Chiral N-Heterocyclic Carbene–Copper(I)-Catalyzed Asymmetric Allylic Arylation of Aliphatic Allylic Bromides: Steric and Electronic Effects on γ-Selectivity

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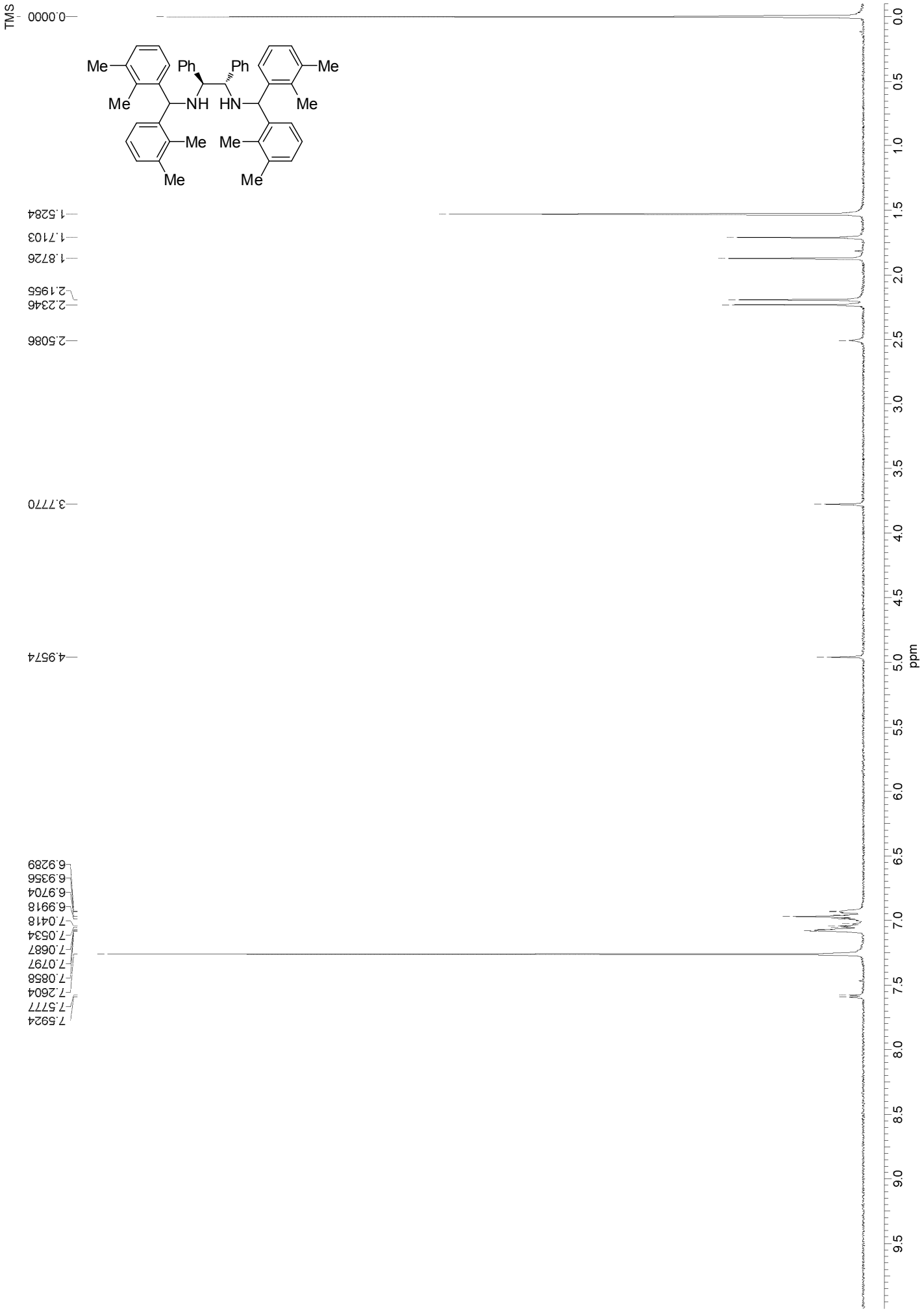
^{1}H-NMR of **C**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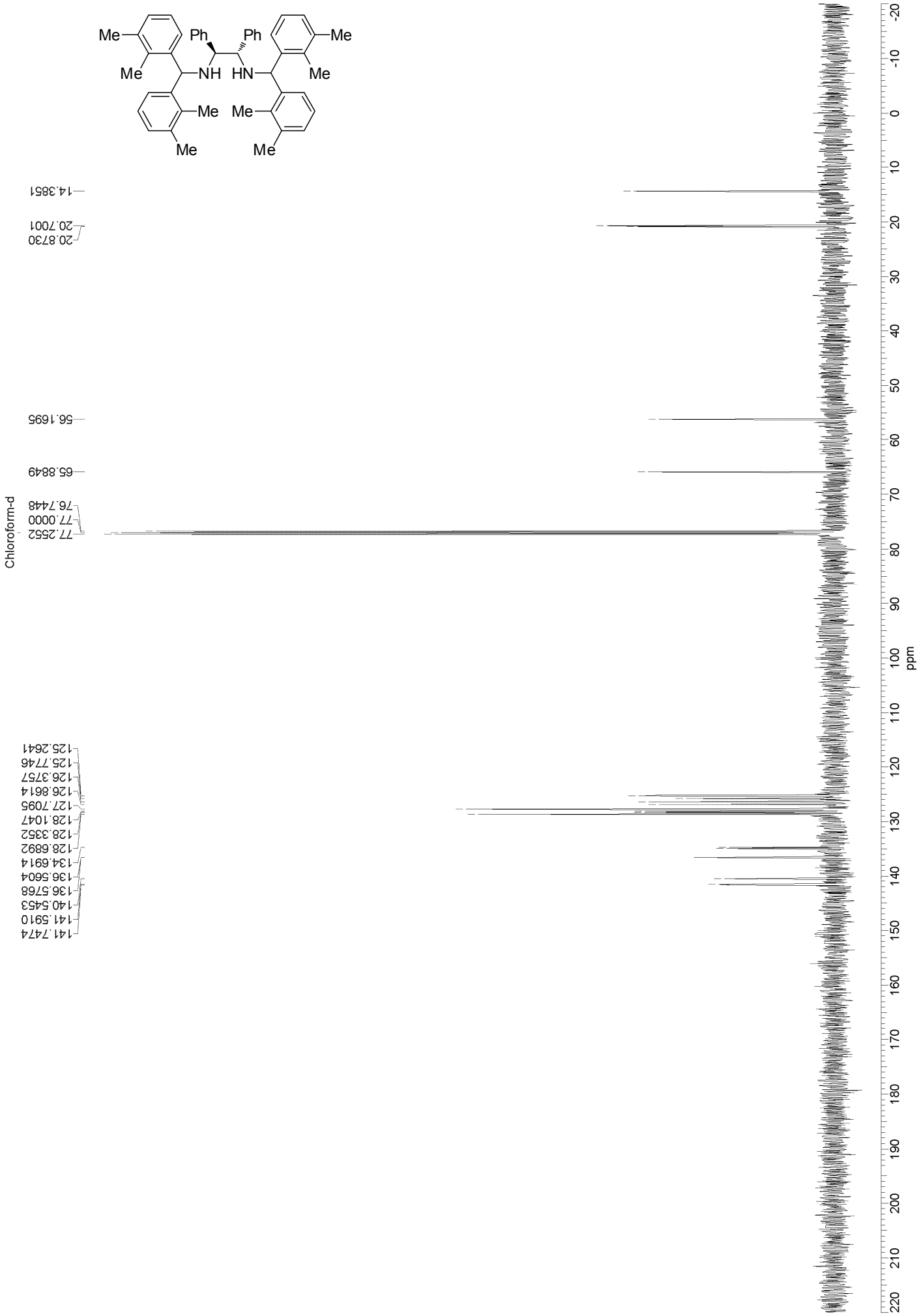
6.9289
6.9356
6.9704
6.9918
7.0418
7.0534
7.0687
7.0797
7.0858
7.2604
7.5777
7.5924
Me
Ph
Ph
Me
Me
NH
HN
Me
Me
Me
Me
Me
ppm

^{13}C-NMR of **C**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65.8849
76.7448
77.0000
77.2552
Chloroform-d
125.2641
125.7746
126.3757
126.8614
127.7095
128.1047
128.3352
128.6892
134.6914
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136.5768
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141.5910
141.7474
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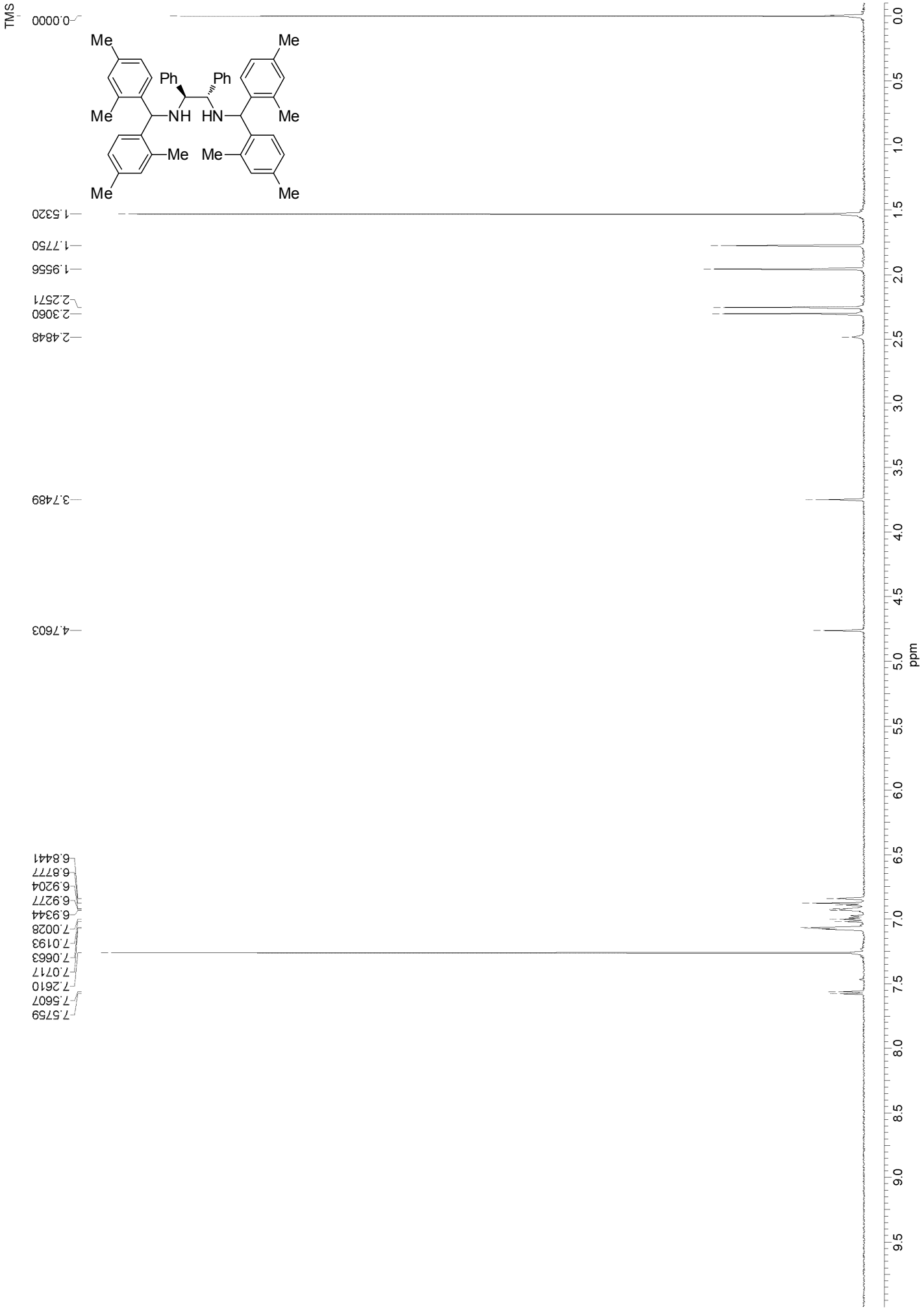
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6.8777
6.9204
6.9277
6.9344
7.0028
7.0193
7.0663
7.0717
7.2610
7.5607
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Ph
Ph
NH
HN
Me
Me
Me
Me
Me
Me
Me
Me
ppm

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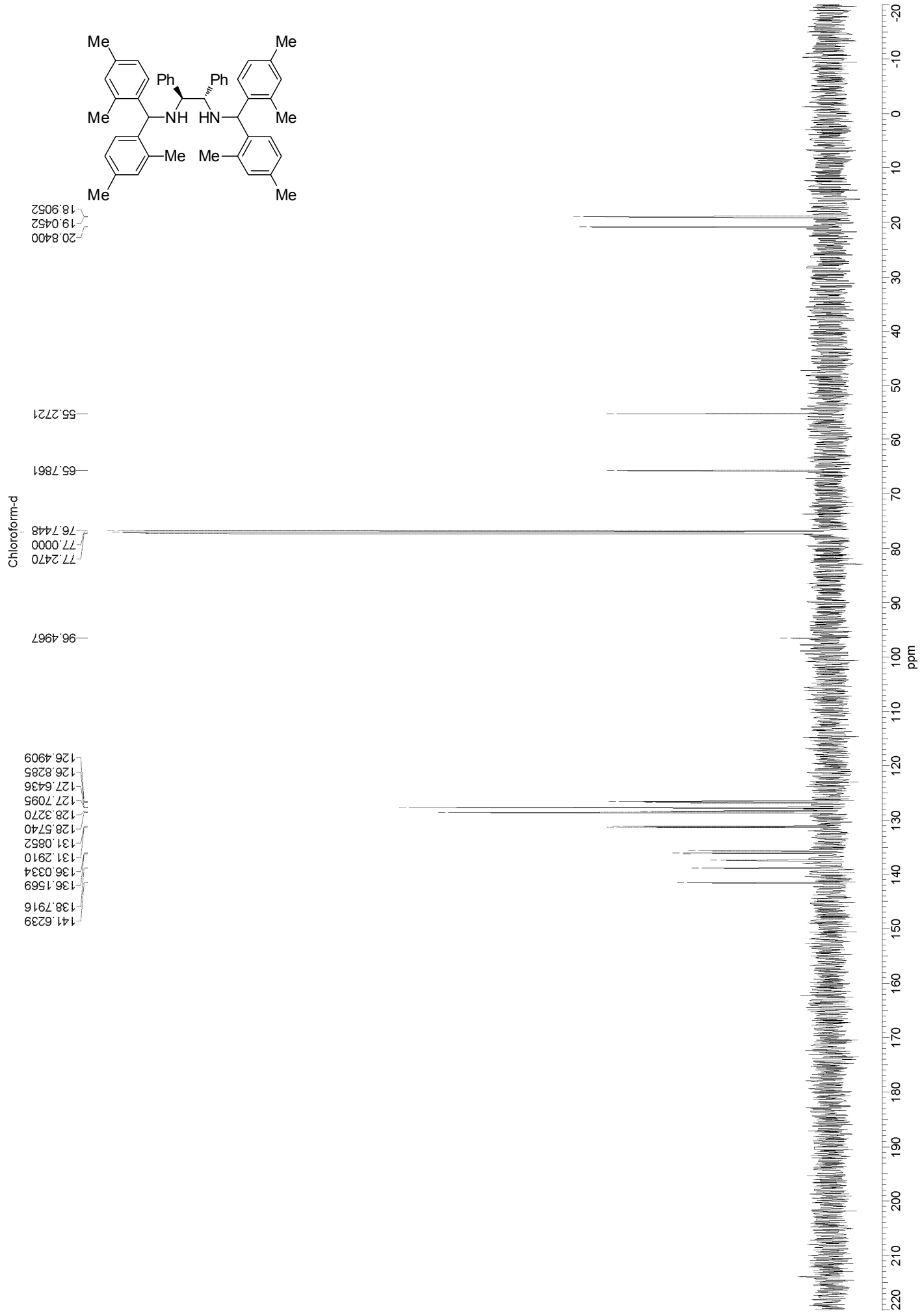
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Me
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65.7861
Chloroform-d
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77.2470
96.4967
126.4909
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128.3270
128.5740
131.0852
131.2910
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138.7916
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-20
-10
0
10
20
30
40
50
60
70
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90
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120
130
140
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180
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200
210
220
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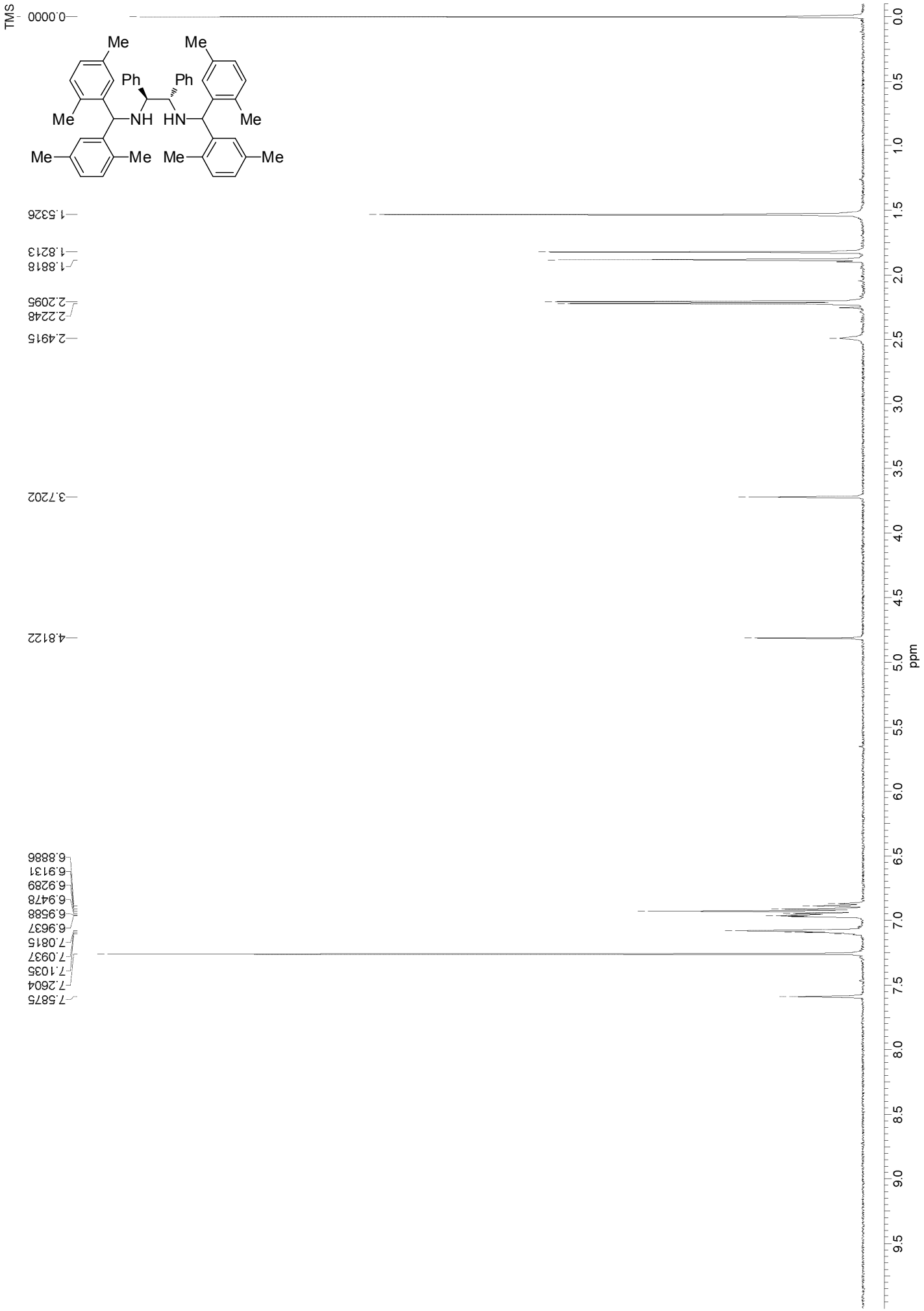
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6.9131
6.9289
6.9478
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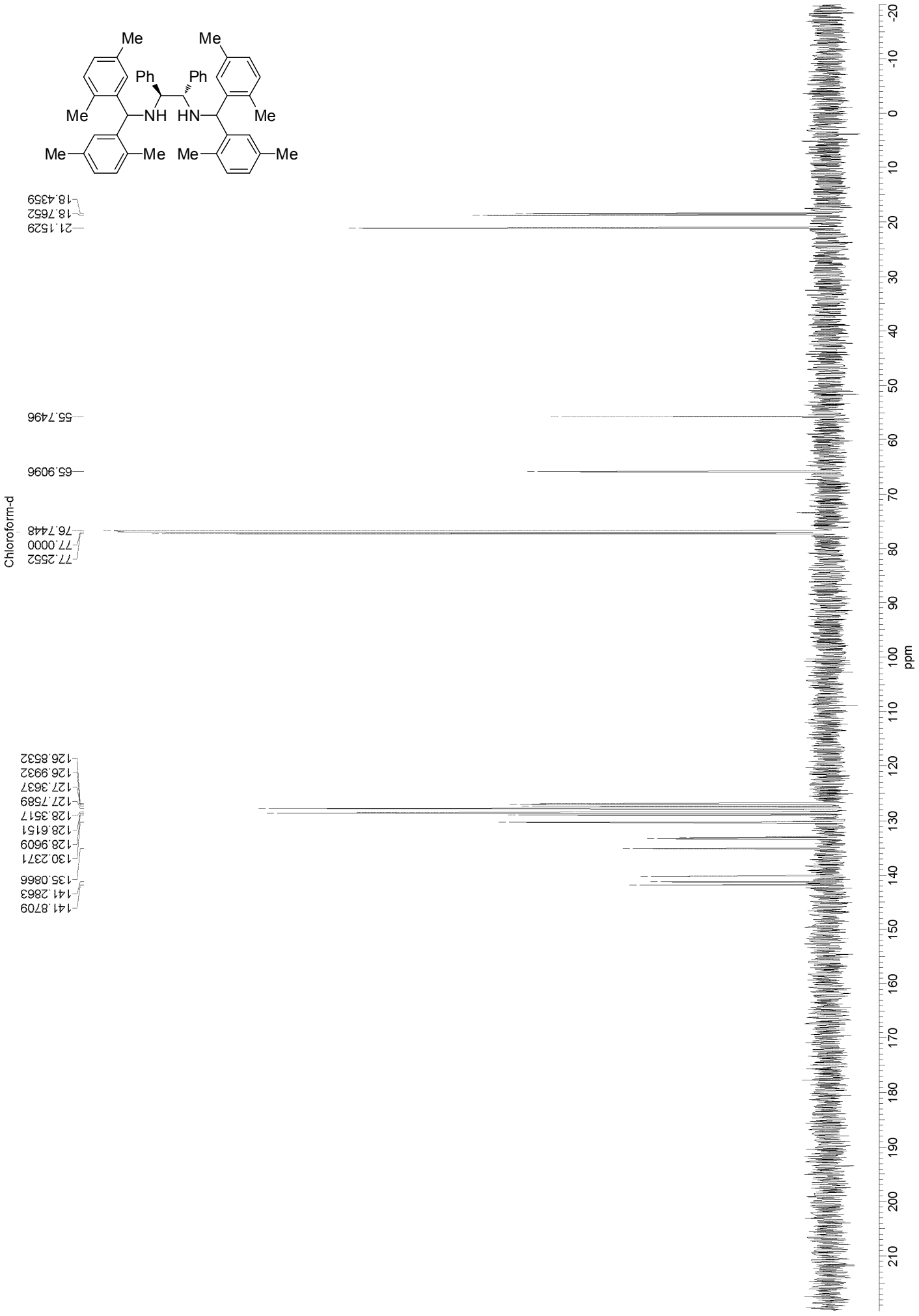
^{13}C-NMR of **E**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Ph
Ph
Me
NH
HN
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Me
Me
Me
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Chloroform-d
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77.2552
126.8532
126.9932
127.3637
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141.8709
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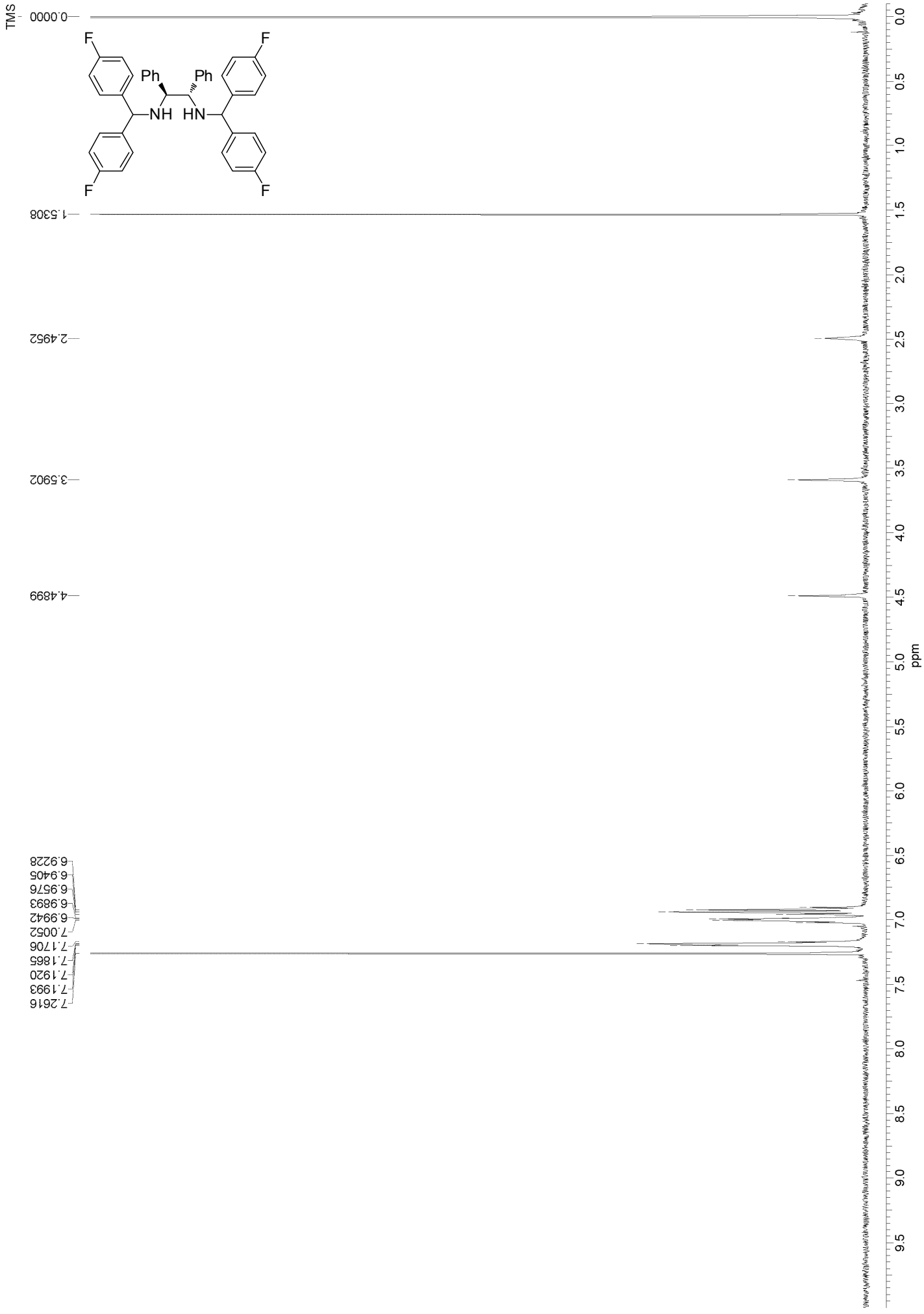
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7.1706
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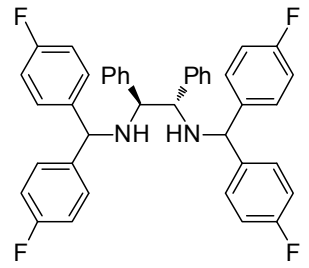
7.1920
7.1993
7.2616
F
F
Ph
Ph
NH
HN
F
F
ppm

^{13}C-NMR of **F**


F
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Ph
Ph
NH
HN
F
F

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115.2523
115.4911
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127.9235
128.1952
128.7222
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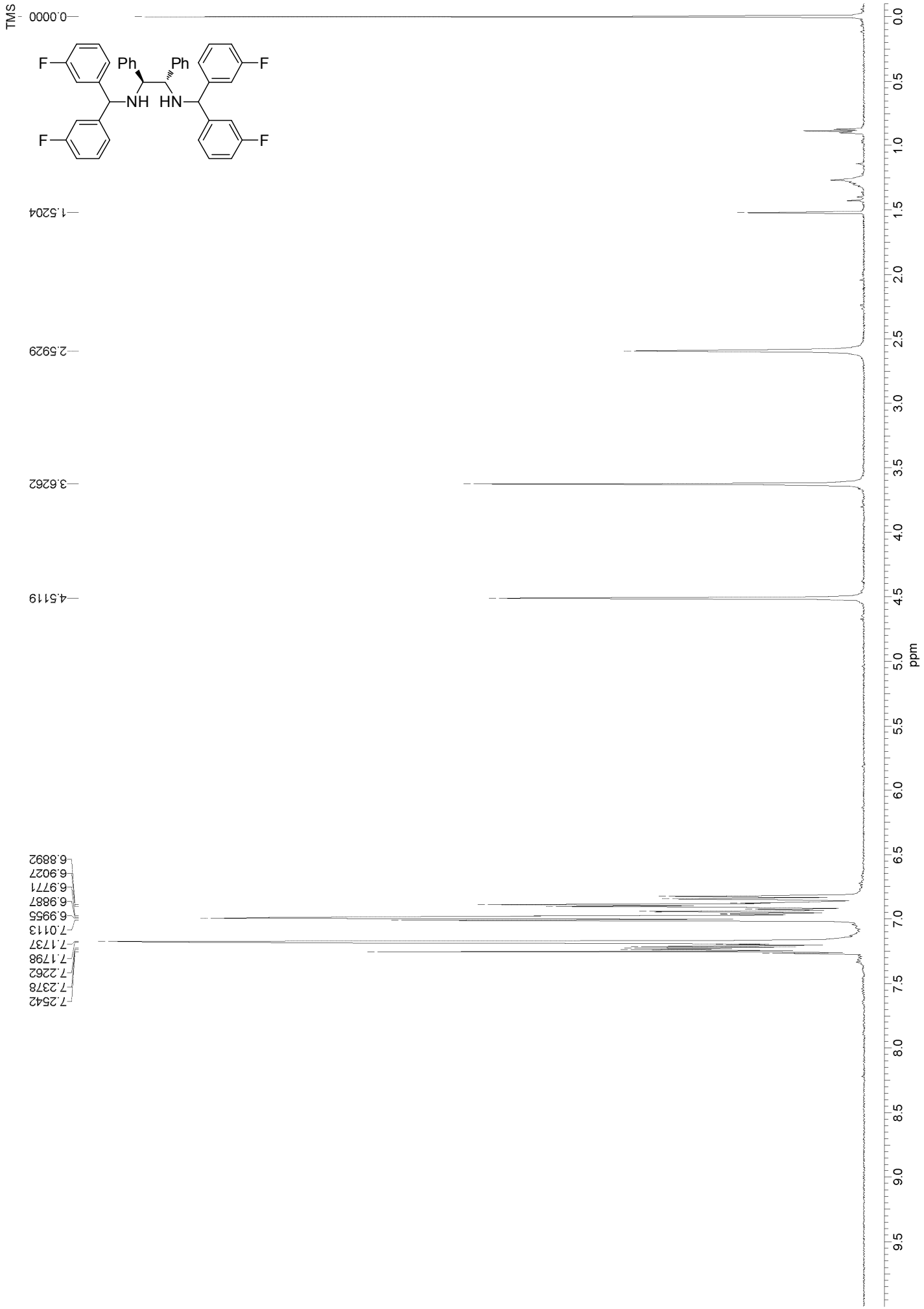
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7.0113
7.1737
7.1798
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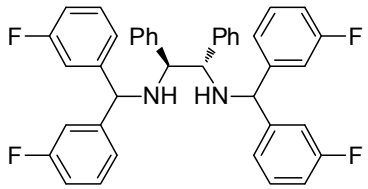
7.2542
F
Ph
Ph
F
NH
HN
F
F
ppm

