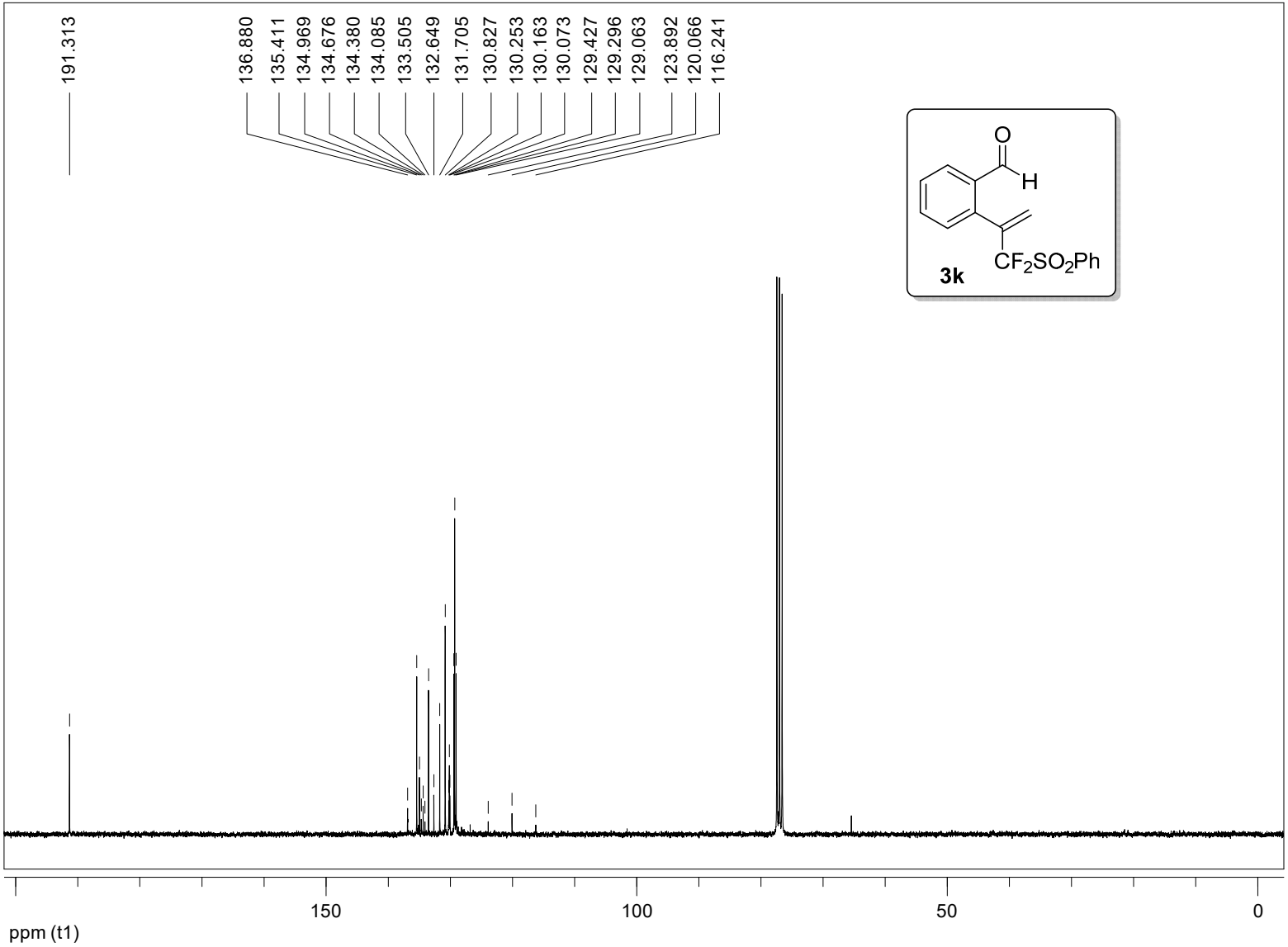
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129.427
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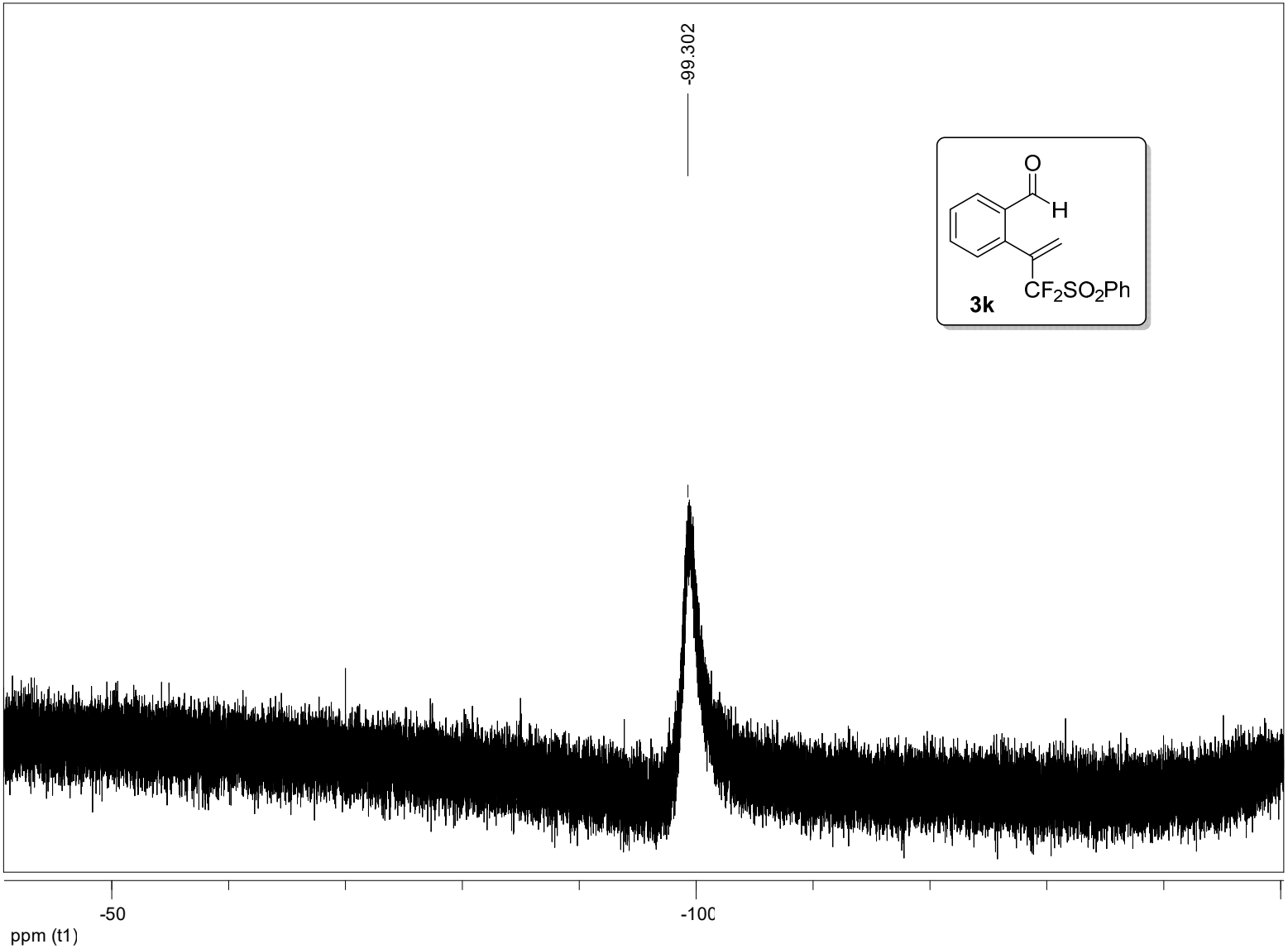
129.063
123.892
120.066
116.241
O
H
CF2SO2Ph
3k
150
100
50
0
ppm (t1)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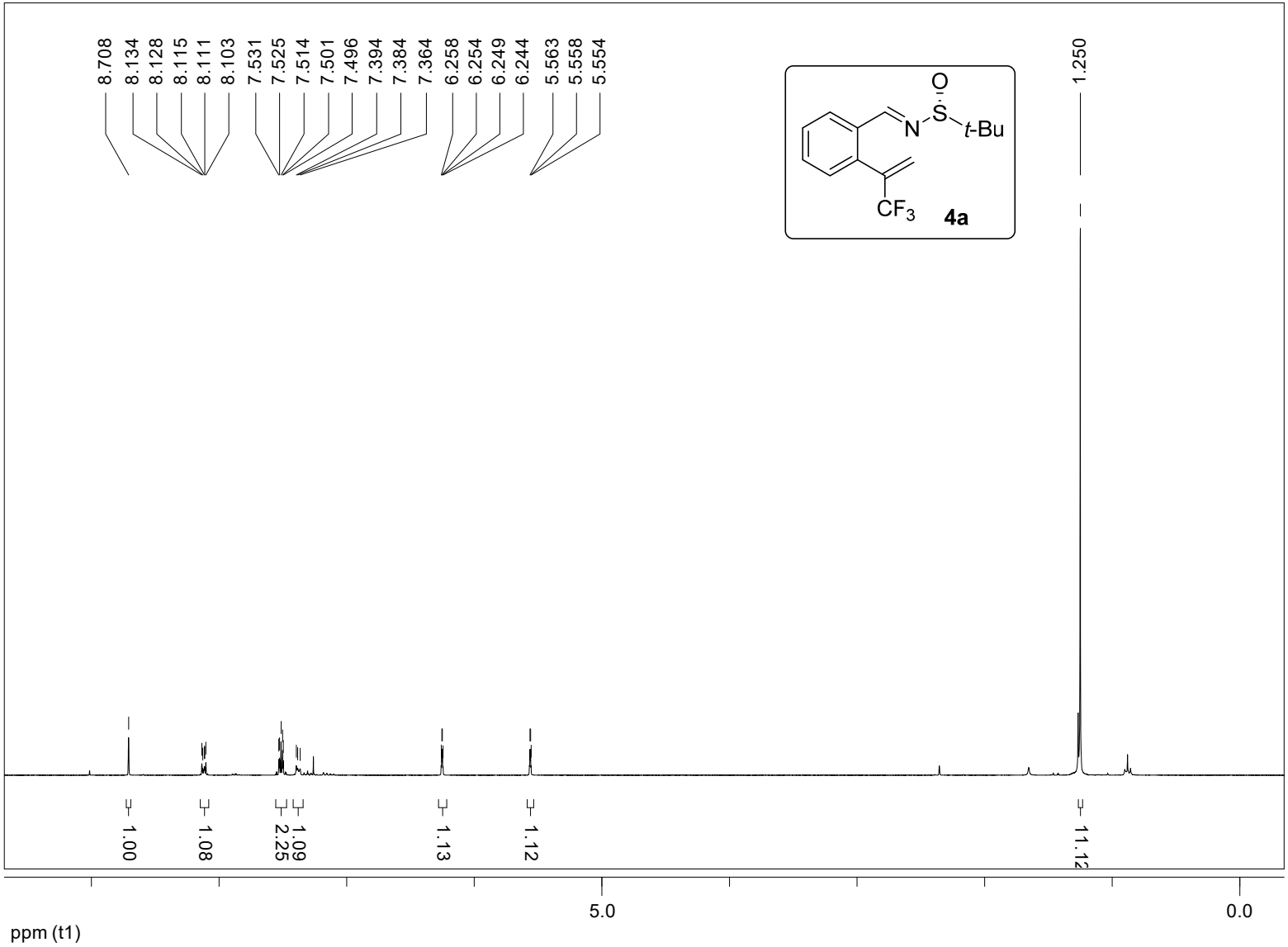
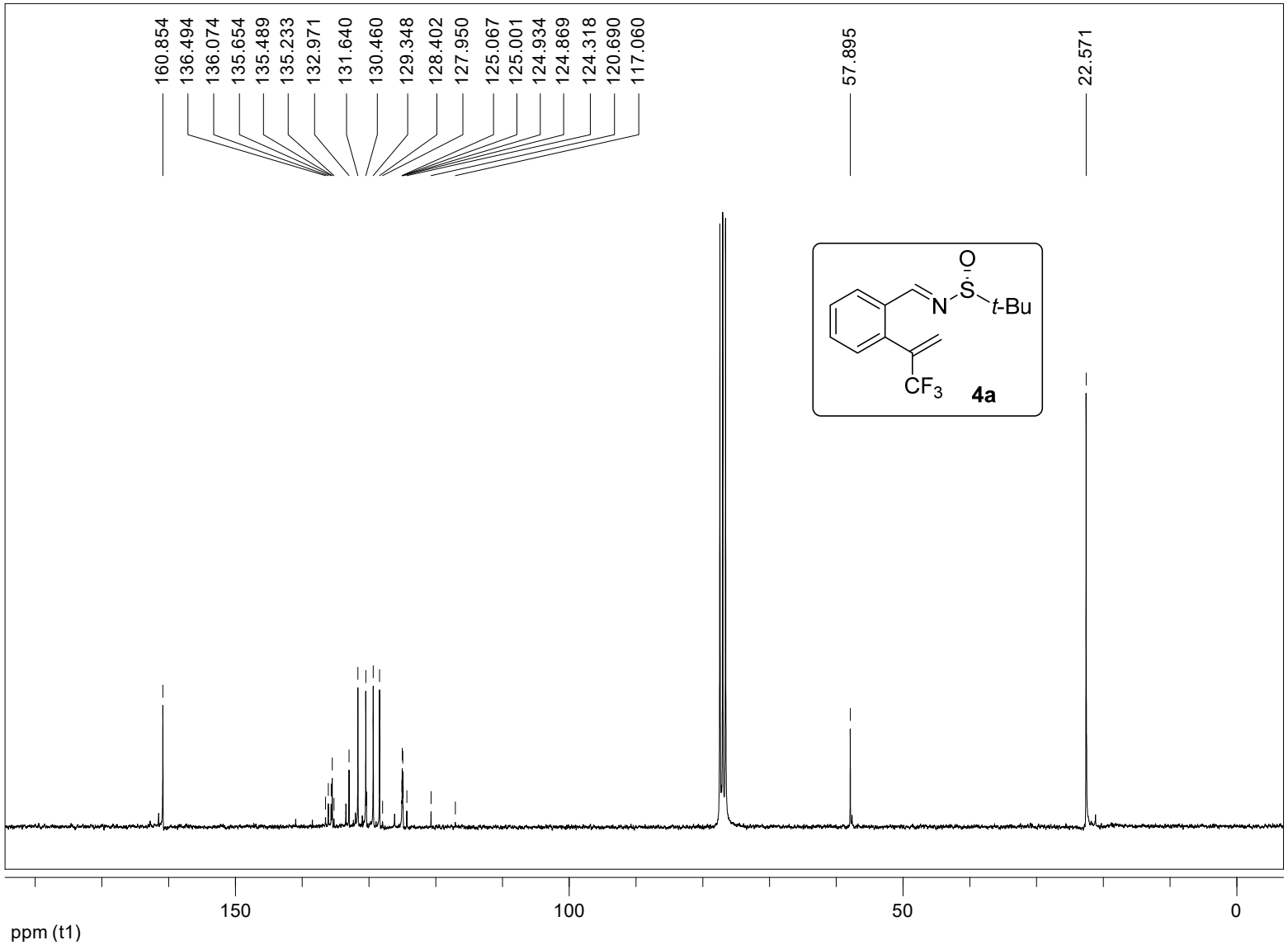
H
CF2SO2Ph
3k
-50
-100
ppm (t1)


8.708
8.134
8.128
8.115
8.111
8.103
7.531
7.525
7.514
7.501
7.496
7.394
7.384
7.364
6.258
6.254
6.249
6.244
5.563
5.558
5.554
1.250
O
S
N
t-Bu
CF3
4a
1.00
1.08
2.25
1.09
1.13
1.12
11.12
5.0
0.0
ppm (t1)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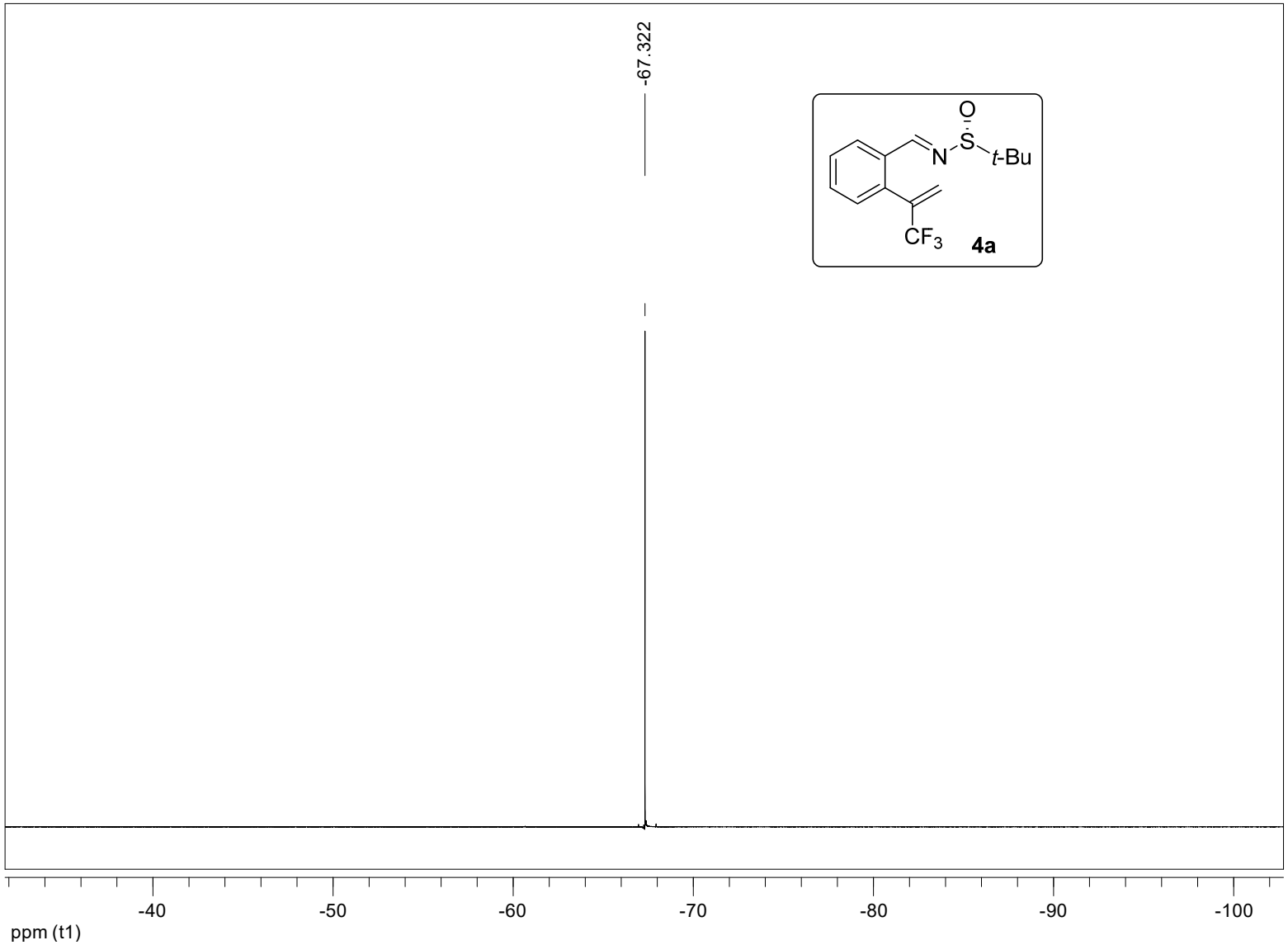
136.074
135.654
135.489
135.233
132.971
131.640
130.460
129.348
128.402
127.950
125.067
125.001
124.934
124.869
124.318
120.690
117.060
57.895
22.571
O
S
N
t-Bu
CF3
4a
150
100
50
0
ppm (t1)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S
N
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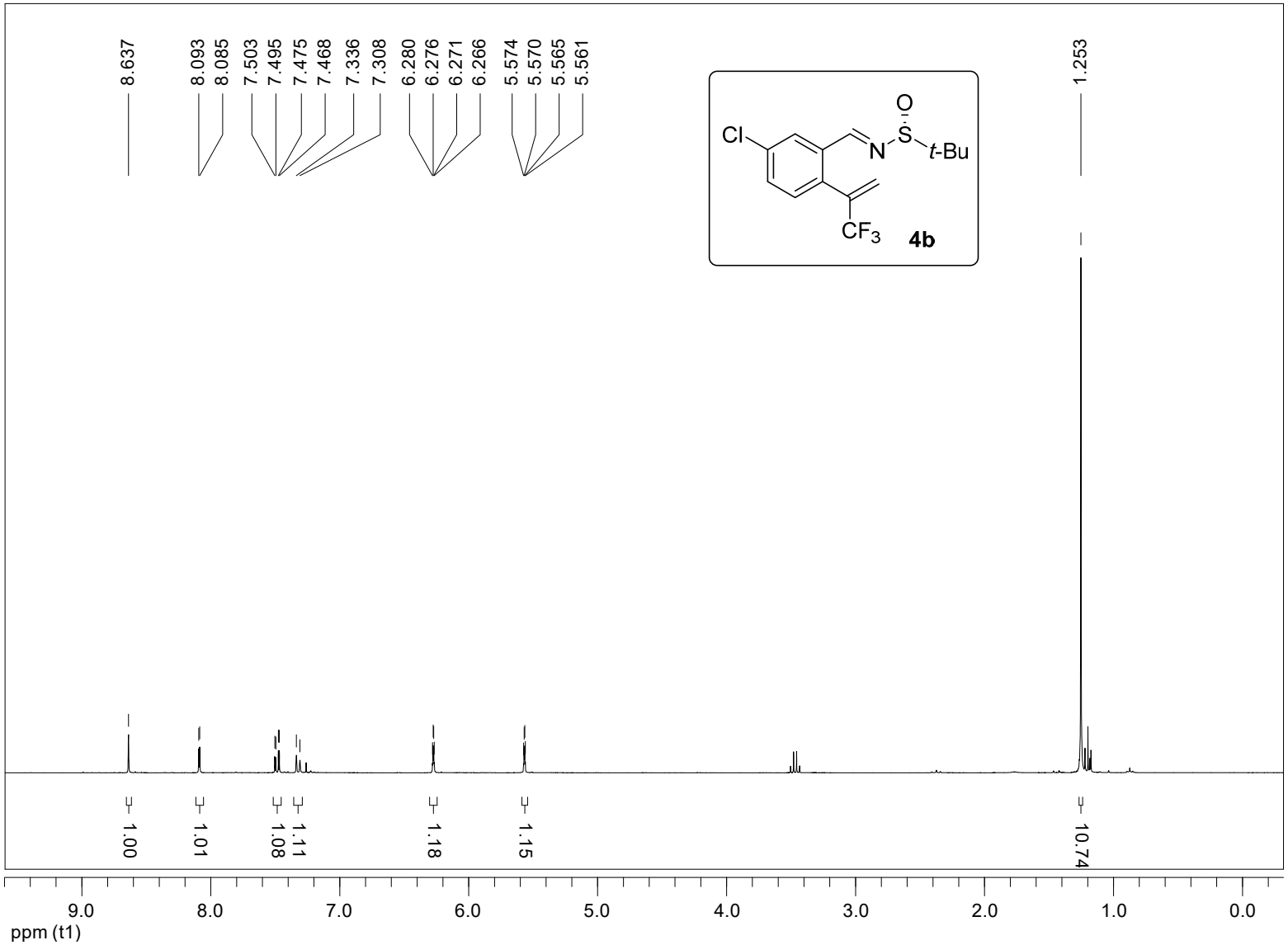
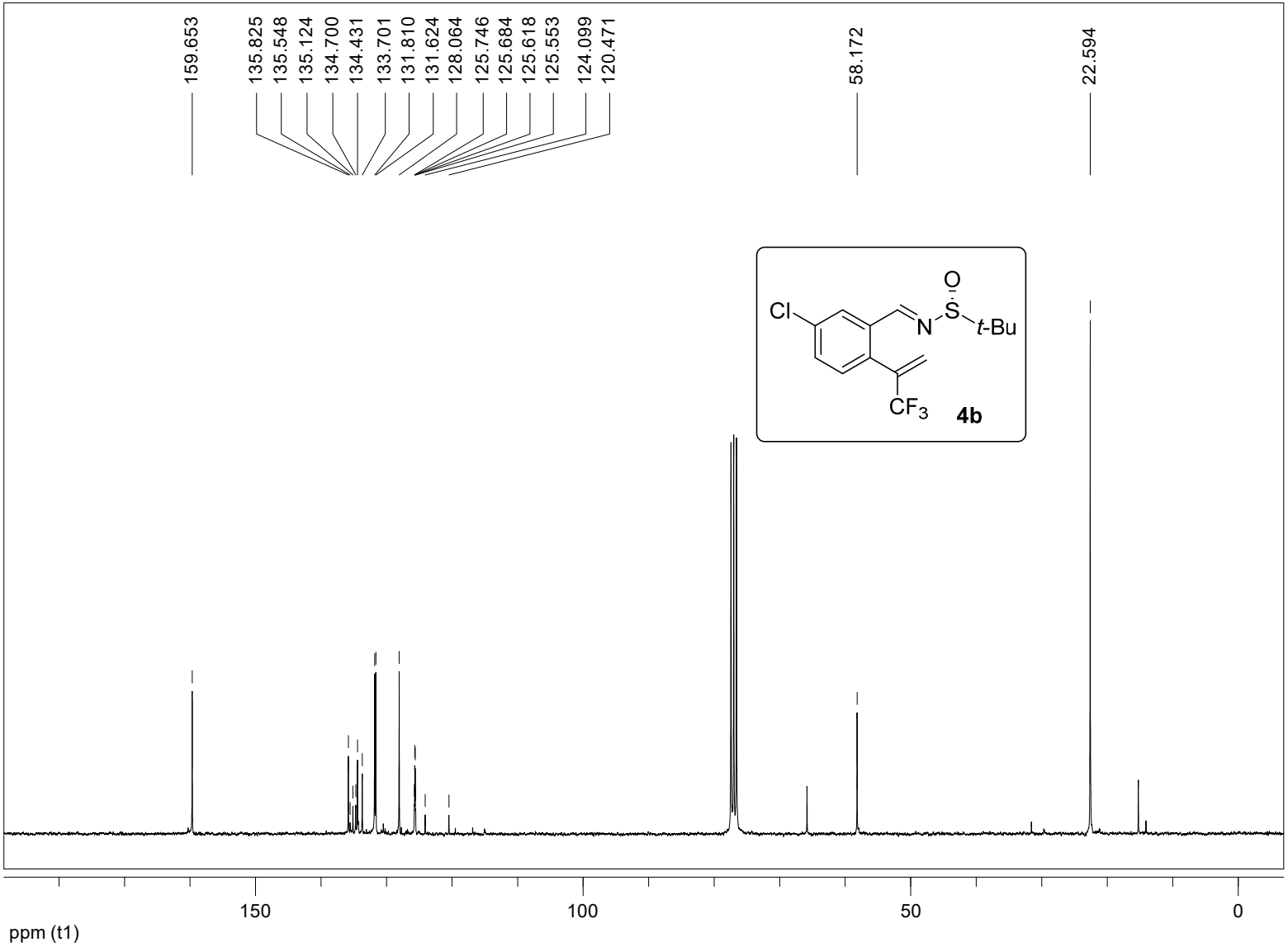
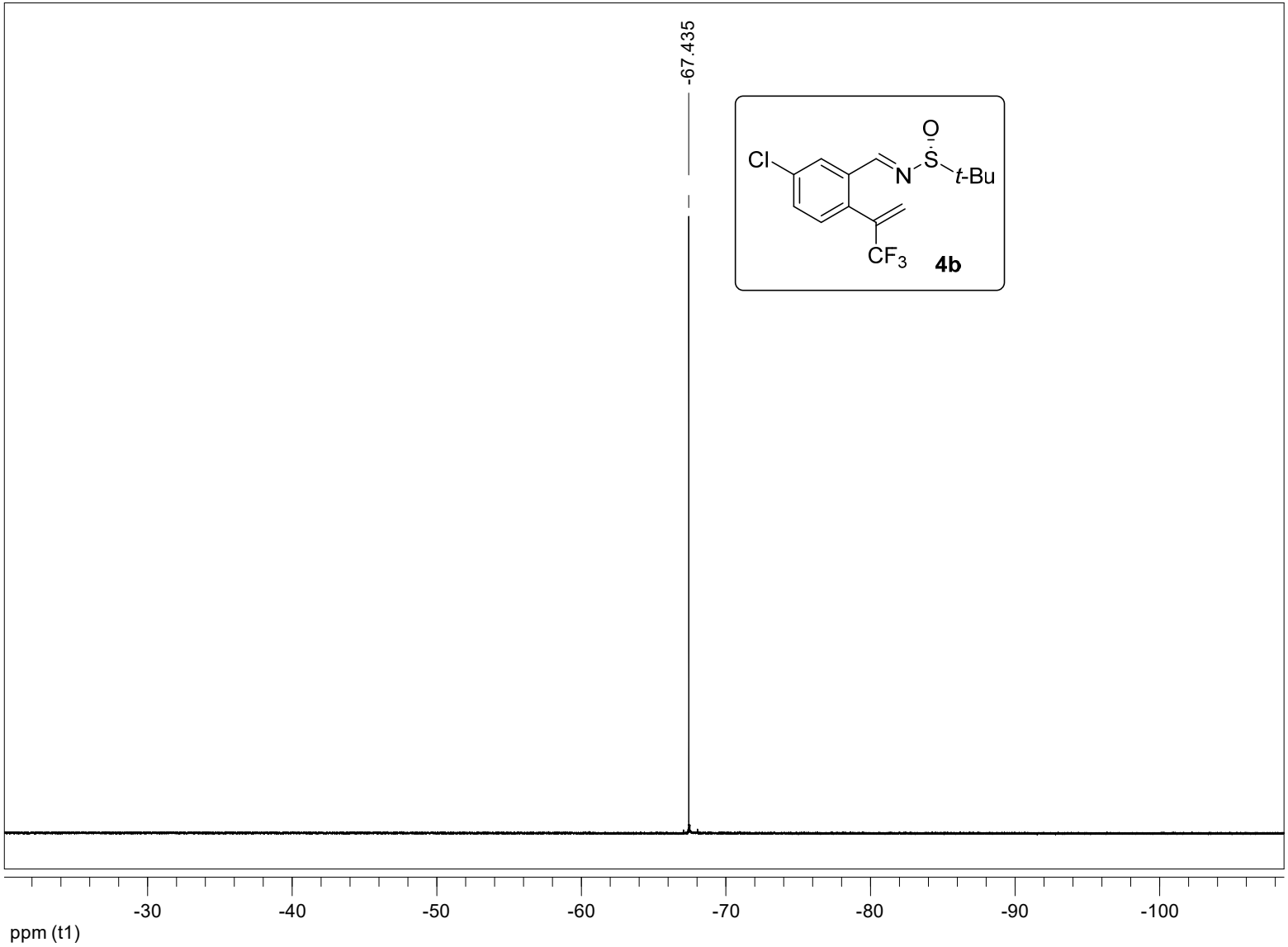
CF3
4a
-40
-50
-60
-70
-80
-90
-100
ppm (t1)


8.637
8.093
8.085
7.503
7.495
7.475
7.468
7.336
7.308
6.280
6.276
6.271
6.266
5.574
5.570
5.565
5.561
1.253
Cl
N
S
O
t-Bu
CF3
4b
1.00
1.01
1.08
1.11
1.18
1.15
10.74
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


159.653
135.825
135.548
135.124
134.700
134.431
133.701
131.810
131.624
128.064
125.746
125.684
125.618
125.553
124.099
120.471
58.172
22.594
Cl
N
S
O
t-Bu
CF3
4b
150
100
50
0
ppm (t1)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Cl
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S
O
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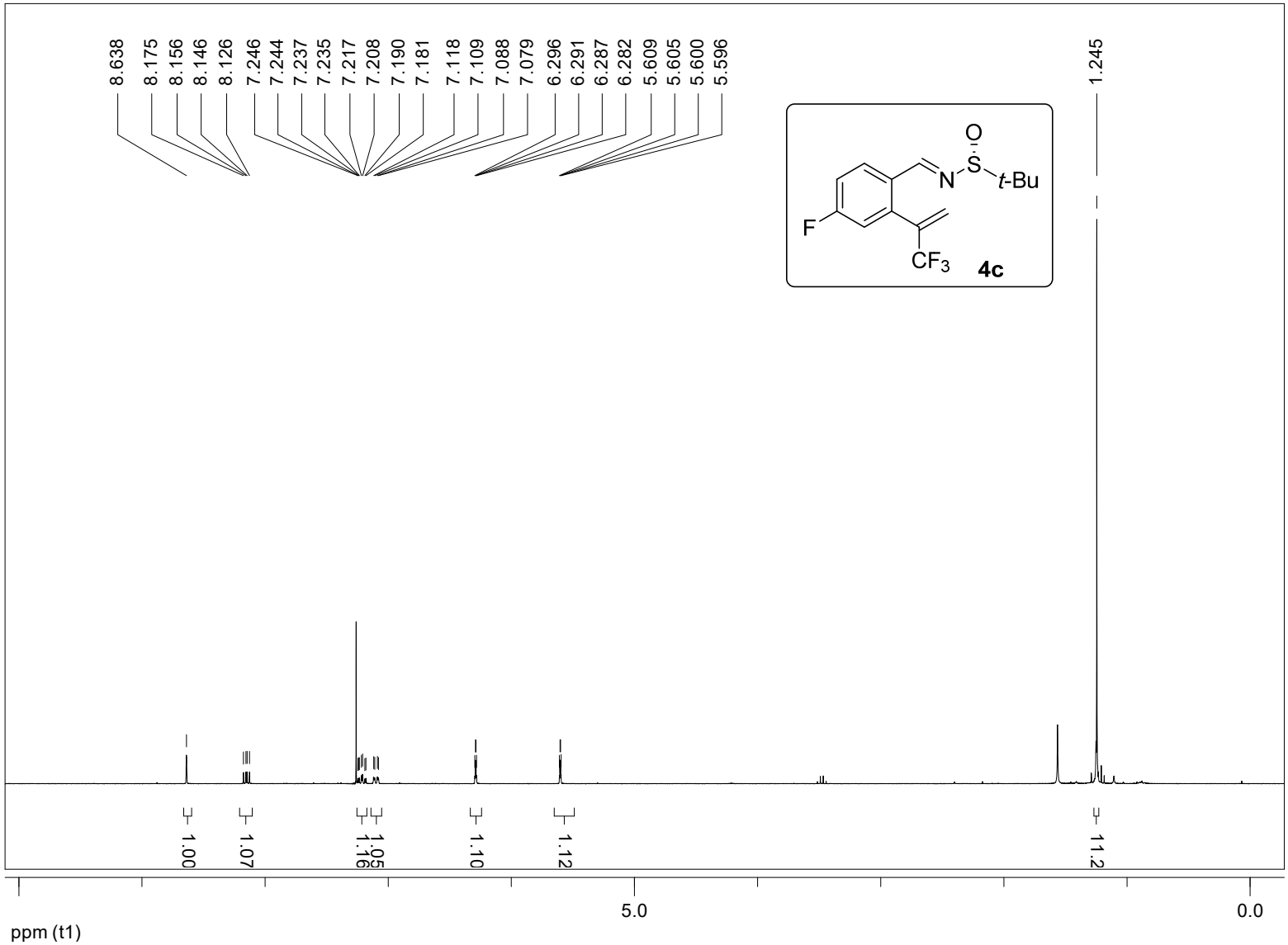
CF3
4b
-30
-40
-50
-60
-70
-80
-90
-100
ppm (t1)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8.175
8.156
8.146
8.126
7.246
7.244
7.237
7.235
7.217
7.208
7.190
7.181
7.118
7.109
7.088
7.079
6.296
6.291
6.287
6.282
5.609
5.605
5.600
5.596
1.245
O
S
N
t-Bu
F
CF3
4c
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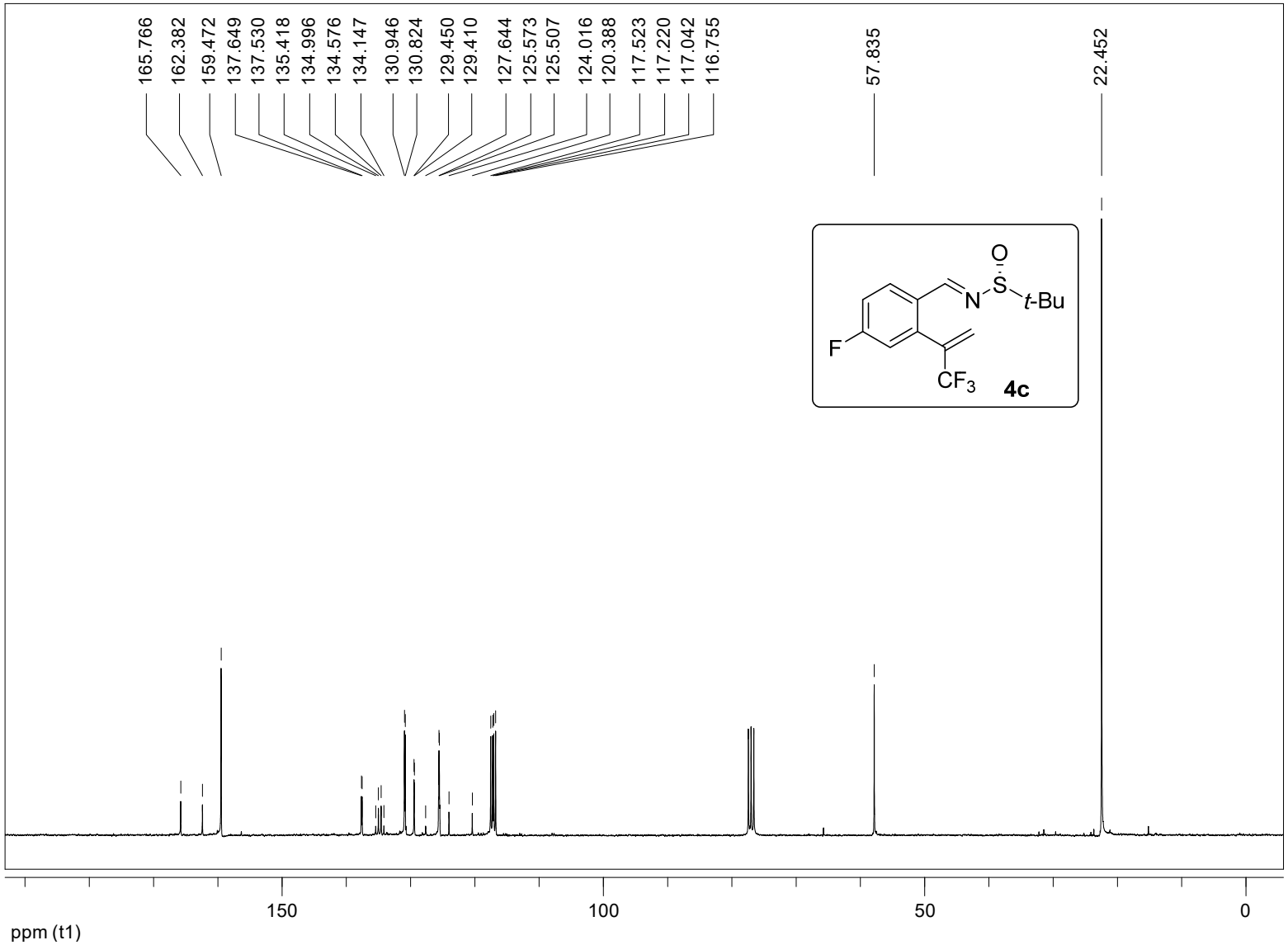
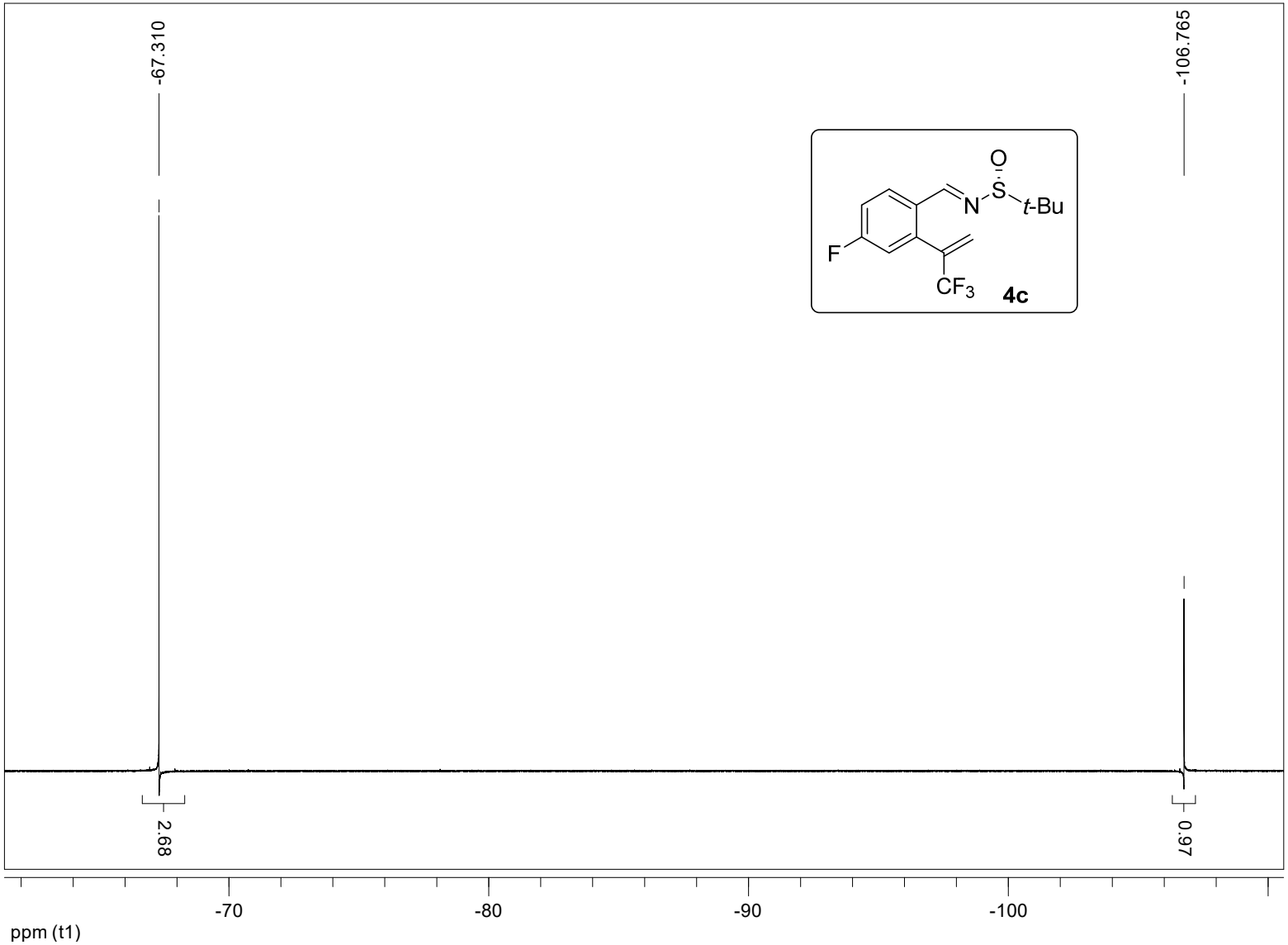
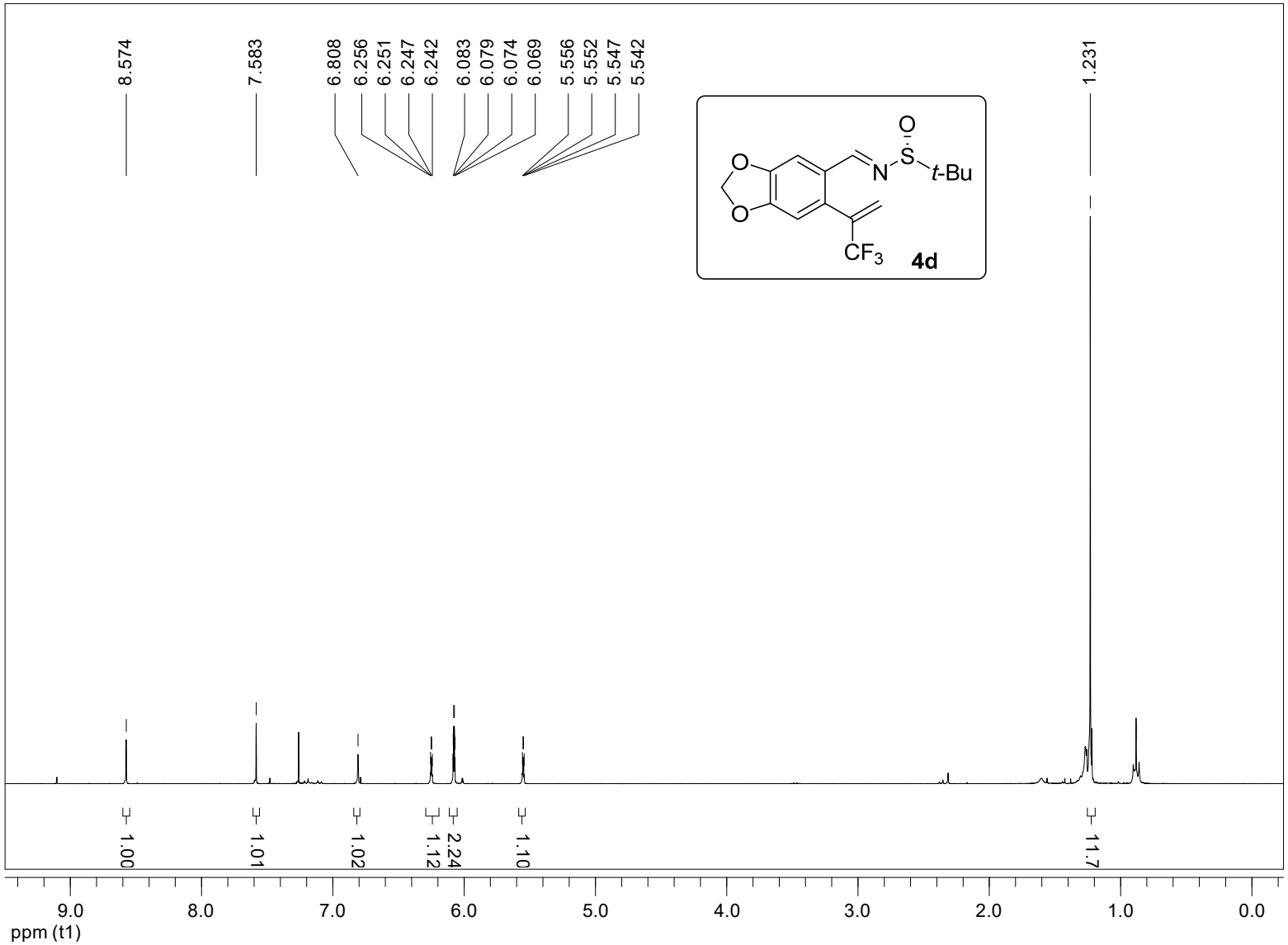
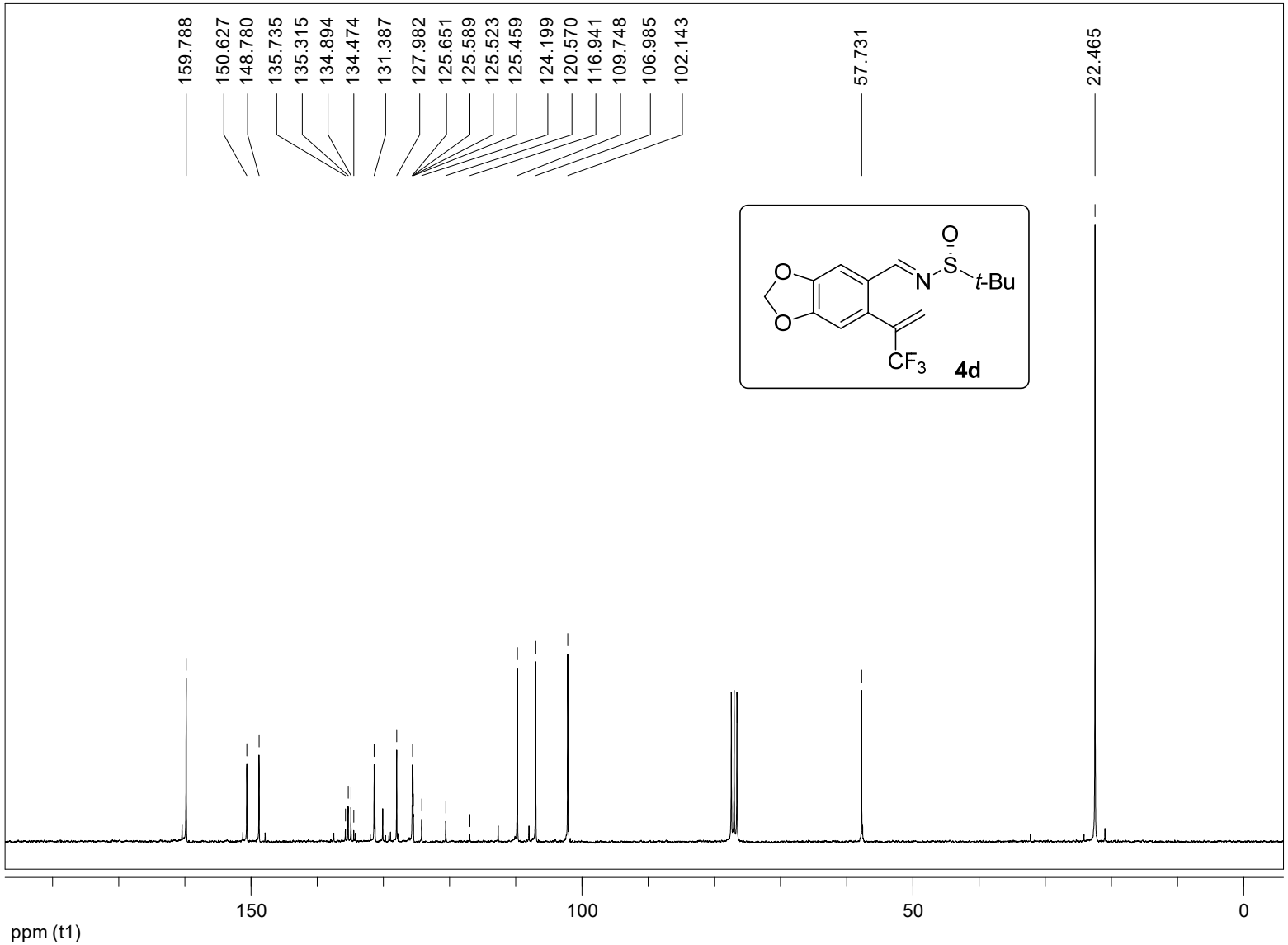
1.07
1.16
1.05
1.10
1.12
11.2
5.0
0.0
ppm (t1)


165.766
162.382
159.472
137.649
137.530
135.418
134.996
134.576
134.147
130.946
130.824
129.450
129.410
127.644
125.573
125.507
124.016
120.388
117.523
117.220
117.042
116.755
57.835
22.452
O
S
N
t-Bu
F
CF3
4c
150
100
50
0
ppm (t1)


-67.310
-106.765
2.68
0.97
-70
-80
-90
-100
ppm (t1)
O
S
N
t-Bu
F
CF3
4c


8.574
7.583
6.808
6.256
6.251
6.247
6.242
6.083
6.079
6.074
6.069
5.556
5.552
5.547
5.542
1.231
O
S
N
t-Bu
O
O
CF3
4d
1.00
1.01
1.02
1.12
2.24
1.10
11.7
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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148.780
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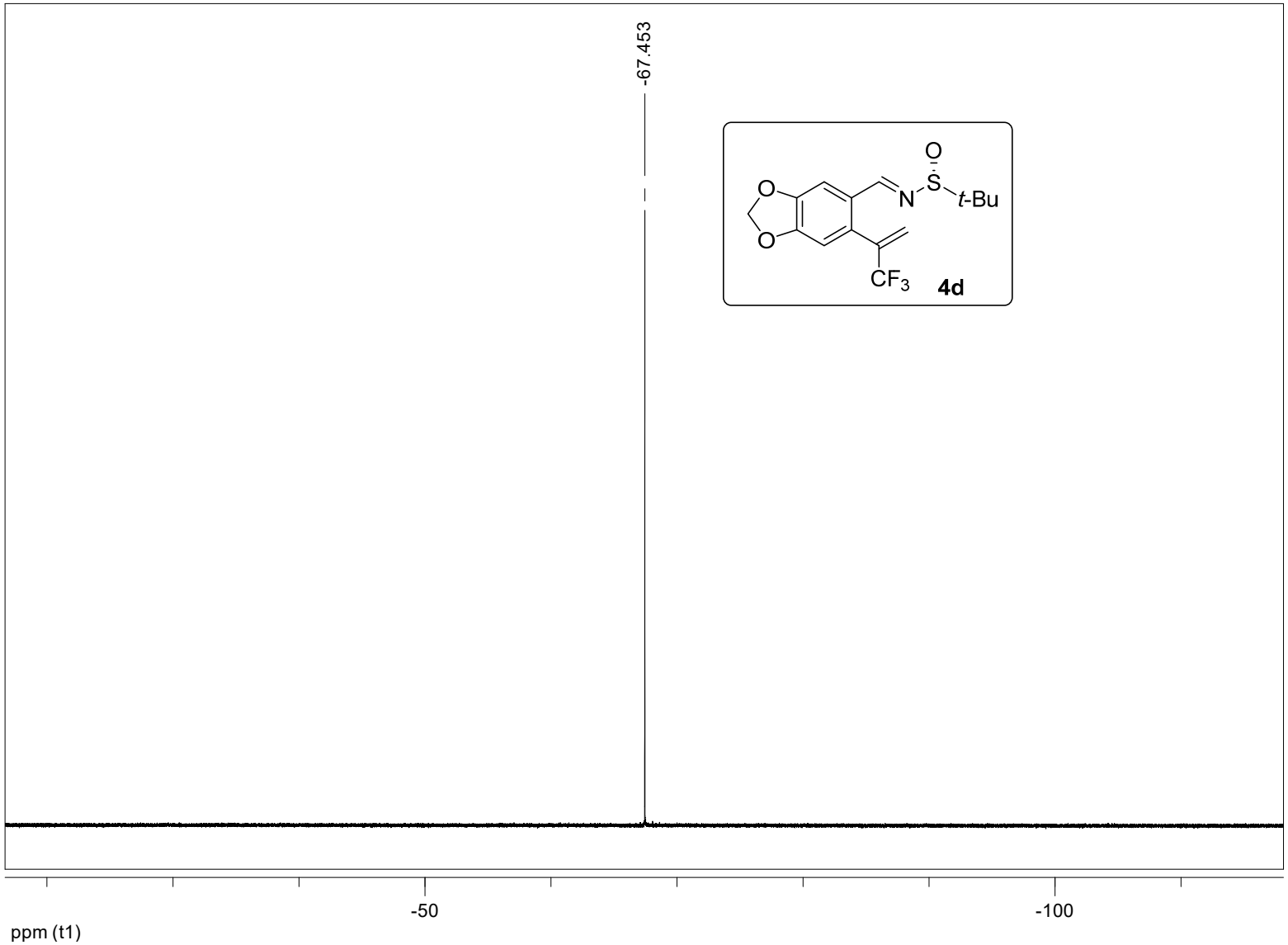
134.474
131.387
127.982
125.651
125.589
125.523
125.459
124.199
120.570
116.941
109.748
106.985
102.143
57.731
22.465
O
S
N
t-Bu
O
O
CF3
4d
150
100
50
0
ppm (t1)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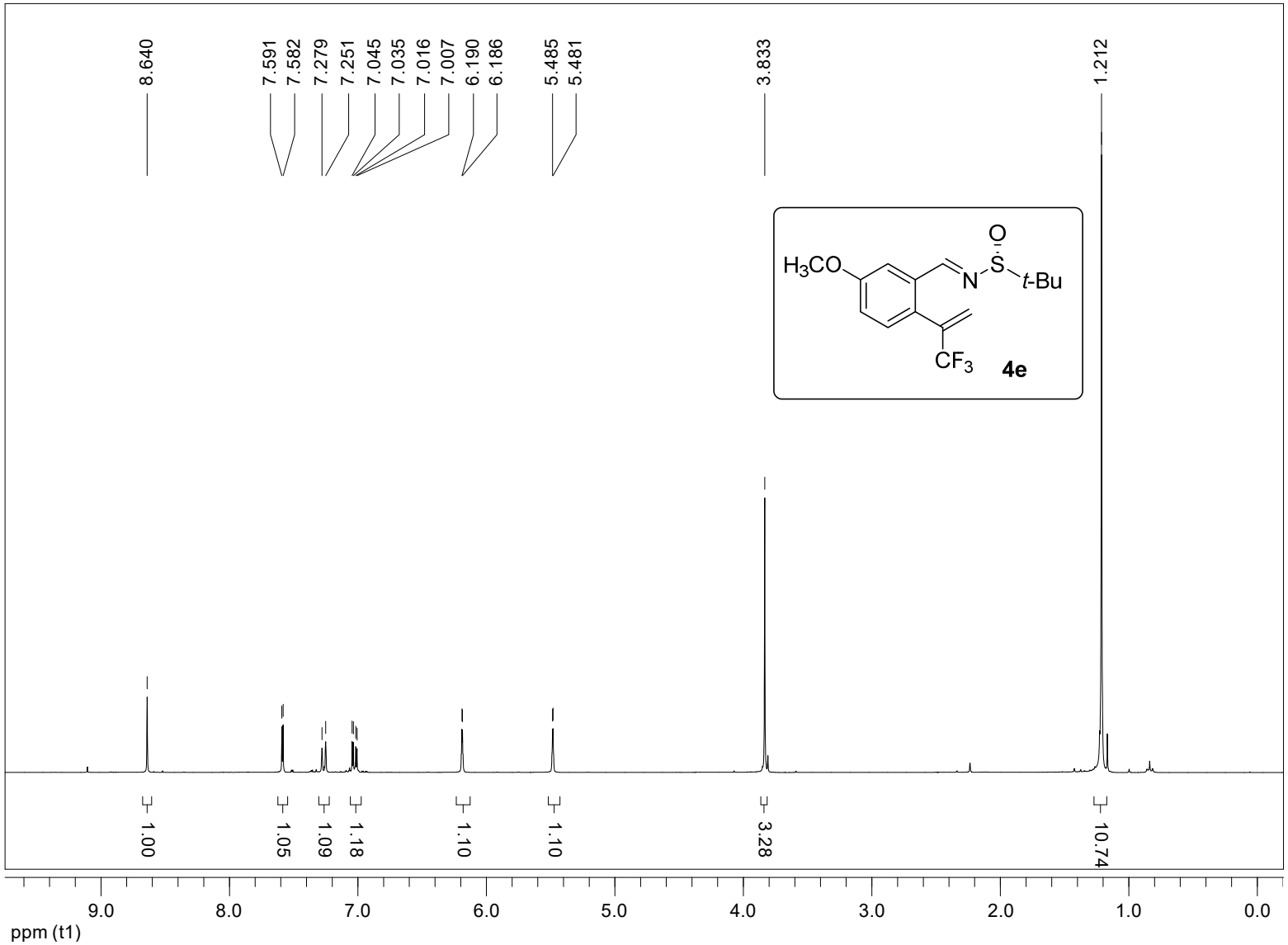
S
N
t-Bu
O
O
CF3
4d
-50
-100
ppm (t1)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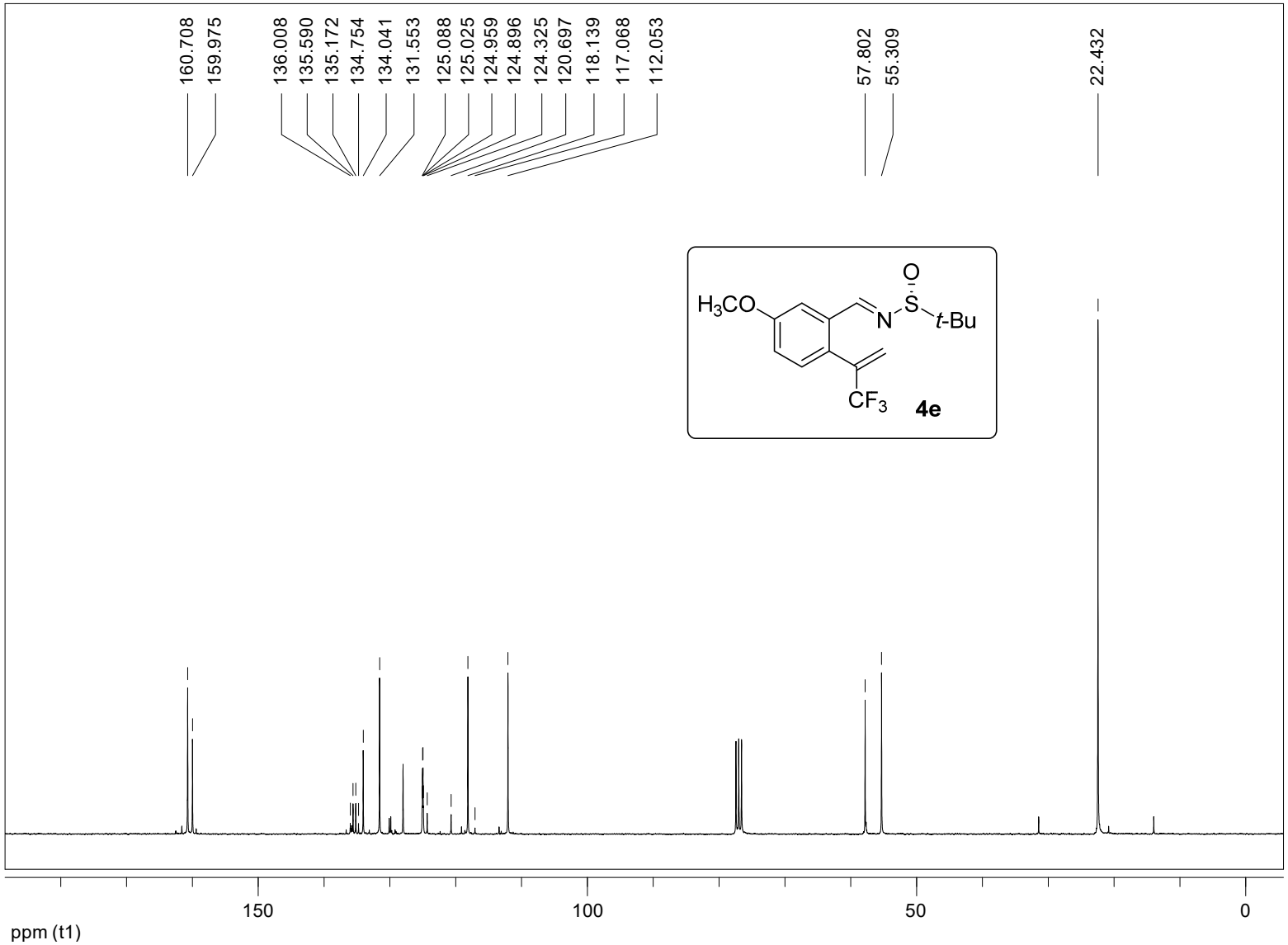
7.279
7.251
7.045
7.035
7.016
7.007
6.190
6.186
5.485
5.481
3.833
1.212
H3CO
N
S
O
t-Bu
CF3
4e
1.00
1.05
1.09
1.18
1.10
1.10
3.28
10.74
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


160.708
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131.553
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125.025
124.959
124.896
124.325
120.697
118.139
117.068
112.053
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55.309
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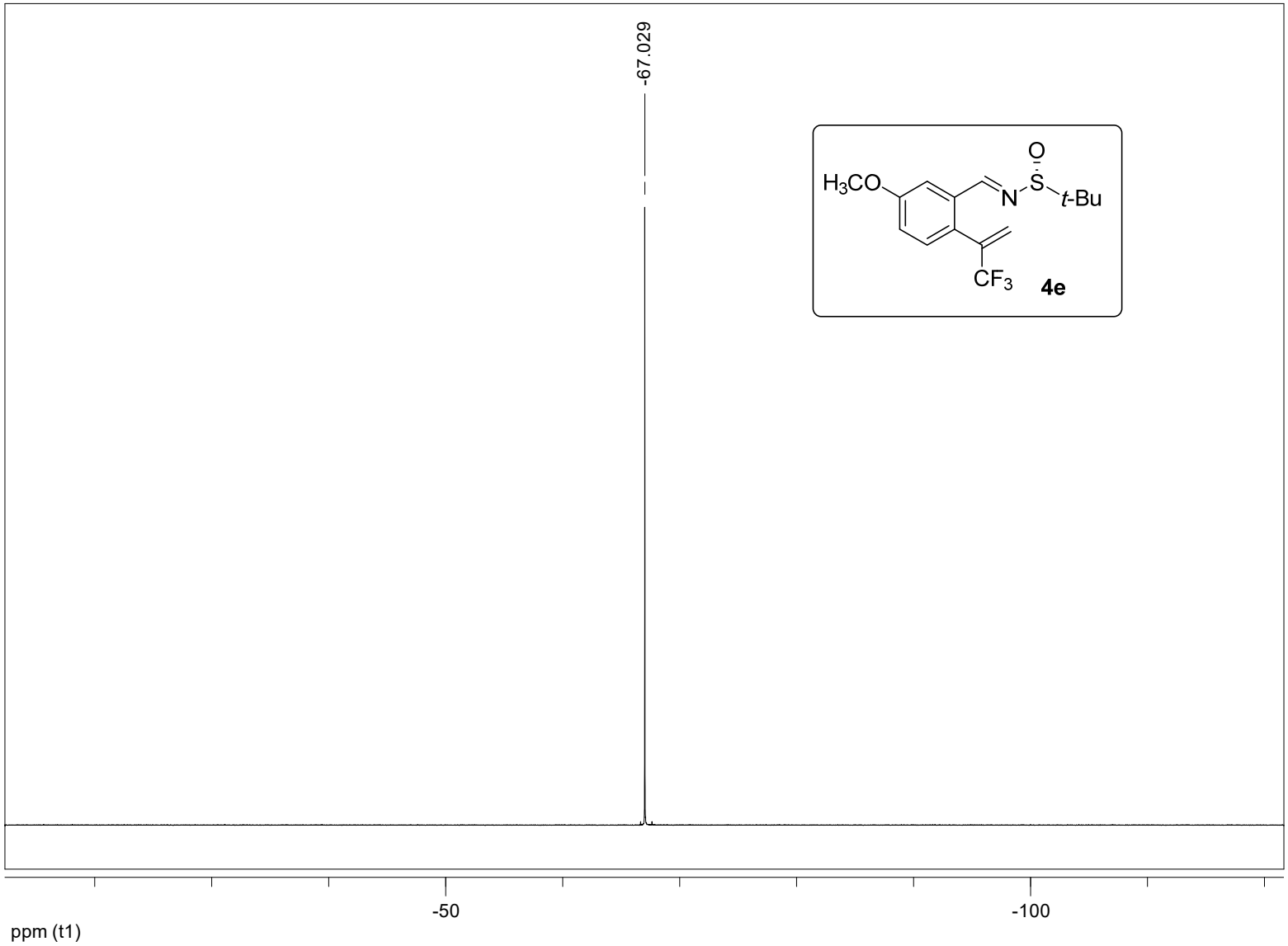
H3CO
N
S
O
t-Bu
CF3
4e
150
100
50
0
ppm (t1)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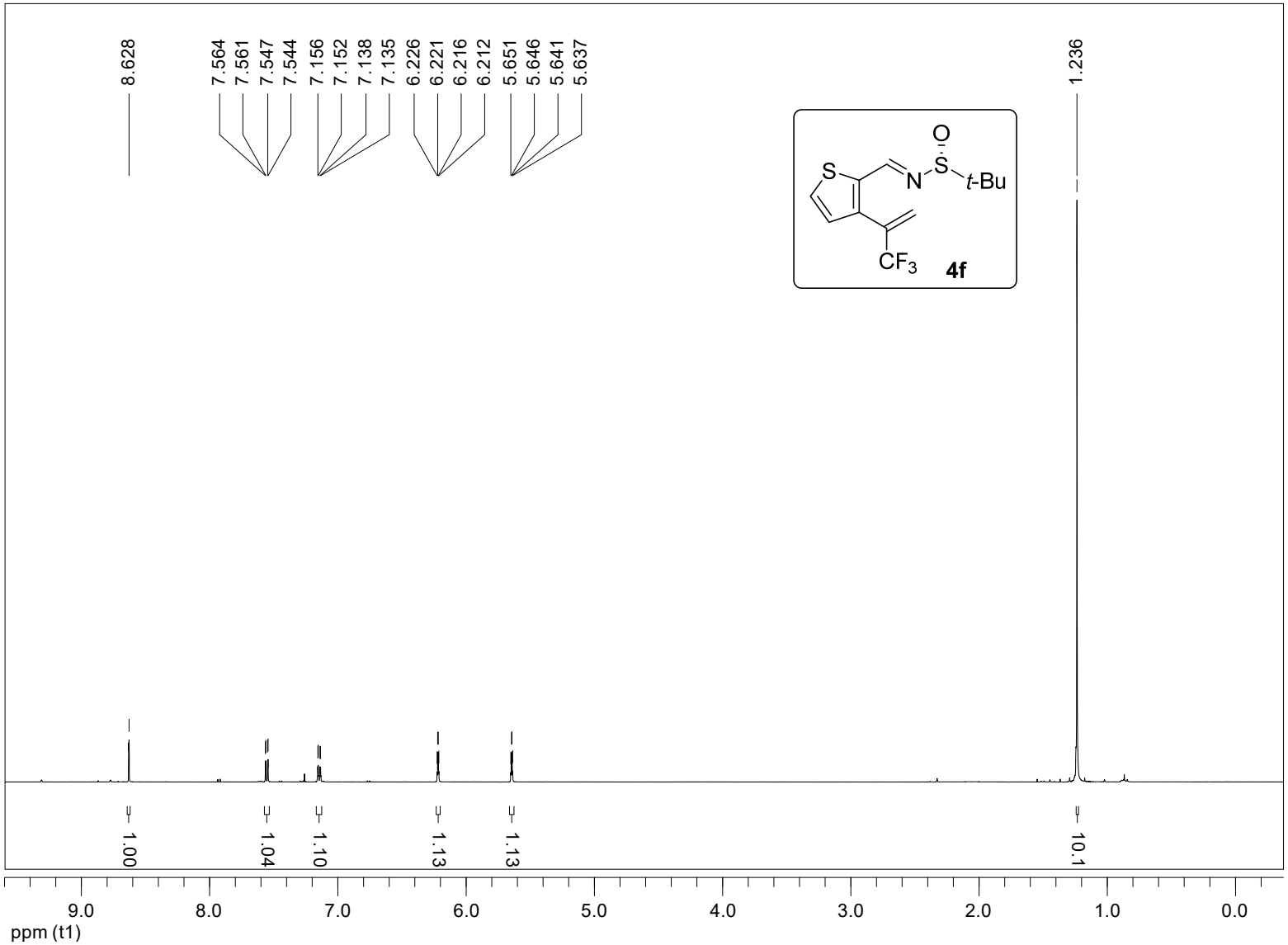
S
O
t-Bu
CF3
4e
-50
-100
ppm (t1)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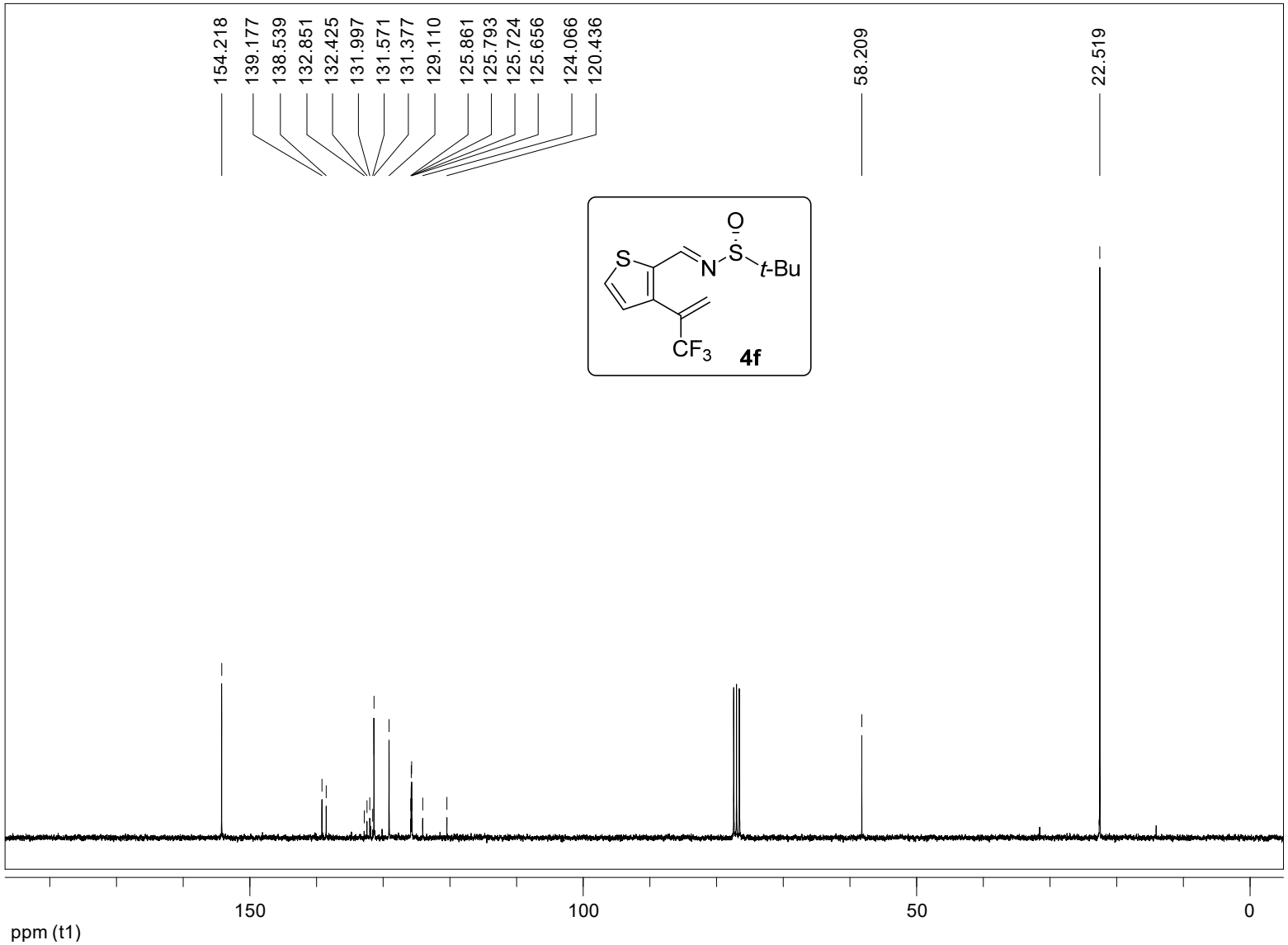
7.547
7.544
7.156
7.152
7.138
7.135
6.226
6.221
6.216
6.212
5.651
5.646
5.641
5.637
1.236
S
N
O
S
t-Bu
CF3
4f
1.00
1.04
1.10
1.13
1.13
10.1
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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131.997
131.571
131.377
129.110
125.861
125.793
125.724
125.656
124.066
120.436
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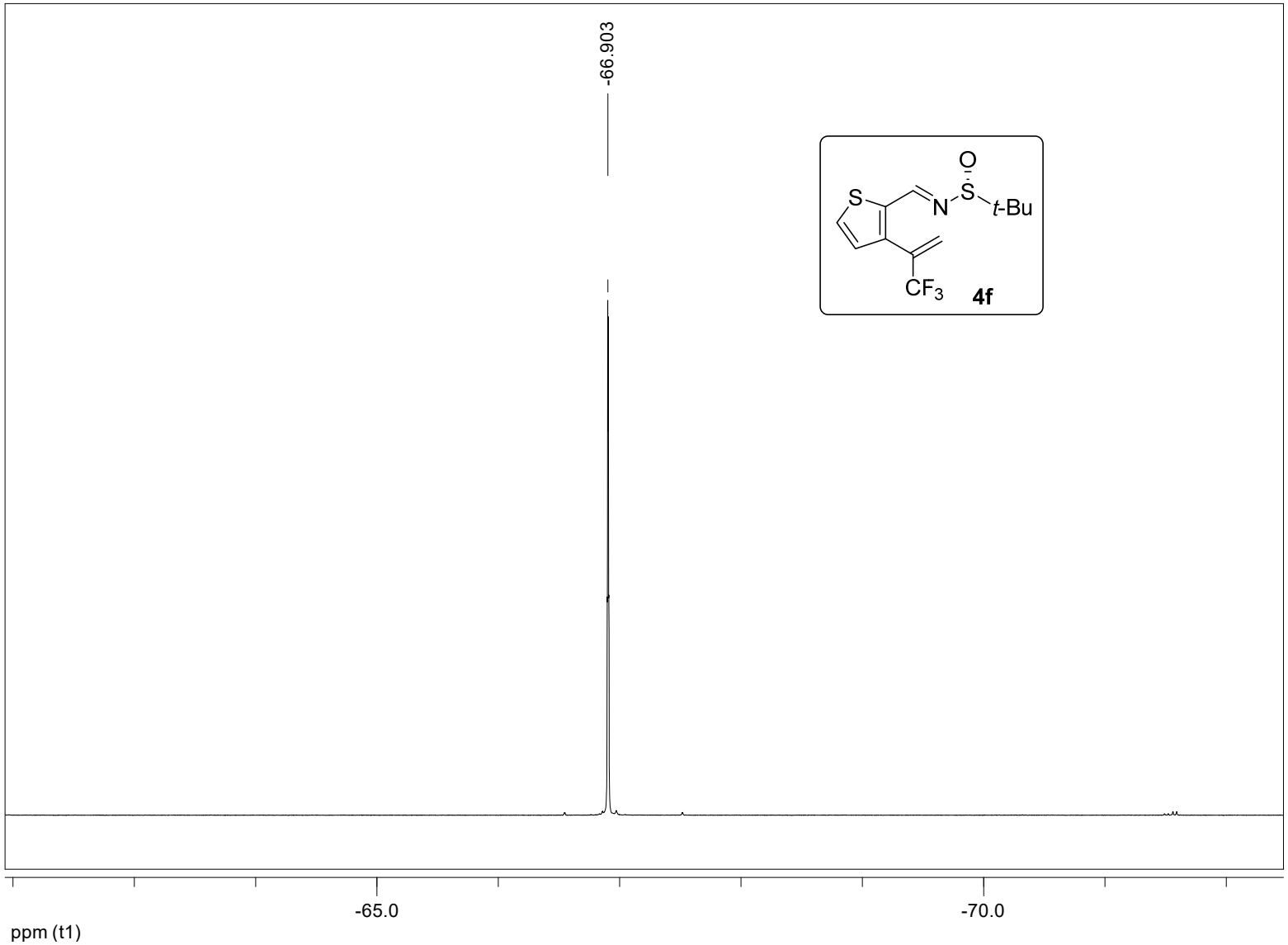
22.519
S
N
O
S
t-Bu
CF3
4f
150
100
50
0
ppm (t1)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N
O
S
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CF3
4f
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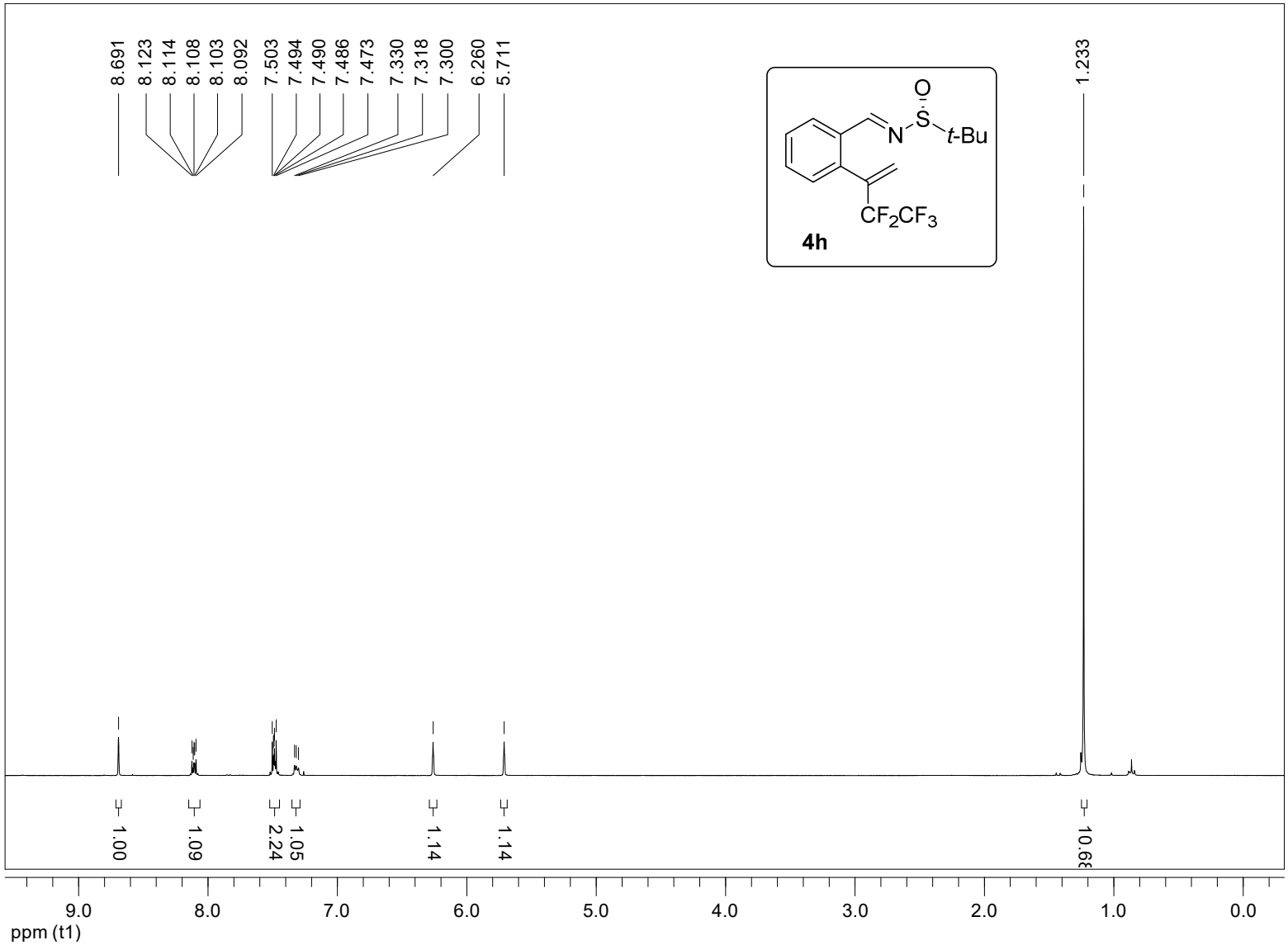
ppm (t1)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8.103
8.092
7.503
7.494
7.490
7.486
7.473
7.330
7.318
7.300
6.260
5.711
1.233
O
S
N
t-Bu
CF2CF3
4h
1.00
1.09
2.24
1.05
1.14
1.14
10.68
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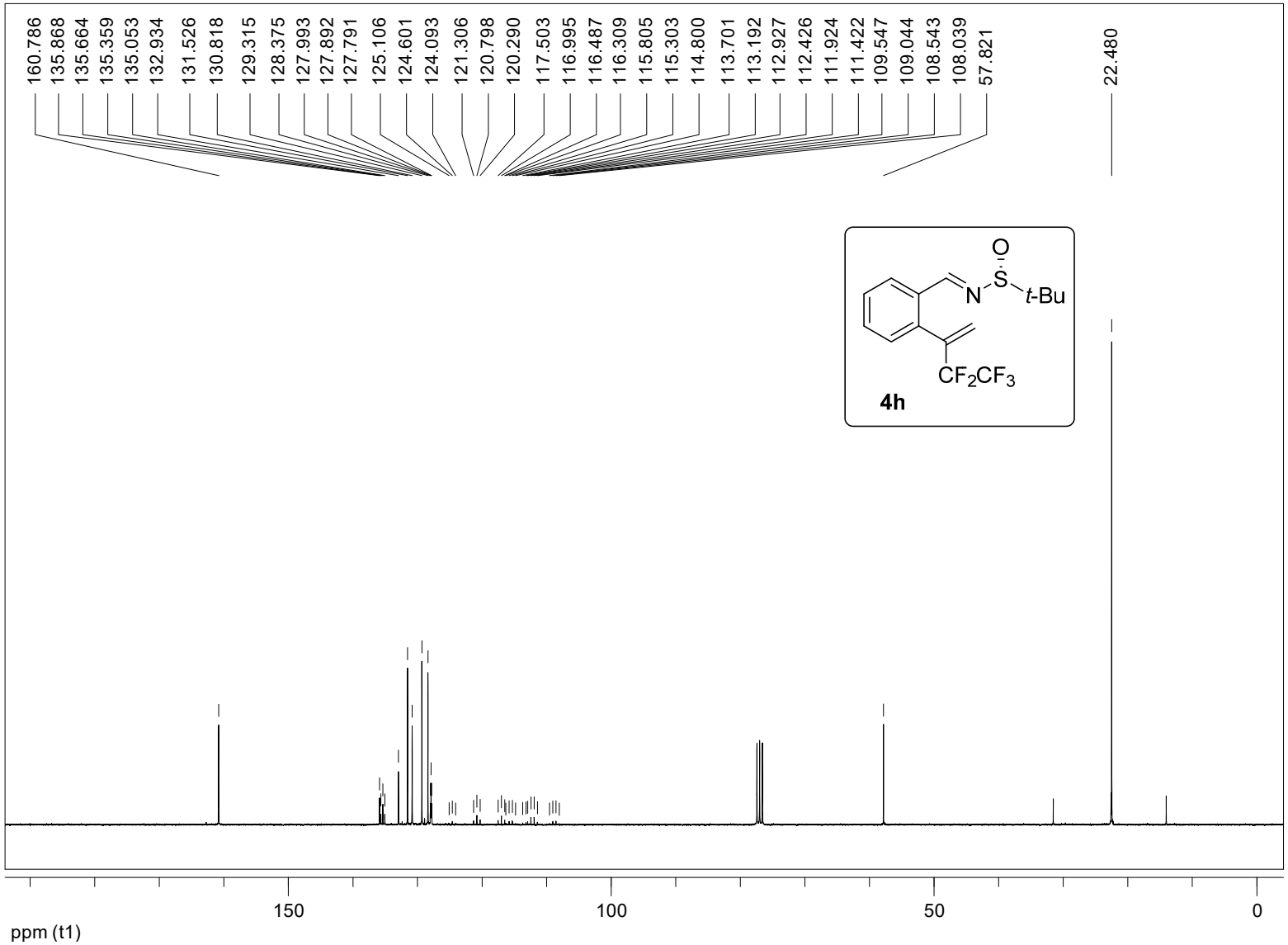
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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128.375
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127.892
127.791
125.106
124.601
124.093
121.306
120.798
120.290
117.503
116.995
116.487
116.309
115.805
115.303
114.800
113.701
113.192
112.927
112.426
111.924
111.422
109.547
109.044
108.543
108.039
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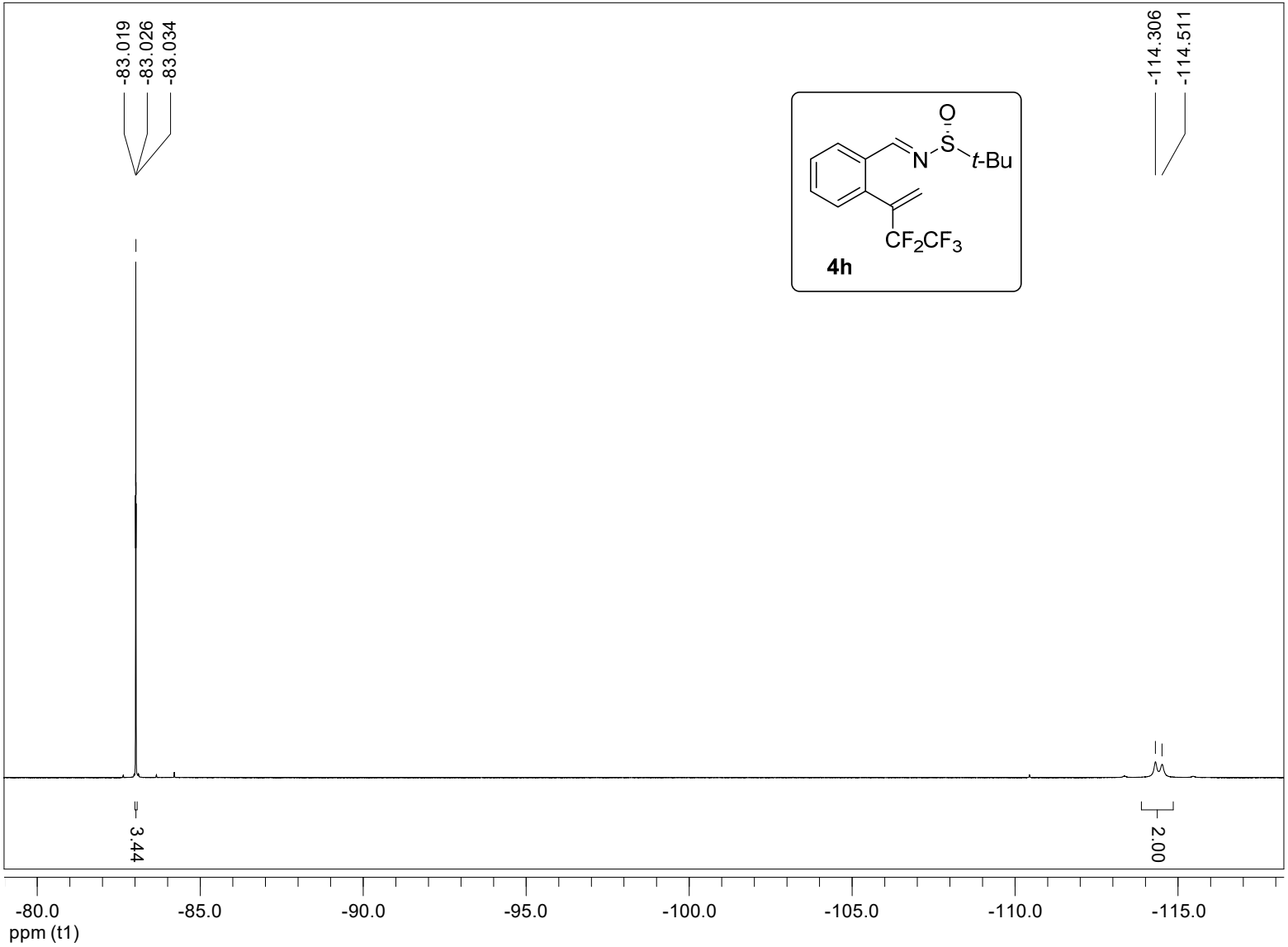
N
t-Bu
CF2CF3
4h
150
100
50
0
ppm (t1)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-83.026
-83.034
-114.306
-114.511
O
S
N
t-Bu
CF2CF3
4h
3.44
2.00
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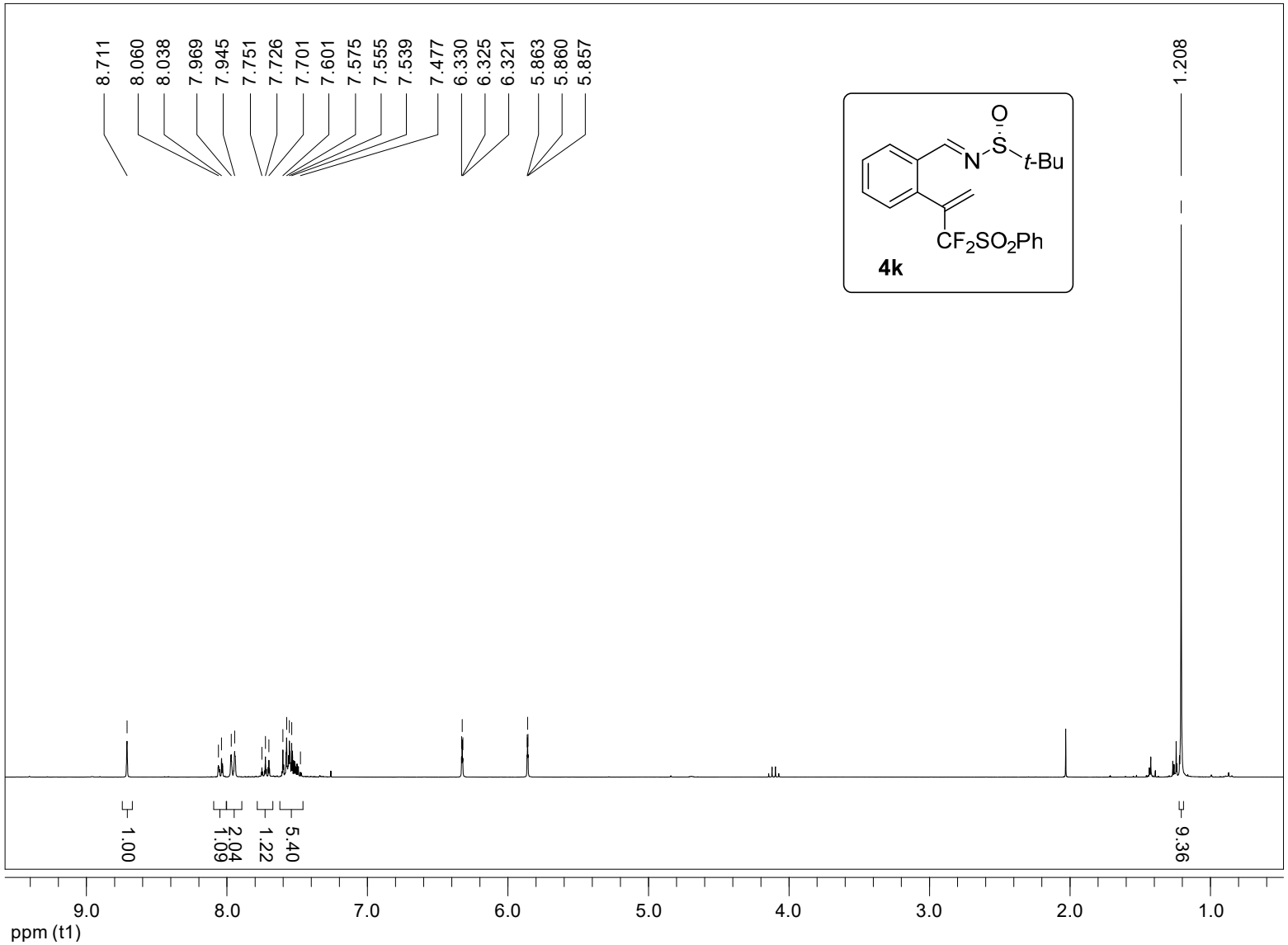
-95.0
-100.0
-105.0
-110.0
-115.0
ppm (t1)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7.945
7.751
7.726
7.701
7.601
7.575
7.555
7.539
7.477
6.330
6.325
6.321
5.863
5.860
5.857
1.208
O
S
N
t-Bu
CF2SO2Ph
4k
1.00
2.04
1.09
1.22
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8.0
7.0
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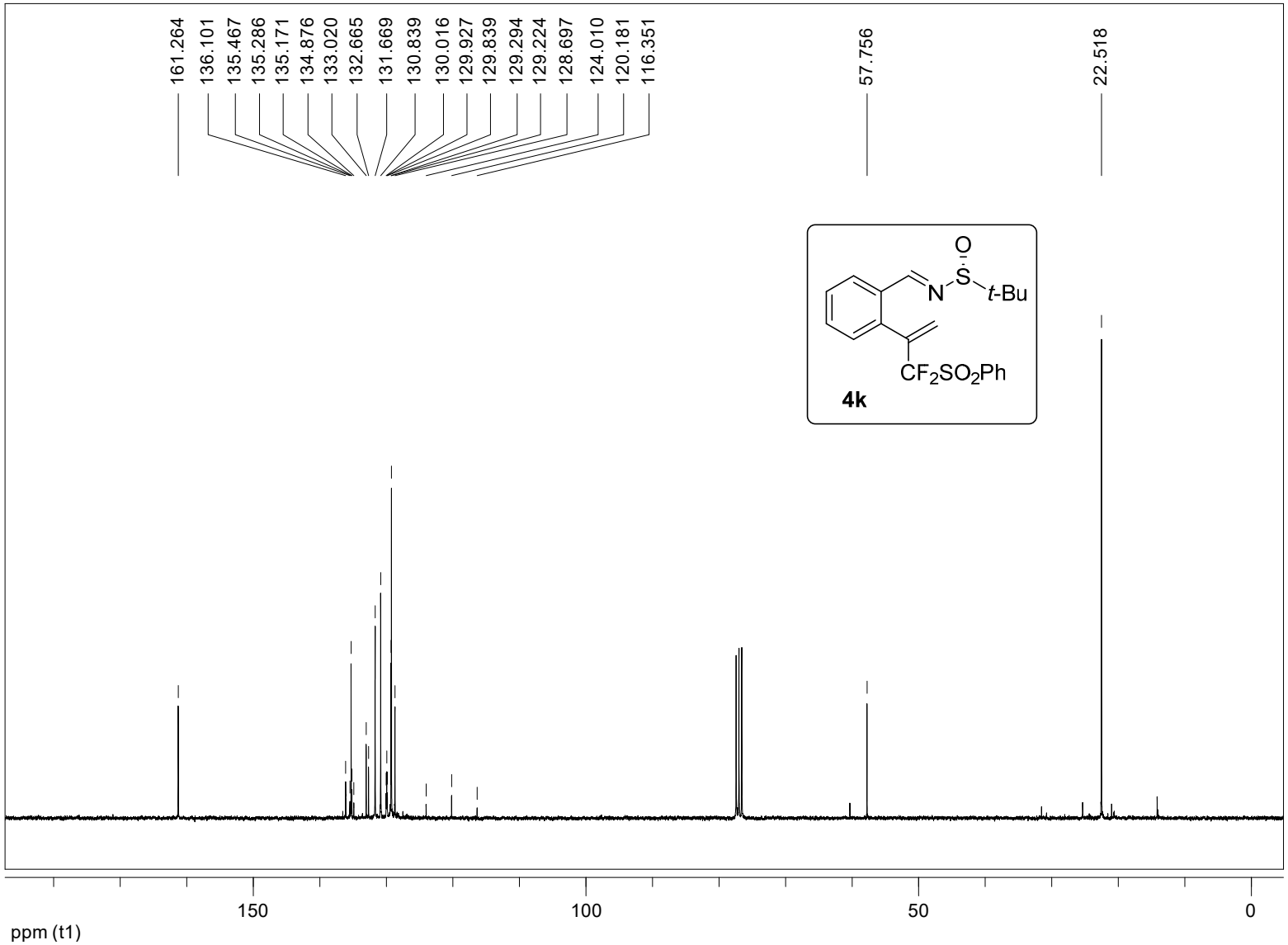
5.0
4.0
3.0
2.0
1.0
ppm (t1)


161.264
136.101
135.467
135.286
135.171
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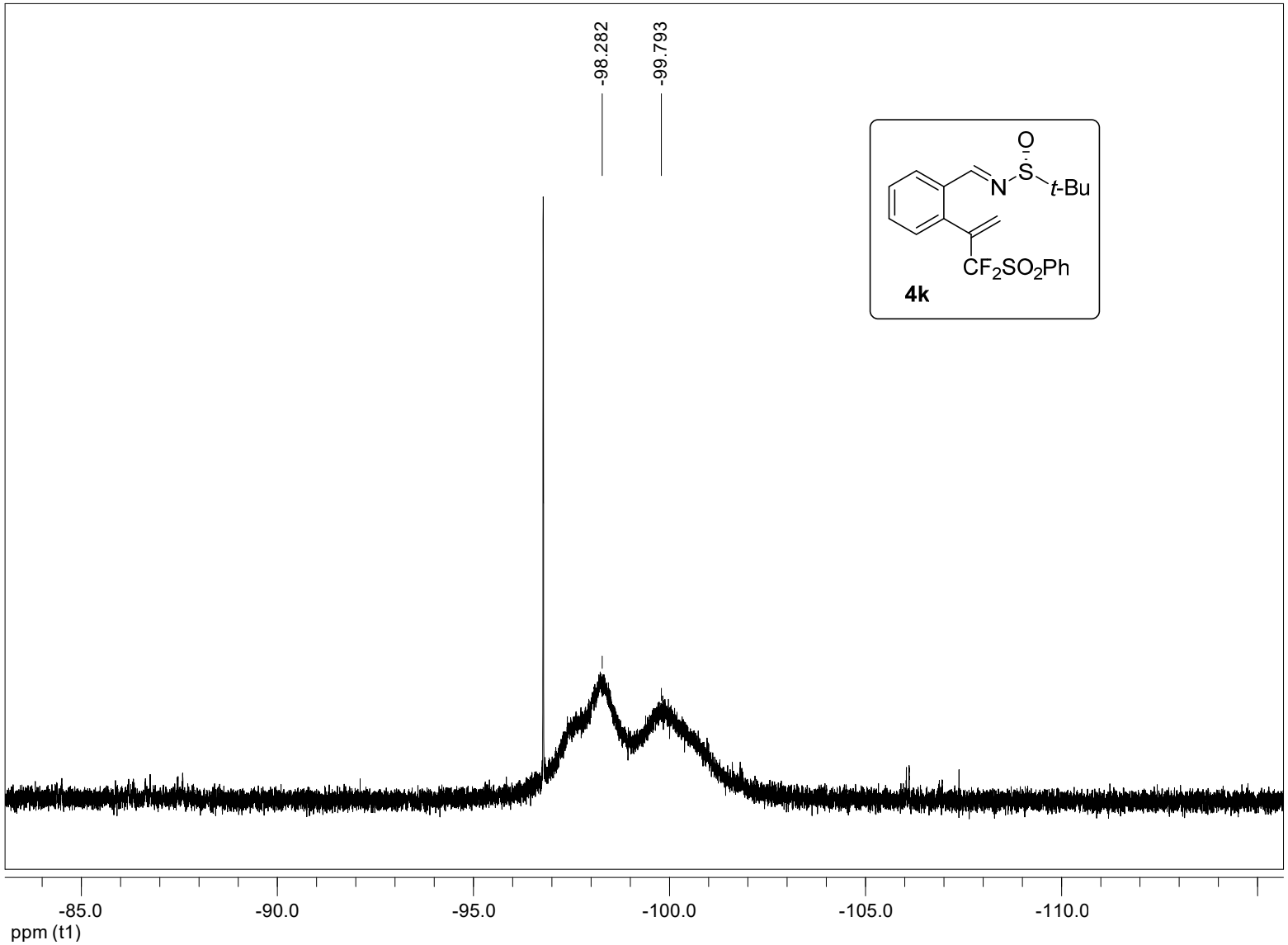
133.020
132.665
131.669
130.839
130.016
129.927
129.839
129.294
129.224
128.697
124.010
120.181
116.351
57.756
22.518
O
S
N
t-Bu
CF2SO2Ph
4k
150
100
50
0
ppm (t1)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-99.793
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S
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t-Bu
CF2SO2Ph
4k
-85.0
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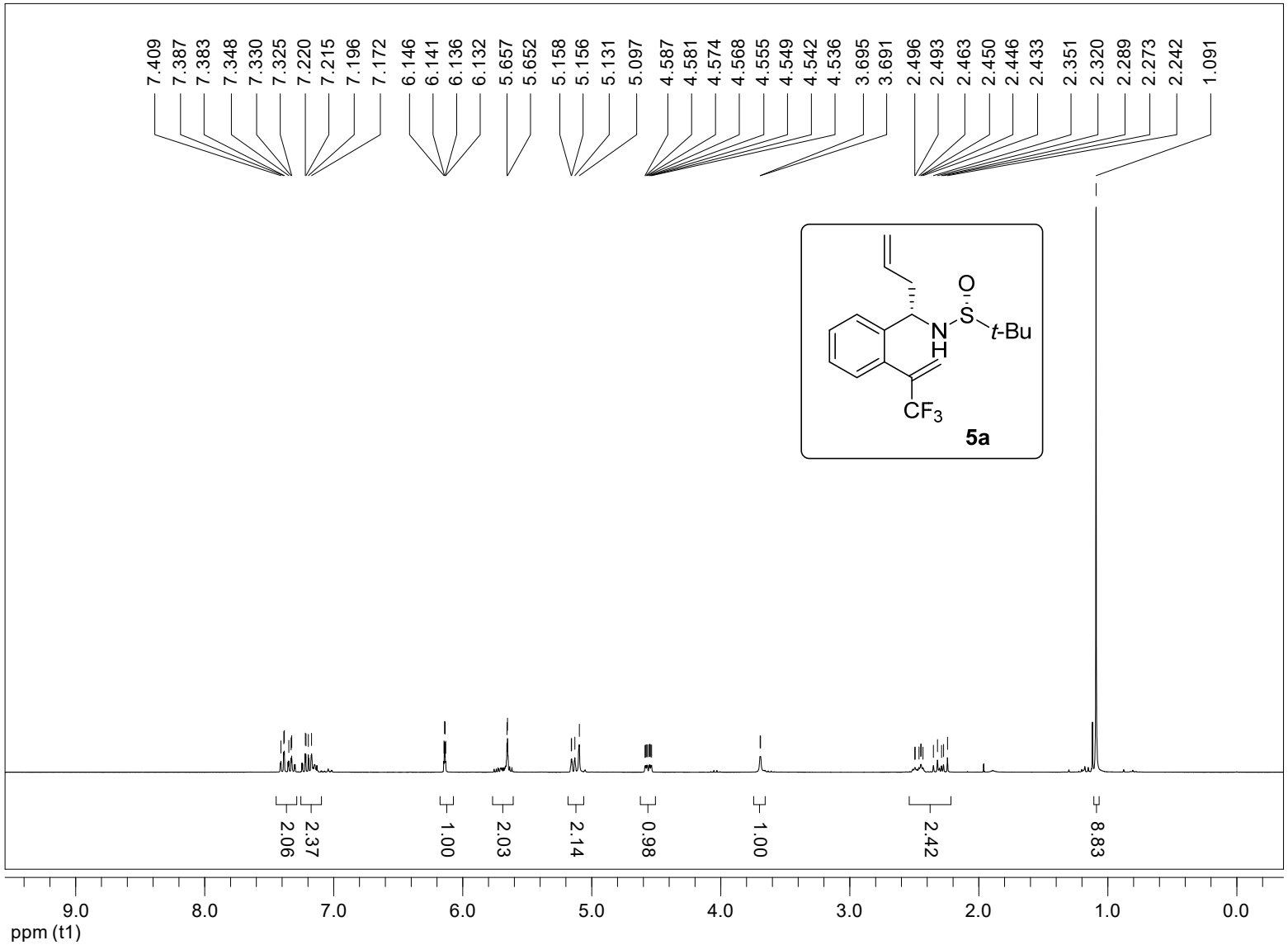
-95.0
-100.0
-105.0
-110.0
ppm (t1)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7.383
7.348
7.330
7.325
7.220
7.215
7.196
7.172
6.146
6.141
6.136
6.132
5.657
5.652
5.158
5.156
5.131
5.097
4.587
4.581
4.574
4.568
4.555
4.549
4.542
4.536
3.695
3.691
2.496
2.493
2.463
2.450
2.446
2.433
2.351
2.320
2.289
2.273
2.242
1.091
O
S
t-Bu
N
H
CF3
5a
2.06
2.37
1.00
2.03
2.14
0.98
1.00
2.42
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7.0
6.0
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3.0
2.0
1.0
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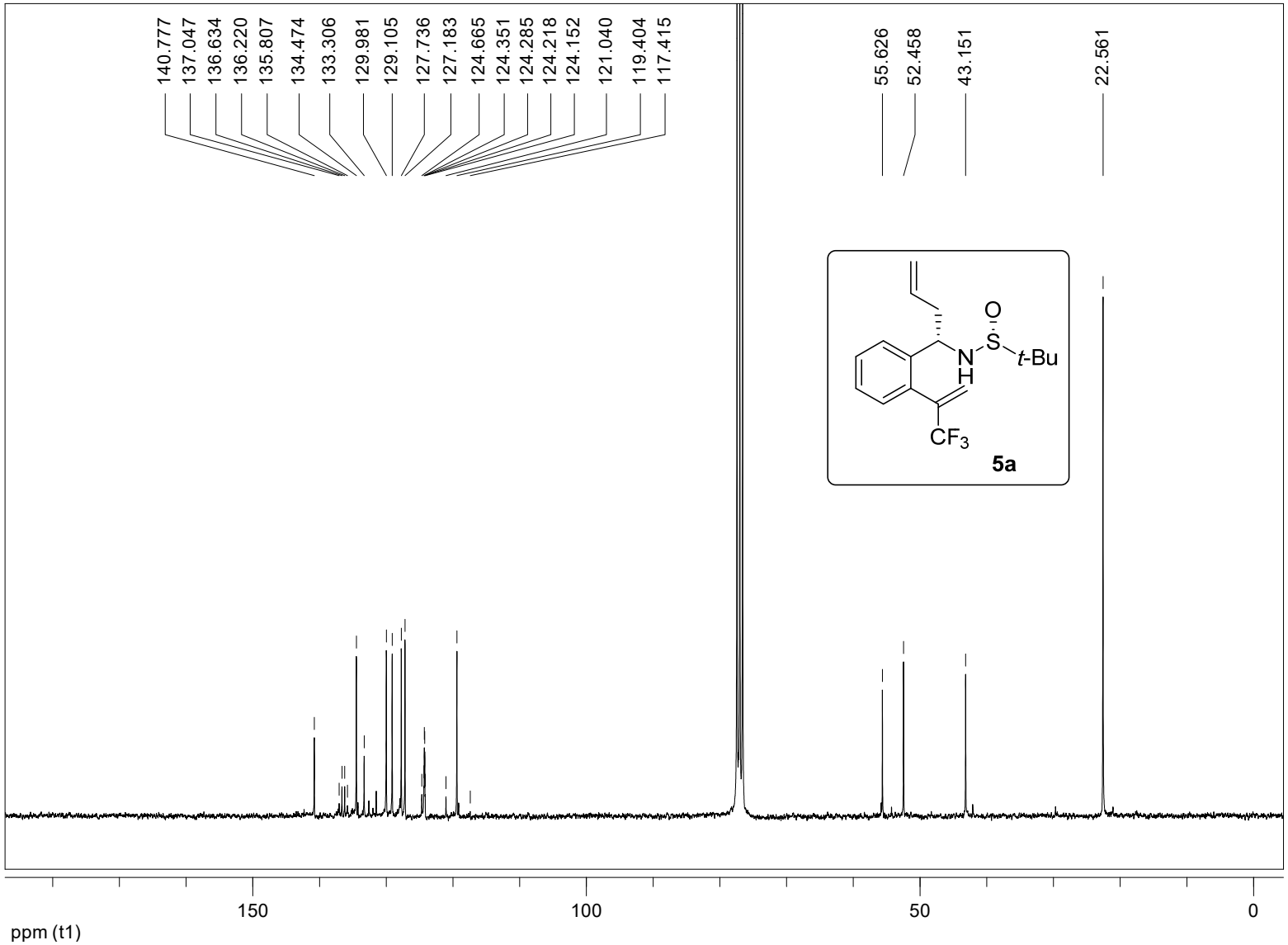
ppm (t1)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136.634
136.220
135.807
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129.981
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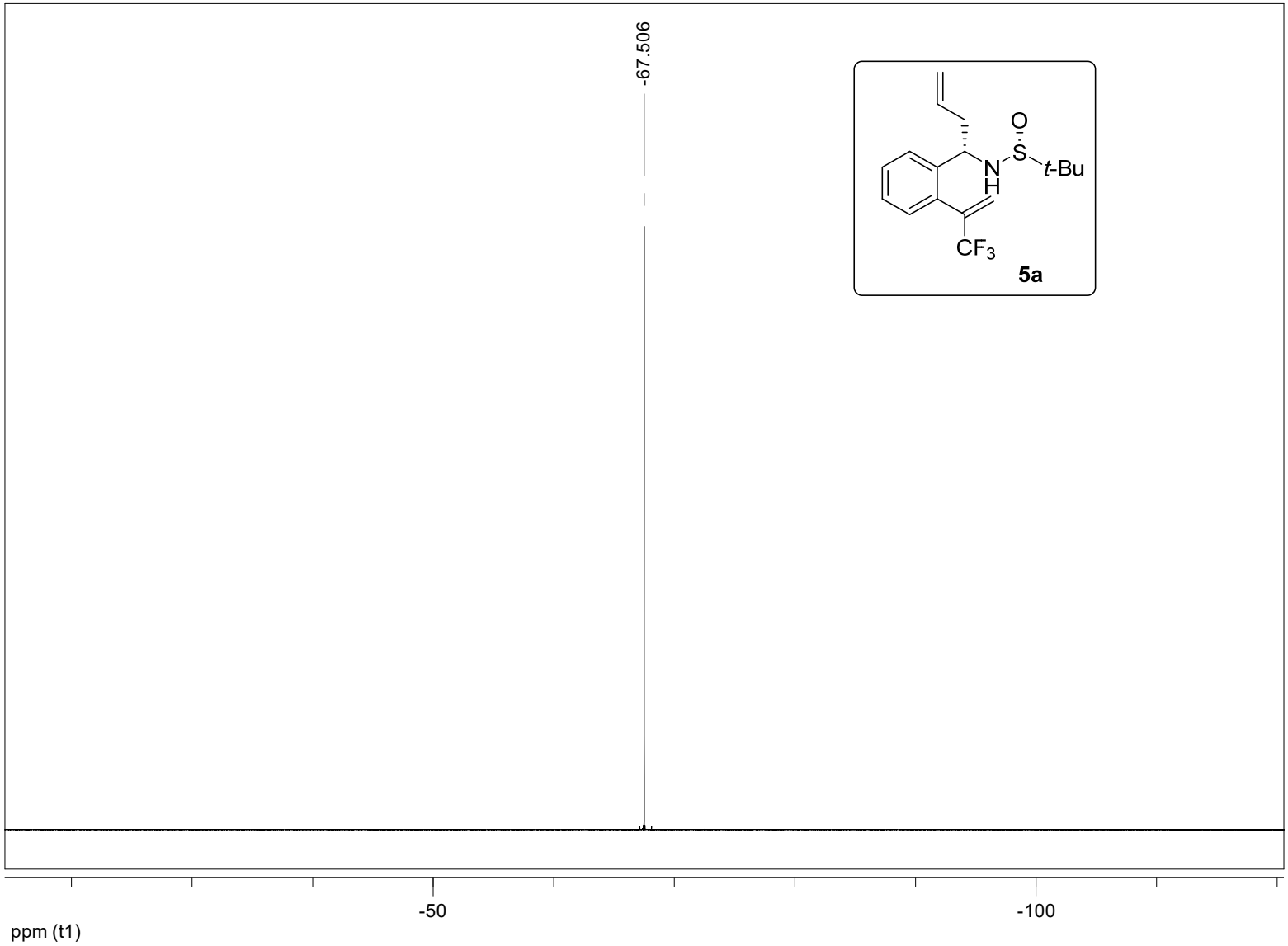
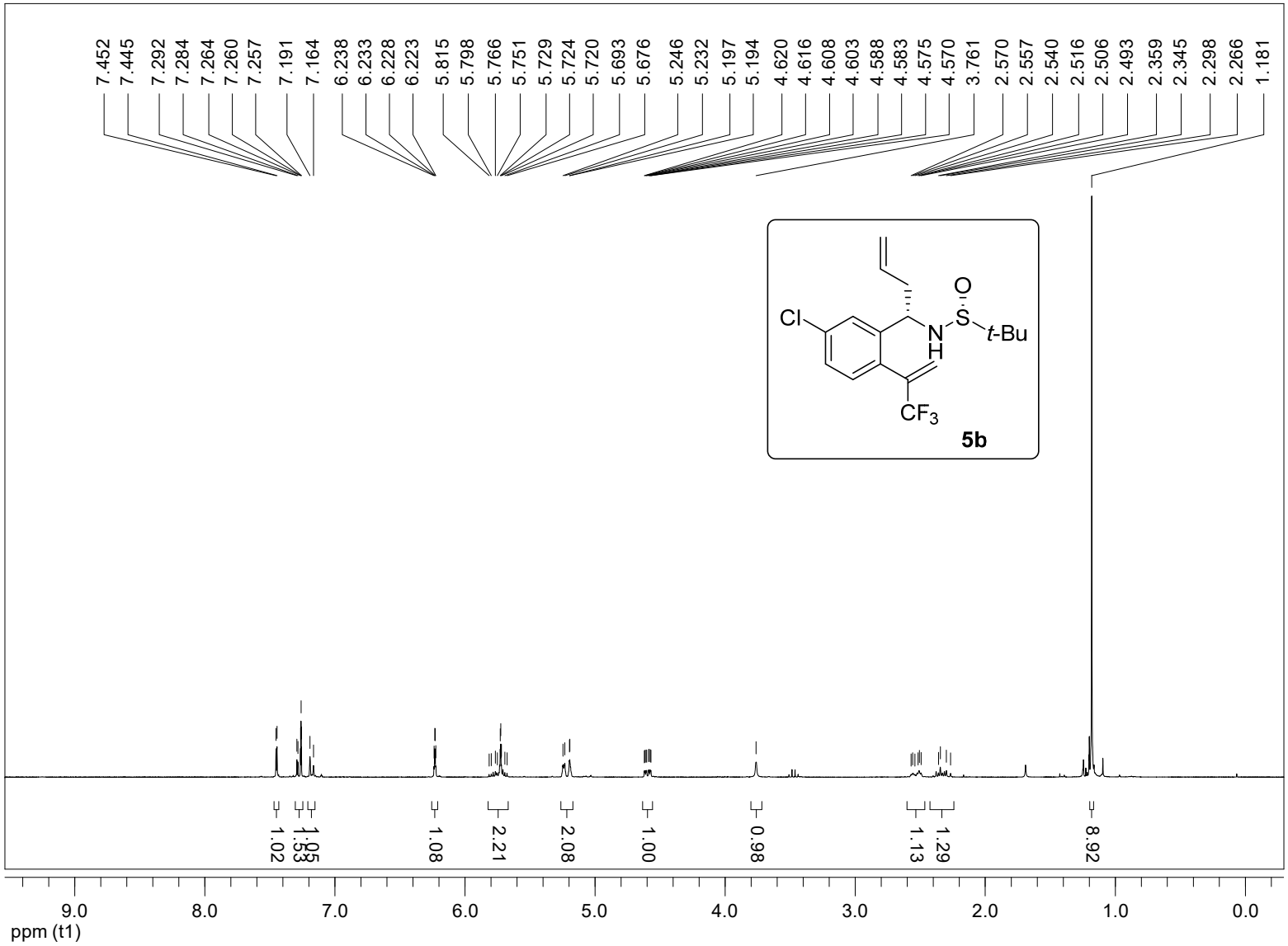
127.183
124.665
124.351
124.285
124.218
124.152
121.040
119.404
117.415
55.626
52.458
43.151
22.561
O
S
N
H
t-Bu
CF3
5a
150
100
50
0
ppm (t1)


-67.506
O
S
t-Bu
N
H
CF3
5a
-50
-100
ppm (t1)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7.284
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7.191
7.164
6.238
6.233
6.228
6.223
5.815
5.798
5.766
5.751
5.729
5.724
5.720
5.693
5.676
5.246
5.232
5.197
5.194
4.620
4.616
4.608
4.603
4.588
4.583
4.575
4.570
3.761
2.570
2.557
2.540
2.516
2.506
2.493
2.359
2.345
2.298
2.266
1.181
Cl
N
H
S
O
t-Bu
CF3
5b
1.02
1.53
1.05
1.08
2.21
2.08
1.00
0.98
1.13
1.29
8.92
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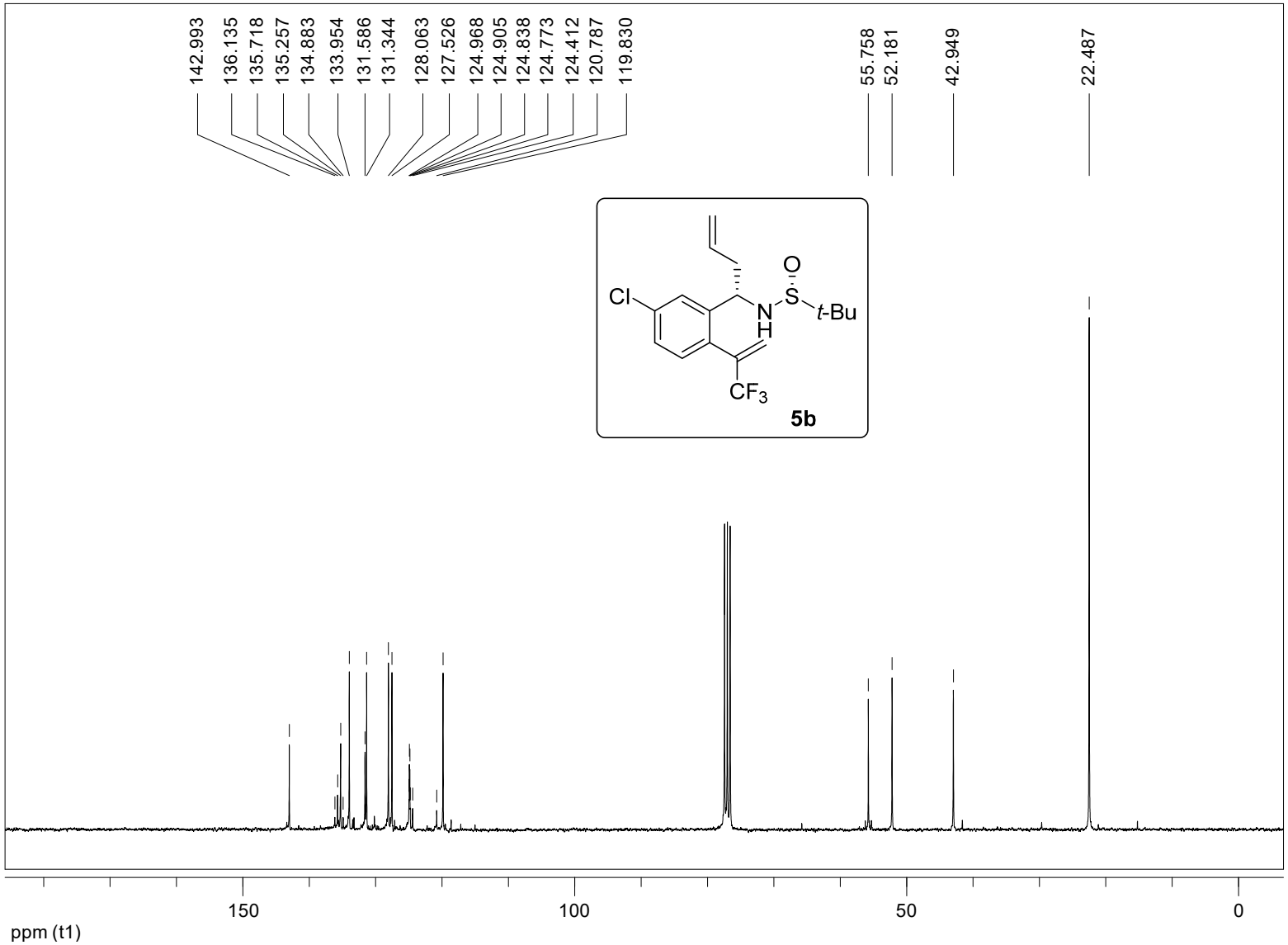
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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135.718
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133.954
131.586
131.344
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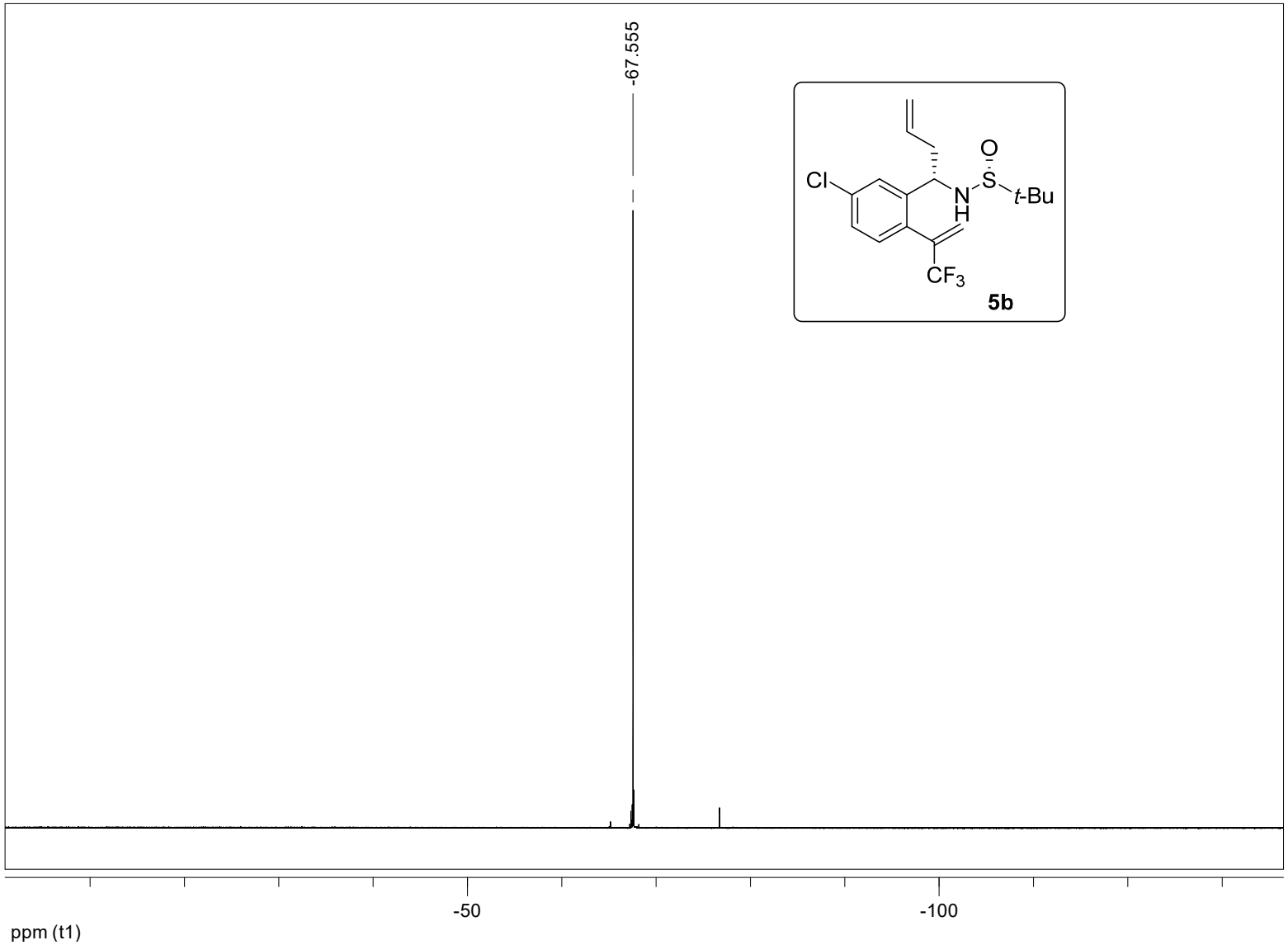
127.526
124.968
124.905
124.838
124.773
124.412
120.787
119.830
55.758
52.181
42.949
22.487
Cl
N
H
S
O
t-Bu
CF3
5b
150
100
50
0
ppm (t1)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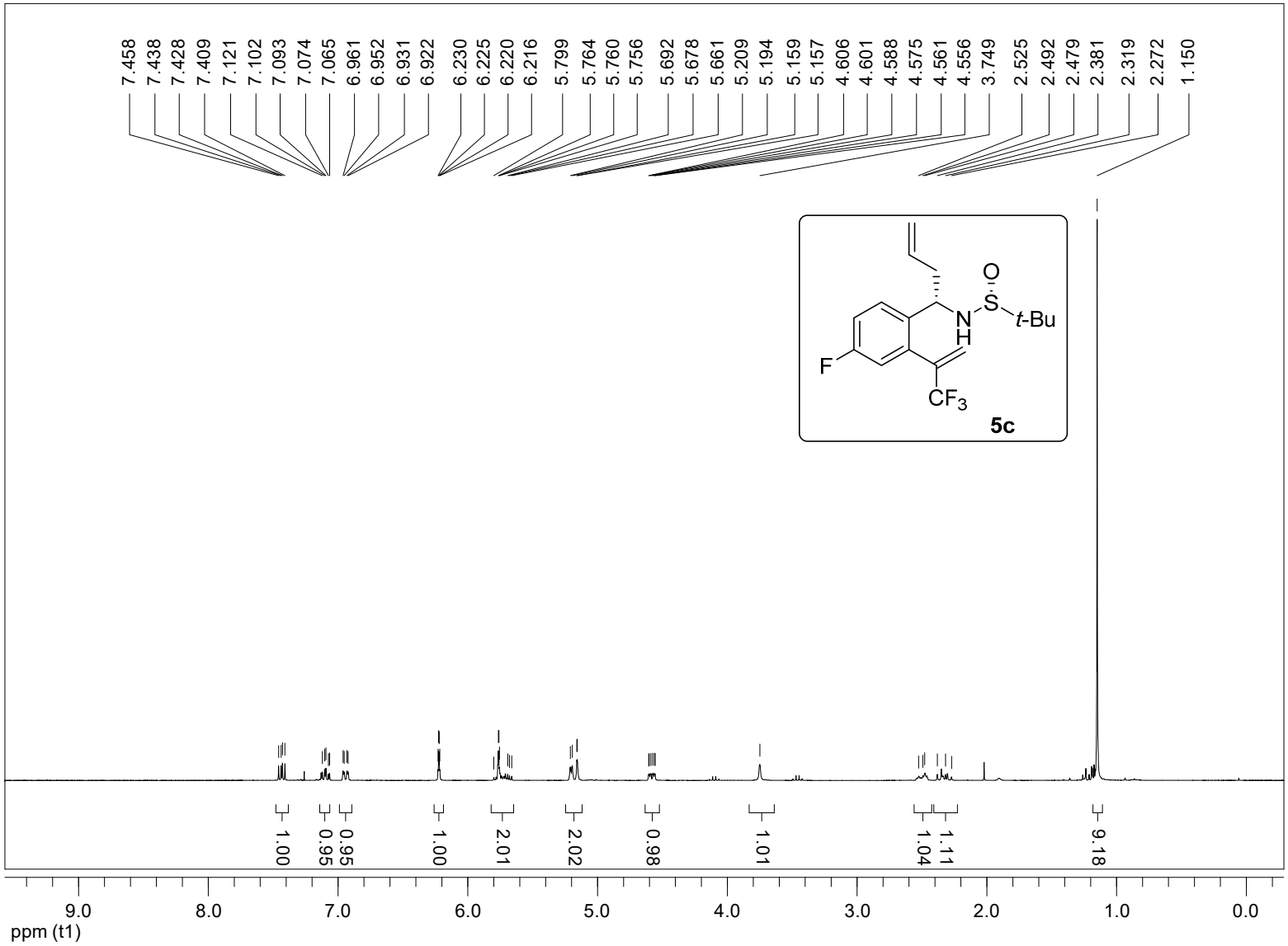
H
O
S
t-Bu
CF3
5b
-50
-100
ppm (t1)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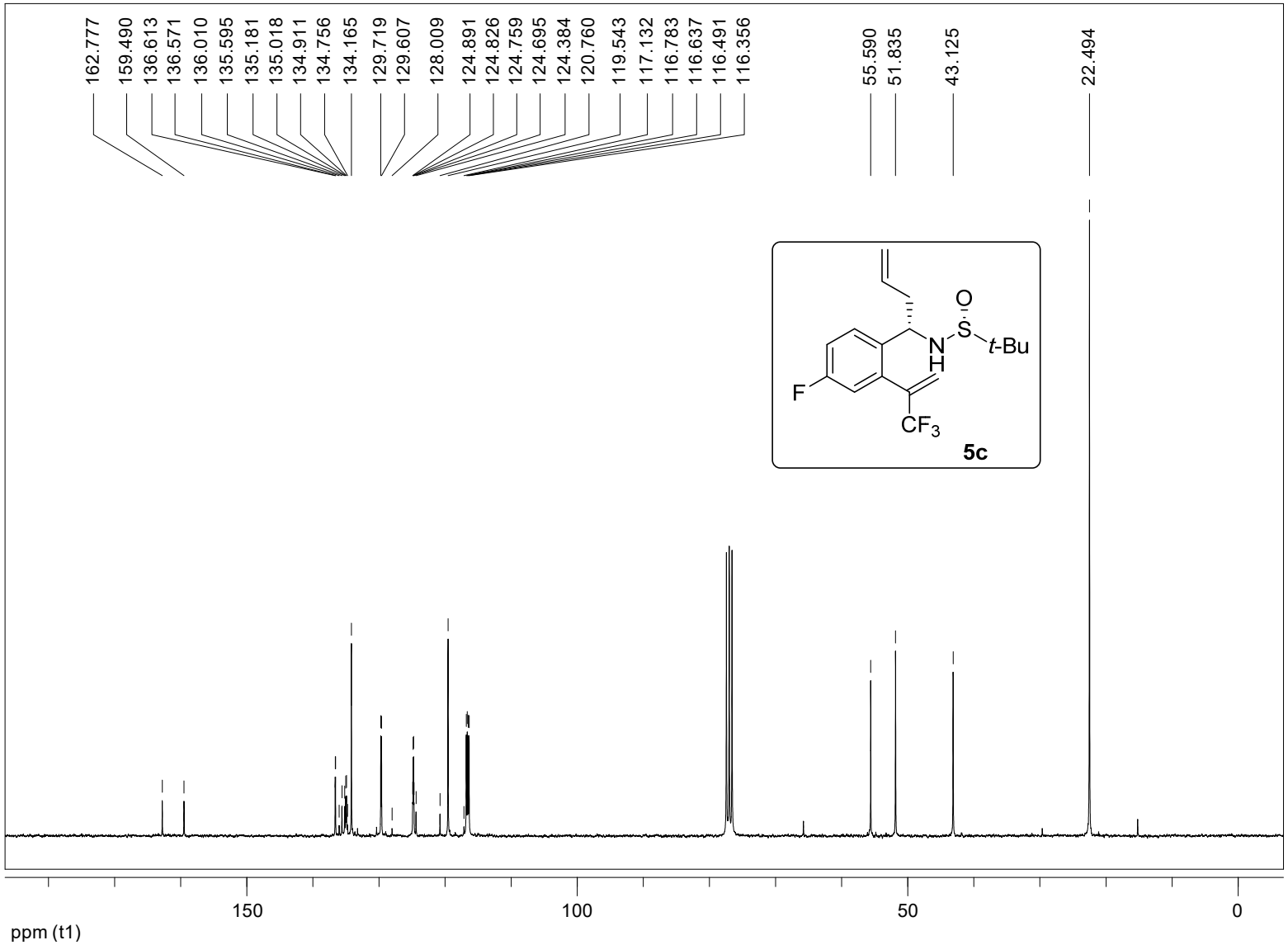
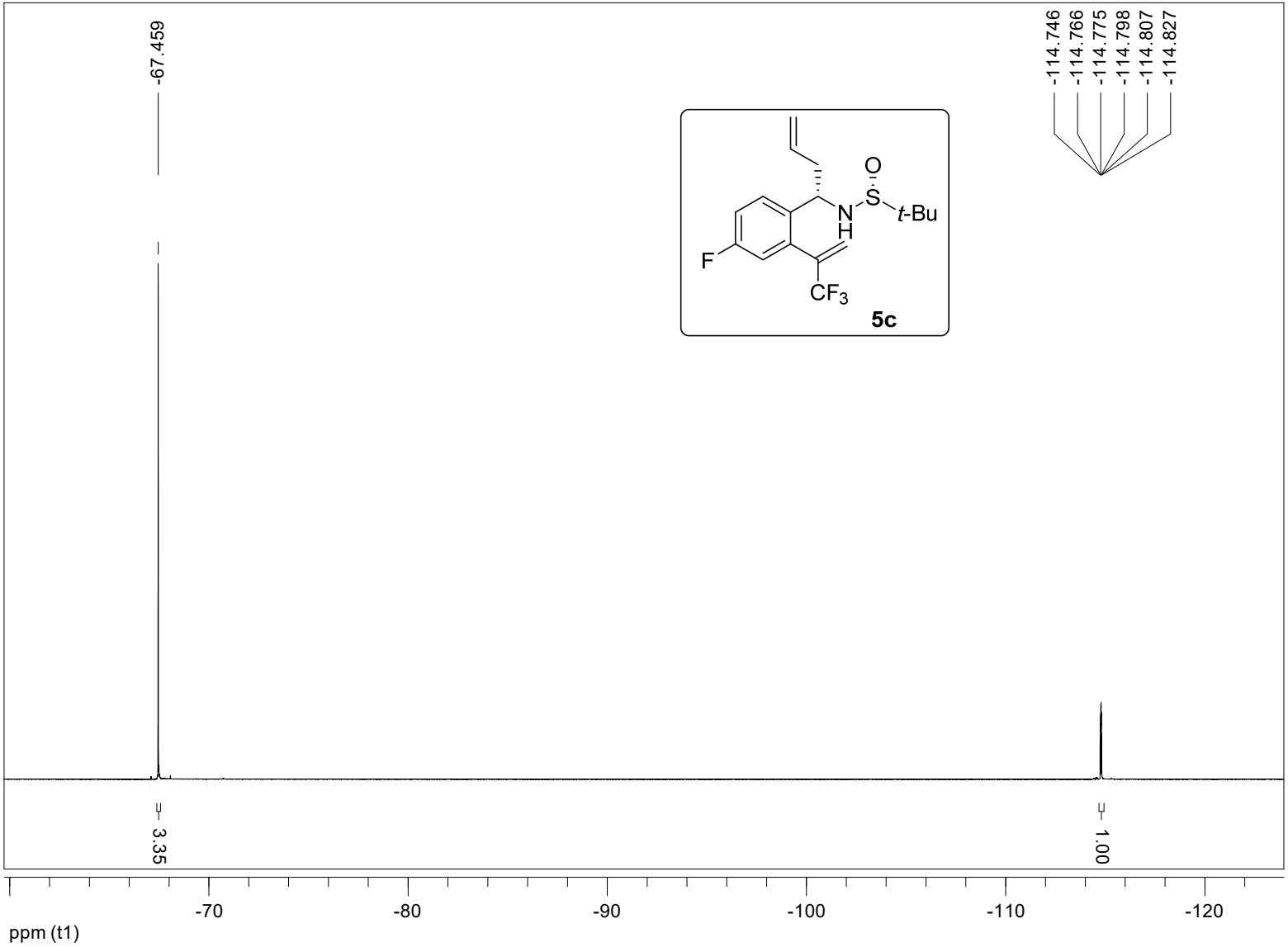
7.428
7.409
7.121
7.102
7.093
7.074
7.065
6.961
6.952
6.931
6.922
6.230
6.225
6.220
6.216
5.799
5.764
5.760
5.756
5.692
5.678
5.661
5.209
5.194
5.159
5.157
4.606
4.601
4.588
4.575
4.561
4.556
3.749
2.525
2.492
2.479
2.381
2.319
2.272
1.150
O
S
t-Bu
N
H
F
CF3
5c
1.00
0.95
0.95
1.00
2.01
2.02
0.98
1.01
1.04
1.11
9.18
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


162.777
159.490
136.613
136.571
136.010
135.595
135.181
135.018
134.911
134.756
134.165
129.719
129.607
128.009
124.891
124.826
124.759
124.695
124.384
120.760
119.543
117.132
116.783
116.637
116.491
116.356
55.590
51.835
43.125
22.494
O
S
N
H
t-Bu
F
CF3
5c
150
100
50
0
ppm (t1)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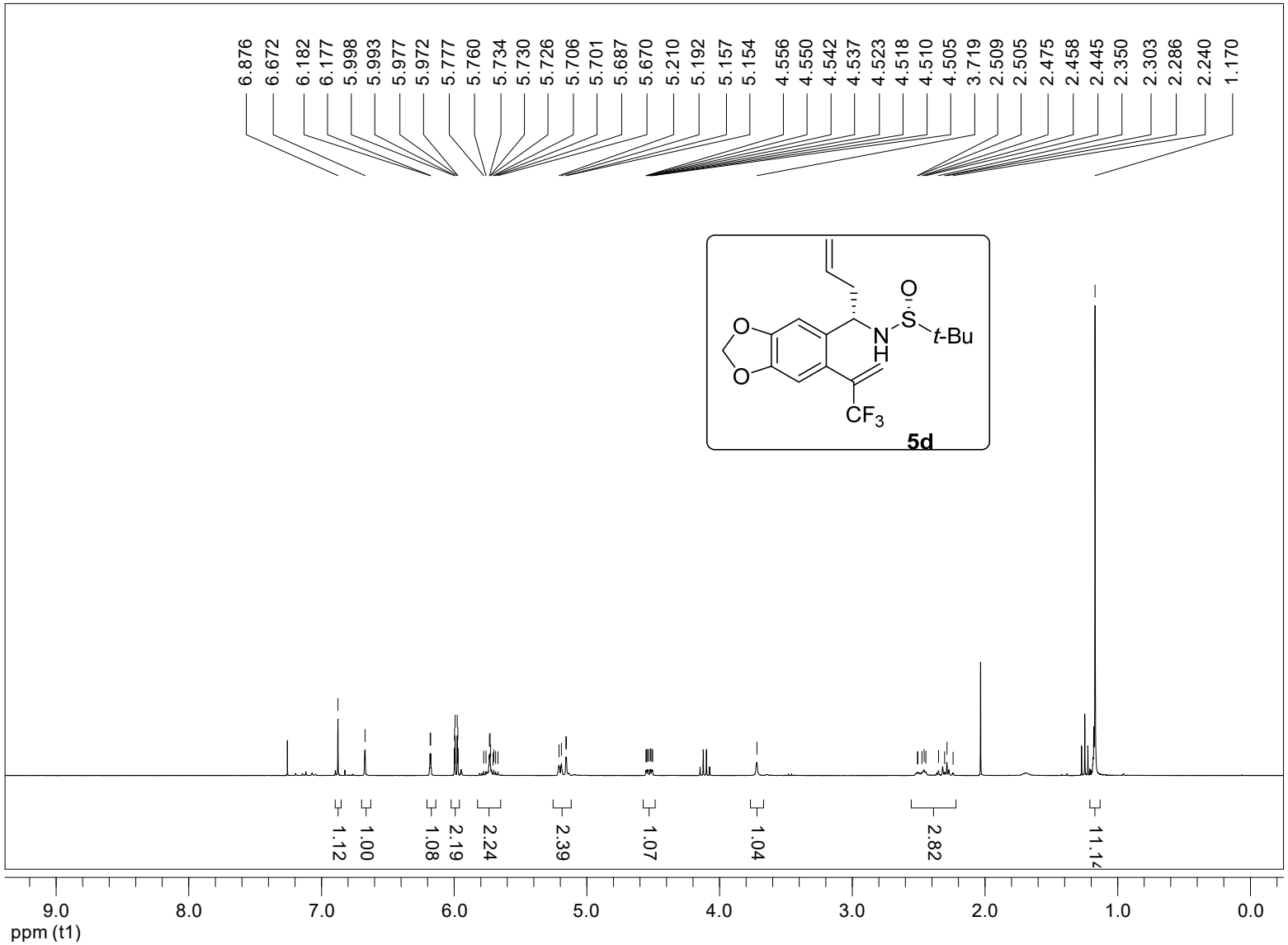
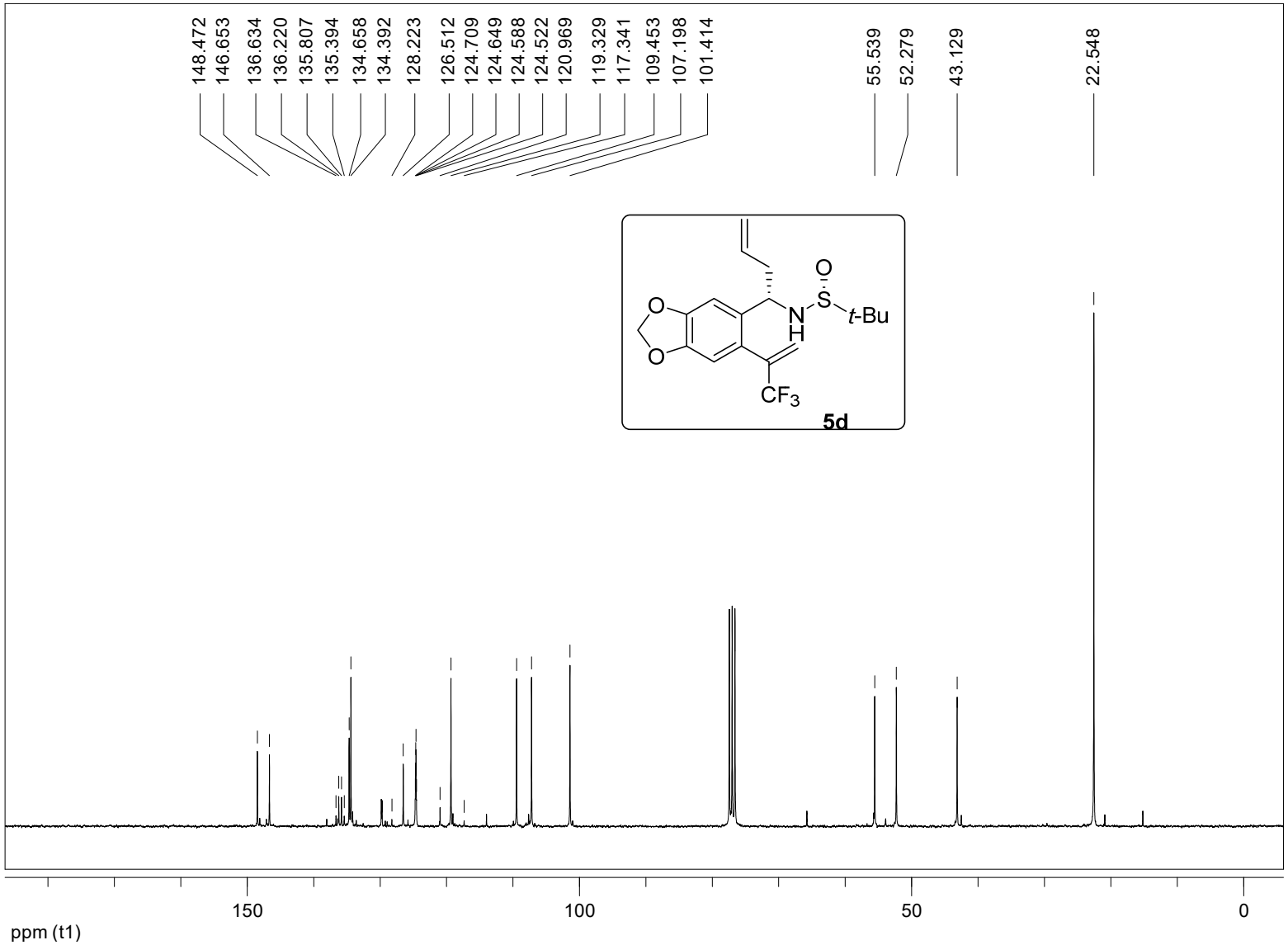
-114.746
-114.766
-114.775
-114.798
-114.807
-114.827
O
S
t-Bu
N
H
F
CF3
5c
3.35
1.00
-70
-80
-90
-100
-110
-120
ppm (t1)


6.876
6.672
6.182
6.177
5.998
5.993
5.977
5.972
5.777
5.760
5.734
5.730
5.726
5.706
5.701
5.687
5.670
5.210
5.192
5.157
5.154
4.556
4.550
4.542
4.537
4.523
4.518
4.510
4.505
3.719
2.509
2.505
2.475
2.458
2.445
2.350
2.303
2.286
2.240
1.170
O
S
t-Bu
N
H
O
O
CF3
5d
1.12
1.00
1.08
2.19
2.24
2.39
1.07
1.04
2.82
11.14
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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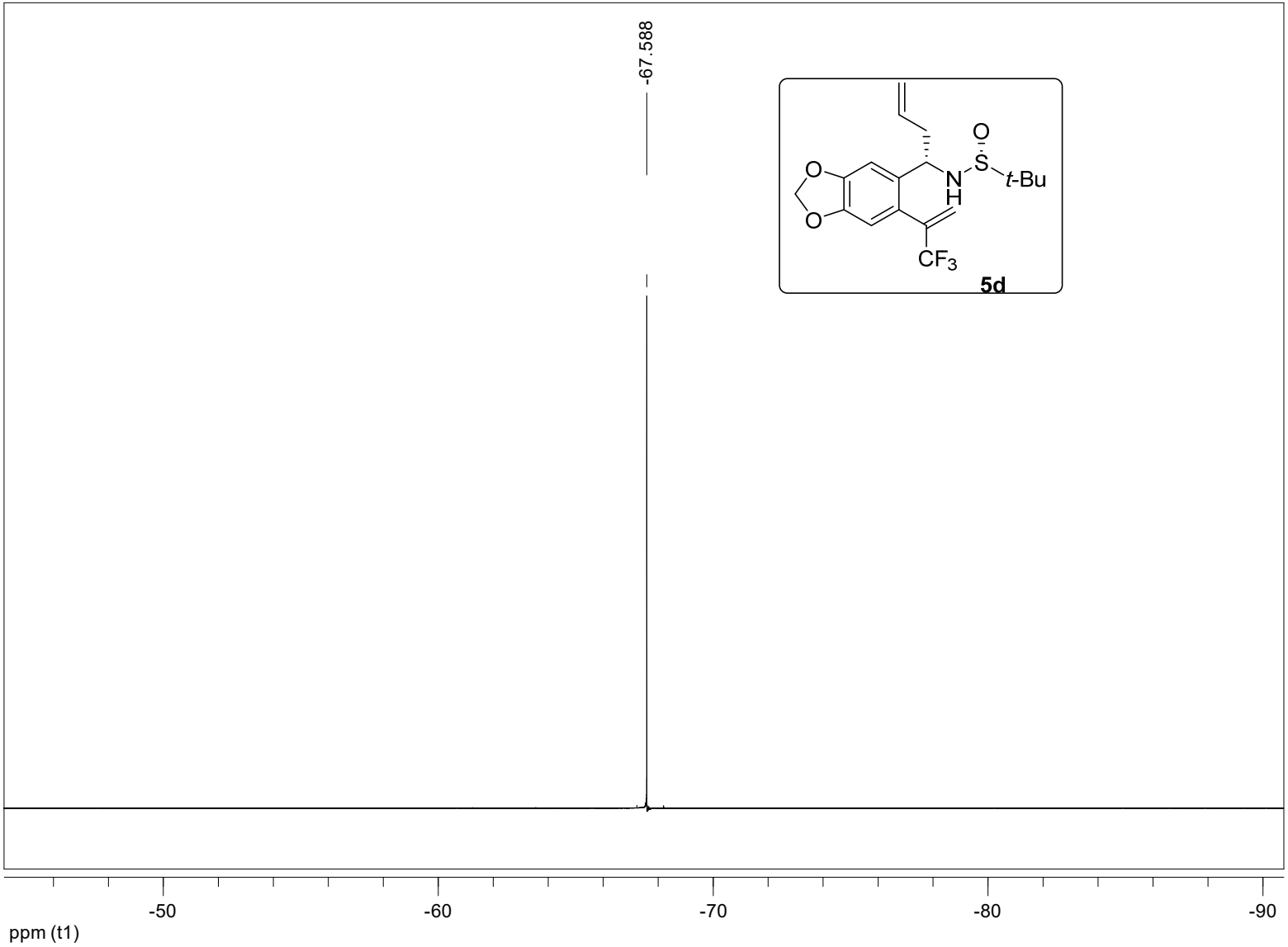
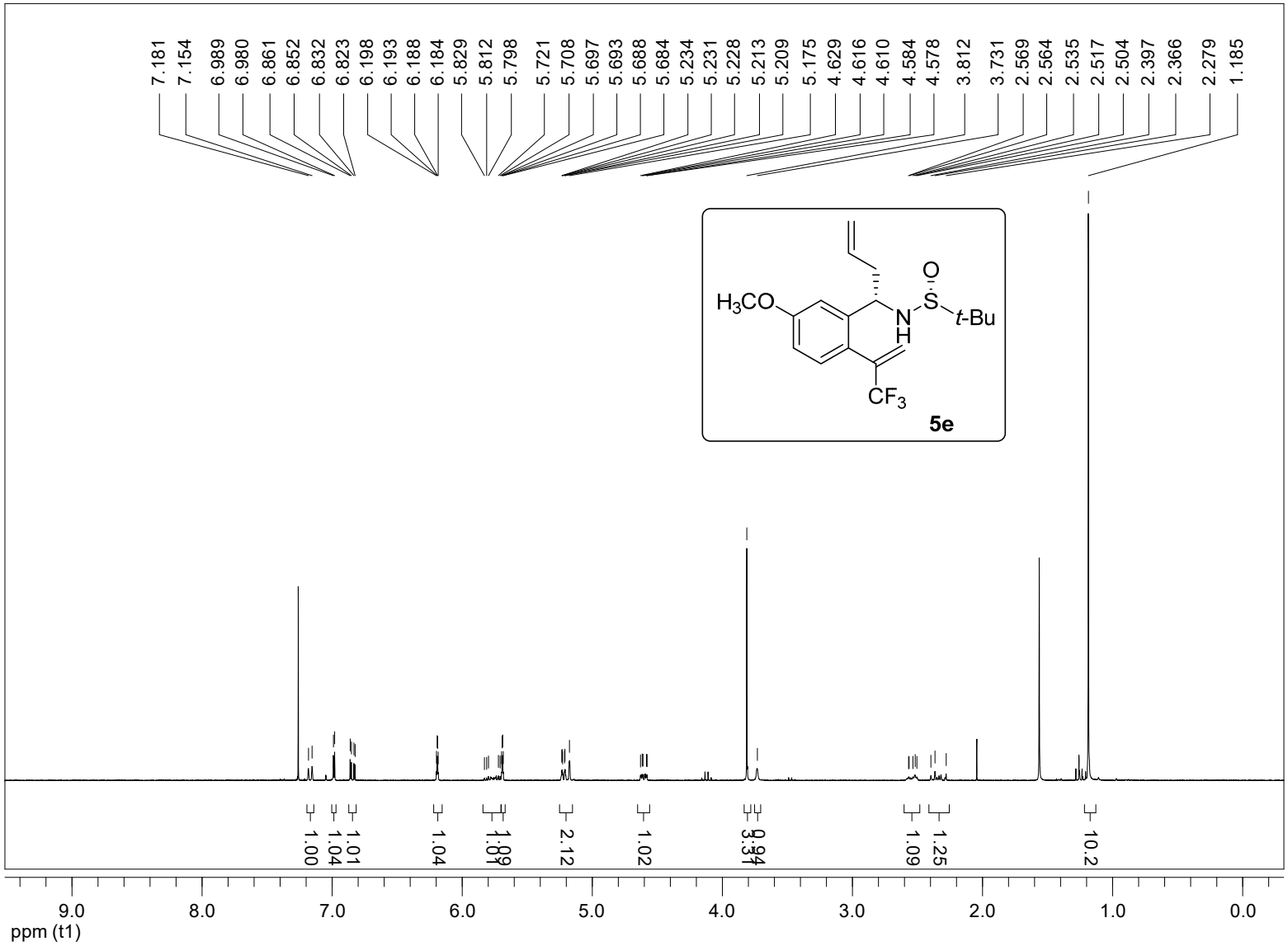
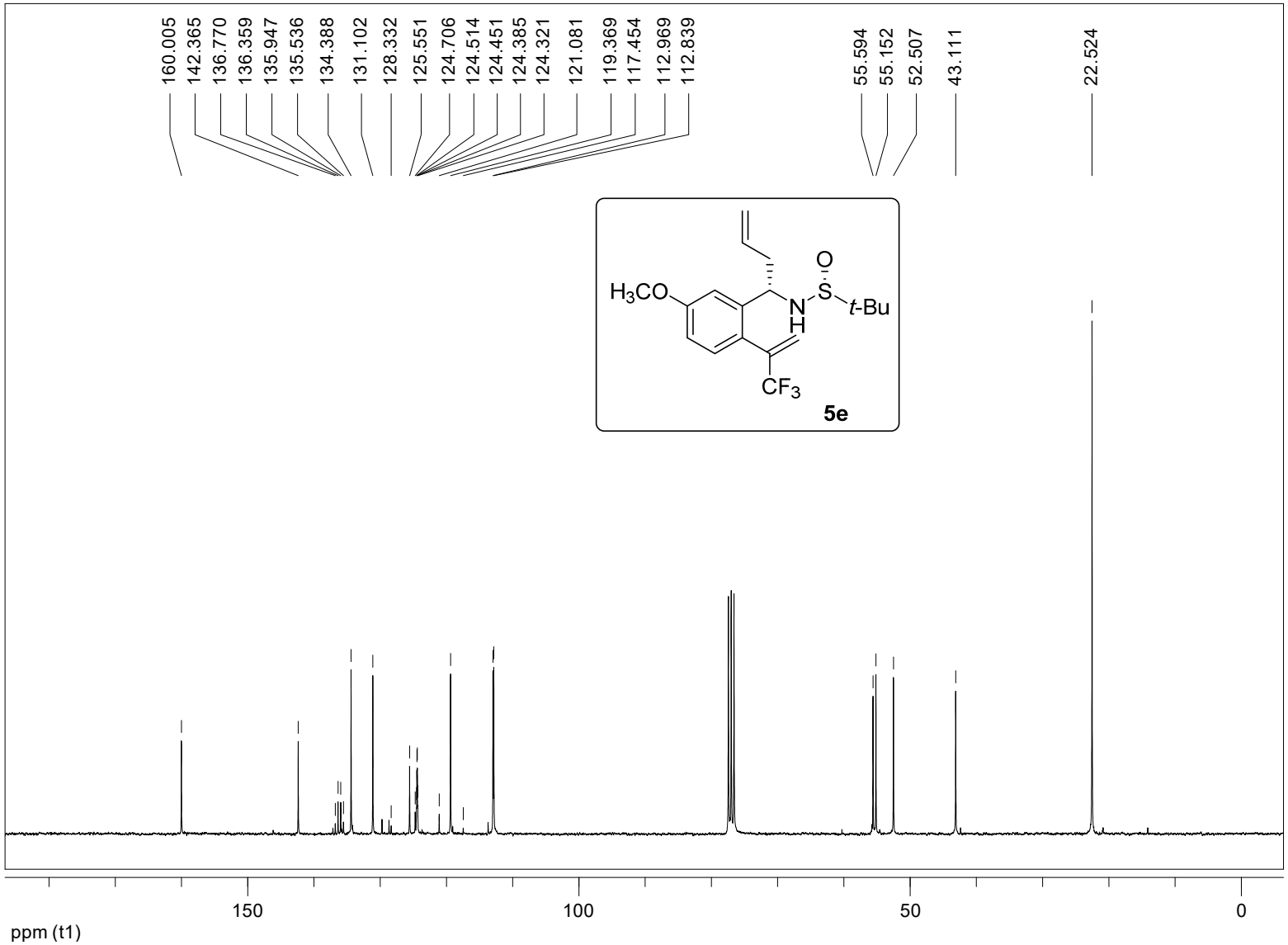
146.653
136.634
136.220
135.807
135.394
134.658
134.392
128.223
126.512
124.709
124.649
124.588
124.522
120.969
119.329
117.341
109.453
107.198
101.414
55.539
52.279
43.129
22.548
O
S
t-Bu
N
H
O
O
CF3
5d
150
100
50
0
ppm (t1)


-67.588
O
S
t-Bu
N
H
O
O
CF3
5d
-50
-60
-70
-80
-90
ppm (t1)