^{13}C-NMR of **G**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NH
HN
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127.3719
127.8988
128.2446
129.8913
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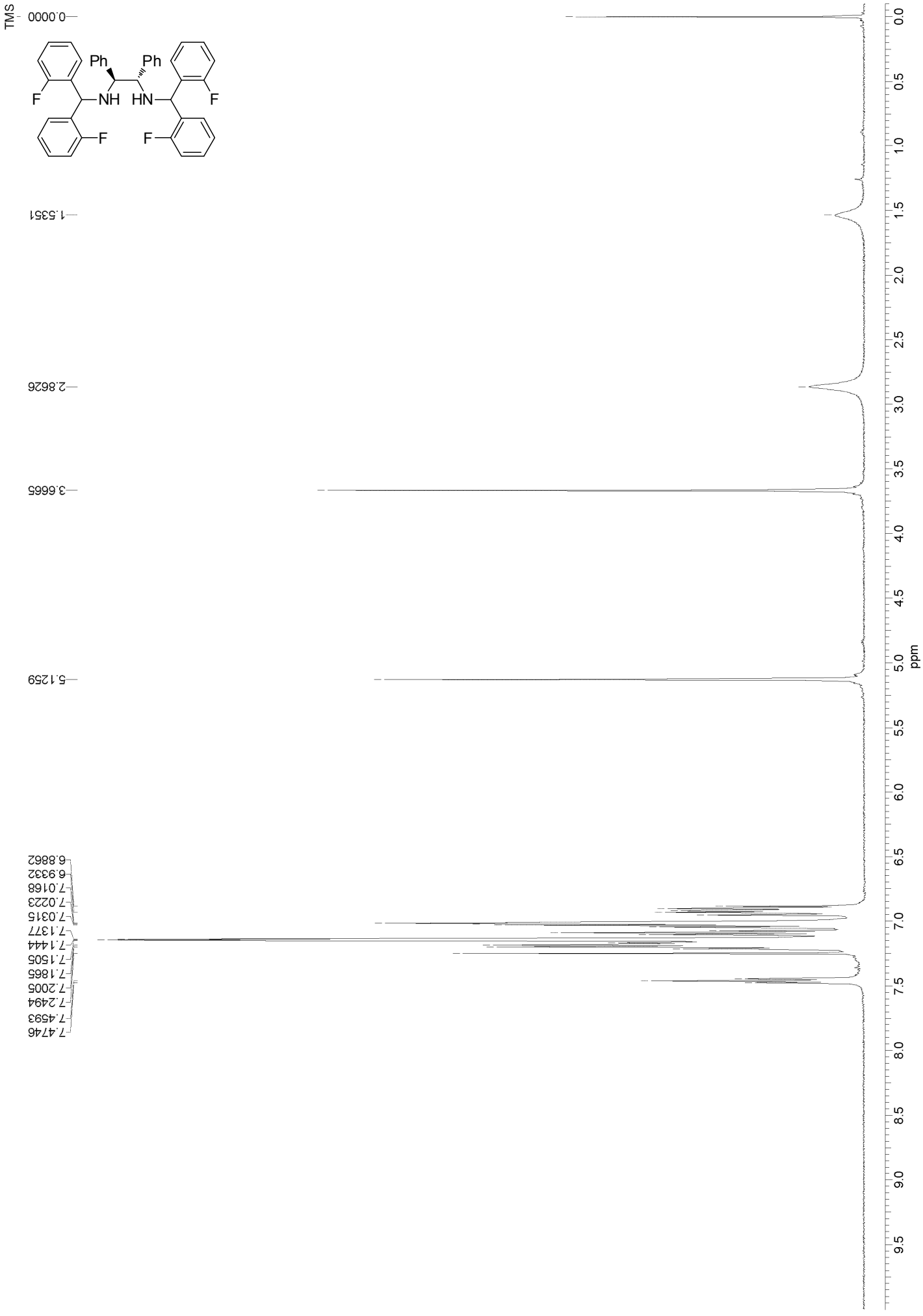
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7.1377
7.1444
7.1505
7.1865
7.2005
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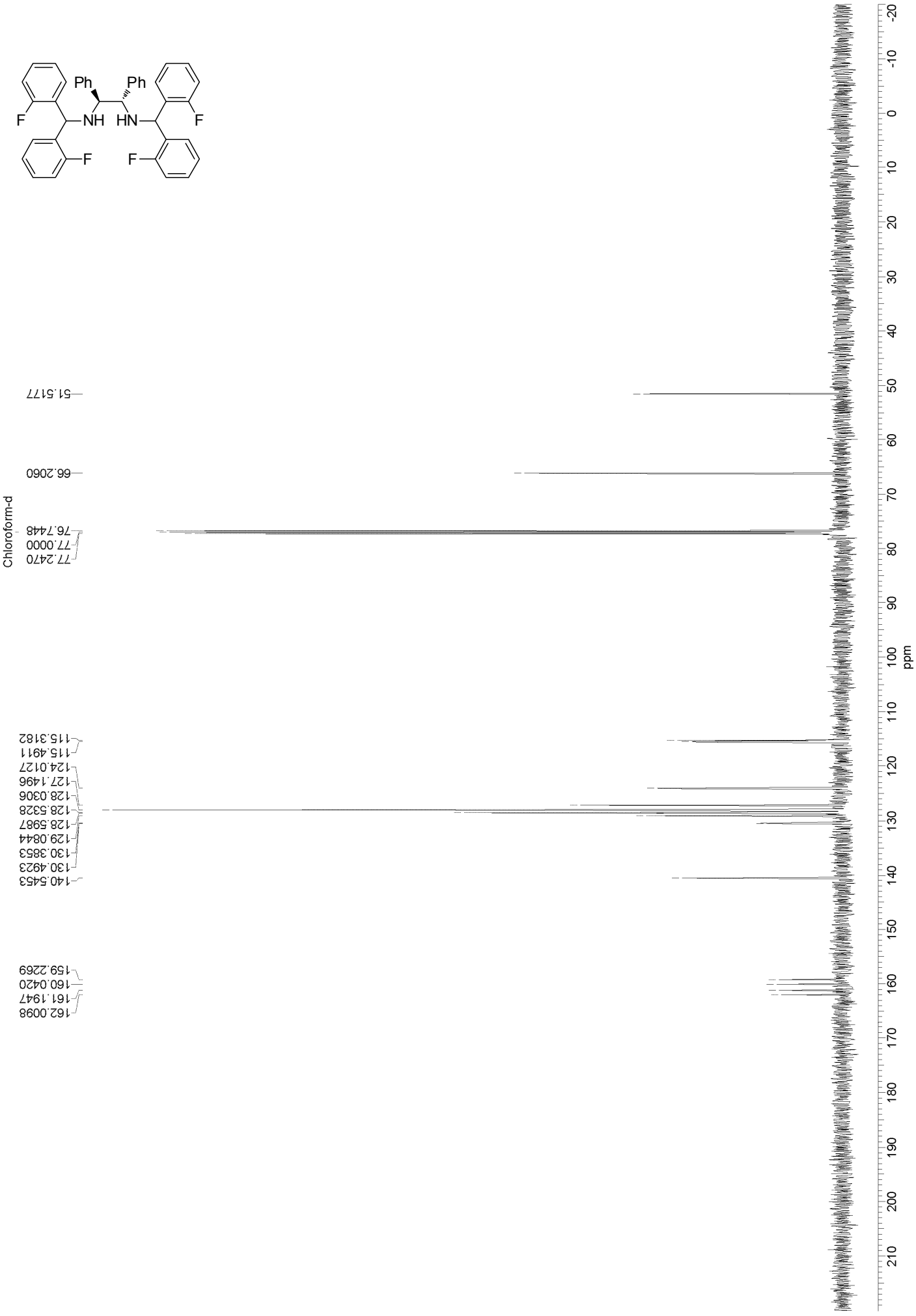
7.4593
7.4746
Ph
Ph
NH
HN
F
F
F
F
ppm

^{13}C-NMR of **H**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115.4911
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128.0306
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128.5987
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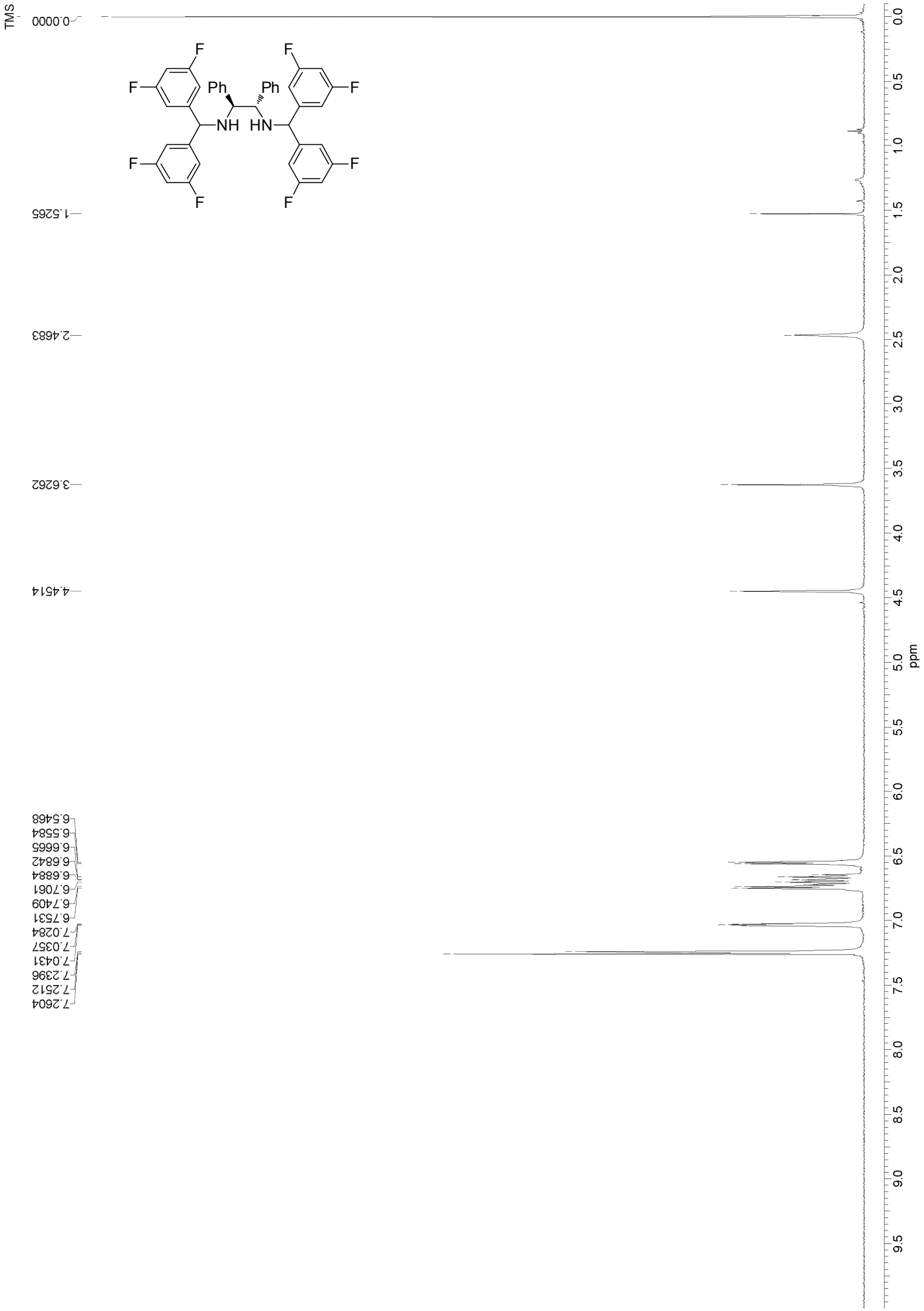
^{1}H-NMR of **I**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6.7409
6.7531
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7.2396
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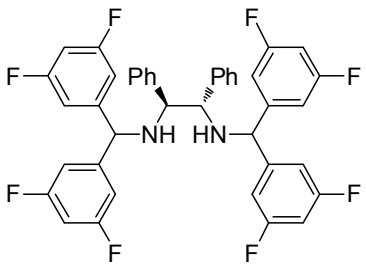
7.2604
F
Ph
NH
HN
ppm

^{13}C-NMR of **I**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F
F
Ph
Ph
F
NH
HN
F
F
F
F

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103.4127
109.9089
110.1147
110.3864
127.6354
127.8577
128.5740
139.5326
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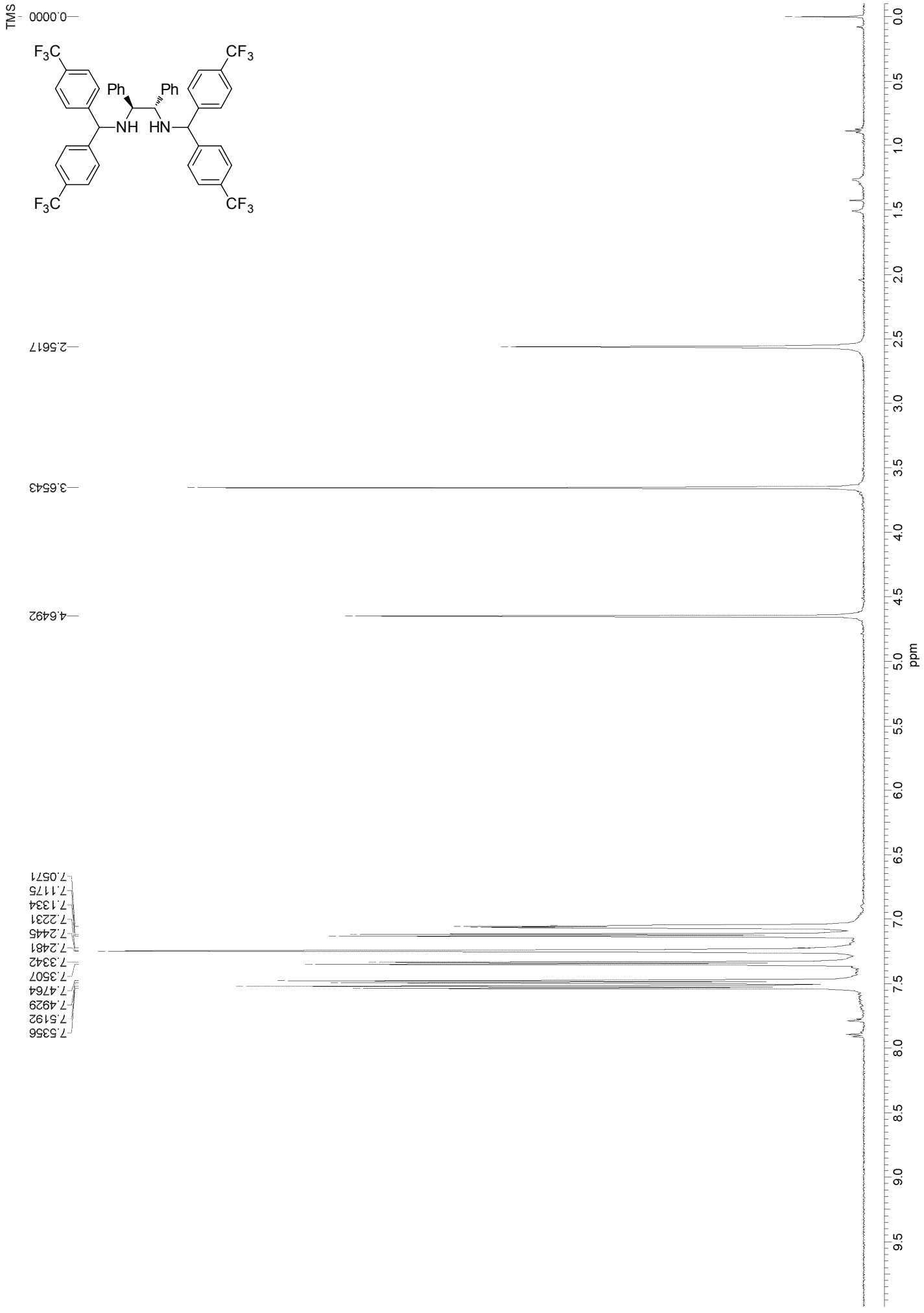
^{1}H-NMR of **J**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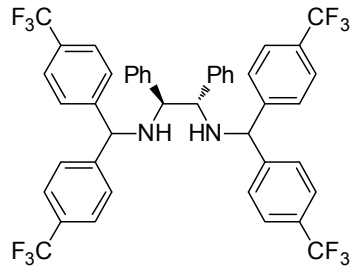
7.2445
7.2481
7.3342
7.3507
7.4764
7.4929
7.5192
7.5356
Ph
Ph
NH
HN
F3C
CF3
F3C
CF3
ppm

^{13}C-NMR of **J**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CF3
Ph
Ph
NH
HN
F3C
CF3

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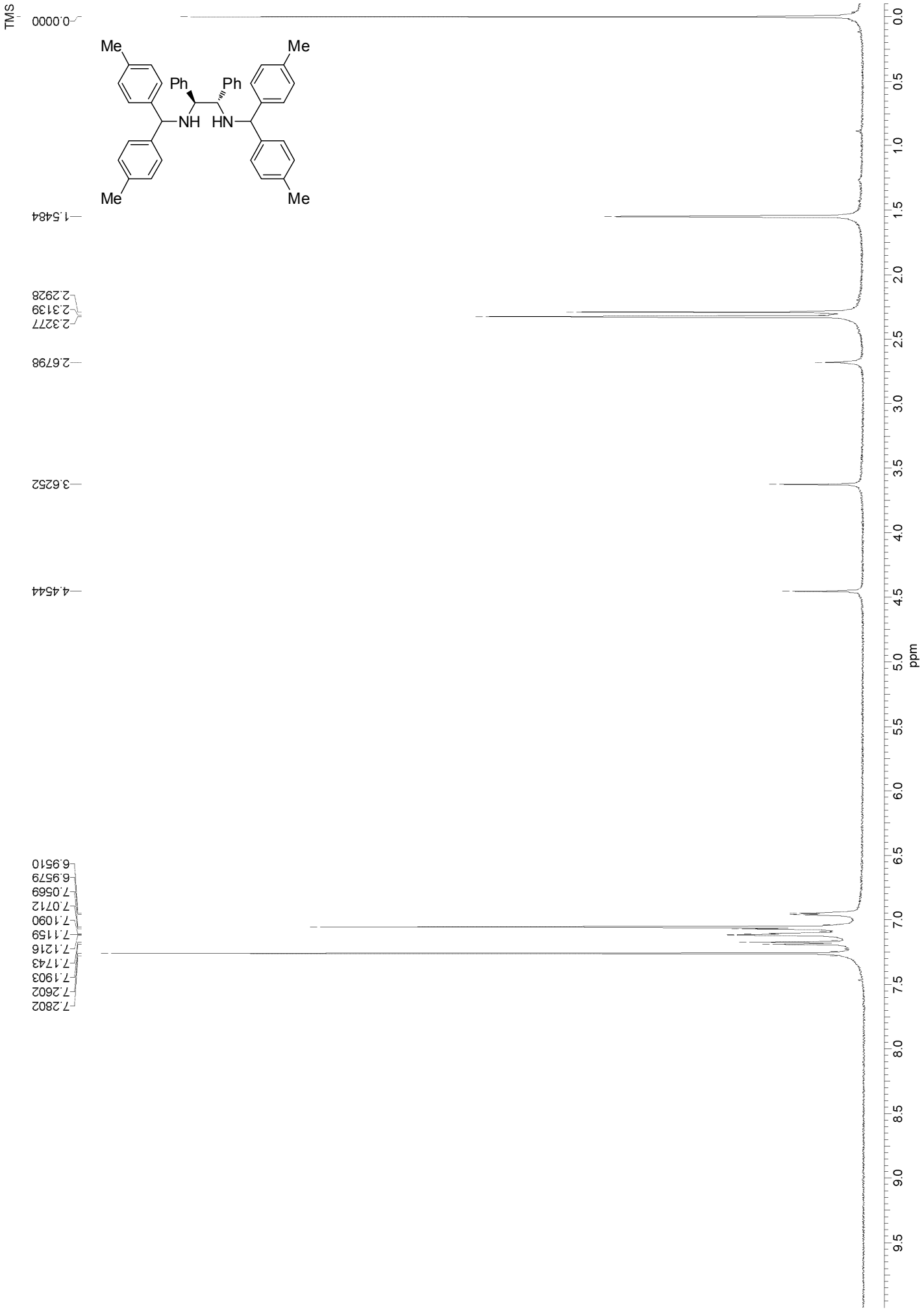
127.5283
127.8659
128.4916
129.5537
129.8831
140.0019
146.3087
147.4202
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
ppm

^{1}H-NMR of **K**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Me
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6.9579
7.0569
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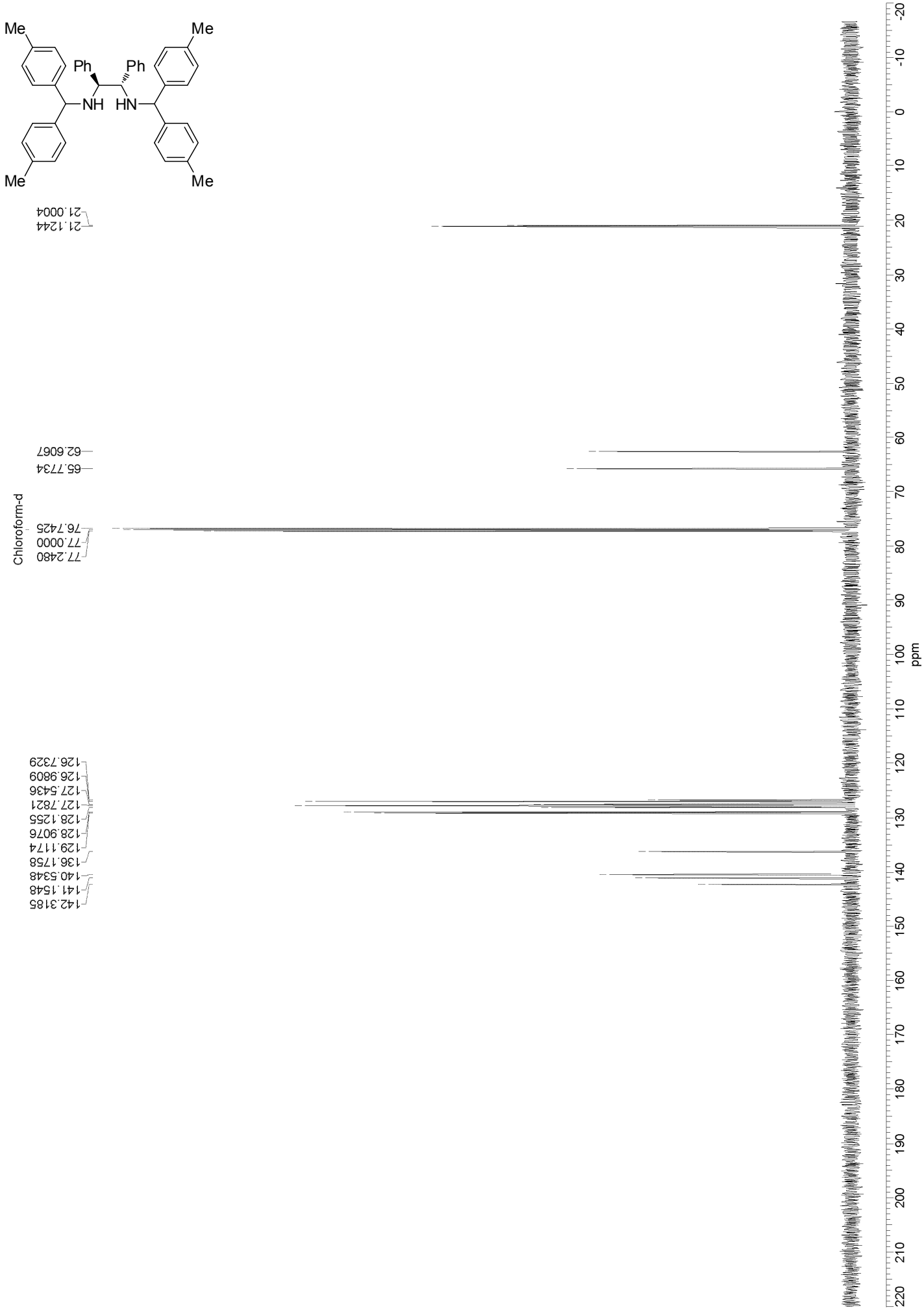
^{13}C-NMR of **K**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77.0000
77.2480
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126.9809
127.5436
127.7821
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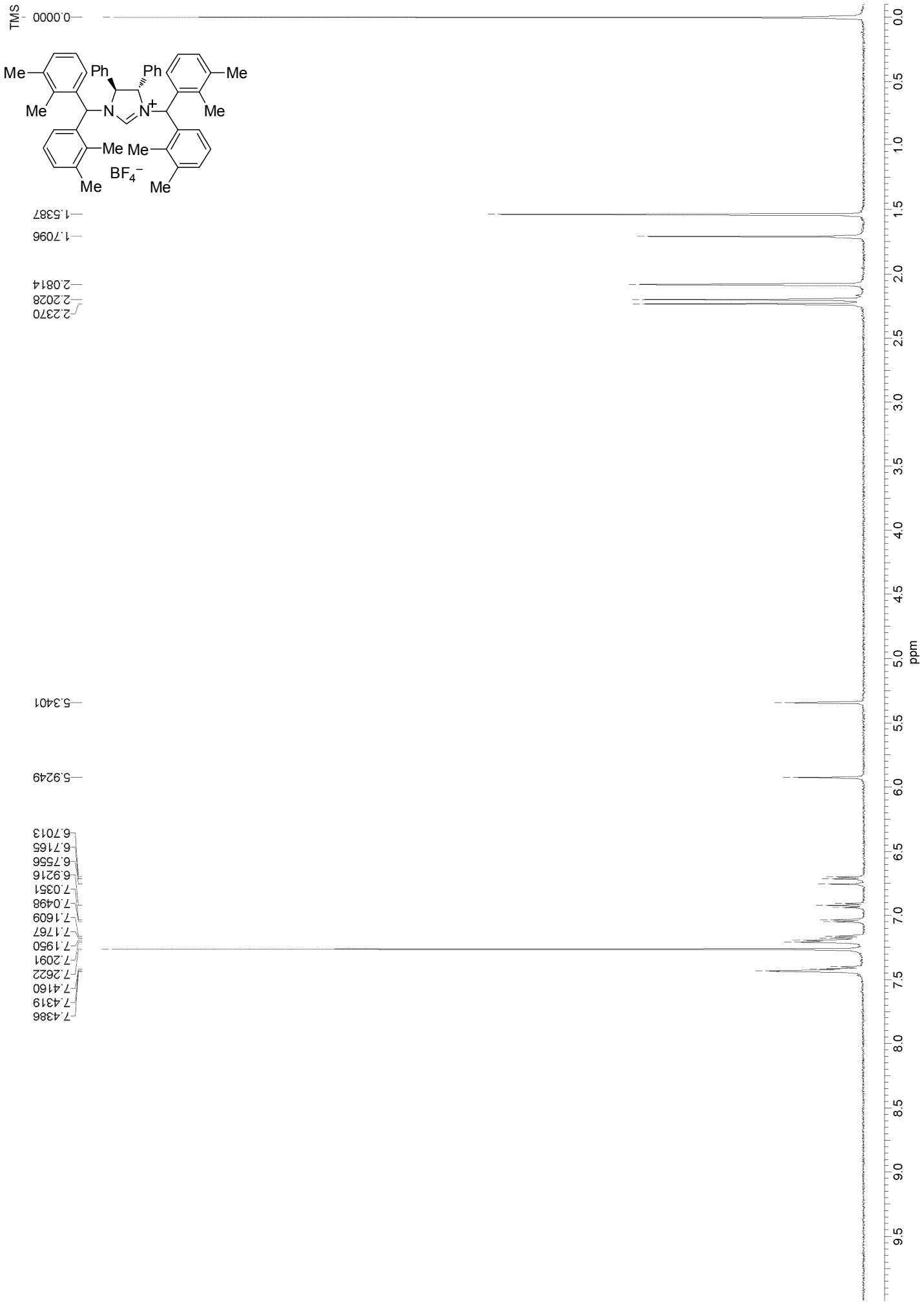
^{1}H-NMR of **C1**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6.7556
6.9216
7.0351
7.0498
7.1609
7.1767
7.1950
7.2091
7.2622
7.4160
7.4319
7.4386
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Ph
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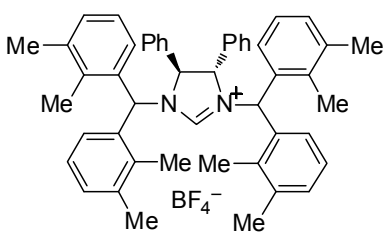
Me
Me
Me
Me
Me
Me
Me
N
N+
BF4−
ppm