7.181
7.154
6.989
6.980
6.861
6.852
6.832
6.823
6.198
6.193
6.188
6.184
5.829
5.812
5.798
5.721
5.708
5.697
5.693
5.688
5.684
5.234
5.231
5.228
5.213
5.209
5.175
4.629
4.616
4.610
4.584
4.578
3.812
3.731
2.569
2.564
2.535
2.517
2.504
2.397
2.366
2.279
1.185
H3CO
N
H
O
S
t-Bu
CF3
5e
1.00
1.04
1.01
1.04
1.09
1.01
2.12
1.02
3.31
0.94
1.09
1.25
10.2
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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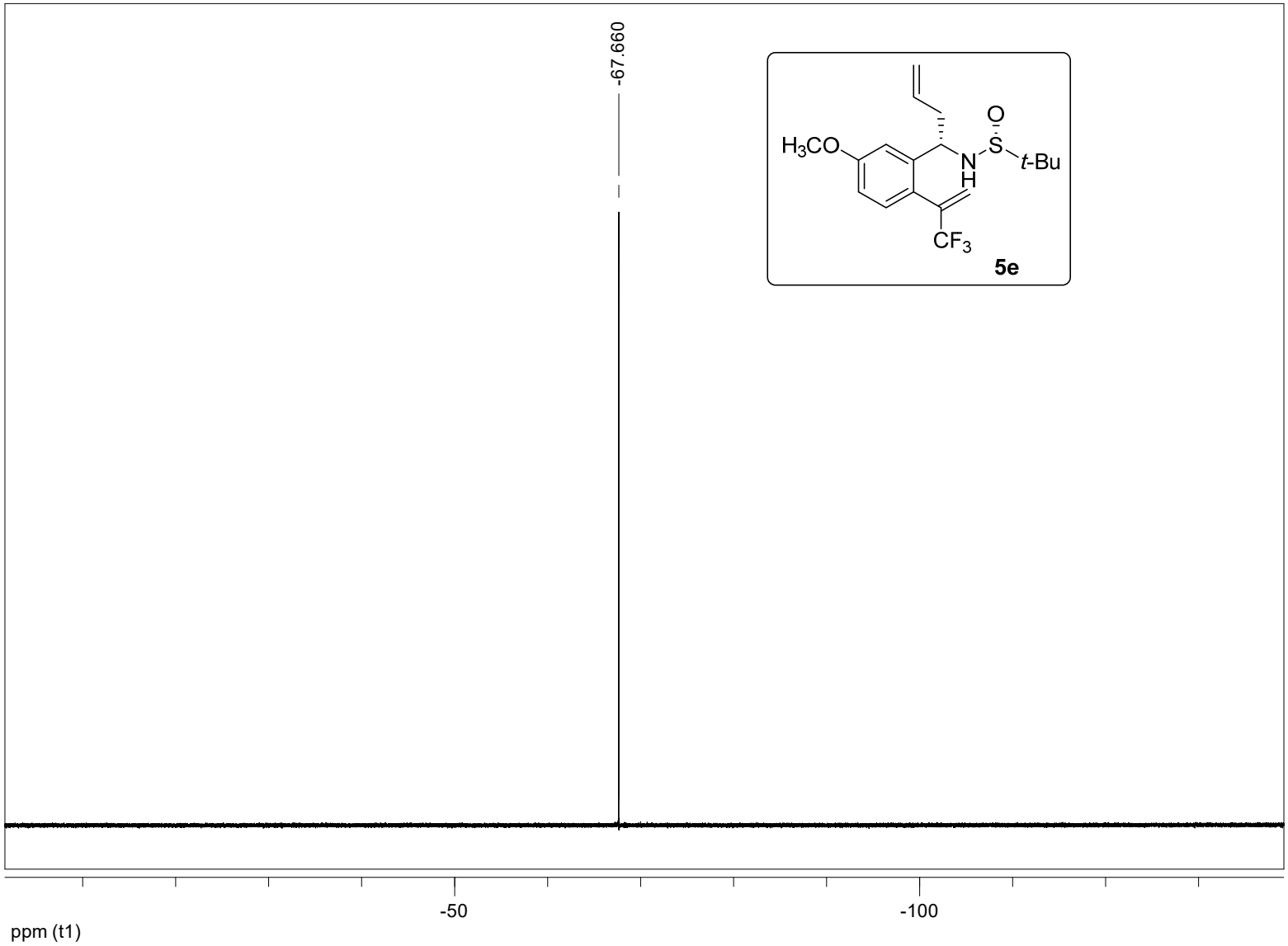
136.770
136.359
135.947
135.536
134.388
131.102
128.332
125.551
124.706
124.514
124.451
124.385
124.321
121.081
119.369
117.454
112.969
112.839
55.594
55.152
52.507
43.111
22.524
H3CO
N
H
S
O
t-Bu
CF3
5e
150
100
50
0
ppm (t1)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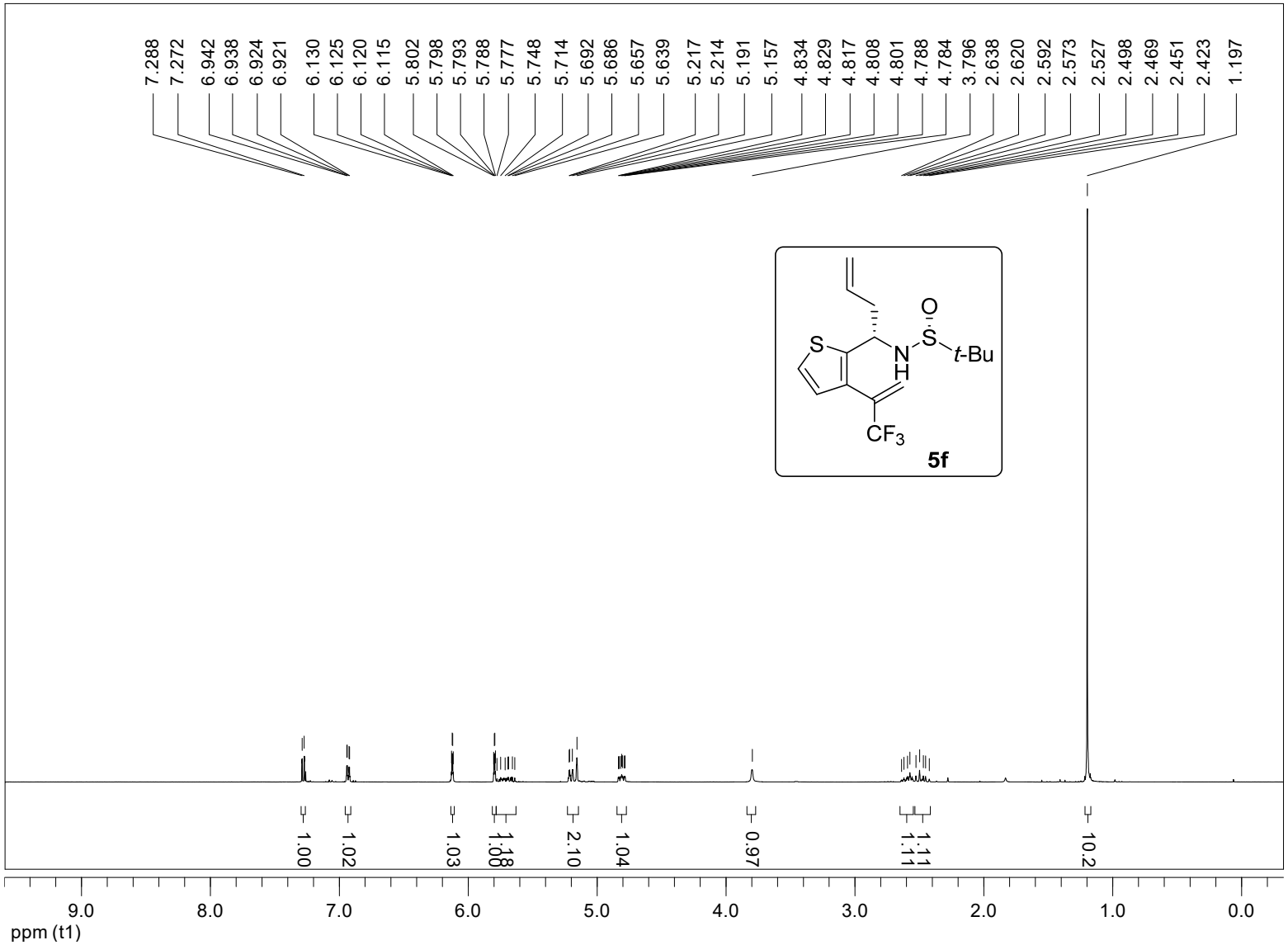
H3CO
O
S
N
H
t-Bu
CF3
5e
-50
-100
ppm (t1)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7.272
6.942
6.938
6.924
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6.130
6.125
6.120
6.115
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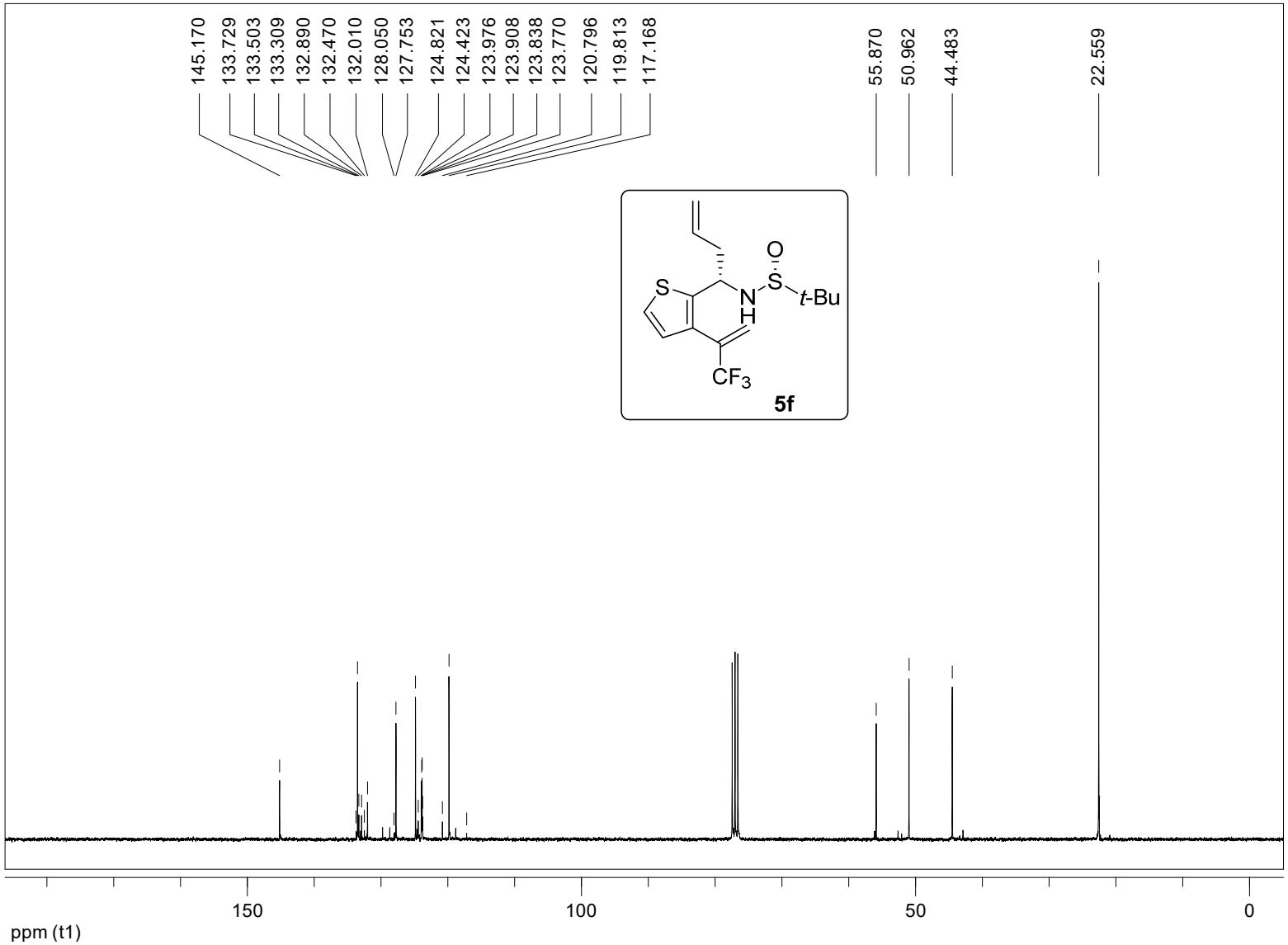
5.798
5.793
5.788
5.777
5.748
5.714
5.692
5.686
5.657
5.639
5.217
5.214
5.191
5.157
4.834
4.829
4.817
4.808
4.801
4.788
4.784
3.796
2.638
2.620
2.592
2.573
2.527
2.498
2.469
2.451
2.423
1.197
S
N
H
O
S
t-Bu
CF3
5f
1.00
1.02
1.03
1.18
1.08
2.10
1.04
0.97
1.11
1.11
10.2
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


145.170
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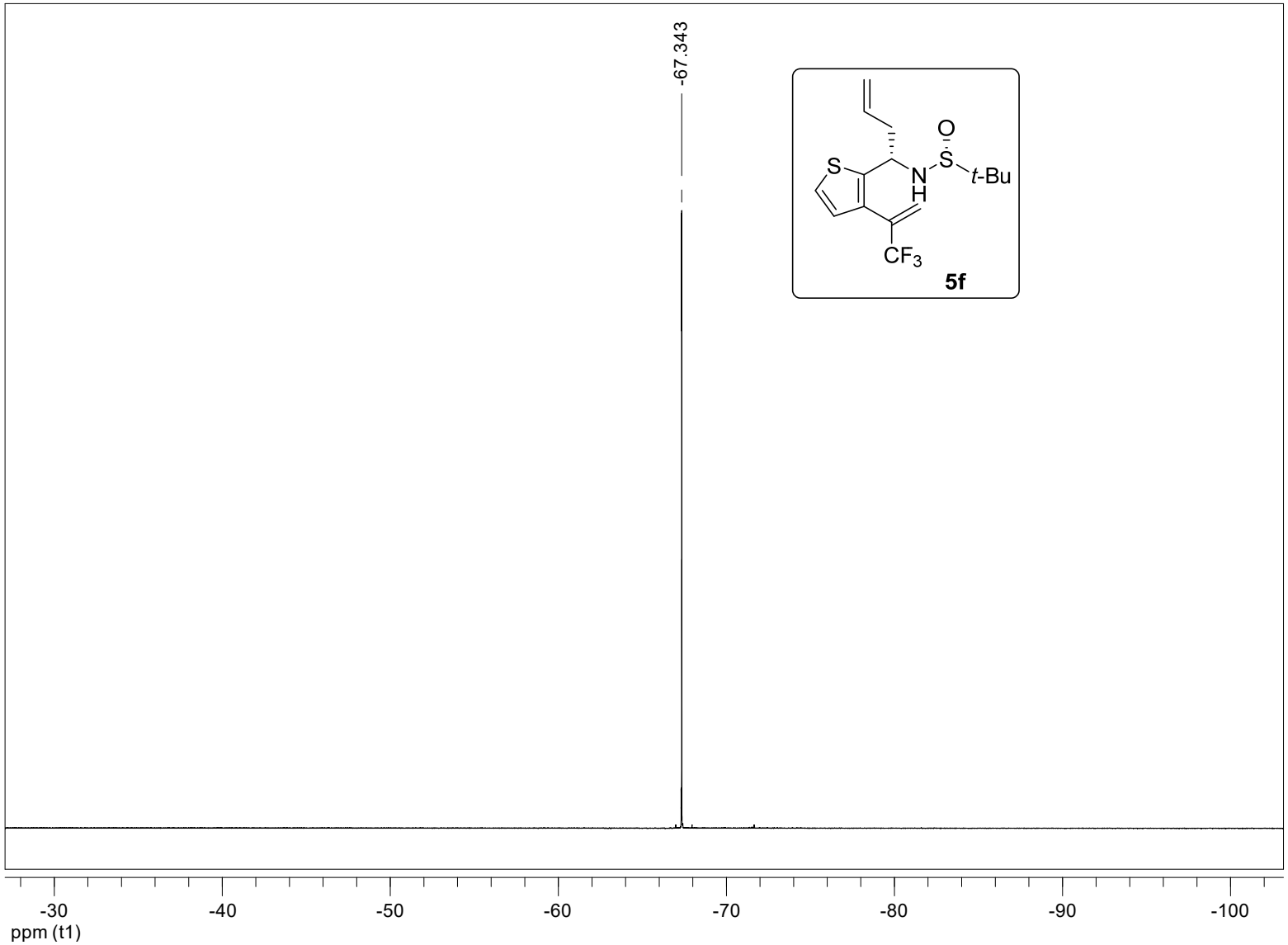
133.503
133.309
132.890
132.470
132.010
128.050
127.753
124.821
124.423
123.976
123.908
123.838
123.770
120.796
119.813
117.168
55.870
50.962
44.483
22.559
S
N
H
O
S
t-Bu
CF3
5f
150
100
50
0
ppm (t1)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S
N
H
O
S
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CF3
5f
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-40
-50
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-70
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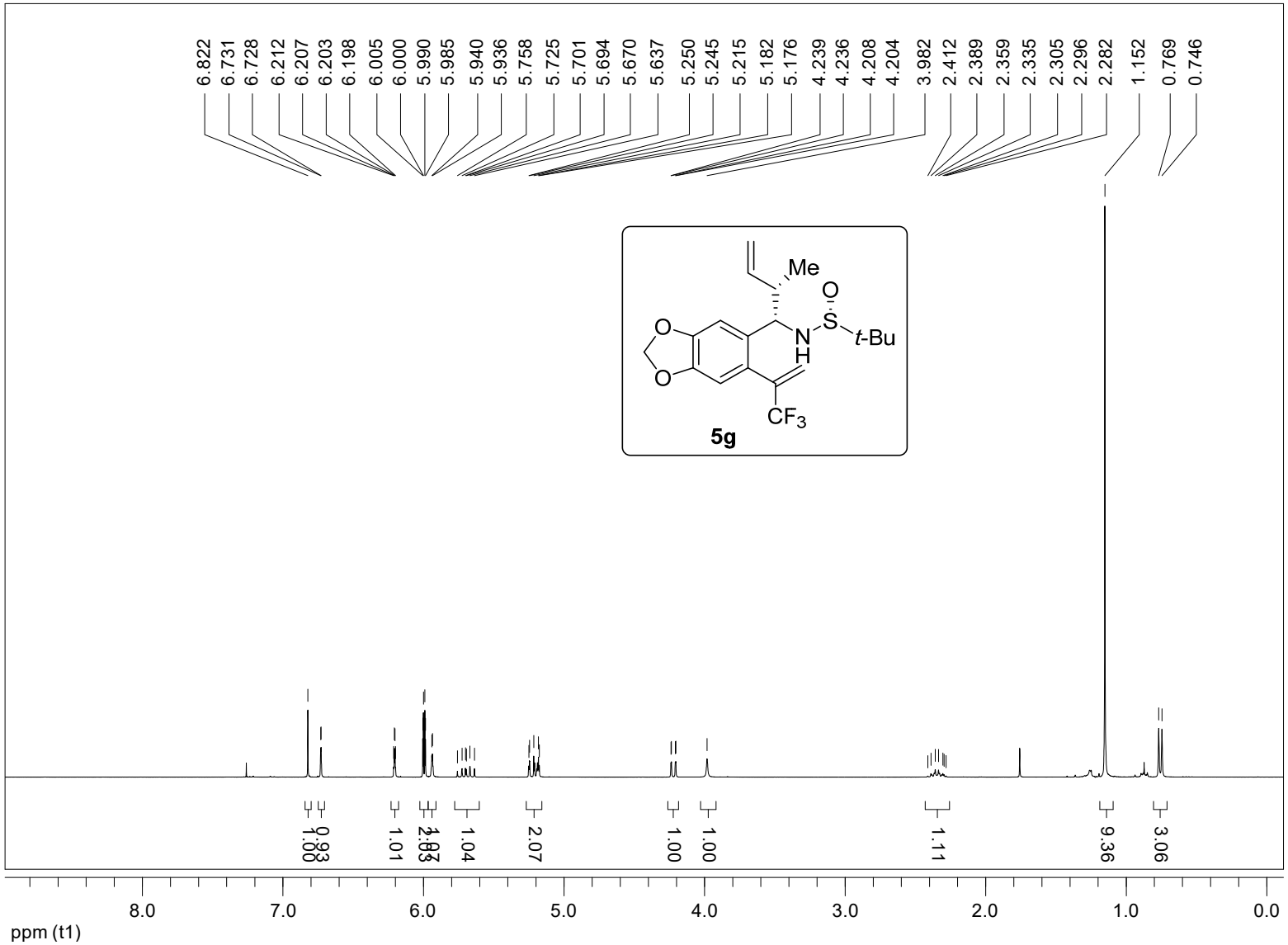
-90
-100
ppm (t1)


6.822
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6.728
6.212
6.207
6.203
6.198
6.005
6.000
5.990
5.985
5.940
5.936
5.758
5.725
5.701
5.694
5.670
5.637
5.250
5.245
5.215
5.182
5.176
4.239
4.236
4.208
4.204
3.982
2.412
2.389
2.359
2.335
2.305
2.296
2.282
1.152
0.769
0.746
Me
O
S
t-Bu
N
H
O
O
CF3
5g
1.00
0.93
1.01
2.03
2.07
1.04
2.07
1.00
1.00
1.11
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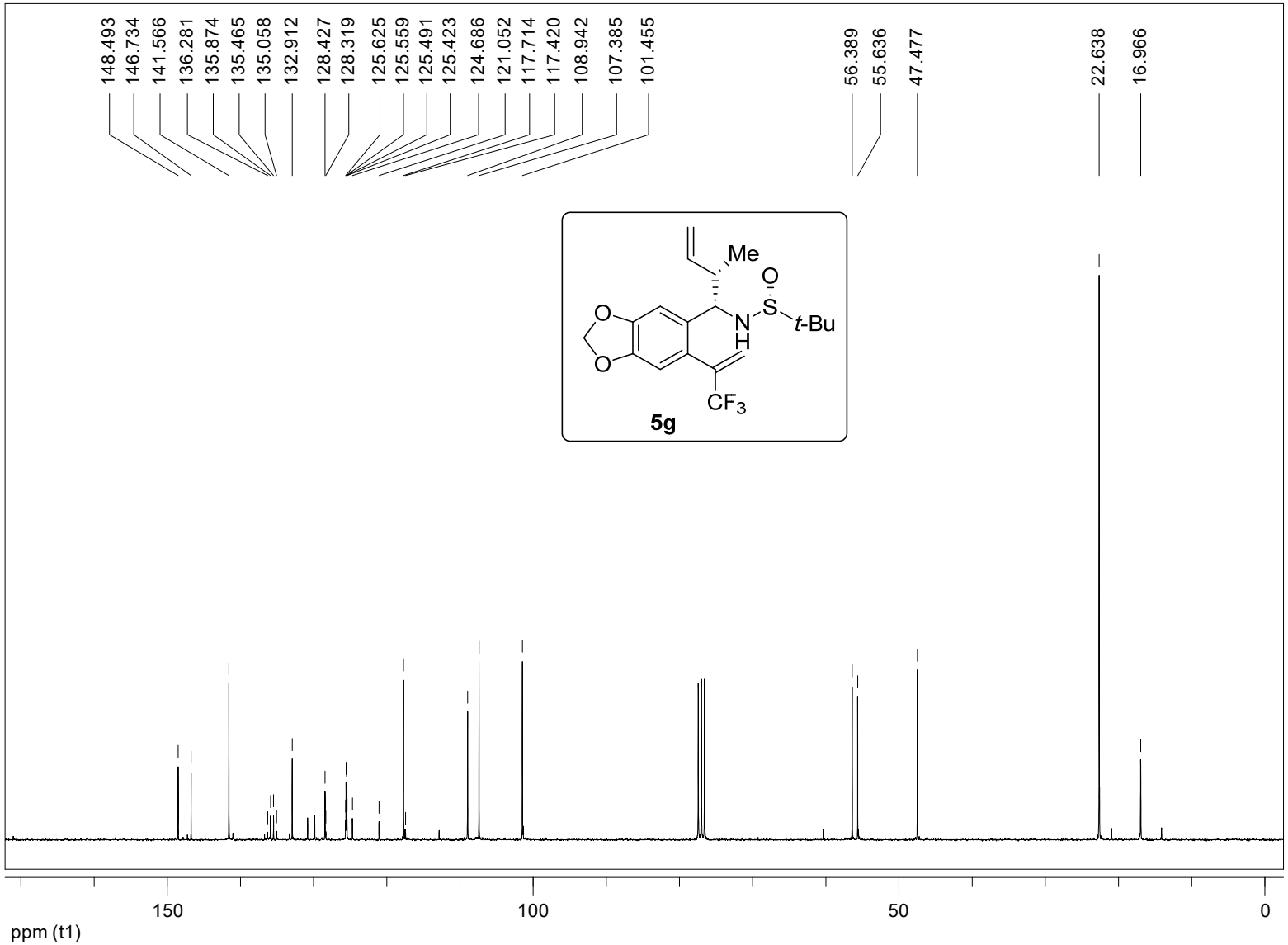
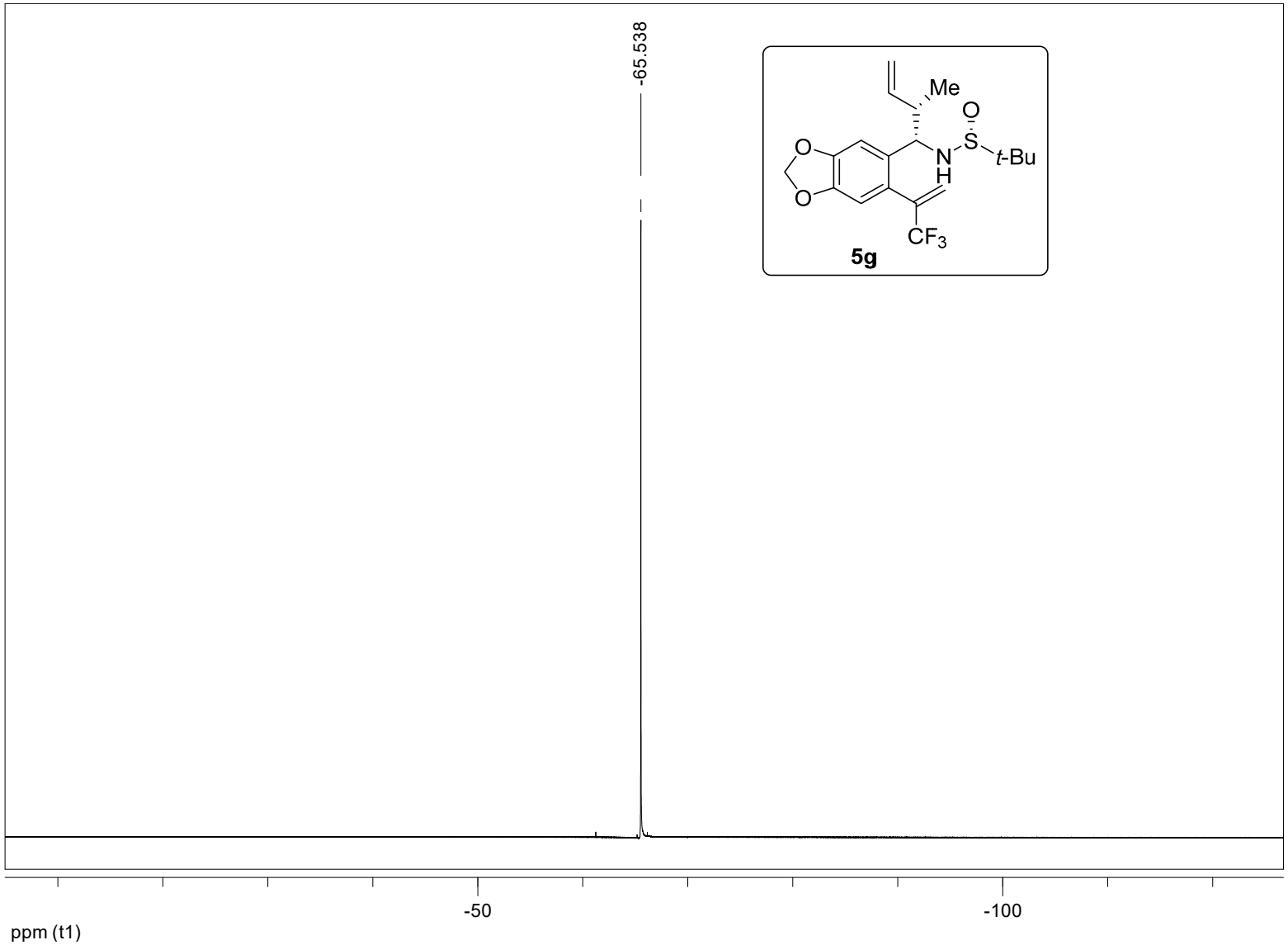
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


148.493
146.734
141.566
136.281
135.874
135.465
135.058
132.912
128.427
128.319
125.625
125.559
125.491
125.423
124.686
121.052
117.714
117.420
108.942
107.385
101.455
56.389
55.636
47.477
22.638
16.966
Me
O
S
t-Bu
N
H
O
O
O
CF3
5g
150
100
50
0
ppm (t1)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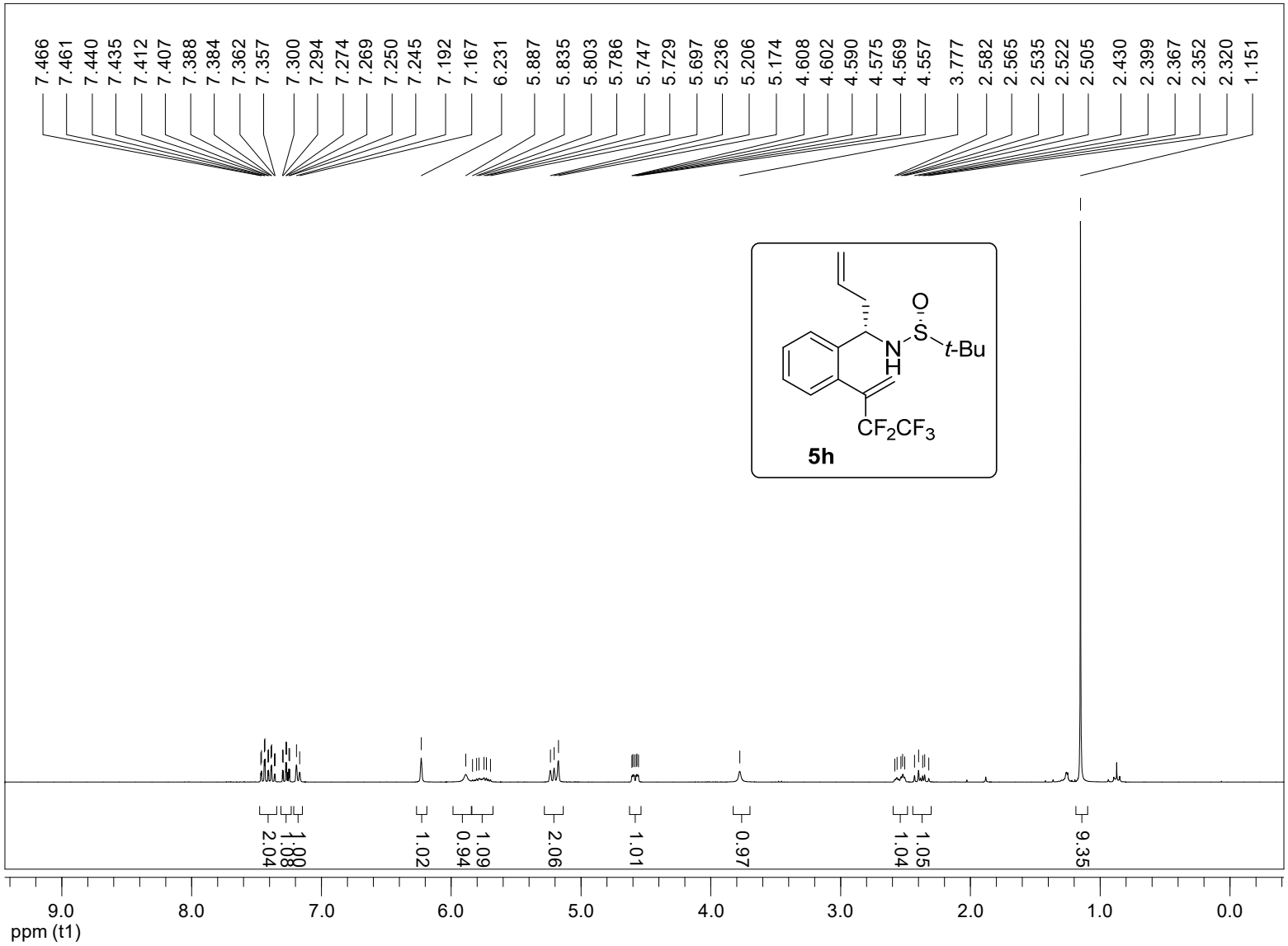
Me
O
S
t-Bu
N
H
O
O
CF3
5g
-50
-100
ppm (t1)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7.435
7.412
7.407
7.388
7.384
7.362
7.357
7.300
7.294
7.274
7.269
7.250
7.245
7.192
7.167
6.231
5.887
5.835
5.803
5.786
5.747
5.729
5.697
5.236
5.206
5.174
4.608
4.602
4.590
4.575
4.569
4.557
3.777
2.582
2.565
2.535
2.522
2.505
2.430
2.399
2.367
2.352
2.320
1.151
O
S
N
H
t-Bu
CF2CF3
5h
2.04
1.00
1.08
1.02
0.94
1.09
2.06
1.01
0.97
1.04
1.05
9.35
9.0
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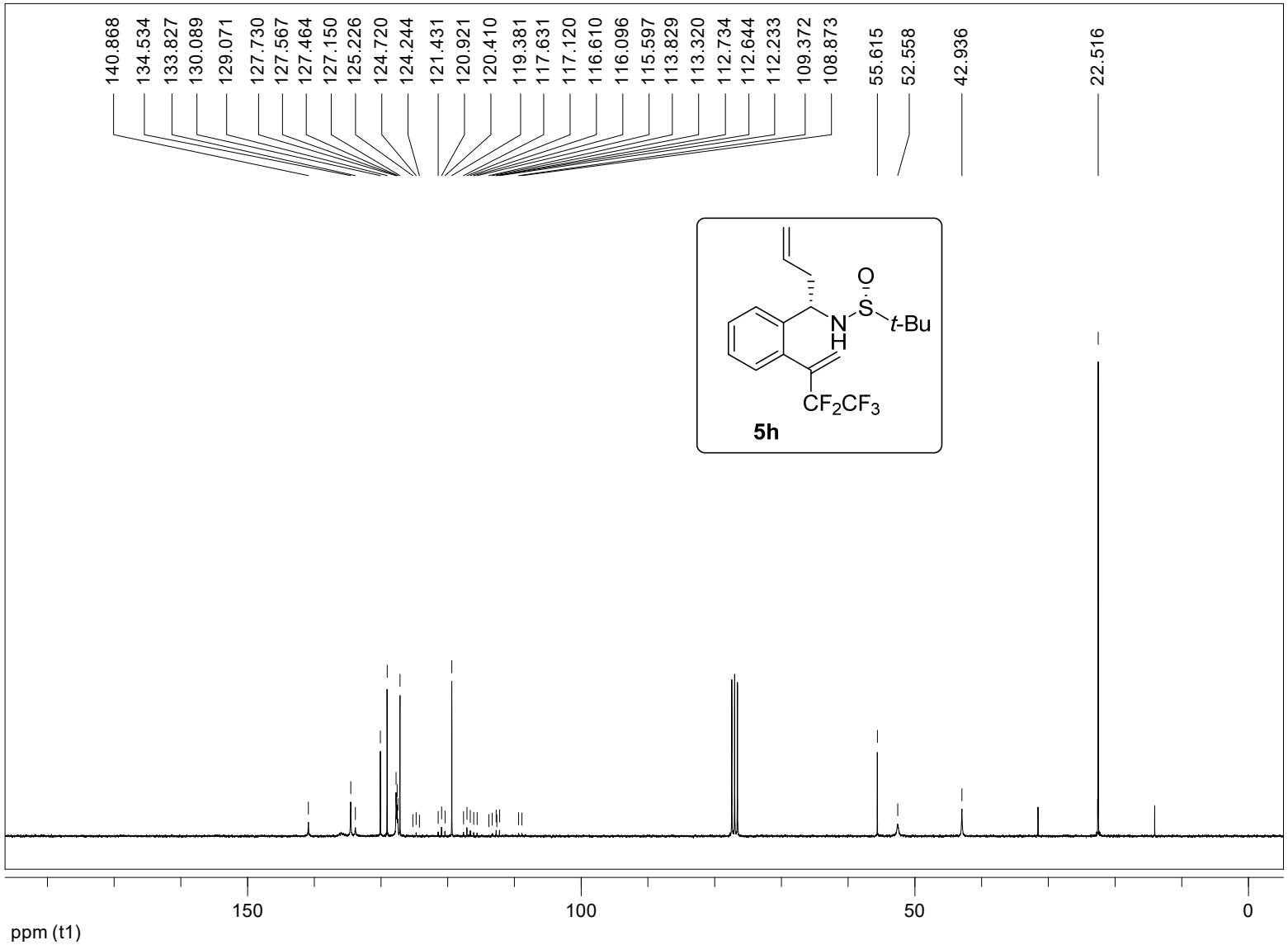
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


140.868
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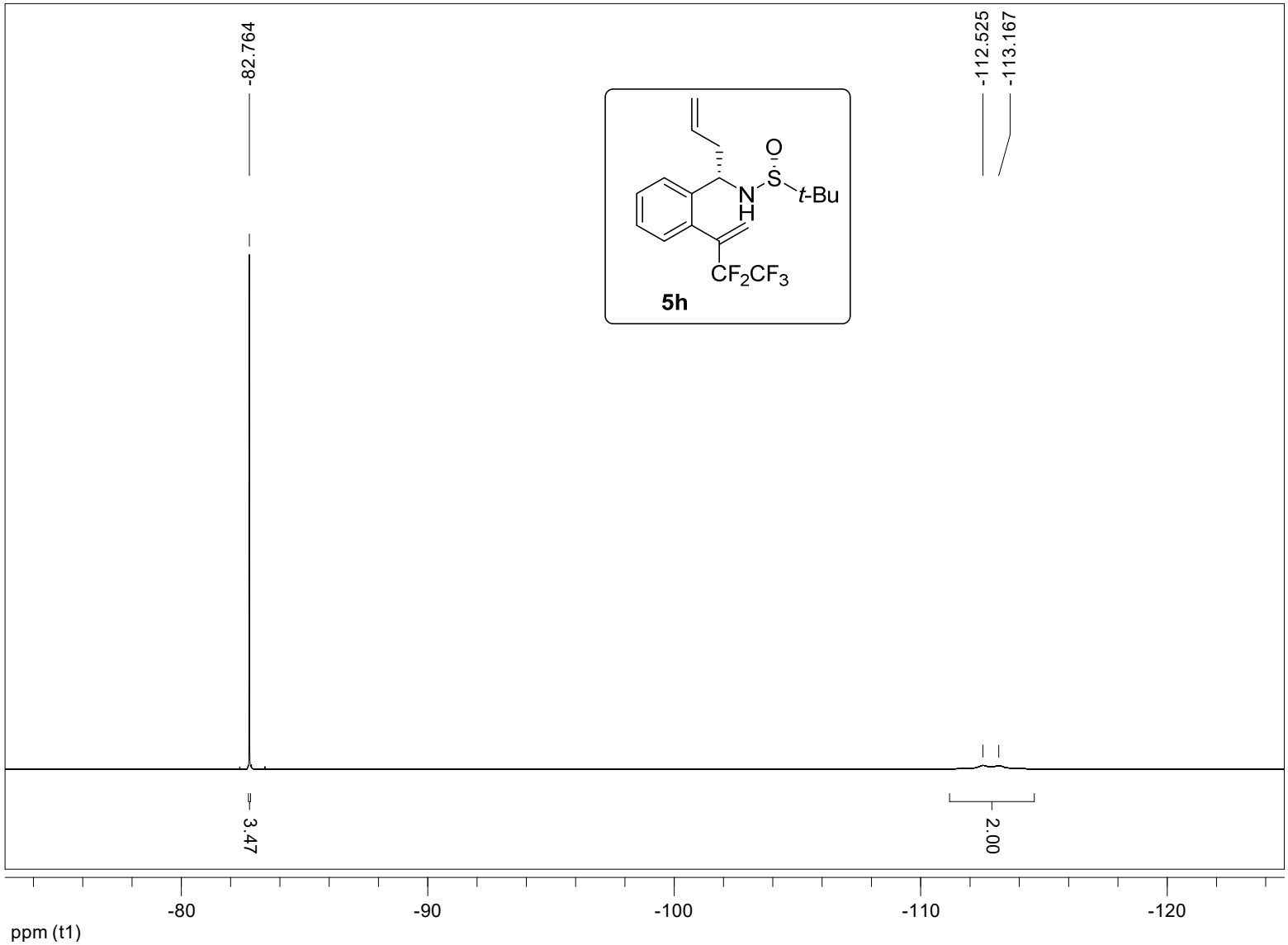
133.827
130.089
129.071
127.730
127.567
127.464
127.150
125.226
124.720
124.244
121.431
120.921
120.410
119.381
117.631
117.120
116.610
116.096
115.597
113.829
113.320
112.734
112.644
112.233
109.372
108.873
55.615
52.558
42.936
22.516
O
S
t-Bu
N
H
CF2CF3
5h
150
100
50
0
ppm (t1)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-112.525
-113.167
O
S
N
H
t-Bu
CF2CF3
5h
3.47
2.00
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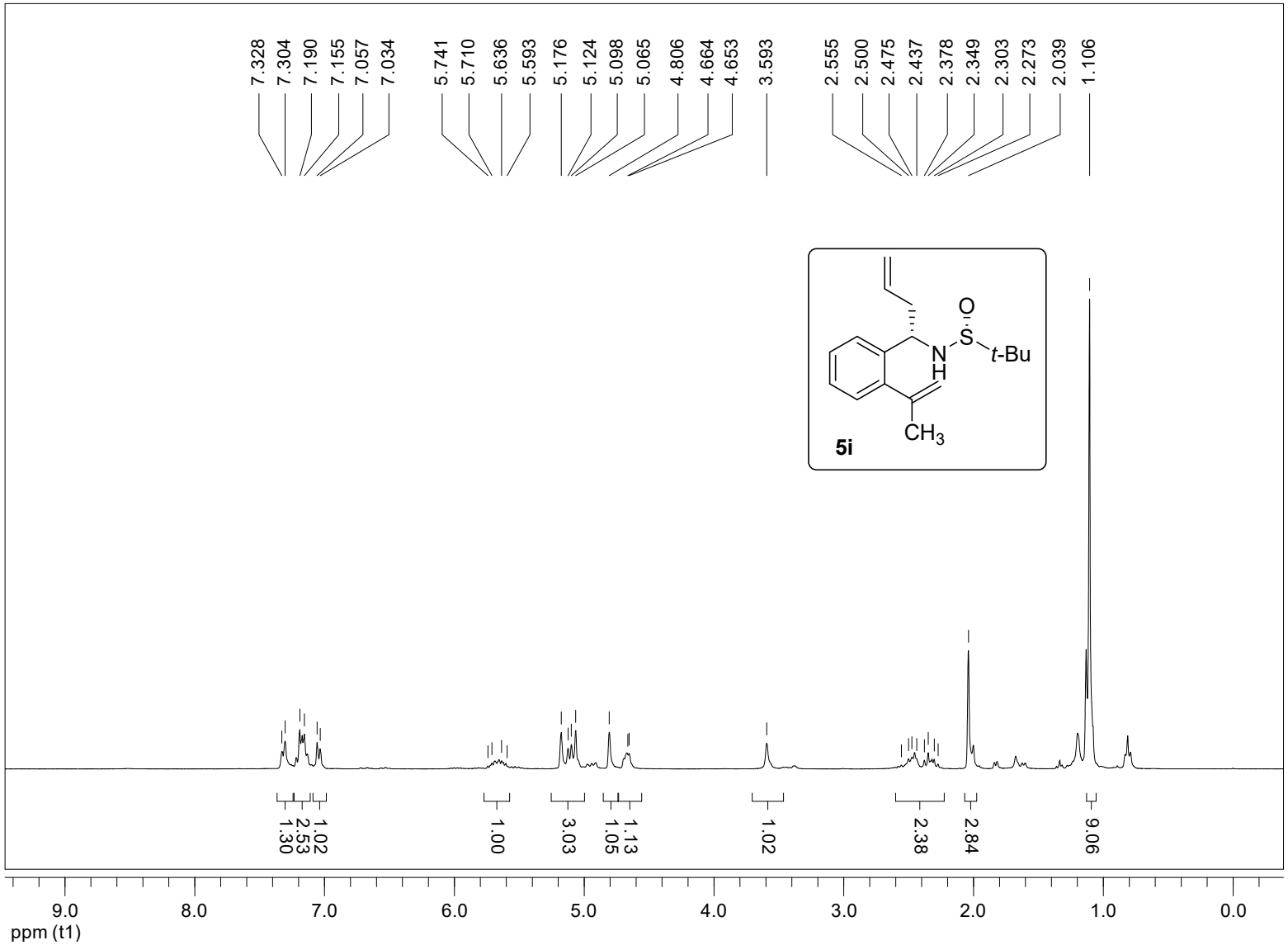
-90
-100
-110
-120
ppm (t1)


7.328
7.304
7.190
7.155
7.057
7.034
5.741
5.710
5.636
5.593
5.176
5.124
5.098
5.065
4.806
4.664
4.653
3.593
2.555
2.500
2.475
2.437
2.378
2.349
2.303
2.273
2.039
1.106
O
S
t-Bu
N
H
CH3
5i
1.30
2.53
1.02
1.00
3.03
1.05
1.13
1.02
2.38
2.84
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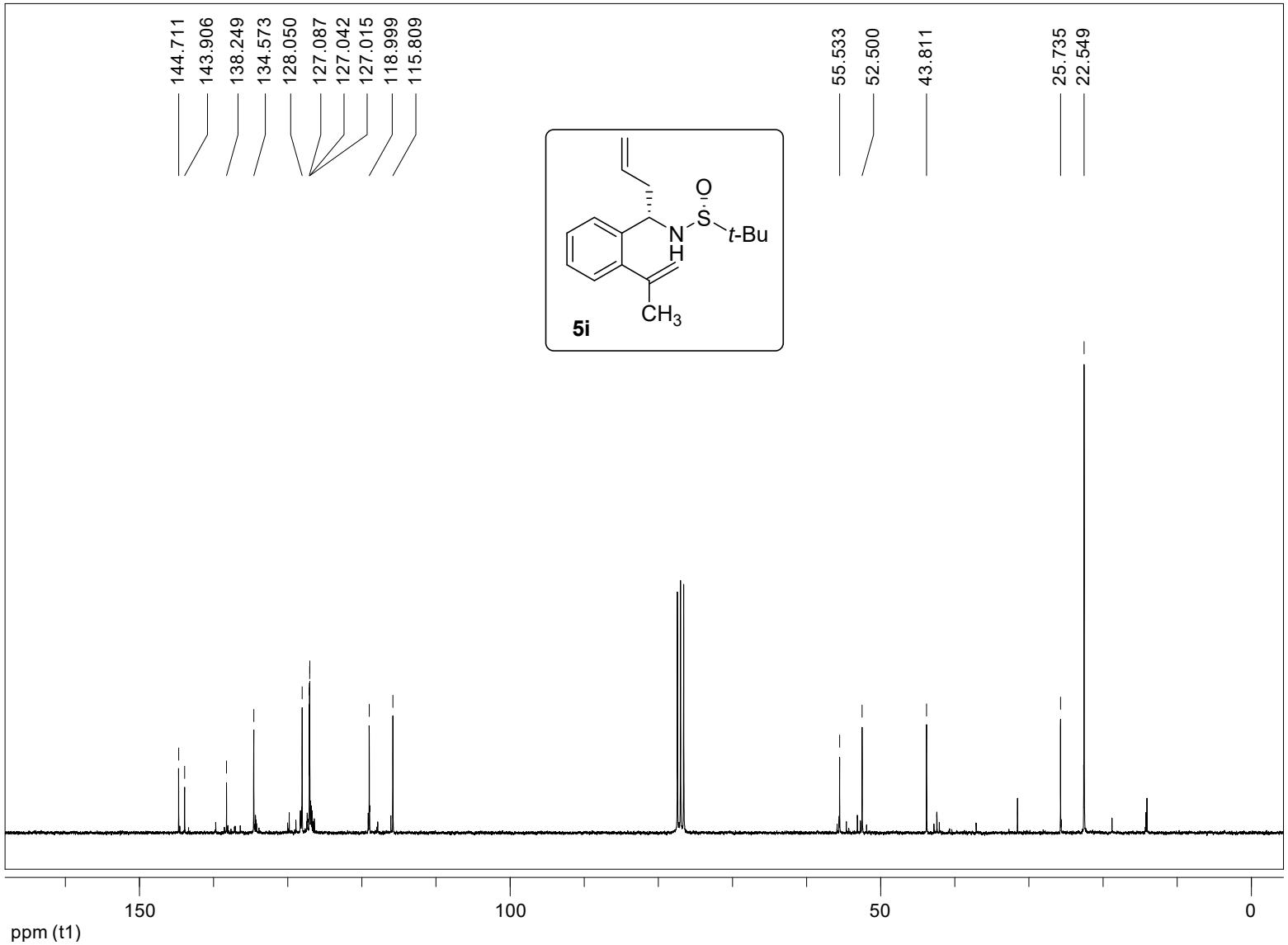
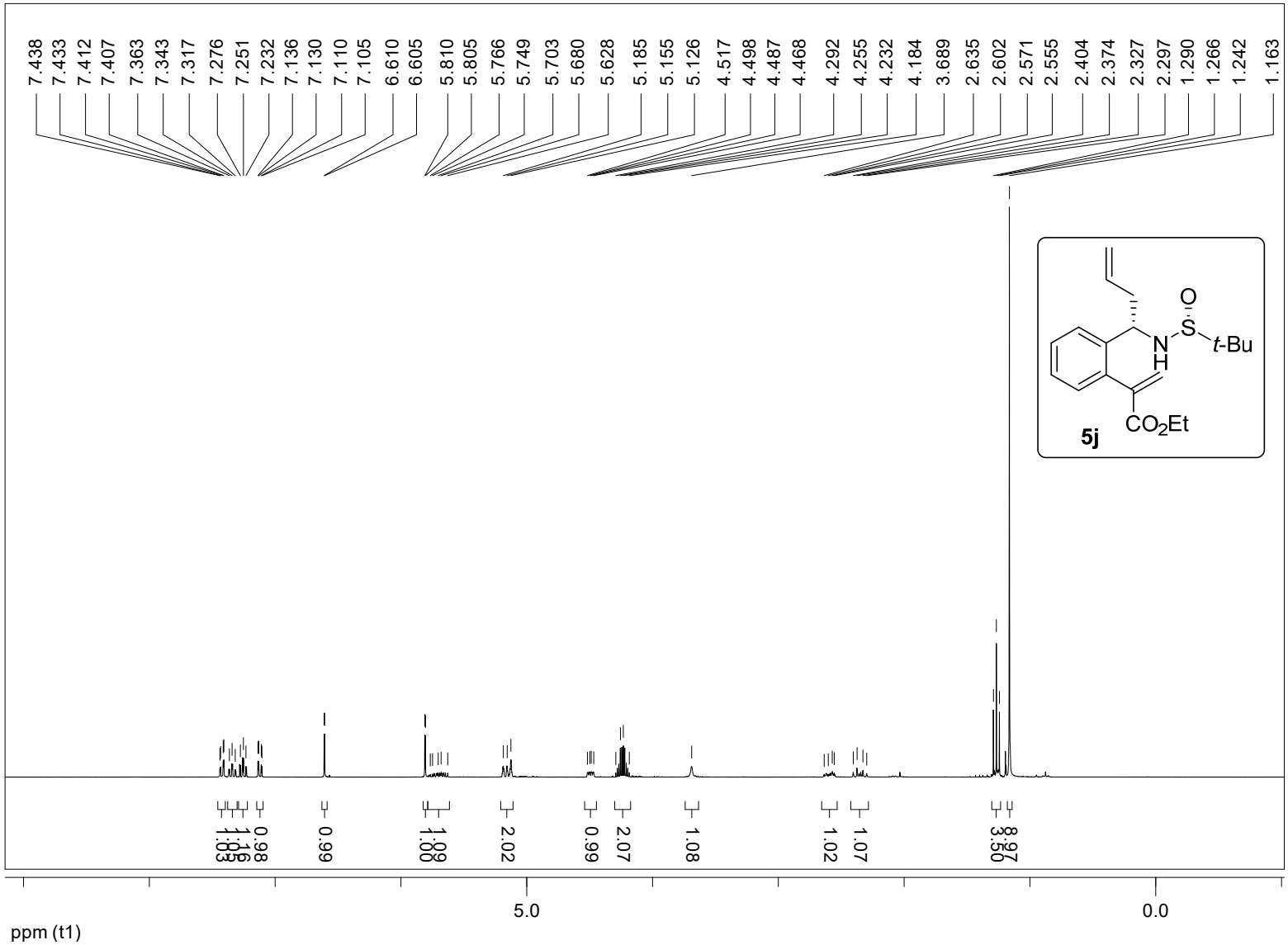
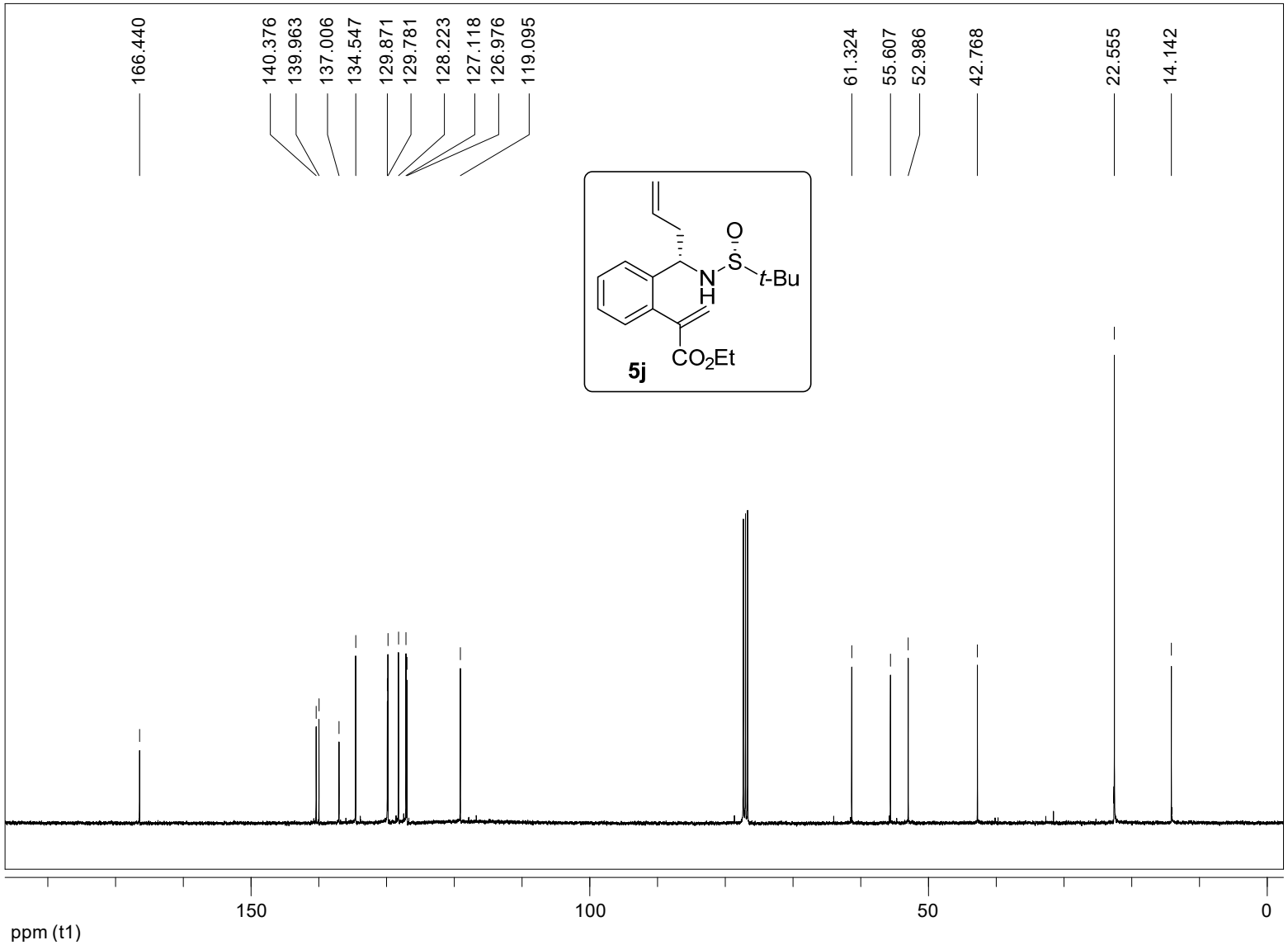
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


144.711
143.906
138.249
134.573
128.050
127.087
127.042
127.015
118.999
115.809
55.533
52.500
43.811
25.735
22.549
O
S
N
H
t-Bu
CH3
5i
150
100
50
0
ppm (t1)


7.438
7.433
7.412
7.407
7.363
7.343
7.317
7.276
7.251
7.232
7.136
7.130
7.110
7.105
6.610
6.605
5.810
5.805
5.766
5.749
5.703
5.680
5.628
5.185
5.155
5.126
4.517
4.498
4.487
4.468
4.292
4.255
4.232
4.184
3.689
2.635
2.602
2.571
2.555
2.404
2.374
2.327
2.297
1.290
1.266
1.242
1.163
1.03
1.00
1.16
0.98
0.99
1.00
1.09
2.02
0.99
2.07
1.08
1.02
1.07
3.50
8.97
5.0
0.0
ppm (t1)
O
S
t-Bu
N
H
CO2Et
5j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134.547
129.871
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128.223
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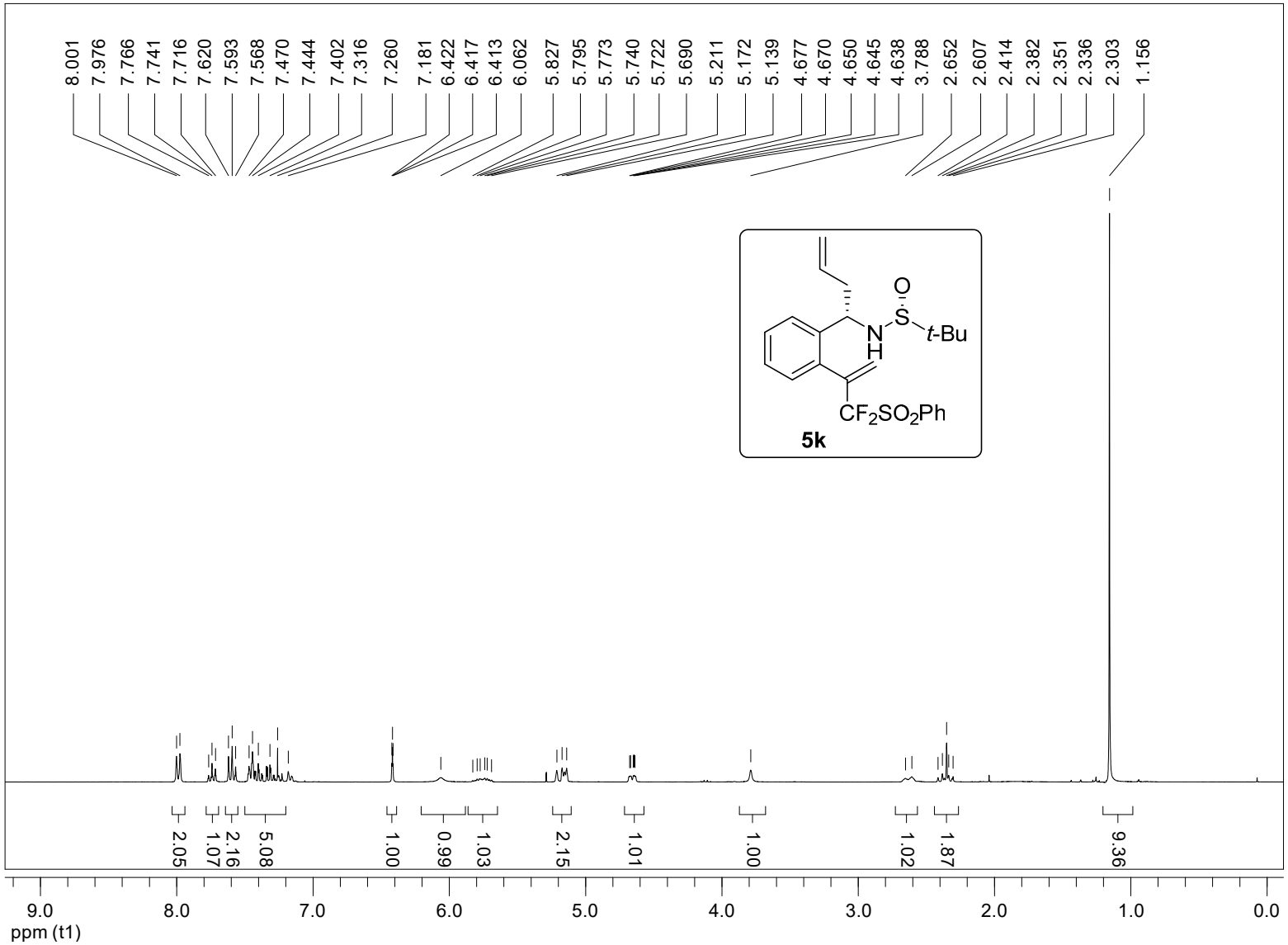
126.976
119.095
61.324
55.607
52.986
42.768
22.555
14.142
O
S
N
H
t-Bu
CO2Et
5j
150
100
50
0
ppm (t1)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7.976
7.766
7.741
7.716
7.620
7.593
7.568
7.470
7.444
7.402
7.316
7.260
7.181
6.422
6.417
6.413
6.062
5.827
5.795
5.773
5.740
5.722
5.690
5.211
5.172
5.139
4.677
4.670
4.650
4.645
4.638
3.788
2.652
2.607
2.414
2.382
2.351
2.336
2.303
1.156
O
S
N
H
t-Bu
CF2SO2Ph
5k
2.05
1.07
2.16
5.08
1.00
0.99
1.03
2.15
1.01
1.00
1.02
1.87
9.36
9.0
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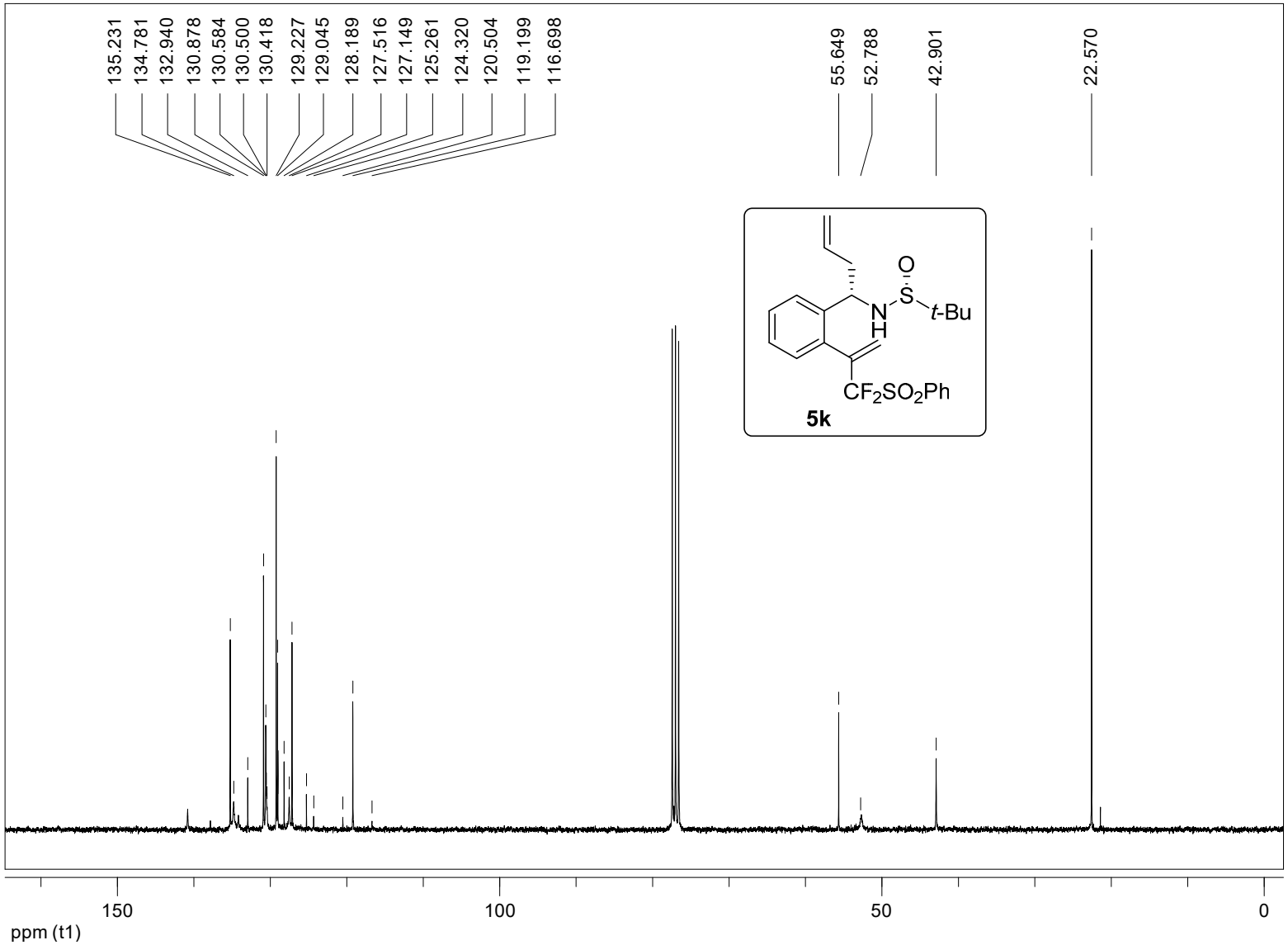
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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134.781
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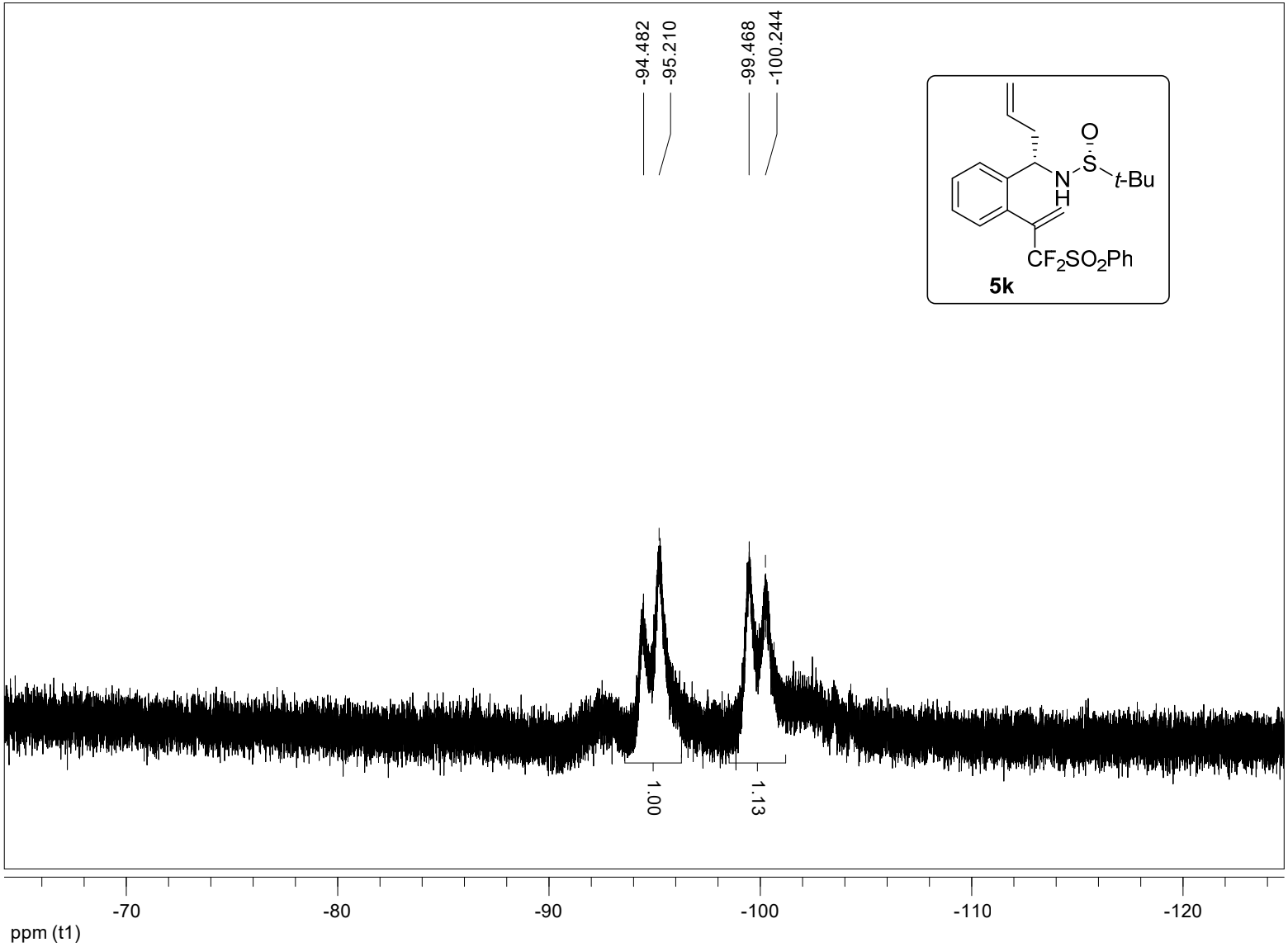
128.189
127.516
127.149
125.261
124.320
120.504
119.199
116.698
55.649
52.788
42.901
22.570
O
S
N
H
t-Bu
CF2SO2Ph
5k
150
100
50
0
ppm (t1)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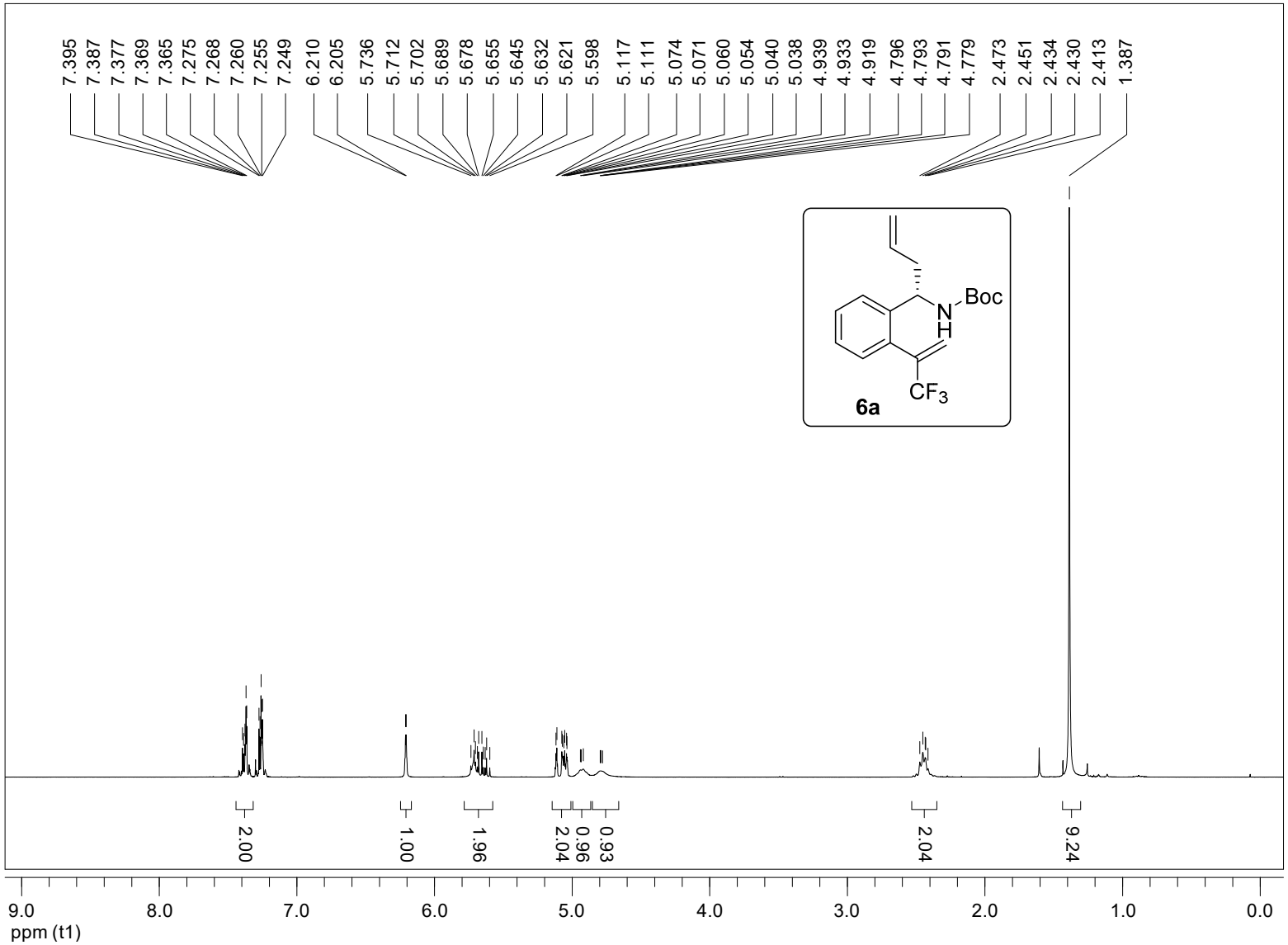
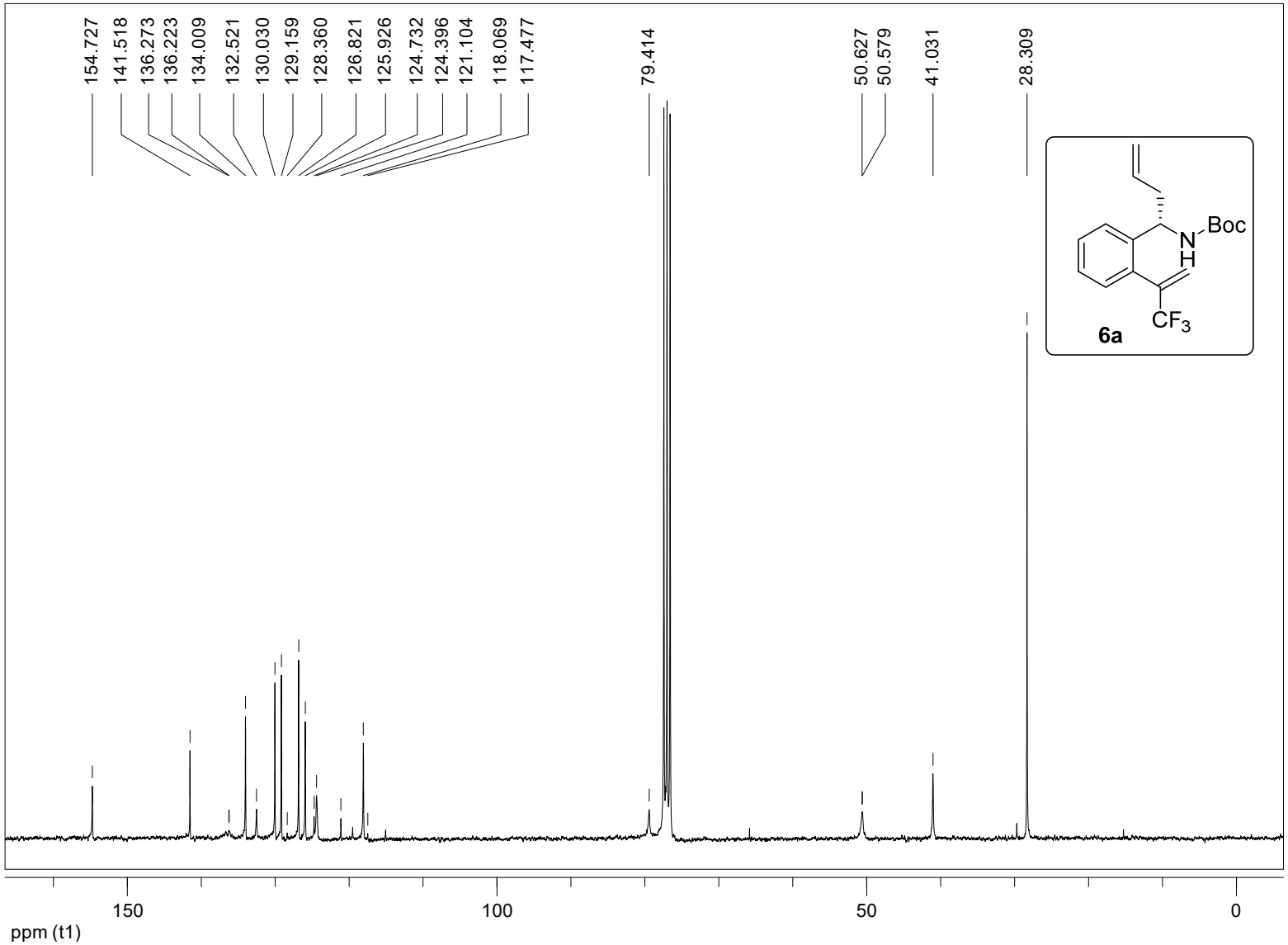
-95.210
-99.468
-100.244
1.00
1.13
O
S
t-Bu
N
H
CF2SO2Ph
5k
-70
-80
-90
-100
-110
-120
ppm (t1)


7.395
7.387
7.377
7.369
7.365
7.275
7.268
7.260
7.255
7.249
6.210
6.205
5.736
5.712
5.702
5.689
5.678
5.655
5.645
5.632
5.621
5.598
5.117
5.111
5.074
5.071
5.060
5.054
5.040
5.038
4.939
4.933
4.919
4.796
4.793
4.791
4.779
2.473
2.451
2.434
2.430
2.413
1.387
Boc
N
H
CF3
6a
2.00
1.00
1.96
2.04
0.96
0.93
2.04
9.24
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


154.727
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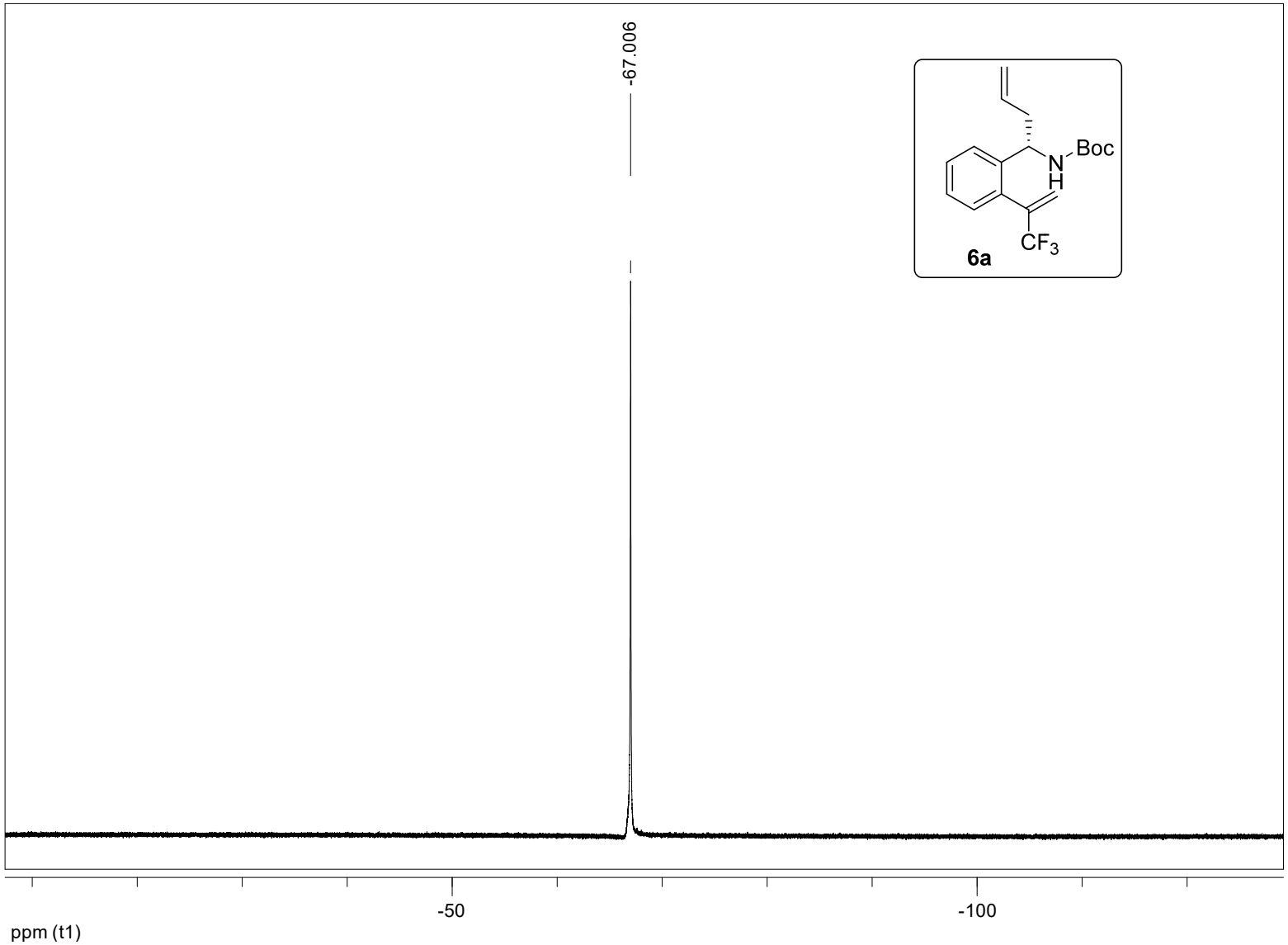
136.273
136.223
134.009
132.521
130.030
129.159
128.360
126.821
125.926
124.732
124.396
121.104
118.069
117.477
79.414
50.627
50.579
41.031
28.309
Boc
N
H
CF3
6a
150
100
50
0
ppm (t1)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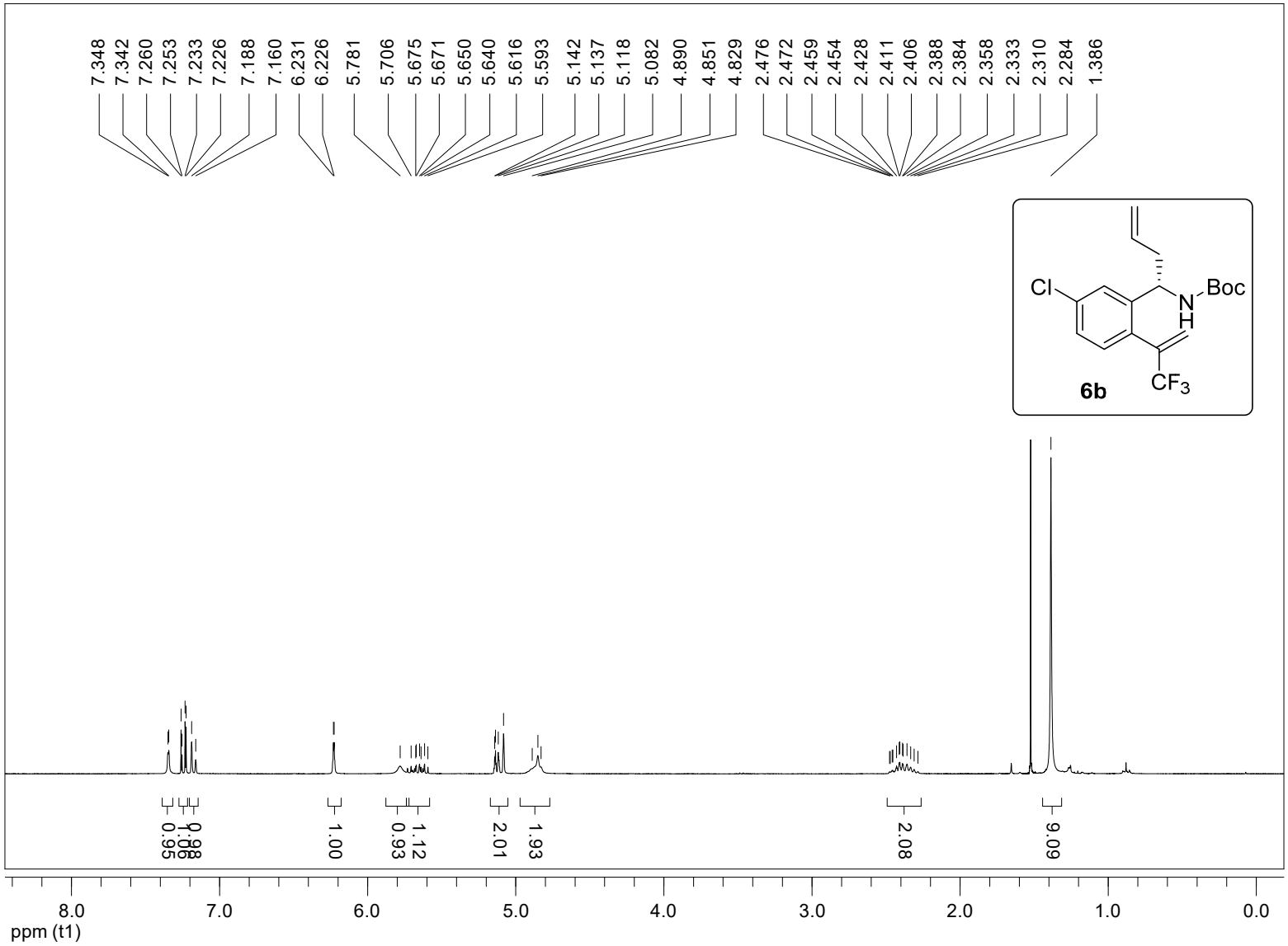
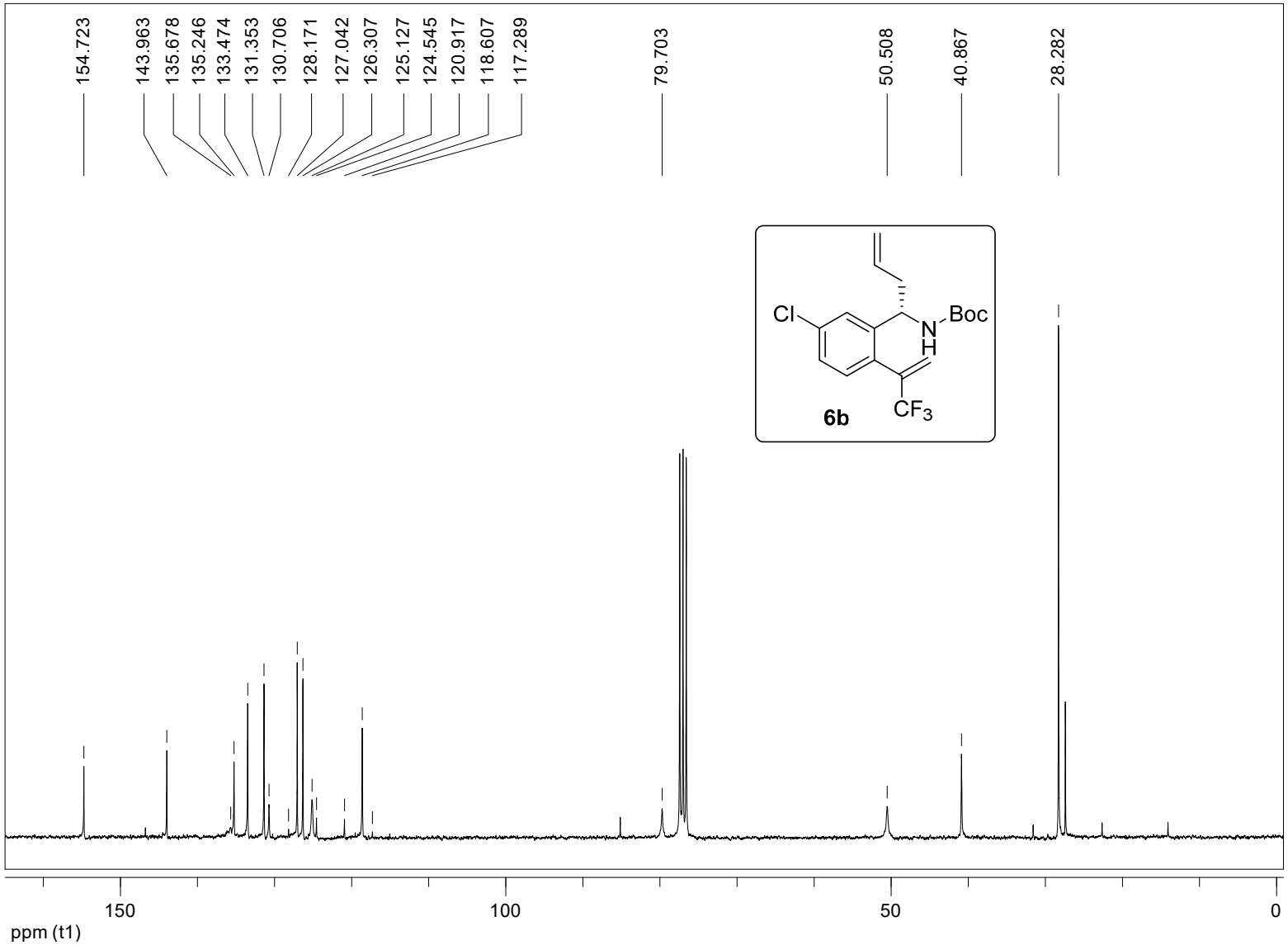
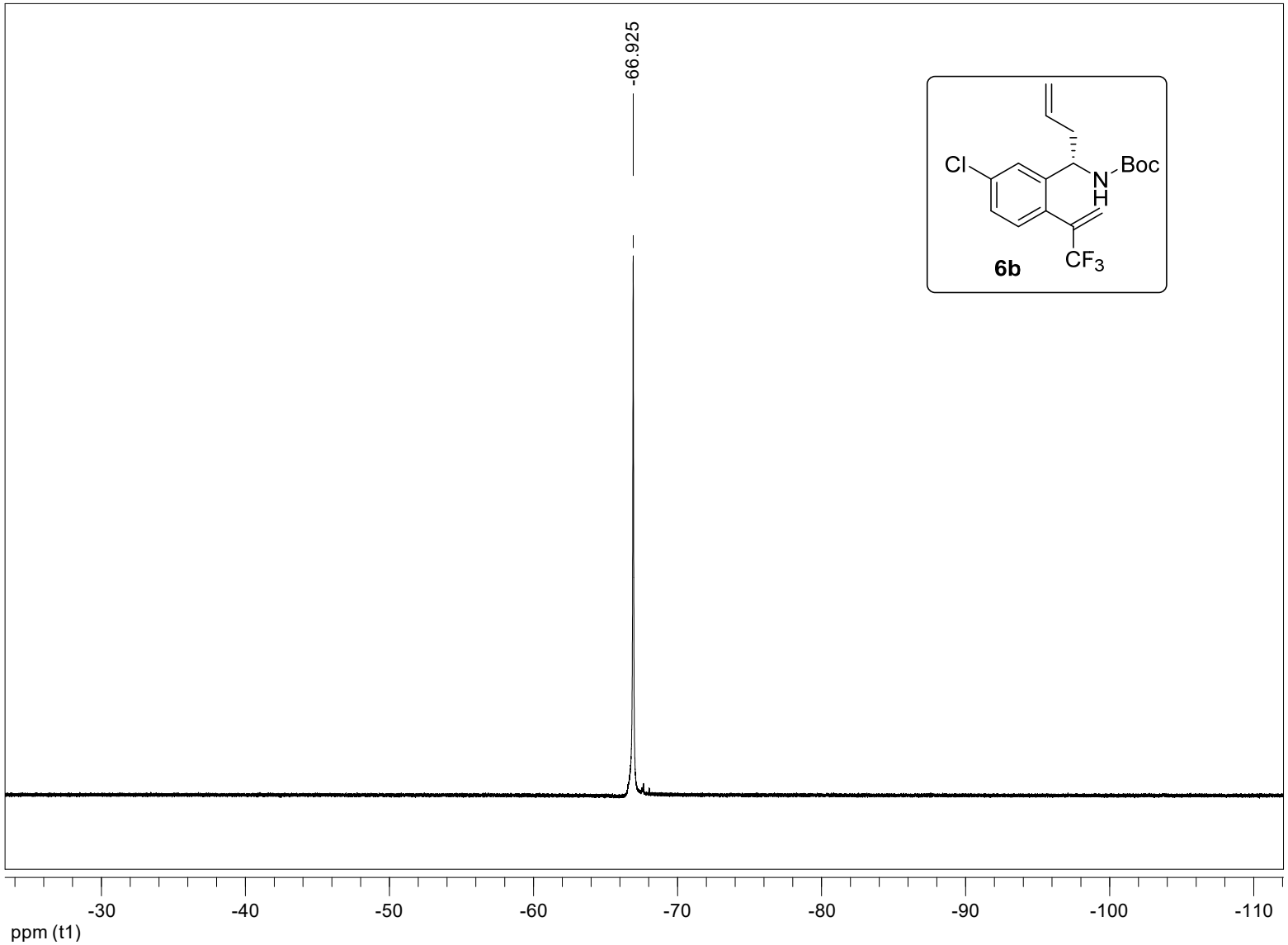
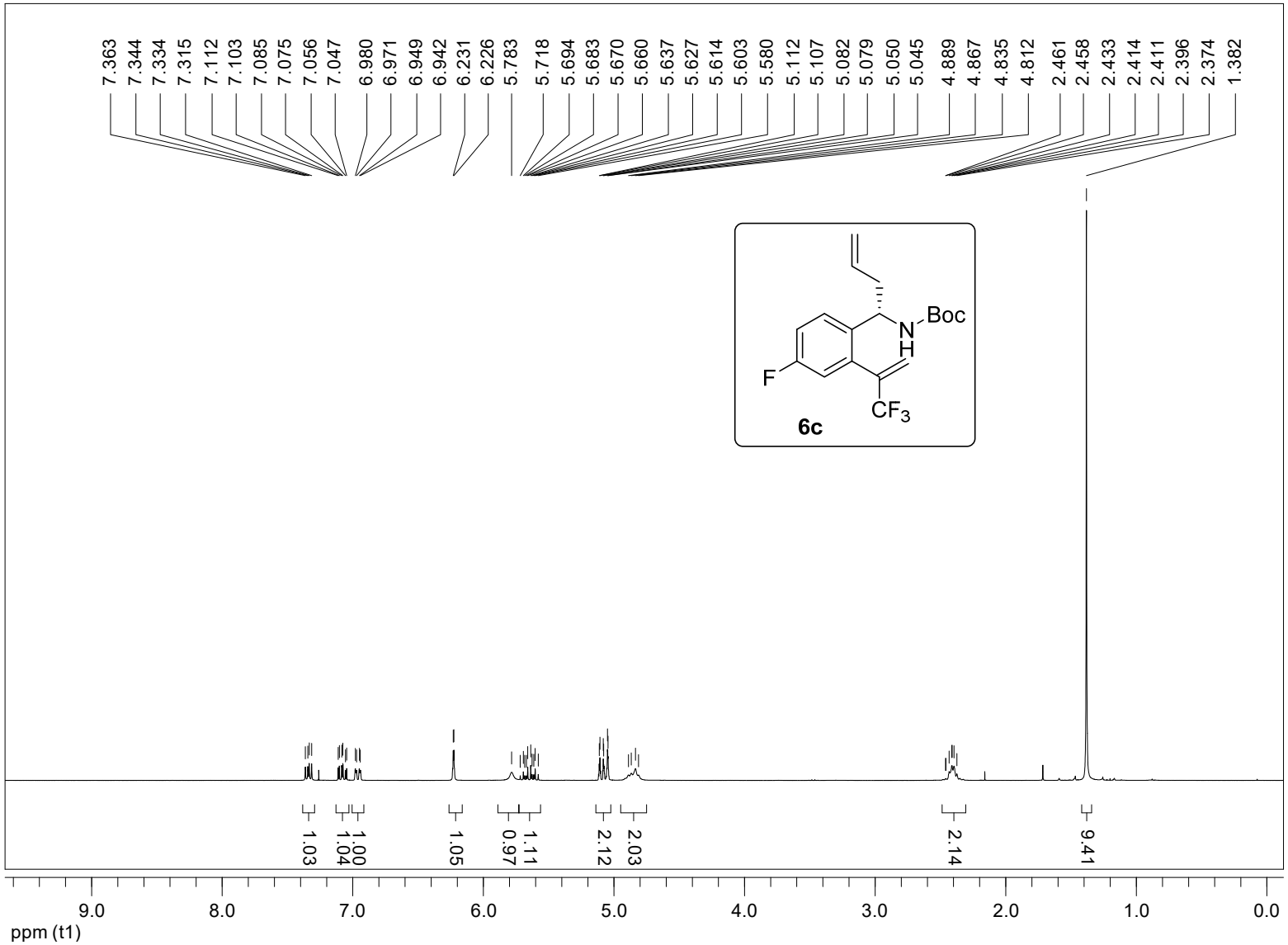
Boc
N
H
CF3
6a
-50
-100
ppm (t1)


7.348
7.342
7.260
7.253
7.233
7.226
7.188
7.160
6.231
6.226
5.781
5.706
5.675
5.671
5.650
5.640
5.616
5.593
5.142
5.137
5.118
5.082
4.890
4.851
4.829
2.476
2.472
2.459
2.454
2.428
2.411
2.406
2.388
2.384
2.358
2.333
2.310
2.284
1.386
Cl
N
Boc
H
CF3
6b
0.95
1.00
0.93
1.12
2.01
1.93
2.08
9.09
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


154.723
143.963
135.678
135.246
133.474
131.353
130.706
128.171
127.042
126.307
125.127
124.545
120.917
118.607
117.289
79.703
50.508
40.867
28.282
Cl
N
H
Boc
CF3
6b
150
100
50
0
ppm (t1)


-66.925
Cl
N
H
Boc
CF3
6b
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm (t1)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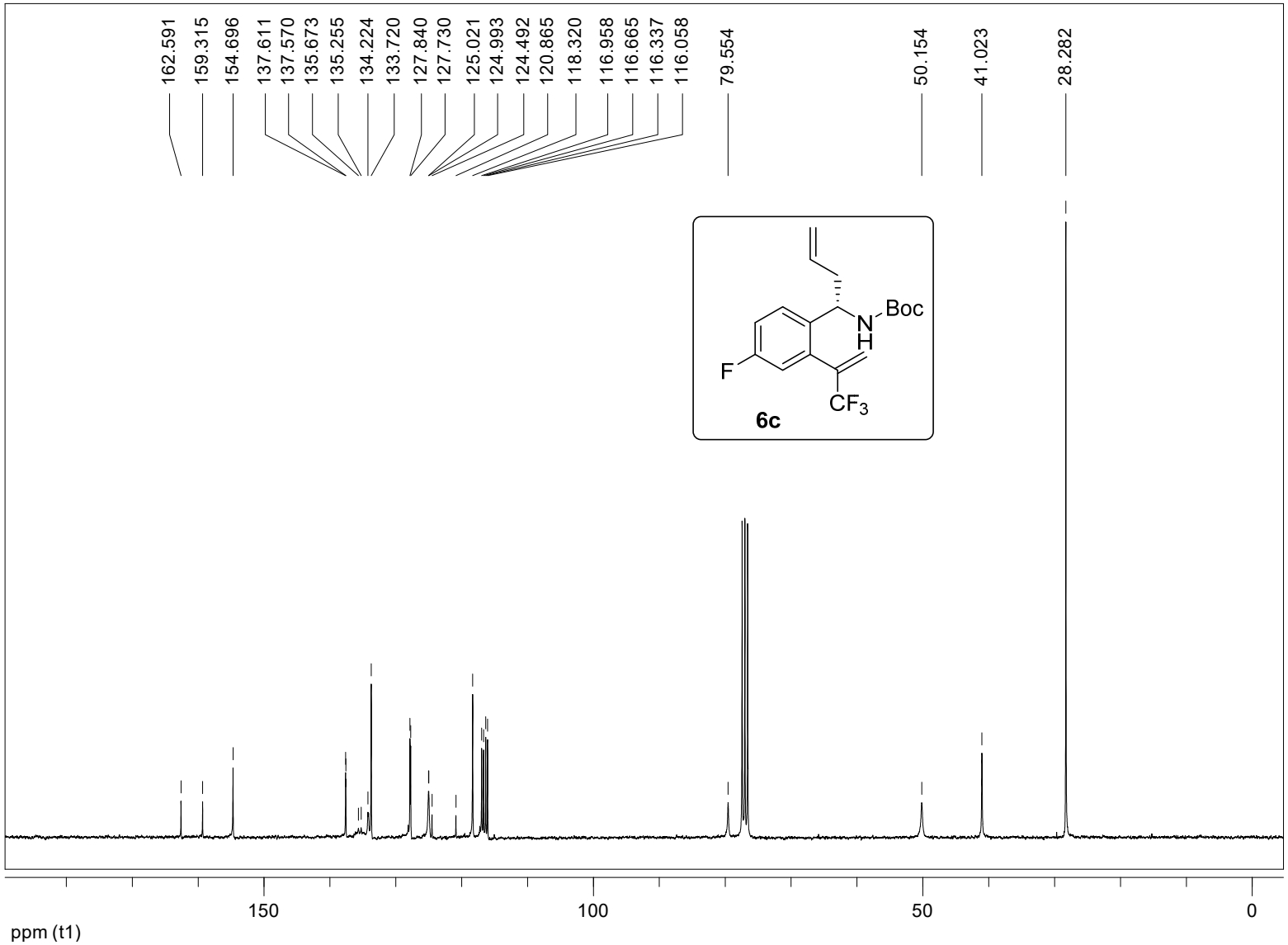
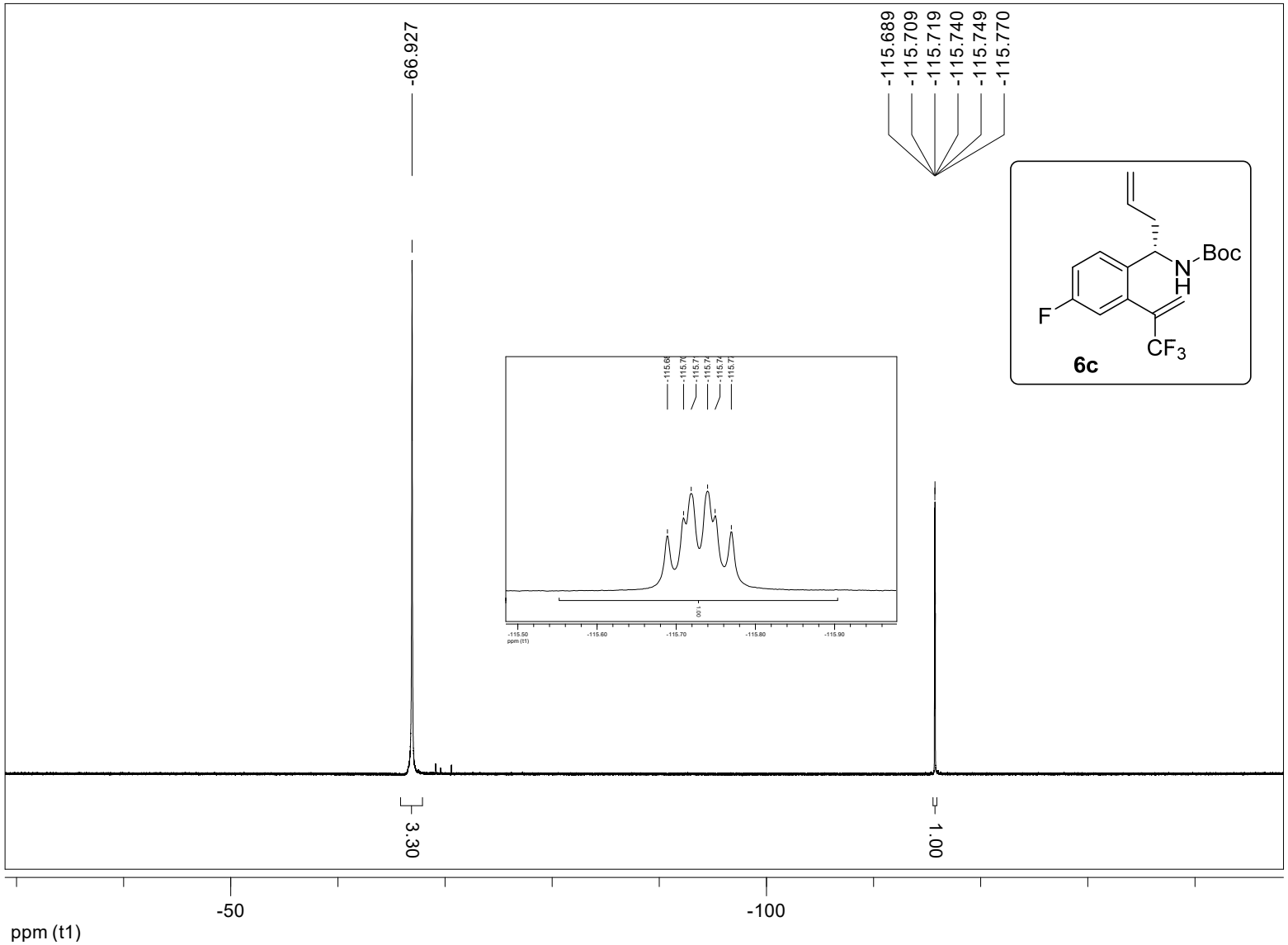
7.334
7.315
7.112
7.103
7.085
7.075
7.056
7.047
6.980
6.971
6.949
6.942
6.231
6.226
5.783
5.718
5.694
5.683
5.670
5.660
5.637
5.627
5.614
5.603
5.580
5.112
5.107
5.082
5.079
5.050
5.045
4.889
4.867
4.835
4.812
2.461
2.458
2.433
2.414
2.411
2.396
2.374
1.382
Boc
N
H
F
CF3
6c
1.03
1.00
1.04
1.05
0.97
1.11
2.12
2.03
2.14
9.41
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


162.591
159.315
154.696
137.611
137.570
135.673
135.255
134.224
133.720
127.840
127.730
125.021
124.993
124.492
120.865
118.320
116.958
116.665
116.337
116.058
79.554
50.154
41.023
28.282
Boc
N
H
F
CF3
6c
150
100
50
0
ppm (t1)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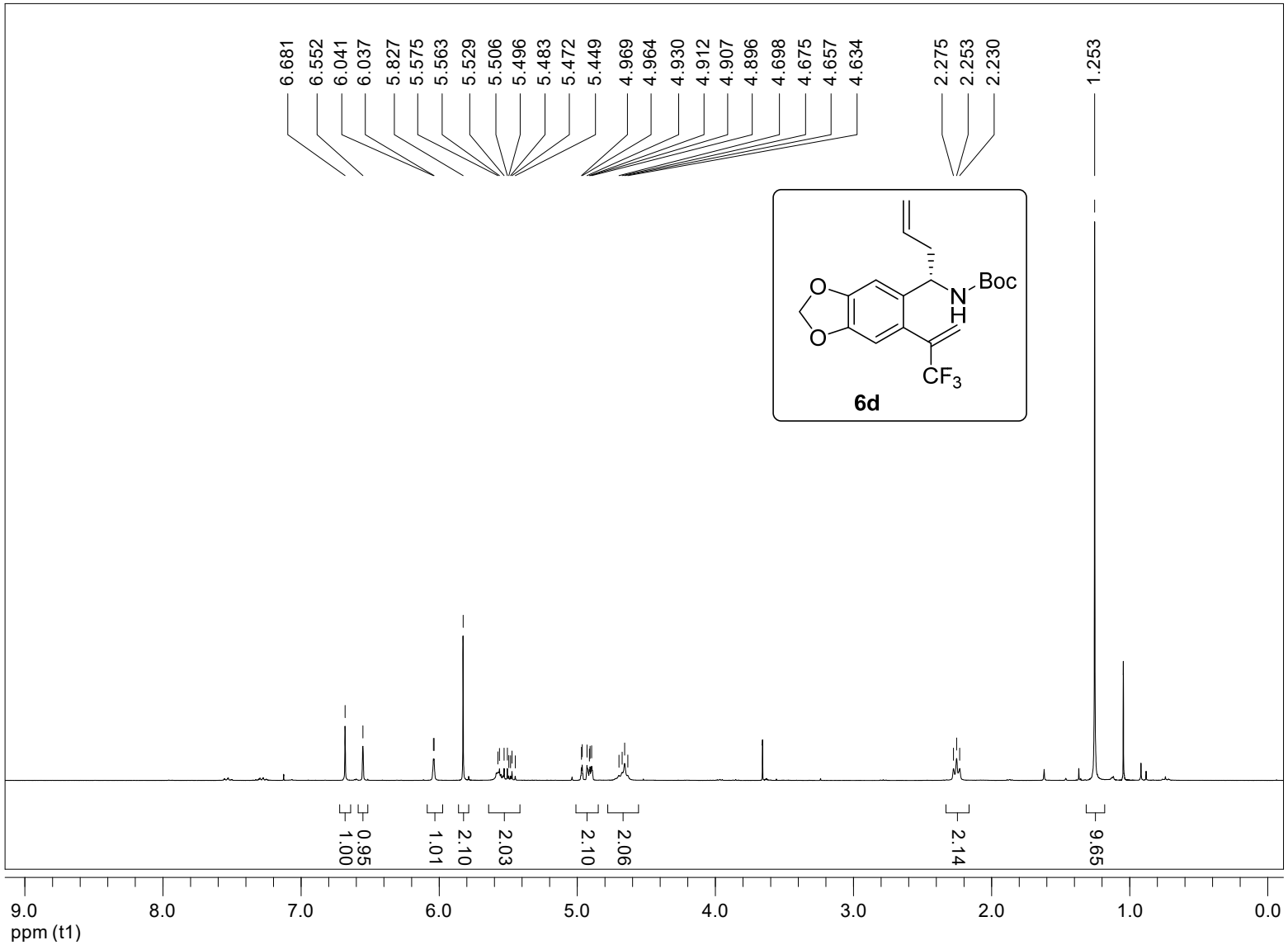
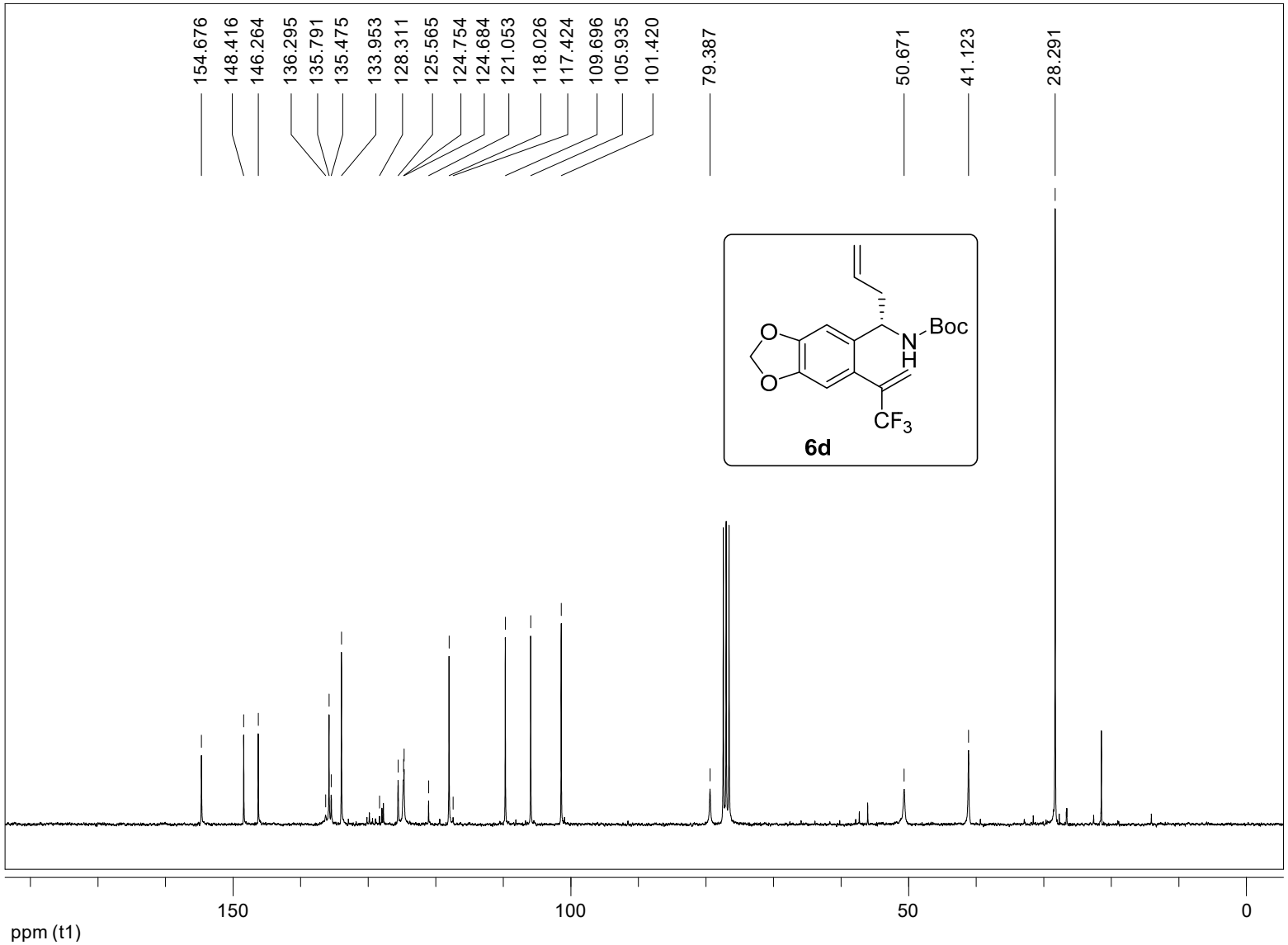
-115.689
-115.709
-115.719
-115.740
-115.749
-115.770
Boc
N
H
F
CF3
6c
3.30
1.00
-50
-100
ppm (t1)


6.681
6.552
6.041
6.037
5.827
5.575
5.563
5.529
5.506
5.496
5.483
5.472
5.449
4.969
4.964
4.930
4.912
4.907
4.896
4.698
4.675
4.657
4.634
2.275
2.253
2.230
1.253
O
O
N
H
Boc
CF3
6d
1.00
0.95
1.01
2.10
2.03
2.10
2.06
2.14
9.65
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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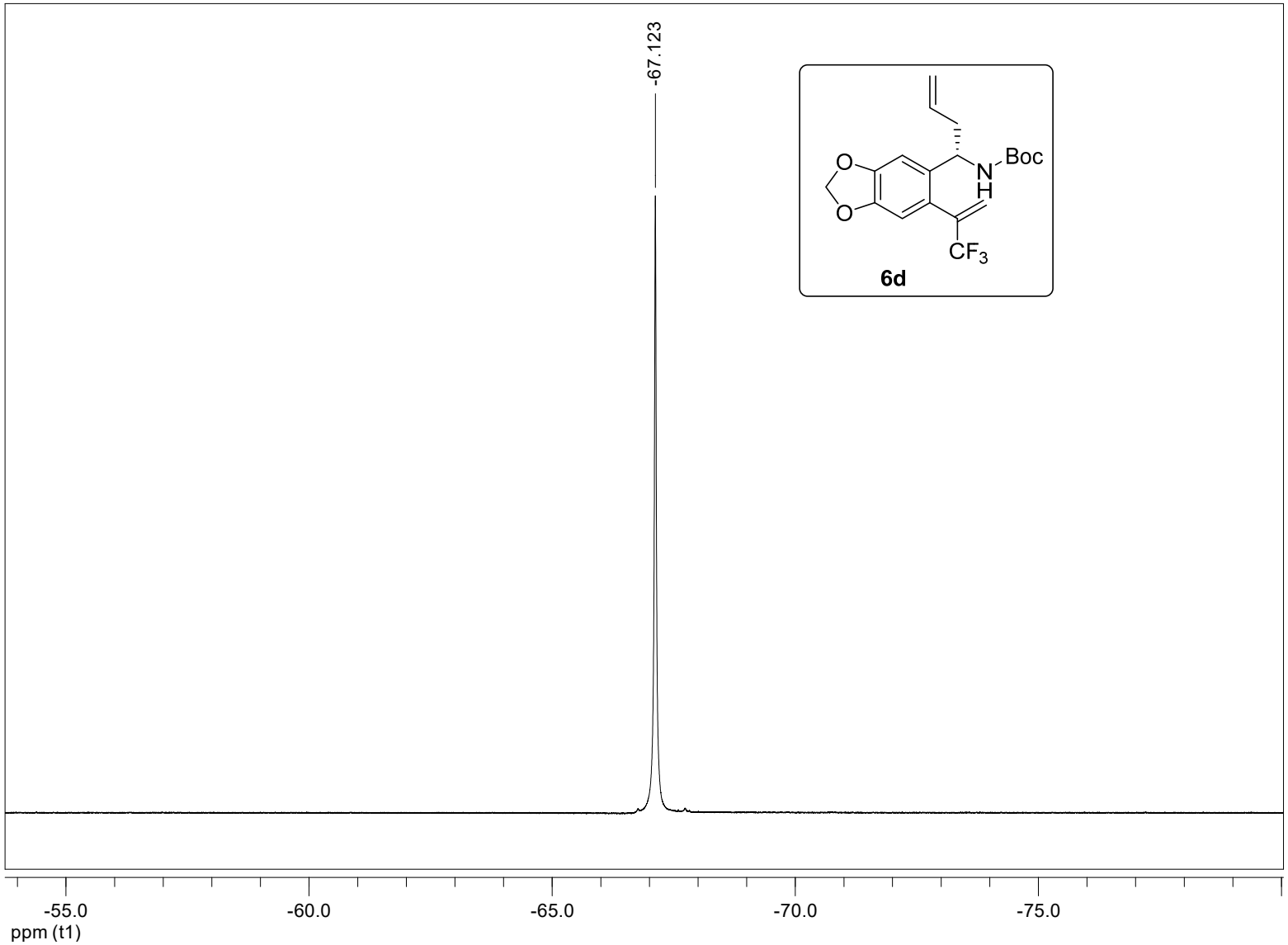
146.264
136.295
135.791
135.475
133.953
128.311
125.565
124.754
124.684
121.053
118.026
117.424
109.696
105.935
101.420
79.387
50.671
41.123
28.291
O
O
N
H
Boc
CF3
6d
150
100
50
0
ppm (t1)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N
H
O
O
CF3
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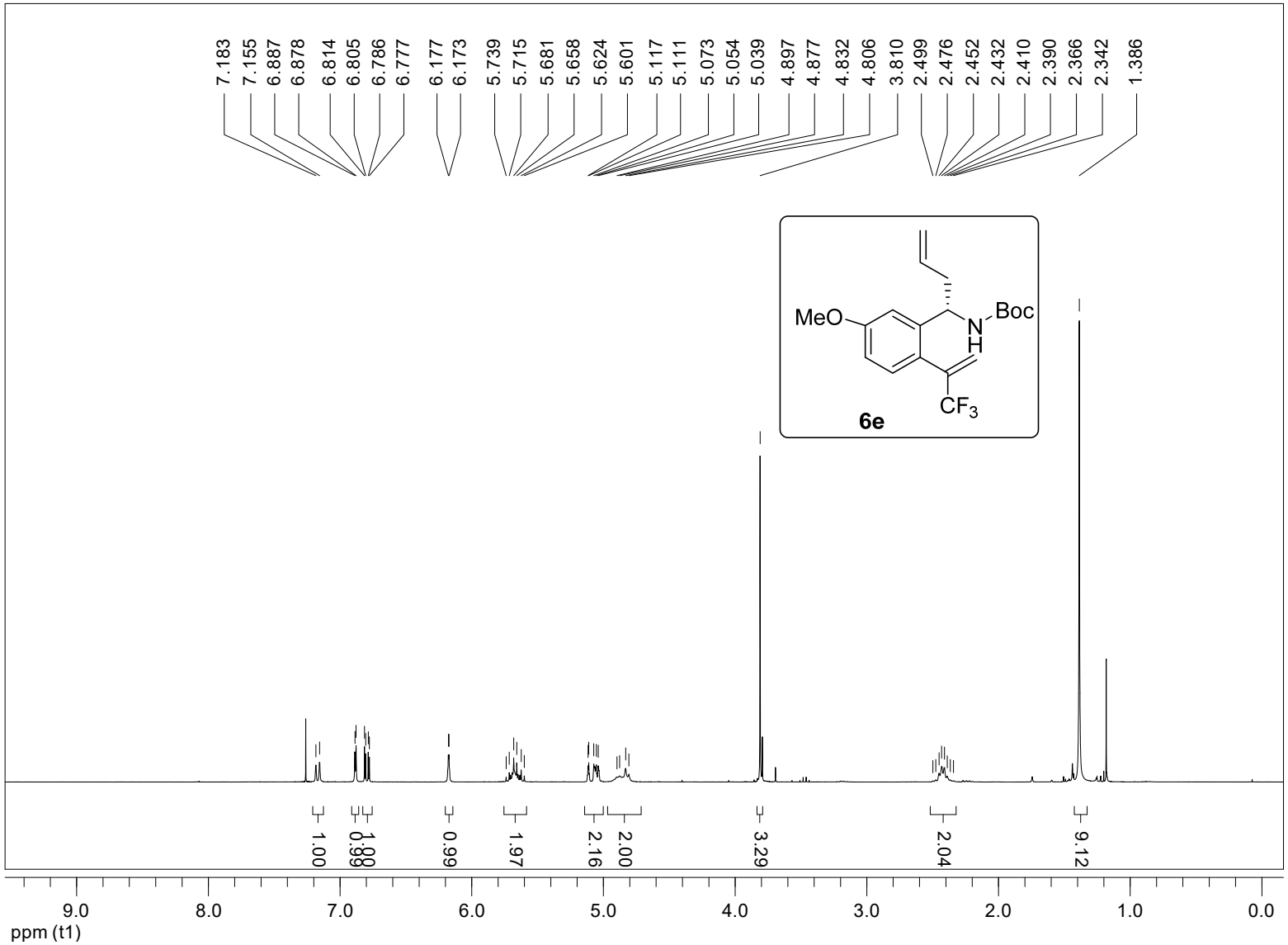
-60.0
-65.0
-70.0
-75.0
ppm (t1)


7.183
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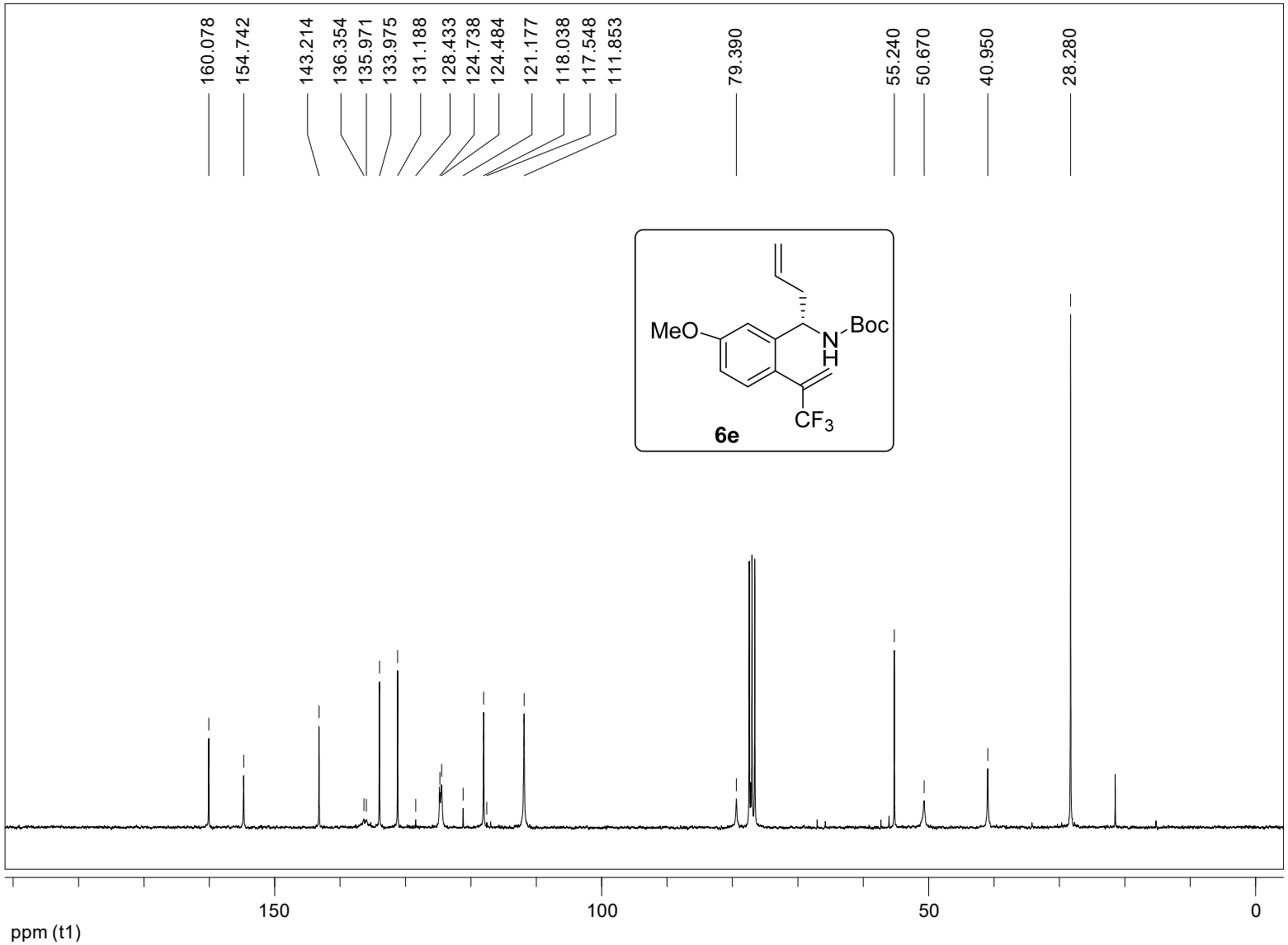
6.814
6.805
6.786
6.777
6.177
6.173
5.739
5.715
5.681
5.658
5.624
5.601
5.117
5.111
5.073
5.054
5.039
4.897
4.877
4.832
4.806
3.810
2.499
2.476
2.452
2.432
2.410
2.390
2.366
2.342
1.386
MeO
Boc
N
H
CF3
6e
1.00
1.00
0.88
0.99
1.97
2.16
2.00
3.29
2.04
9.12
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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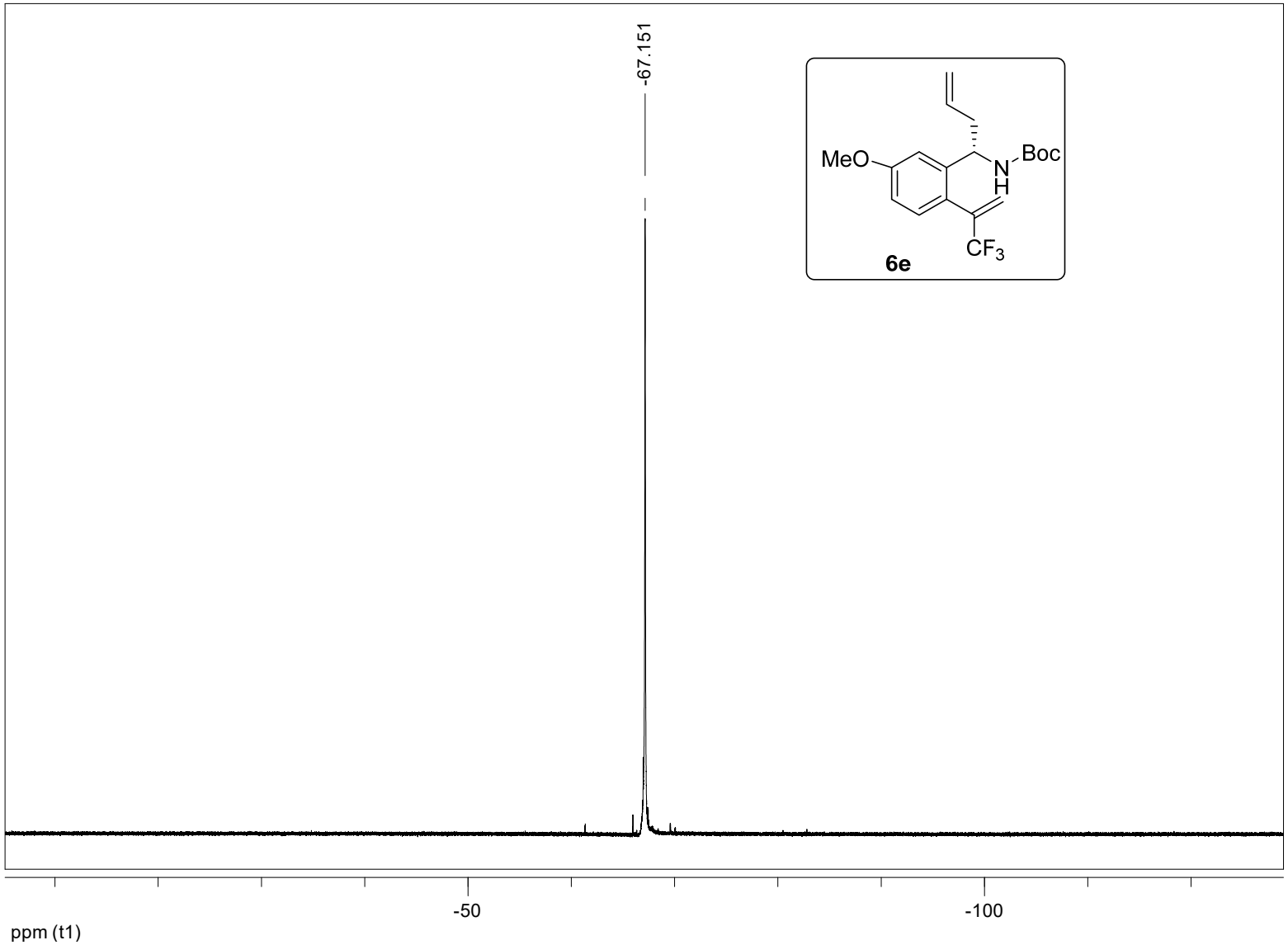
131.188
128.433
124.738
124.484
121.177
118.038
117.548
111.853
79.390
55.240
50.670
40.950
28.280
MeO
N
H
Boc
CF3
6e
150
100
50
0
ppm (t1)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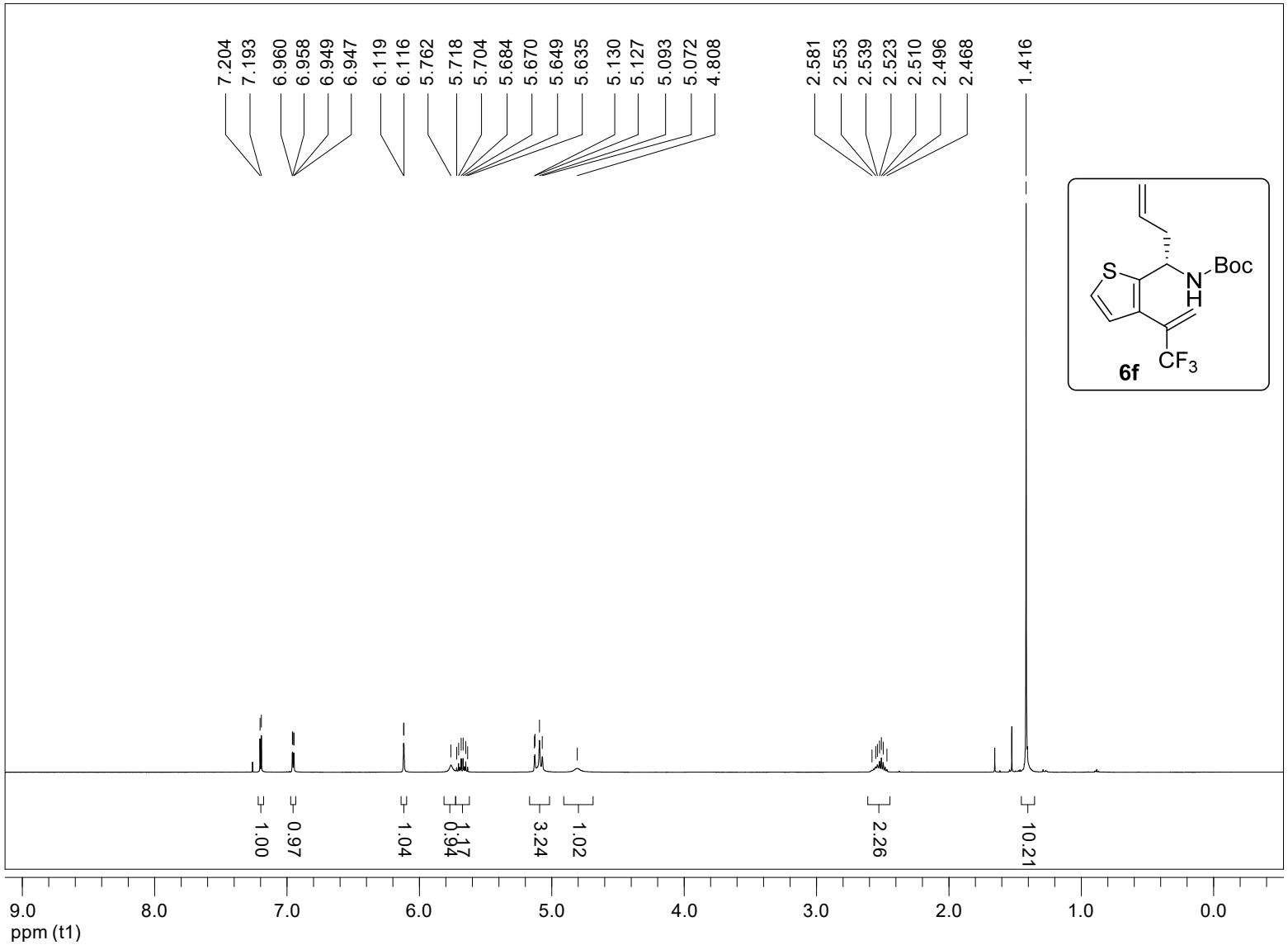
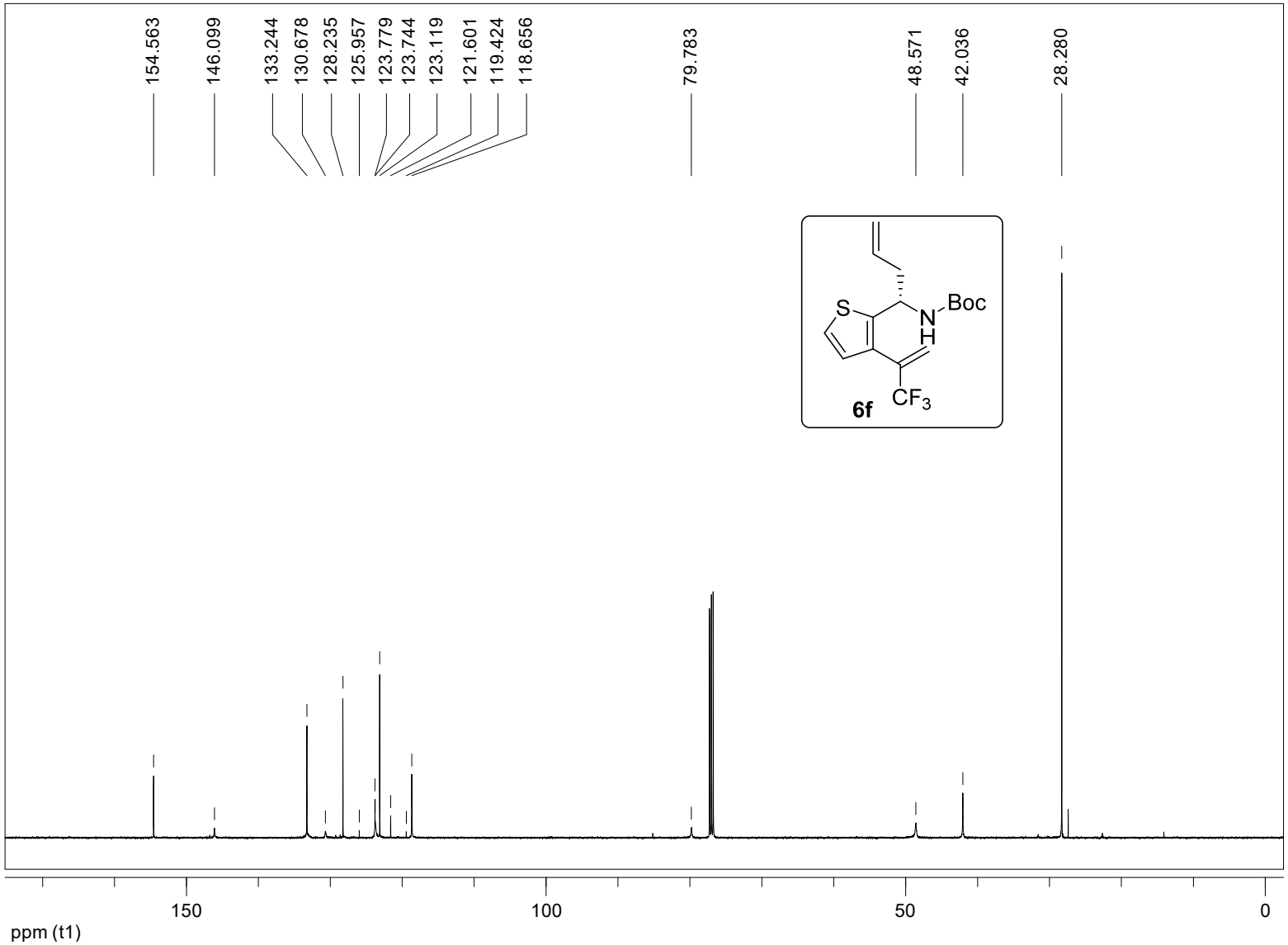
N
H
Boc
CF3
6e
-50
-100
ppm (t1)


7.204
7.193
6.960
6.958
6.949
6.947
6.119
6.116
5.762
5.718
5.704
5.684
5.670
5.649
5.635
5.130
5.127
5.093
5.072
4.808
2.581
2.553
2.539
2.523
2.510
2.496
2.468
1.416
1.00
0.97
1.04
1.17
0.94
3.24
1.02
2.26
10.21
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
S
N
H
Boc
CF3
6f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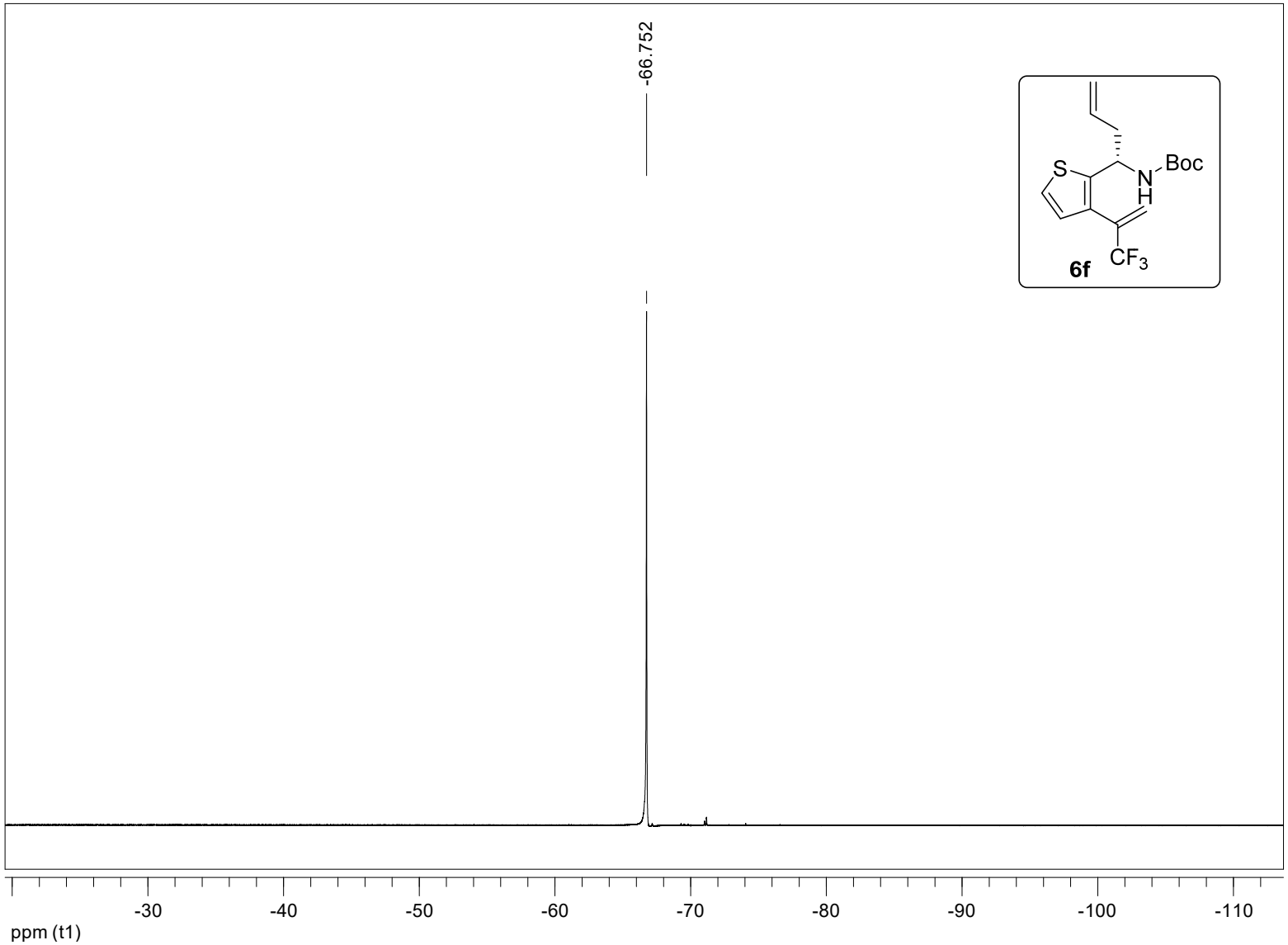
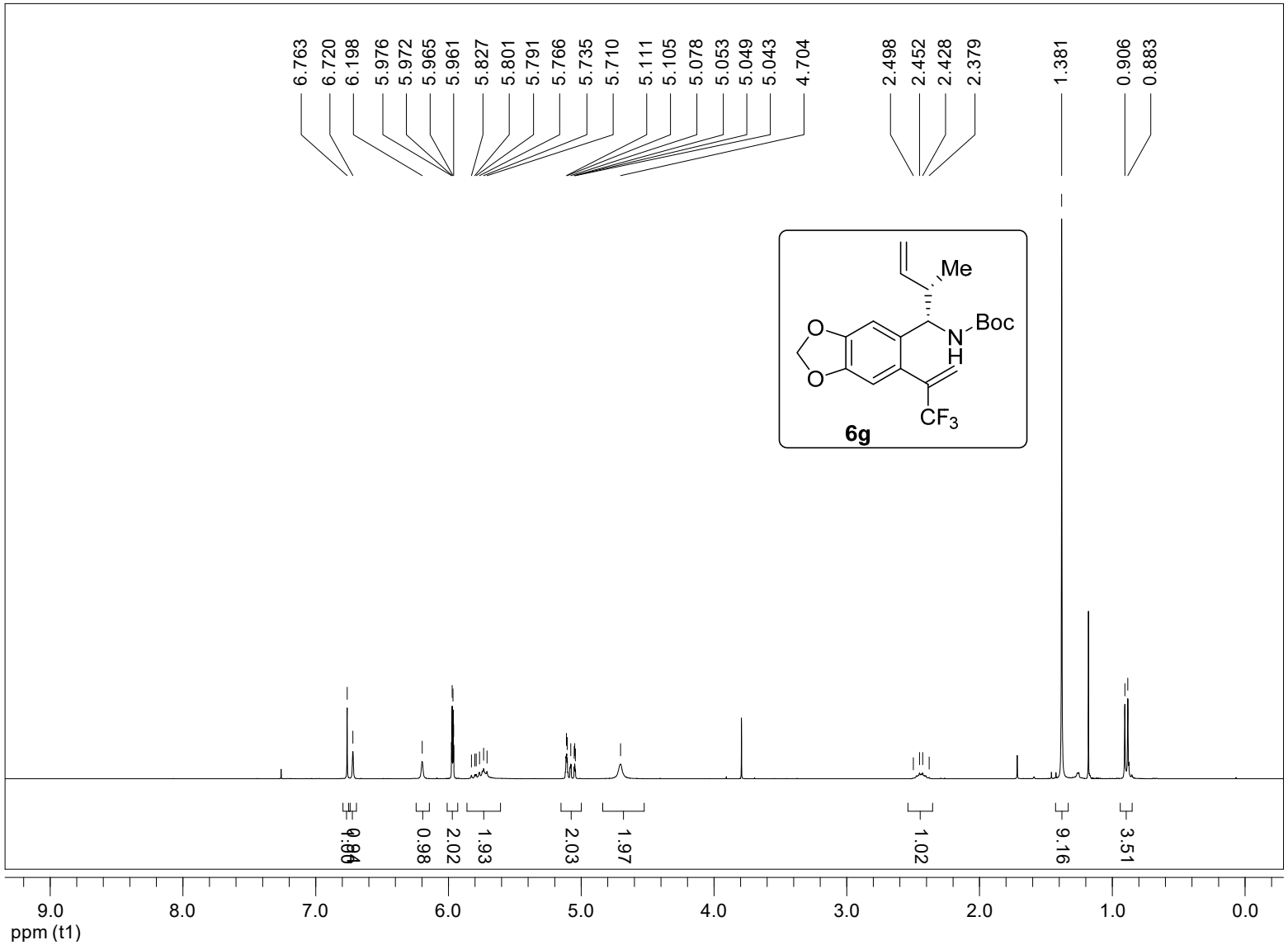
146.099
133.244
130.678
128.235
125.957
123.779
123.744
123.119
121.601
119.424
118.656
79.783
48.571
42.036
28.280
S
N
H
Boc
CF3
6f
150
100
50
0
ppm (t1)


-66.752
S
N
Boc
H
CF3
6f
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm (t1)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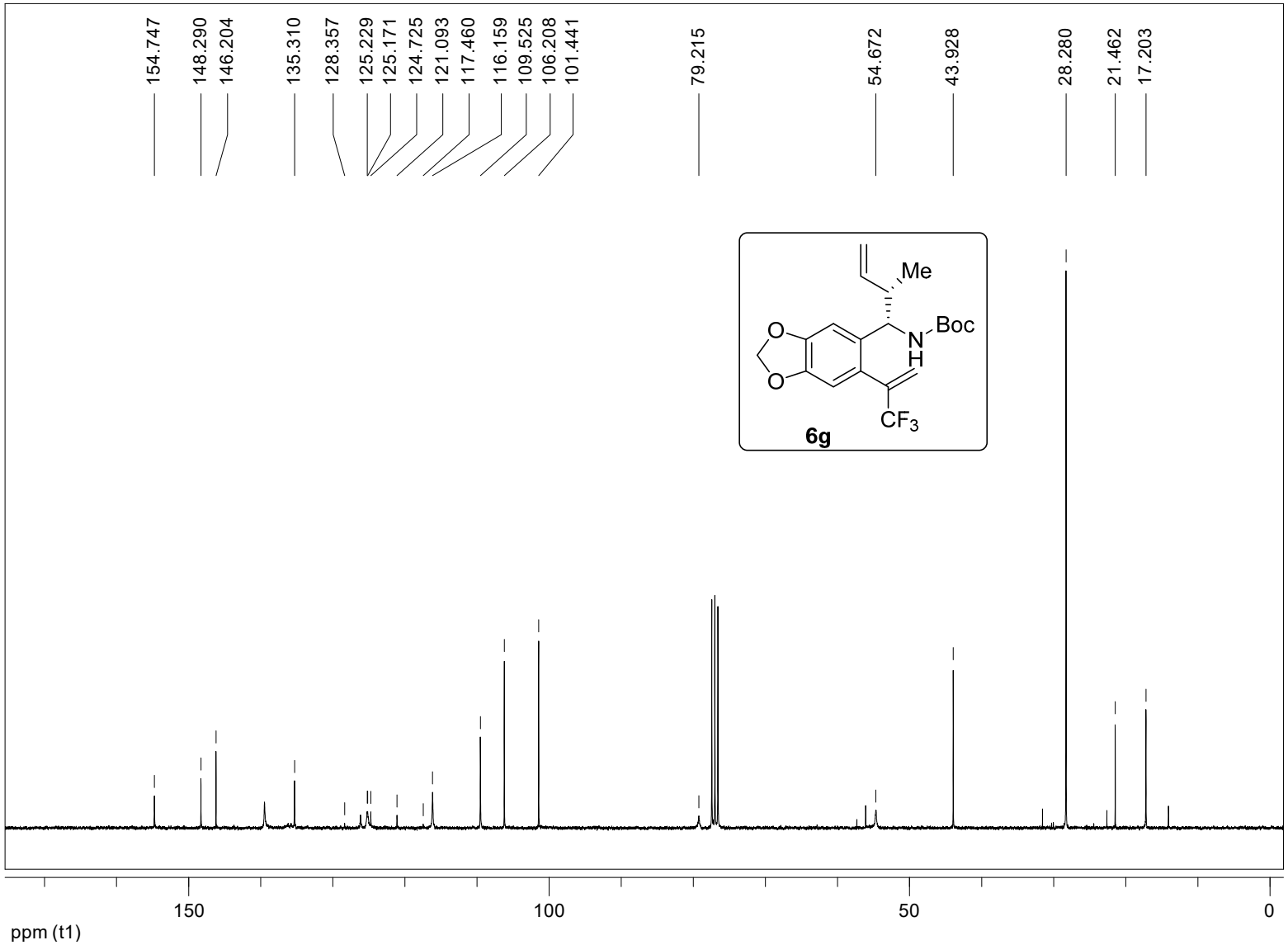
6.720
6.198
5.976
5.972
5.965
5.961
5.827
5.801
5.791
5.766
5.735
5.710
5.111
5.105
5.078
5.053
5.049
5.043
4.704
2.498
2.452
2.428
2.379
1.381
0.906
0.883
Me
Boc
N
H
O
O
CF3
6g
1.04
0.98
2.02
1.93
2.03
1.97
1.02
9.16
3.51
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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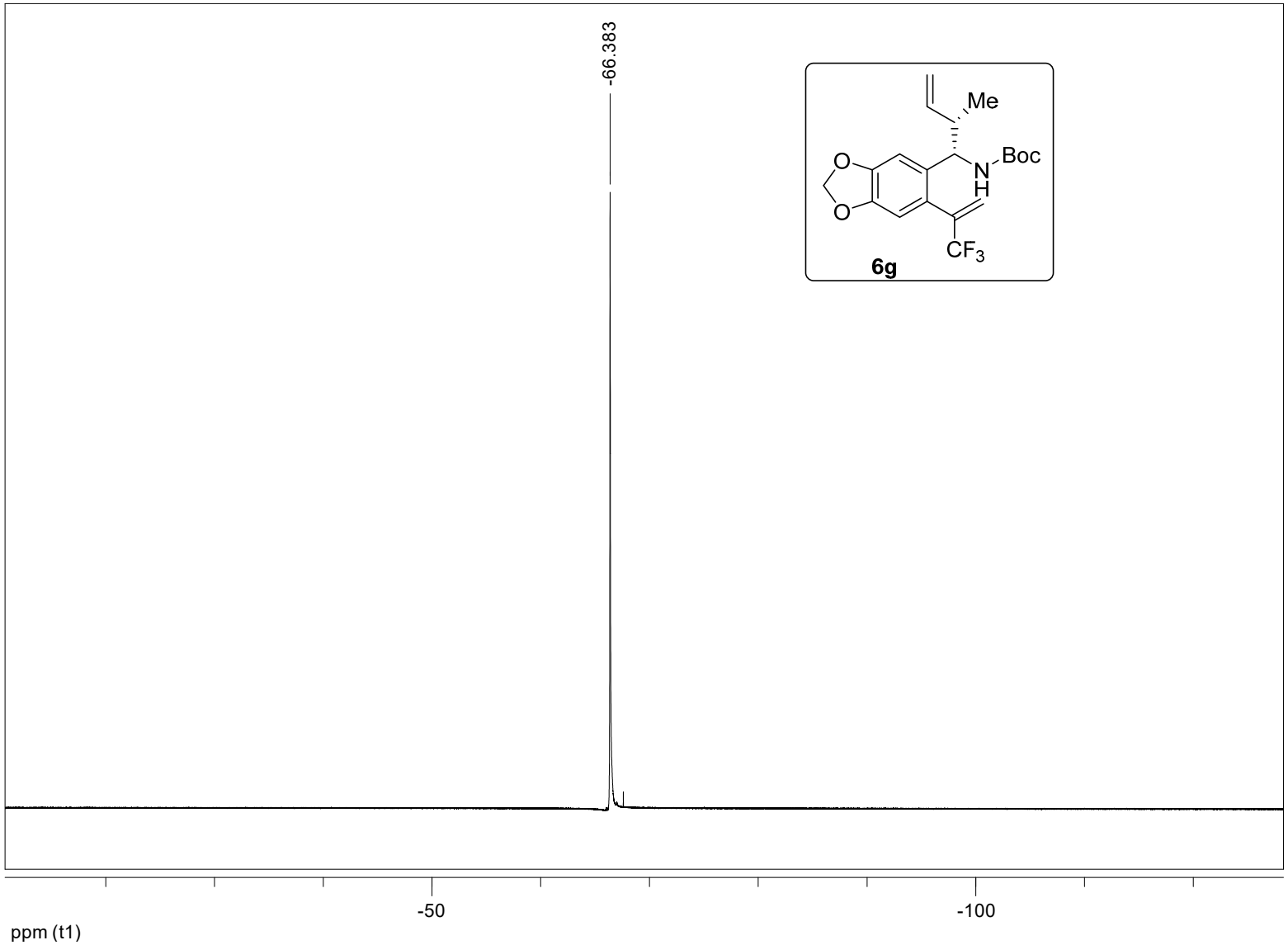
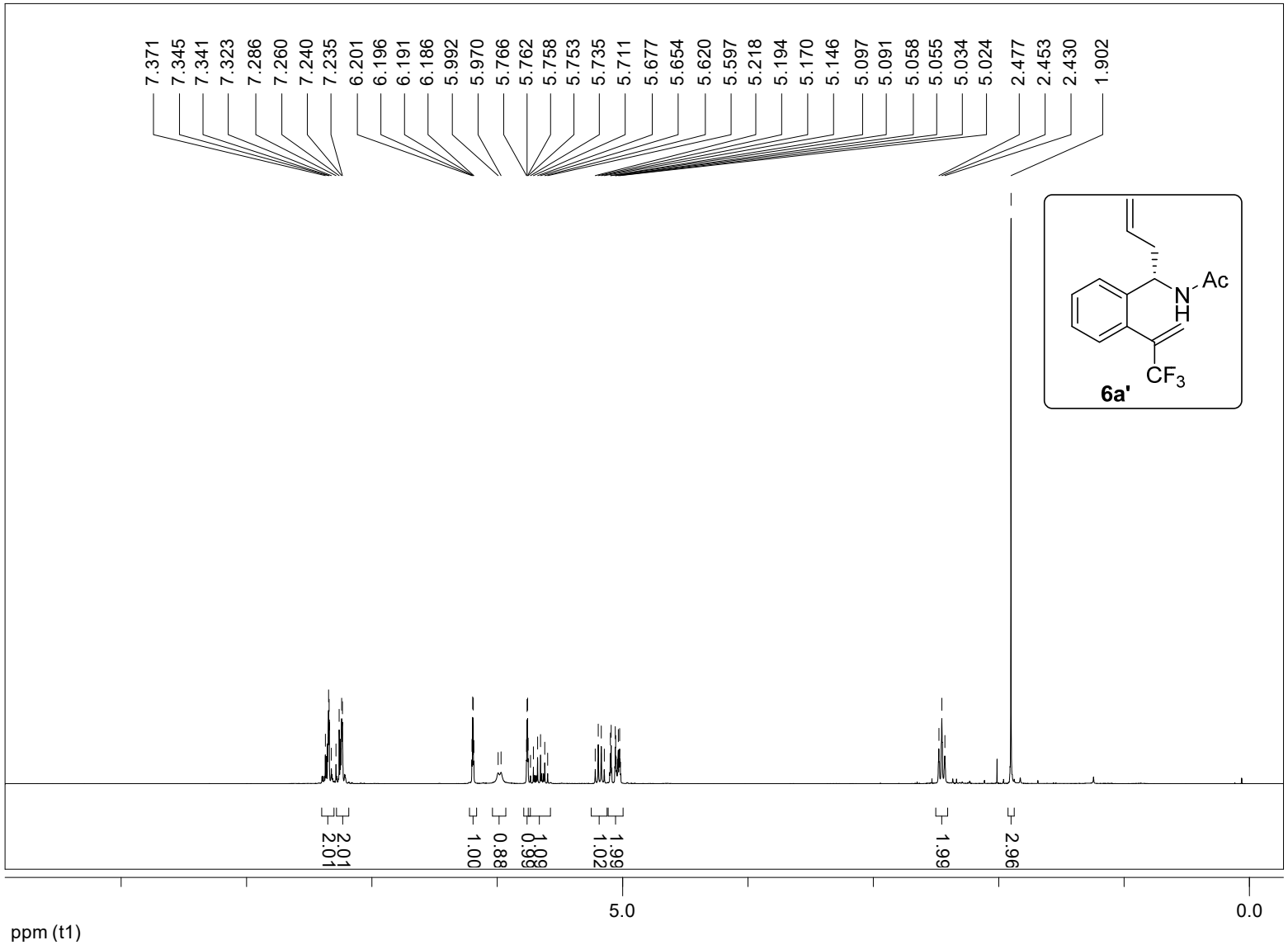
146.204
135.310
128.357
125.229
125.171
124.725
121.093
117.460
116.159
109.525
106.208
101.441
79.215
54.672
43.928
28.280
21.462
17.203
Me
Boc
N
H
O
O
CF3
6g
150
100
50
0
ppm (t1)


-66.383
Me
Boc
N
H
O
O
CF3
6g
-50
-100
ppm (t1)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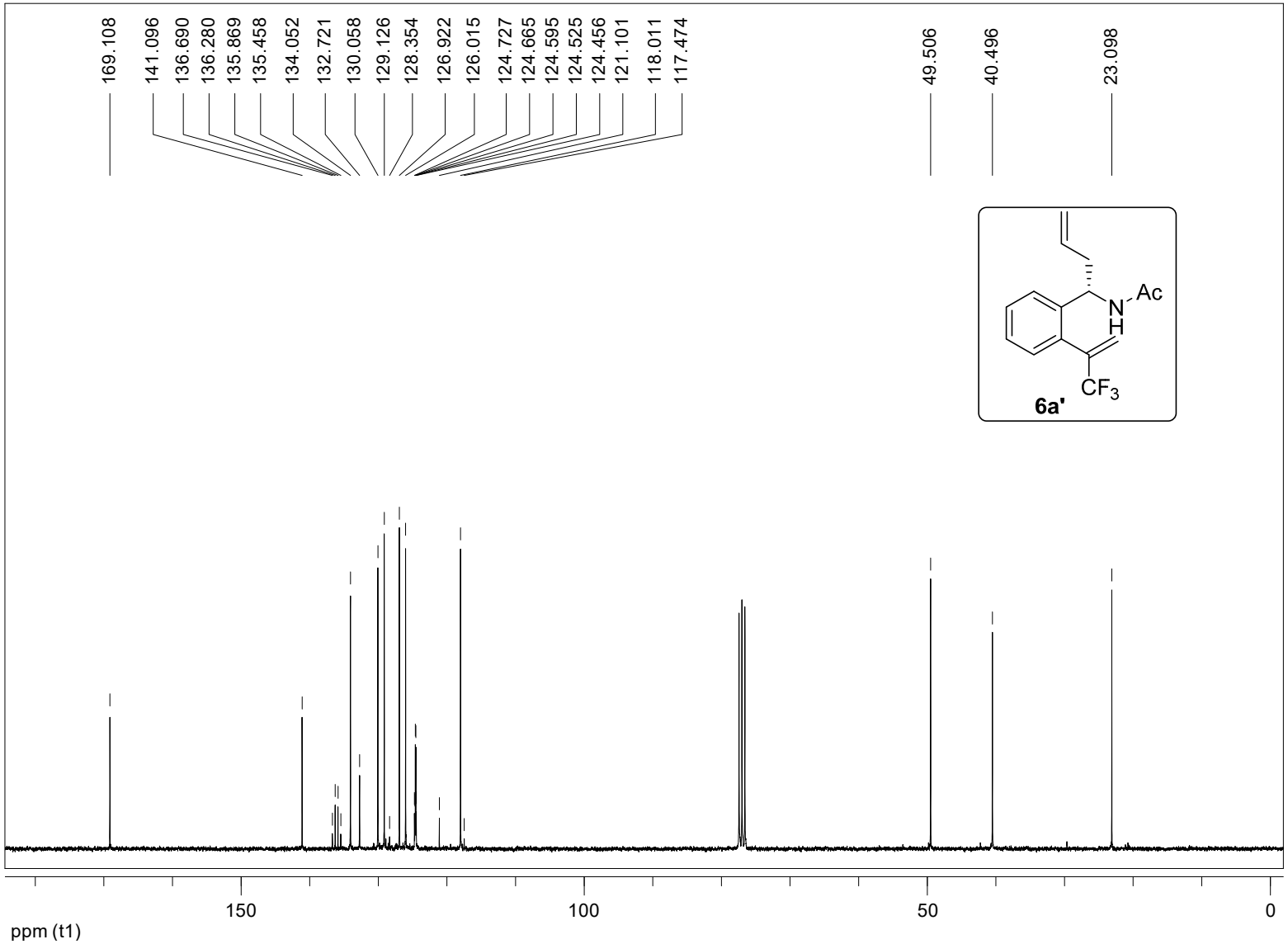
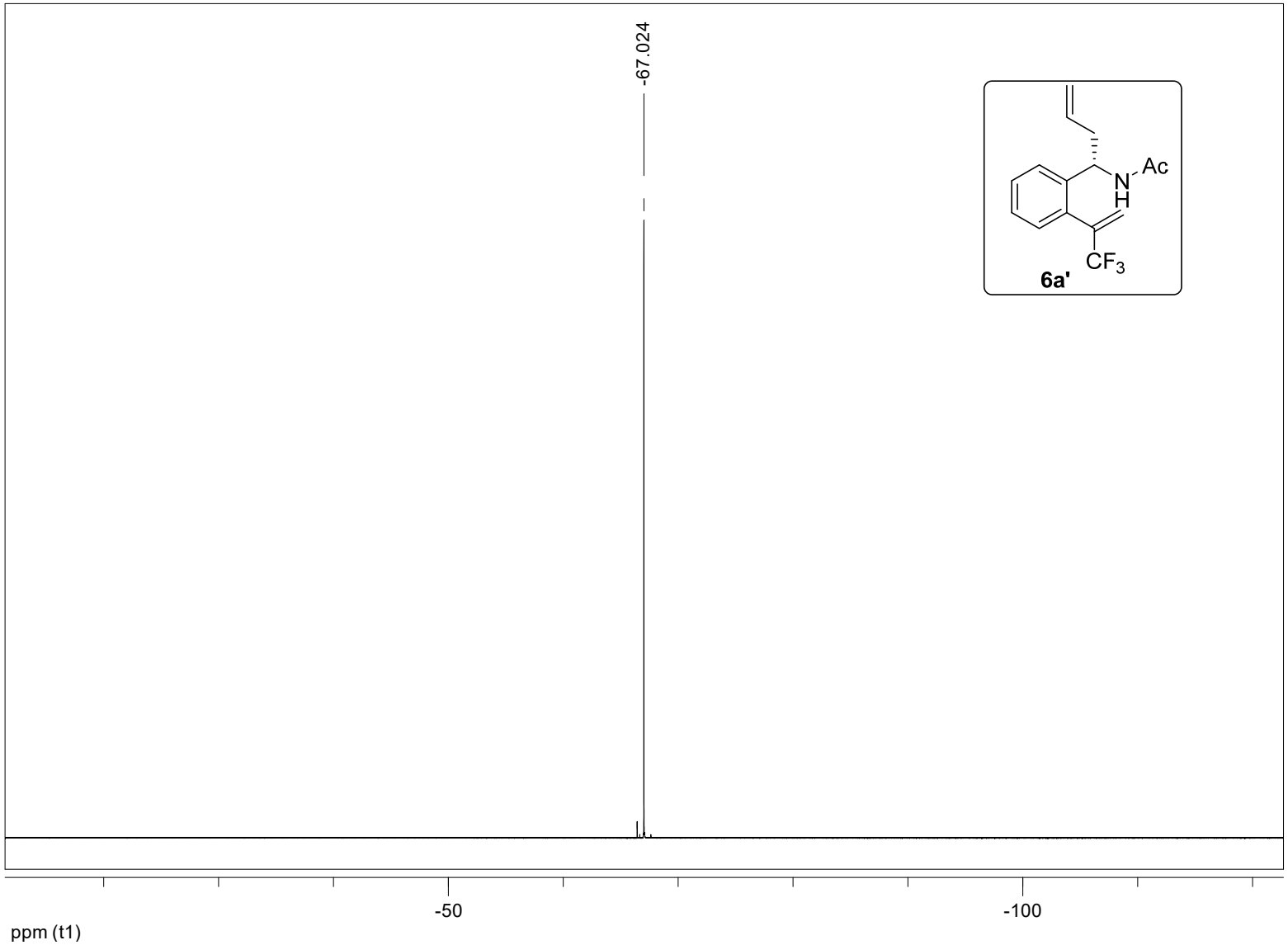
7.345
7.341
7.323
7.286
7.260
7.240
7.235
6.201
6.196
6.191
6.186
5.992
5.970
5.766
5.762
5.758
5.753
5.735
5.711
5.677
5.654
5.620
5.597
5.218
5.194
5.170
5.146
5.097
5.091
5.058
5.055
5.034
5.024
2.477
2.453
2.430
1.902
Ac
N
H
CF3
6a'
2.01
2.01
1.00
0.88
0.98
1.09
1.02
1.99
1.99
2.96
5.0
0.0
ppm (t1)