^{13}C-NMR of **C1**


Me
Ph
Ph
Me
Me
N
N+
Me
Me Me
BF4−
Me
Me

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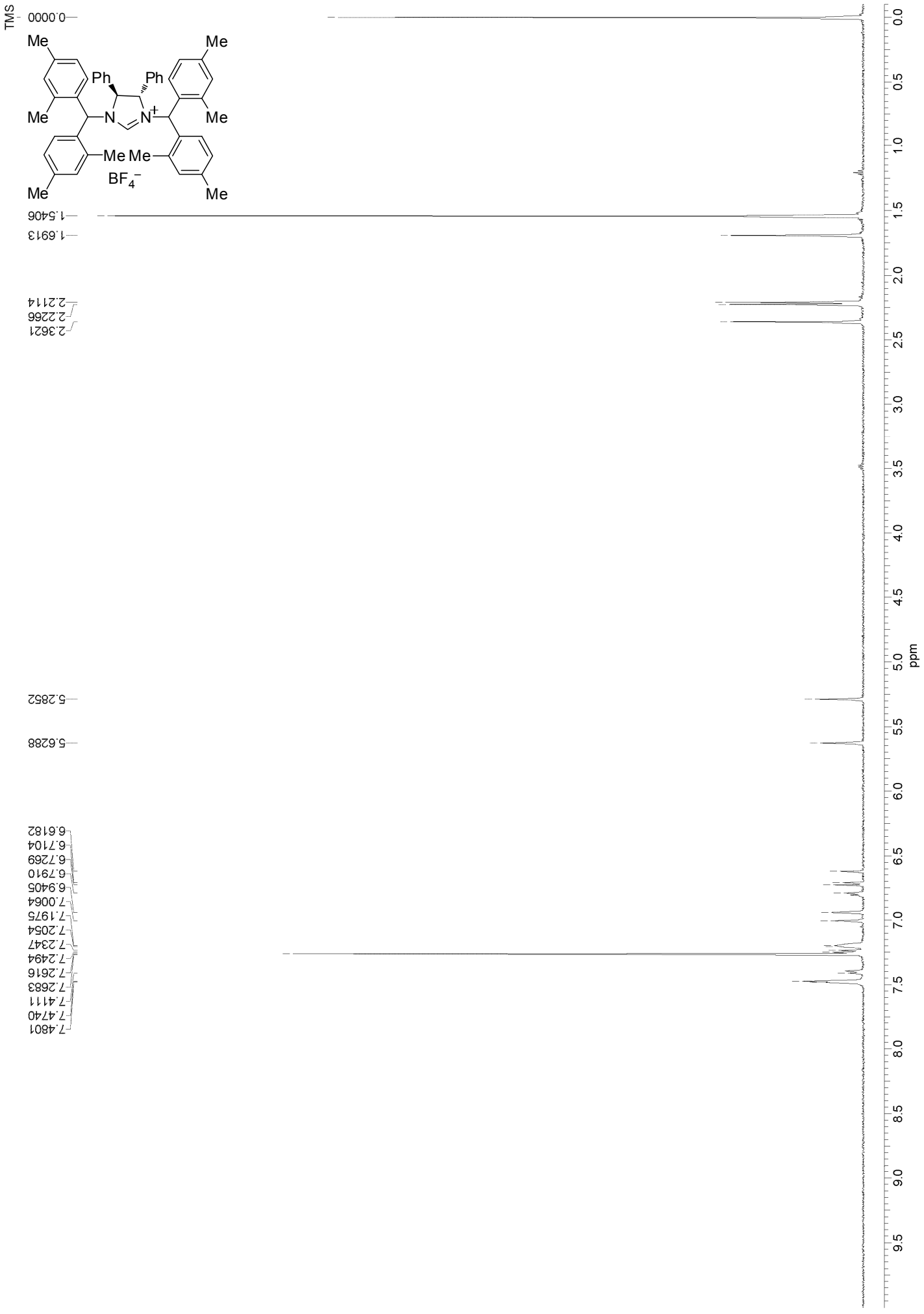
73.1797
76.7448
77.0000
77.2552
Chloroform-d
124.6137
126.2192
126.4498
126.4992
128.5410
129.8501
130.9040
131.2663
131.8262
132.1637
135.1442
138.6105
138.7257
154.6491
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
ppm

^{1}H-NMR of **D1**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6.9405
7.0064
7.1975
7.2054
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7.4801
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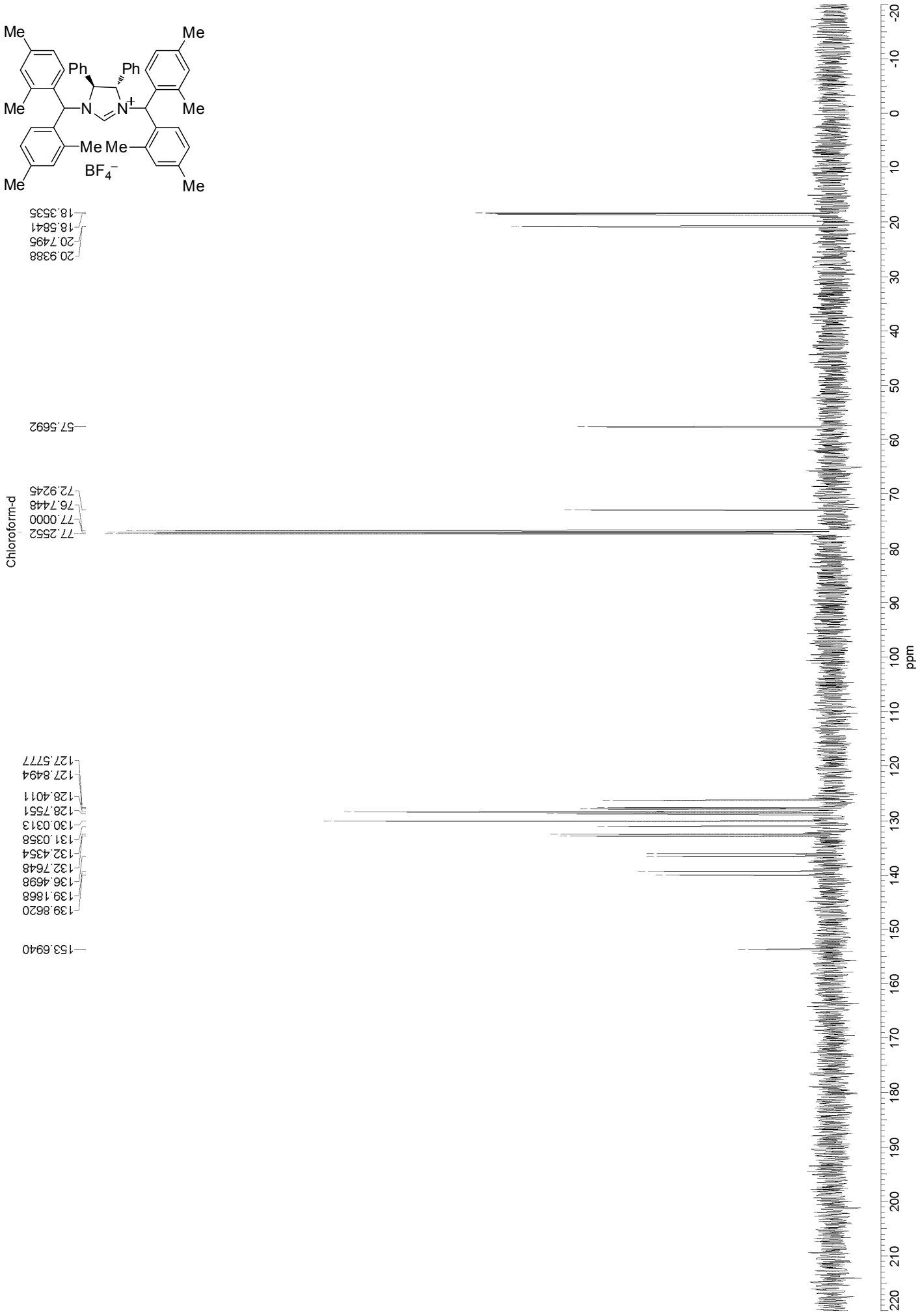
^{13}C-NMR of **D1**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Ph
Ph
Me
N
N+
Me
Me Me
BF4−
Me
Me
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20.9388
57.5692
Chloroform-d
72.9245
76.7448
77.0000
77.2552
127.5777
127.8494
128.4011
128.7551
130.0313
131.0358
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132.7648
136.4698
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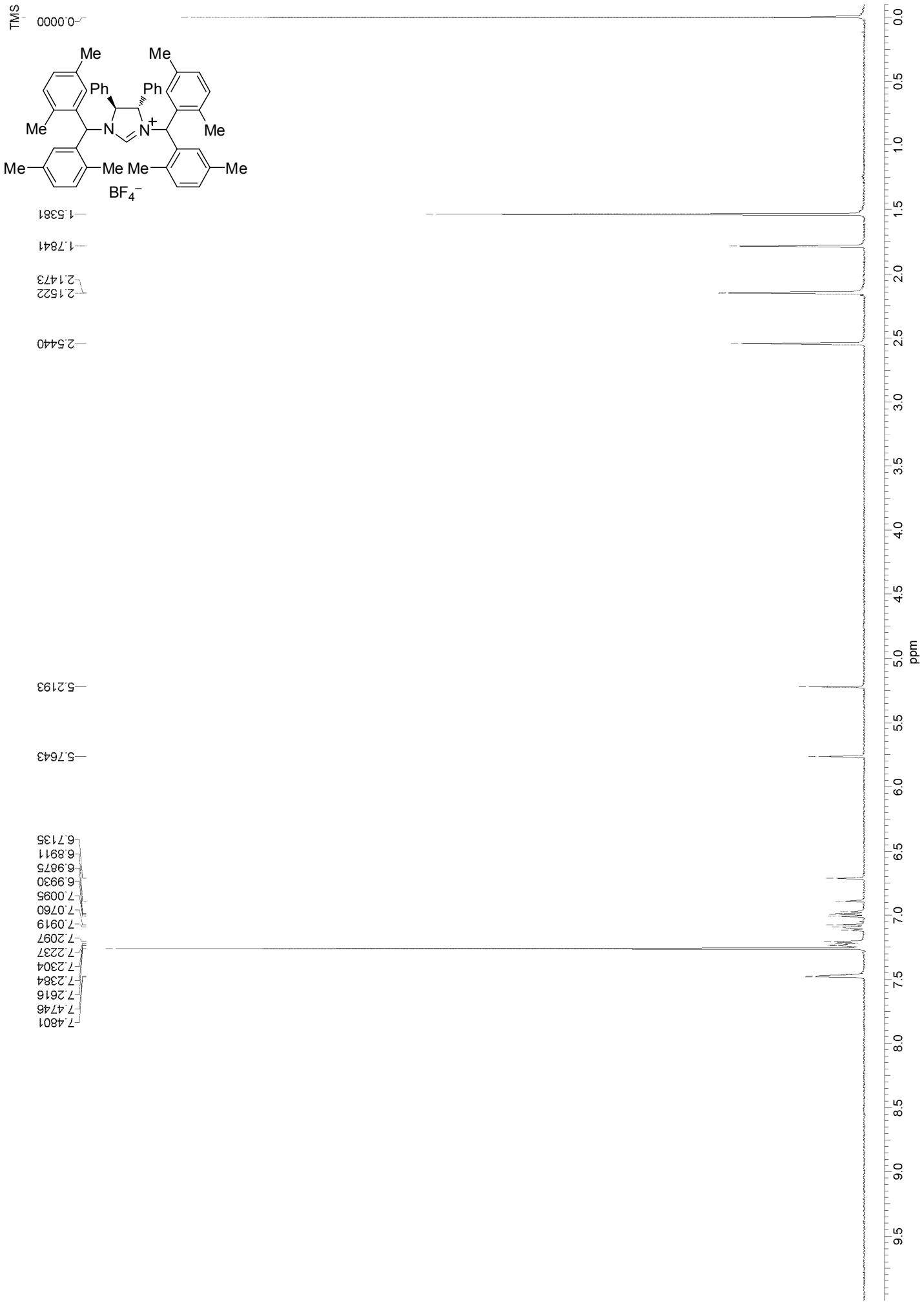
139.8620
153.6940
ppm

^{1}H-NMR of **E1**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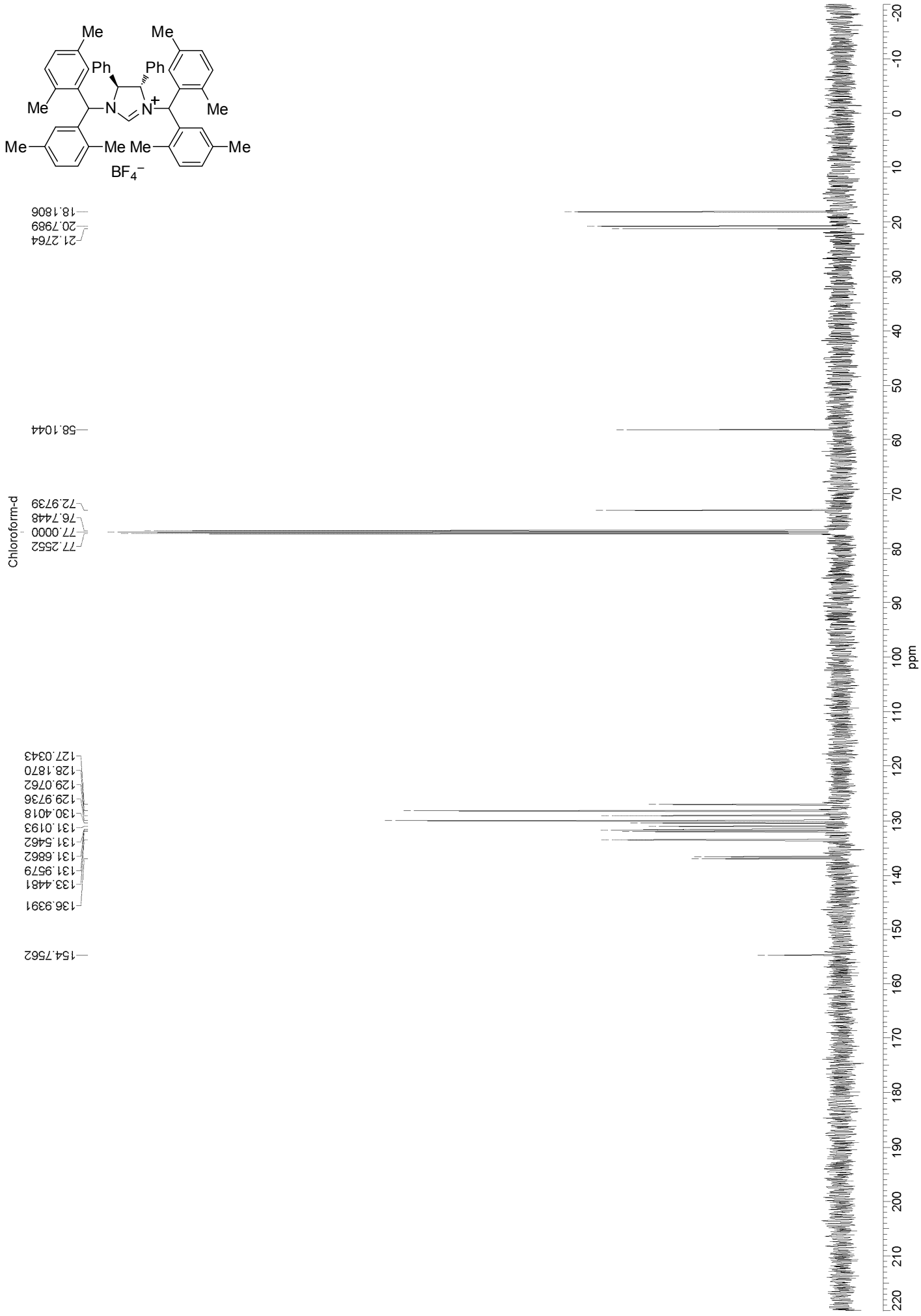
6.7135
6.8911
6.9875
6.9930
7.0095
7.0760
7.0919
7.2097
7.2237
7.2304
7.2384
7.2616
7.4746
7.4801
Me
Ph
N
N+
BF4−
ppm

^{13}C-NMR of **E1**


Me
Me
Ph
Ph
Me
N
N+
Me
Me
Me Me
Me
BF4−
18.1806
20.7989
21.2764
58.1044
Chloroform-d
72.9739
76.7448
77.0000
77.2552
127.0343
128.1870
129.0762
129.9736
130.4018
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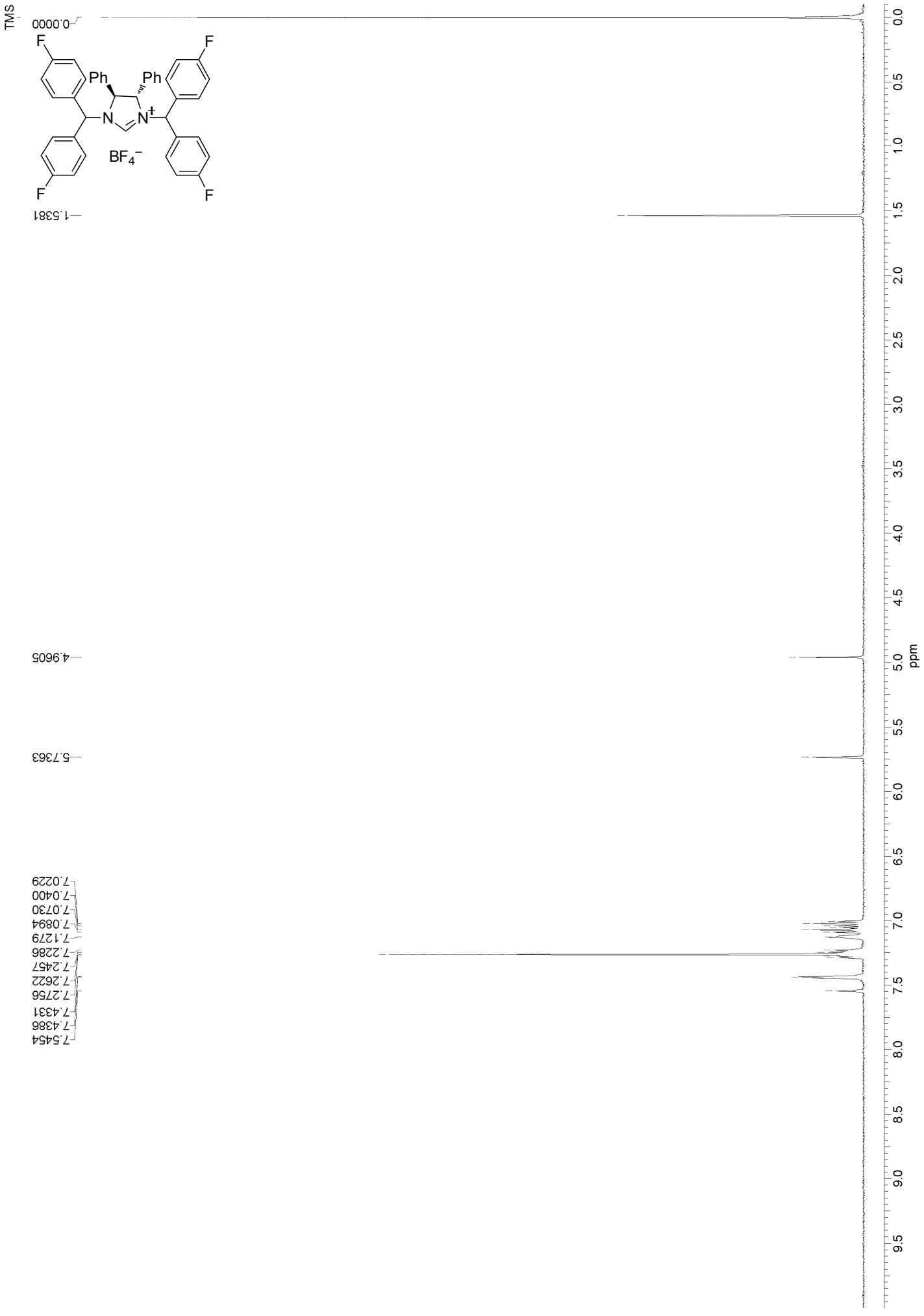
^{1}H-NMR of **F1**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7.0400
7.0730
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7.1279
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7.2622
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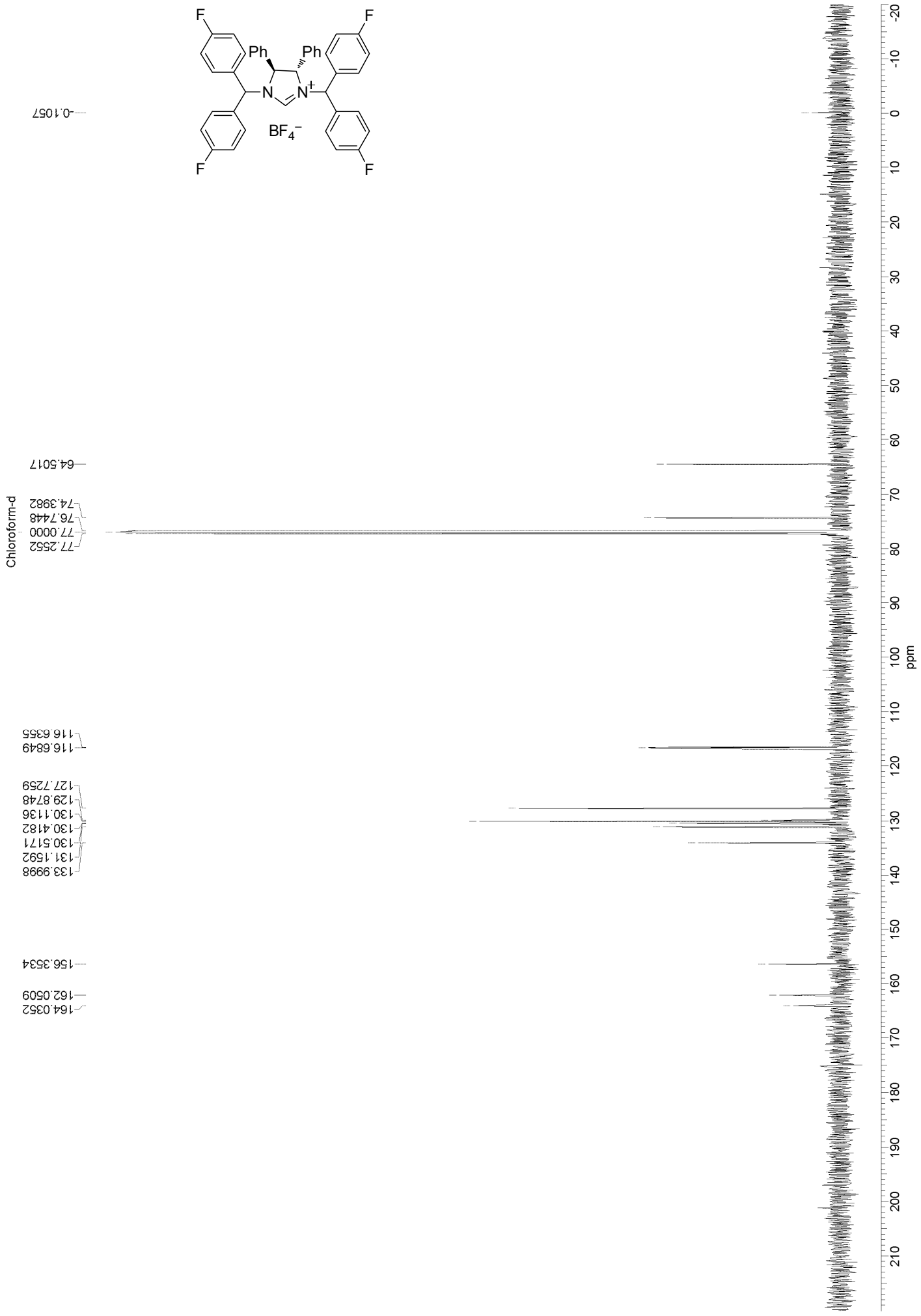
^{13}C-NMR of **F1**


F
F
Ph
Ph
N
N+
BF4−
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Chloroform-d
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77.0000
77.2552
116.6355
116.6849
127.7259
129.8748
130.1136
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156.3534
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164.0352
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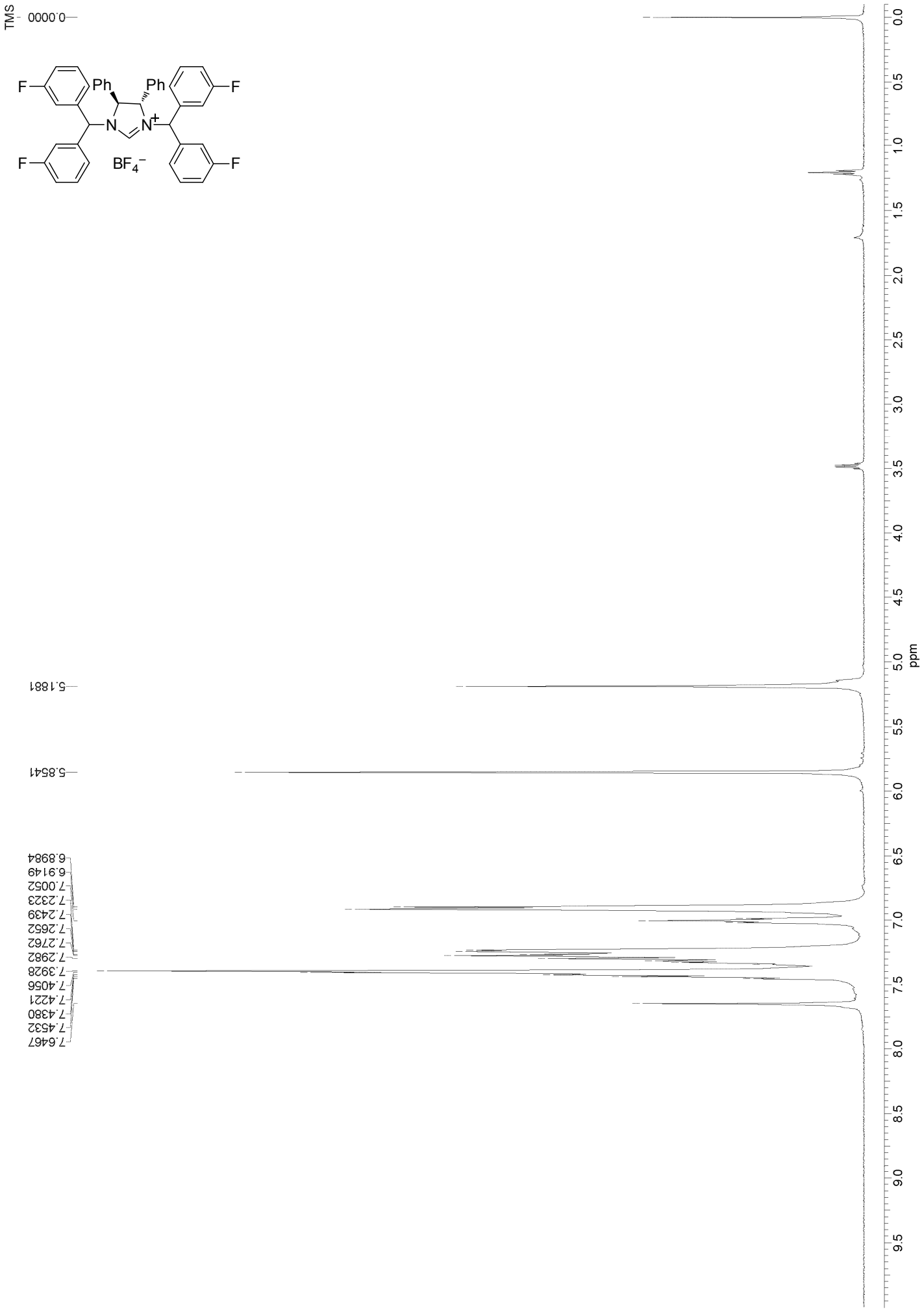
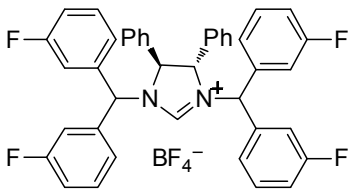
^{1}H-NMR of **G1**

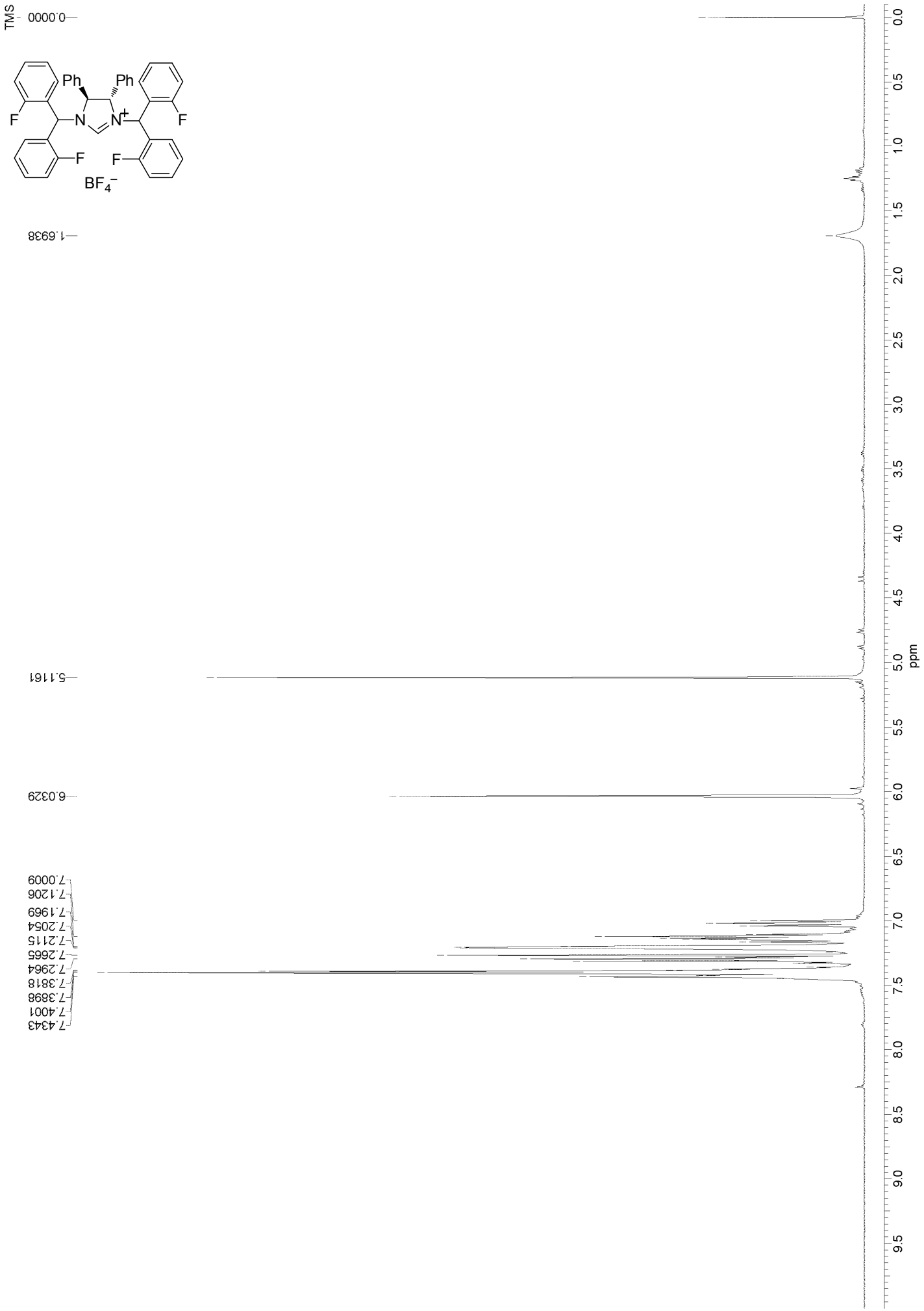

TMS
0.0000
F
Ph
Ph
F
N
N+
F
BF4−
F
5.1881
5.8541
6.8984
6.9149
7.0052
7.2323
7.2439
7.2652
7.2762
7.2982
7.3928
7.4056
7.4221
7.4380
7.4532
7.6467
ppm

^{13}C-NMR of **G1**

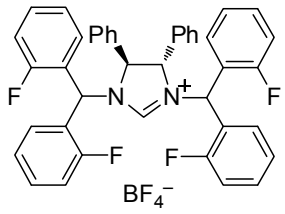

F
Ph
Ph
F
N
N+
F
BF4−
F

64.7734
Chloroform-d
74.4641
76.7448
77.0000
77.2552
115.2606
115.5652
115.7463
116.6026
116.7673
124.0374
125.0501
127.6683
130.0560
130.4429
131.5709
134.0245
136.3463
136.7827
136.8321
157.4485
161.8863
163.8705
164.0599
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
ppm

^{1}H-NMR of **H1**

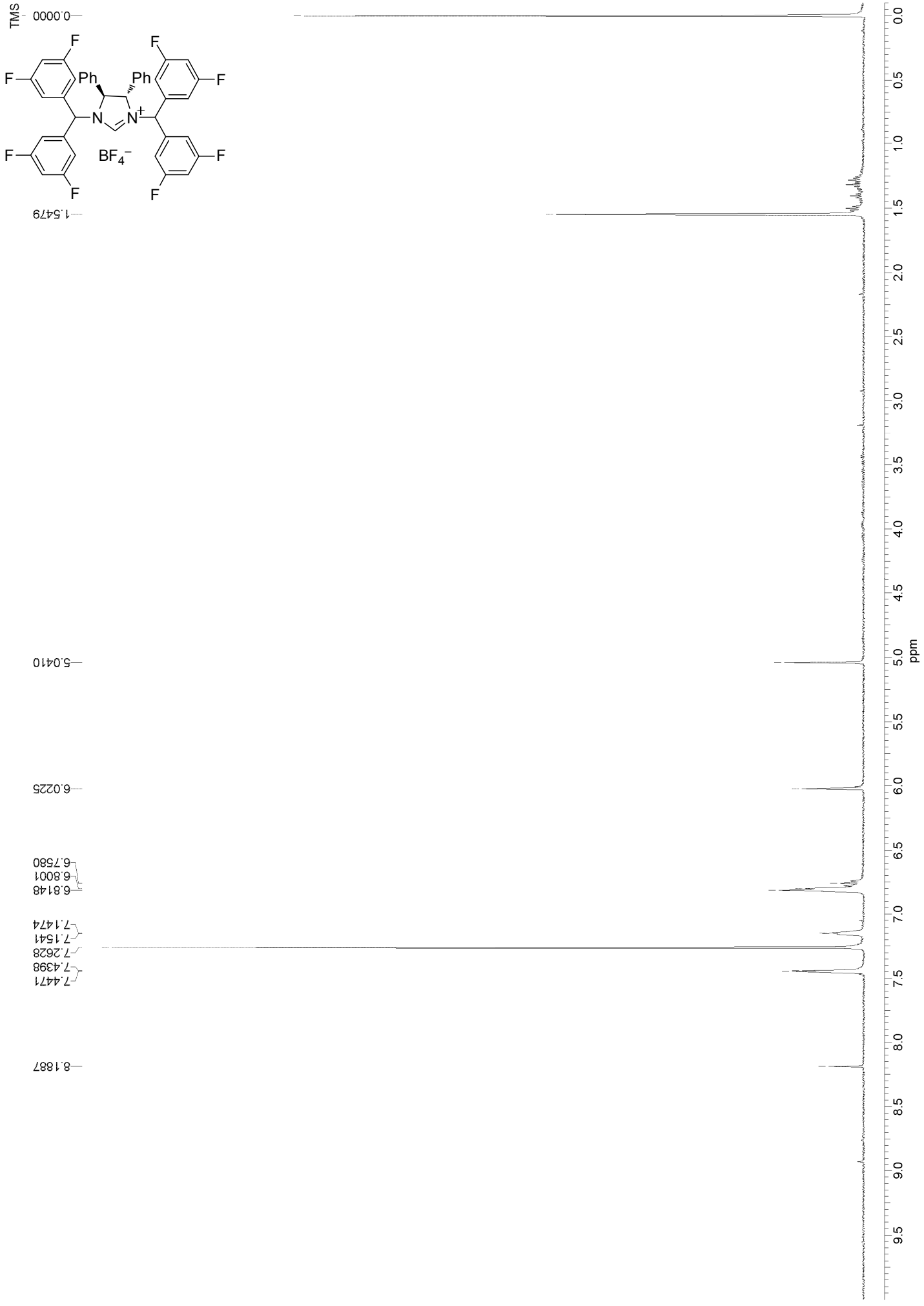

TMS
0.0000
1.6938
5.1161
6.0329
7.0009
7.1206
7.1969
7.2054
7.2115
7.2665
7.2964
7.3818
7.3898
7.4001
7.4343
Ph
Ph
F
F
F
F
N
N+
BF4−
ppm

^{13}C-NMR of **H1**

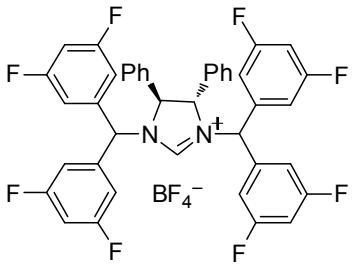

Ph
Ph
F
N
N+
F
F
F
BF4−

54.8028
Chloroform-d
77.2552
77.0000
76.7448
75.0569
133.1435
131.9332
131.1181
130.5747
130.3359
129.8501
127.9565
125.8075
125.6182
120.5958
120.2582
116.1992
115.8287
115.6640
161.2605
160.8983
159.2845
158.9223
155.7771
ppm

^{1}H-NMR of **I1**

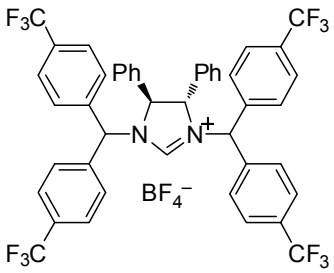

TMS
0.0000
1.5479
5.0410
6.0225
6.7580
6.8001
6.8148
7.1474
7.1541
7.2628
7.4398
7.4471
8.1887
ppm

^{13}C-NMR of **I1**


F
F
F
Ph
Ph
F
N
N
F
F
BF4−
F
F

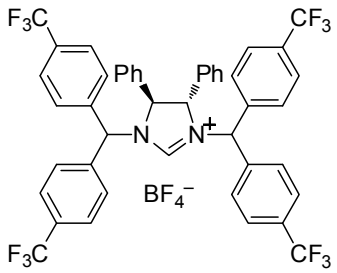
53.3581
53.5804
53.7944
54.0085
54.2308
64.6872
74.9625
105.4919
105.6895
105.8954
112.1116
112.3256
112.4491
112.6714
127.9526
130.5132
131.0895
134.1194
137.7009
137.7668
138.1373
138.2114
158.6879
162.9445
164.8464
164.9535
ppm

^{1}H-NMR of **J1**


F3C
CF3
Ph
Ph
N
N+
BF4−
F3C
CF3

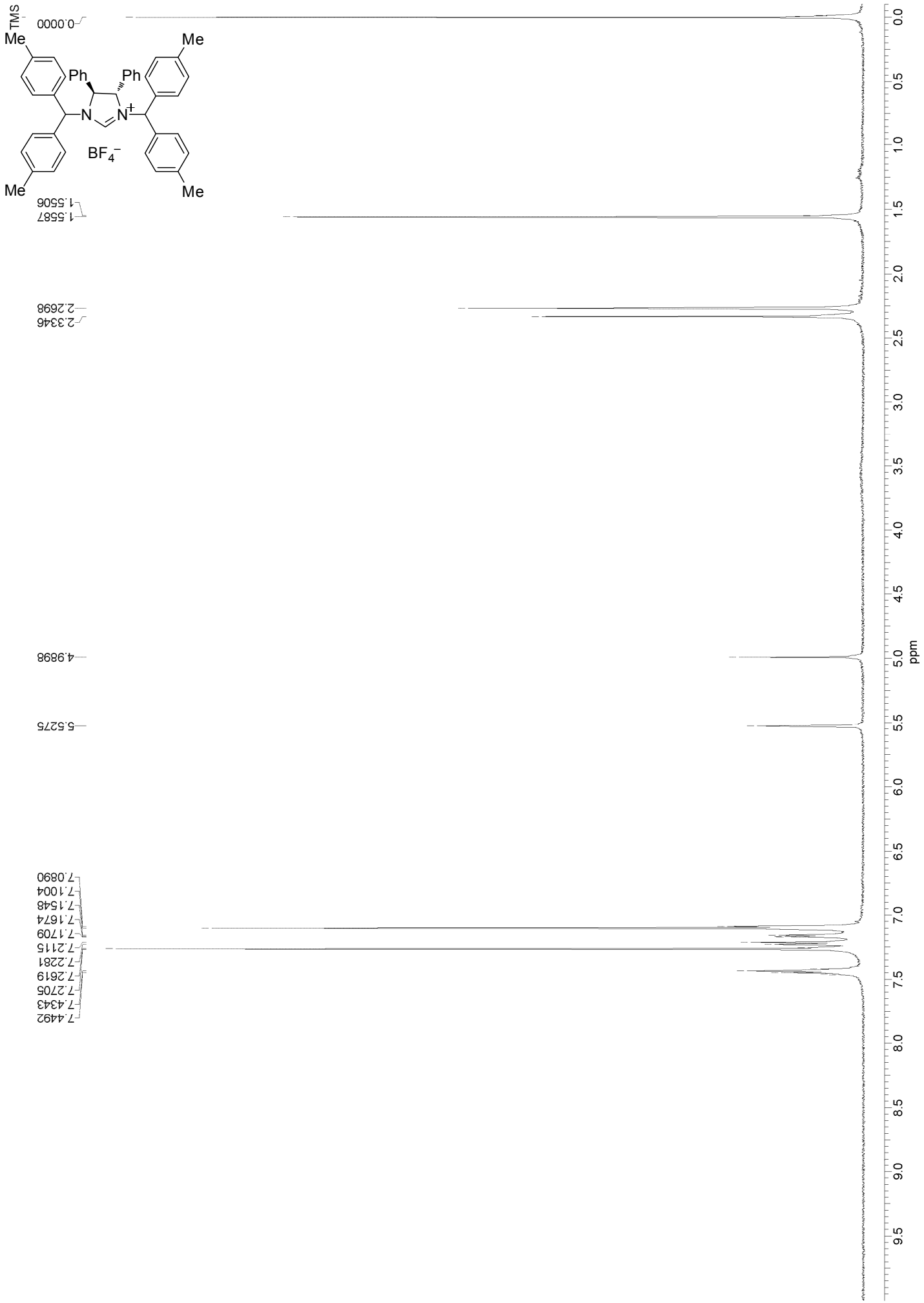
1.5510
Dichloromethane-d2
5.1424
5.3200
5.3304
5.9603
7.1859
7.4410
7.4539
7.4642
7.4722
7.5973
7.6132
7.6504
7.6663
ppm

^{13}C-NMR of **J1**

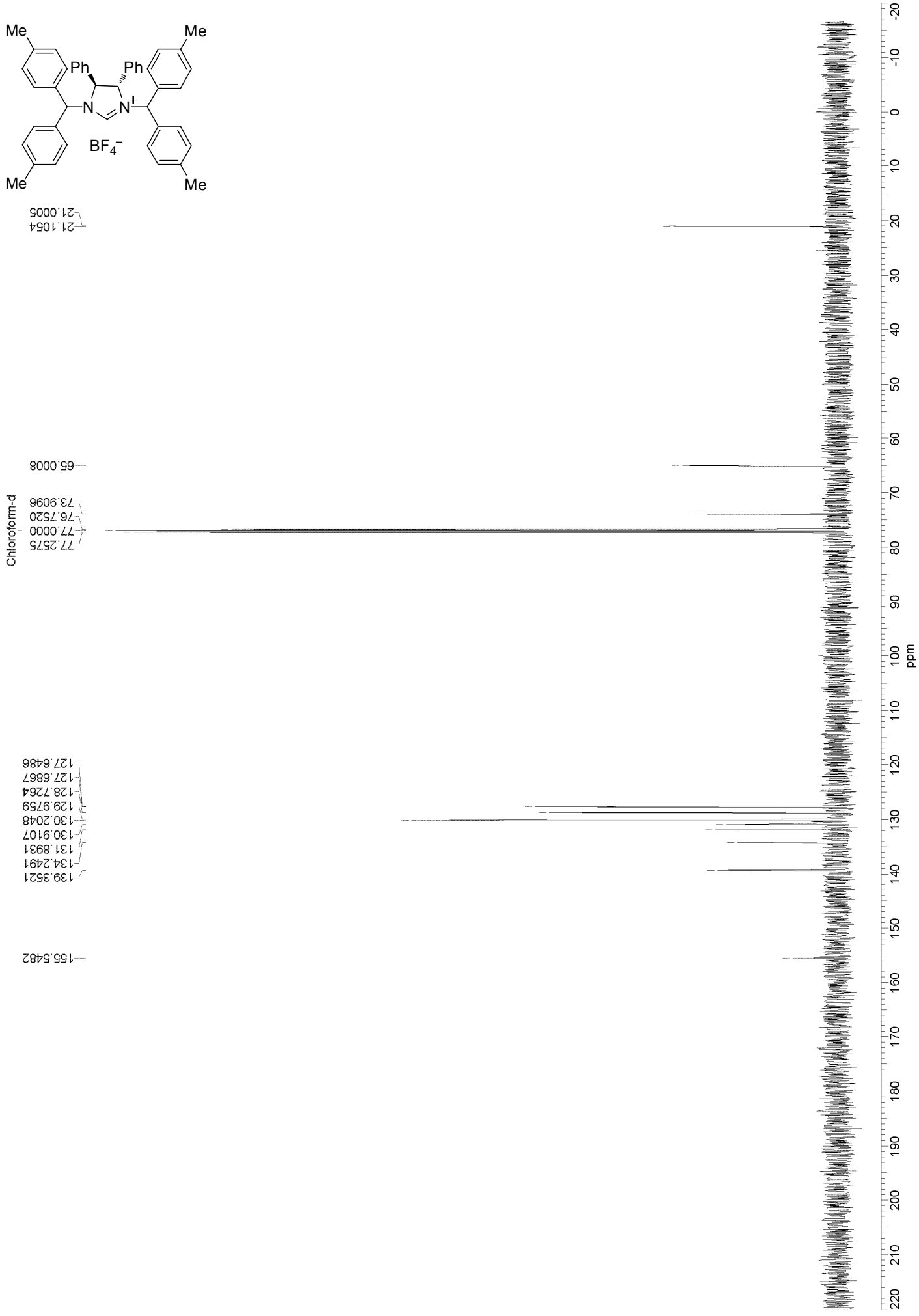

F3C
CF3
Ph
Ph
N
N+
BF4−
F3C
CF3

53.3581
53.5721
53.7944
54.0085
54.2226
65.3294
74.9707
122.8726
122.9961
125.0462
127.0469
128.1337
129.3111
130.0356
130.5955
131.0895
131.8882
132.1434
133.9877
137.9397
138.5572
157.5846
ppm

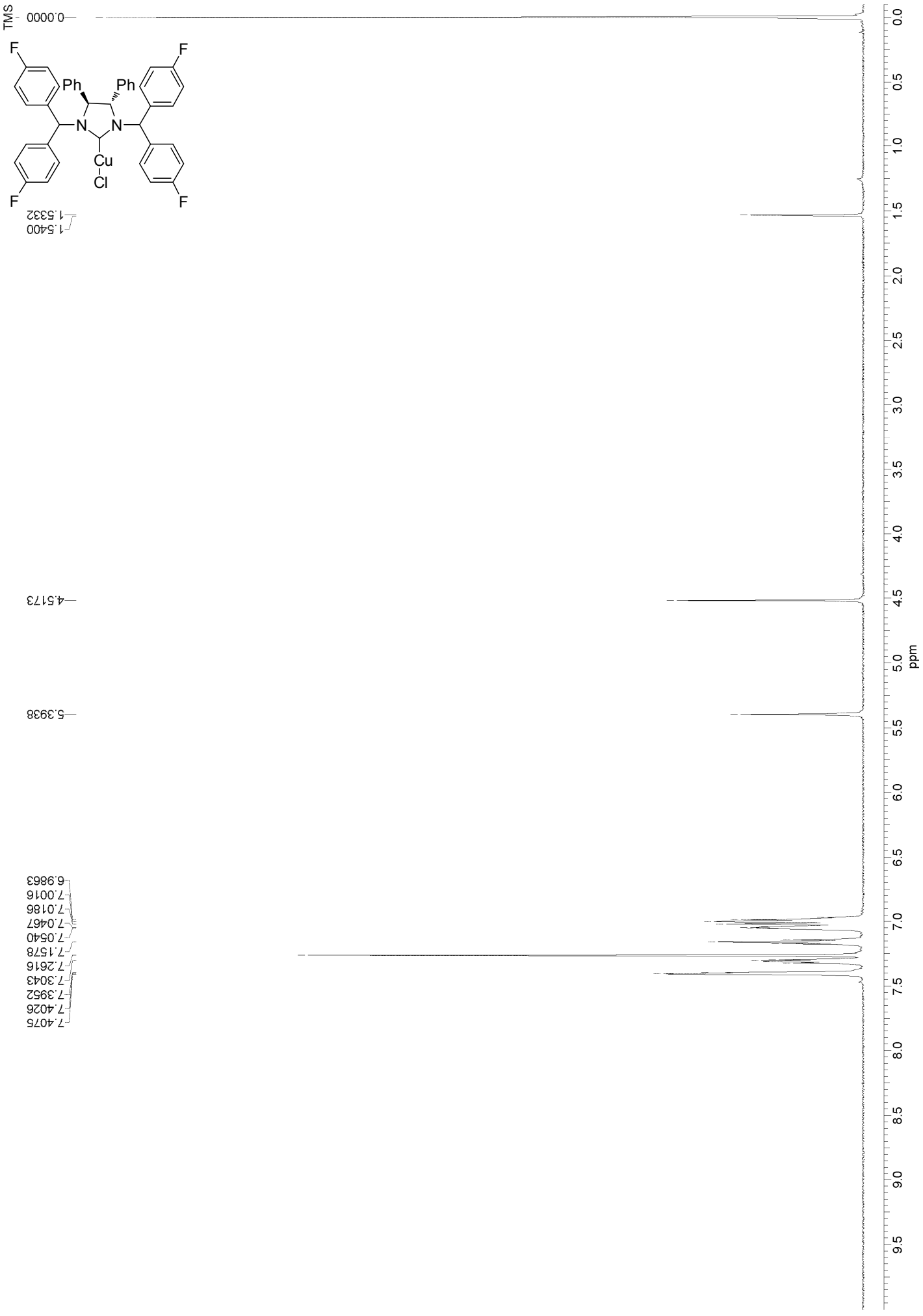
^{1}H-NMR of **K1**


TMS
0.0000
Me
Me
Ph
Ph
N
N+
BF4−
Me
Me
1.5506
1.5587
2.2698
2.3346
4.9898
5.5275
7.0890
7.1004
7.1548
7.1674
7.1709
7.2115
7.2281
7.2619
7.2705
7.4343
7.4492
ppm

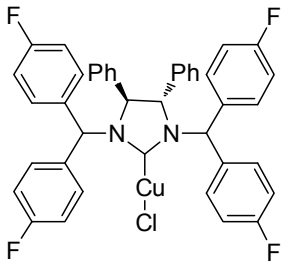
^{13}C-NMR of **K1**


Me
Me
Ph
Ph
N
N+
BF4−
Me
Me
21.0005
21.1054
65.0008
Chloroform-d
73.9096
76.7520
77.0000
77.2575
127.6486
127.6867
128.7264
129.9759
130.2048
130.9107
131.8931
134.2491
139.3521
155.5482
ppm

^{1}H-NMR of **1f**

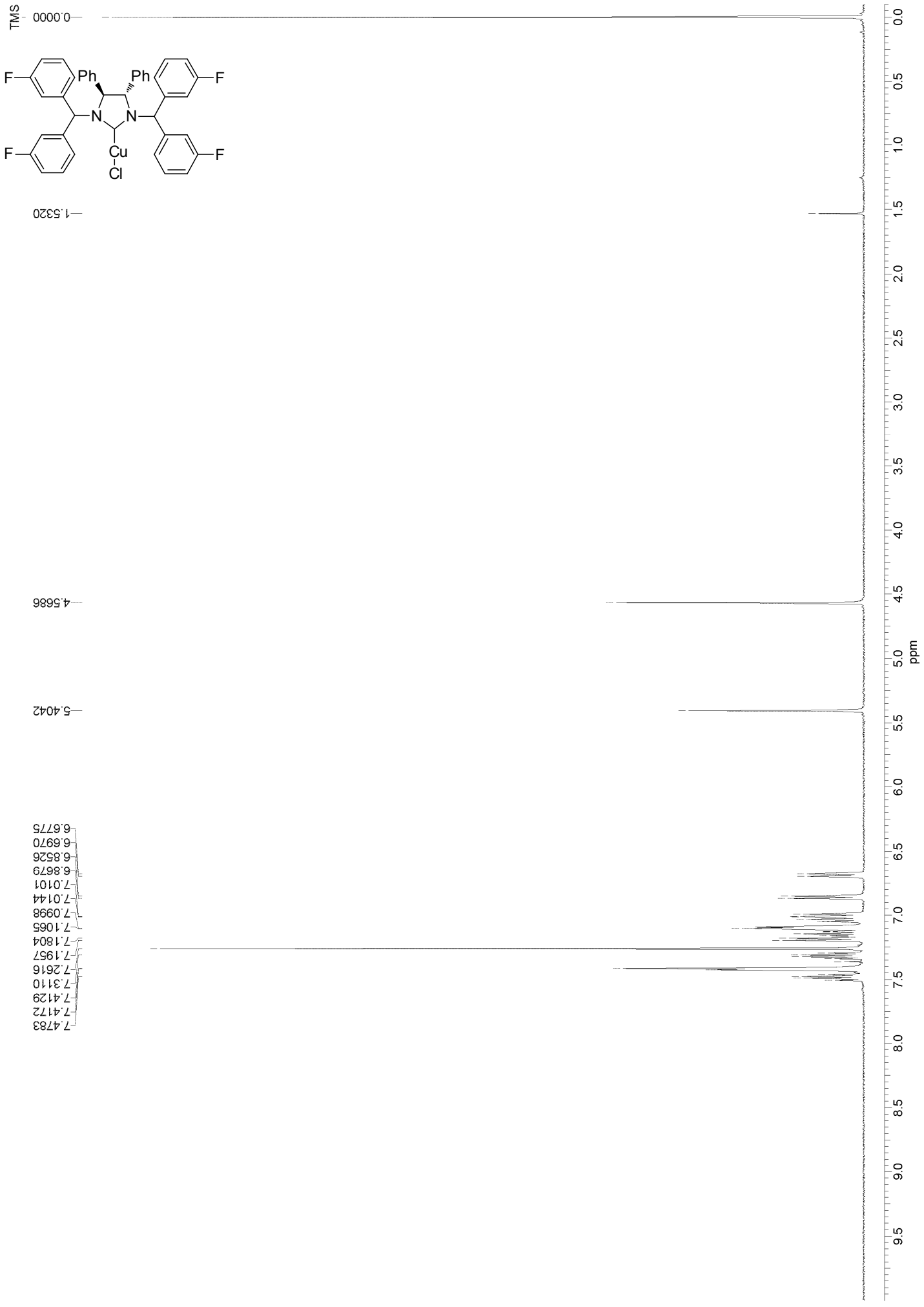

TMS
0.0000
F
F
Ph
Ph
N
N
Cu
Cl
F
F
1.5332
1.5400
4.5173
5.3938
6.9863
7.0016
7.0186
7.0467
7.0540
7.1578
7.2616
7.3043
7.3952
7.4026
7.4075
ppm

^{13}C-NMR of **1f**

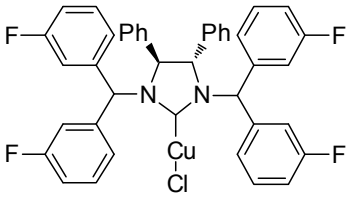

F
F
Ph
Ph
N
N
Cu
Cl
F
F

63.8266
Chloroform-d
74.5959
76.7448
77.0000
77.2552
116.4050
116.5779
127.4131
129.7266
130.0971
130.4676
132.4025
133.7610
137.5072
161.7957
162.0427
163.7717
164.0187
198.6401
ppm

^{1}H-NMR of **1g**

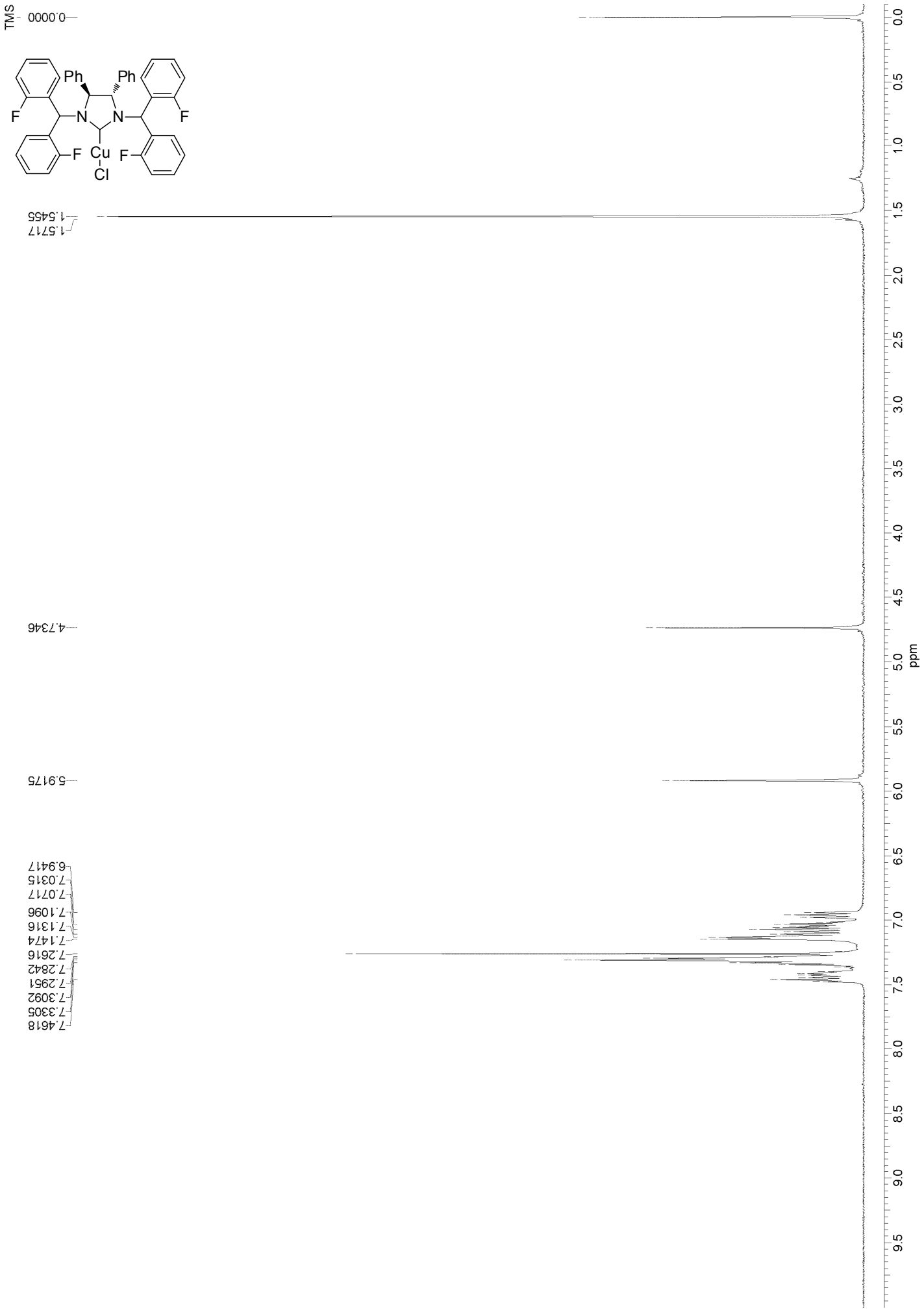

TMS
0.0000
1.5320
4.5686
5.4042
6.6775
6.6970
6.8526
6.8679
7.0101
7.0144
7.0998
7.1065
7.1804
7.1957
7.2616
7.3110
7.4129
7.4172
7.4783
F
Ph
Ph
F
N
N
Cu
Cl
F
F
ppm

^{13}C-NMR of **1g**

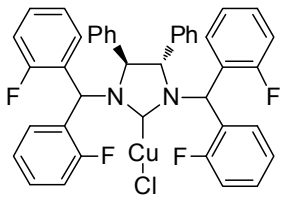

F
Ph
Ph
F
N
N
F
Cu
Cl
F

64.1065
Chloroform-d
74.6699
76.7448
77.0000
77.2552
115.3923
115.5734
115.9192
116.1086
123.9550
124.3173
127.4542
129.7019
129.7843
131.1099
131.1757
137.1696
138.7751
139.9196
162.3309
164.1669
164.3069
199.3235
ppm