169.108
141.096
136.690
136.280
135.869
135.458
134.052
132.721
130.058
129.126
128.354
126.922
126.015
124.727
124.665
124.595
124.525
124.456
121.101
118.011
117.474
49.506
40.496
23.098
Ac
N
H
CF3
6a'
150
100
50
0
ppm (t1)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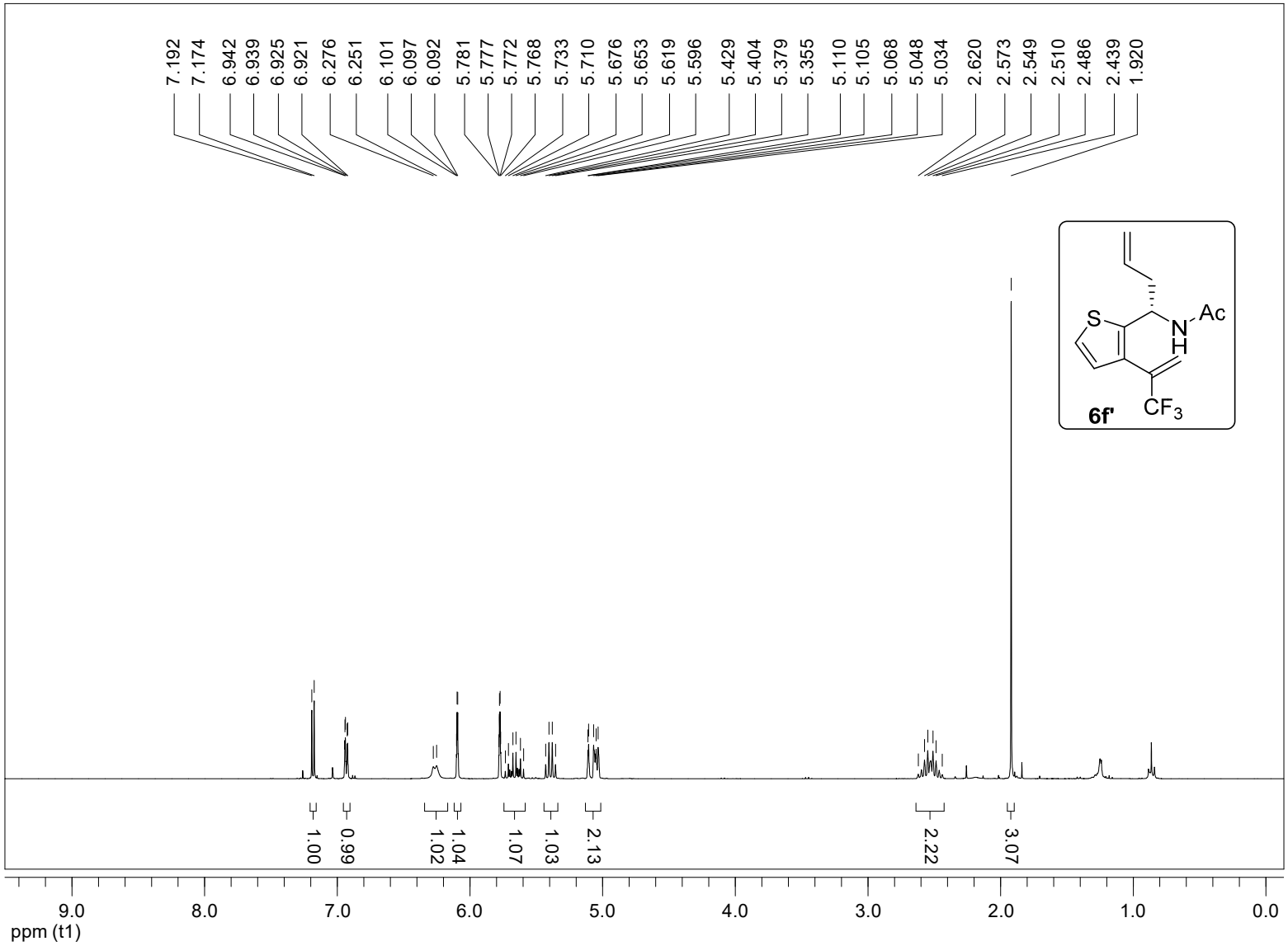
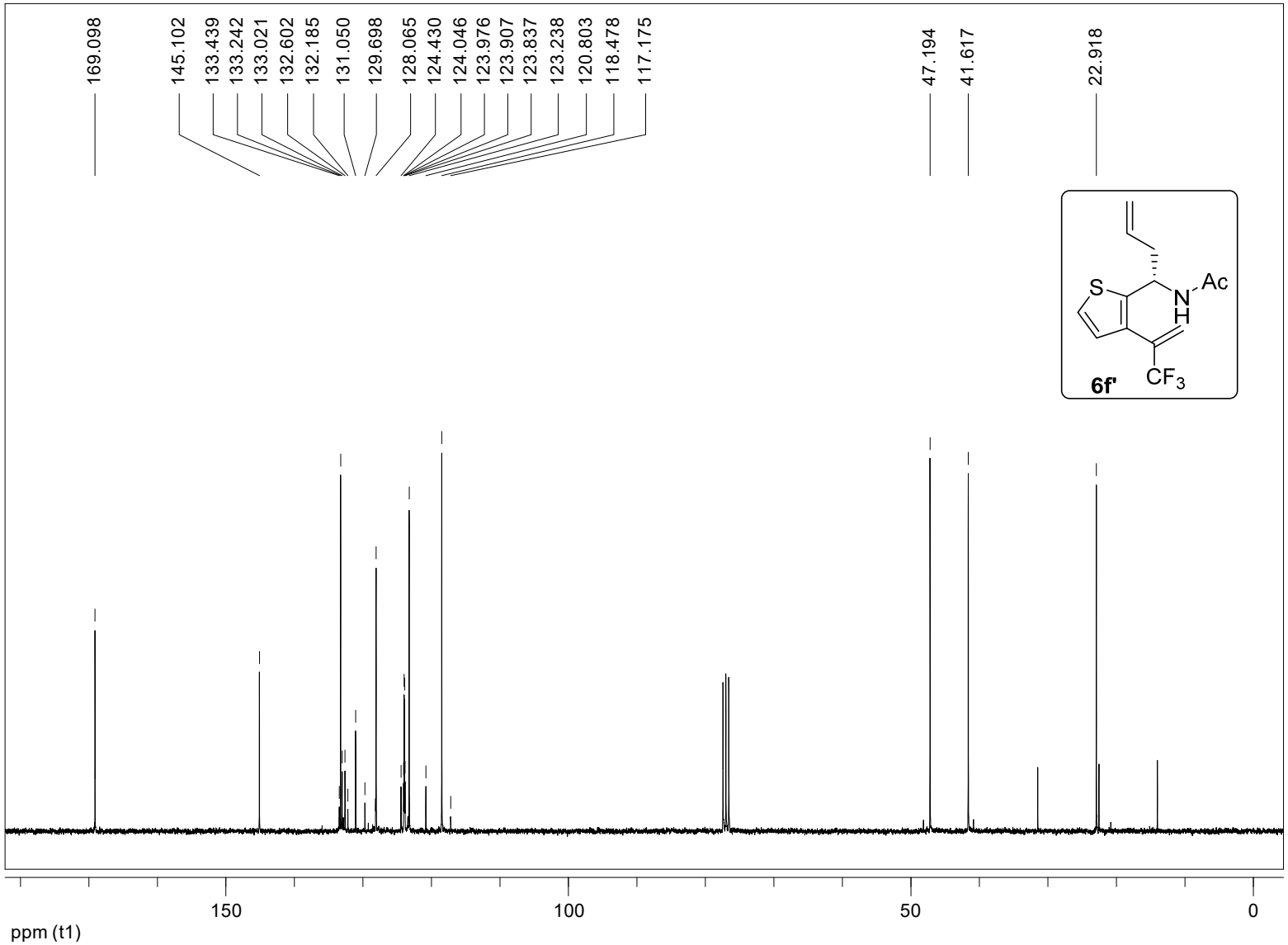
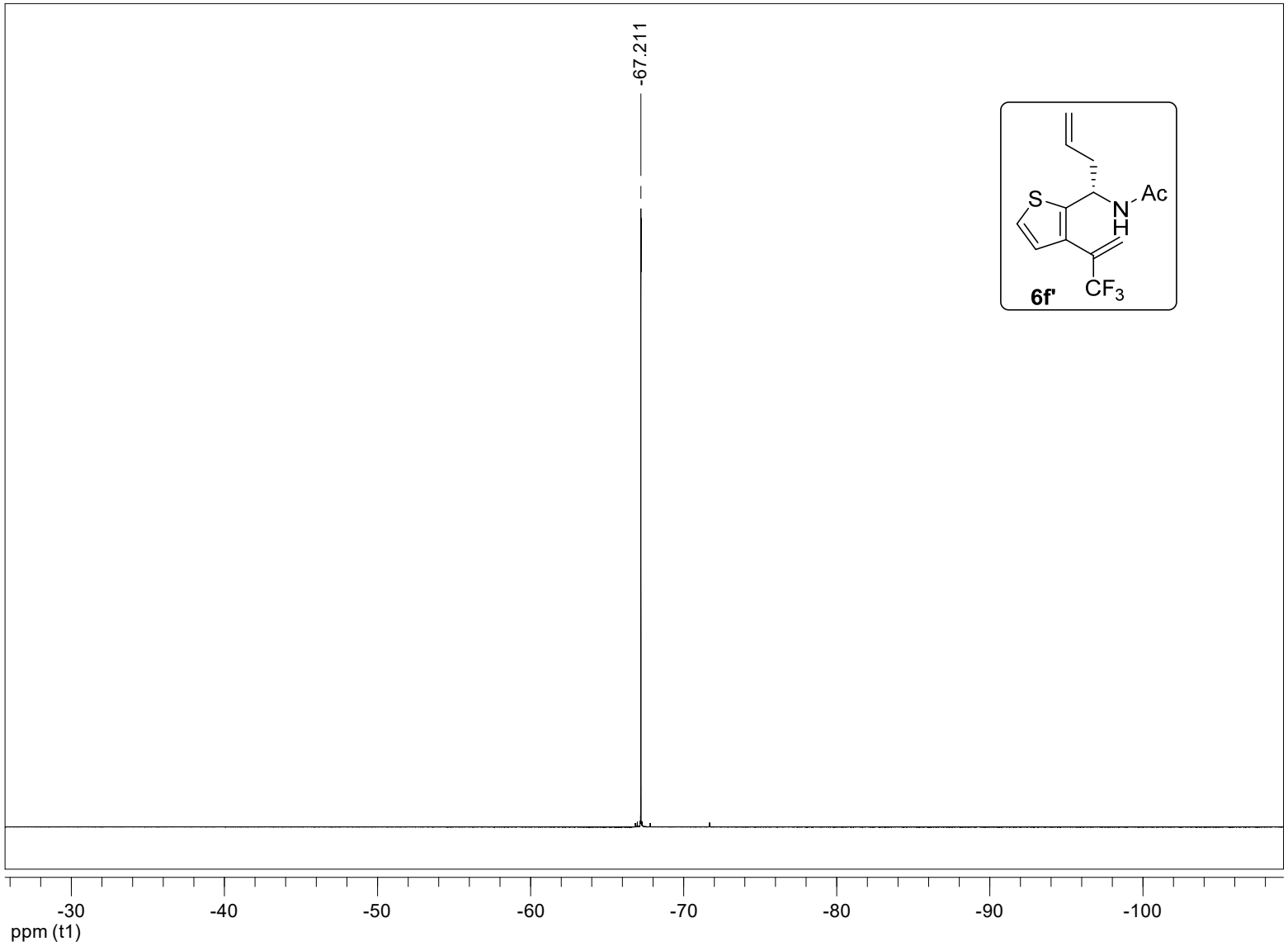
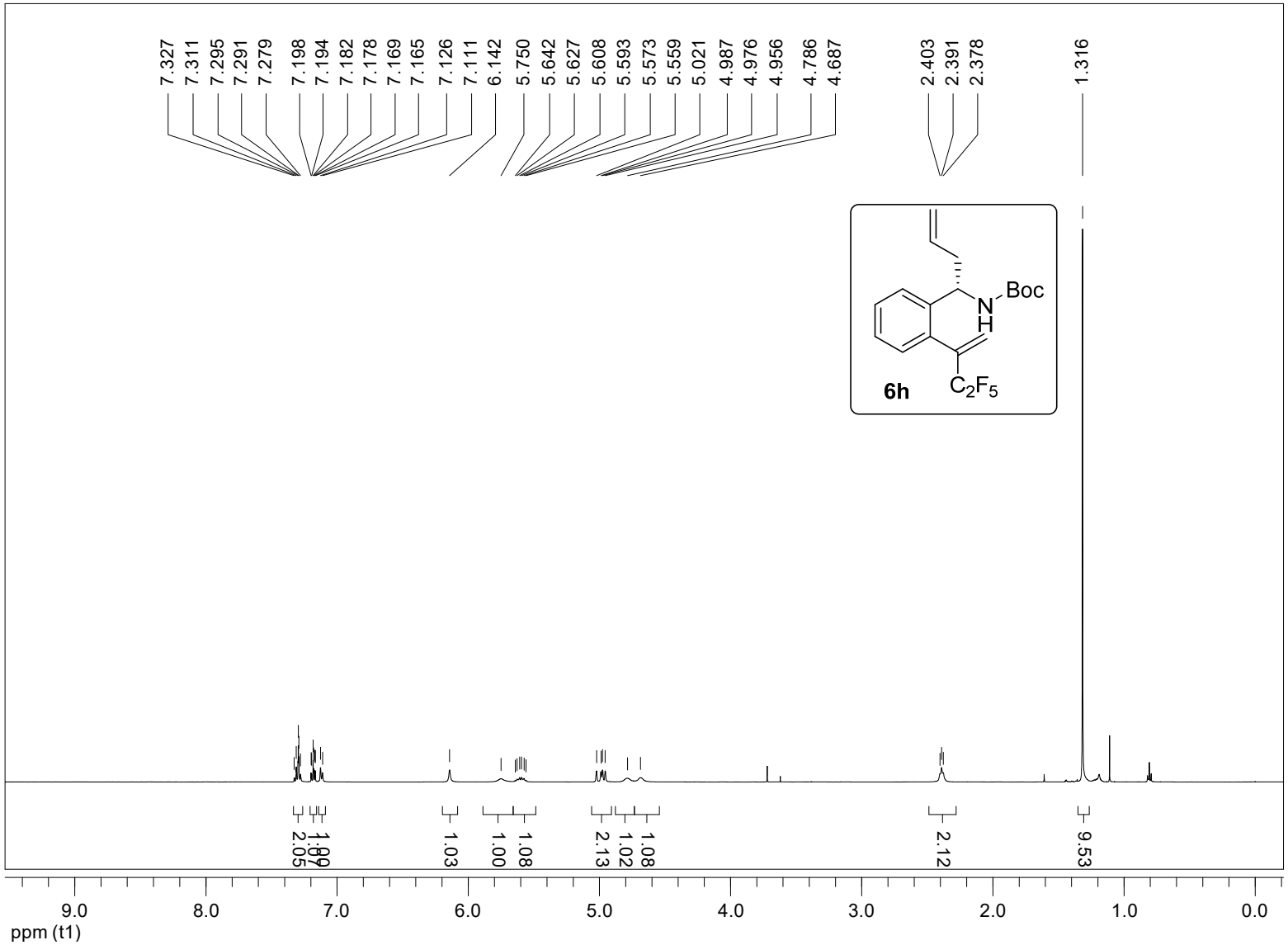
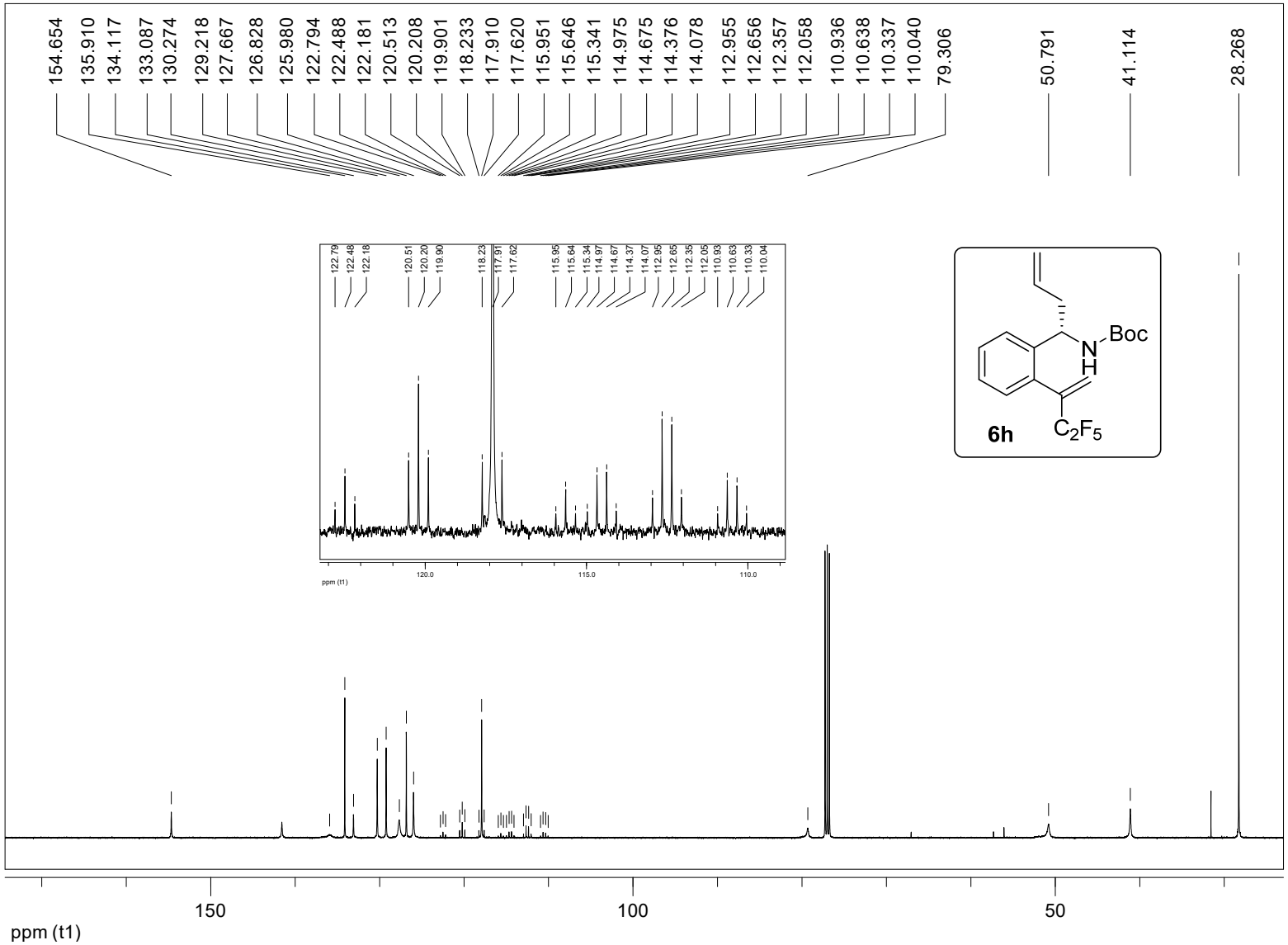
Ac
N
H
CF3
6a'
-50
-100
ppm (t1)

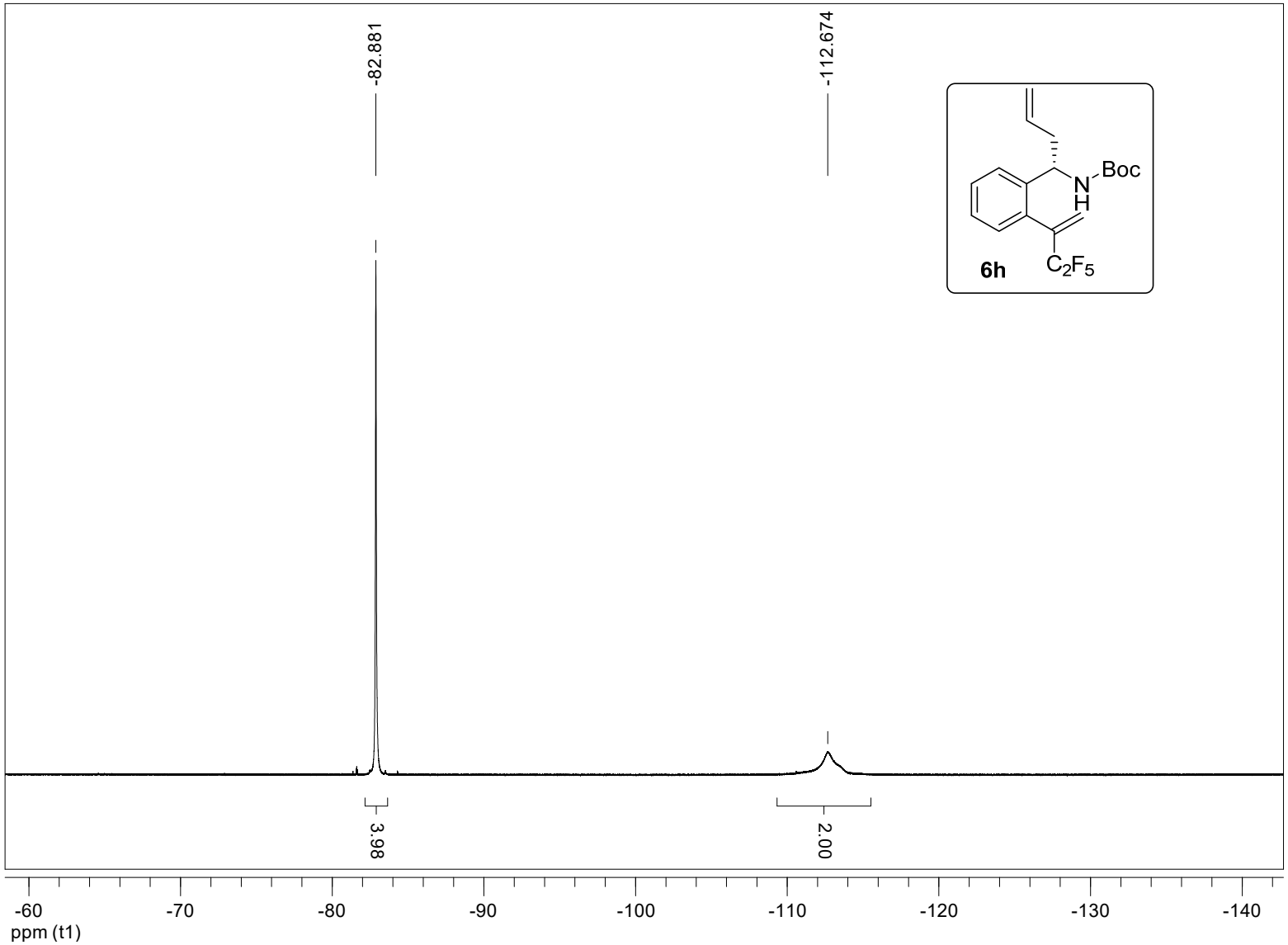

7.192
7.174
6.942
6.939
6.925
6.921
6.276
6.251
6.101
6.097
6.092
5.781
5.777
5.772
5.768
5.733
5.710
5.676
5.653
5.619
5.596
5.429
5.404
5.379
5.355
5.110
5.105
5.068
5.048
5.034
2.620
2.573
2.549
2.510
2.486
2.439
1.920
S
N
H
Ac
CF3
6f'
1.00
0.99
1.02
1.04
1.07
1.03
2.13
2.22
3.07
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

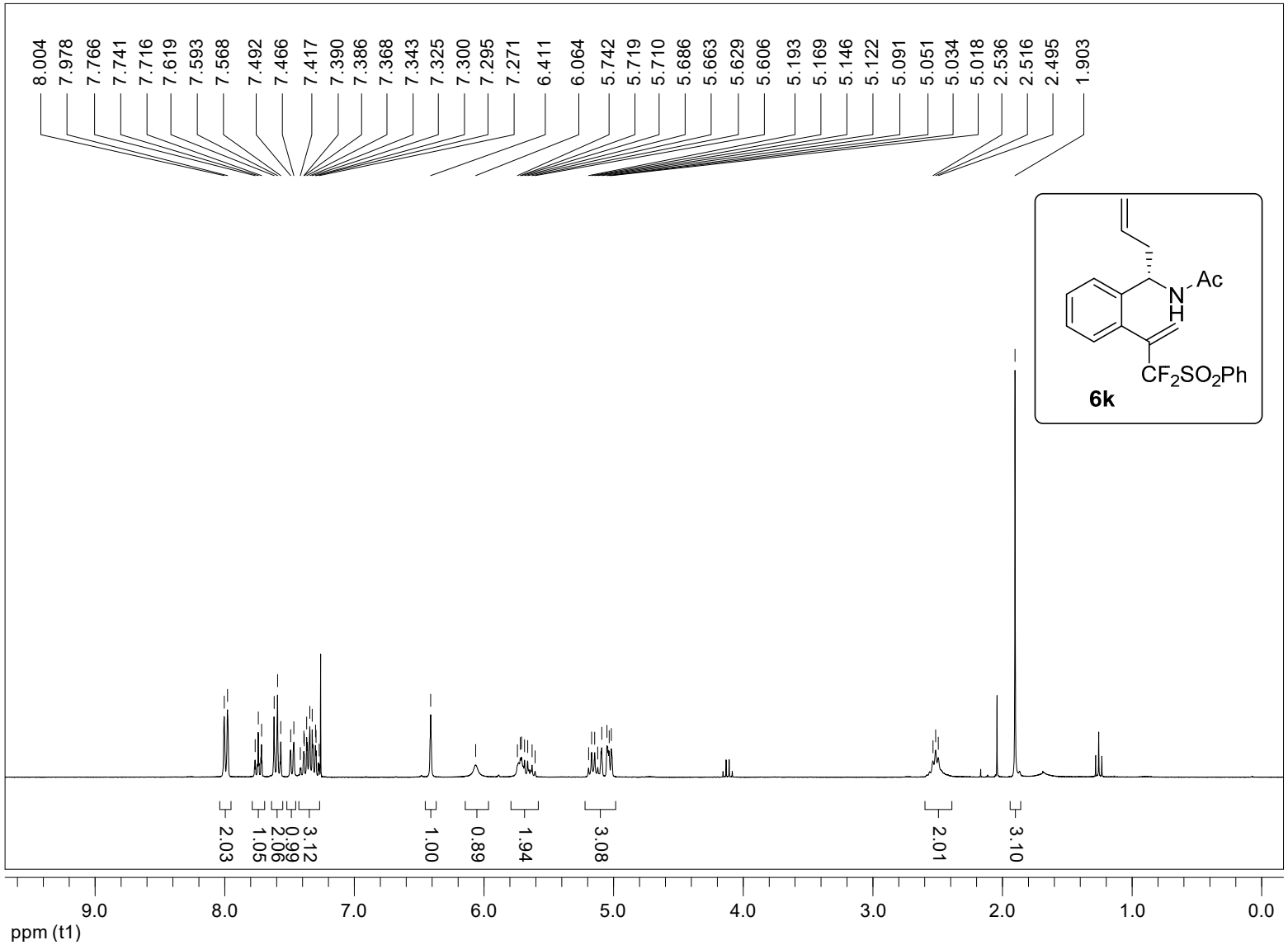

169.098
145.102
133.439
133.242
133.021
132.602
132.185
131.050
129.698
128.065
124.430
124.046
123.976
123.907
123.837
123.238
120.803
118.478
117.175
47.194
41.617
22.918
S
N
H
Ac
CF3
6f'
150
100
50
0
ppm (t1)


-67.211
S
N
Ac
H
CF3
6f'
-30
-40
-50
-60
-70
-80
-90
-100
ppm (t1)


7.327
7.311
7.295
7.291
7.279
7.198
7.194
7.182
7.178
7.169
7.165
7.126
7.111
6.142
5.750
5.642
5.627
5.608
5.593
5.573
5.559
5.021
4.987
4.976
4.956
4.786
4.687
2.403
2.391
2.378
1.316
Boc
N
H
6h
C2F5
2.05
1.03
1.00
1.08
2.13
1.02
1.08
2.12
9.53
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


154.654
135.910
134.117
133.087
130.274
129.218
127.667
126.828
125.980
122.794
122.488
122.181
120.513
120.208
119.901
118.233
117.910
117.620
115.951
115.646
115.341
114.975
114.675
114.376
114.078
112.955
112.656
112.357
112.058
110.936
110.638
110.337
110.040
79.306
50.791
41.114
28.268
Boc
N
H
6h
C_2F_5
150
100
50
ppm (t1)


-82.881
-112.674
Boc
N
H
6h
C_2F_5
3.98
2.00
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm (t1)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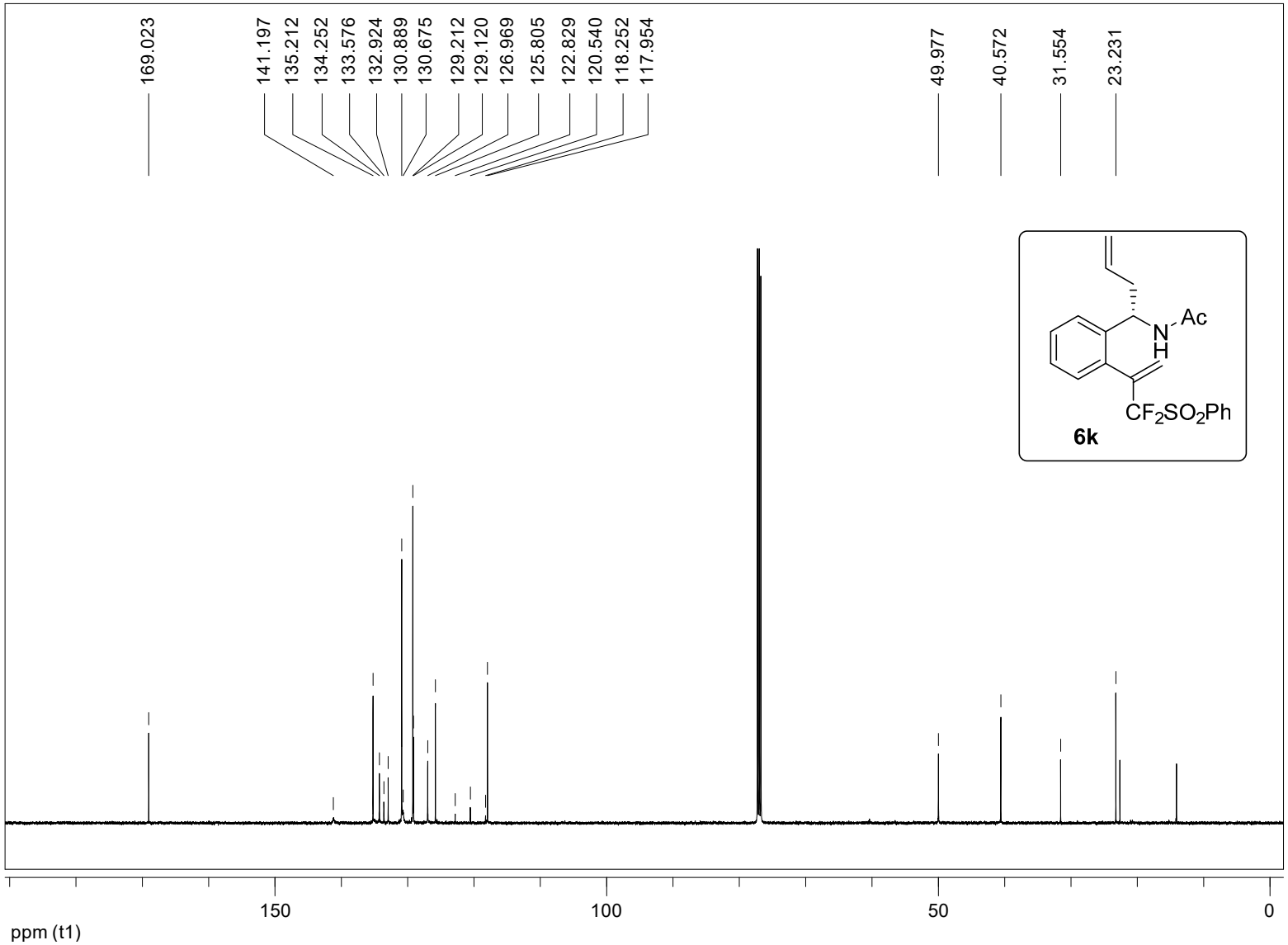
7.978
7.766
7.741
7.716
7.619
7.593
7.568
7.492
7.466
7.417
7.390
7.386
7.368
7.343
7.325
7.300
7.295
7.271
6.411
6.064
5.742
5.719
5.710
5.686
5.663
5.629
5.606
5.193
5.169
5.146
5.122
5.091
5.051
5.034
5.018
2.536
2.516
2.495
1.903
Ac
N
H
CF2SO2Ph
6k
2.03
1.05
2.06
0.99
3.12
1.00
0.89
1.94
3.08
2.01
3.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


169.023
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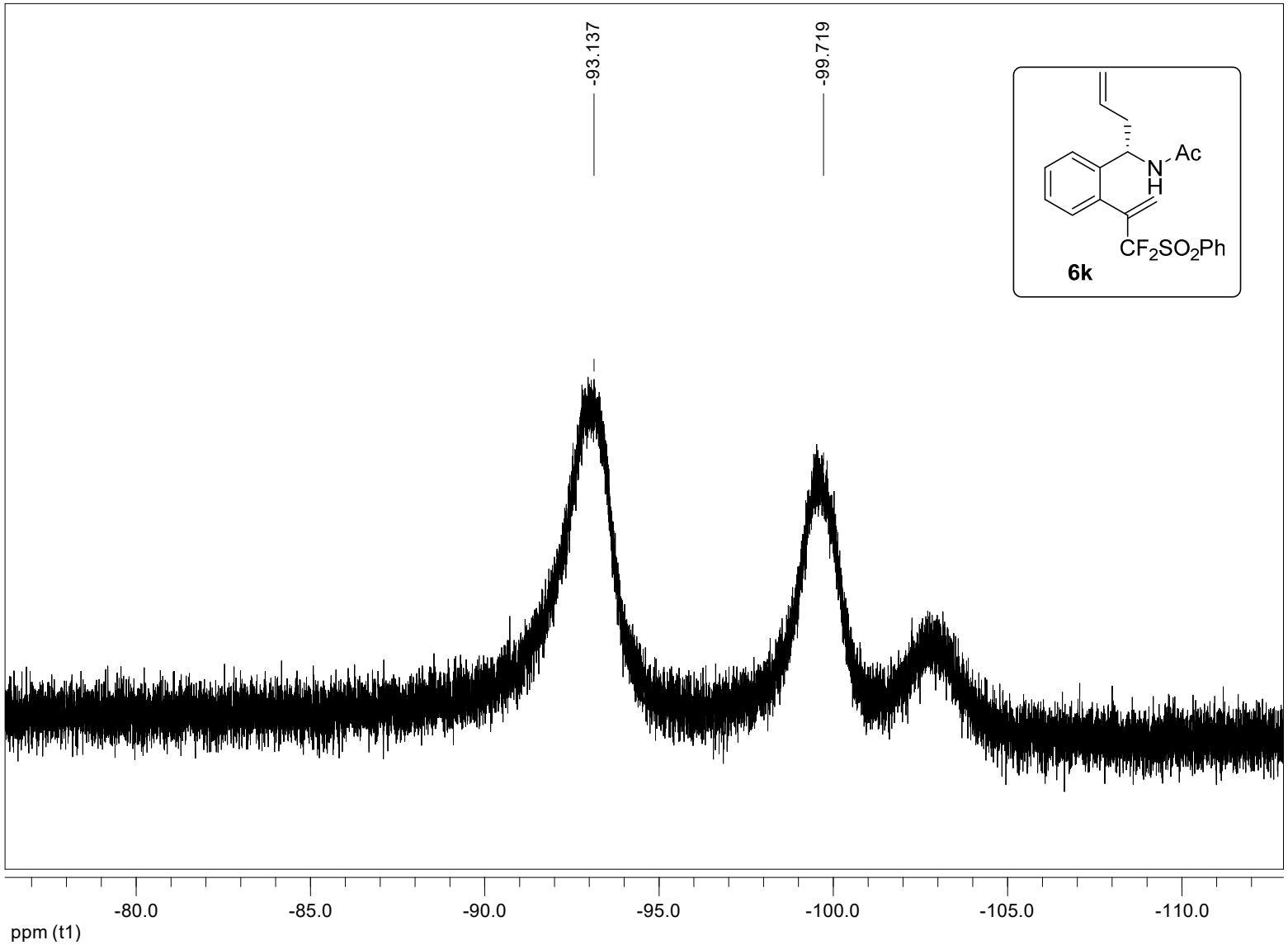
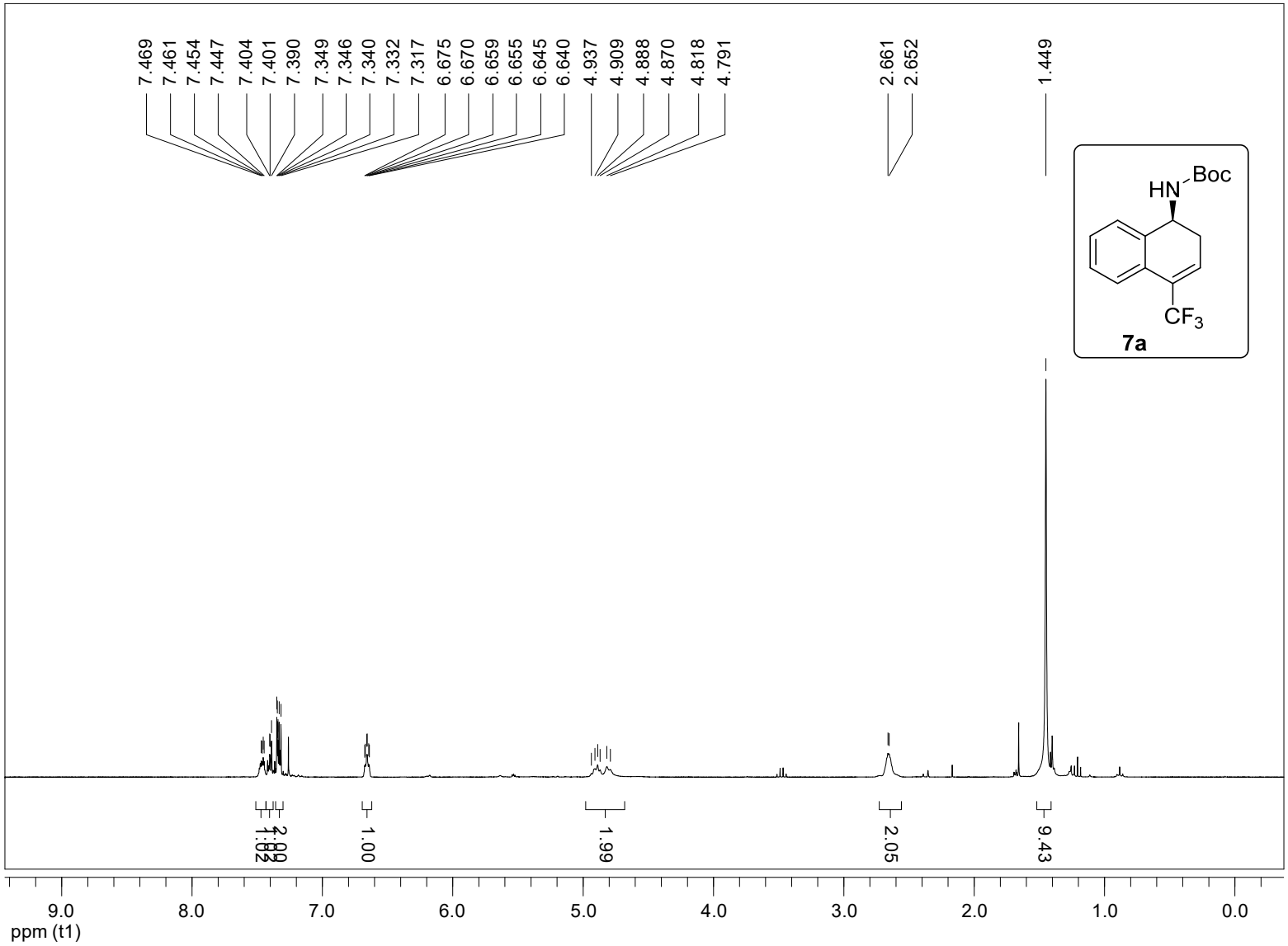
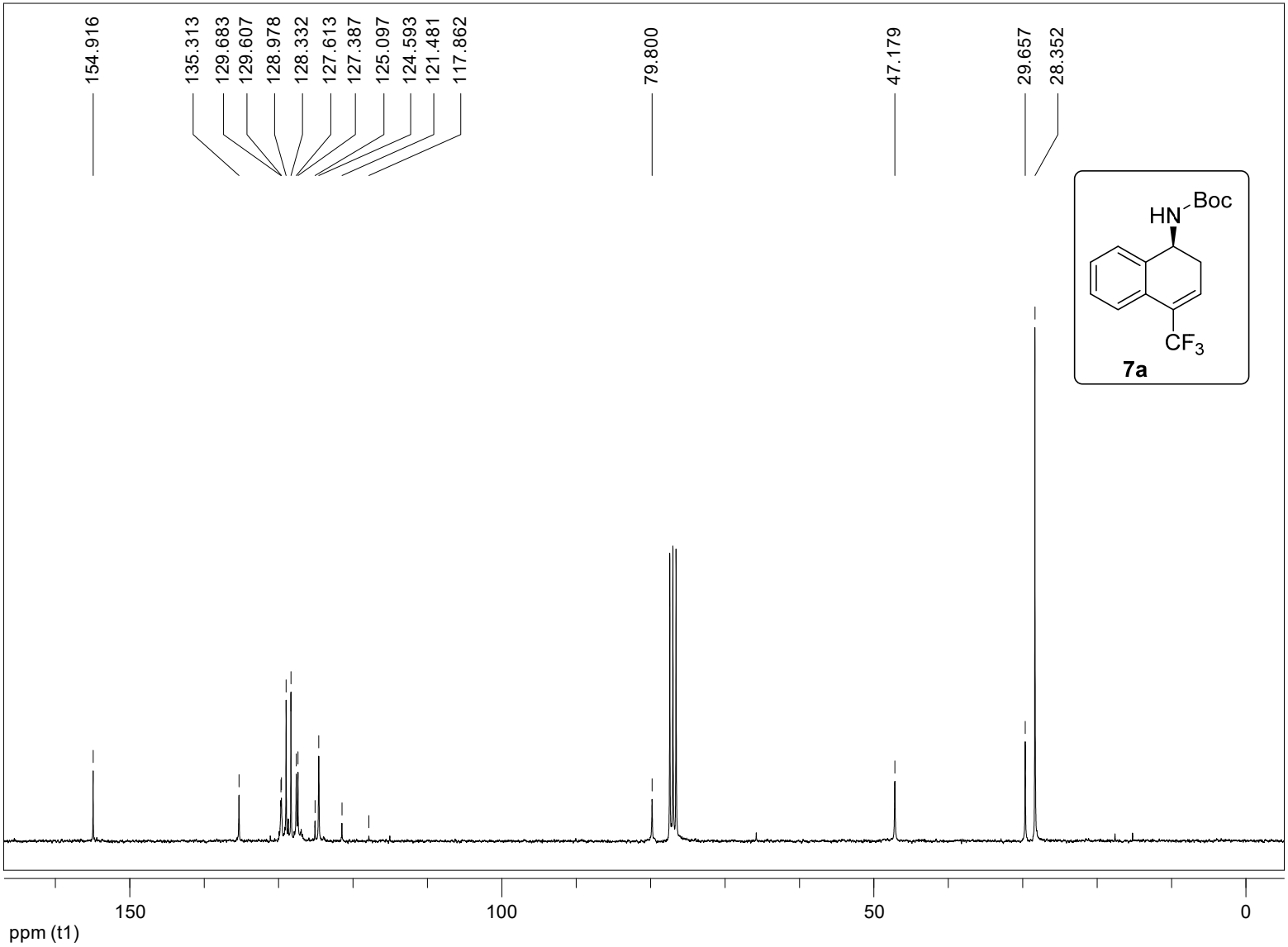
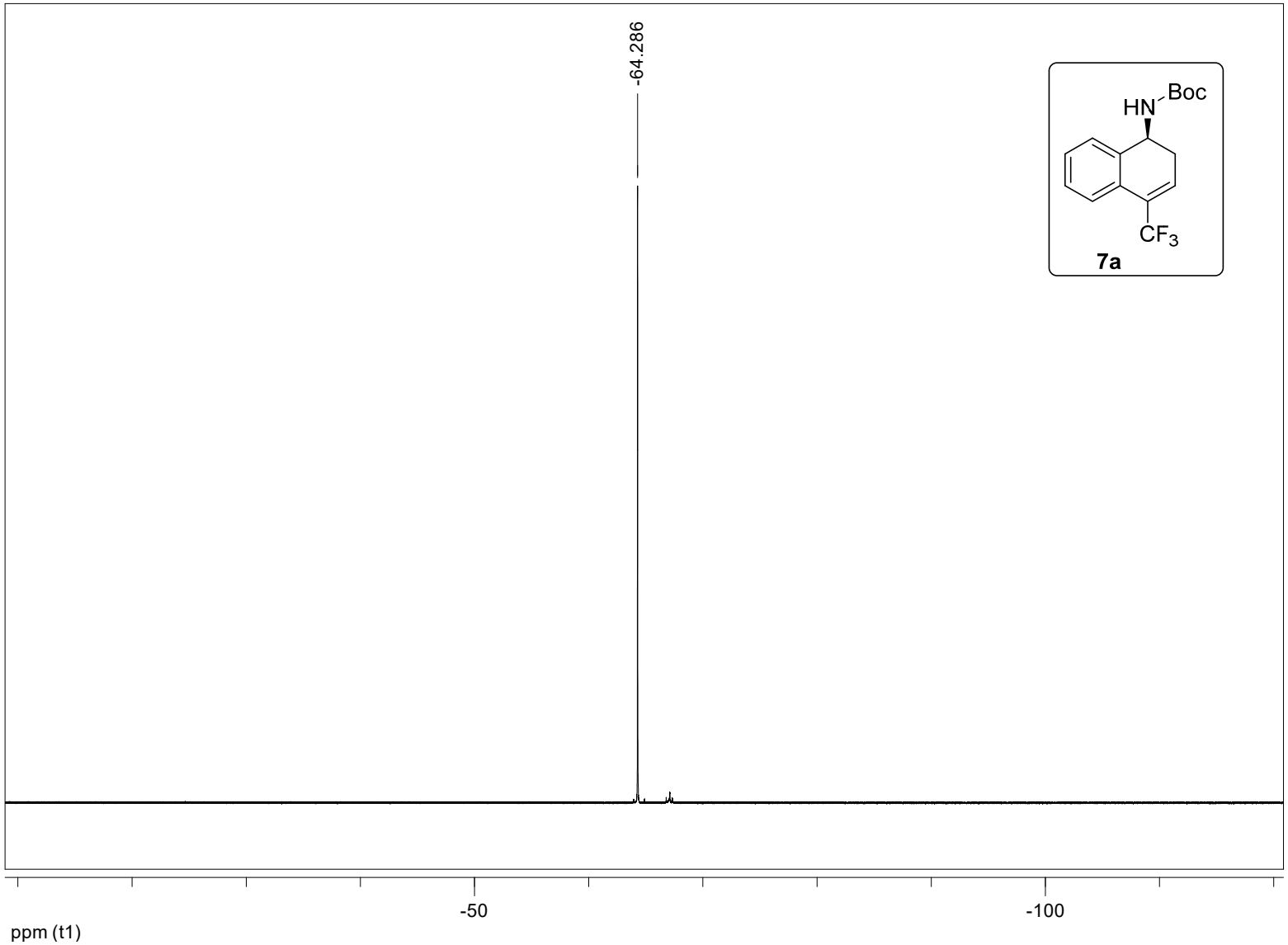
135.212
134.252
133.576
132.924
130.889
130.675
129.212
129.120
126.969
125.805
122.829
120.540
118.252
117.954
49.977
40.572
31.554
23.231
Ac
N
H
CF2SO2Ph
6k
150
100
50
0
ppm (t1)


-93.137
-99.719
Ac
N
H
CF2SO2Ph
6k
-80.0
-85.0
-90.0
-95.0
-100.0
-105.0
-110.0
ppm (t1)


7.469
7.461
7.454
7.447
7.404
7.401
7.390
7.349
7.346
7.340
7.332
7.317
6.675
6.670
6.659
6.655
6.645
6.640
4.937
4.909
4.888
4.870
4.818
4.791
2.661
2.652
1.449
HN
Boc
CF3
7a
1.00
1.99
2.05
9.43
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


154.916
135.313
129.683
129.607
128.978
128.332
127.613
127.387
125.097
124.593
121.481
117.862
79.800
47.179
29.657
28.352
HN
Boc
CF3
7a
150
100
50
0
ppm (t1)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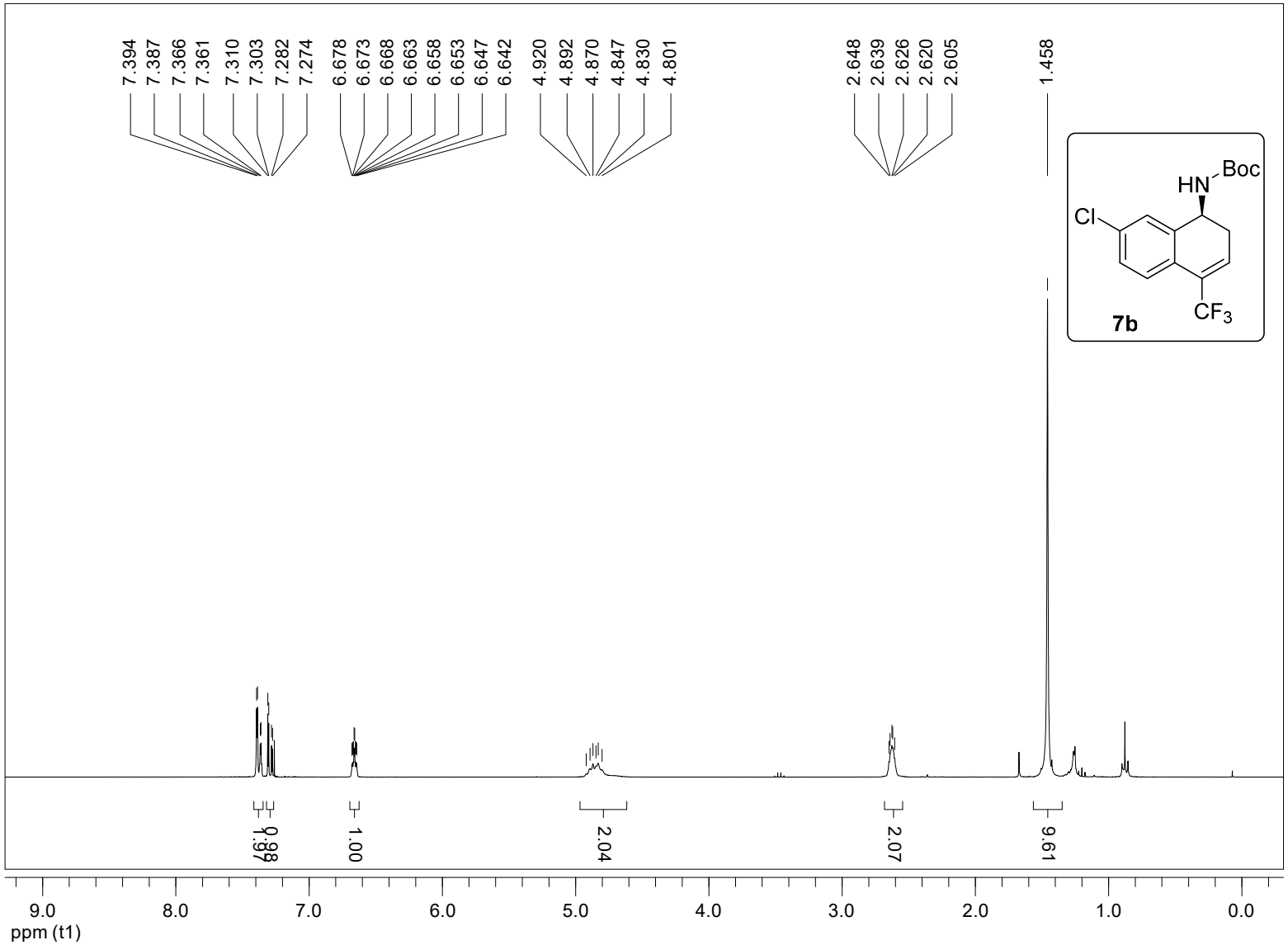
HN
Boc
CF3
7a
-50
-100
ppm (t1)


7.394
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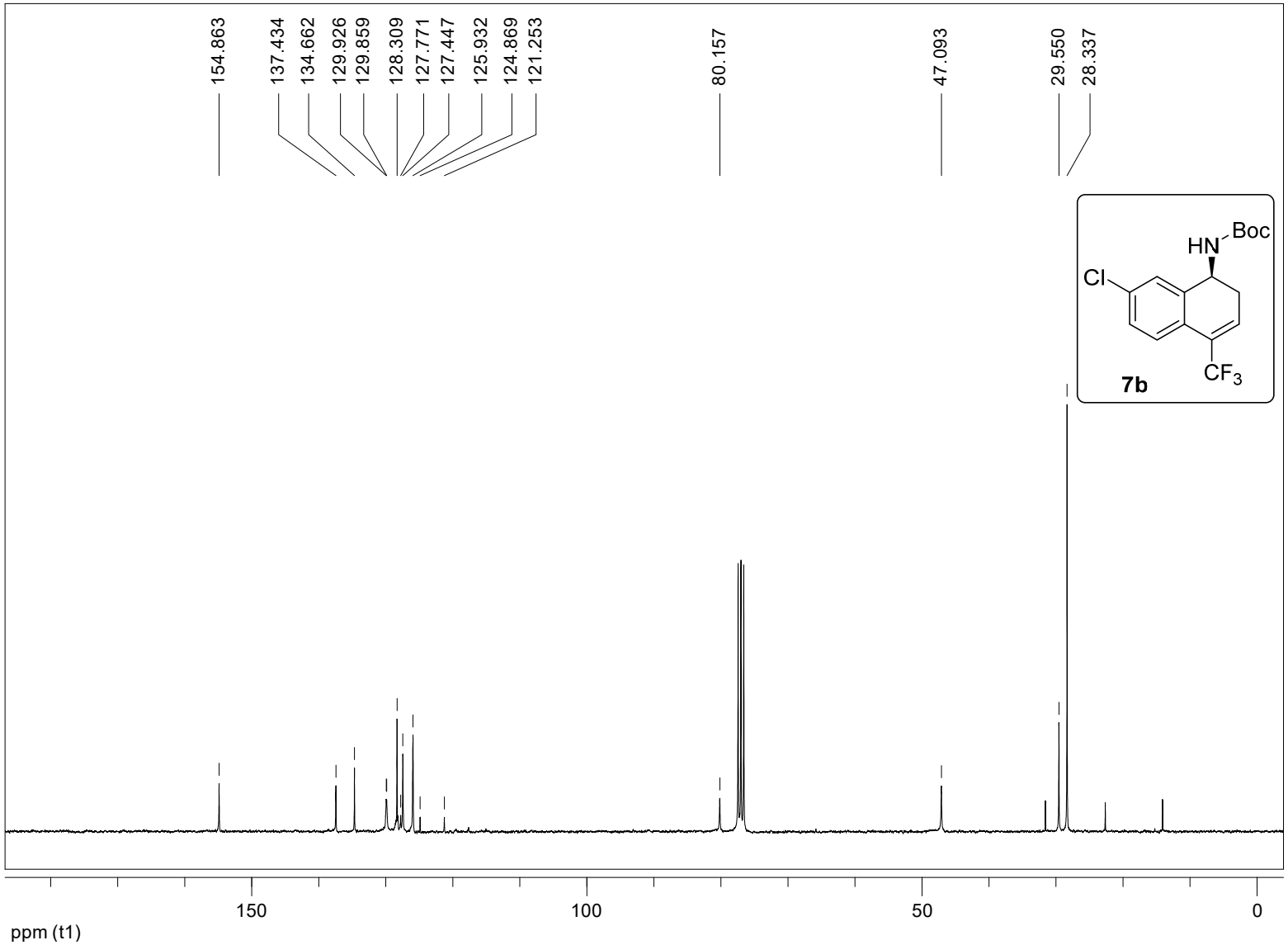
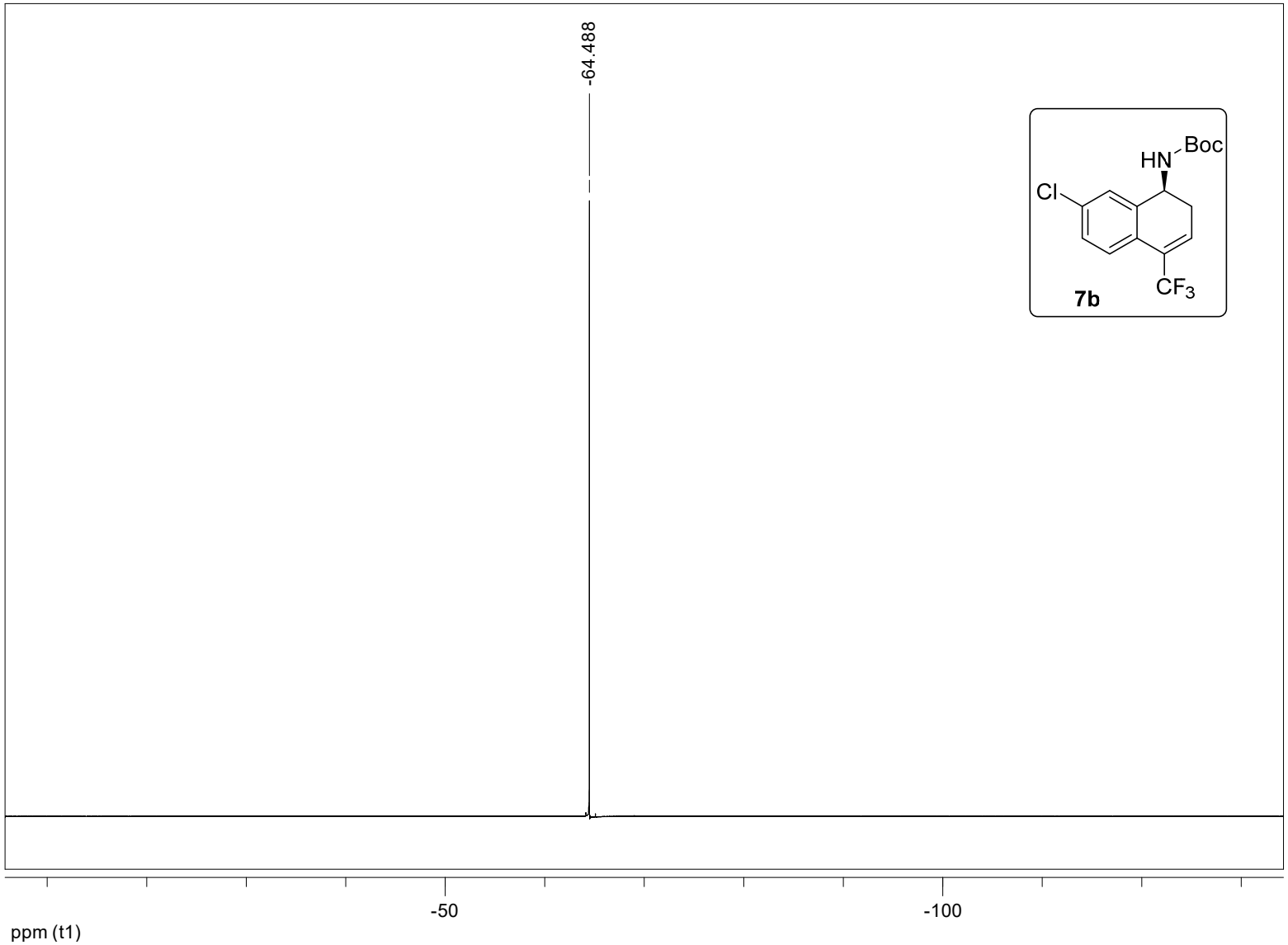
7.361
7.310
7.303
7.282
7.274
6.678
6.673
6.668
6.663
6.658
6.653
6.647
6.642
4.920
4.892
4.870
4.847
4.830
4.801
2.648
2.639
2.626
2.620
2.605
1.458
HN
Boc
Cl
CF3
7b
1.97
0.98
1.00
2.04
2.07
9.61
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


154.863
137.434
134.662
129.926
129.859
128.309
127.771
127.447
125.932
124.869
121.253
80.157
47.093
29.550
28.337
HN
Boc
Cl
CF3
7b
150
100
50
0
ppm (t1)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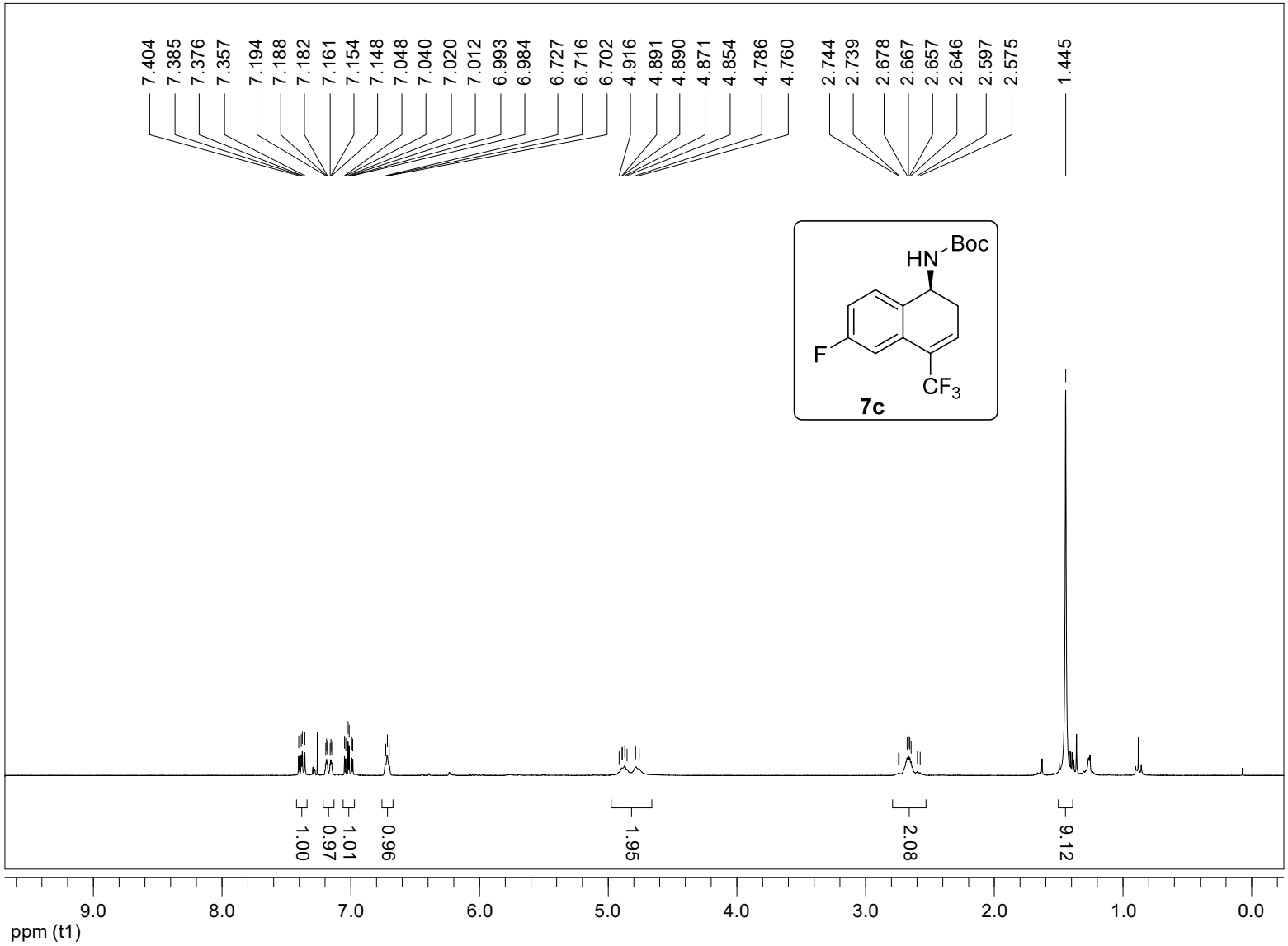
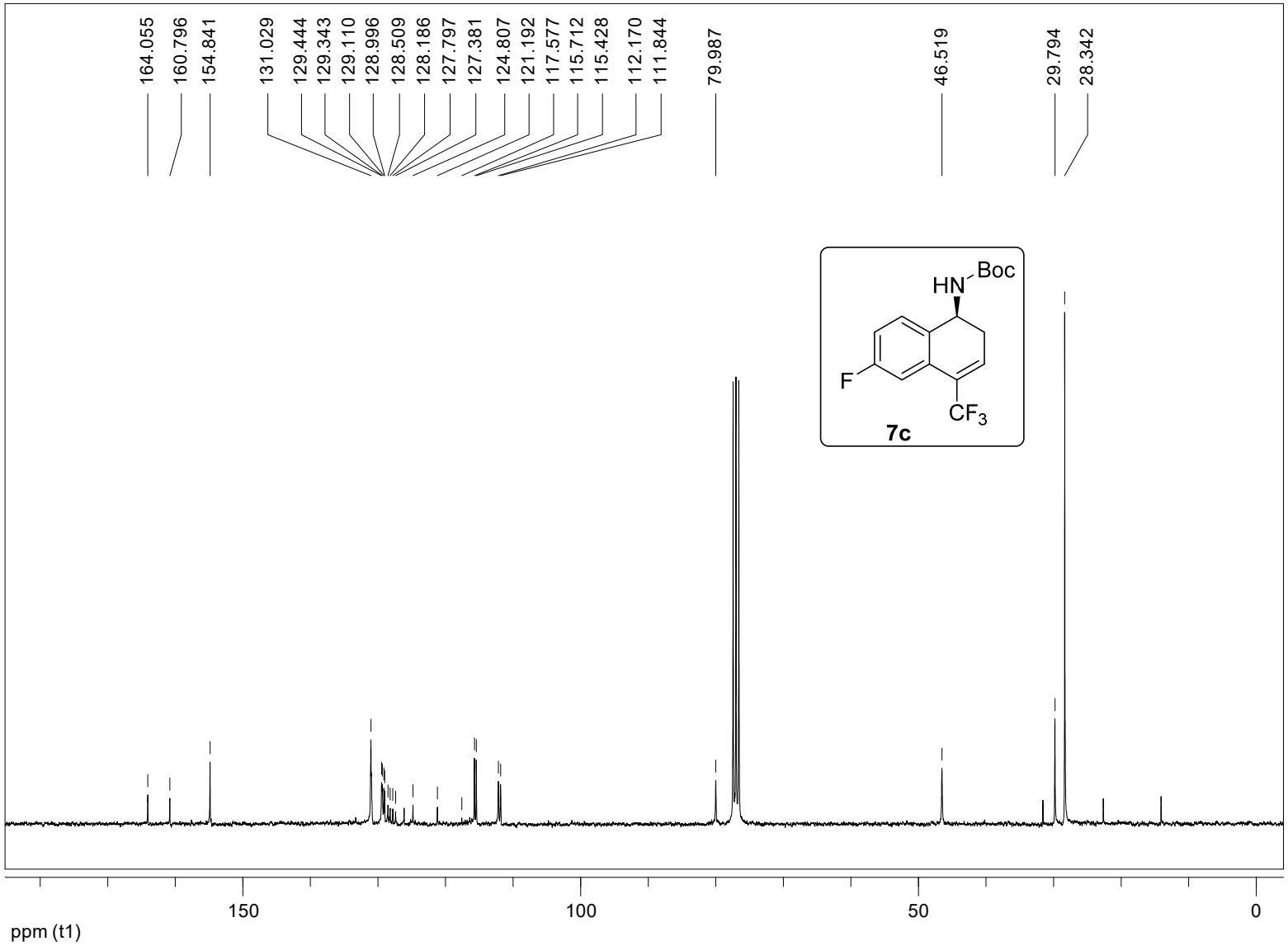
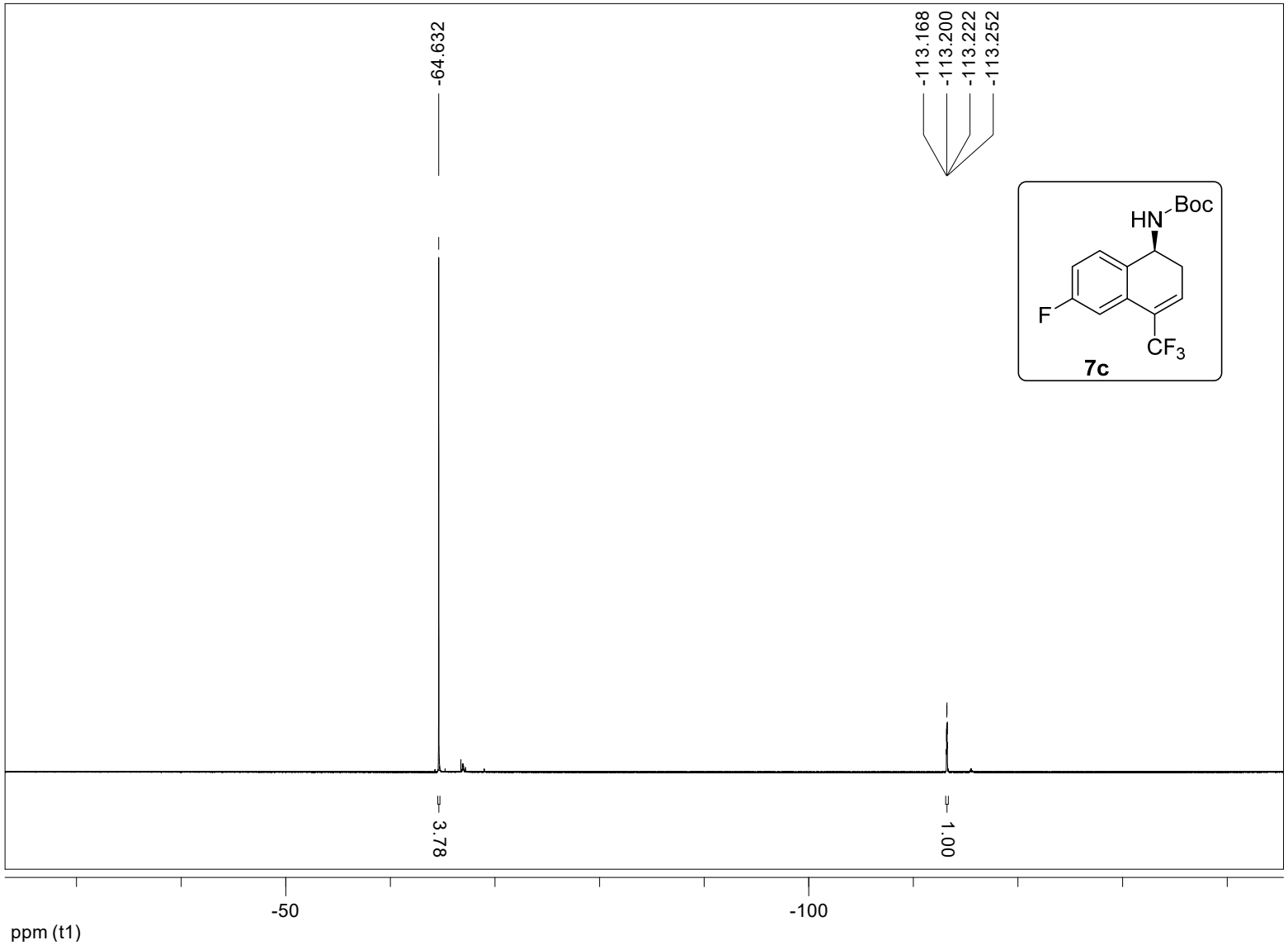
Boc
Cl
CF3
7b
-50
-100
ppm (t1)


7.404
7.385
7.376
7.357
7.194
7.188
7.182
7.161
7.154
7.148
7.048
7.040
7.020
7.012
6.993
6.984
6.727
6.716
6.702
4.916
4.891
4.890
4.871
4.854
4.786
4.760
2.744
2.739
2.678
2.667
2.657
2.646
2.597
2.575
1.445
HN
Boc
F
CF3
7c
1.00
0.97
1.01
0.96
1.95
2.08
9.12
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


164.055
160.796
154.841
131.029
129.444
129.343
129.110
128.996
128.509
128.186
127.797
127.381
124.807
121.192
117.577
115.712
115.428
112.170
111.844
79.987
46.519
29.794
28.342
HN
Boc
F
CF3
7c
150
100
50
0
ppm (t1)


-64.632
-113.168
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-113.222
-113.252
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Boc
F
CF3
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3.78
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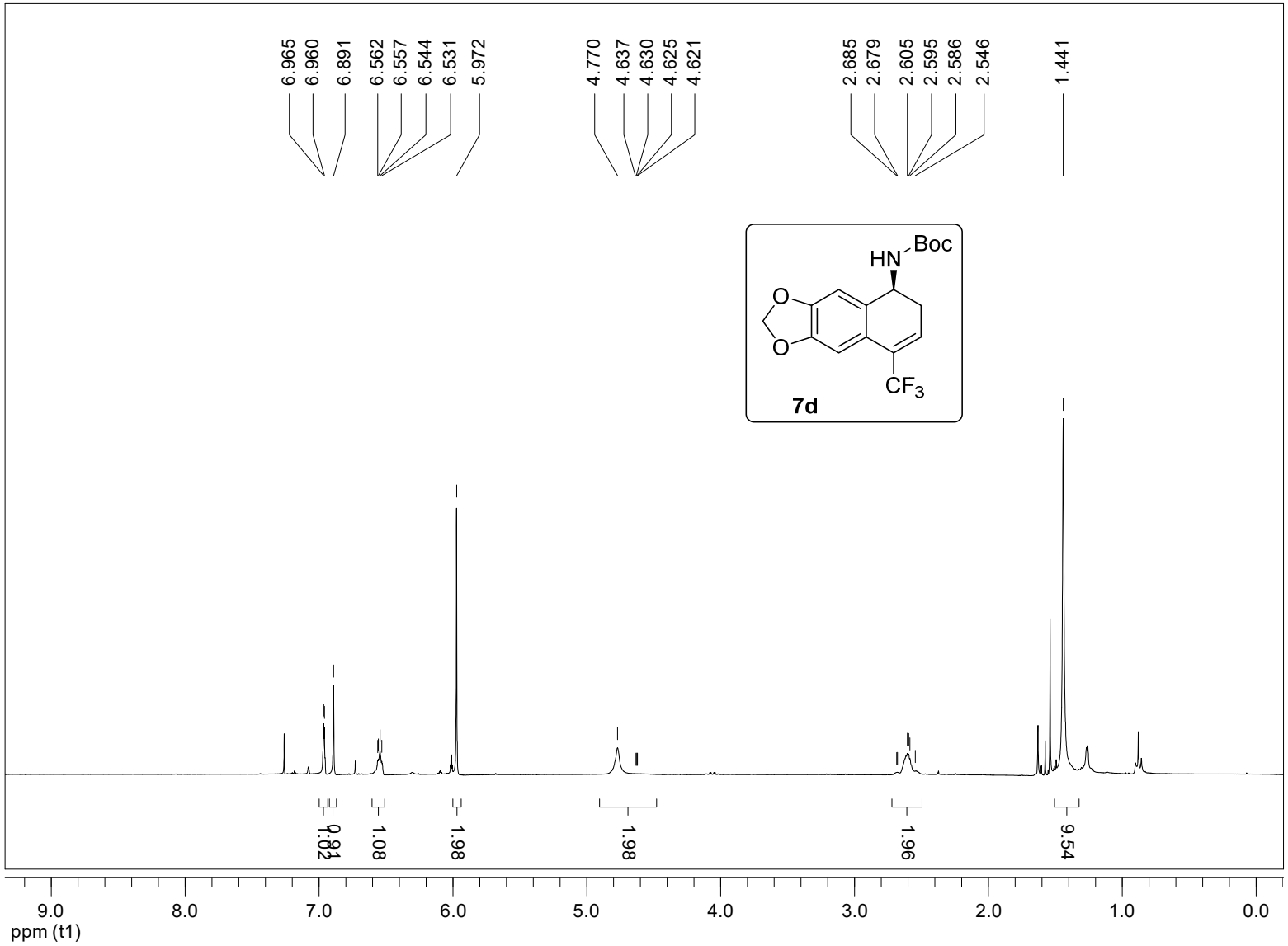
-50
-100
ppm (t1)