^{1}H-NMR of **1h**

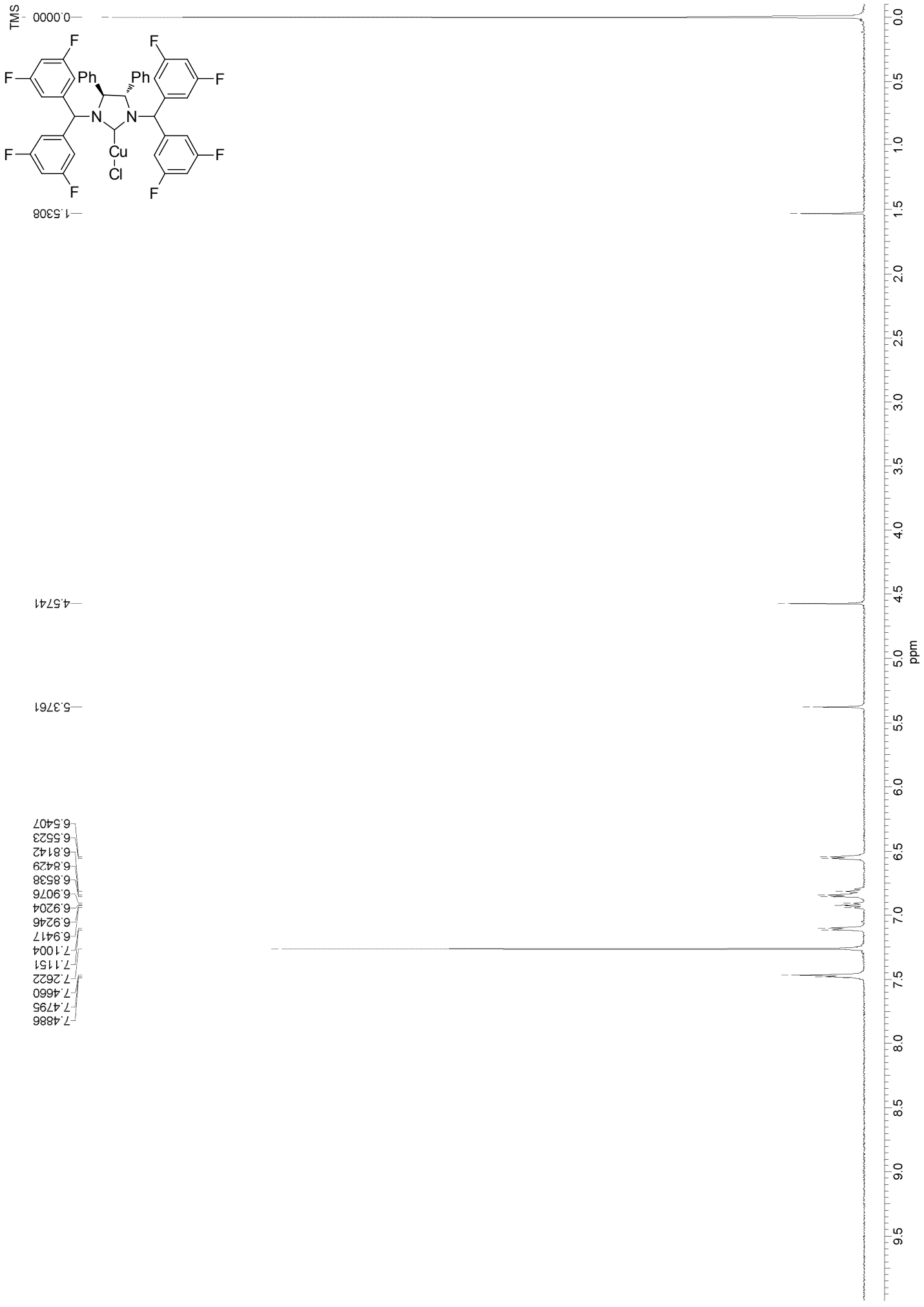

TMS
0.0000
Ph
Ph
F
N
N
F
F
Cu
Cl
F
1.5455
1.5717
4.7346
5.9175
6.9417
7.0315
7.0717
7.1096
7.1316
7.1474
7.2616
7.2842
7.2951
7.3092
7.3305
7.4618
ppm

^{13}C-NMR of **1h**

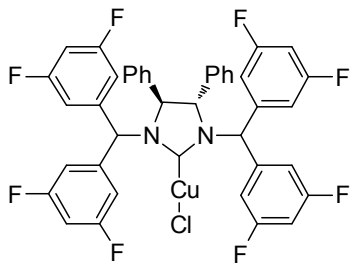

Ph
Ph
F
N
N
F
F
Cu
F
Cl

53.0161
Chloroform-d
77.2552
77.0000
76.7448
75.7238
136.3216
130.9534
130.8876
130.5335
129.4879
129.2903
129.0021
128.3187
125.3135
125.1242
124.2926
116.0263
115.7793
115.6064
161.7051
161.2605
159.7209
159.2845
197.5122
ppm

^{1}H-NMR of **1i**

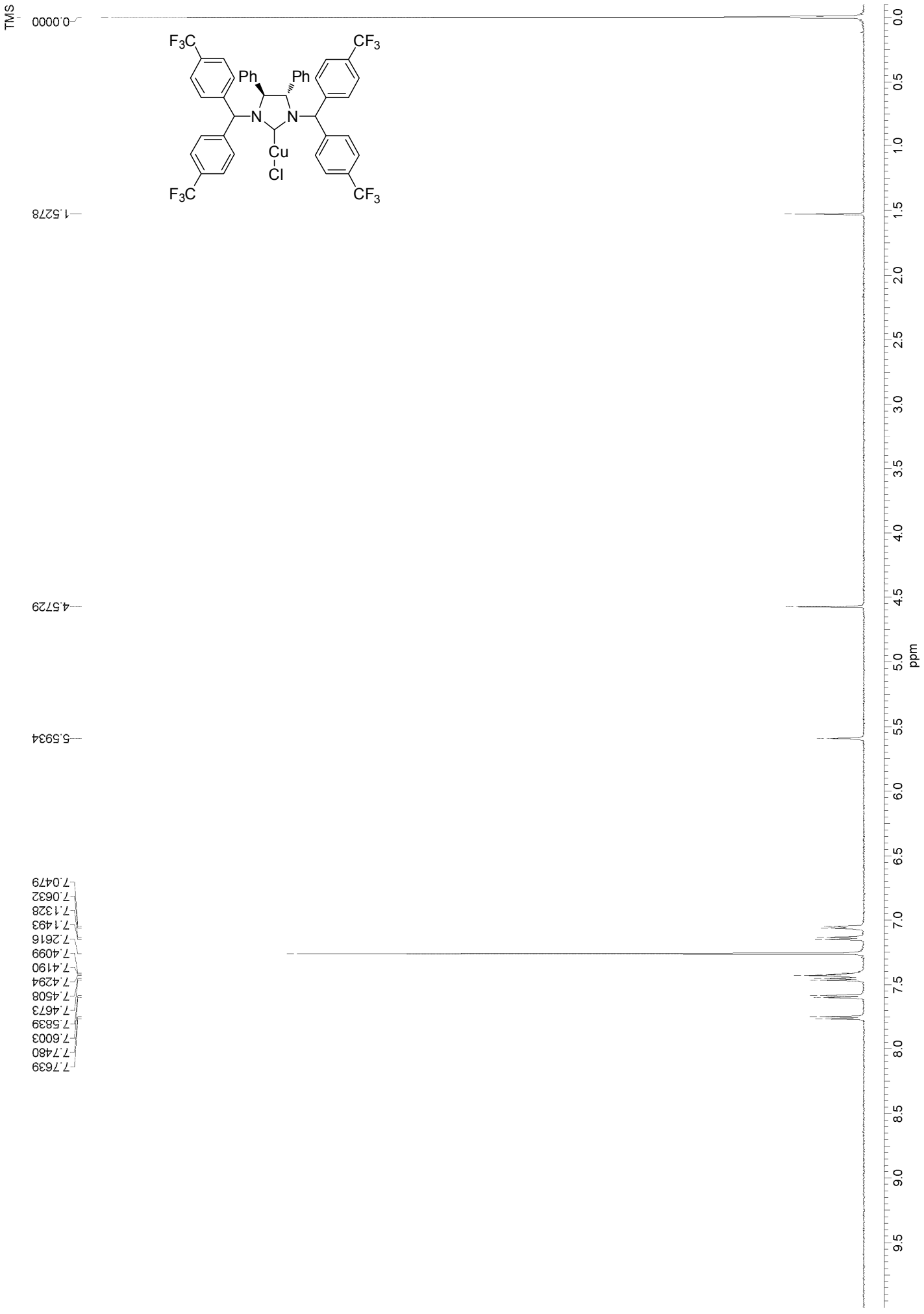

TMS
0.0000
1.5308
4.5741
5.3761
6.5407
6.5523
6.8142
6.8429
6.8538
6.9076
6.9204
6.9246
6.9417
7.1004
7.1151
7.2622
7.4660
7.4795
7.4886
ppm

^{13}C-NMR of **1i**

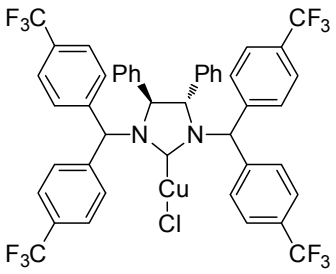

F
F
Ph
Ph
F
N
N
Cu
Cl
F
F
F
F
F

63.6207
Chloroform-d
74.8264
76.7448
77.0000
77.2552
104.8618
105.0594
105.2323
105.4299
111.2015
111.4156
111.9343
112.1483
127.3060
130.1383
136.4204
139.5408
139.6149
140.2819
140.3477
162.7755
162.8743
164.6362
164.7762
199.6528
ppm

^{1}H-NMR of **1j**

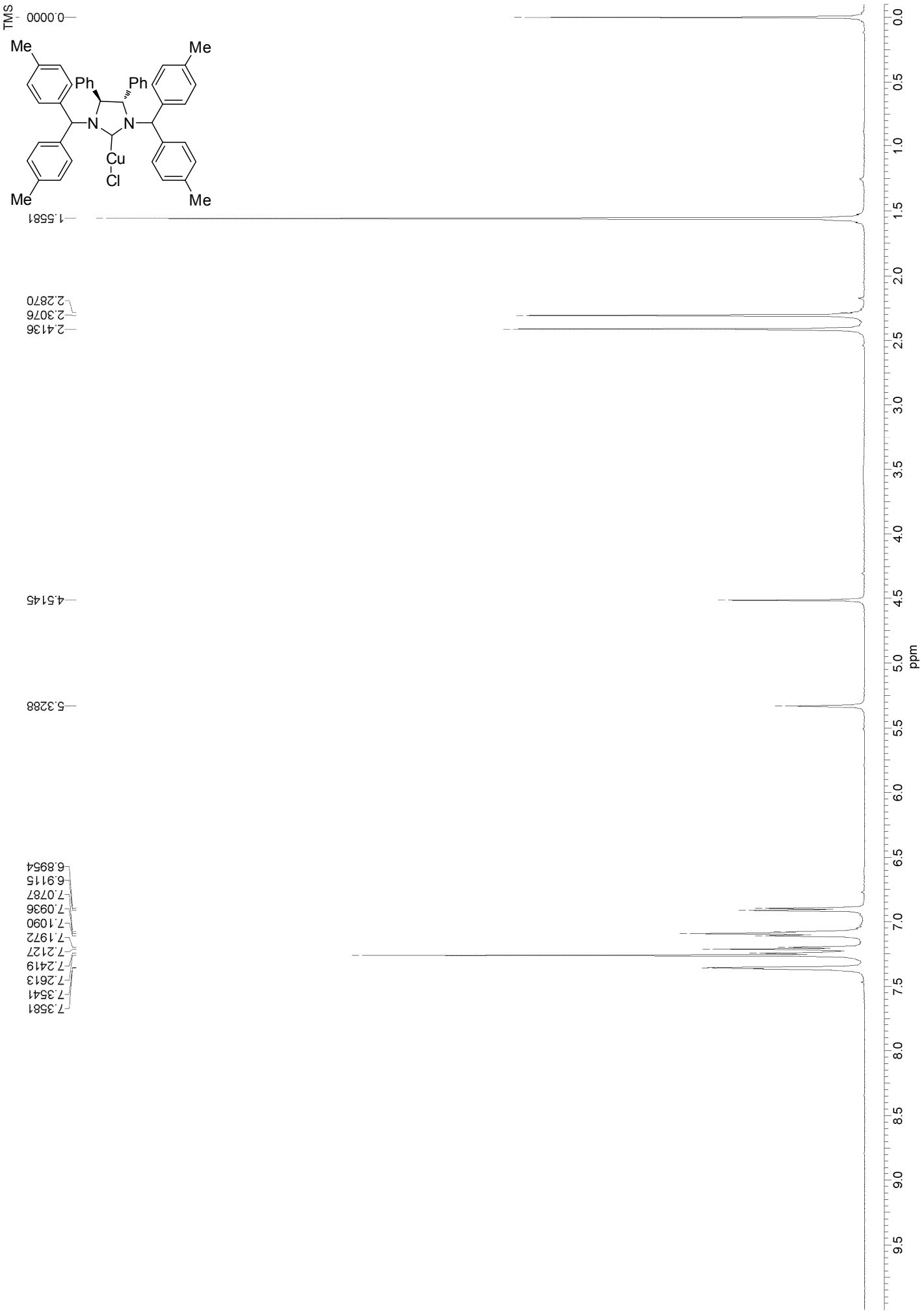

TMS
0.0000
1.5278
4.5729
5.5934
7.0479
7.0632
7.1328
7.1493
7.2616
7.4099
7.4190
7.4294
7.4508
7.4673
7.5839
7.6003
7.7480
7.7639
F3C
CF3
Ph
Ph
N
N
Cu
Cl
F3C
CF3
ppm

^{13}C-NMR of **1j**

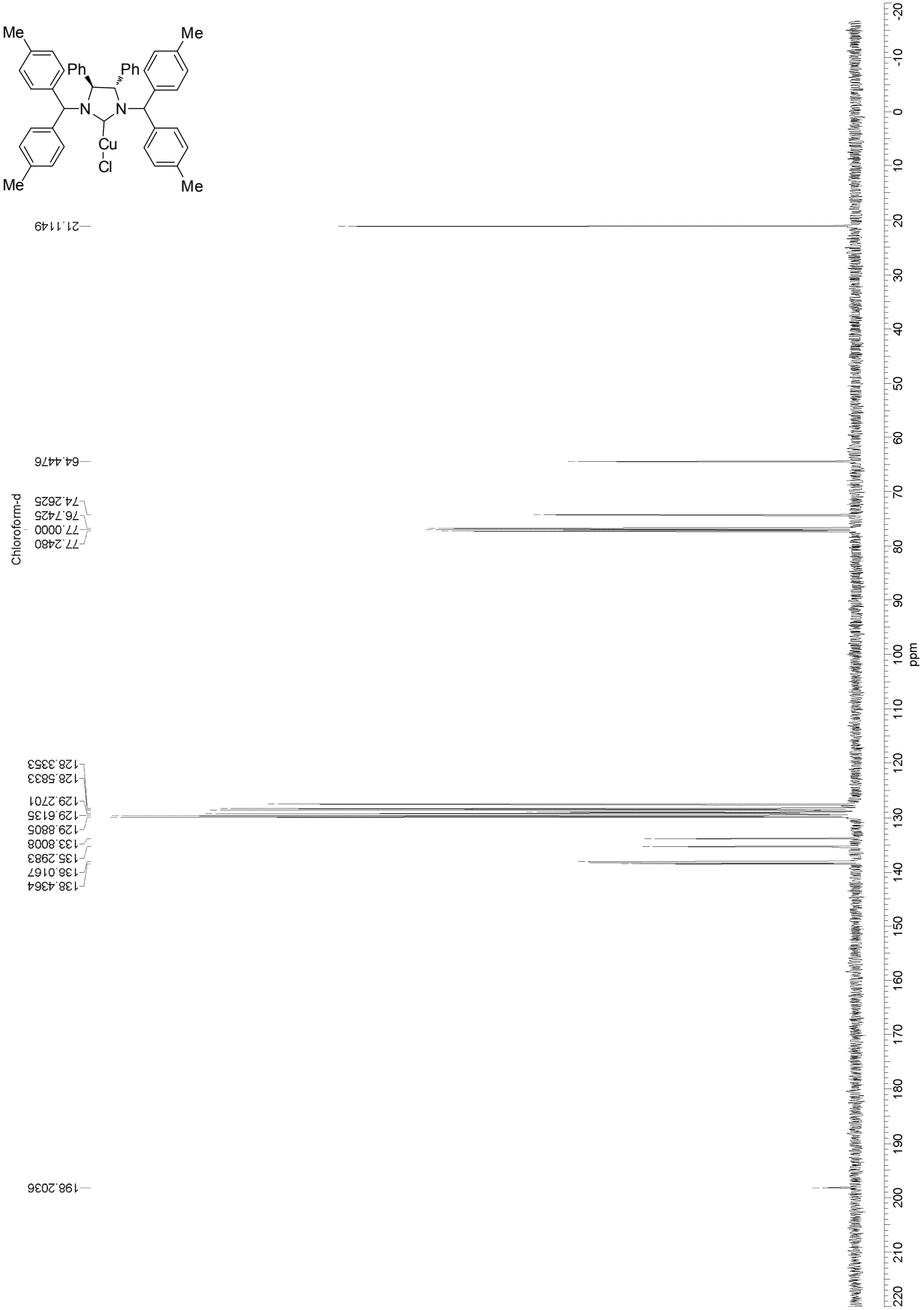

F3C
CF3
Ph
Ph
N
N
Cu
Cl
F3C
CF3

64.4852
Chloroform-d
74.8182
76.7448
77.0000
77.2552
122.6706
126.4827
126.6803
127.3225
128.8951
129.1091
129.9572
131.3569
131.5956
131.8756
136.8650
139.9854
140.9899
199.4717
ppm

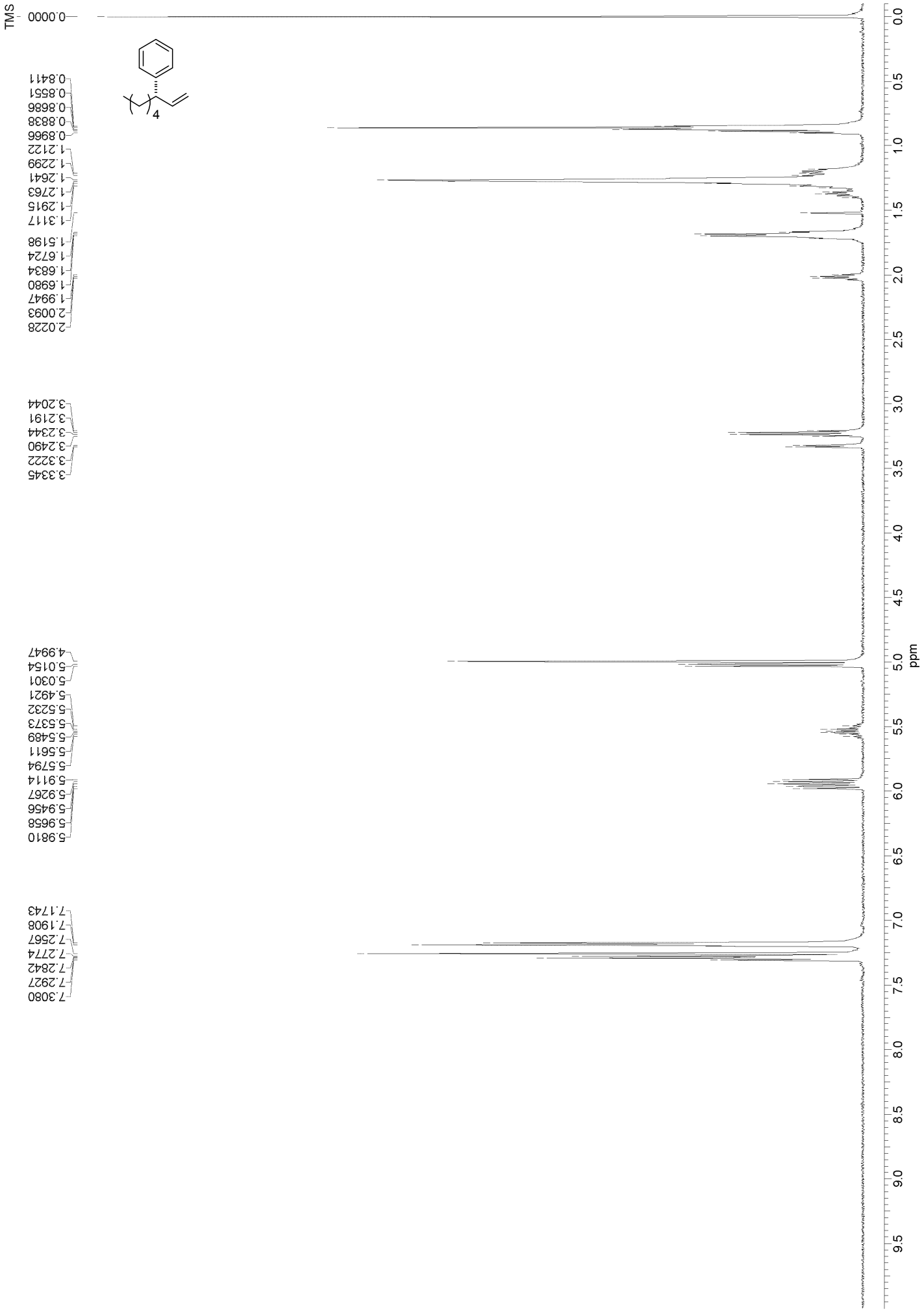
^{1}H-NMR of **1k**


TMS
0.0000
Me
Me
Ph
Ph
N
N
Cu
Cl
Me
Me
1.5581
2.2870
2.3076
2.4136
4.5145
5.3288
6.8954
6.9115
7.0787
7.0936
7.1090
7.1972
7.2127
7.2419
7.2613
7.3541
7.3581
ppm

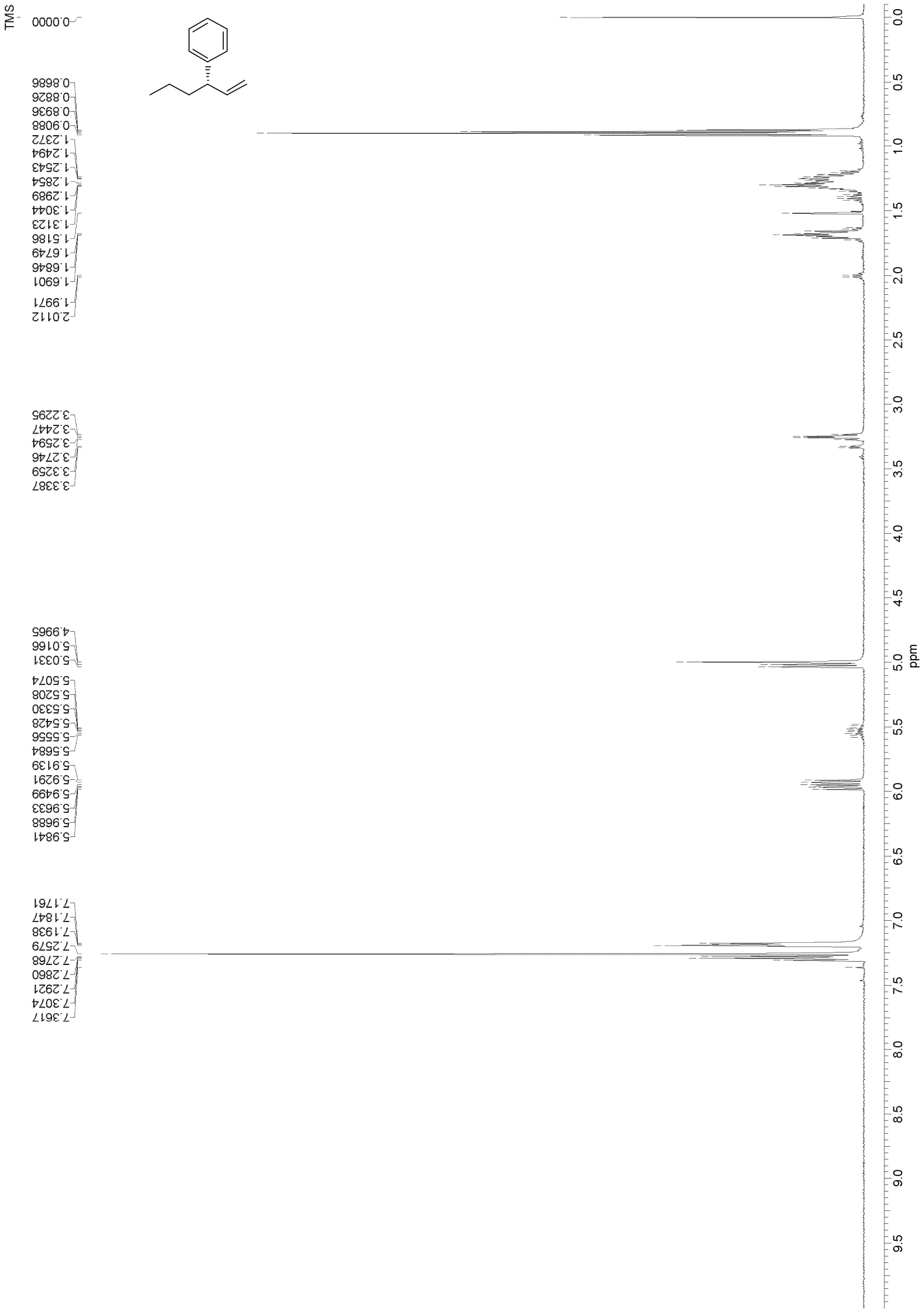
^{13}C-NMR of **1k**


Me
Me
Ph
Ph
N
N
Cu
Cl
Me
Me
21.1149
64.4476
Chloroform-d
74.2625
76.7425
77.0000
77.2480
128.3353
128.5833
129.2701
129.6135
129.8805
133.8008
135.2983
138.0167
138.4364
198.2036
ppm

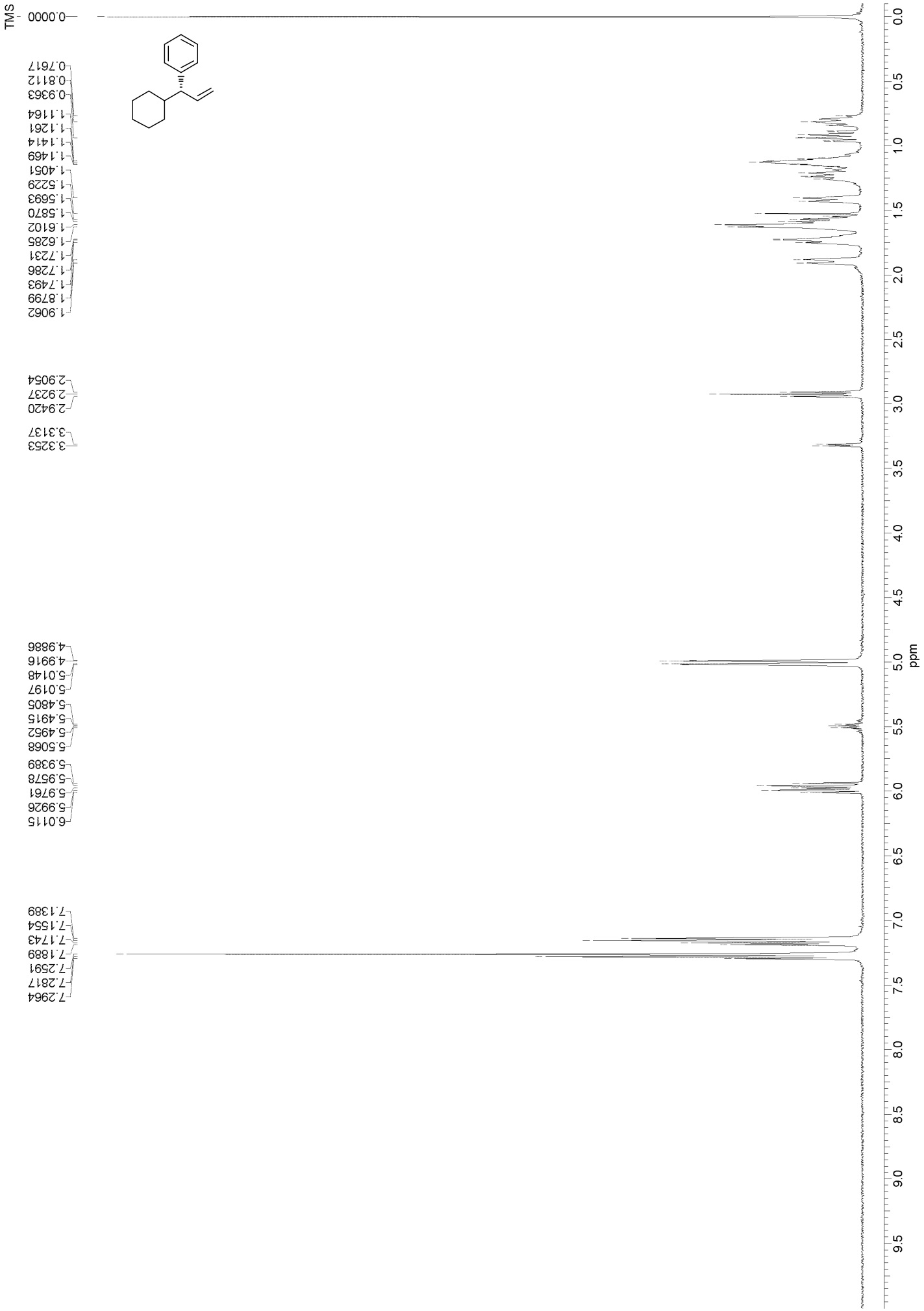
^{1}H-NMR of **3aa** (γ:α = 84:16)



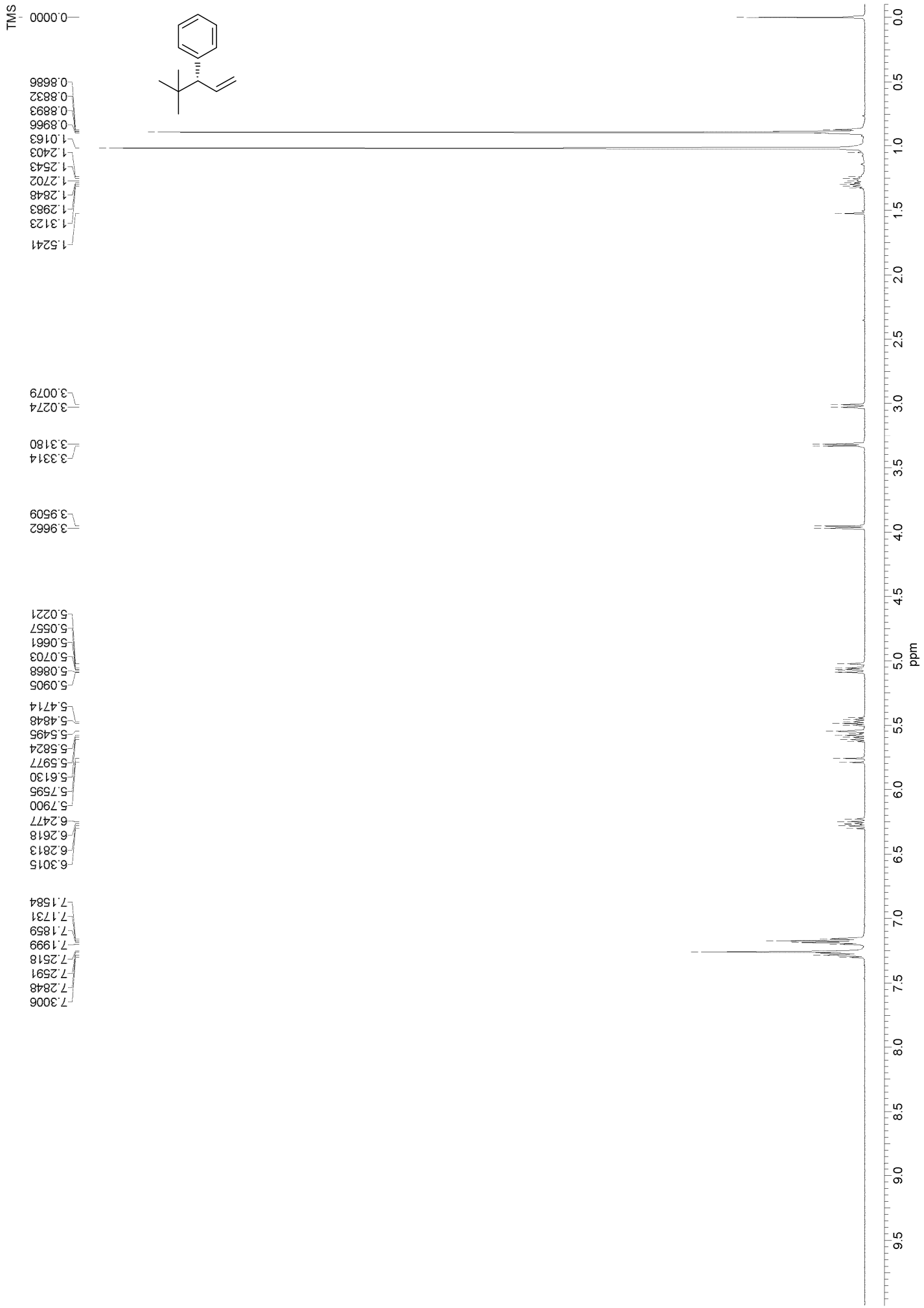
^{1}H-NMR of **3ba** (γ:α = 91:9)



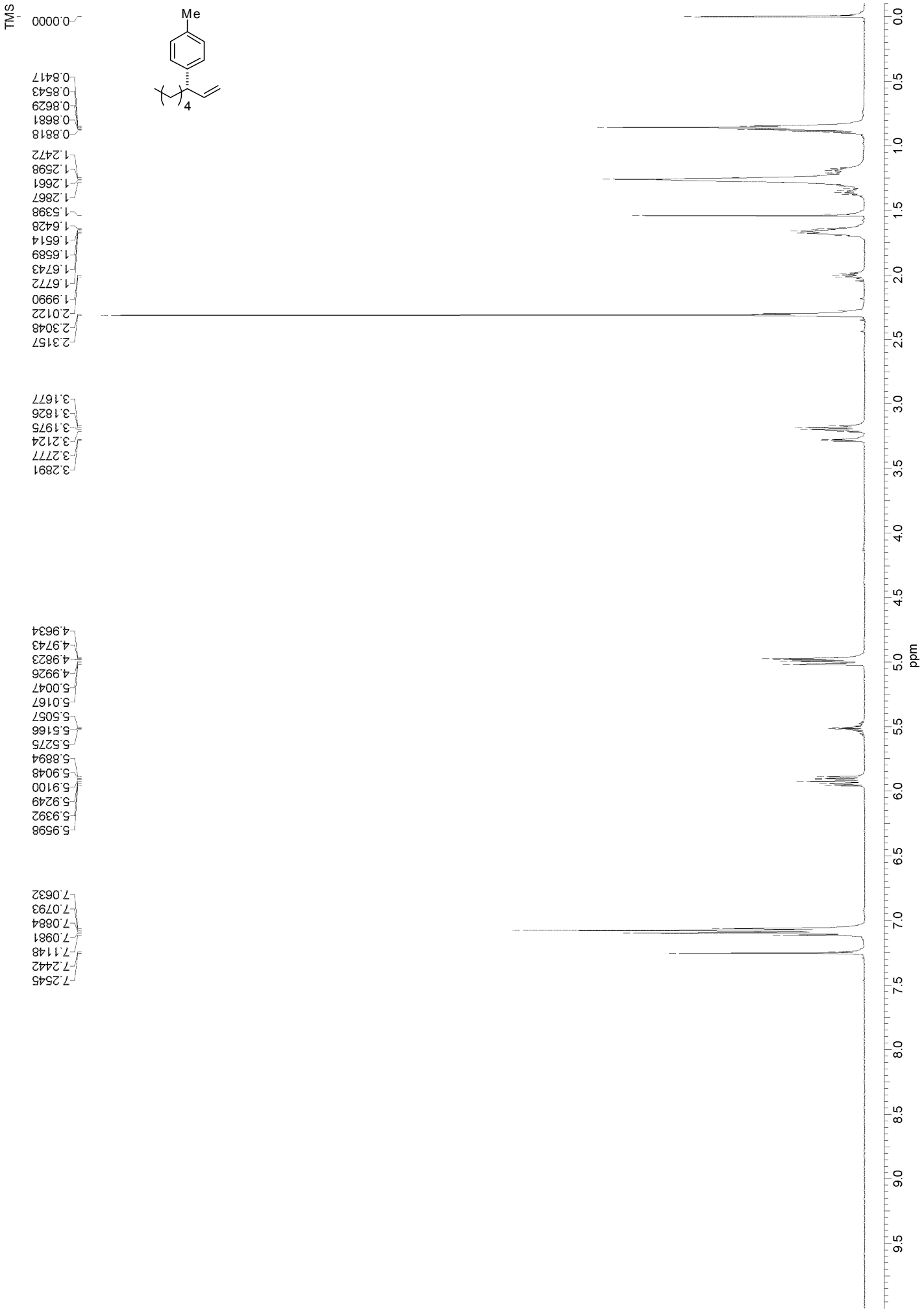
^{1}H-NMR of **3ca** (γ:α = 89:11)



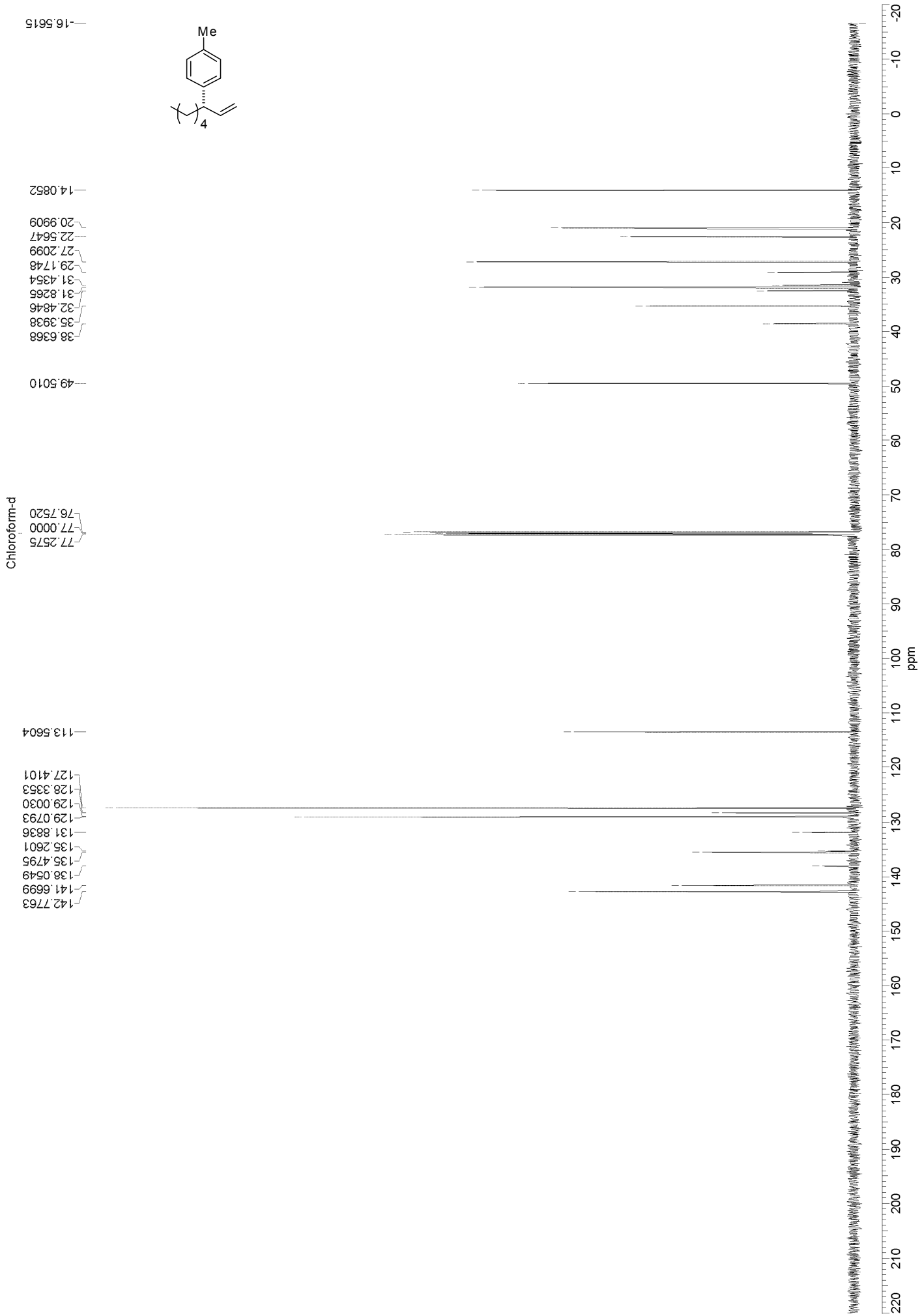
^{1}H-NMR of **3da** (γ:α = 53:47)



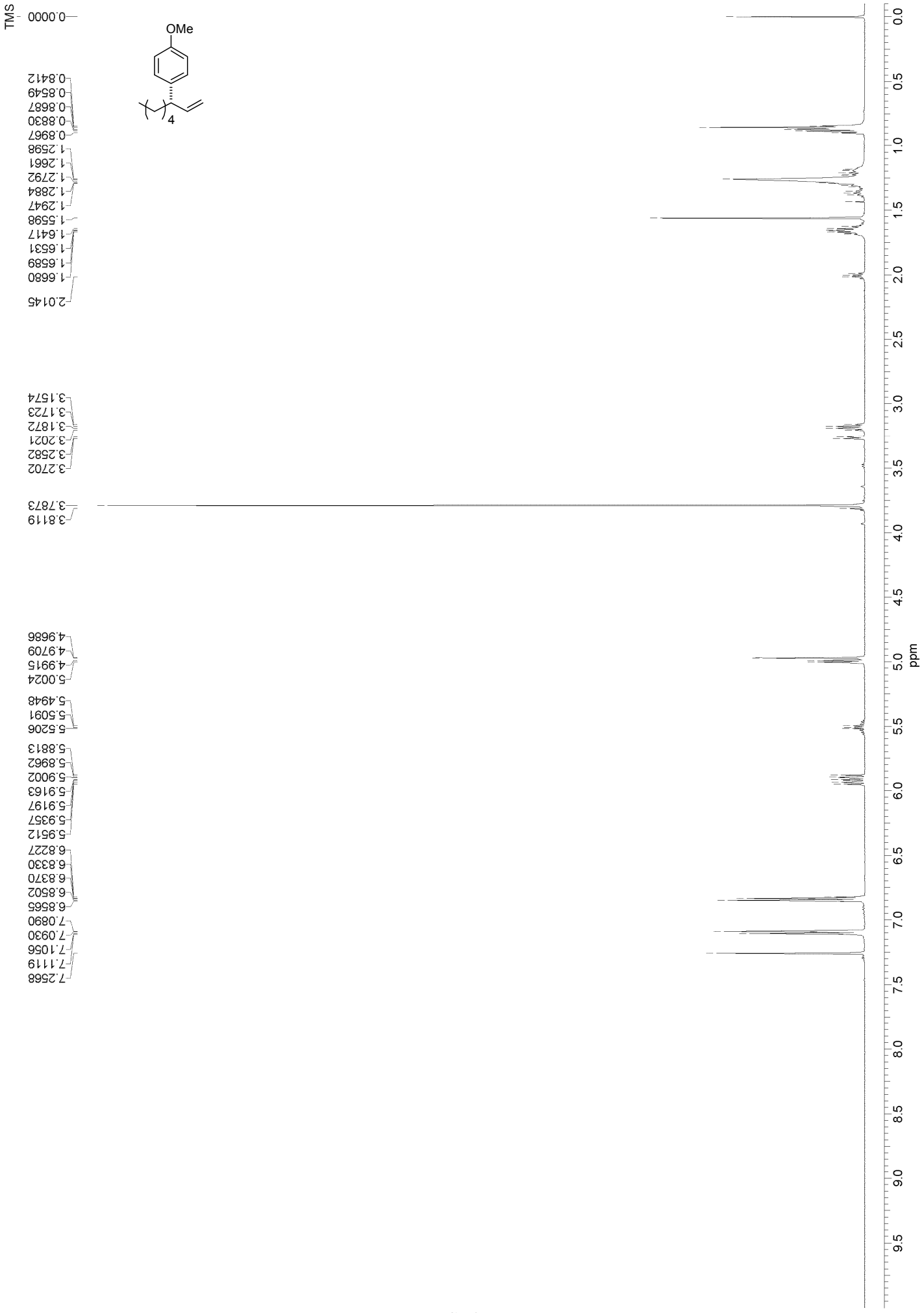
^{1}H-NMR of **3ab** (γ:α = 82:18)



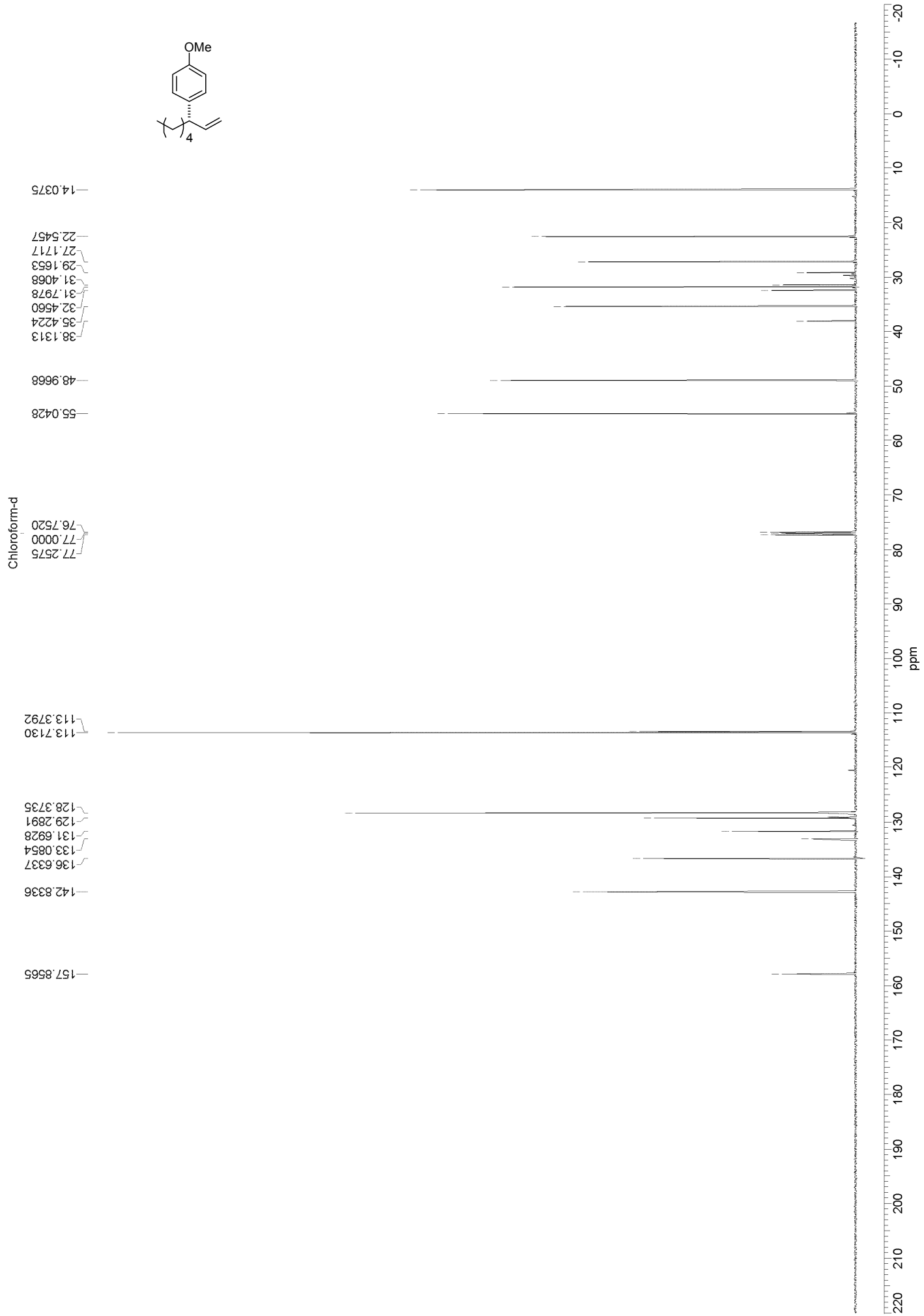
^{13}C-NMR of **3ab** (γ:α = 82:18)



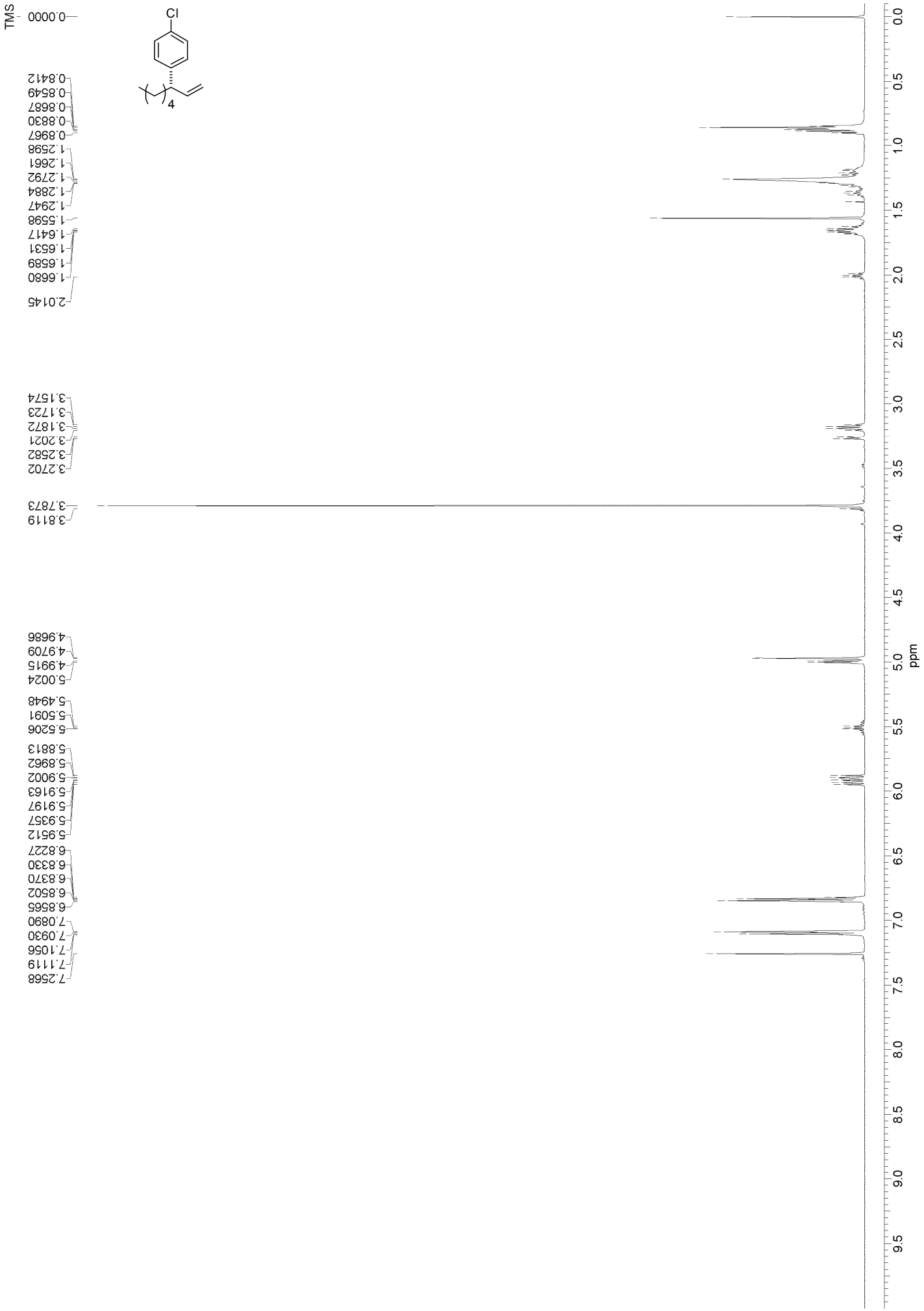
^{1}H-NMR of **3ac** (γ:α = 79:21)



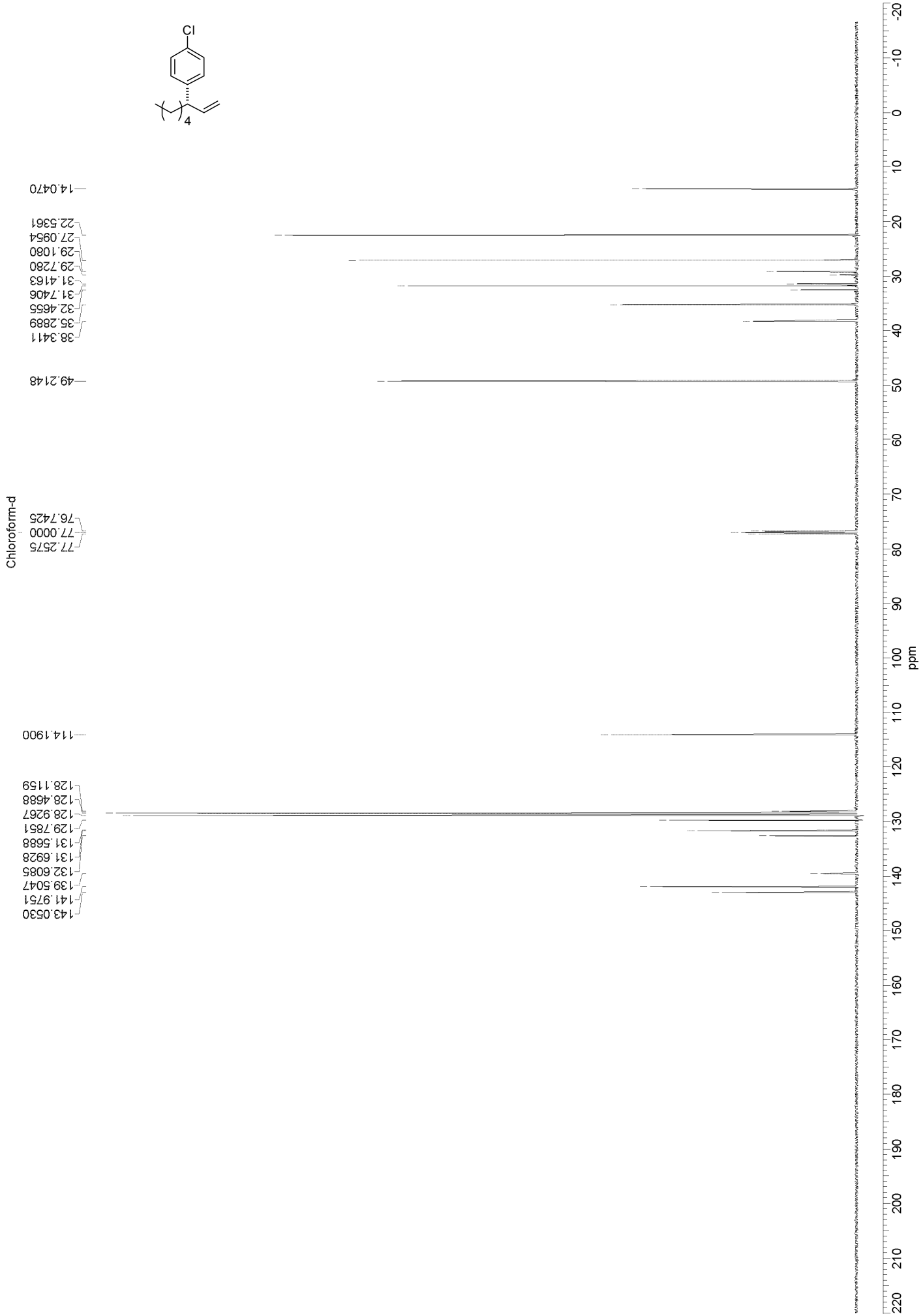
^{13}C-NMR of **3ac** (γ:α = 79:21)



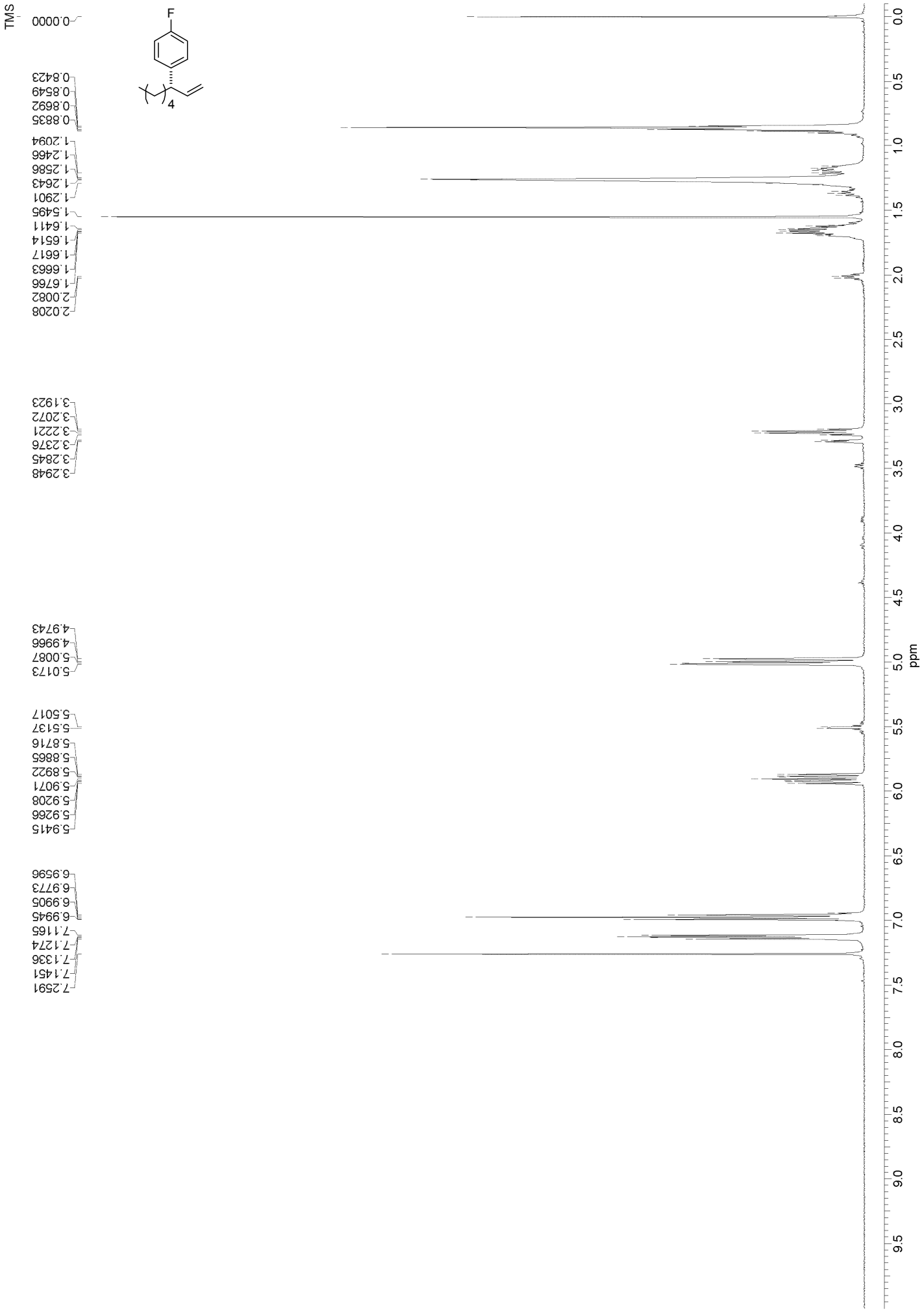
^{1}H-NMR of **3ad** (γ:α = 87:13)