6.965
6.960
6.891
6.562
6.557
6.544
6.531
5.972
4.770
4.637
4.630
4.625
4.621
2.685
2.679
2.605
2.595
2.586
2.546
1.441
HN
Boc
O
O
CF3
7d
0.91
1.02
1.08
1.98
1.98
1.96
9.54
9.0
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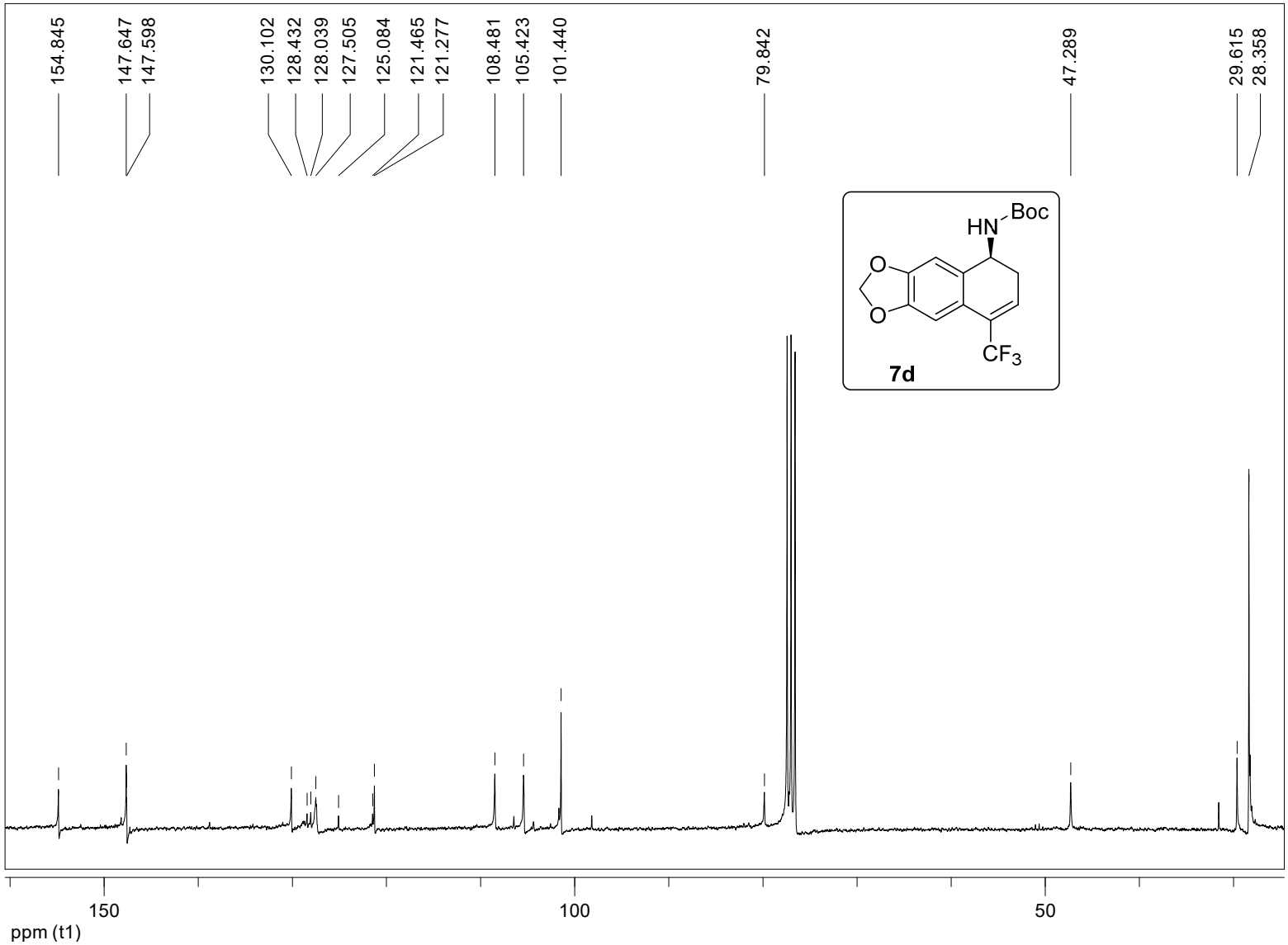
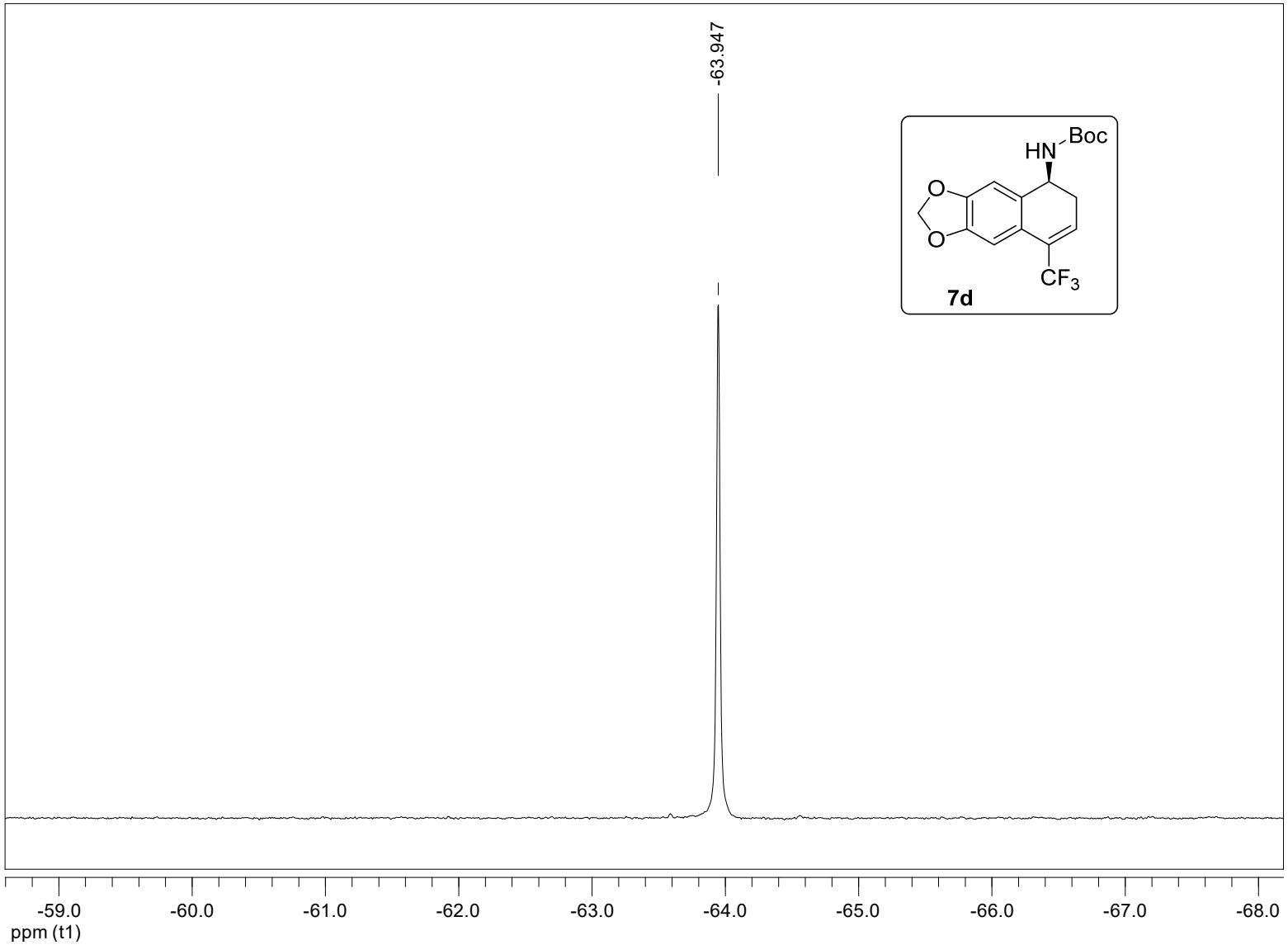
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


154.845
147.647
147.598
130.102
128.432
128.039
127.505
125.084
121.465
121.277
108.481
105.423
101.440
79.842
47.289
29.615
28.358
HN
Boc
O
O
CF3
7d
150
100
50
ppm (t1)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Boc
O
O
CF3
7d
-59.0
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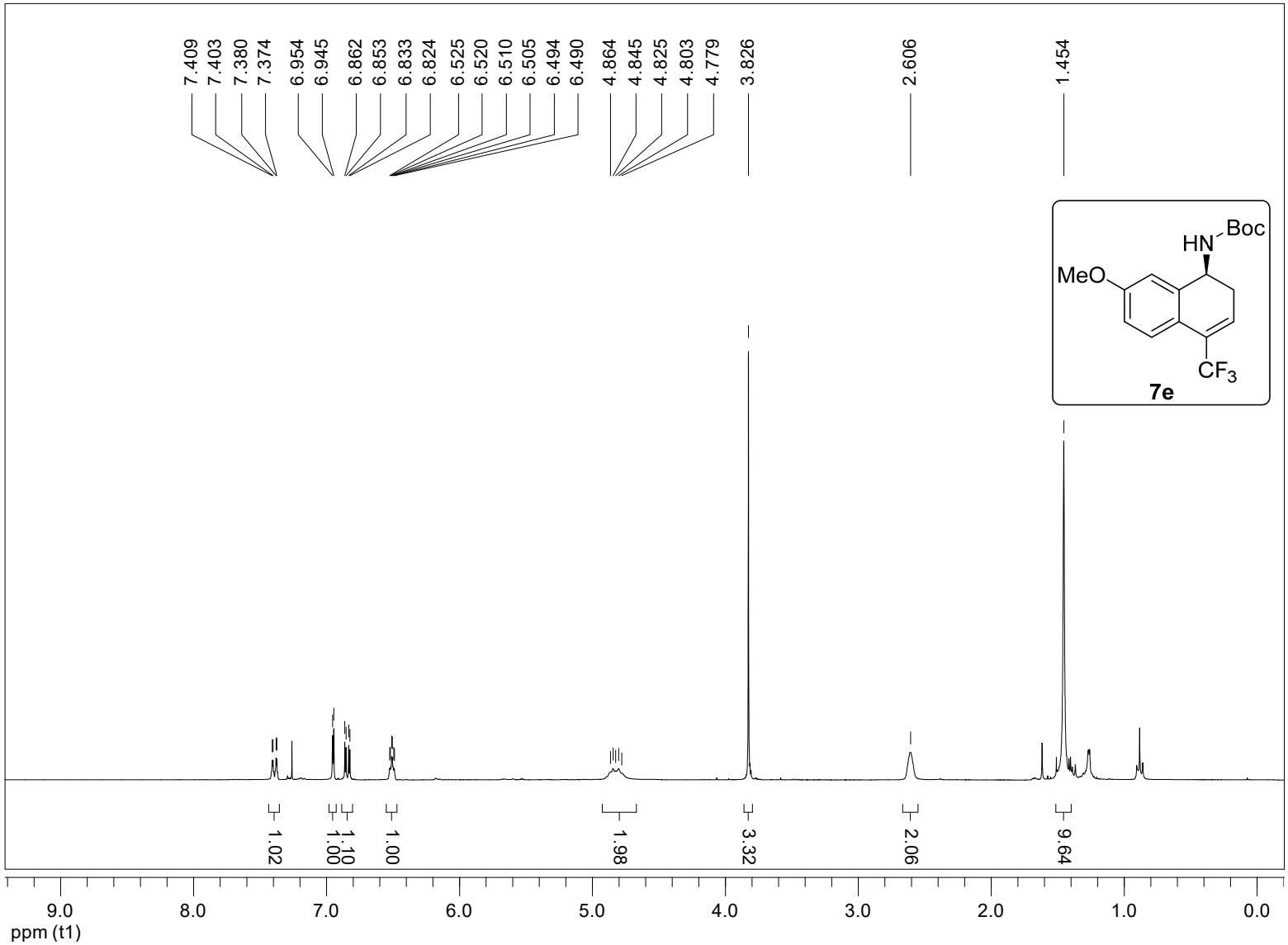
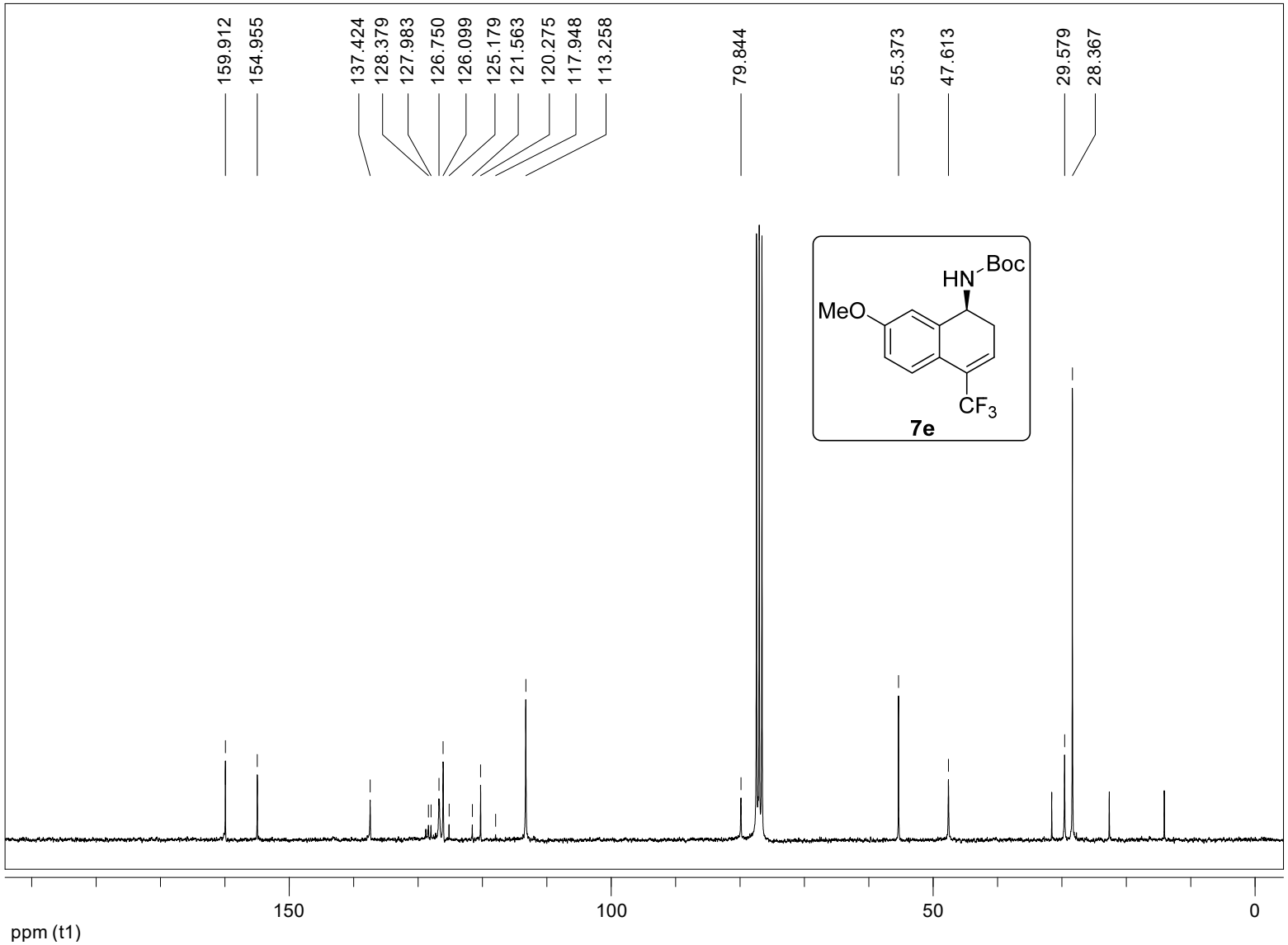
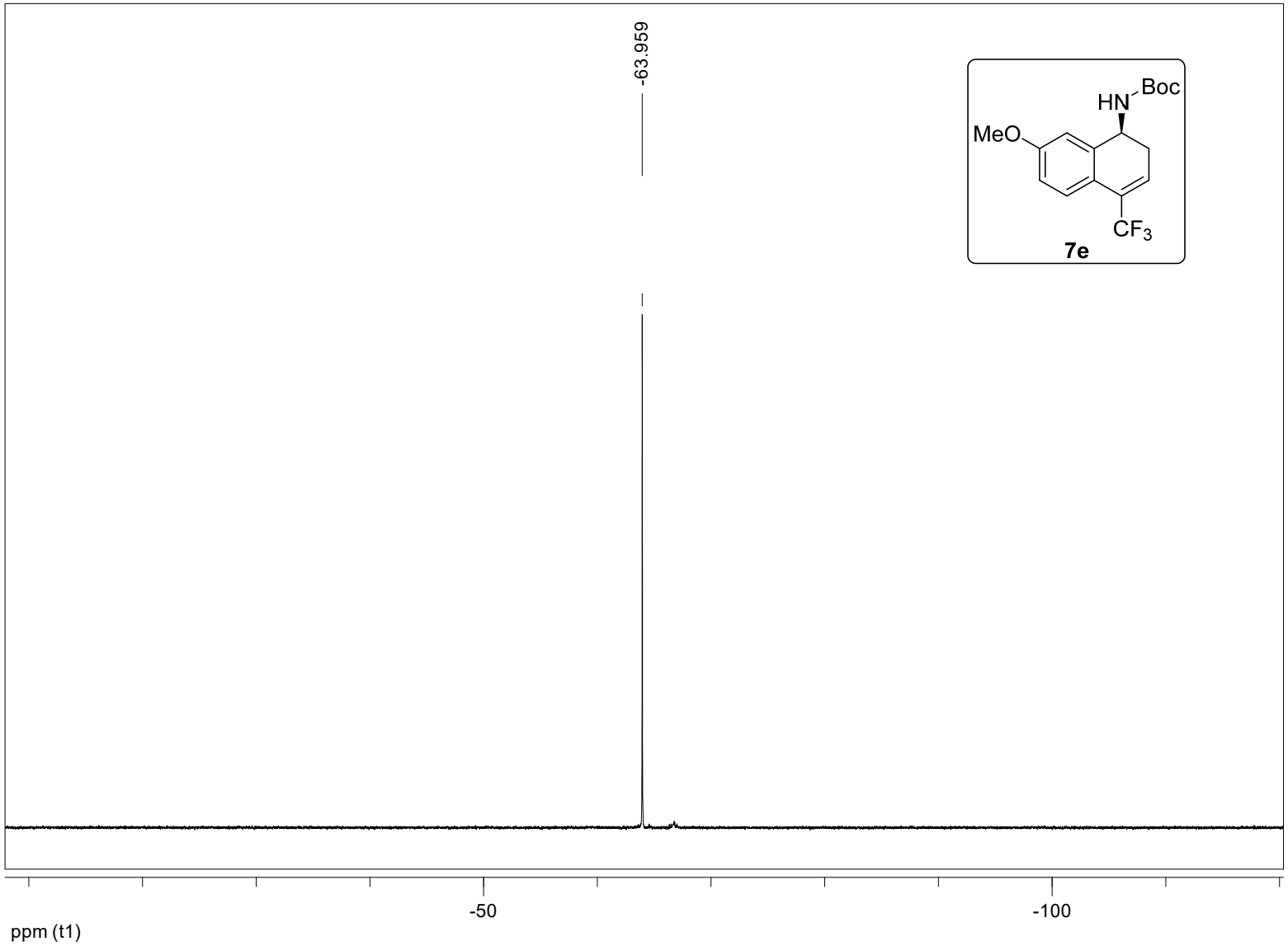
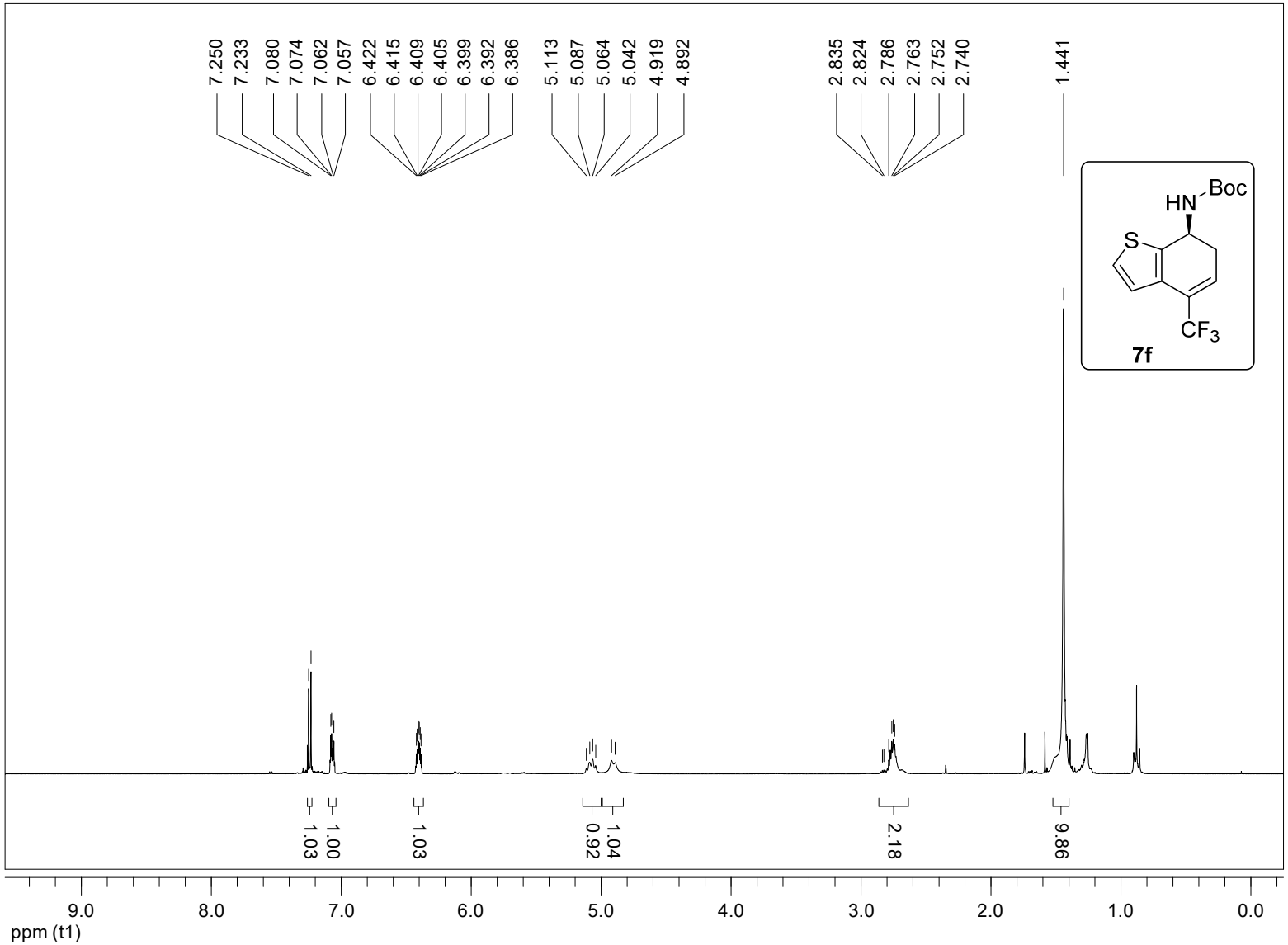
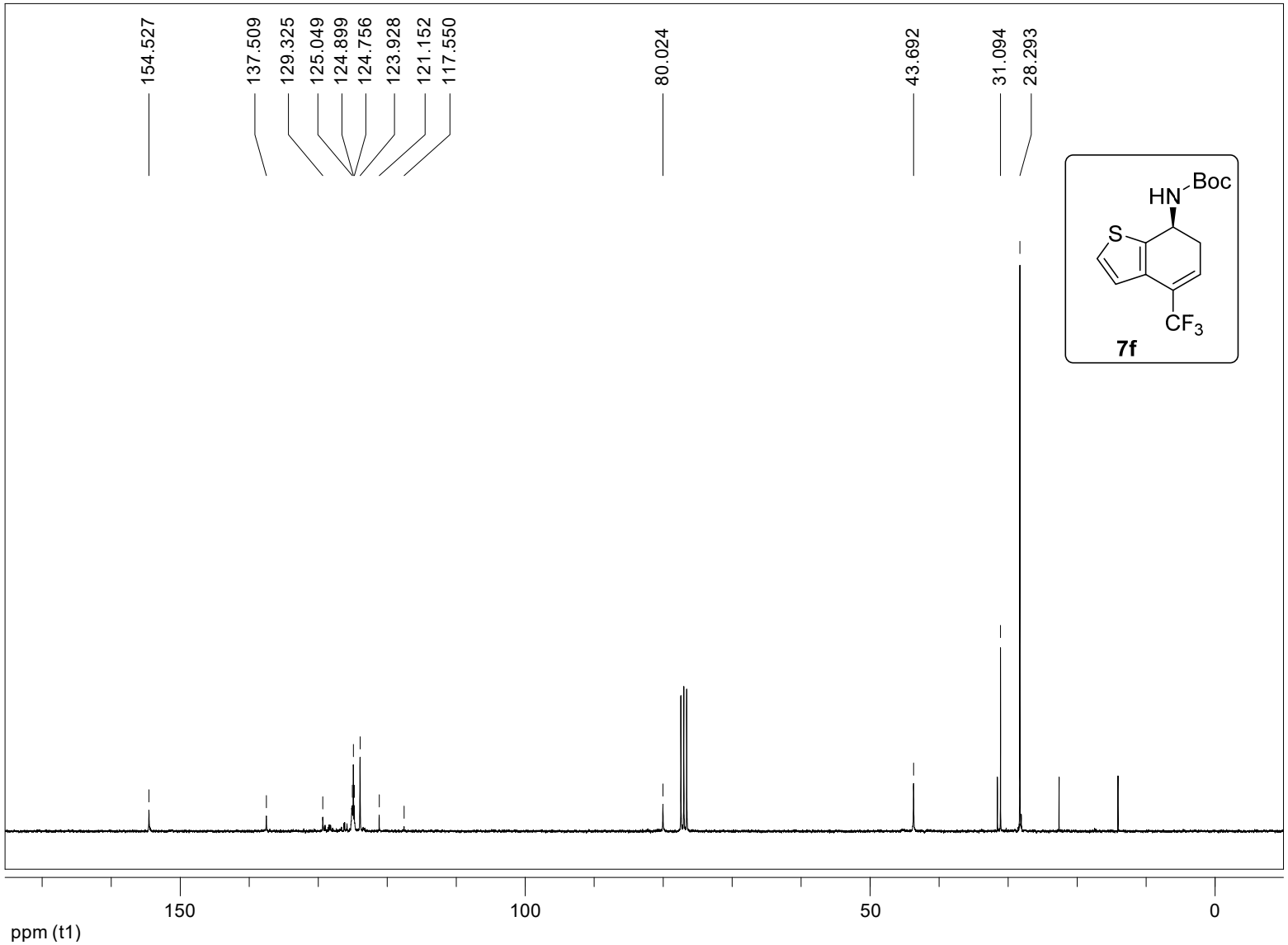
-61.0
-62.0
-63.0
-64.0
-65.0
-66.0
-67.0
-68.0
ppm (t1)

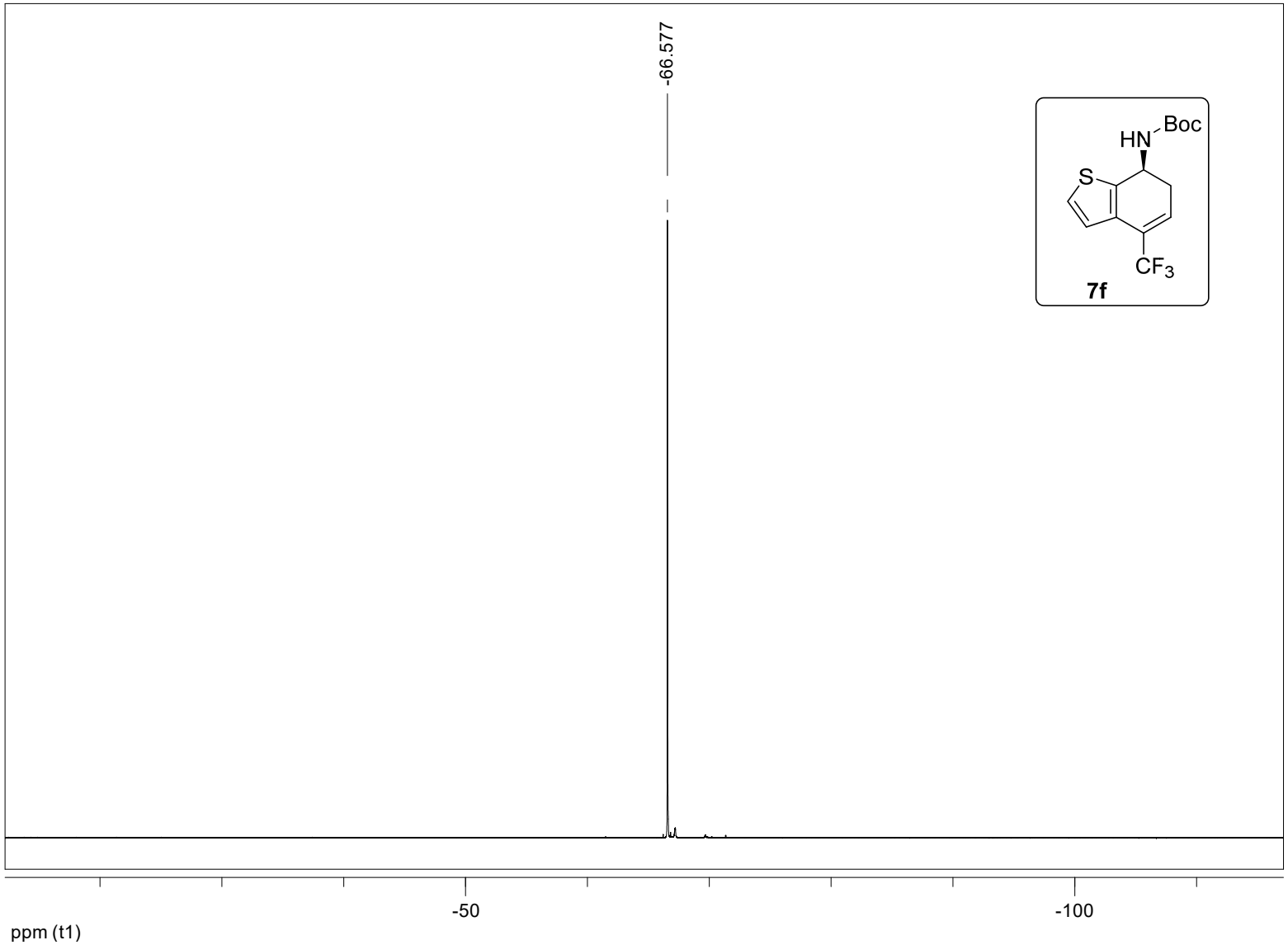

7.409
7.403
7.380
7.374
6.954
6.945
6.862
6.853
6.833
6.824
6.525
6.520
6.510
6.505
6.494
6.490
4.864
4.845
4.825
4.803
4.779
3.826
2.606
1.454
HN
Boc
MeO
CF3
7e
1.02
1.10
1.00
1.00
1.98
3.32
2.06
9.64
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

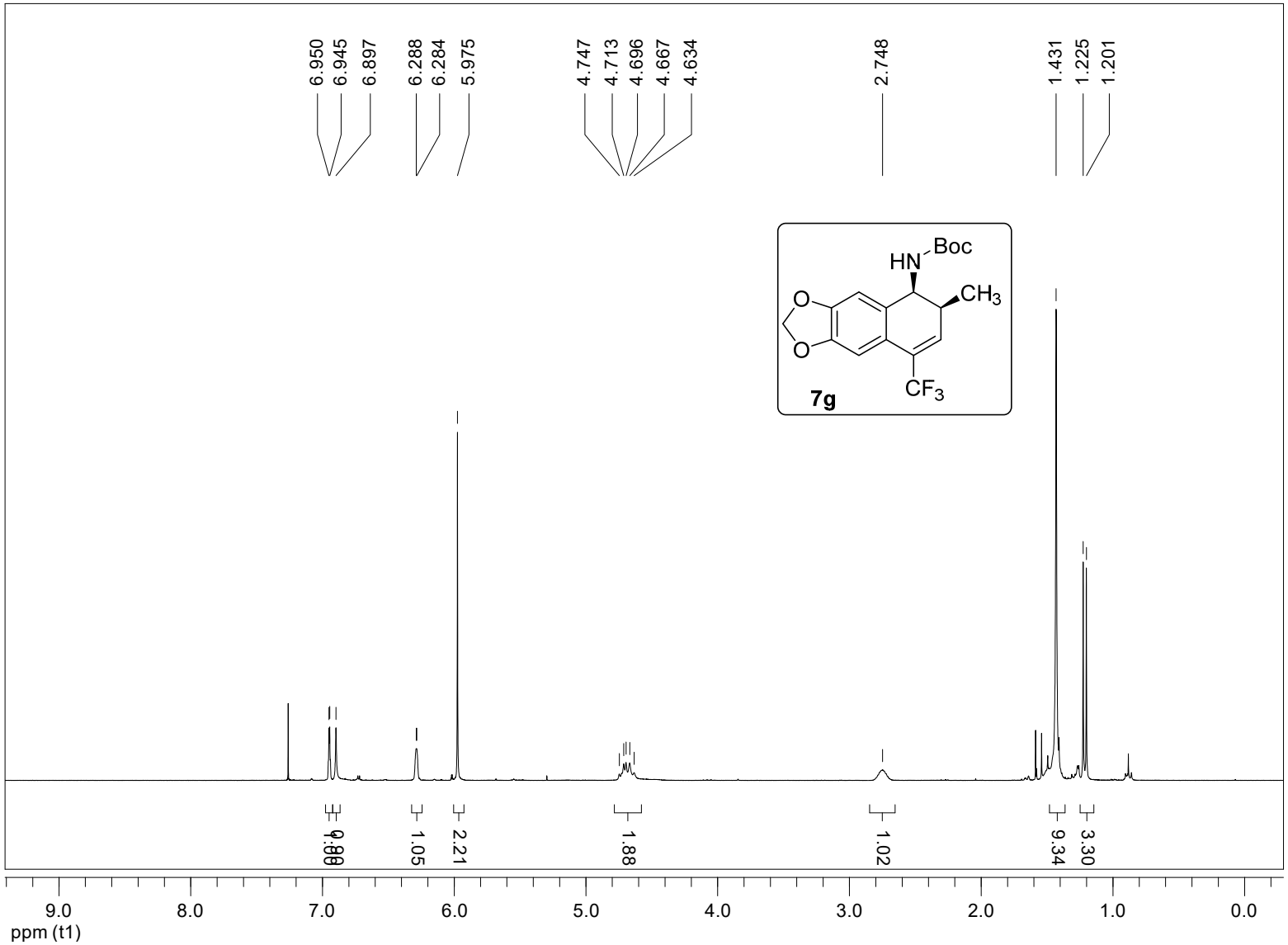

159.912
154.955
137.424
128.379
127.983
126.750
126.099
125.179
121.563
120.275
117.948
113.258
79.844
55.373
47.613
29.579
28.367
HN
Boc
MeO
CF3
7e
150
100
50
0
ppm (t1)

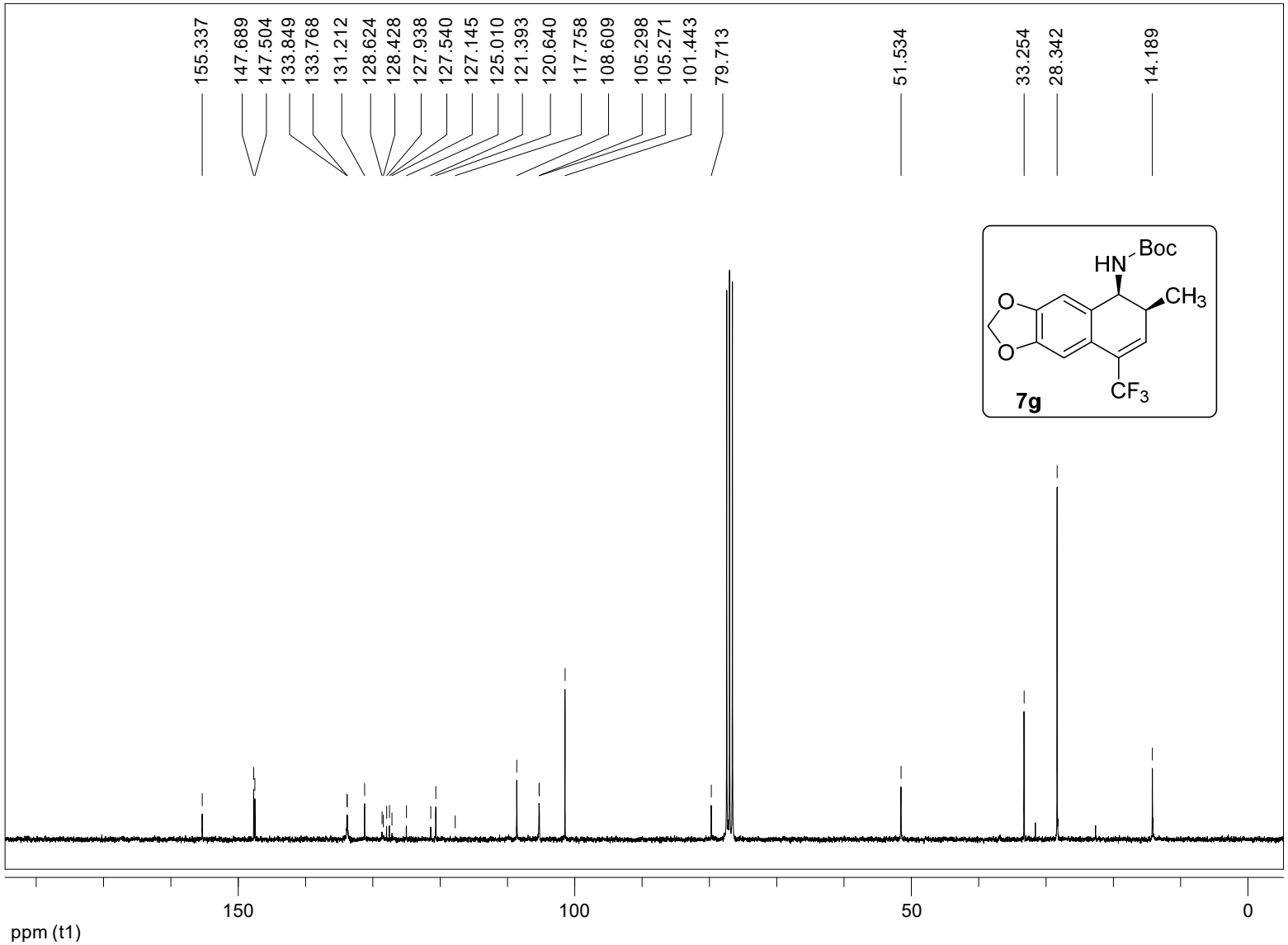

-63.959
HN
Boc
MeO
CF3
7e
-50
-100
ppm (t1)

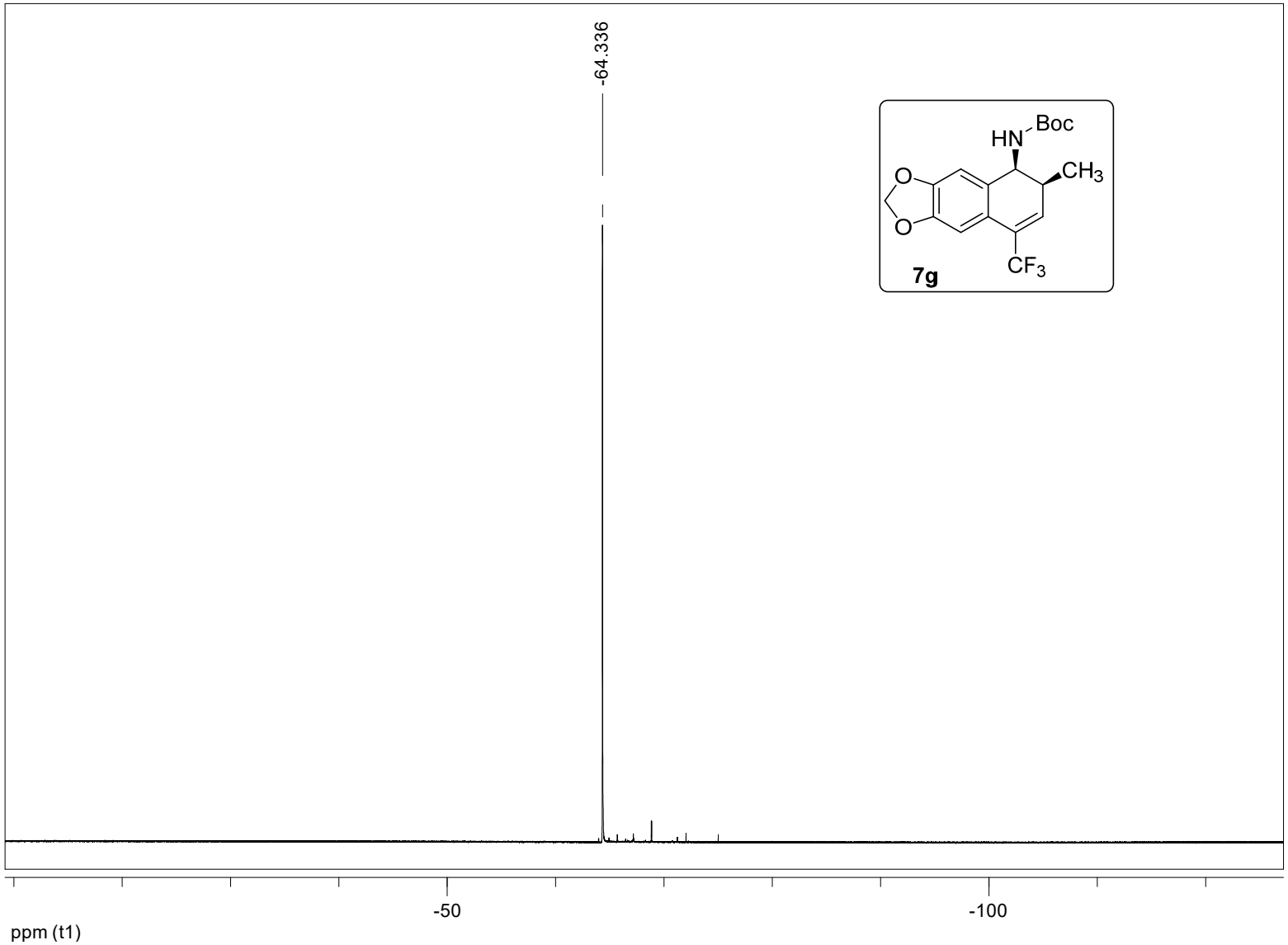

7.250
7.233
7.080
7.074
7.062
7.057
6.422
6.415
6.409
6.405
6.399
6.392
6.386
5.113
5.087
5.064
5.042
4.919
4.892
2.835
2.824
2.786
2.763
2.752
2.740
1.441
HN
Boc
S
CF3
7f
1.03
1.00
1.03
0.92
1.04
2.18
9.86
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

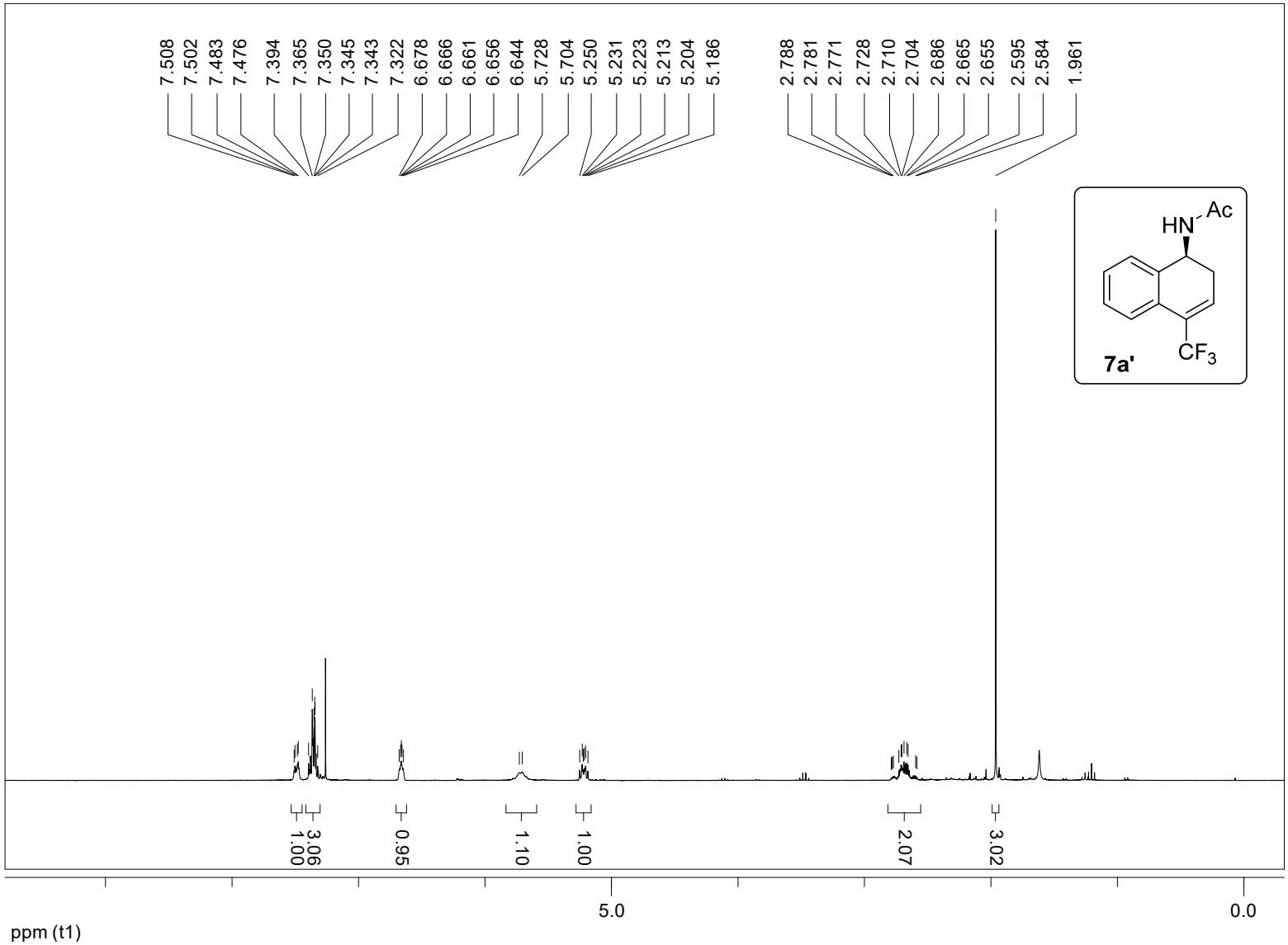

154.527
137.509
129.325
125.049
124.899
124.756
123.928
121.152
117.550
80.024
43.692
31.094
28.293
HN
Boc
S
CF3
7f
150
100
50
0
ppm (t1)

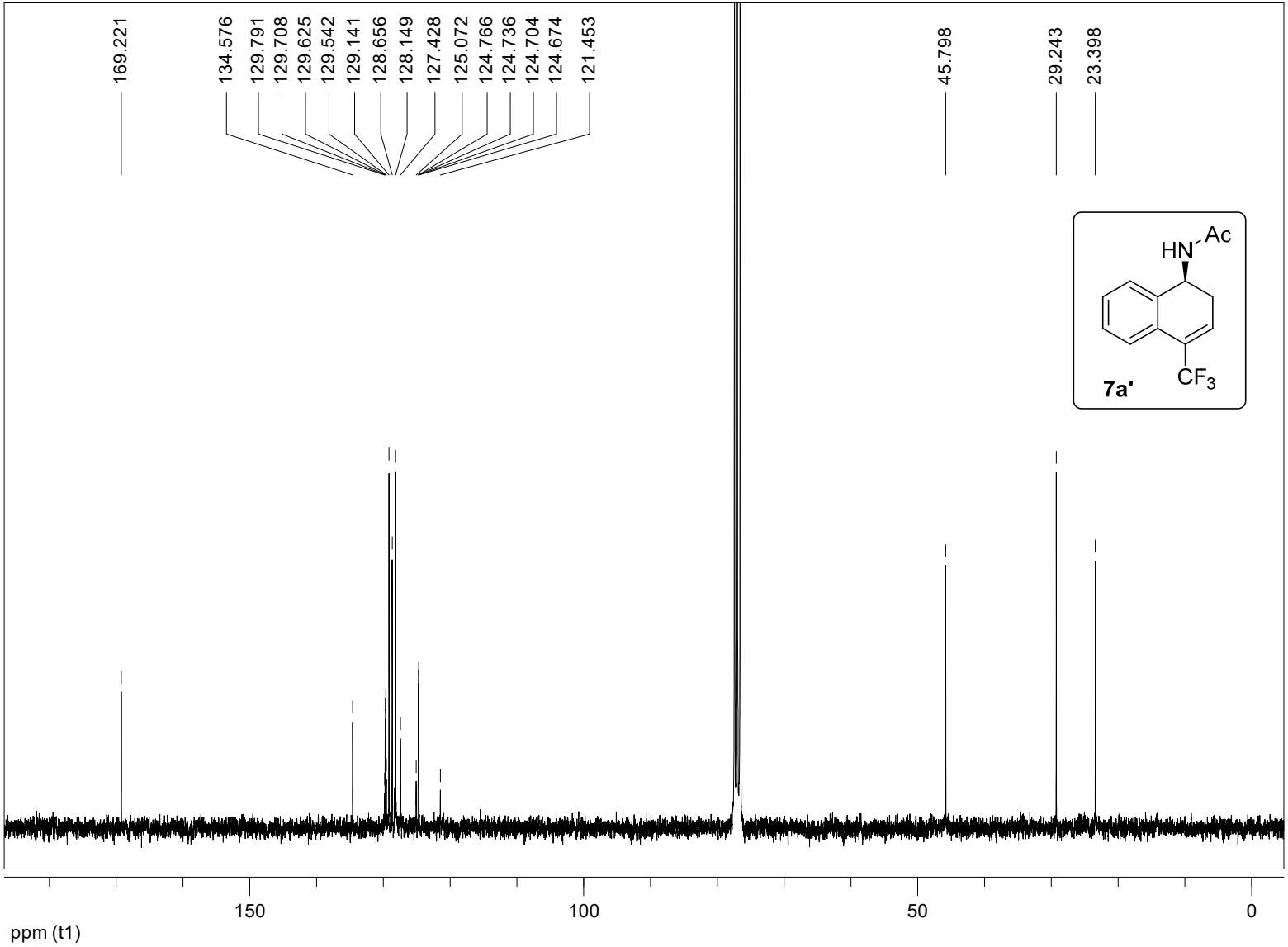

-66.577
HN
Boc
S
CF3
7f
-50
-100
ppm (t1)

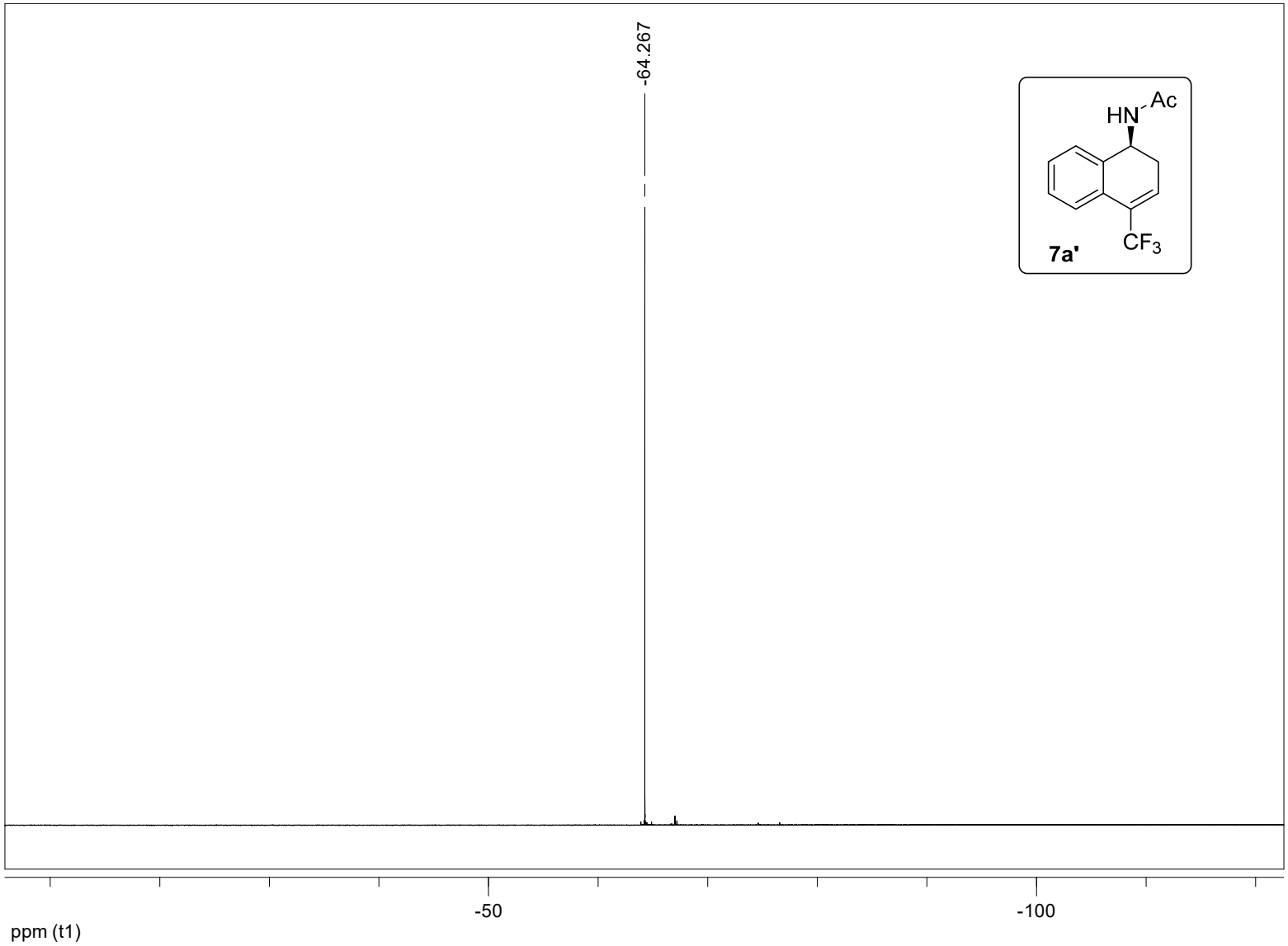

6.950
6.945
6.897
6.288
6.284
5.975
4.747
4.713
4.696
4.667
4.634
2.748
1.431
1.225
1.201
HN
Boc
CH3
O
O
CF3
7g
1.05
2.21
1.88
1.02
9.34
3.30
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

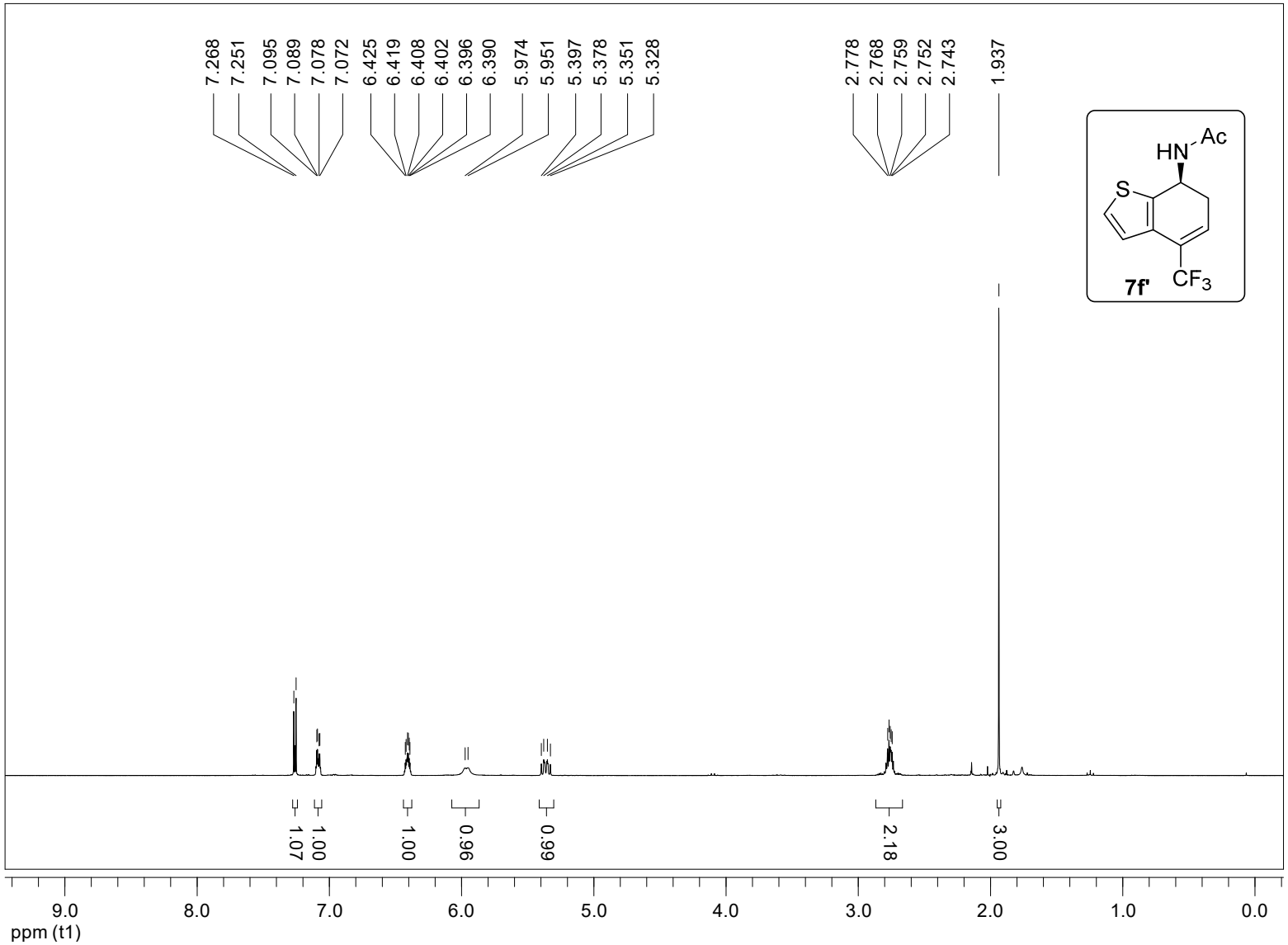

155.337
147.689
147.504
133.849
133.768
131.212
128.624
128.428
127.938
127.540
127.145
125.010
121.393
120.640
117.758
108.609
105.298
105.271
101.443
79.713
51.534
33.254
28.342
14.189
HN
Boc
CH3
O
O
CF3
7g
150
100
50
0
ppm (t1)

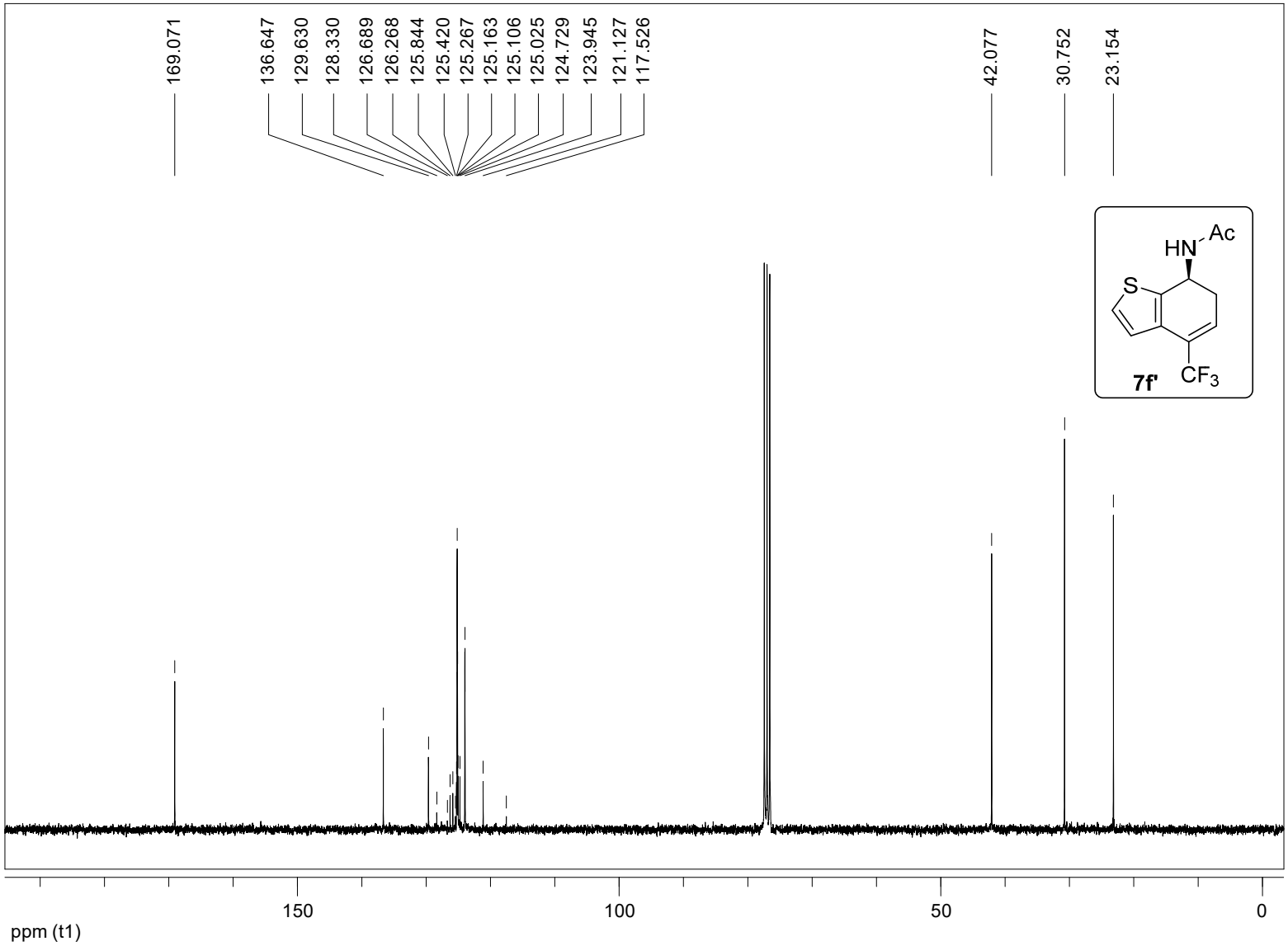

-64.336
HN
Boc
CH3
O
O
CF3
7g
-50
-100
ppm (t1)

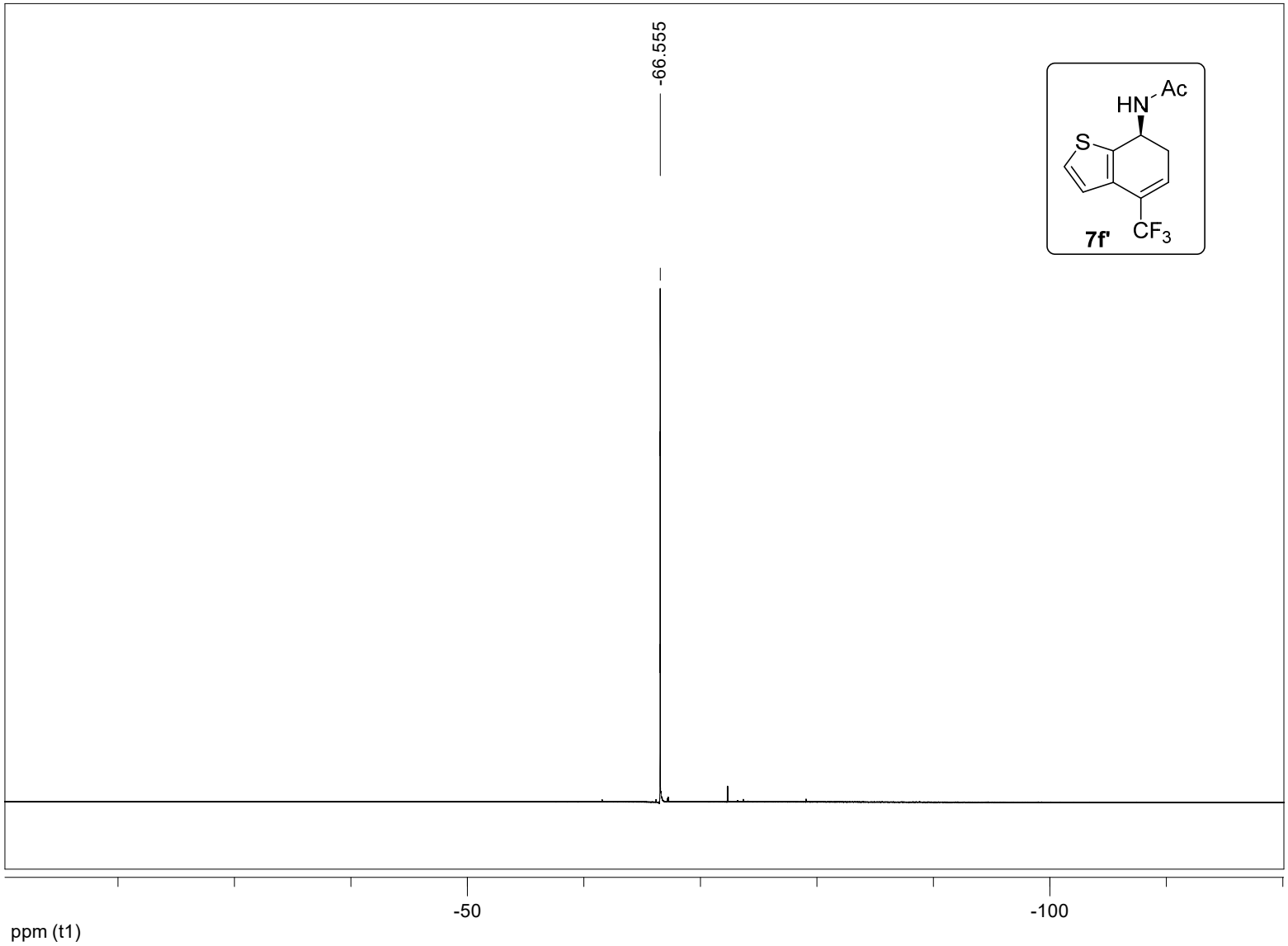

7.508
7.502
7.483
7.476
7.394
7.365
7.350
7.345
7.343
7.322
6.678
6.666
6.661
6.656
6.644
5.728
5.704
5.250
5.231
5.223
5.213
5.204
5.186
2.788
2.781
2.771
2.728
2.710
2.704
2.686
2.665
2.655
2.595
2.584
1.961
HN
Ac
CF3
7a'
1.00
3.06
0.95
1.10
1.00
2.07
3.02
5.0
0.0
ppm (t1)

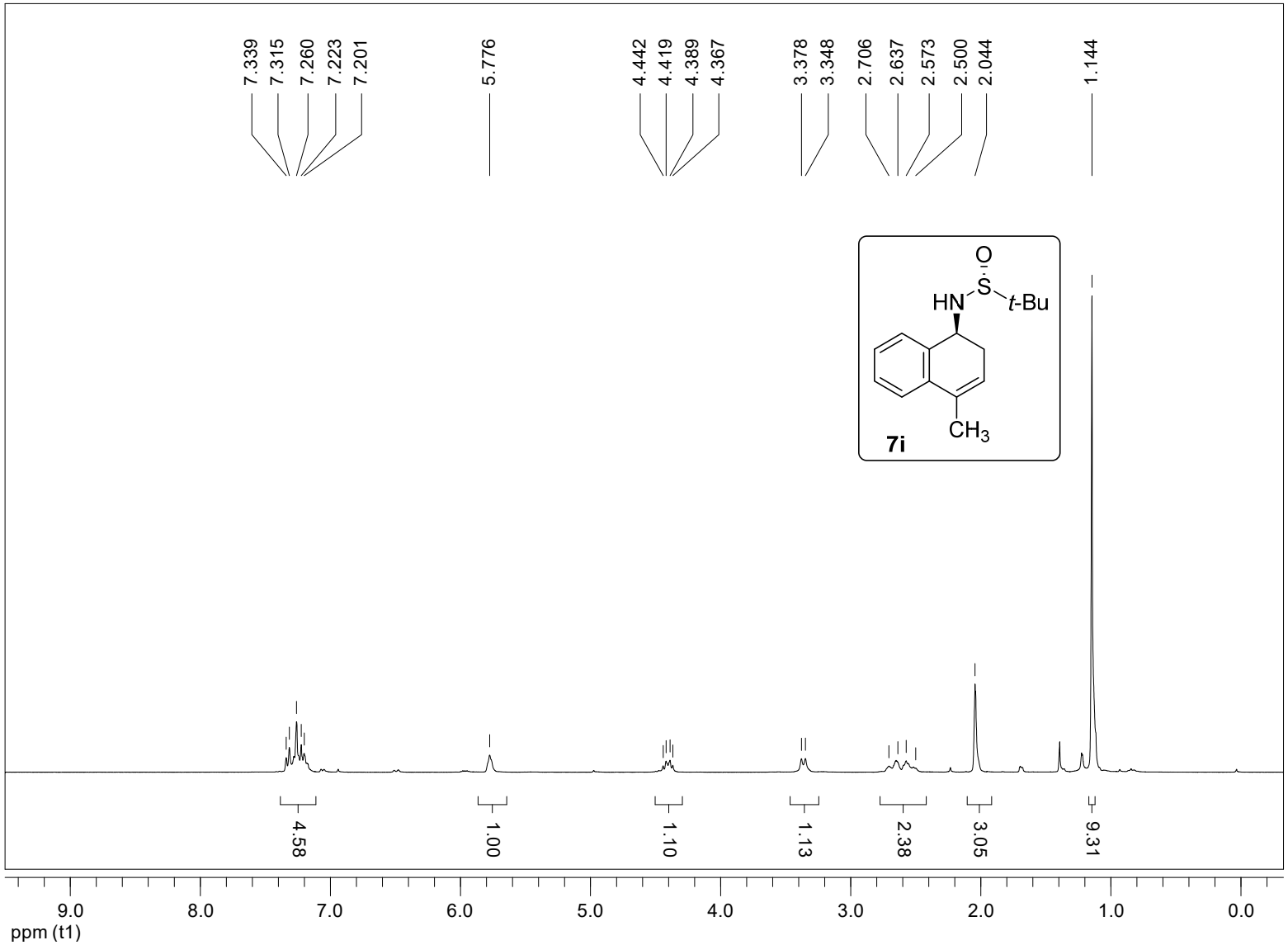

169.221
134.576
129.791
129.708
129.625
129.542
129.141
128.656
128.149
127.428
125.072
124.766
124.736
124.704
124.674
121.453
45.798
29.243
23.398
HN
Ac
CF3
7a'
150
100
50
0
ppm (t1)

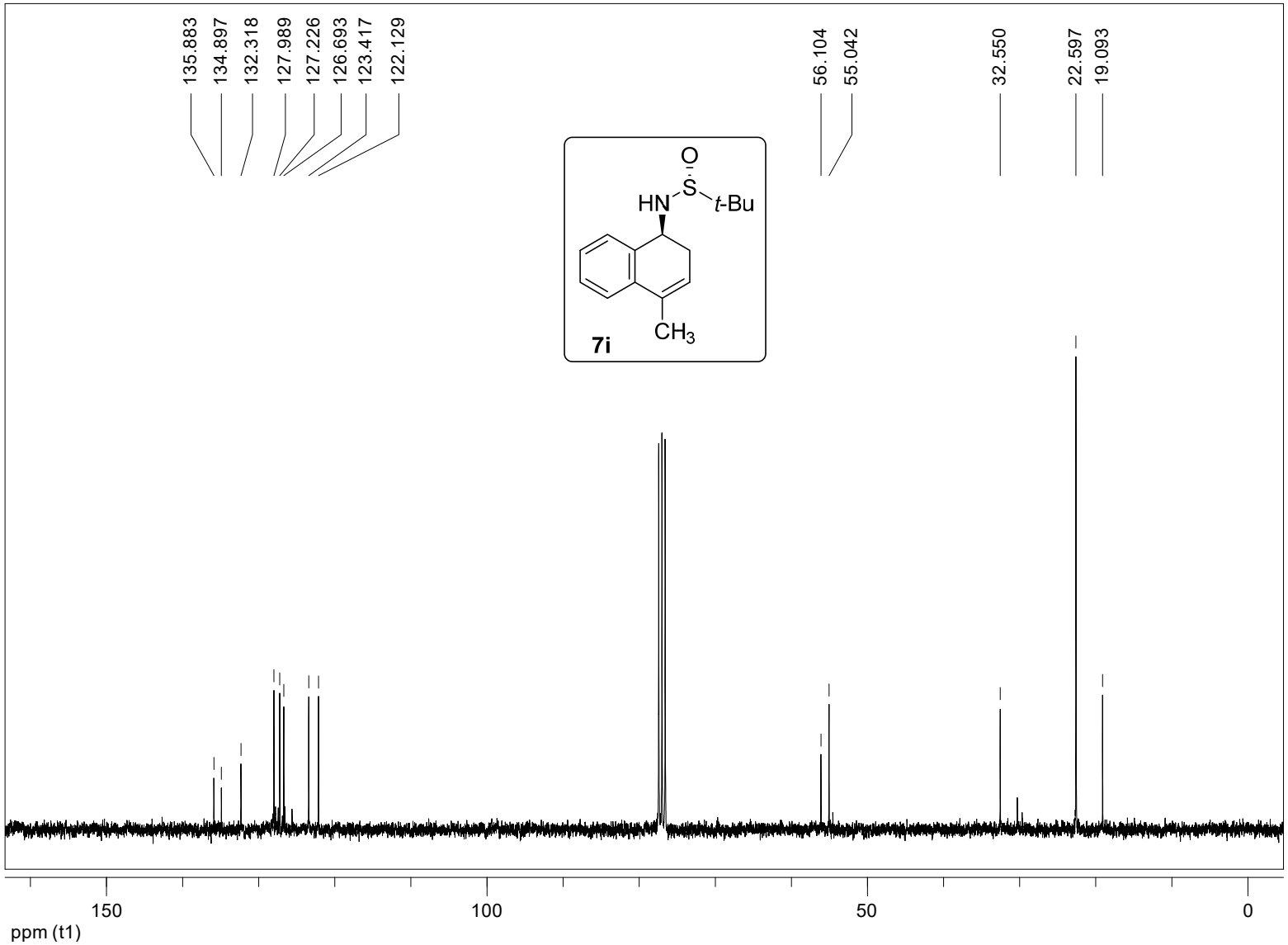

-64.267
HN
Ac
CF3
7a'
-50
-100
ppm (t1)

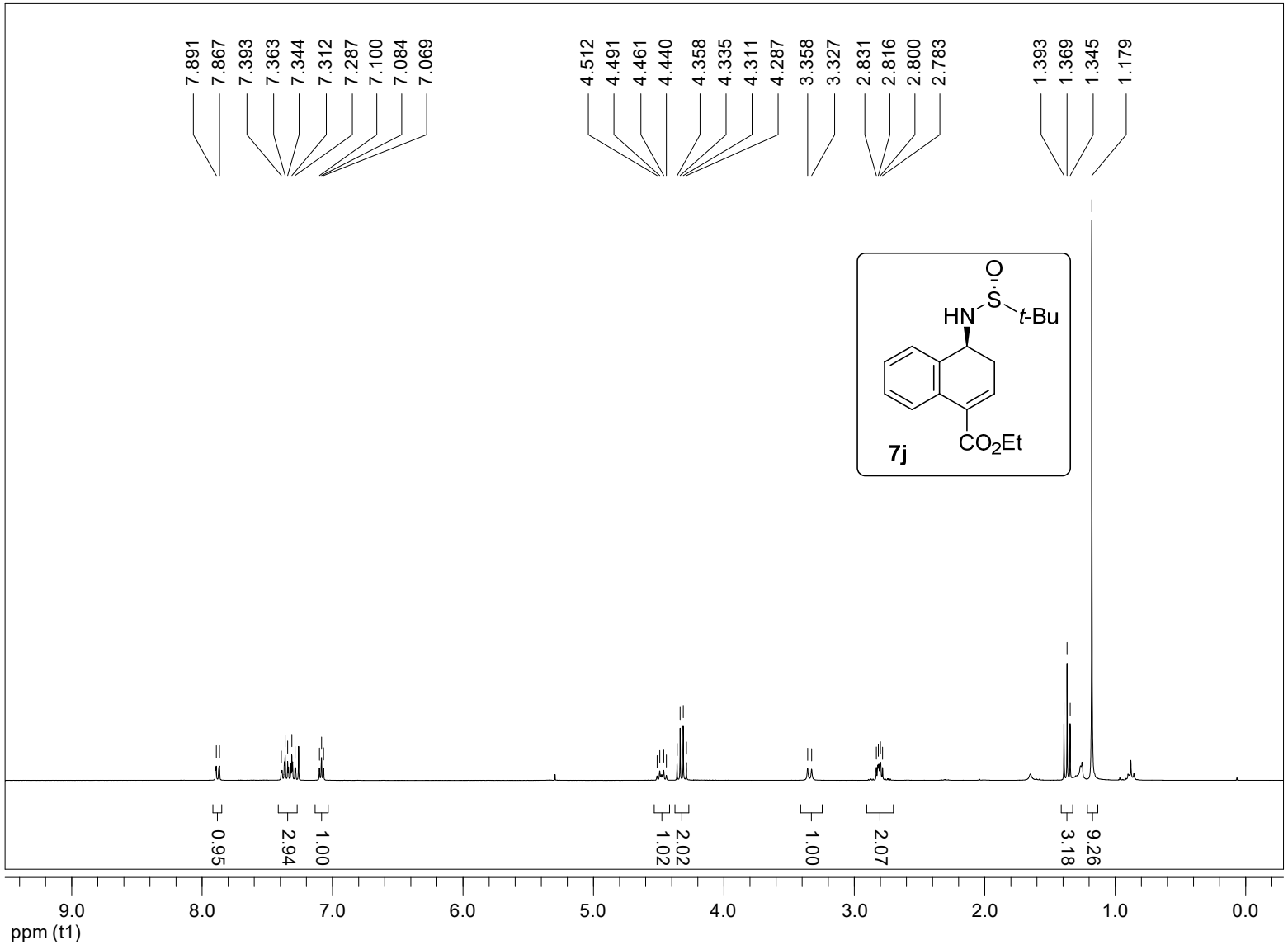

7.268
7.251
7.095
7.089
7.078
7.072
6.425
6.419
6.408
6.402
6.396
6.390
5.974
5.951
5.397
5.378
5.351
5.328
2.778
2.768
2.759
2.752
2.743
1.937
HN
Ac
S
CF3
7f'
1.07
1.00
1.00
0.96
0.99
2.18
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

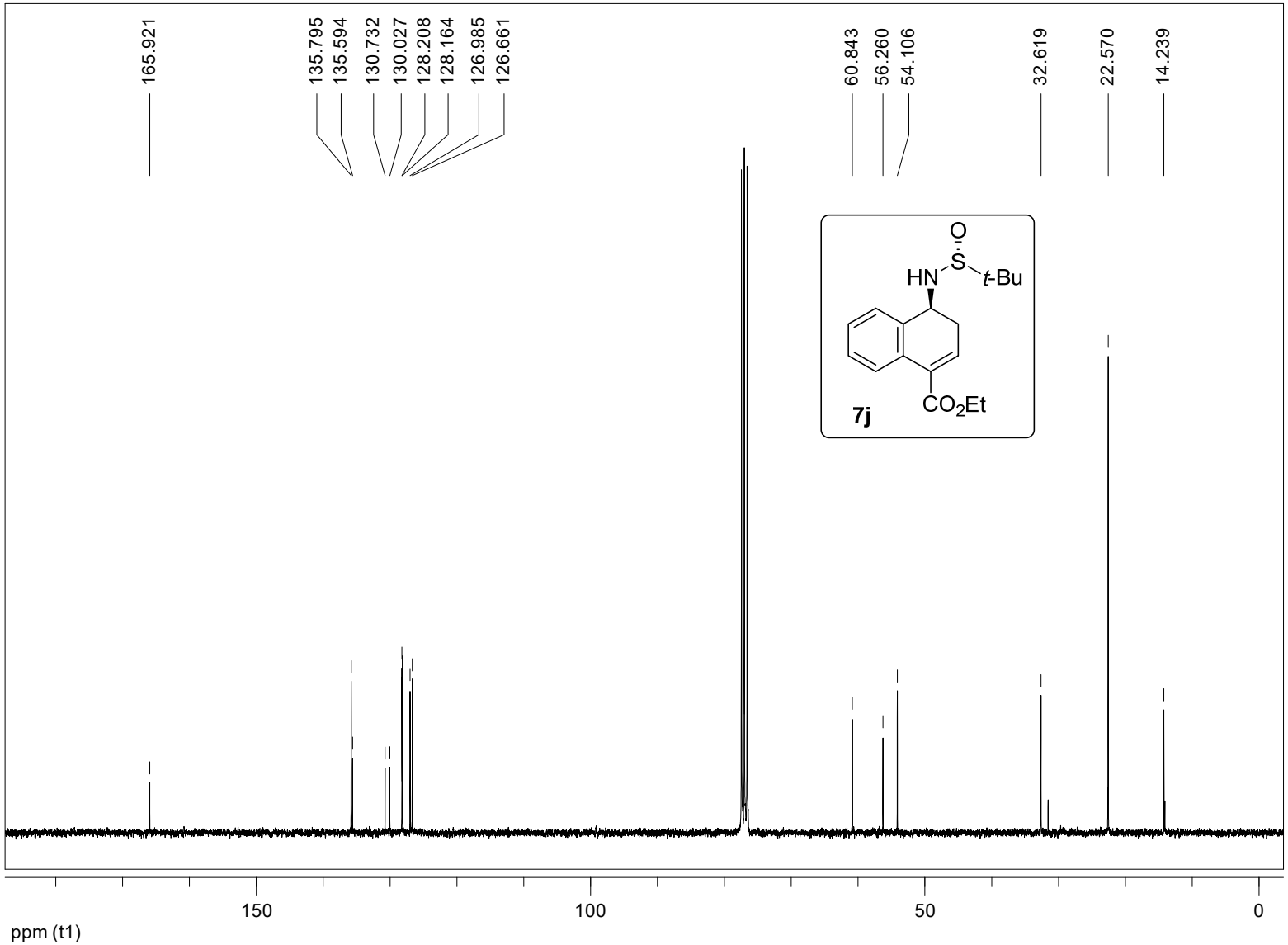

169.071
136.647
129.630
128.330
126.689
126.268
125.844
125.420
125.267
125.163
125.106
125.025
124.729
123.945
121.127
117.526
42.077
30.752
23.154
HN
Ac
S
CF3
7f'
150
100
50
0
ppm (t1)