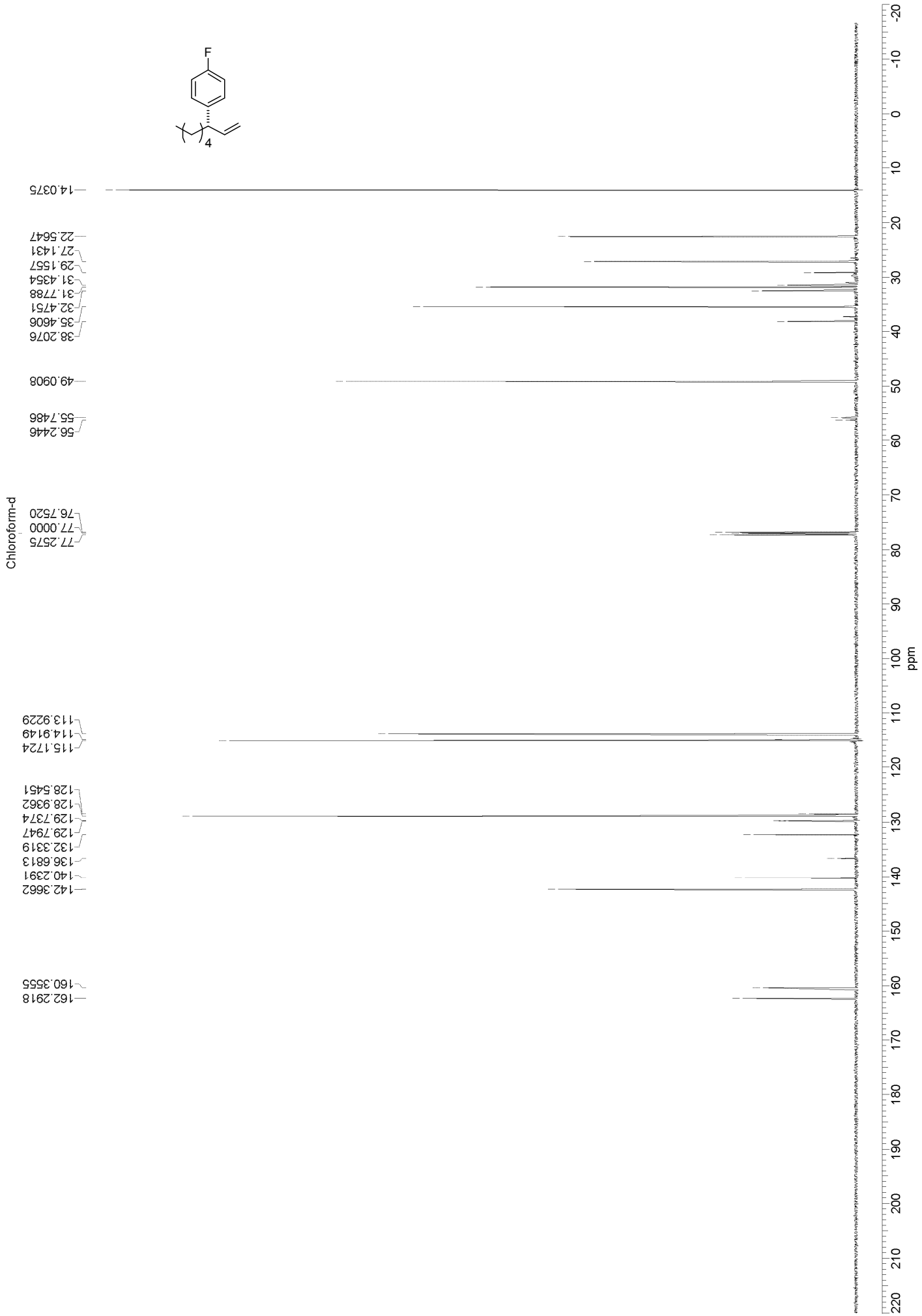
^{13}C-NMR of **3ad** (γ:α = 83:17)



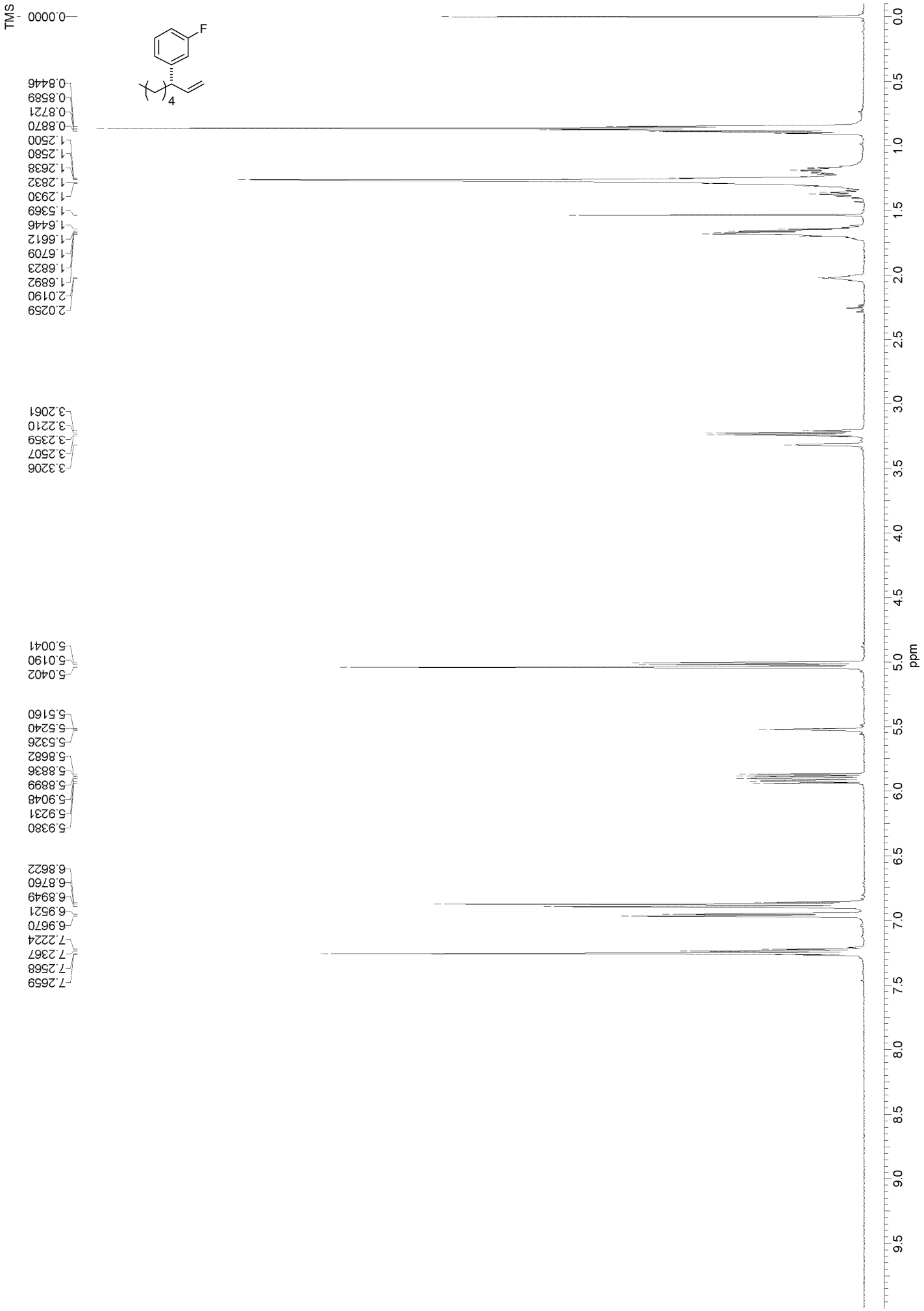
^{1}H-NMR of **3ae** (γ:α = 88:12)



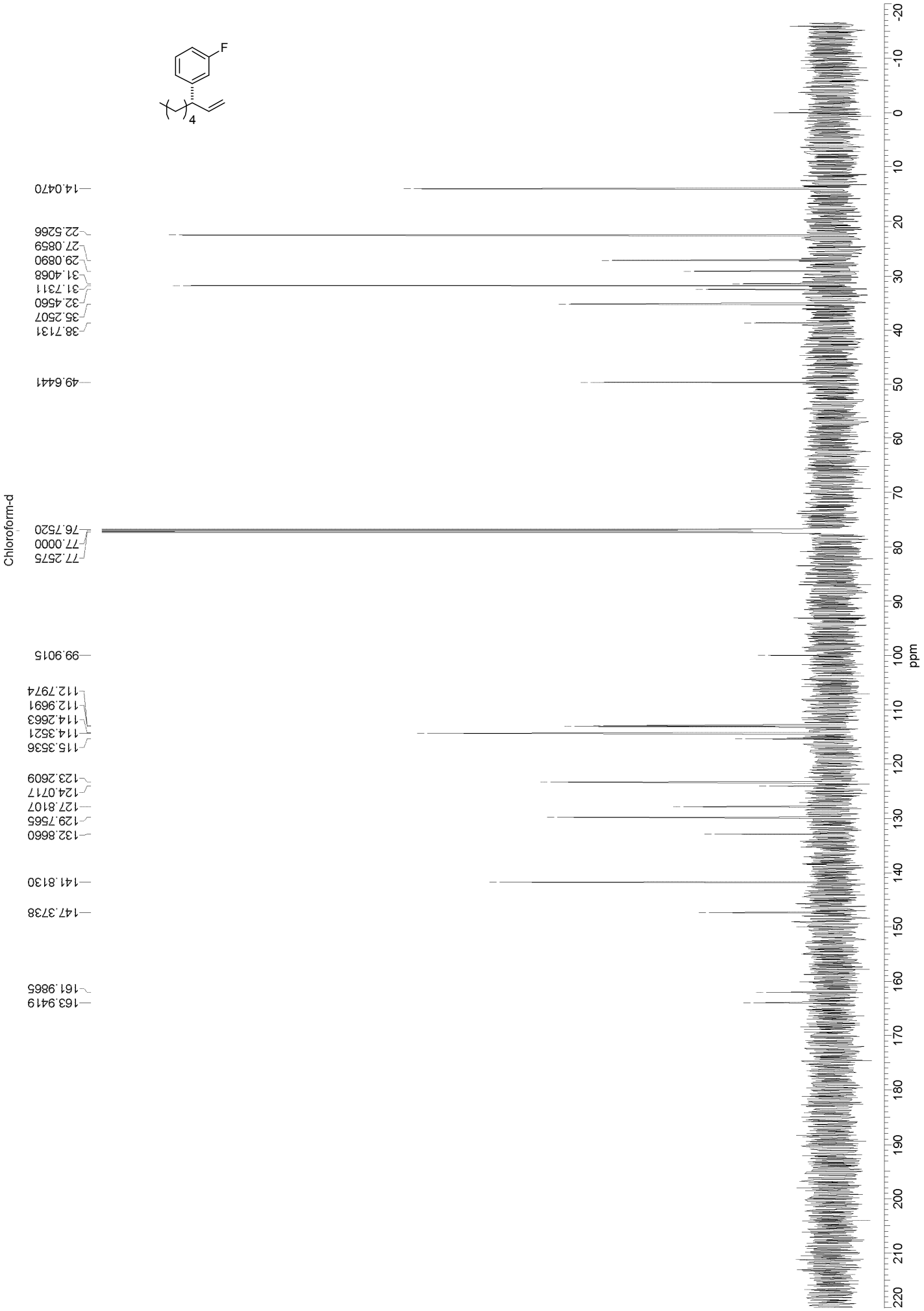
^{13}C-NMR of **3ae** (γ:α = 88:12)



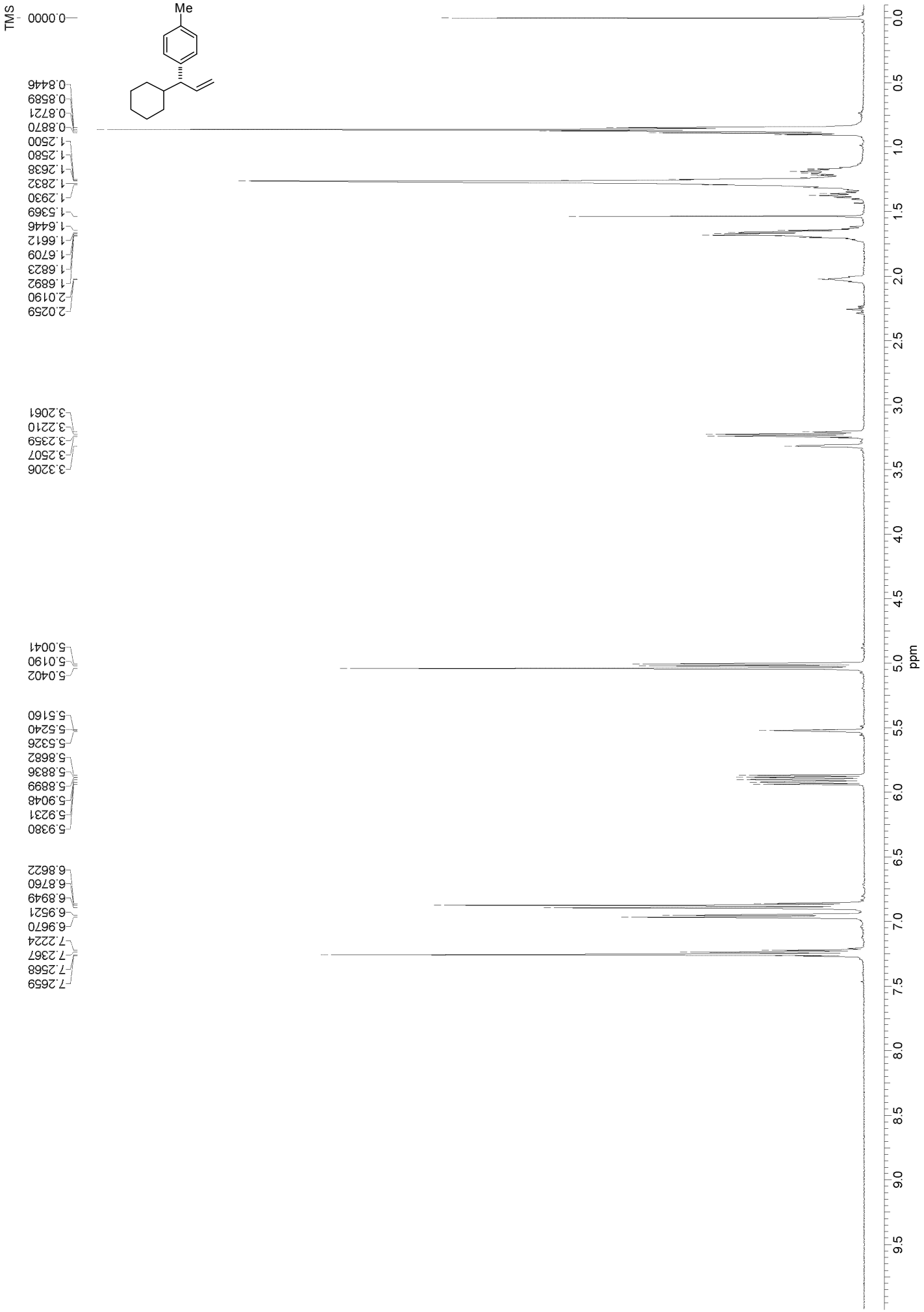
^{1}H-NMR of **3af** (γ:α = 84:16)



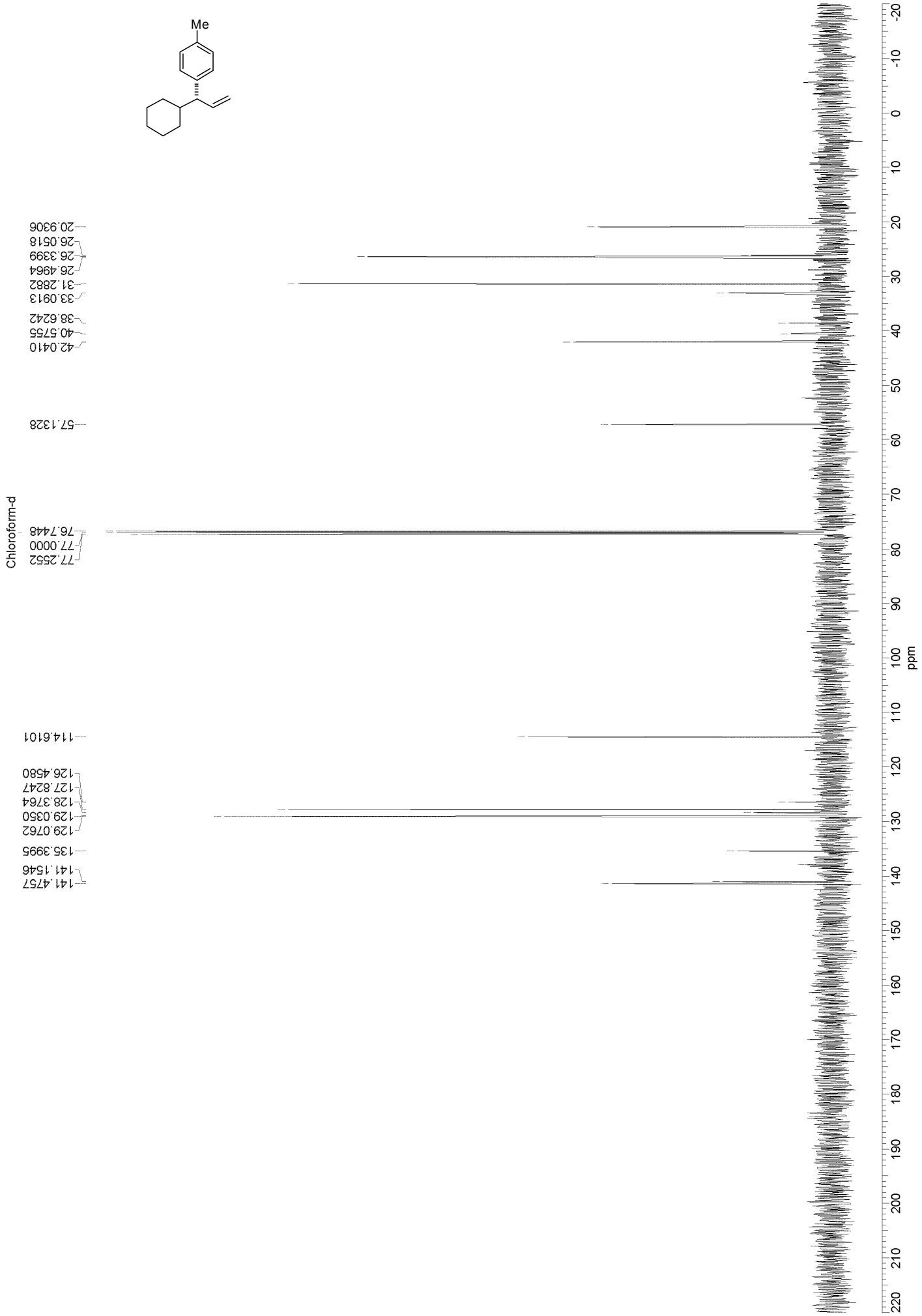
^{13}C-NMR of **3af** (γ:α = 79:21)



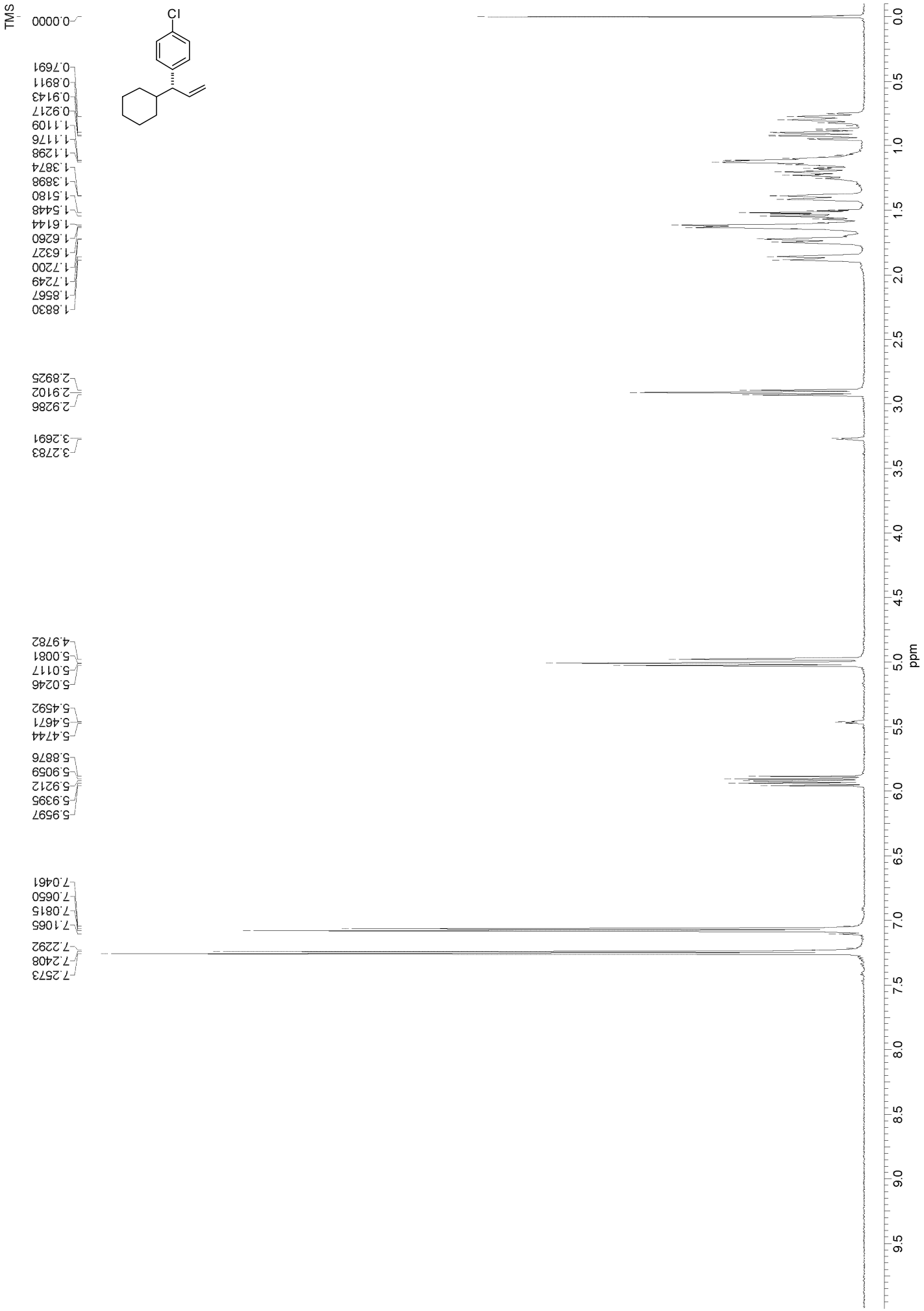
^{1}H-NMR of **3cb** (γ:α = 87:13)



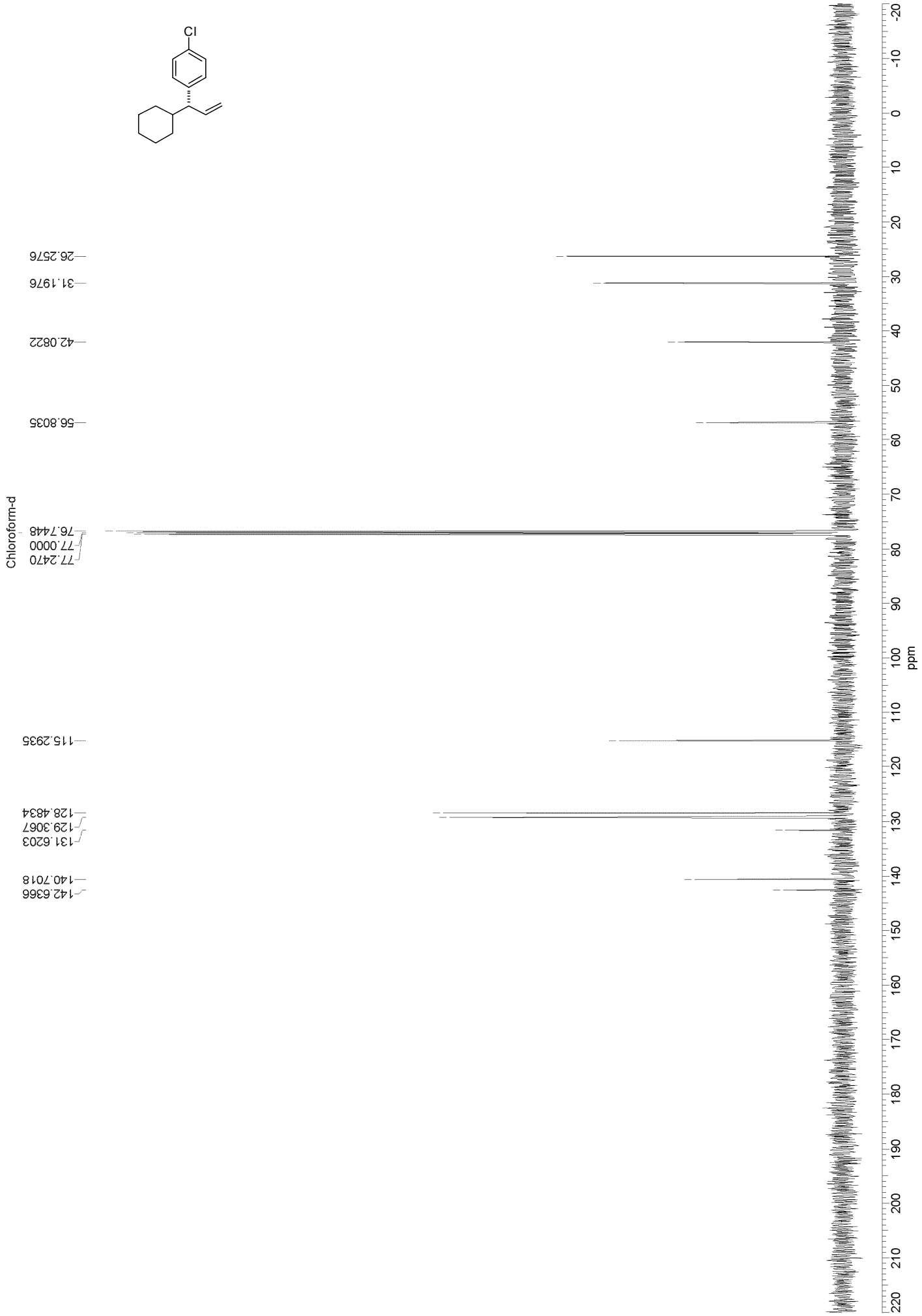
^{13}C-NMR of **3cb** (γ:α = 87:13)



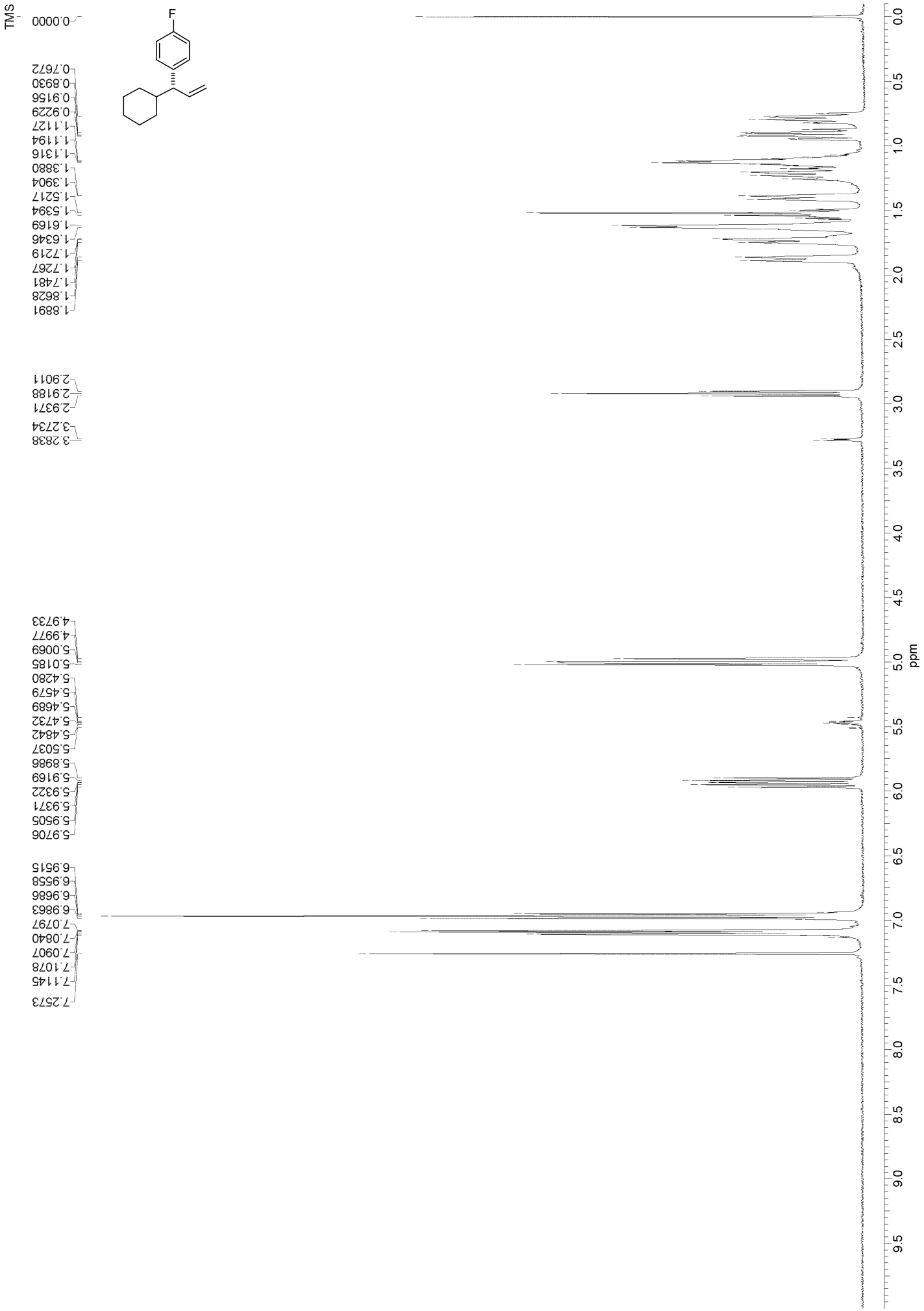
^{1}H-NMR of **3cd** (γ:α = 96:4)