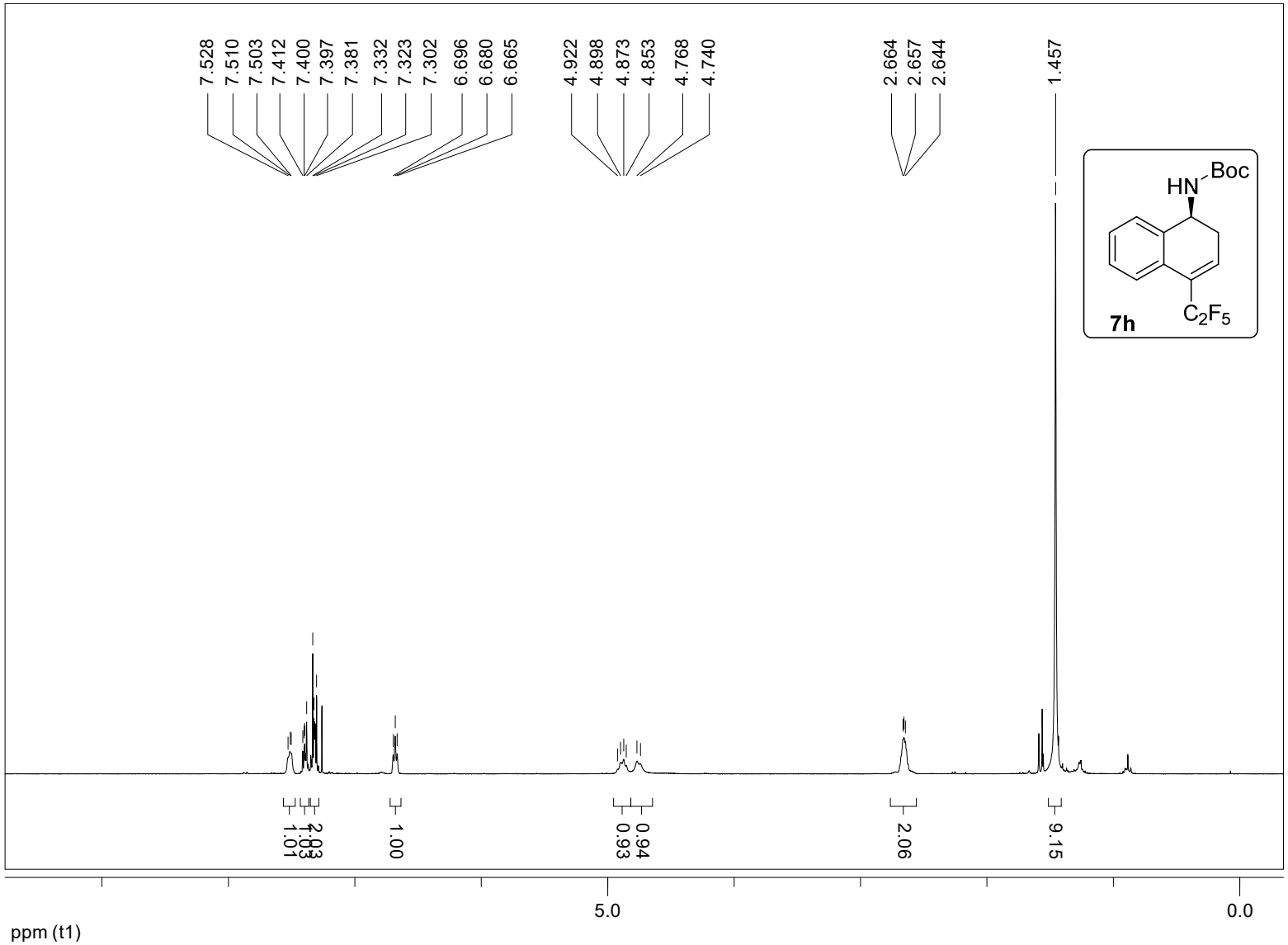

-66.555
HN
Ac
S
CF3
7f'
-50
-100
ppm (t1)

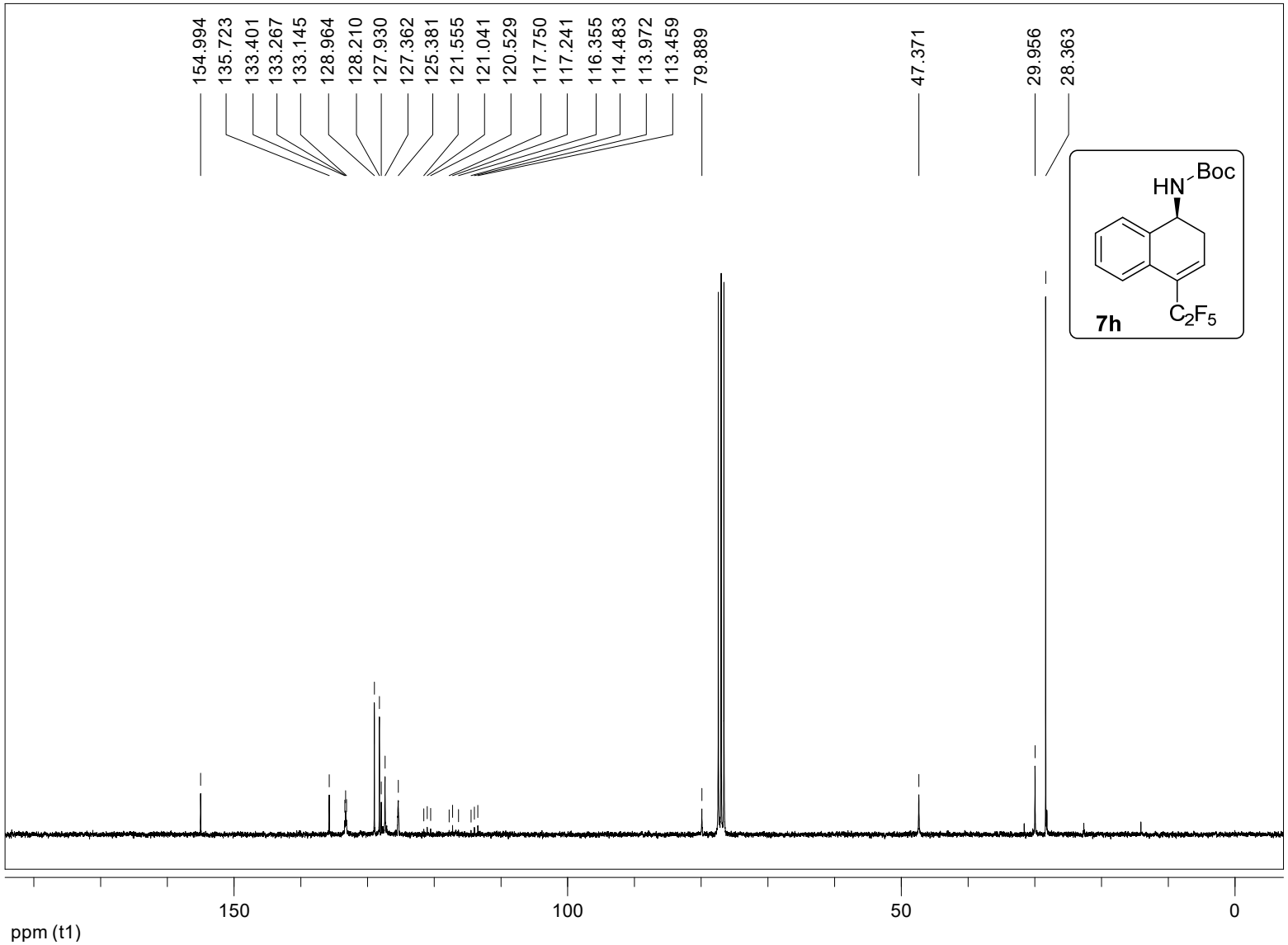

7.339
7.315
7.260
7.223
7.201
5.776
4.442
4.419
4.389
4.367
3.378
3.348
2.706
2.637
2.573
2.500
2.044
1.144
O
S
HN
t-Bu
CH3
7i
4.58
1.00
1.10
1.13
2.38
3.05
9.31
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

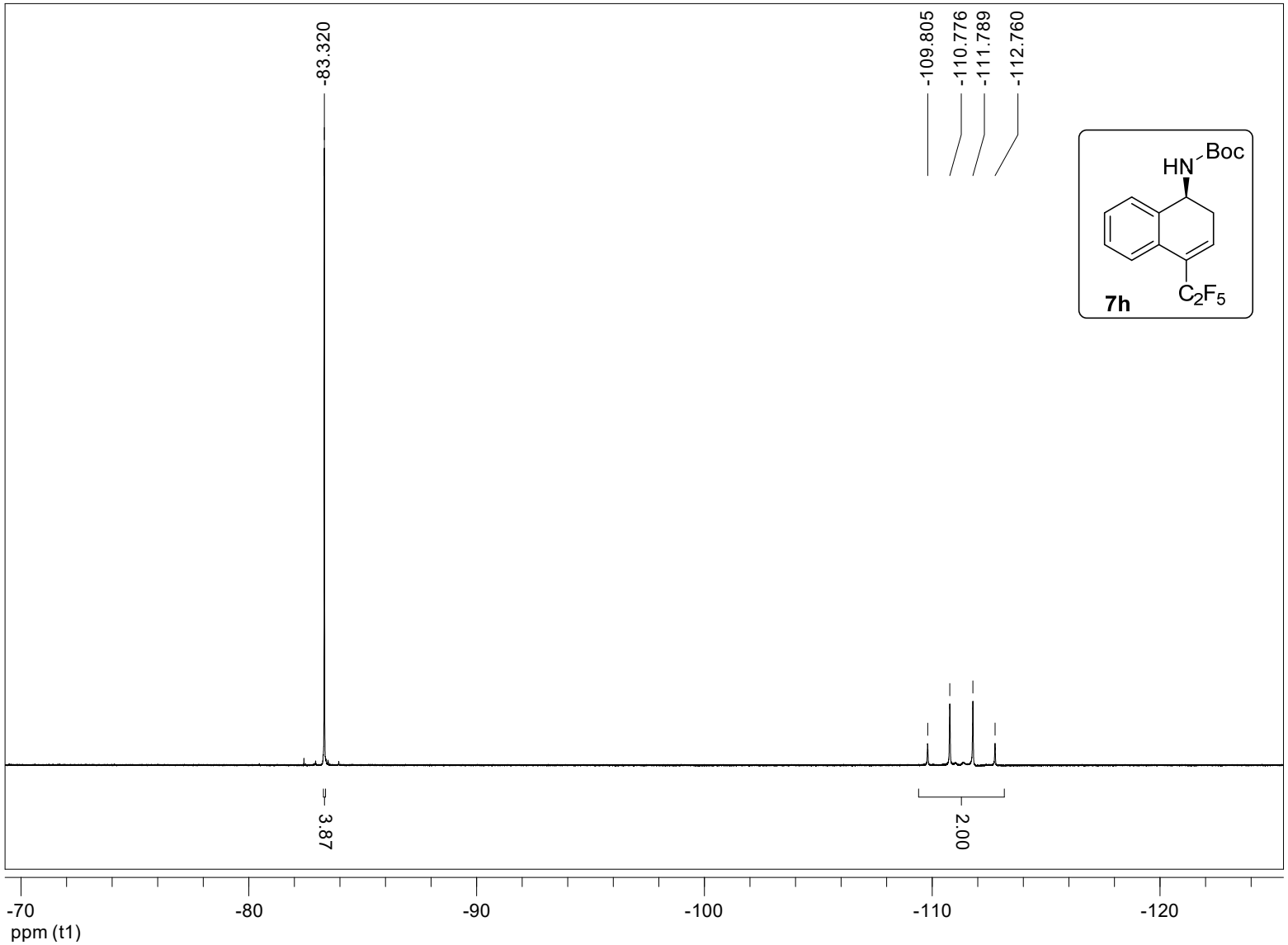

135.883
134.897
132.318
127.989
127.226
126.693
123.417
122.129
56.104
55.042
32.550
22.597
19.093
O
S
HN
t-Bu
CH3
7i
150
100
50
0
ppm (t1)

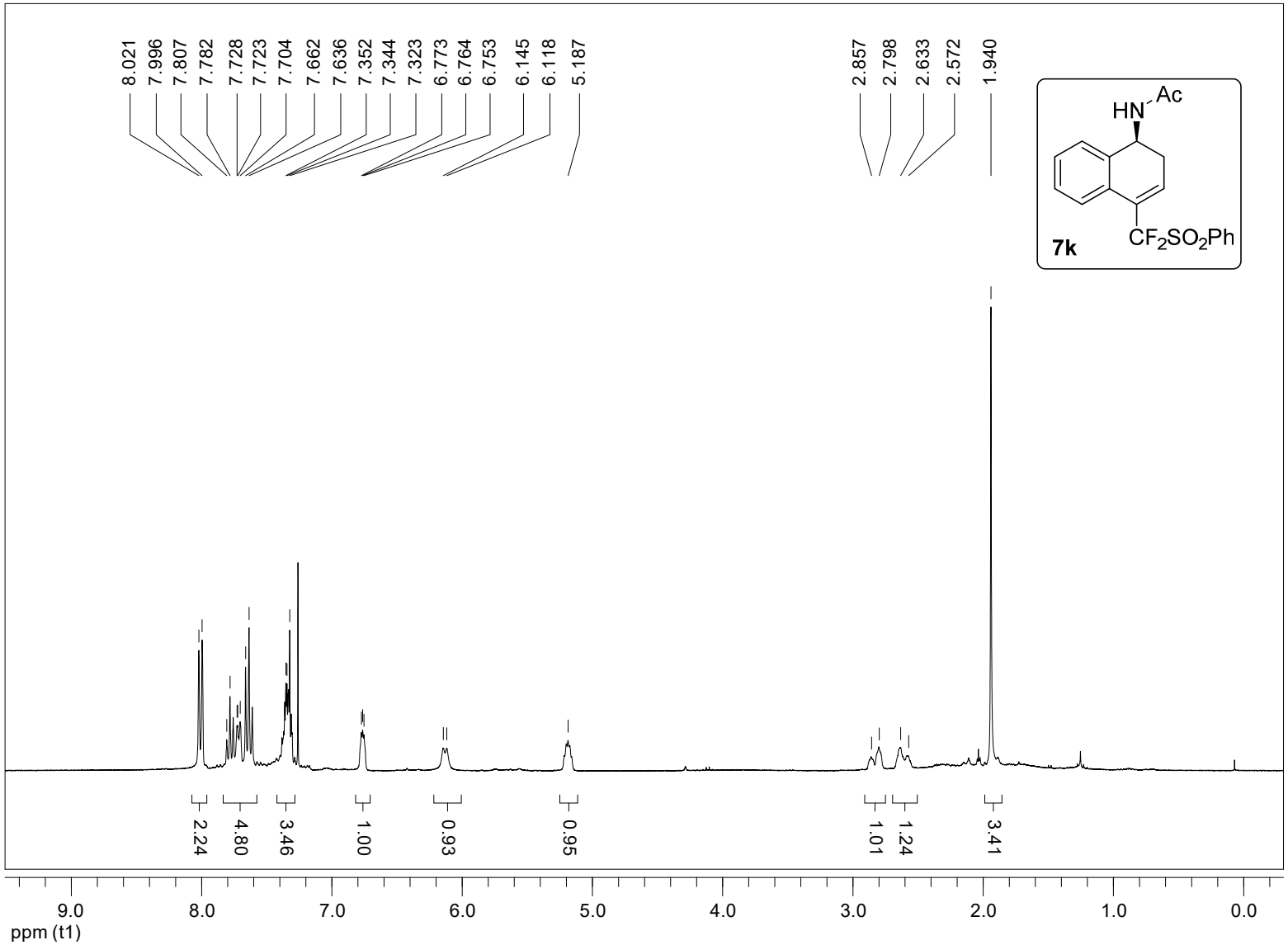

7.891
7.867
7.393
7.363
7.344
7.312
7.287
7.100
7.084
7.069
4.512
4.491
4.461
4.440
4.358
4.335
4.311
4.287
3.358
3.327
2.831
2.816
2.800
2.783
1.393
1.369
1.345
1.179
O
S
HN
t-Bu
CO2Et
7j
0.95
2.94
1.00
1.02
2.02
1.00
2.07
3.18
9.26
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

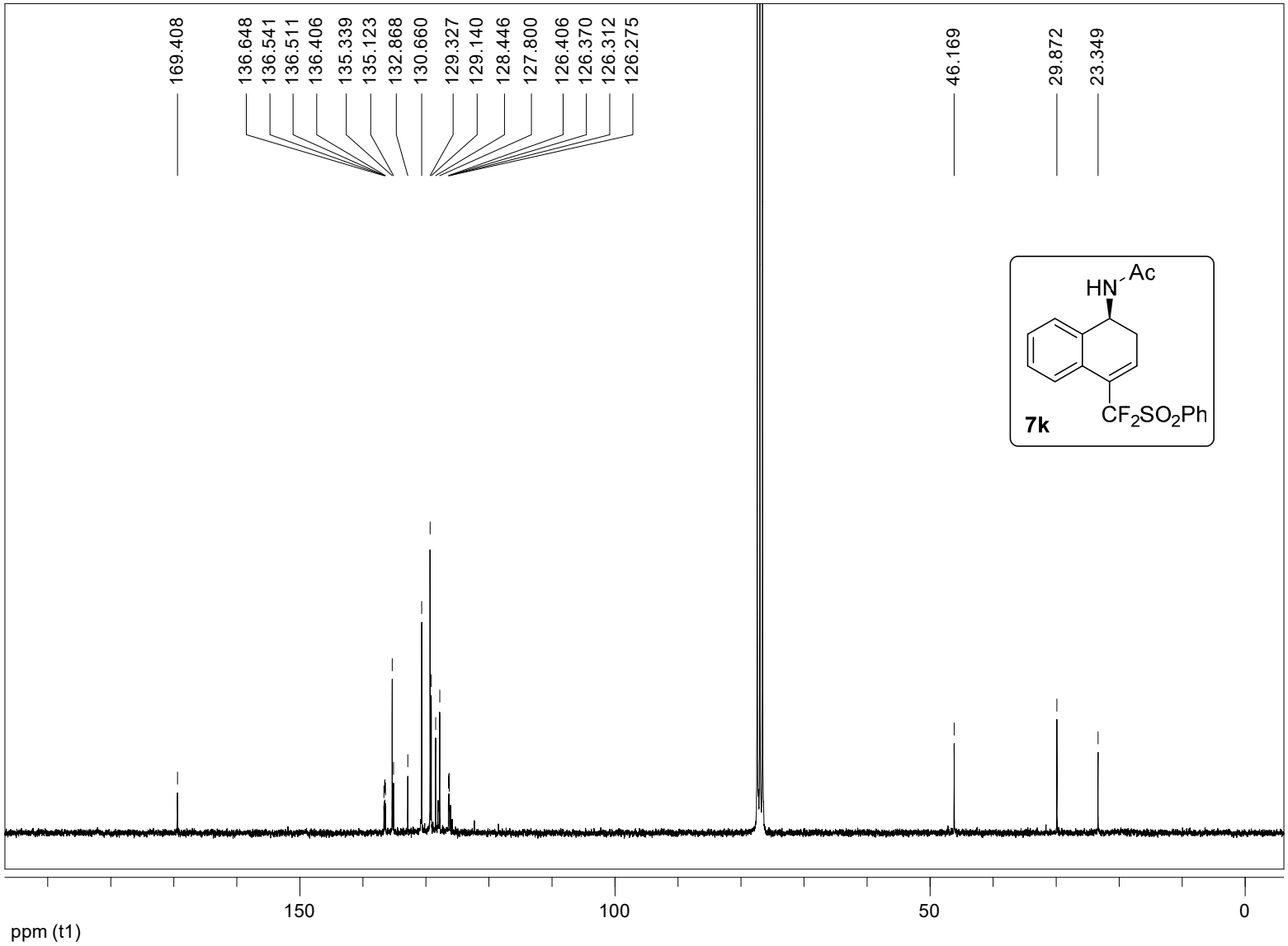

165.921
135.795
135.594
130.732
130.027
128.208
128.164
126.985
126.661
60.843
56.260
54.106
32.619
22.570
14.239
O
S
HN
t-Bu
CO2Et
7j
150
100
50
0
ppm (t1)

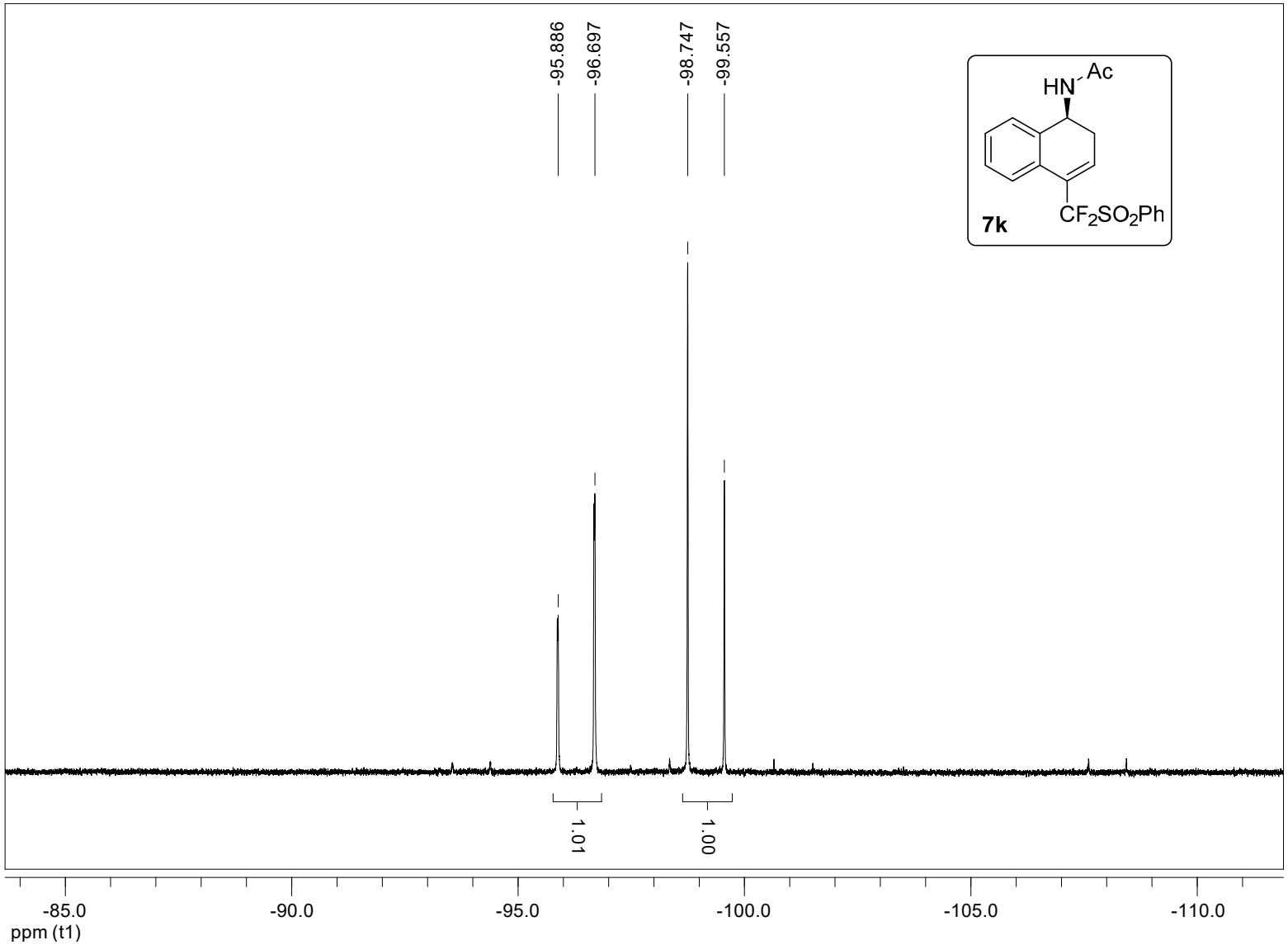

7.528
7.510
7.503
7.412
7.400
7.397
7.381
7.332
7.323
7.302
6.696
6.680
6.665
4.922
4.898
4.873
4.853
4.768
4.740
2.664
2.657
2.644
1.457
HN
Boc
C2F5
7h
1.01
2.03
1.03
1.00
0.93
0.94
2.06
9.15
5.0
0.0
ppm (t1)

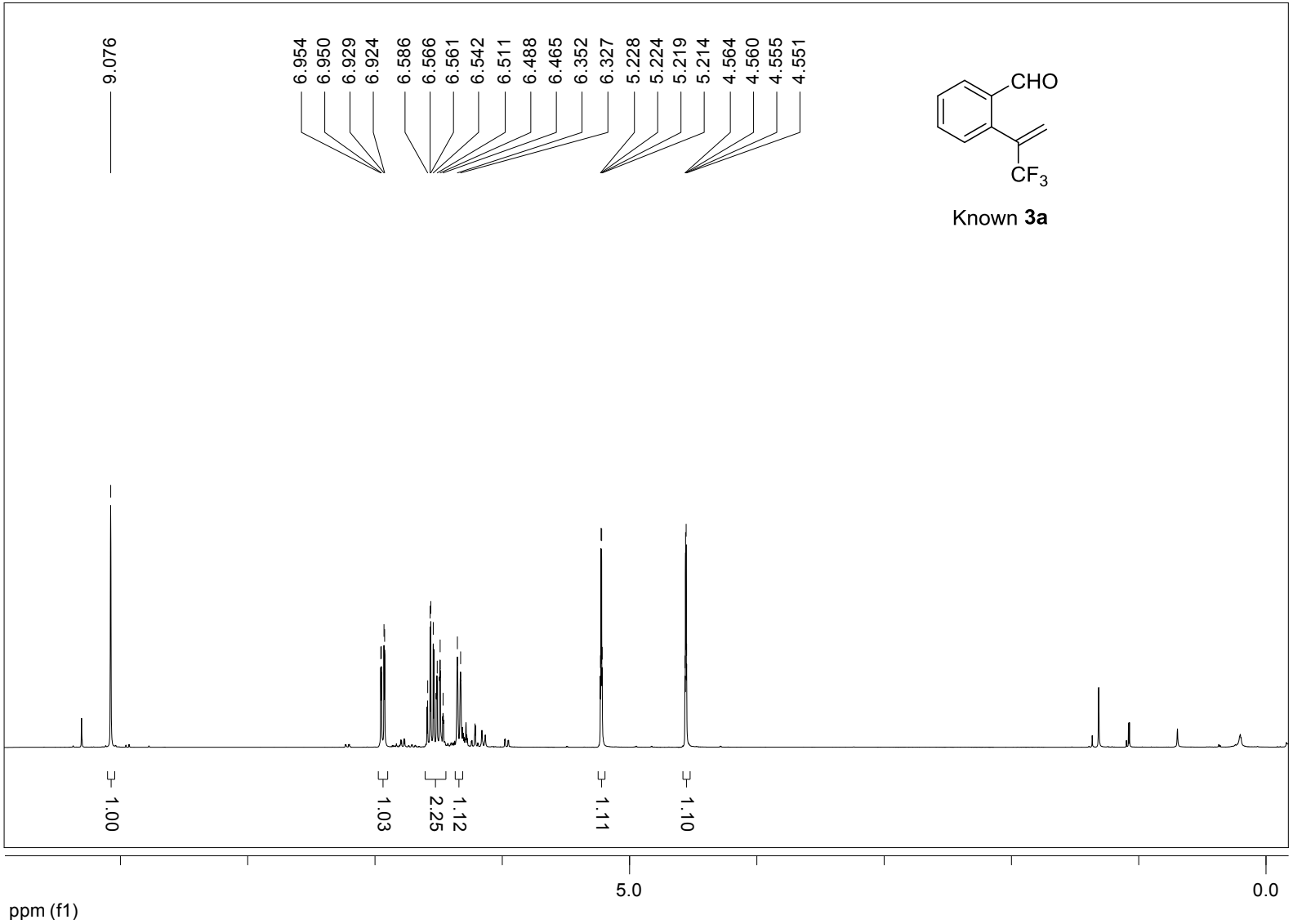

154.994
135.723
133.401
133.267
133.145
128.964
128.210
127.930
127.362
125.381
121.555
121.041
120.529
117.750
117.241
116.355
114.483
113.972
113.459
79.889
47.371
29.956
28.363
HN
Boc
C2F5
7h
150
100
50
0
ppm (t1)

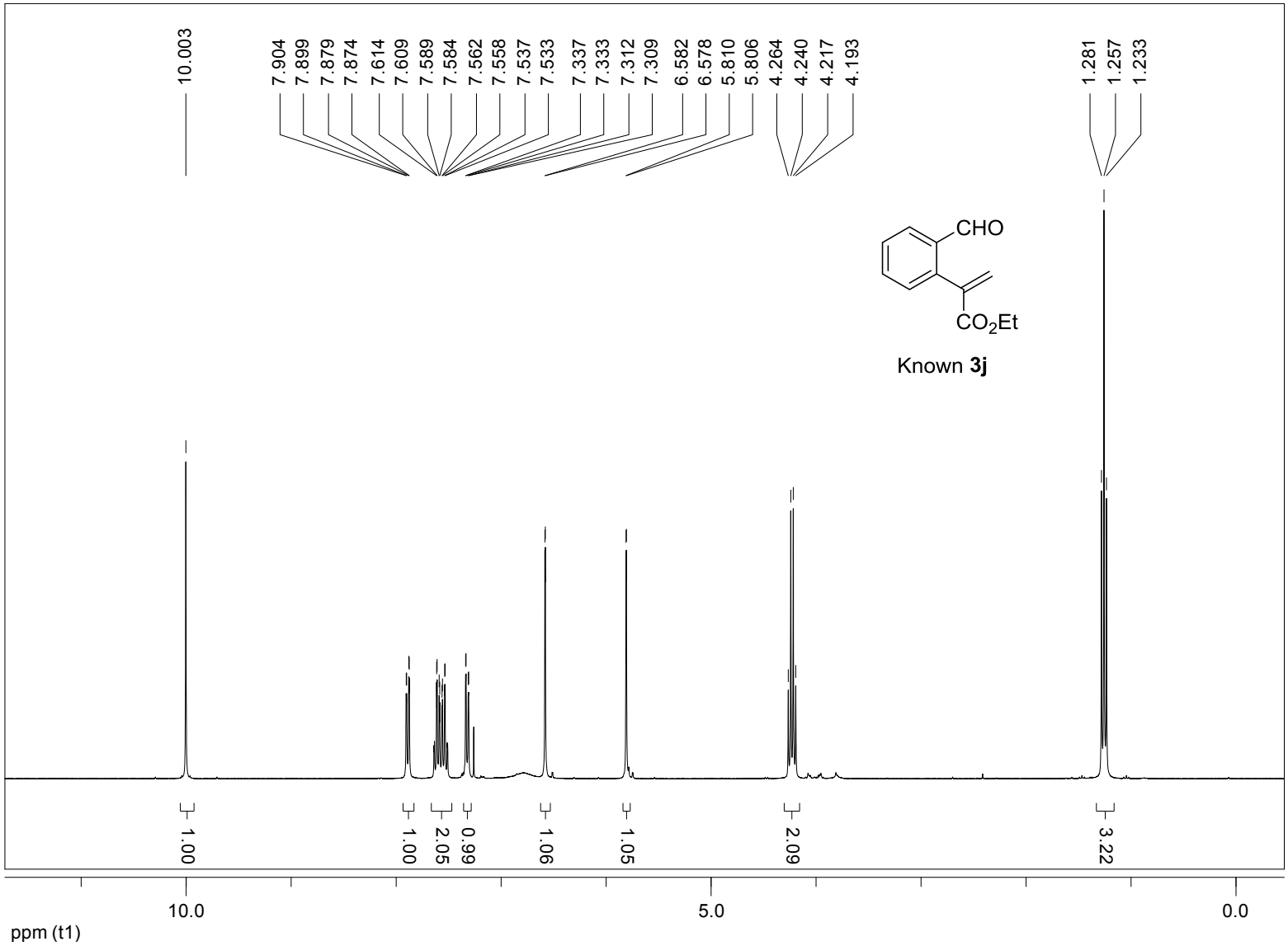

-83.320
-109.805
-110.776
-111.789
-112.760
HN
Boc
C2F5
7h
3.87
2.00
-70
-80
-90
-100
-110
-120
ppm (t1)

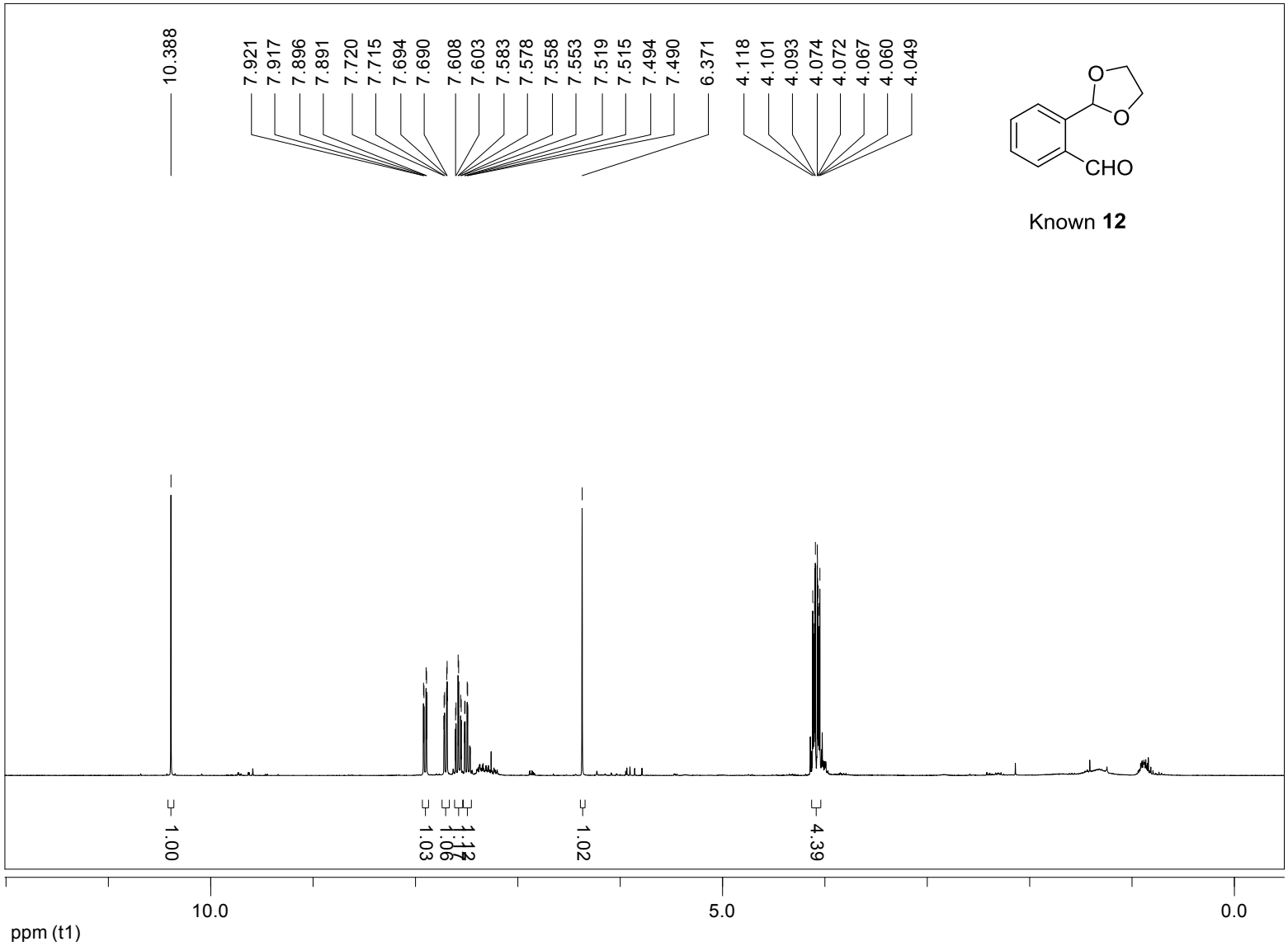

8.021
7.996
7.807
7.782
7.728
7.723
7.704
7.662
7.636
7.352
7.344
7.323
6.773
6.764
6.753
6.145
6.118
5.187
2.857
2.798
2.633
2.572
1.940
HN
Ac
CF2SO2Ph
7k
2.24
4.80
3.46
1.00
0.93
0.95
1.01
1.24
3.41
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

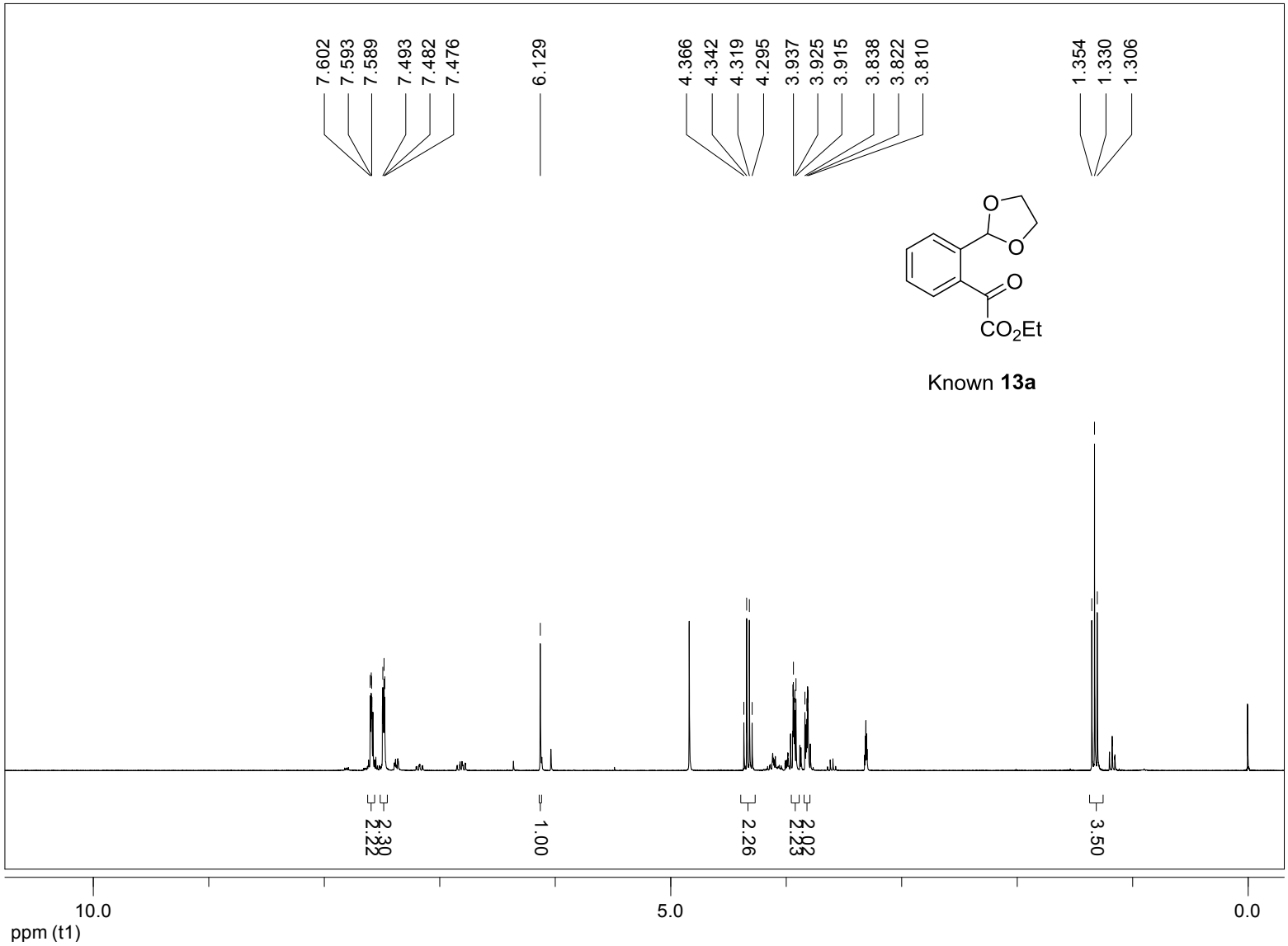

169.408
136.648
136.541
136.511
136.406
135.339
135.123
132.868
130.660
129.327
129.140
128.446
127.800
126.406
126.370
126.312
126.275
46.169
29.872
23.349
HN
Ac
CF2SO2Ph
7k
150
100
50
0
ppm (t1)

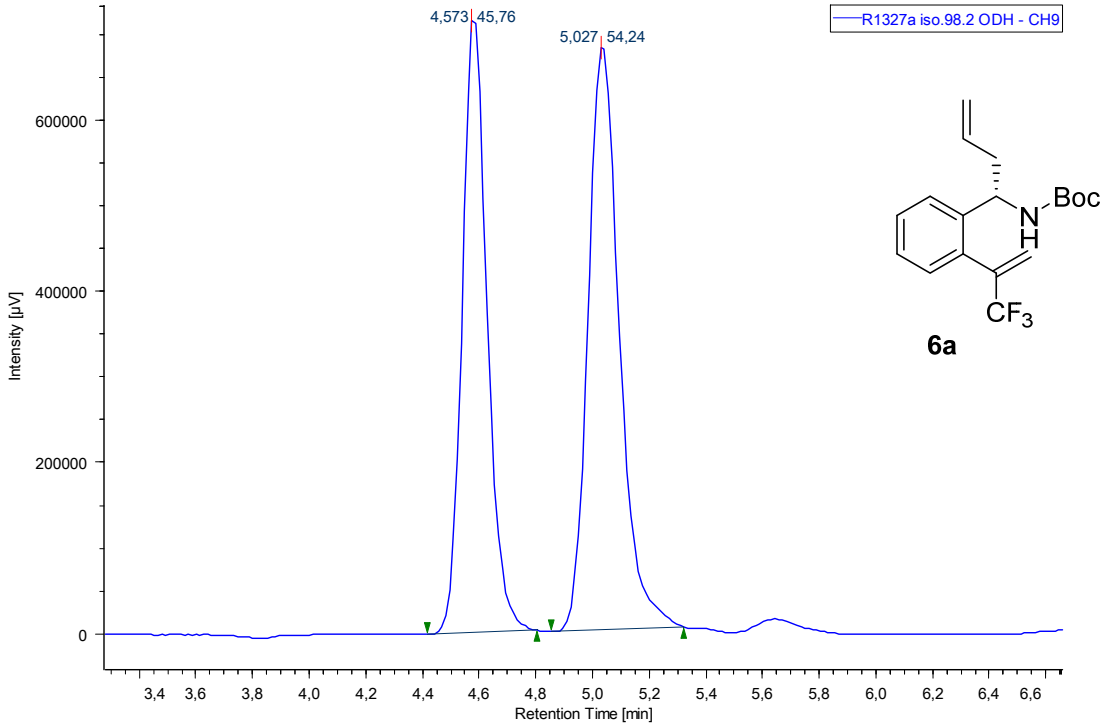

-95.886
-96.697
-98.747
-99.557
HN
Ac
CF2SO2Ph
7k
1.01
1.00
-85.0
-90.0
-95.0
-100.0
-105.0
-110.0
ppm (t1)

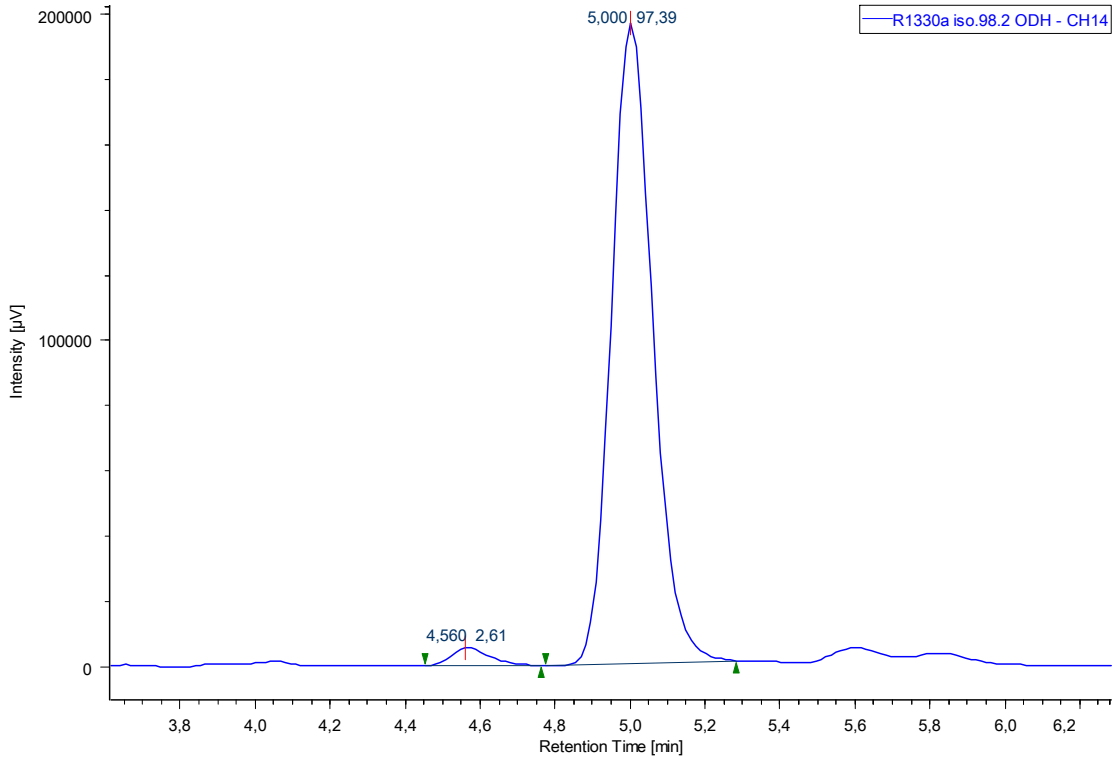

9.076
6.954
6.950
6.929
6.924
6.586
6.566
6.561
6.542
6.511
6.488
6.465
6.352
6.327
5.228
5.224
5.219
5.214
4.564
4.560
4.555
4.551
CHO
CF3
Known 3a
1.00
1.03
2.25
1.12
1.11
1.10
5.0
0.0
ppm (f1)

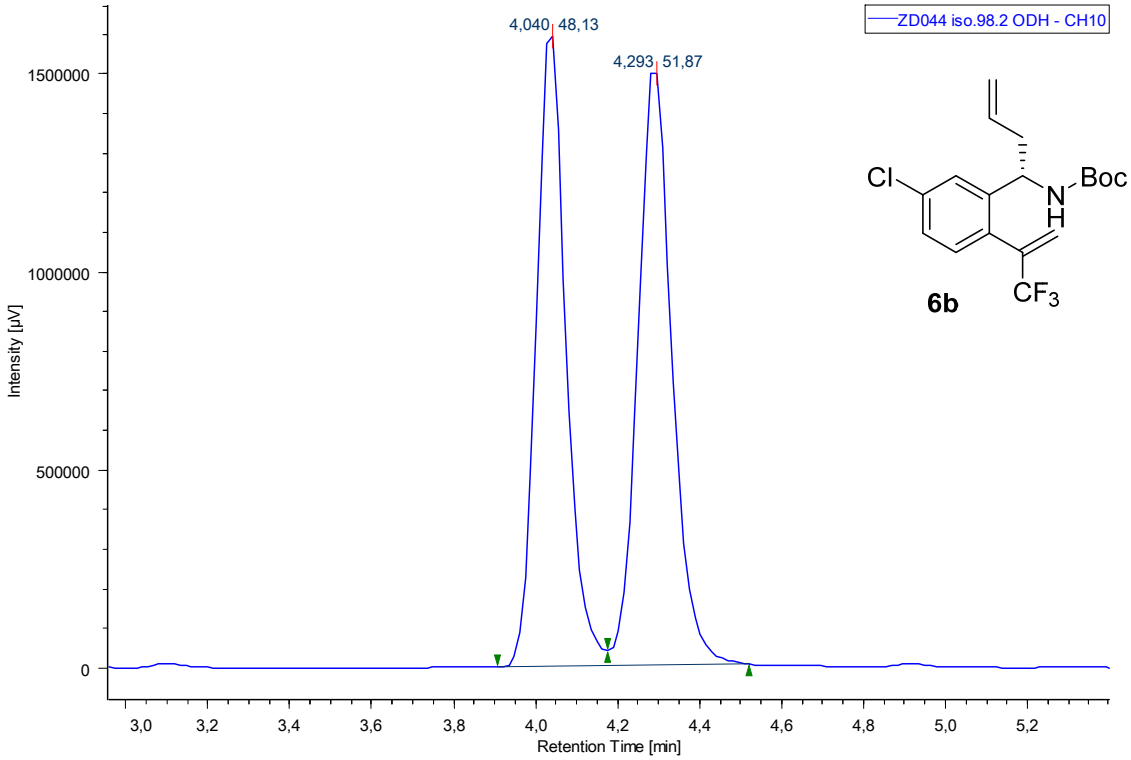

10.003
7.904
7.899
7.879
7.874
7.614
7.609
7.589
7.584
7.562
7.558
7.537
7.533
7.337
7.333
7.312
7.309
6.582
6.578
5.810
5.806
4.264
4.240
4.217
4.193
1.281
1.257
1.233
CHO
CO2Et
Known 3j
1.00
1.00
2.05
0.99
1.06
1.05
2.09
3.22
10.0
5.0
0.0
ppm (t1)

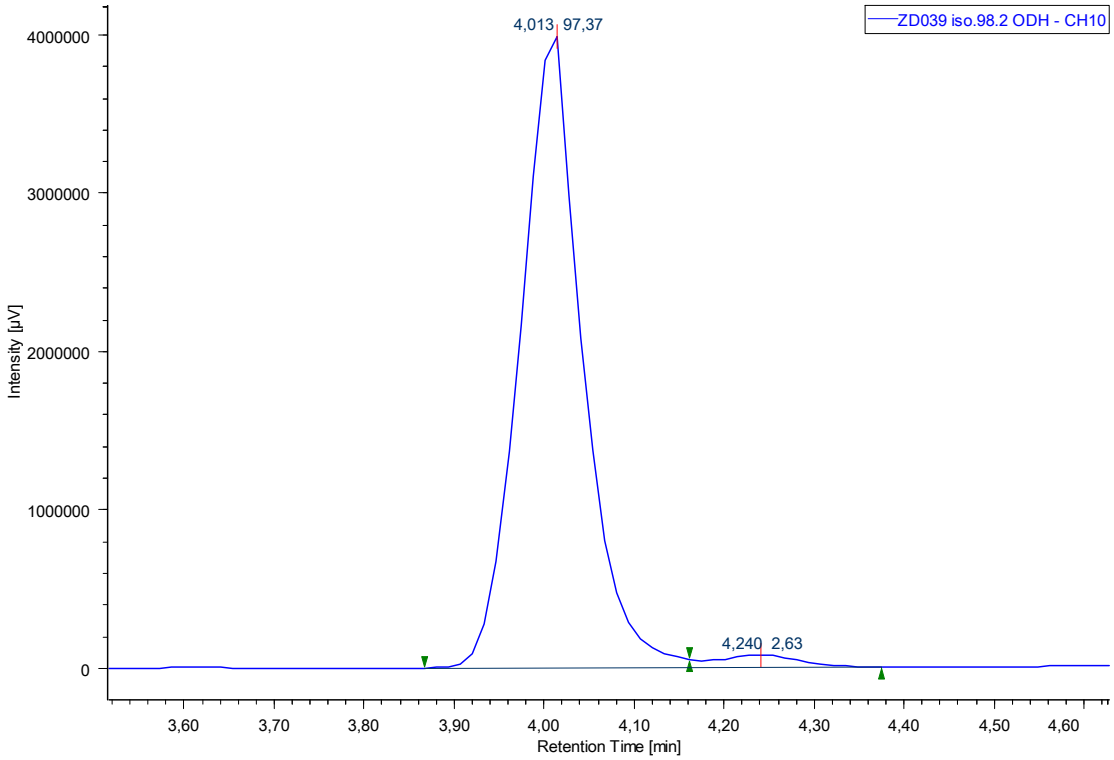

10.388
7.921
7.917
7.896
7.891
7.720
7.715
7.694
7.690
7.608
7.603
7.583
7.578
7.558
7.553
7.519
7.515
7.494
7.490
6.371
4.118
4.101
4.093
4.074
4.072
4.067
4.060
4.049
O
O
CHO
Known 12
1.00
1.03
1.06
1.12
1.02
4.39
10.0
5.0
0.0
ppm (t1)

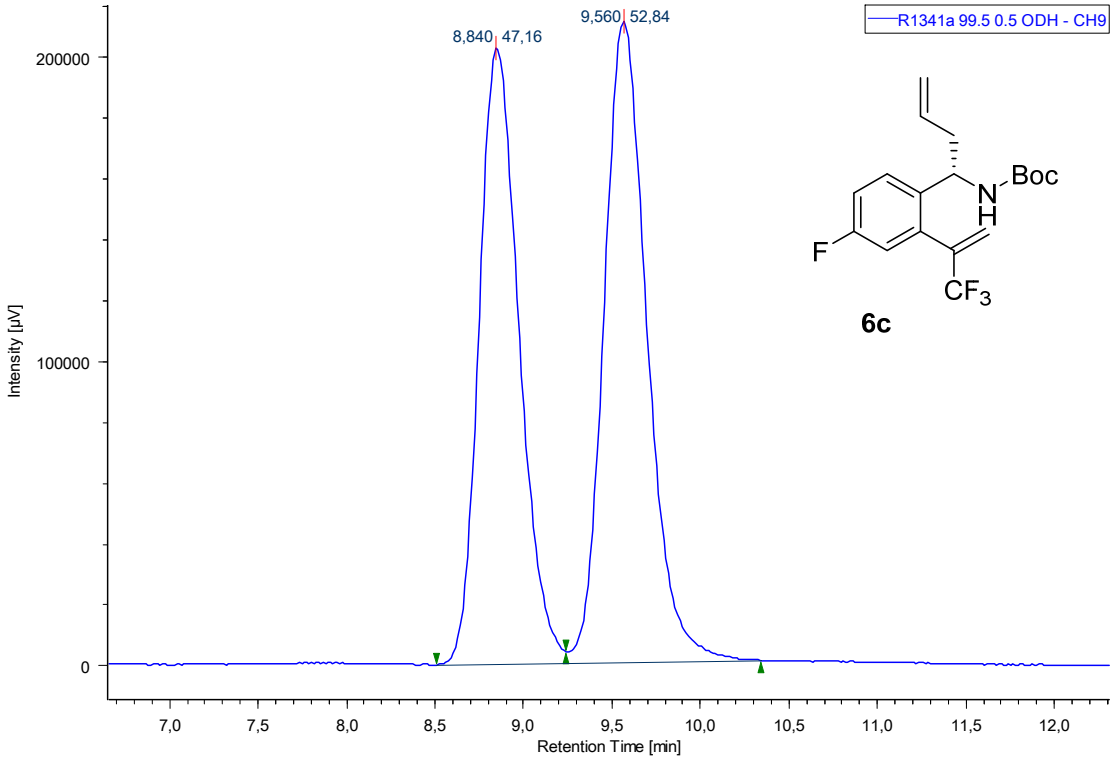

7.602
7.593
7.589
7.493
7.482
7.476
6.129
4.366
4.342
4.319
4.295
3.937
3.925
3.915
3.838
3.822
3.810
1.354
1.330
1.306
O
O
O
CO_2Et
Known **13a**
2.22
2.30
1.00
2.26
2.23
2.02
3.50
10.0
5.0
0.0
ppm (t1)

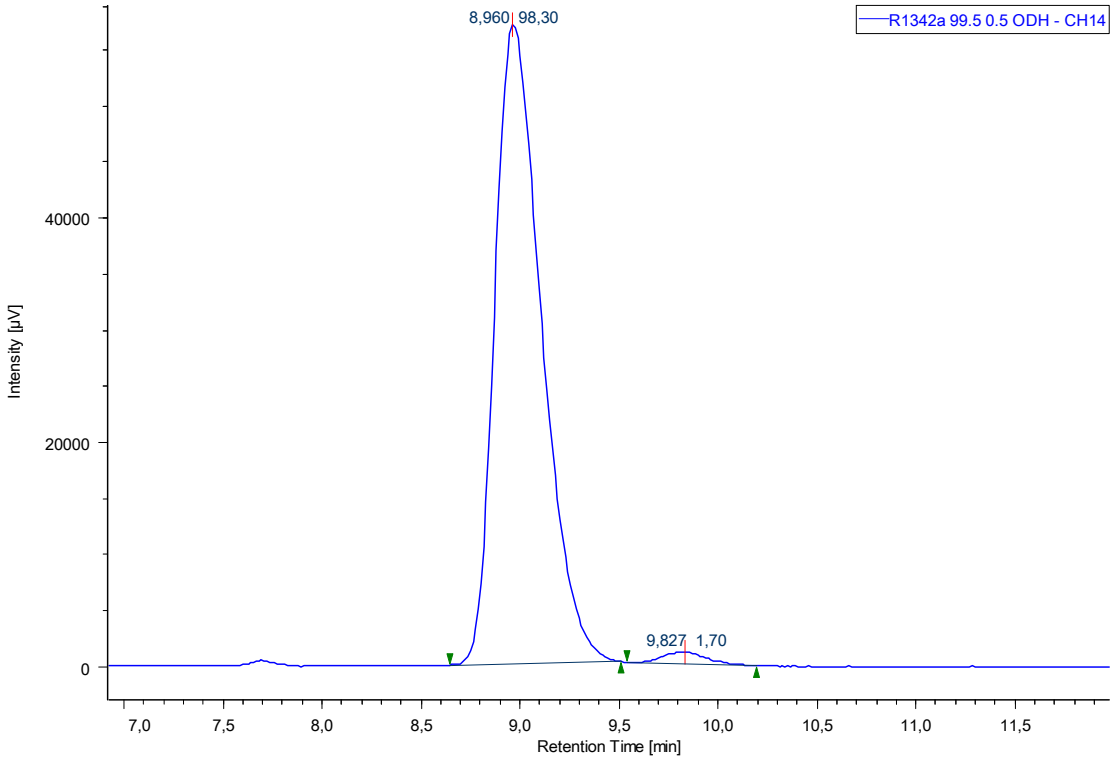

R1327a iso.98.2 ODH - CH9
4,573 45,76
5,027 54,24
Intensity [µV]
600000
400000
200000
0
3,4 3,6 3,8 4,0 4,2 4,4 4,6 4,8 5,0 5,2 5,4 5,6 5,8 6,0 6,2 6,4 6,6
Retention Time [min]
Boc
N
H
CF3
6a

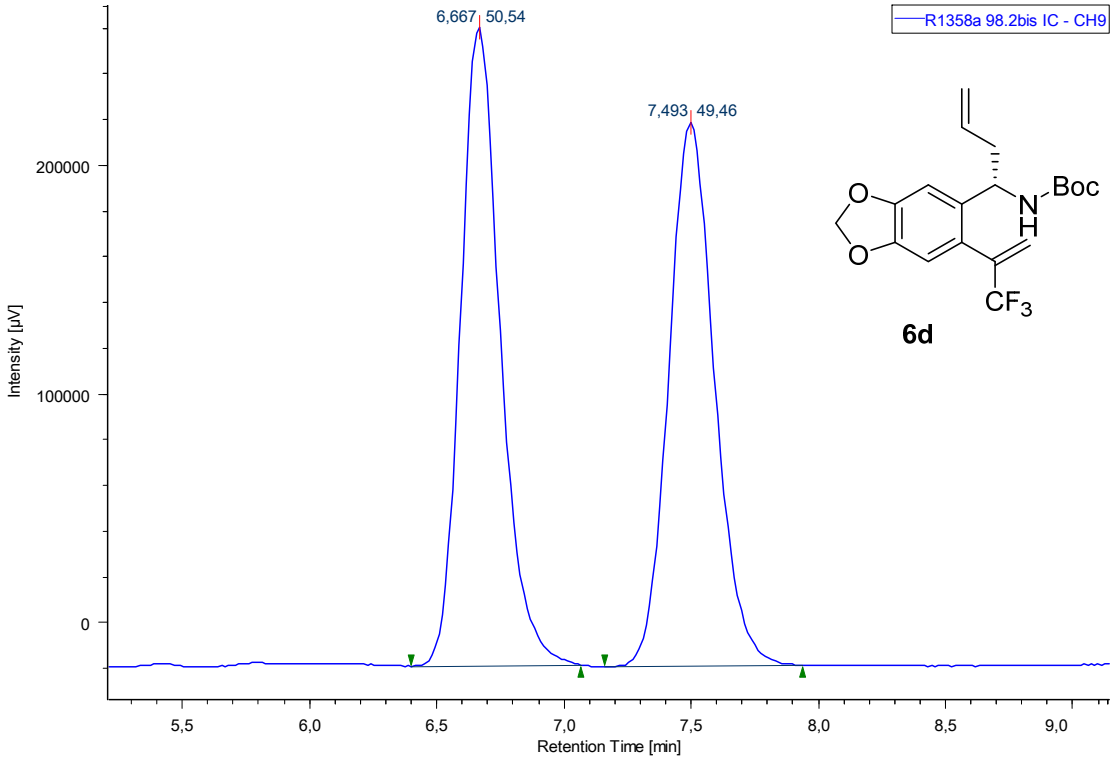

R1330a iso.98.2 ODH - CH14
5,000 97,39
4,560 2,61
Intensity [µV]
200000
100000
0
3,8 4,0 4,2 4,4 4,6 4,8 5,0 5,2 5,4 5,6 5,8 6,0 6,2
Retention Time [min]

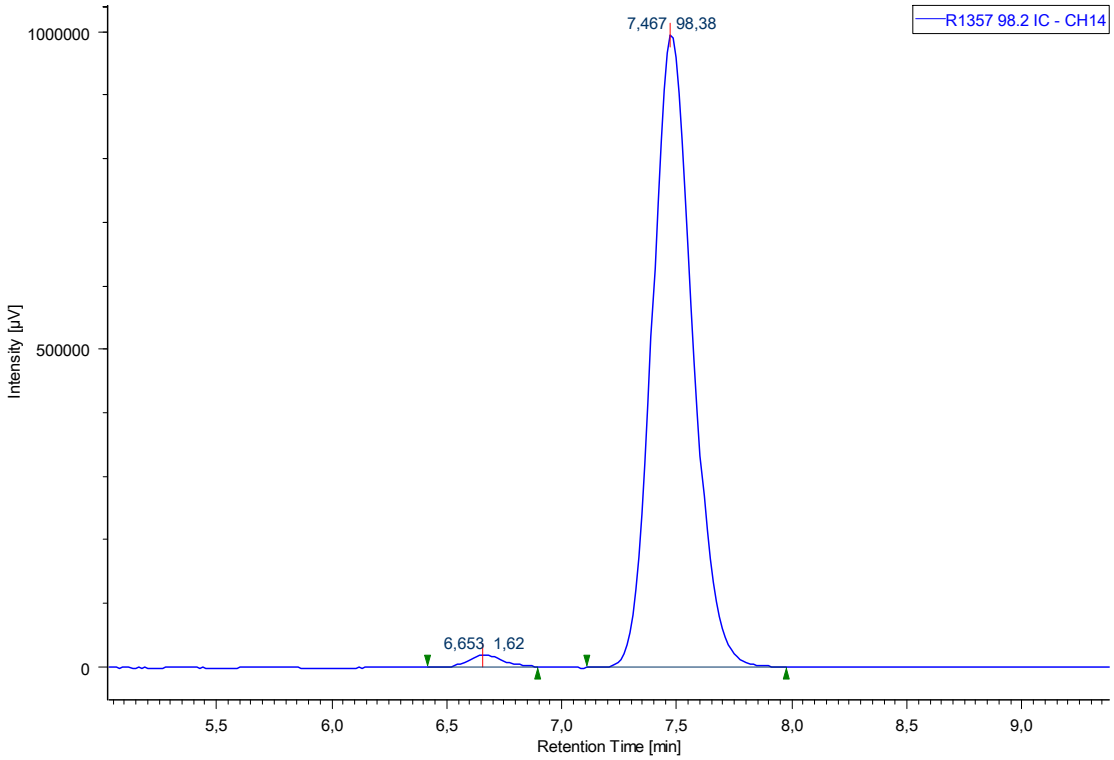

ZD044 iso.98.2 ODH - CH10
4,040 48,13
4,293 51,87
Cl
Boc
N
H
CF3
6b
Intensity [µV]
1500000
1000000
500000
0
3,0
3,2
3,4
3,6
3,8
4,0
4,2
4,4
4,6
4,8
5,0
5,2
Retention Time [min]

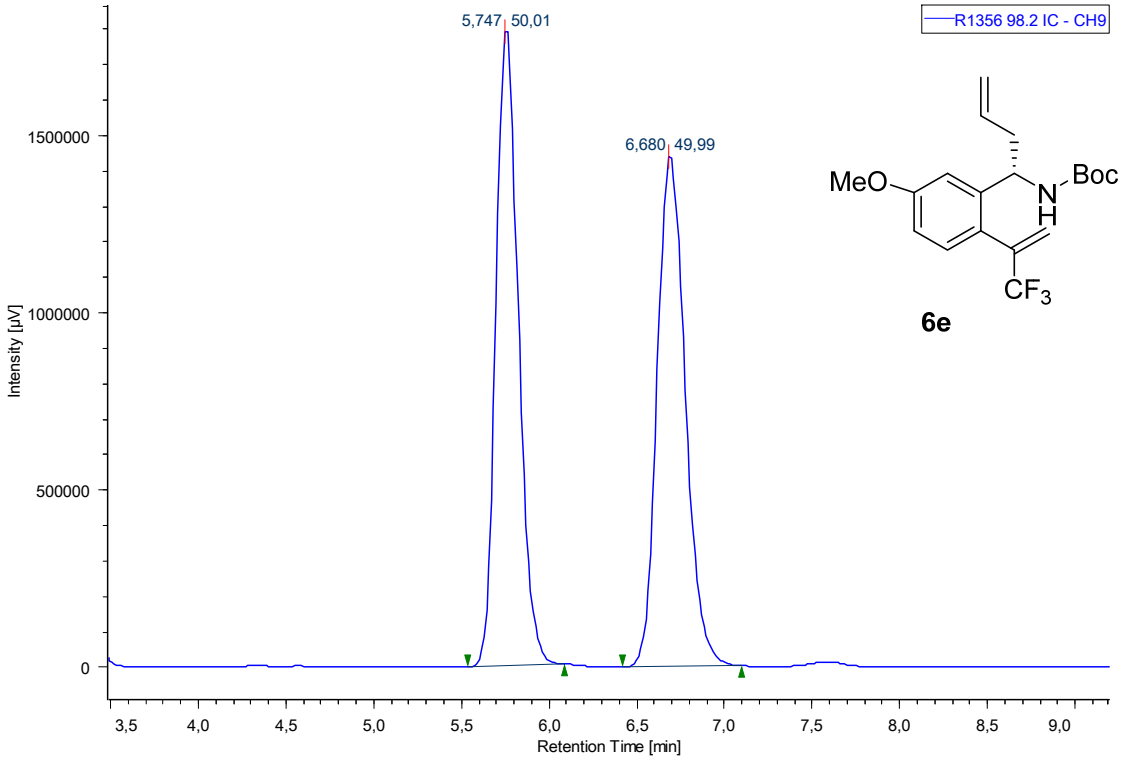

ZD039 iso.98.2 ODH - CH10
4,013 97,37
4,240 2,63
Intensity [µV]
4000000
3000000
2000000
1000000
0
3,60
3,70
3,80
3,90
4,00
4,10
4,20
4,30
4,40
4,50
4,60
Retention Time [min]

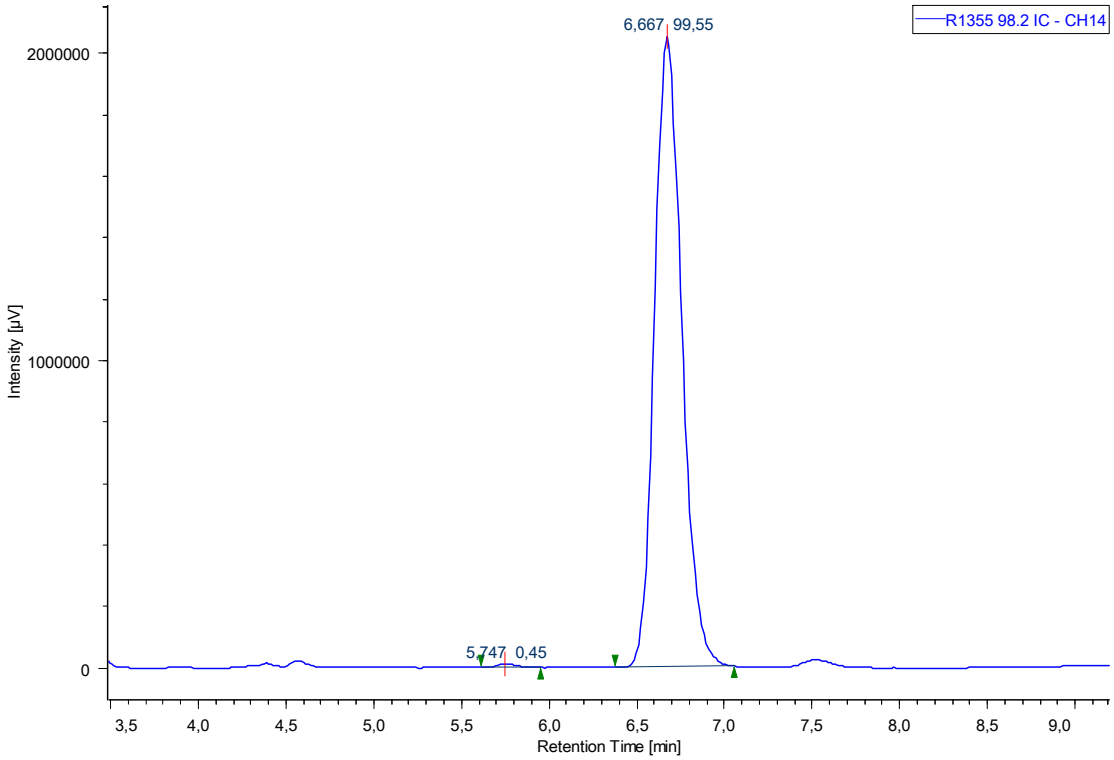

R1341a 99.5 0.5 ODH - CH9
8,840 47,16
9,560 52,84
Intensity [µV]
200000
100000
0
7,0
7,5
8,0
8,5
9,0
9,5
10,0
10,5
11,0
11,5
12,0
Retention Time [min]
Boc
N
H
F
CF3
6c

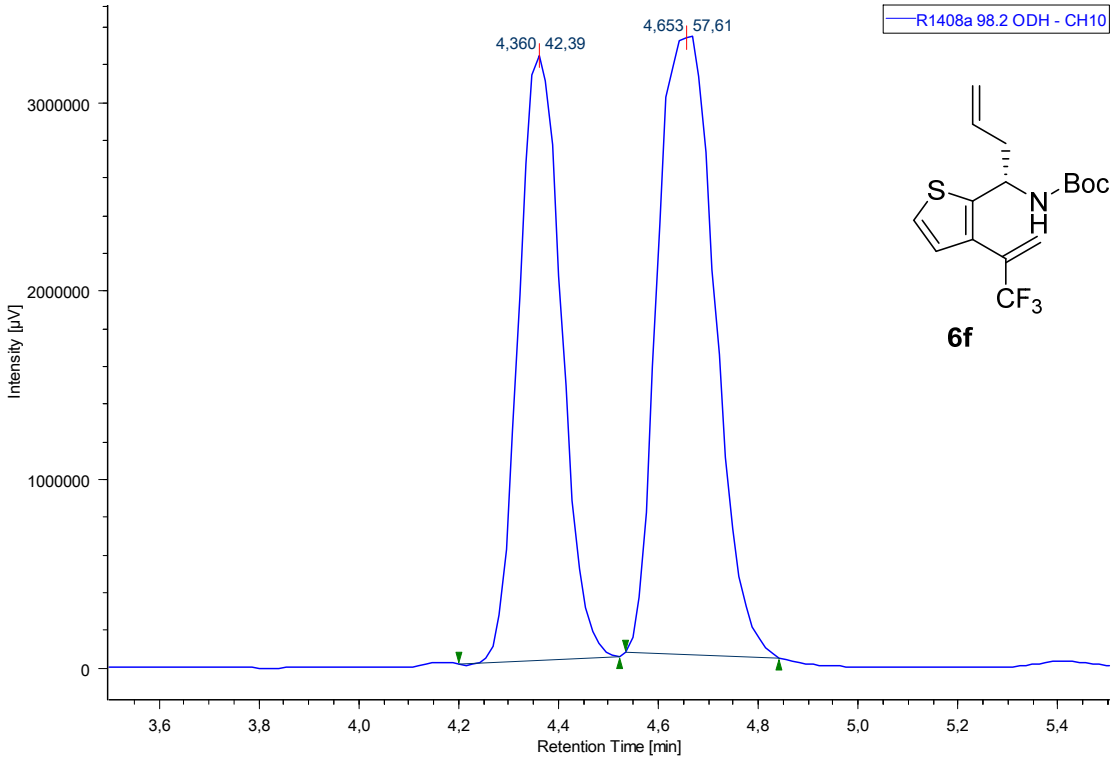

R1342a 99.5 0.5 ODH - CH14
8,960 98,30
9,827 1,70
Intensity [µV]
40000
20000
0
7,0
7,5
8,0
8,5
9,0
9,5
10,0
10,5
11,0
11,5
Retention Time [min]

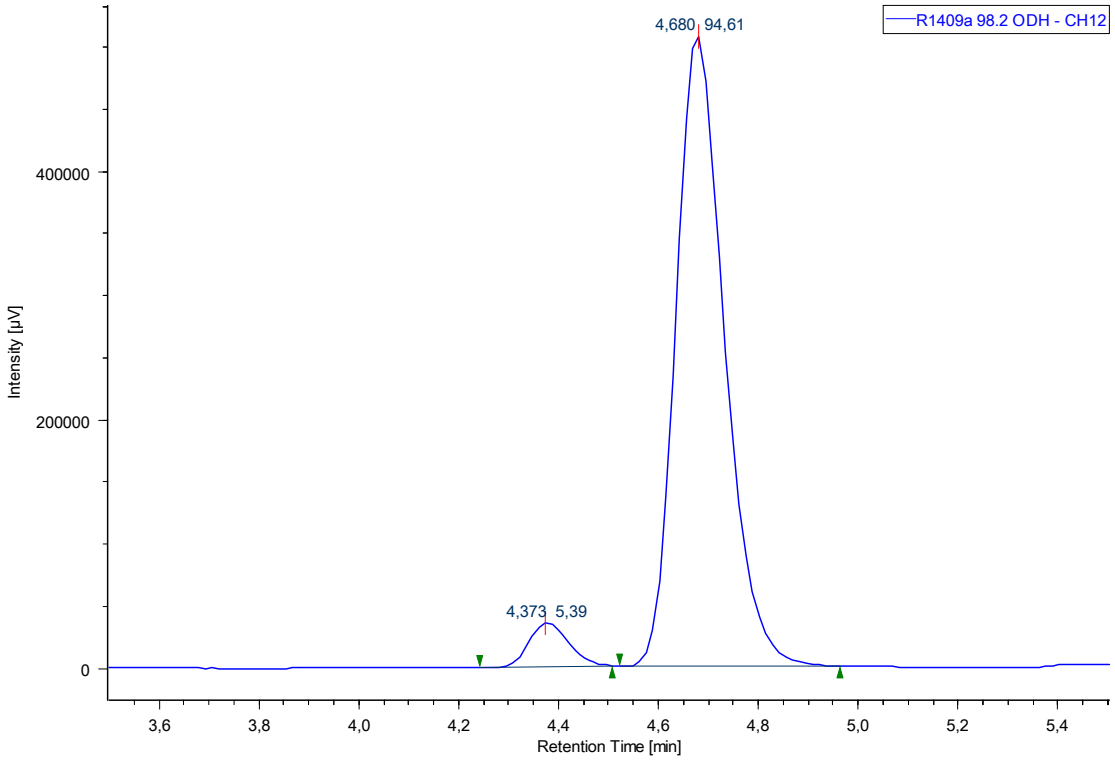

R1358a 98.2bis IC - CH9
6,667 50,54
7,493 49,46
Intensity [µV]
200000
100000
0
5,5
6,0
6,5
7,0
7,5
8,0
8,5
9,0
Retention Time [min]
Boc
N
H
O
O
CF3
6d

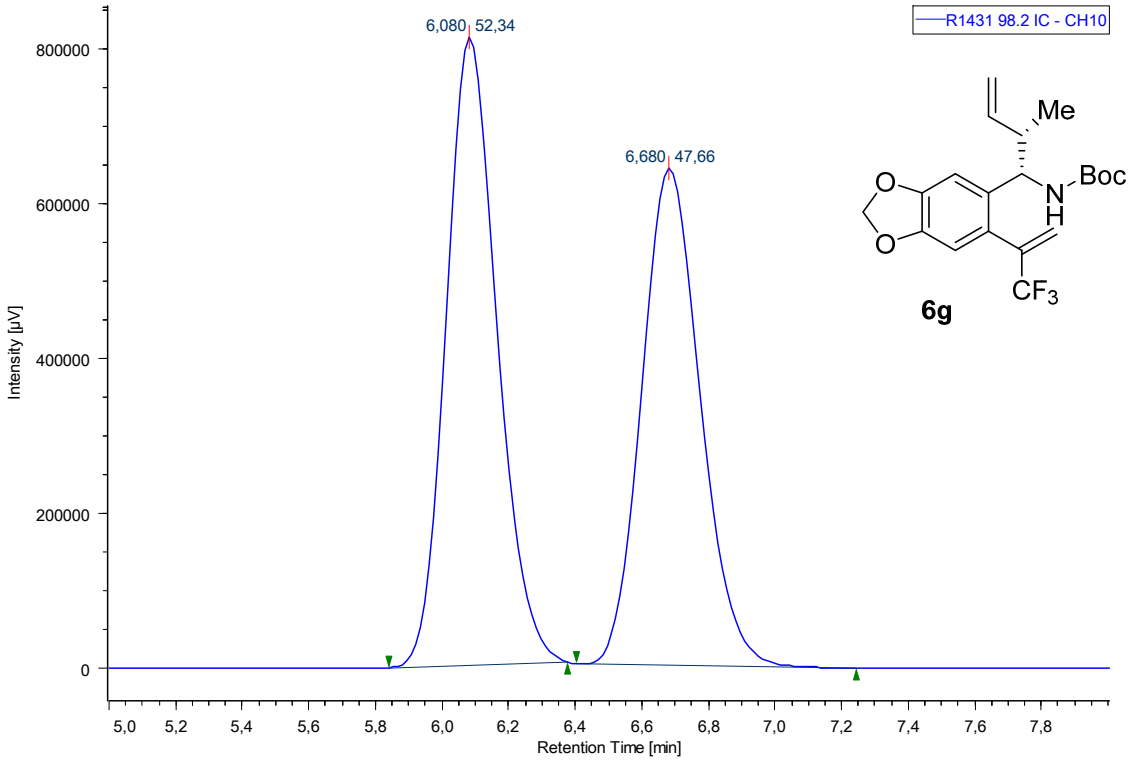

R1357 98.2 IC - CH14
7,467 98,38
6,653 1,62
Intensity [µV]
1000000
500000
0
5,5
6,0
6,5
7,0
7,5
8,0
8,5
9,0
Retention Time [min]

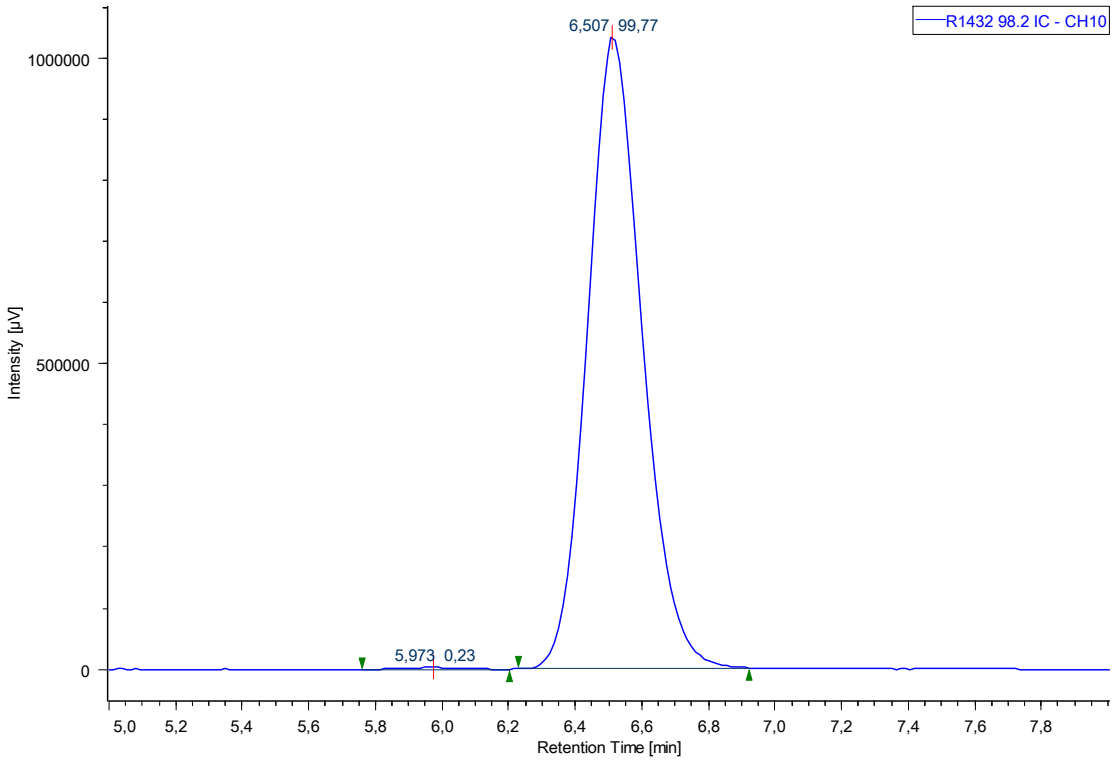

R1356 98.2 IC - CH9
5,747 50,01
6,680 49,99
1500000
1000000
500000
0
Intensity [µV]
3,5
4,0
4,5
5,0
5,5
6,0
6,5
7,0
7,5
8,0
8,5
9,0
Retention Time [min]
MeO
Boc
N
H
CF3
6e

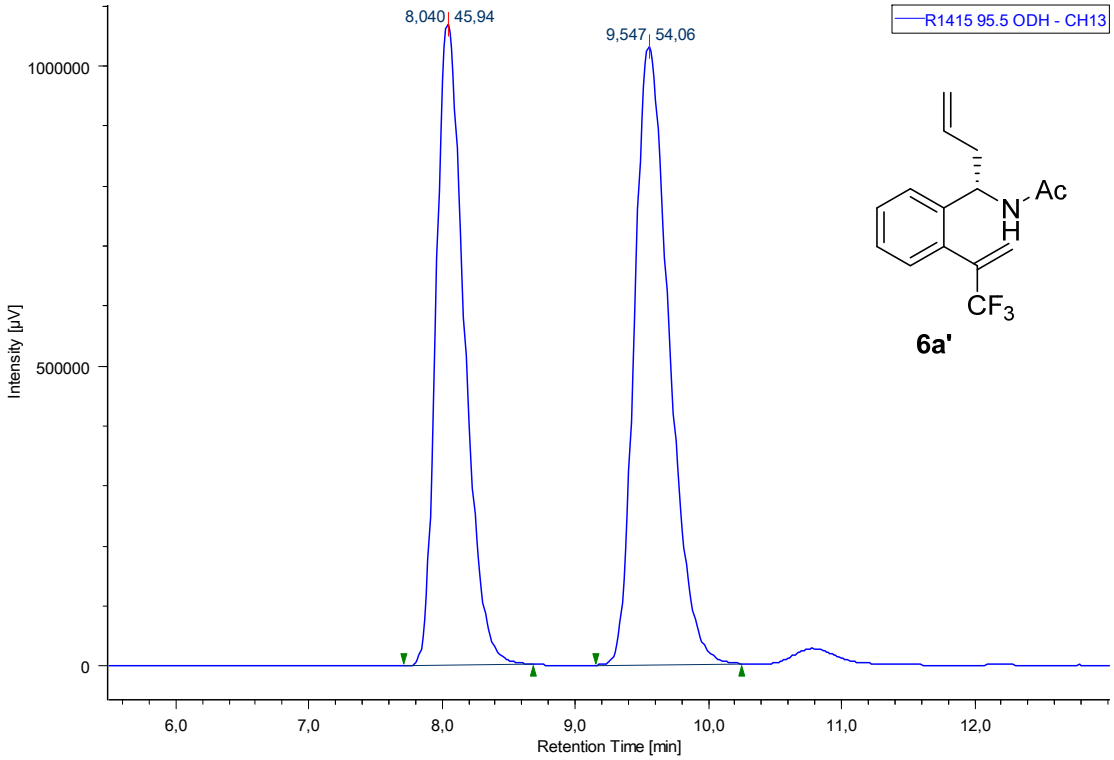

R1355 98.2 IC - CH14
6,667 99,55
5,747 0,45
2000000
1000000
0
Intensity [µV]
3,5
4,0
4,5
5,0
5,5
6,0
6,5
7,0
7,5
8,0
8,5
9,0
Retention Time [min]

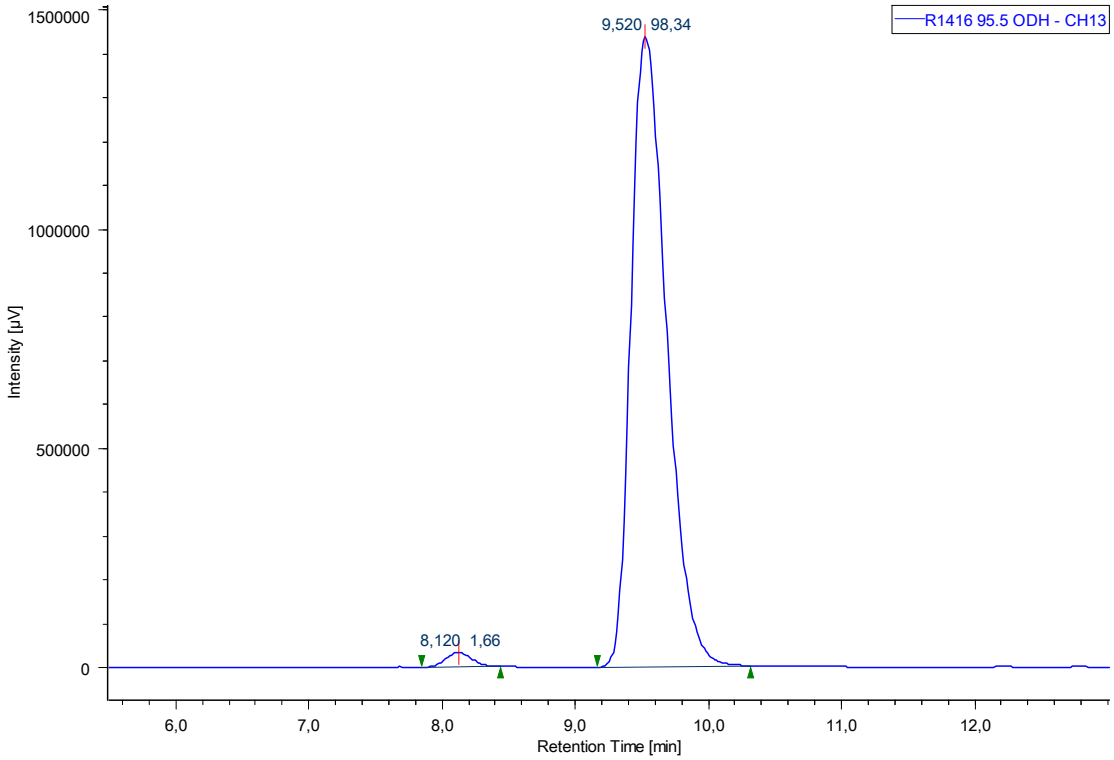

R1408a 98.2 ODH - CH10
4,360 42,39
4,653 57,61
Intensity [µV]
3000000
2000000
1000000
0
3,6
3,8
4,0
4,2
4,4
4,6
4,8
5,0
5,2
5,4
Retention Time [min]
S
N
H
Boc
CF3
6f

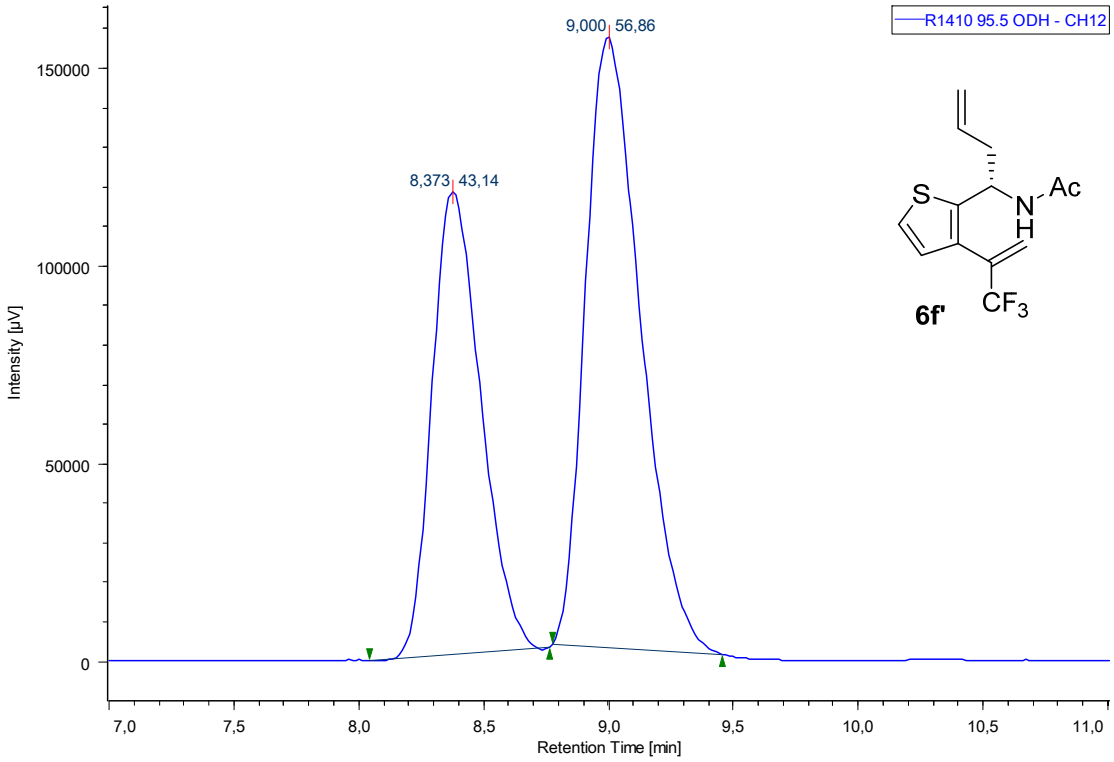

R1409a 98.2 ODH - CH12
4,680 94,61
4,373 5,39
Intensity [µV]
400000
200000
0
3,6
3,8
4,0
4,2
4,4
4,6
4,8
5,0
5,2
5,4
Retention Time [min]

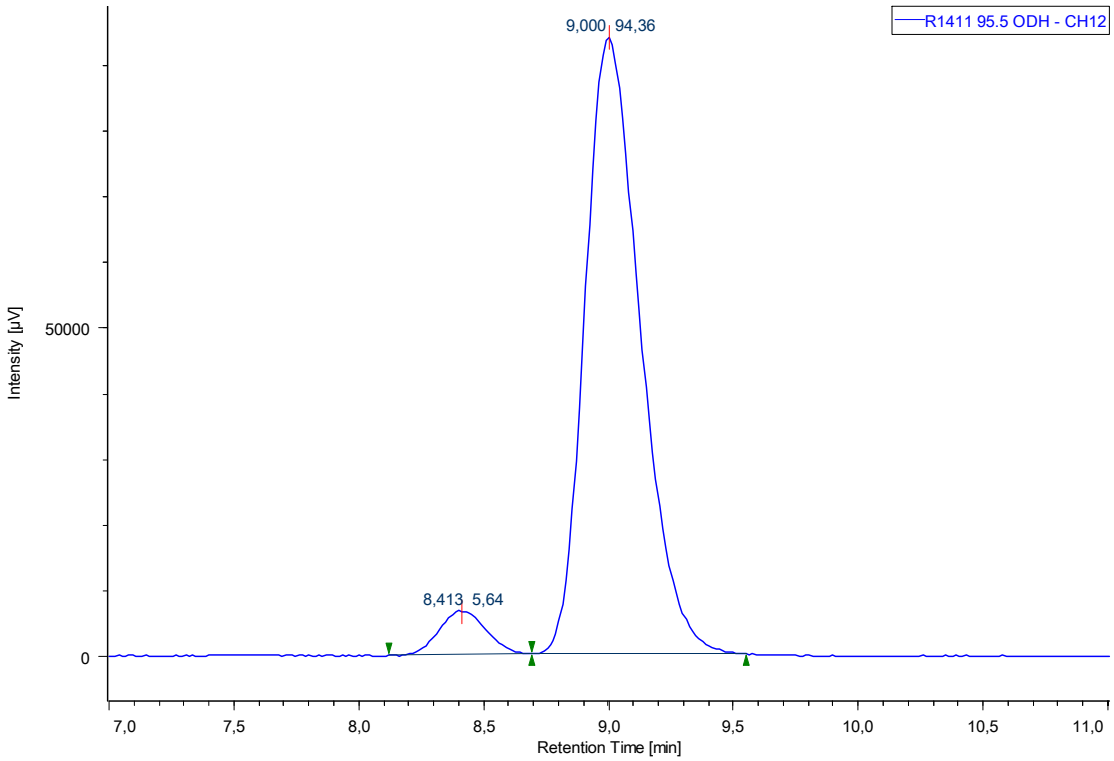

R1431 98.2 IC - CH10
6,080 52,34
6,680 47,66
Intensity [µV]
800000
600000
400000
200000
0
5,0 5,2 5,4 5,6 5,8 6,0 6,2 6,4 6,6 6,8 7,0 7,2 7,4 7,6 7,8
Retention Time [min]
Me
Boc
N
H
O
O
CF3
6g

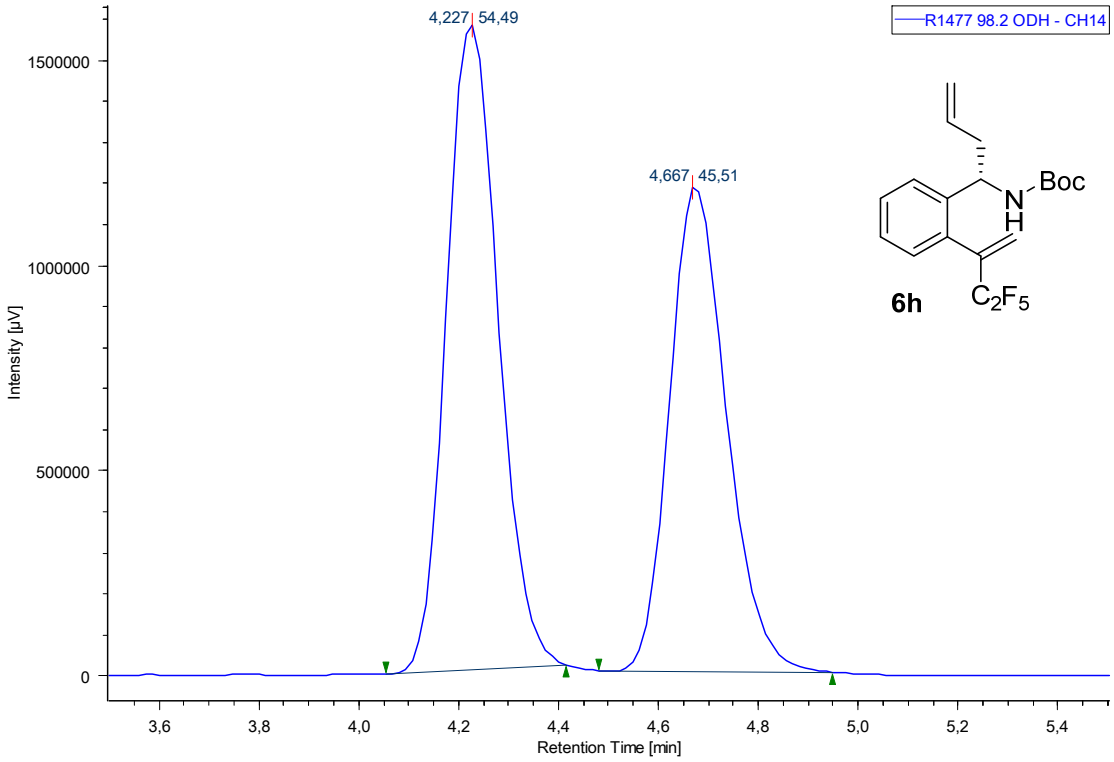

R1432 98.2 IC - CH10
6,507 99,77
5,973 0,23
Intensity [µV]
1000000
500000
0
5,0 5,2 5,4 5,6 5,8 6,0 6,2 6,4 6,6 6,8 7,0 7,2 7,4 7,6 7,8
Retention Time [min]

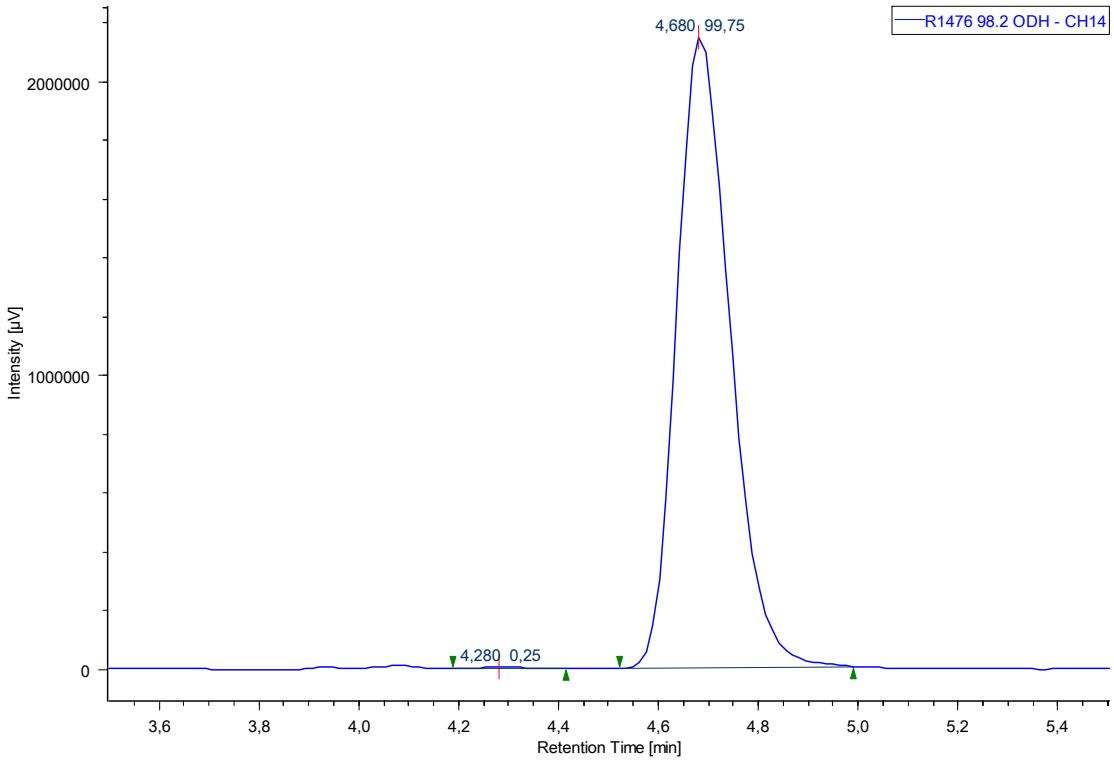

8,040 45,94
9,547 54,06
R1415 95.5 ODH - CH13
Ac
N
H
CF3
6a'
Intensity [µV]
1000000
500000
0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
Retention Time [min]

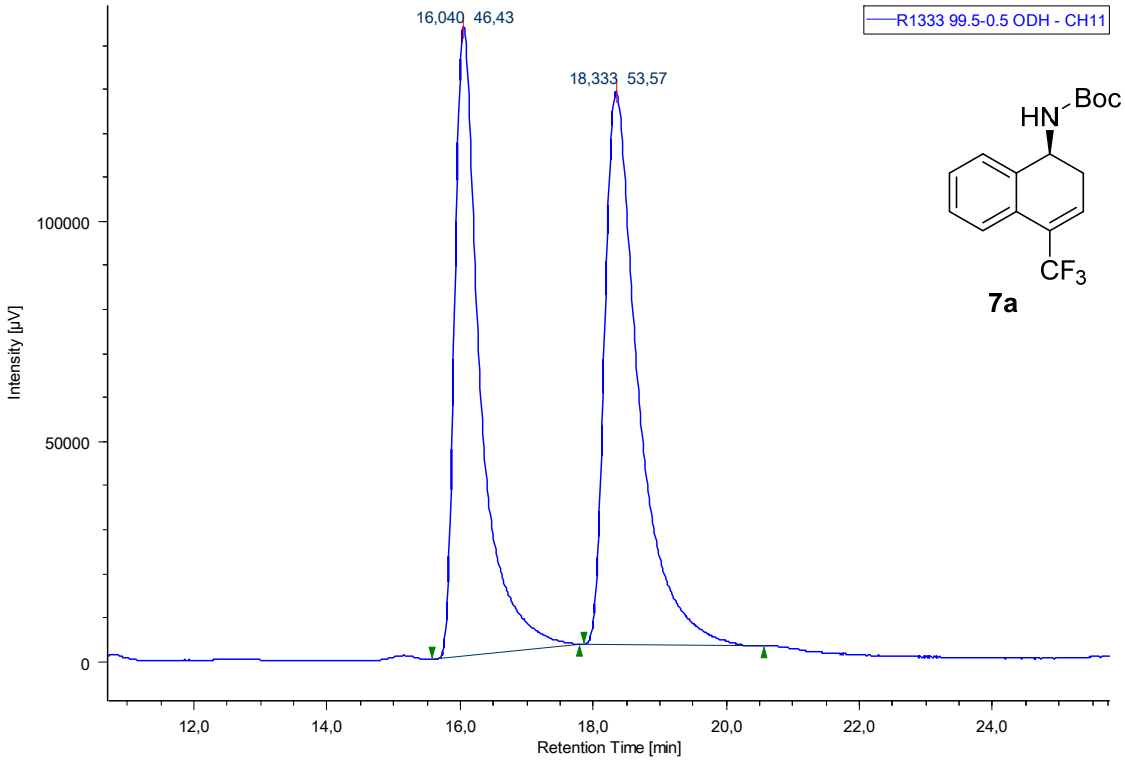

9,520 98,34
R1416 95.5 ODH - CH13
8,120 1,66
Intensity [µV]
1500000
1000000
500000
0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
Retention Time [min]

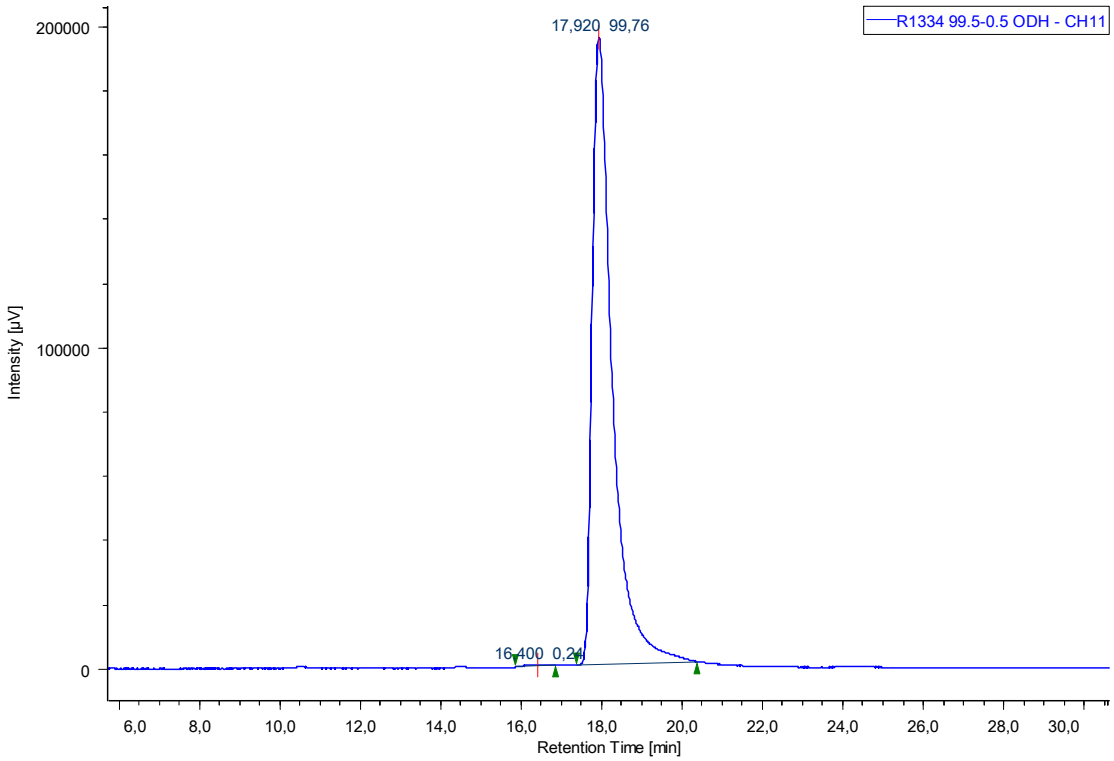

R1410 95.5 ODH - CH12
9,000 56,86
8,373 43,14
150000
100000
50000
0
Intensity [µV]
7,0
7,5
8,0
8,5
9,0
9,5
10,0
10,5
11,0
Retention Time [min]
S
N
Ac
H
CF3
6f'

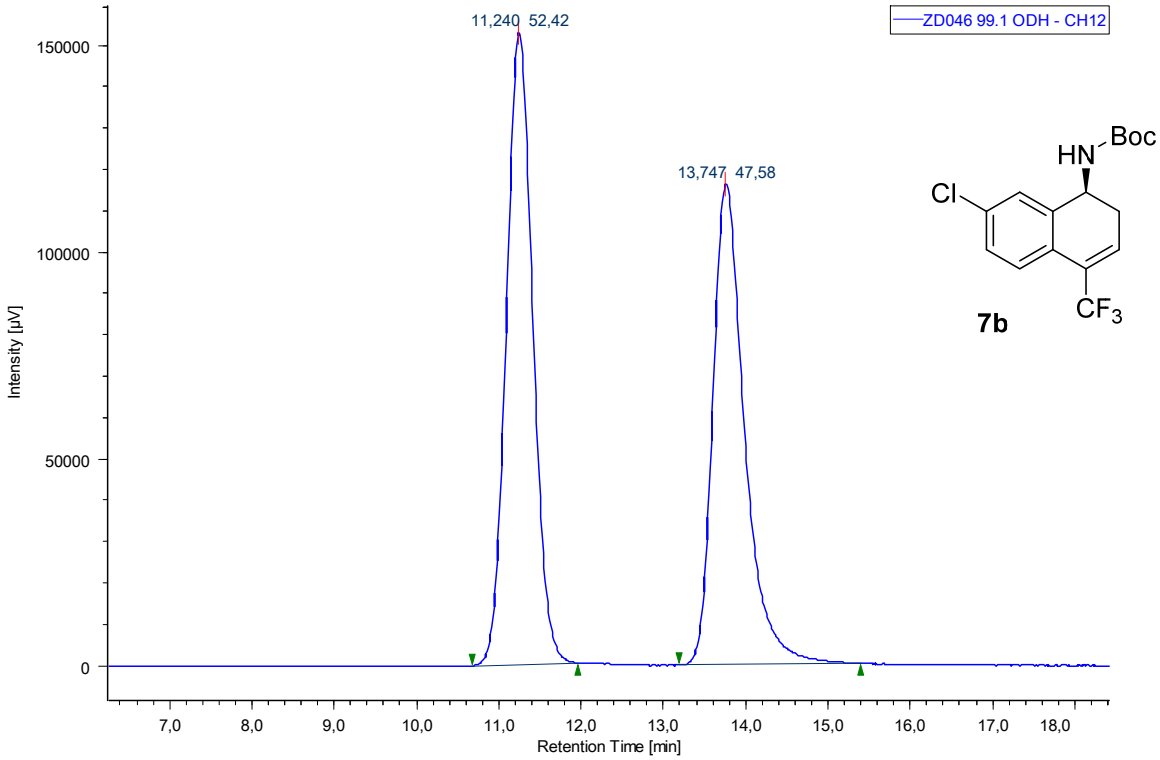

R1411 95.5 ODH - CH12
9,000 94,36
8,413 5,64
50000
0
Intensity [µV]
7,0
7,5
8,0
8,5
9,0
9,5
10,0
10,5
11,0
Retention Time [min]

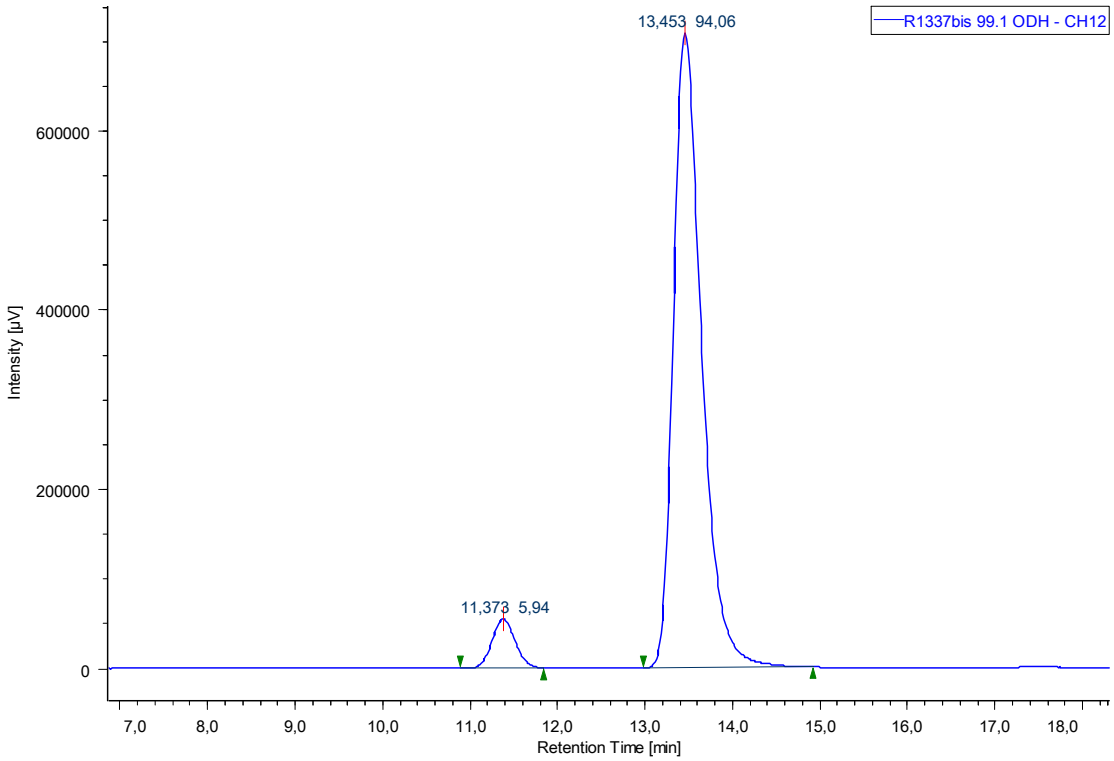

R1477 98.2 ODH - CH14
4,227 54,49
4,667 45,51
Boc
N
H
6h
C_2F_5
Intensity [µV]
1500000
1000000
500000
0
3,6
3,8
4,0
4,2
4,4
4,6
4,8
5,0
5,2
5,4
Retention Time [min]

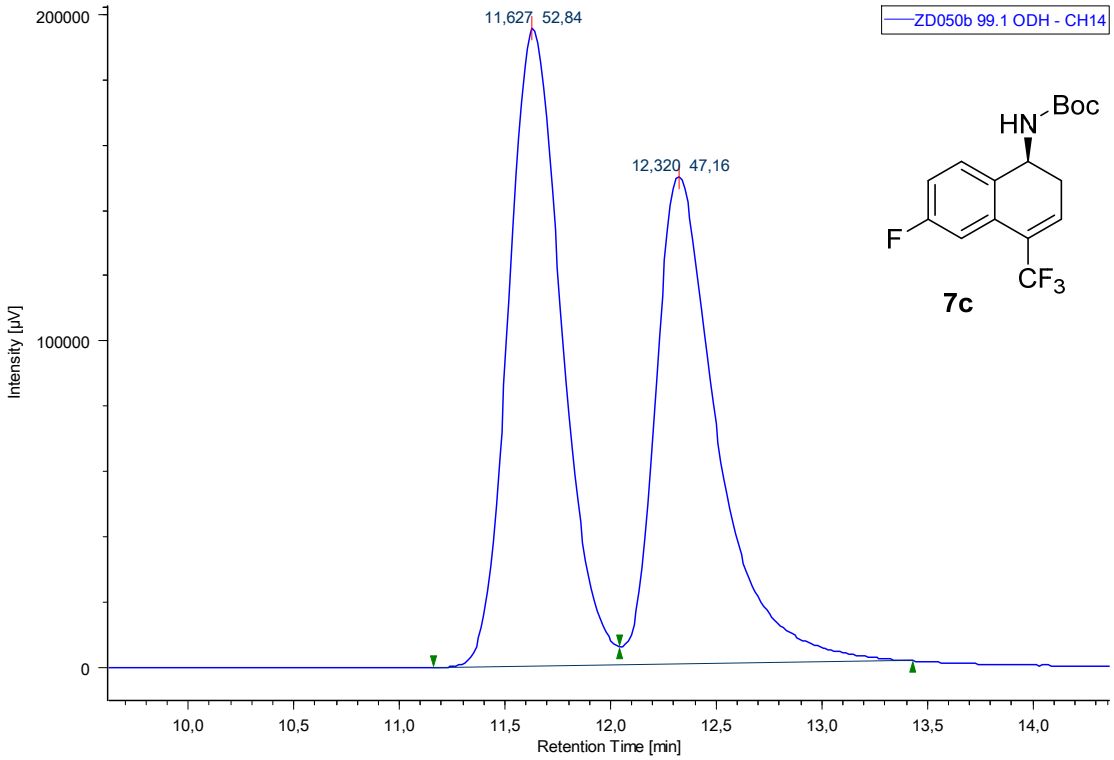

R1476 98.2 ODH - CH14
4,680 99,75
4,280 0,25
Intensity [µV]
2000000
1000000
0
3,6
3,8
4,0
4,2
4,4
4,6
4,8
5,0
5,2
5,4
Retention Time [min]

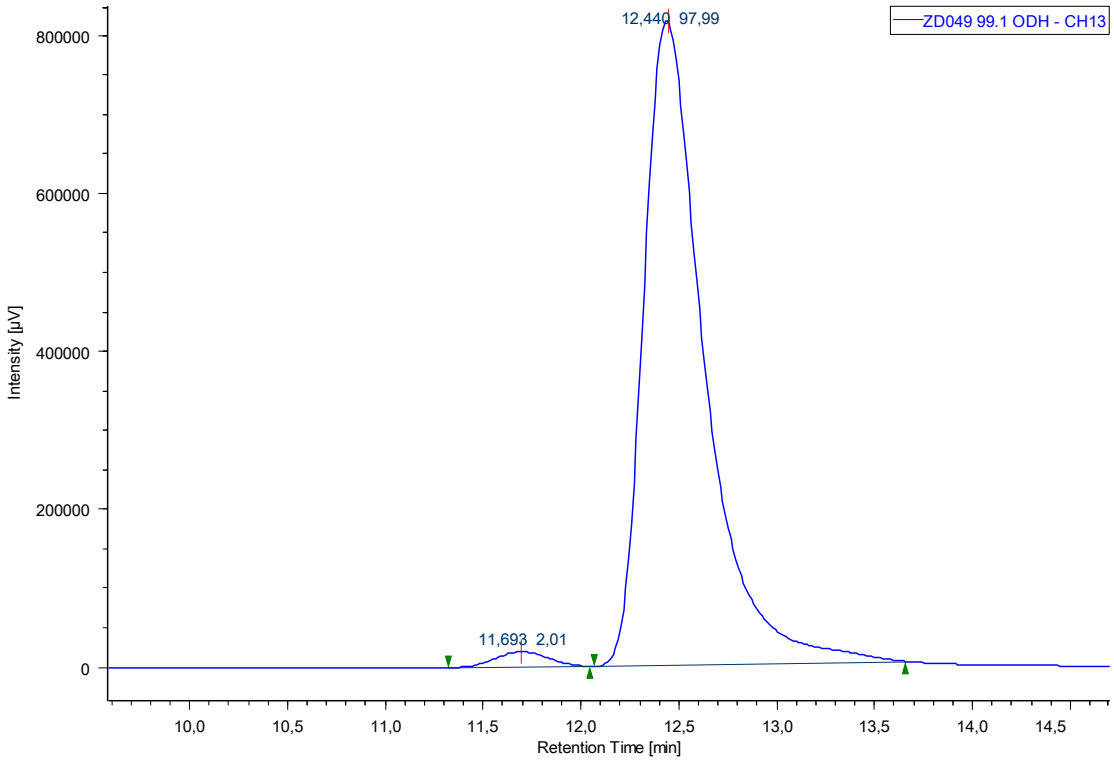

R1333 99.5-0.5 ODH - CH11
16,040 46,43
18,333 53,57
HN
Boc
CF3
7a
Intensity [µV]
100000
50000
0
12,0
14,0
16,0
18,0
20,0
22,0
24,0
Retention Time [min]

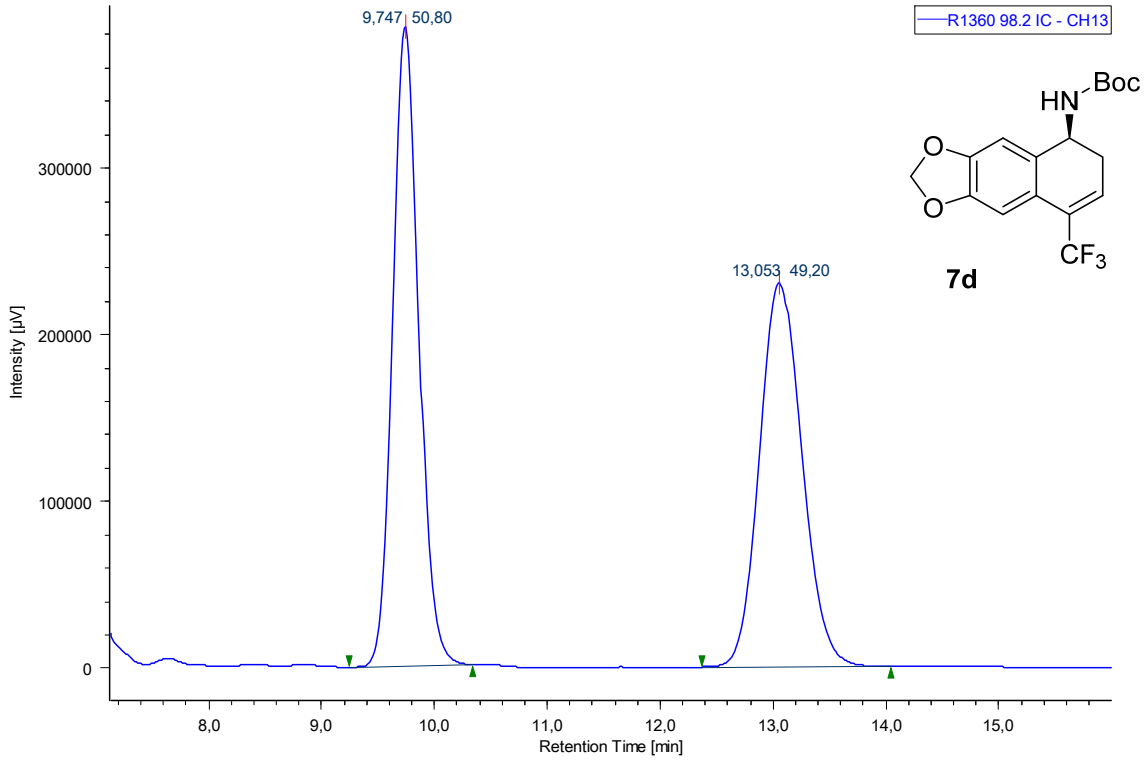

R1334 99.5-0.5 ODH - CH11
17,920 99,76
16,400 0,24
Intensity [µV]
200000
100000
0
6,0
8,0
10,0
12,0
14,0
16,0
18,0
20,0
22,0
24,0
26,0
28,0
30,0
Retention Time [min]

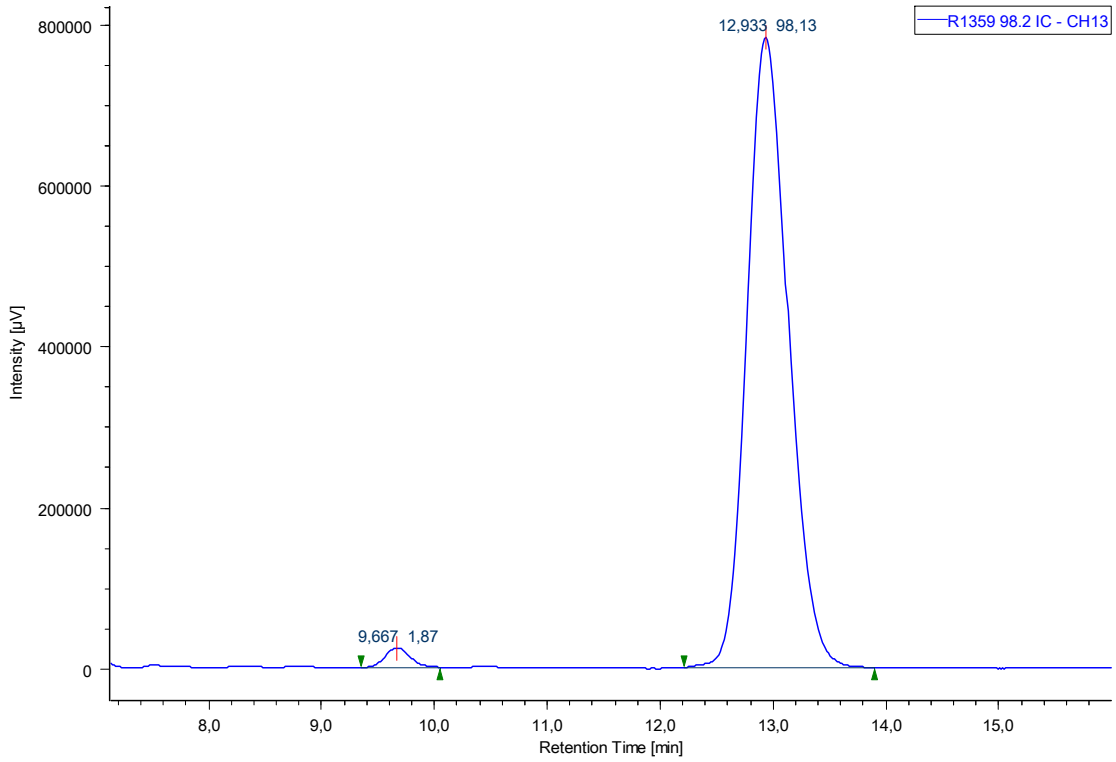

ZD046 99.1 ODH - CH12
11,240 52,42
13,747 47,58
HN
Boc
Cl
CF3
7b
Intensity [µV]
150000
100000
50000
0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
14,0
15,0
16,0
17,0
18,0
Retention Time [min]

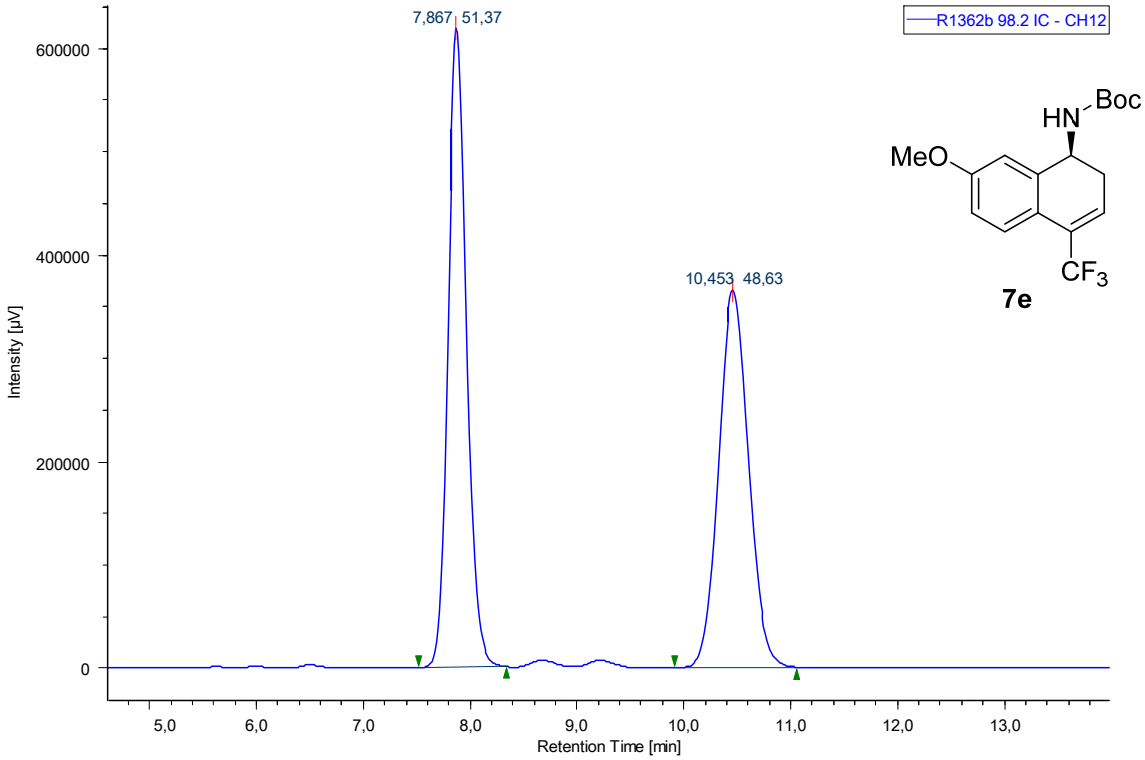

R1337bis 99.1 ODH - CH12
13,453 94,06
11,373 5,94
Intensity [µV]
600000
400000
200000
0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
14,0
15,0
16,0
17,0
18,0
Retention Time [min]

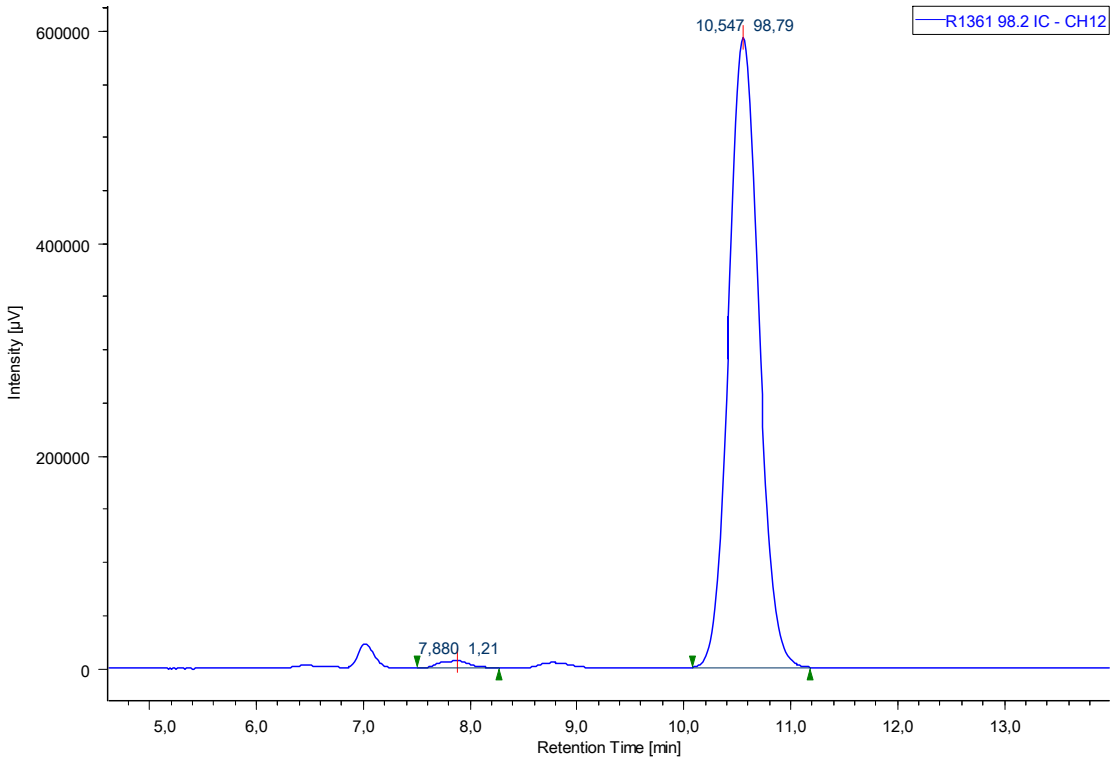

ZD050b 99.1 ODH - CH14
11,627 52,84
12,320 47,16
HN
Boc
F
CF3
7c
Intensity [µV]
200000
100000
0
10,0
10,5
11,0
11,5
12,0
12,5
13,0
13,5
14,0
Retention Time [min]

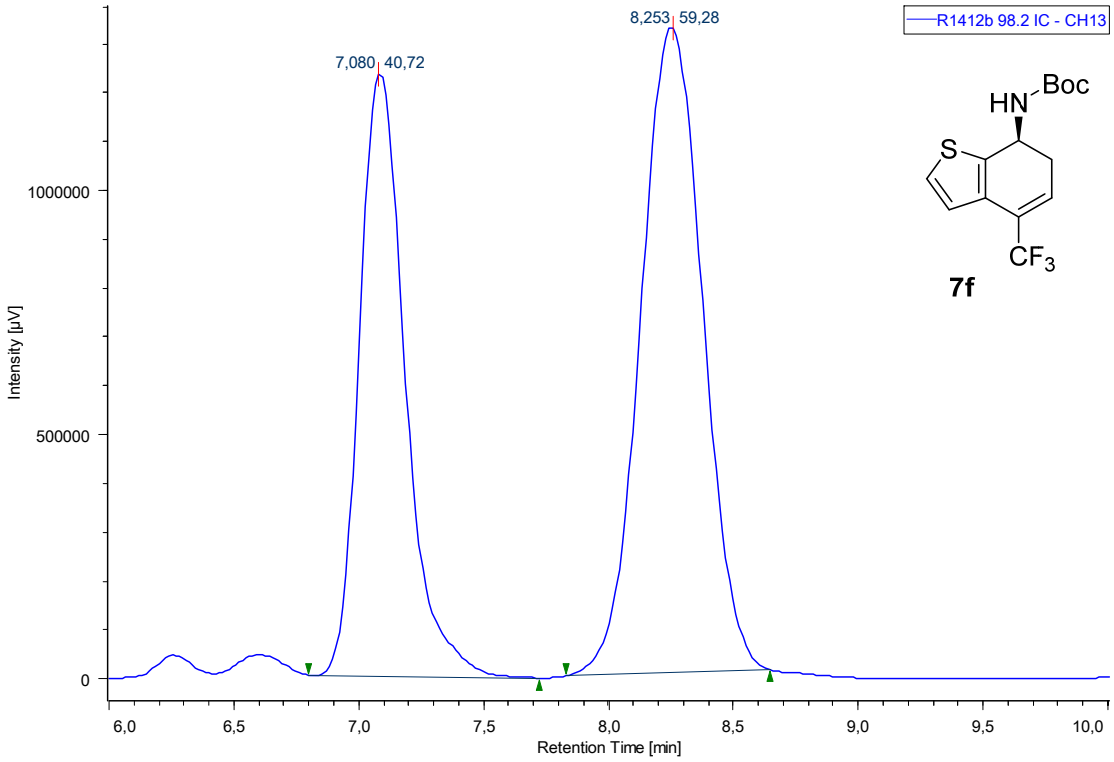

ZD049 99.1 ODH - CH13
12,440 97,99
11,693 2,01
Intensity [µV]
800000
600000
400000
200000
0
10,0
10,5
11,0
11,5
12,0
12,5
13,0
13,5
14,0
14,5
Retention Time [min]

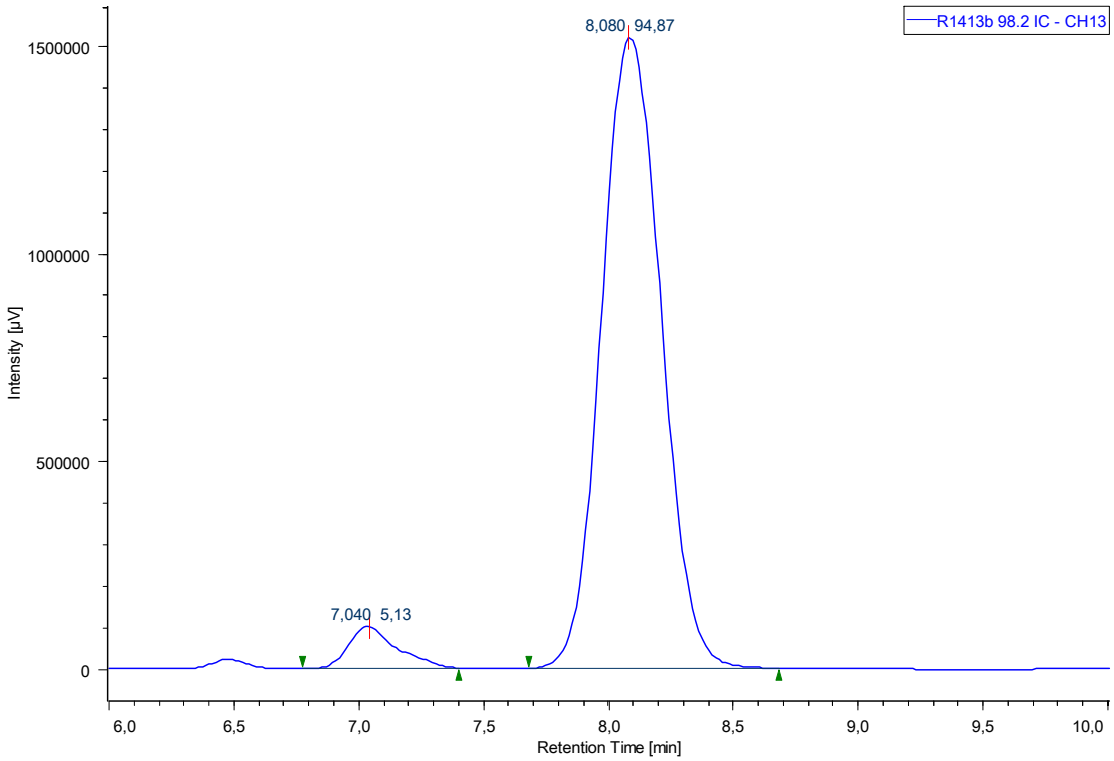

R1360 98.2 IC - CH13
9,747 50,80
13,053 49,20
HN
Boc
O
O
CF3
7d
Intensity [µV]
300000
200000
100000
0
8,0
9,0
10,0
11,0
12,0
13,0
14,0
15,0
Retention Time [min]

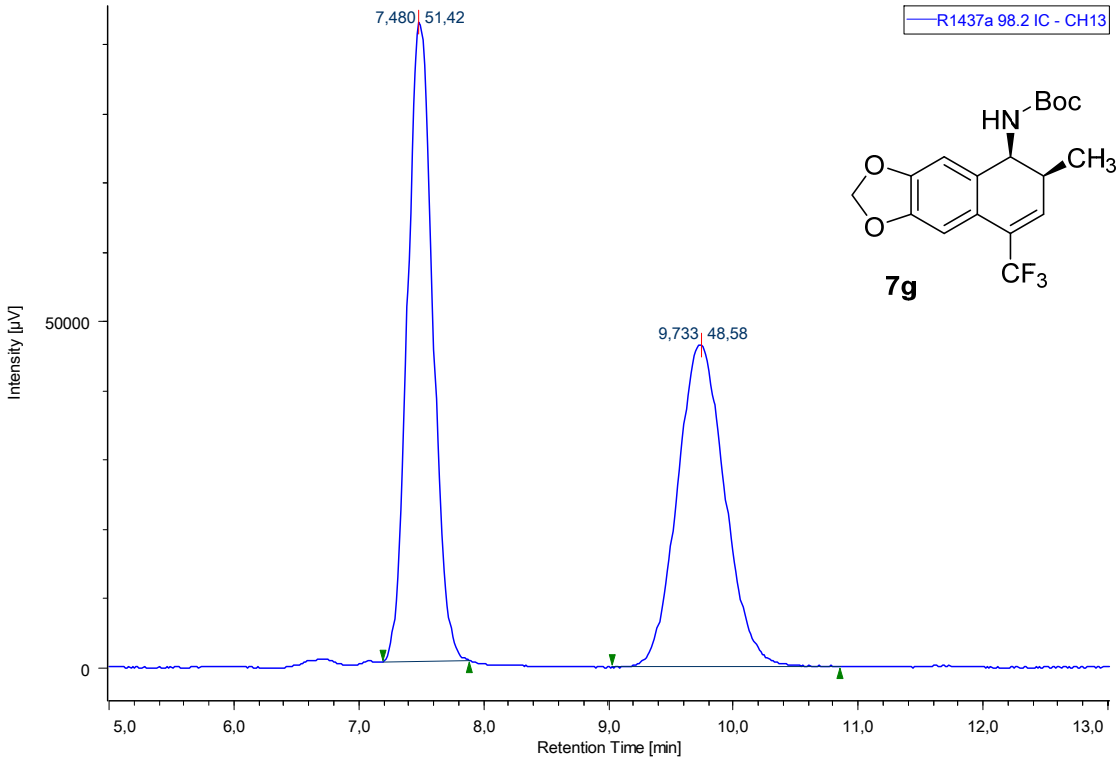

R1359 98.2 IC - CH13
12,933 98,13
9,667 1,87
Intensity [µV]
800000
600000
400000
200000
0
8,0
9,0
10,0
11,0
12,0
13,0
14,0
15,0
Retention Time [min]

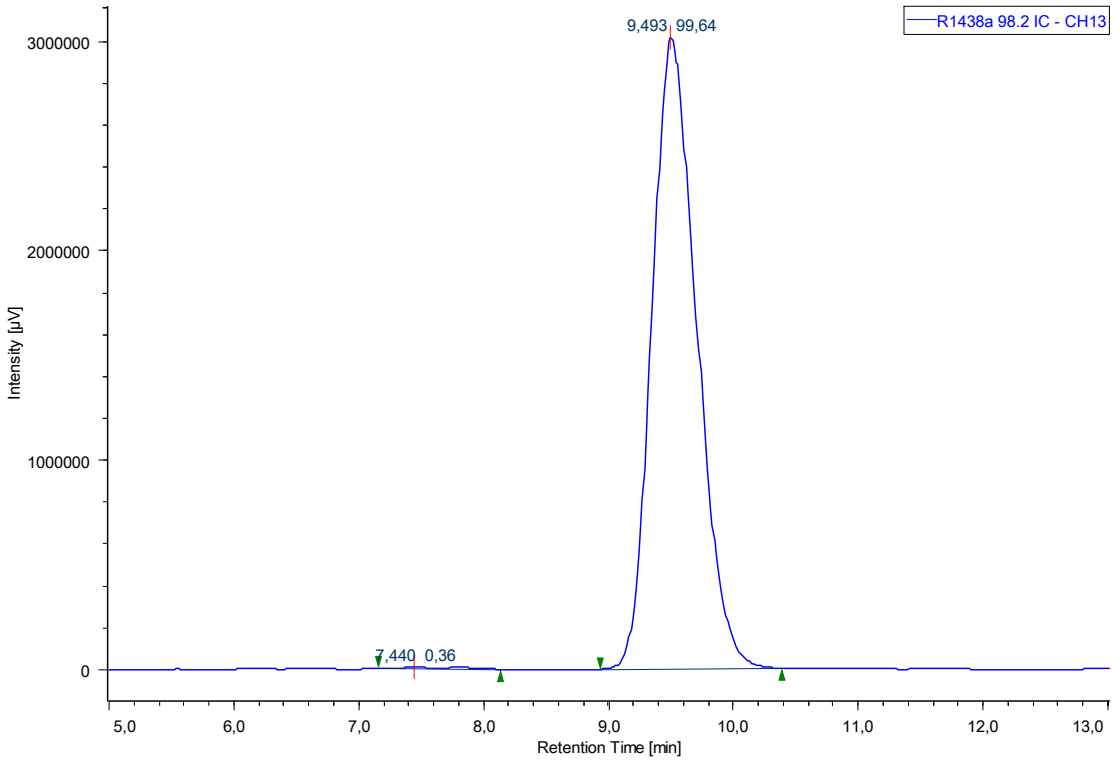

R1362b 98.2 IC - CH12
7,867 51,37
10,453 48,63
HN
Boc
MeO
CF3
7e
Intensity [µV]
600000
400000
200000
0
5,0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
Retention Time [min]

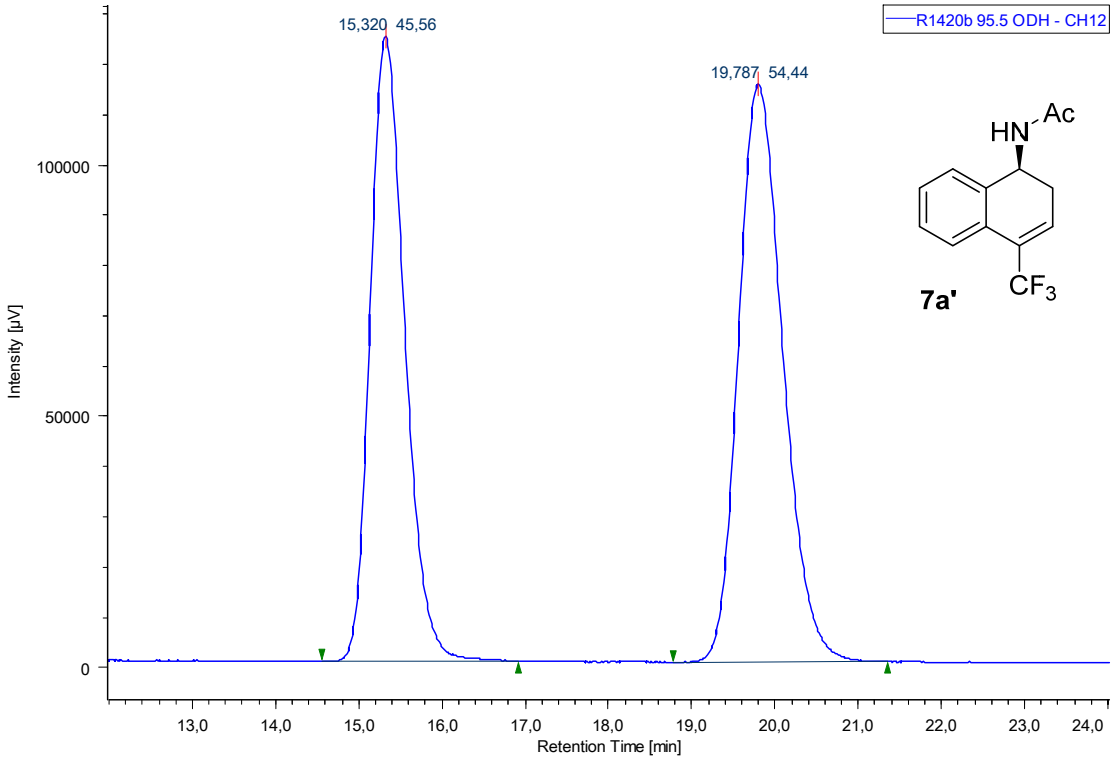

R1361 98.2 IC - CH12
10,547 98,79
7,880 1,21
Intensity [µV]
600000
400000
200000
0
5,0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
Retention Time [min]

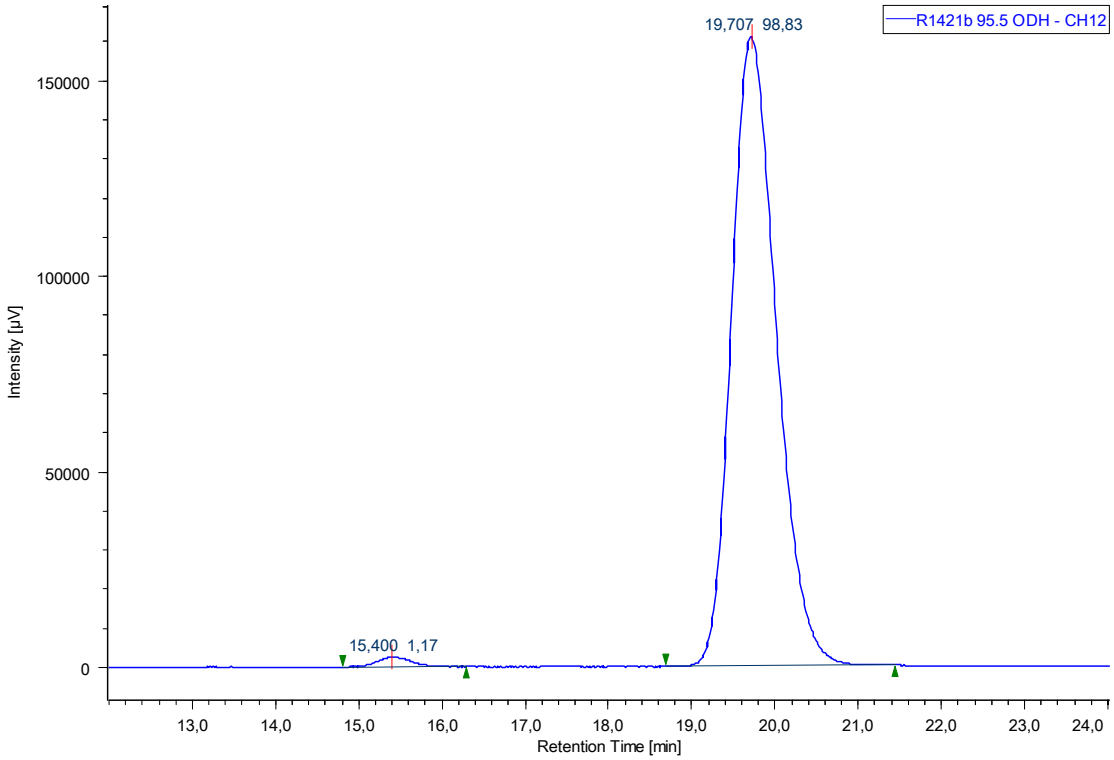

R1412b 98.2 IC - CH13
7,080 40,72
8,253 59,28
HN
Boc
S
CF3
7f
Intensity [µV]
1000000
500000
0
6,0
6,5
7,0
7,5
8,0
8,5
9,0
9,5
10,0
Retention Time [min]

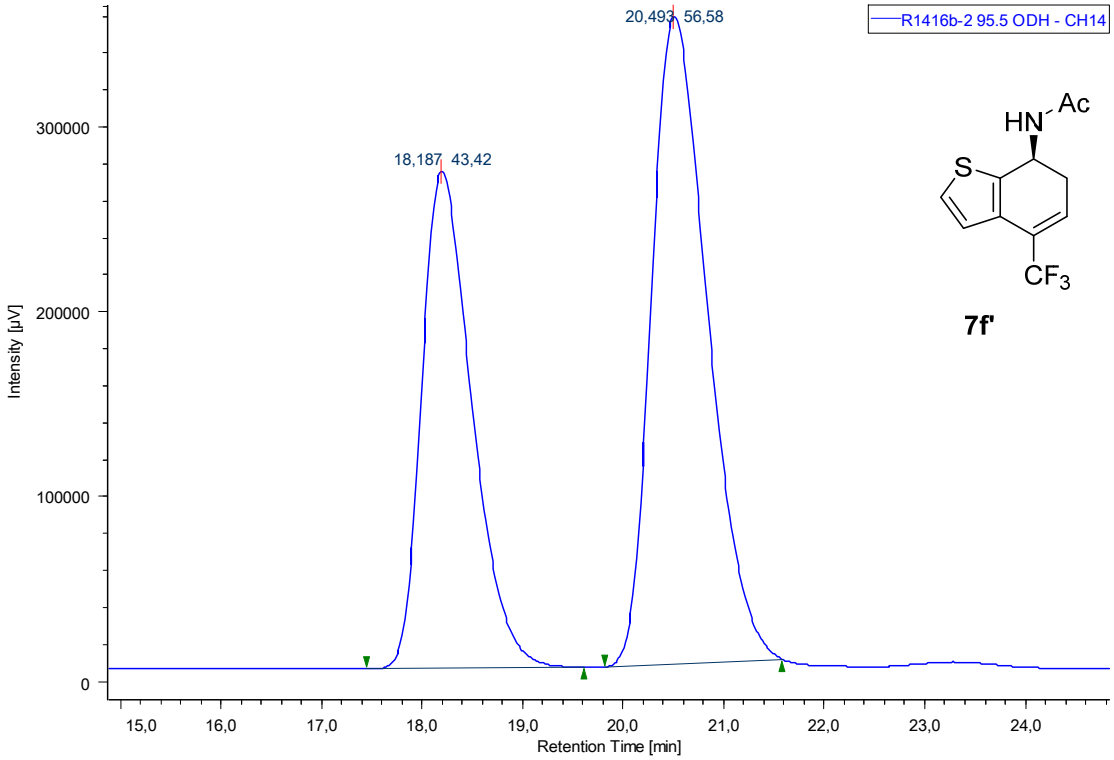

R1413b 98.2 IC - CH13
8,080 94,87
7,040 5,13
Intensity [µV]
1500000
1000000
500000
0
6,0
6,5
7,0
7,5
8,0
8,5
9,0
9,5
10,0
Retention Time [min]

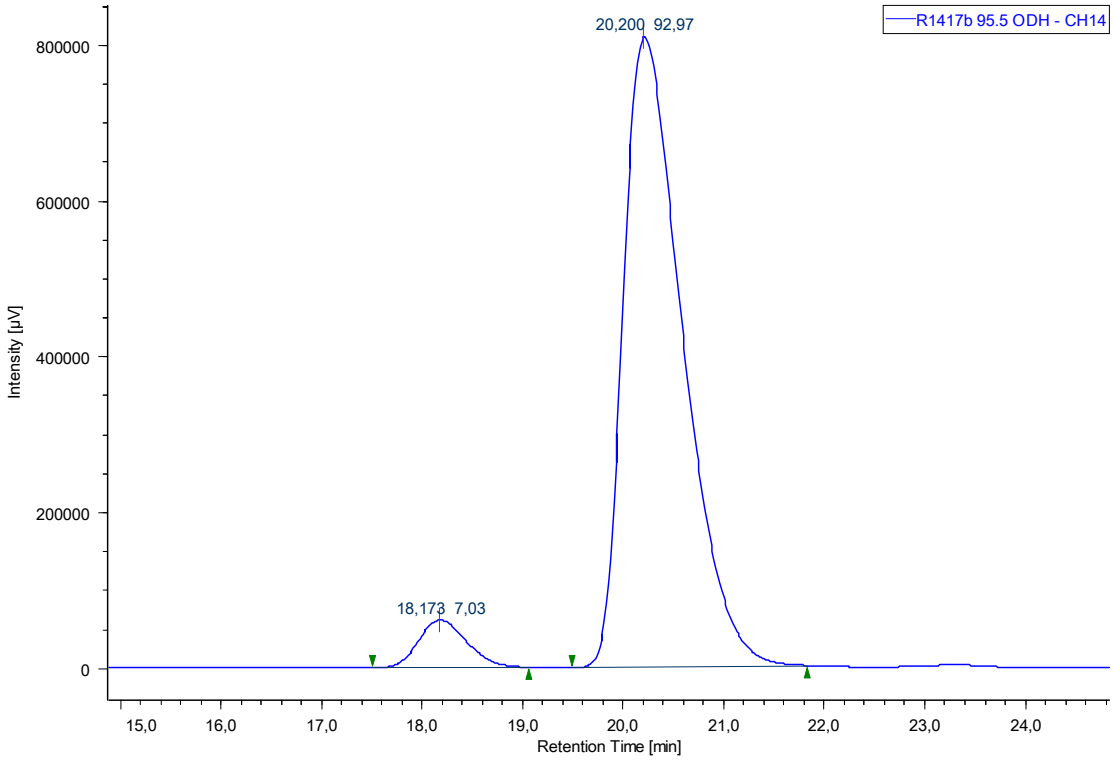

7,480 51,42
9,733 48,58
R1437a 98.2 IC - CH13
HN
Boc
CH3
O
O
CF3
7g
Intensity [µV]
50000
0
5,0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
Retention Time [min]

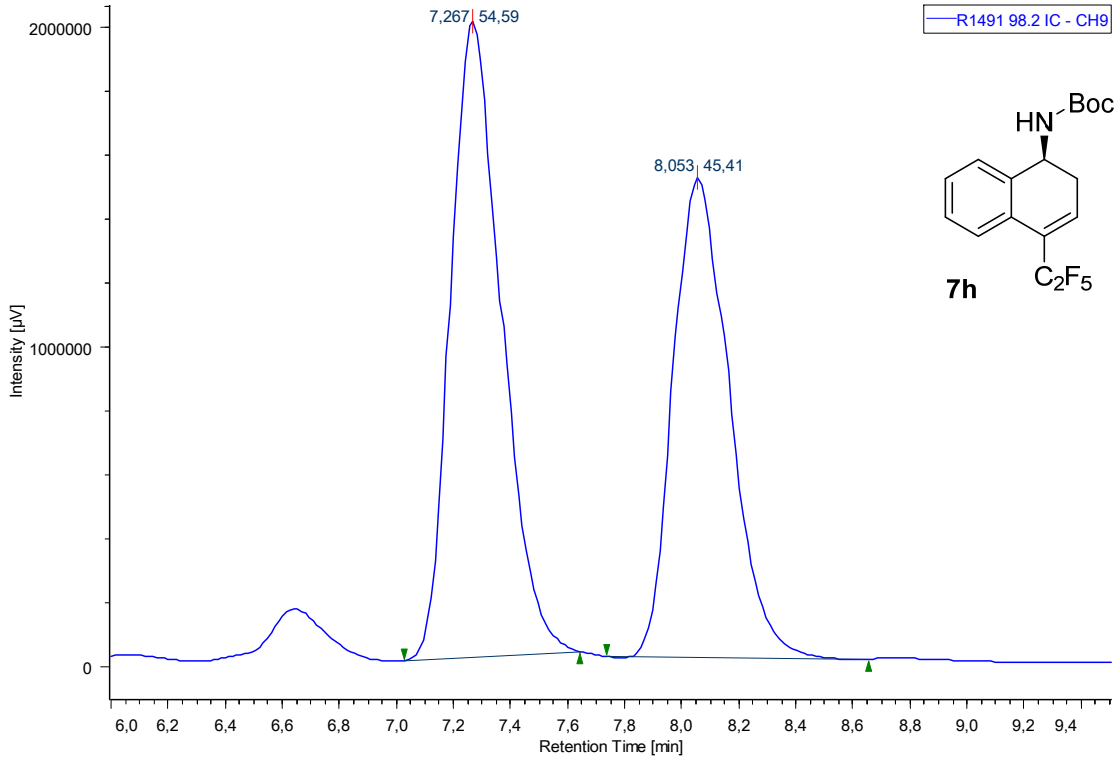

9,493 99,64
R1438a 98.2 IC - CH13
7,440 0,36
Intensity [µV]
3000000
2000000
1000000
0
5,0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
Retention Time [min]

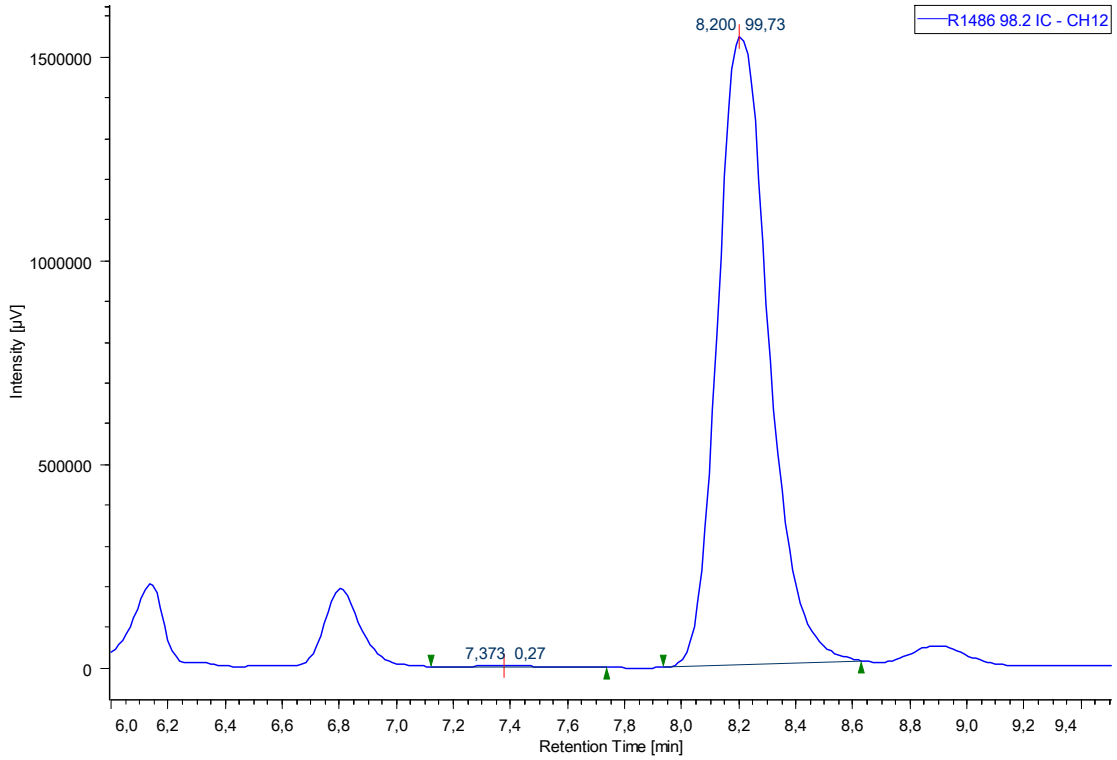

R1420b 95.5 ODH - CH12
15,320 45,56
19,787 54,44
HN
Ac
CF3
7a'
Intensity [µV]
100000
50000
0
13,0
14,0
15,0
16,0
17,0
18,0
19,0
20,0
21,0
22,0
23,0
24,0
Retention Time [min]

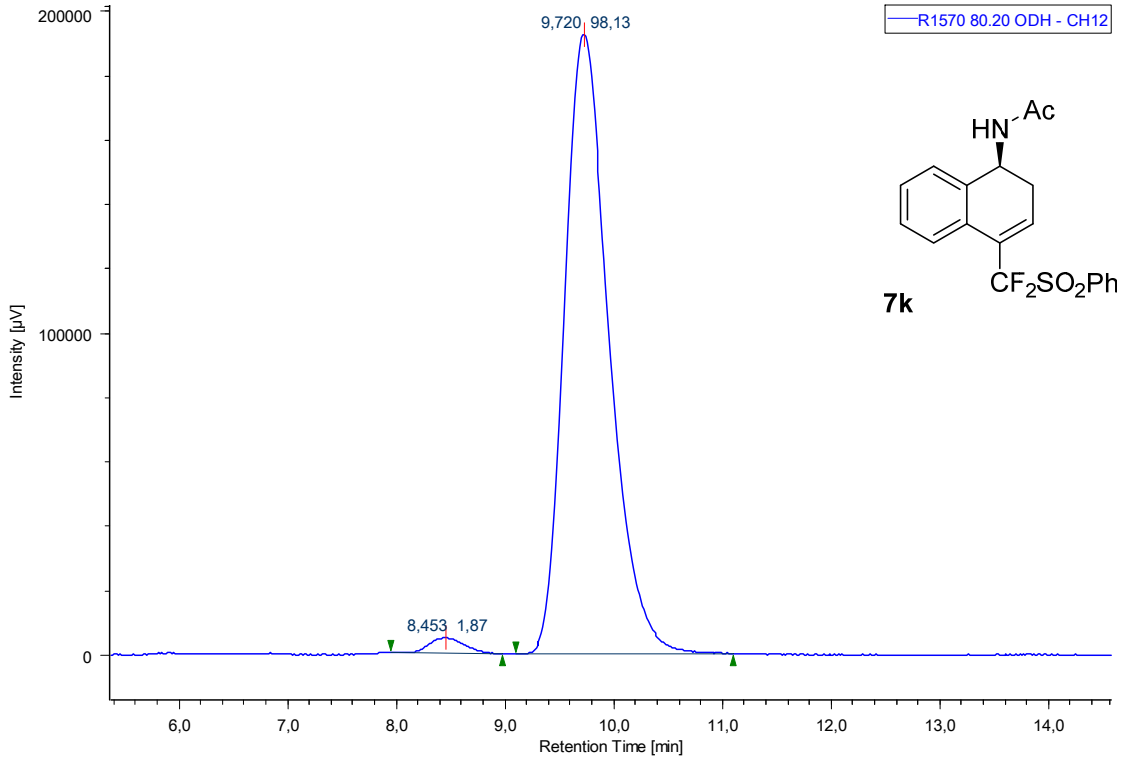

R1421b 95.5 ODH - CH12
19,707 98,83
15,400 1,17
Intensity [µV]
150000
100000
50000
0
13,0
14,0
15,0
16,0
17,0
18,0
19,0
20,0
21,0
22,0
23,0
24,0
Retention Time [min]


R1416b-2 95.5 ODH - CH14
18,187 43,42
20,493 56,58
HN
Ac
S
CF3
7f'
Intensity [µV]
Retention Time [min]


R1417b 95.5 ODH - CH14
18,173 7,03
20,200 92,97
Intensity [µV]
Retention Time [min]


R1491 98.2 IC - CH9
7,267 54,59
8,053 45,41
HN
Boc
C_2F_5
7h
Intensity [µV]
2000000
1000000
0
6,0 6,2 6,4 6,6 6,8 7,0 7,2 7,4 7,6 7,8 8,0 8,2 8,4 8,6 8,8 9,0 9,2 9,4
Retention Time [min]


R1486 98.2 IC - CH12
8,200 99,73
7,373 0,27
Intensity [µV]
1500000
1000000
500000
0
6,0 6,2 6,4 6,6 6,8 7,0 7,2 7,4 7,6 7,8 8,0 8,2 8,4 8,6 8,8 9,0 9,2 9,4
Retention Time [min]


R1570 80.20 ODH - CH12
9,720 98,13
8,453 1,87
Intensity [µV]
200000
100000
0
6,0
7,0
8,0
9,0
10,0
11,0
12,0
13,0
14,0
Retention Time [min]
HN
Ac
CF2SO2Ph
7k