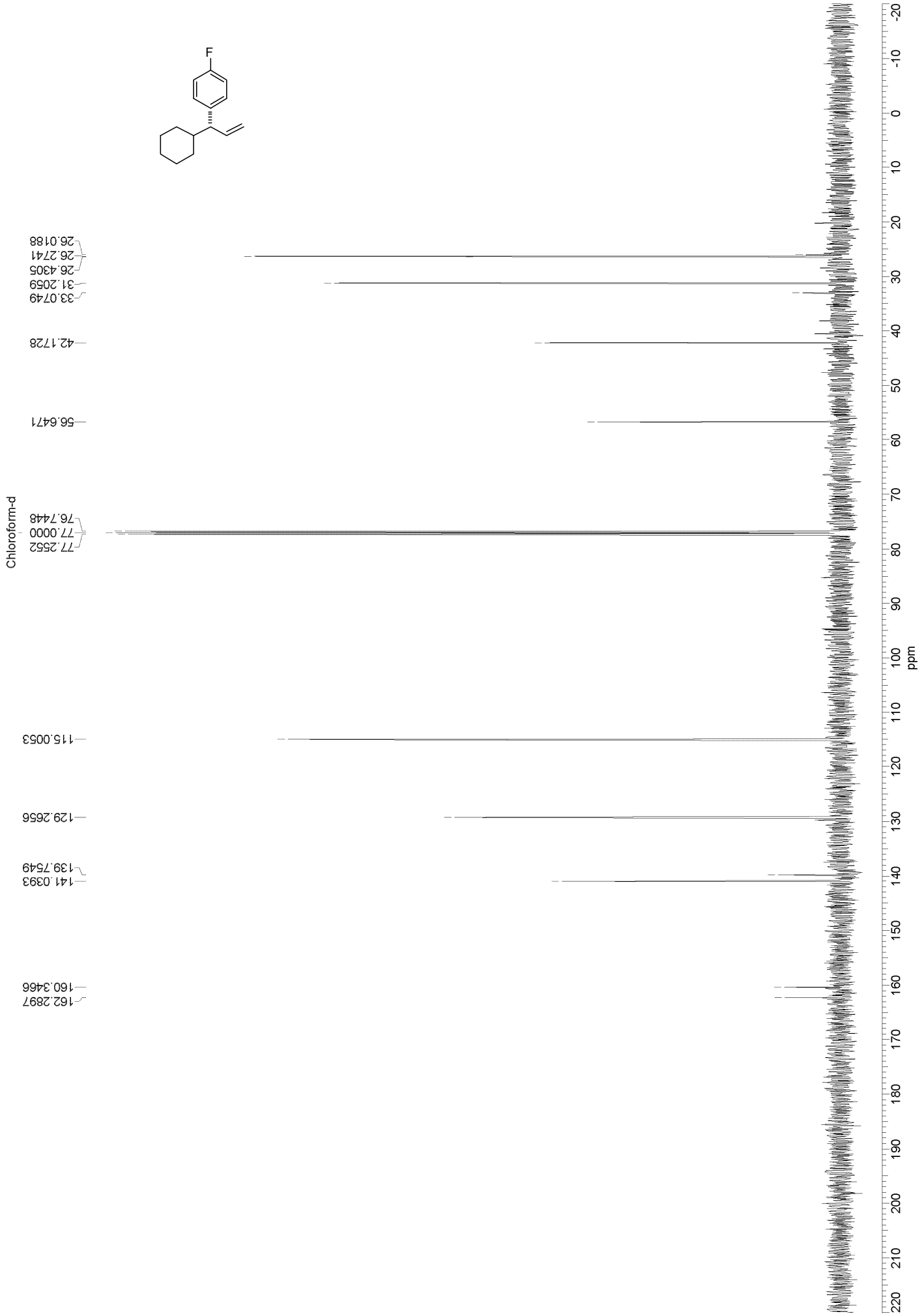
^{13}C-NMR of **3cd** (γ:α = 96:4)



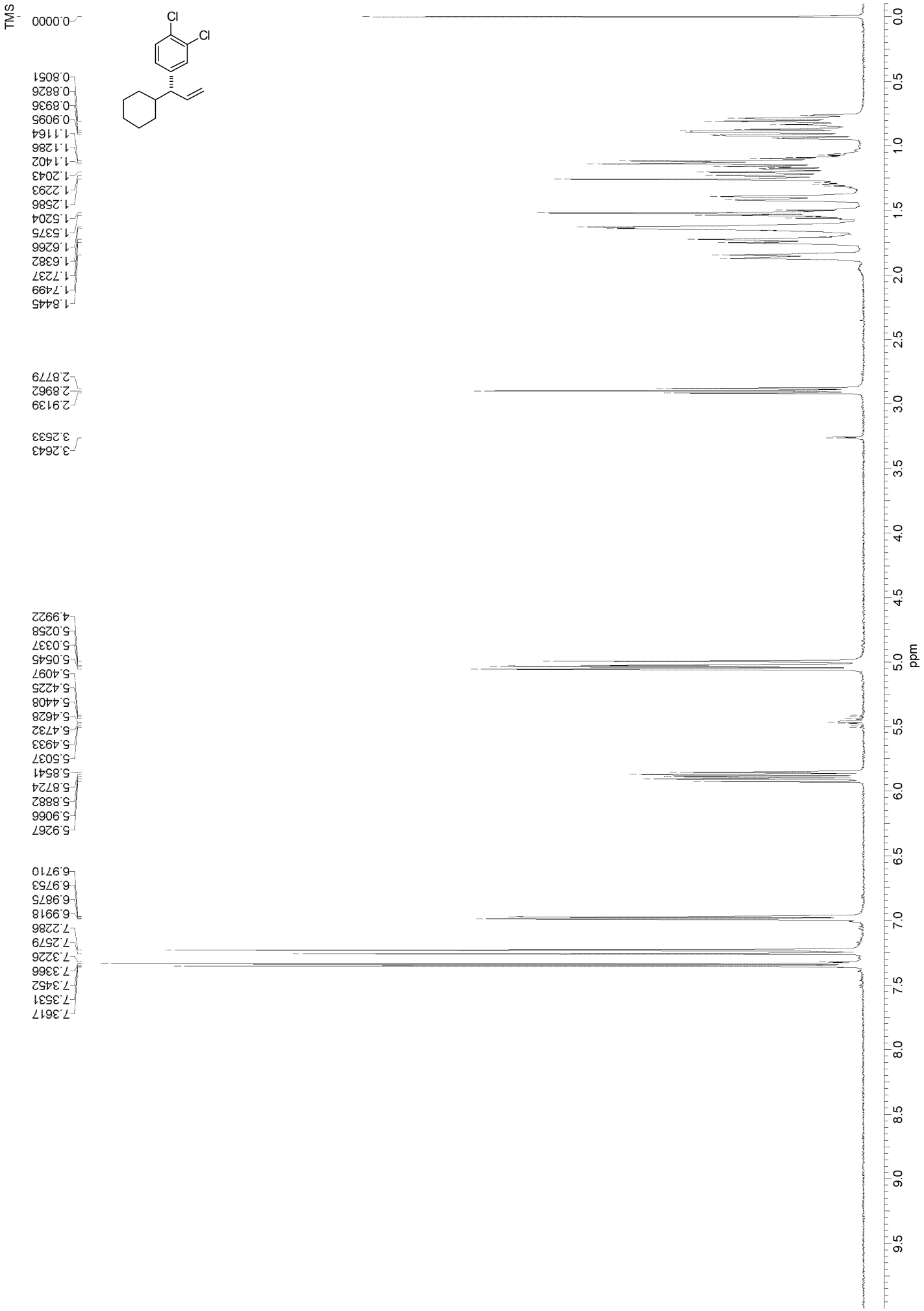
^{1}H-NMR of **3ce** (γ:α = 95:5)



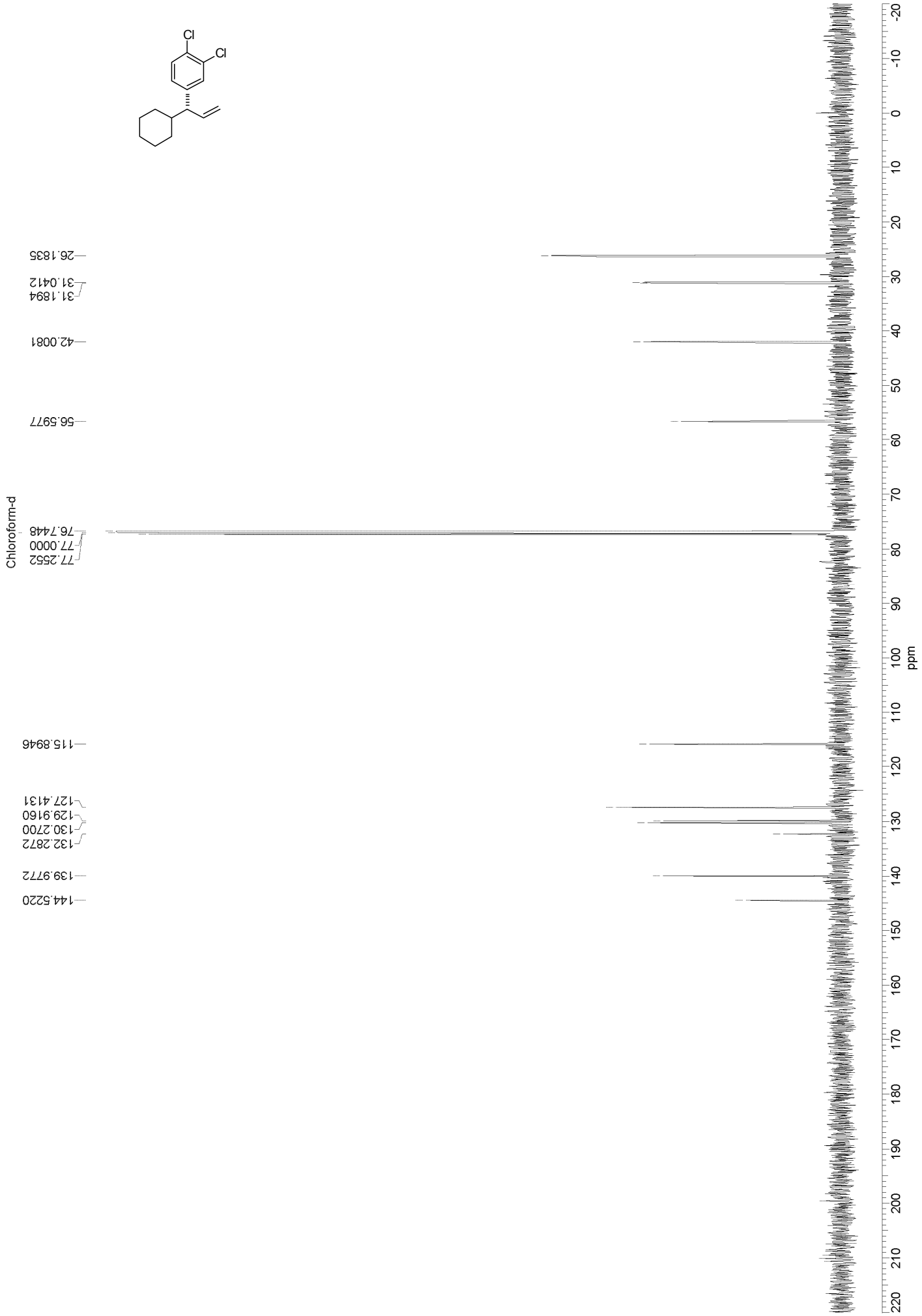
^{13}C-NMR of **3ce** (γ:α = 95:5)



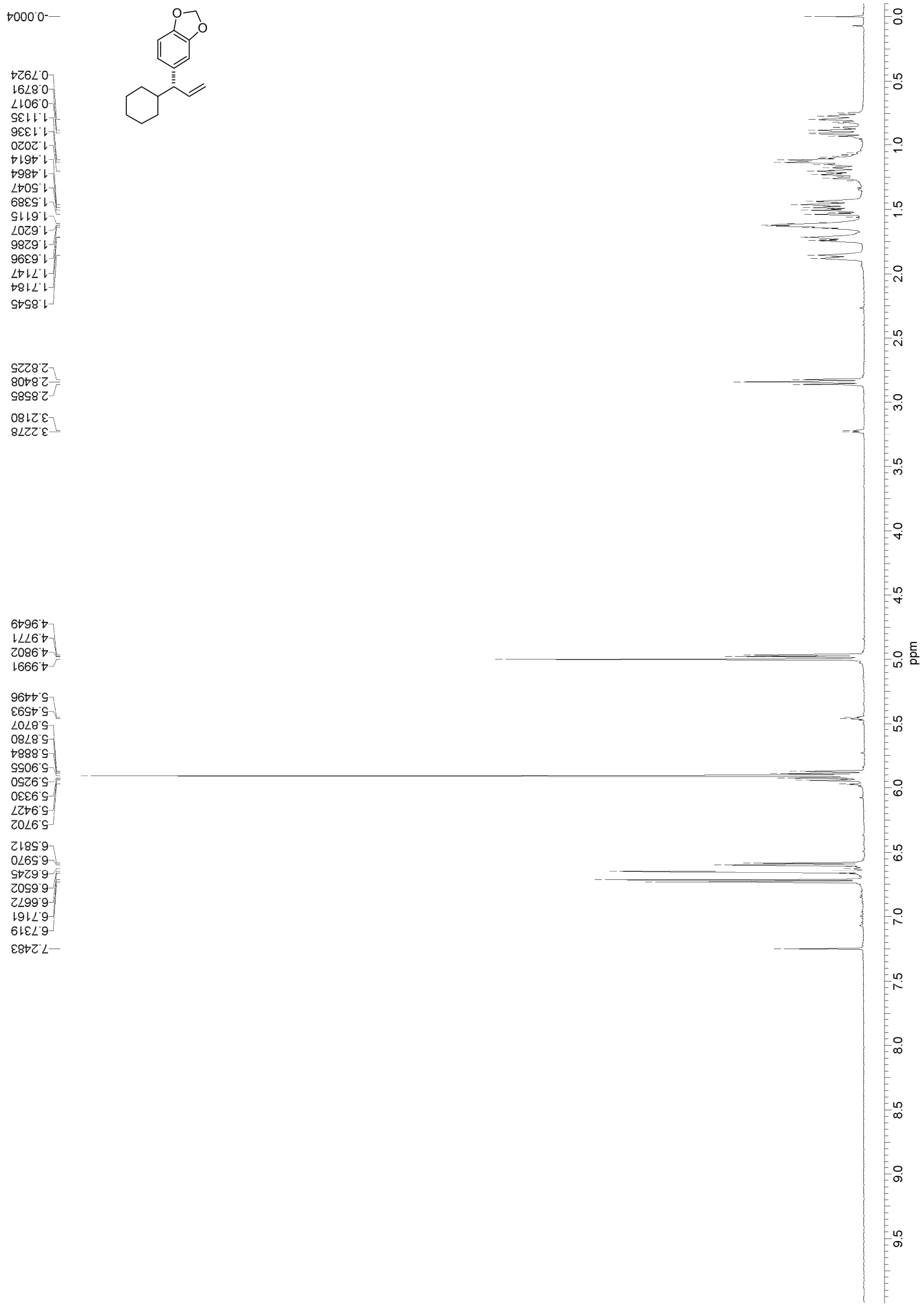
^{1}H-NMR of **3cg** (γ:α = 96:4)



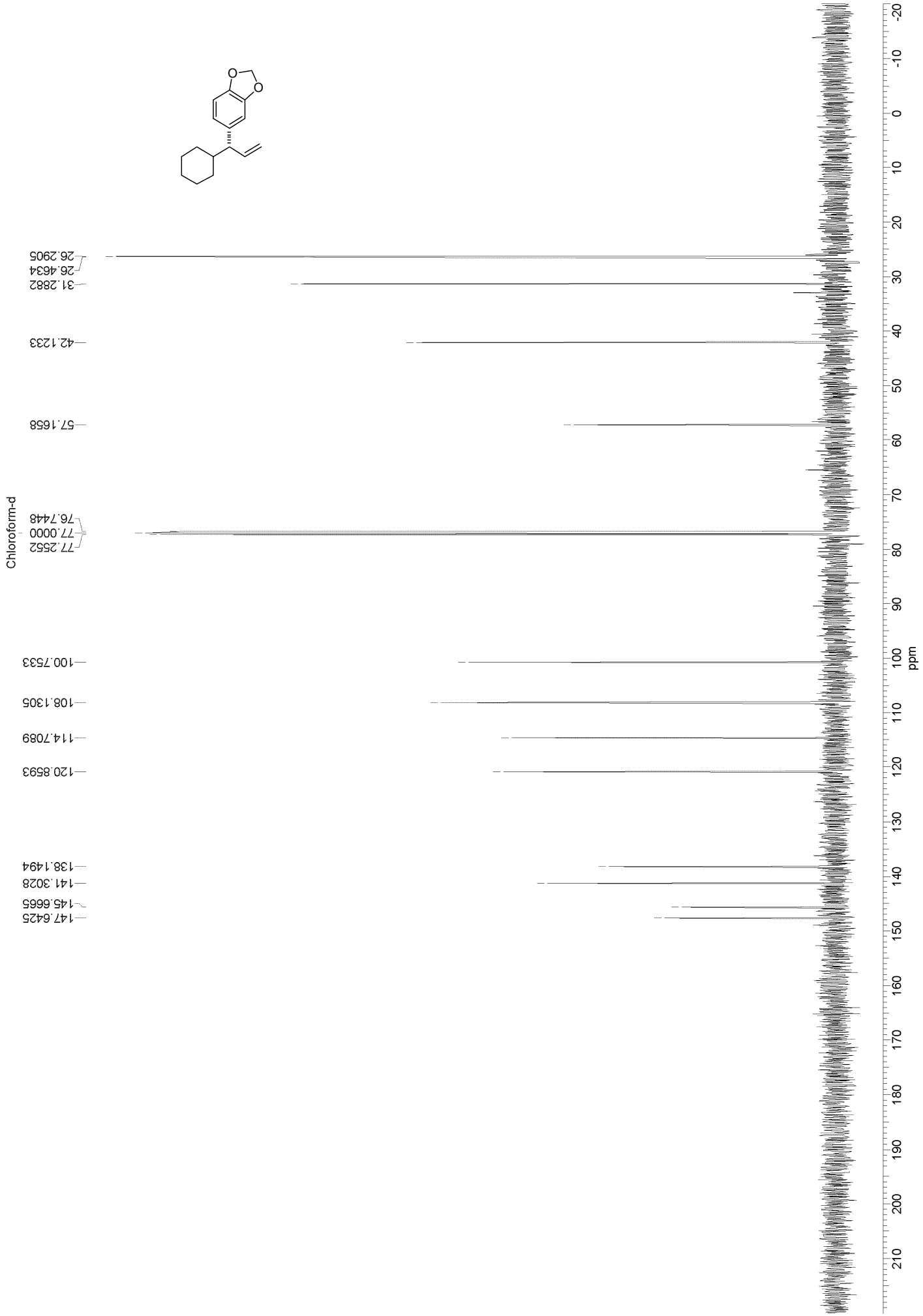
^{13}C-NMR of **3cg** (γ:α = 96:4)



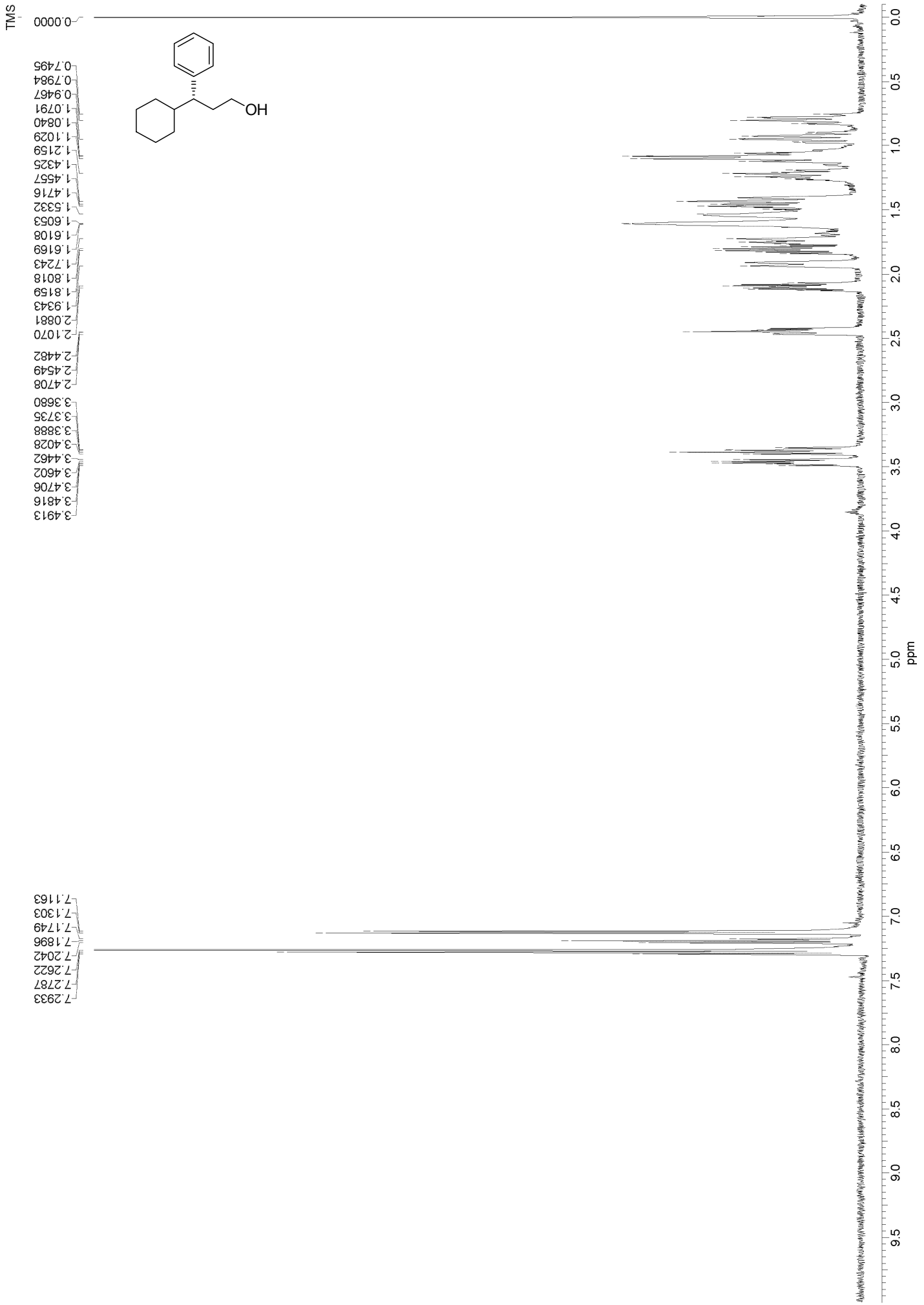
^{1}H-NMR of **3ch** (γ:α = 91:9)



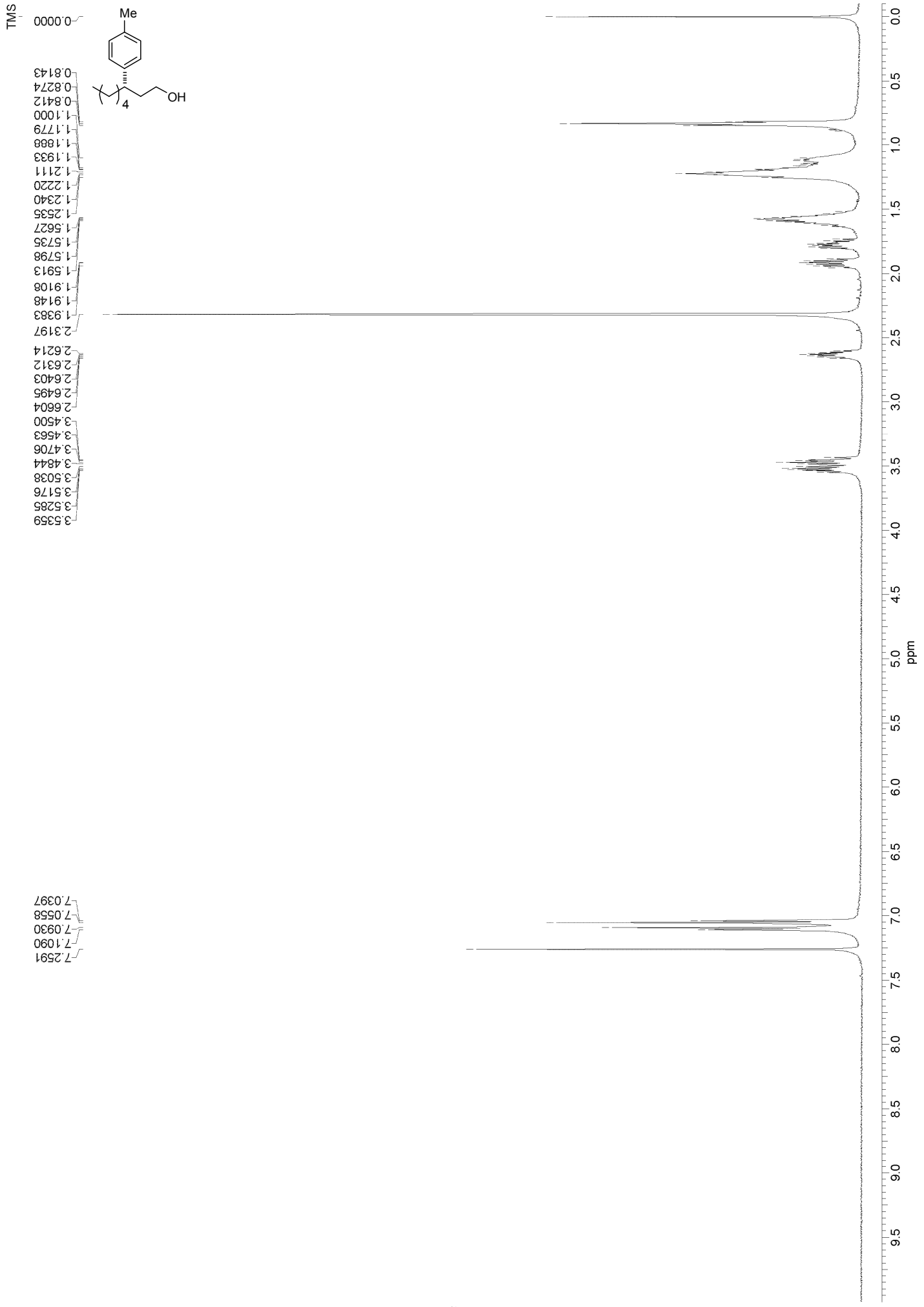
^{13}C-NMR of **3ch** (γ:α = 91:9)



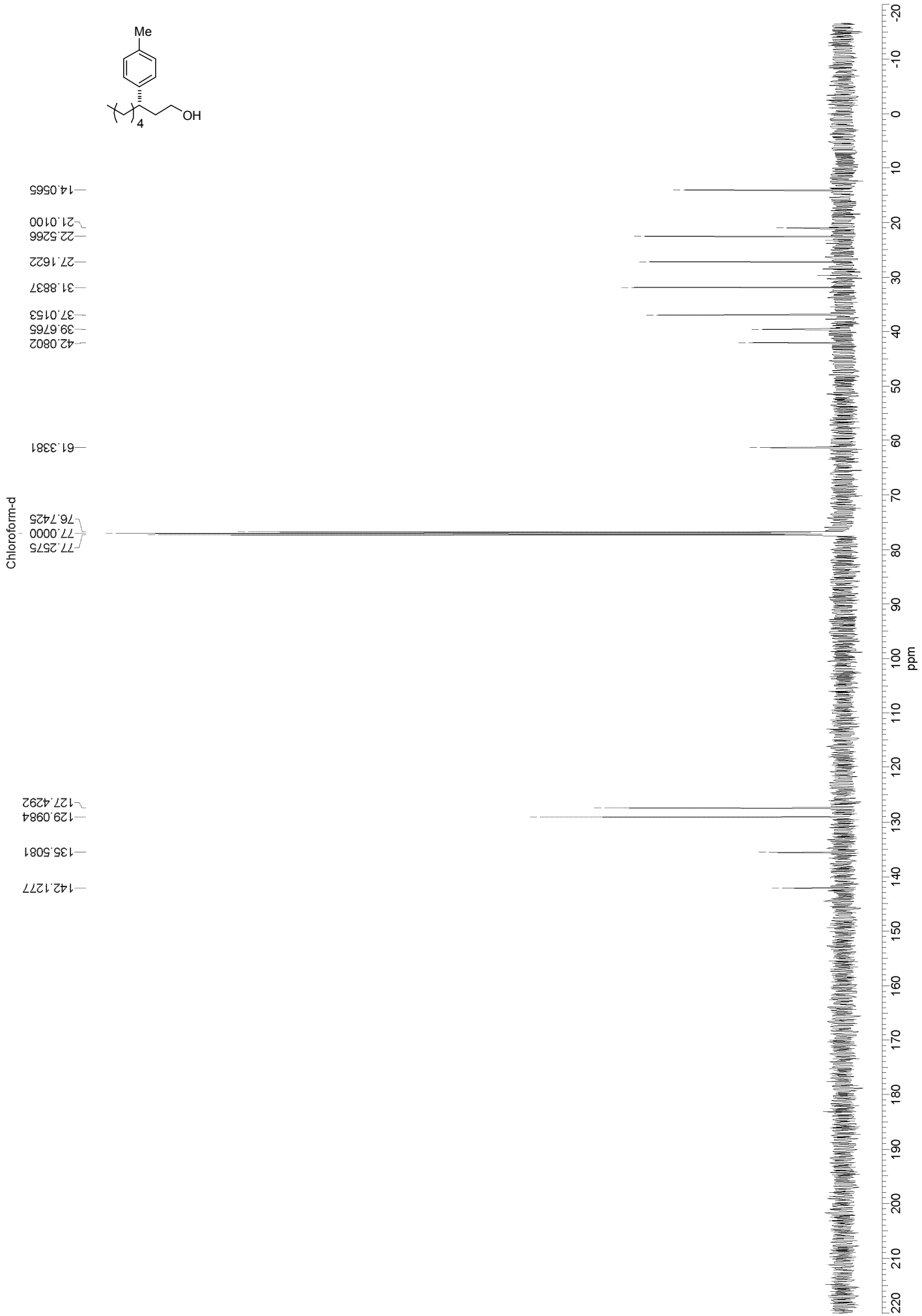
^{1}H-NMR of **4**


TMS
0.0000
0.7495
0.7984
0.9467
1.0791
1.0840
1.1029
1.2159
1.4325
1.4557
1.4716
1.5332
1.6053
1.6108
1.6169
1.7243
1.8018
1.8159
1.9343
2.0881
2.1070
2.4482
2.4549
2.4708
3.3680
3.3735
3.3888
3.4028
3.4462
3.4602
3.4706
3.4816
3.4913
7.1163
7.1303
7.1749
7.1896
7.2042
7.2622
7.2787
7.2933
OH
ppm

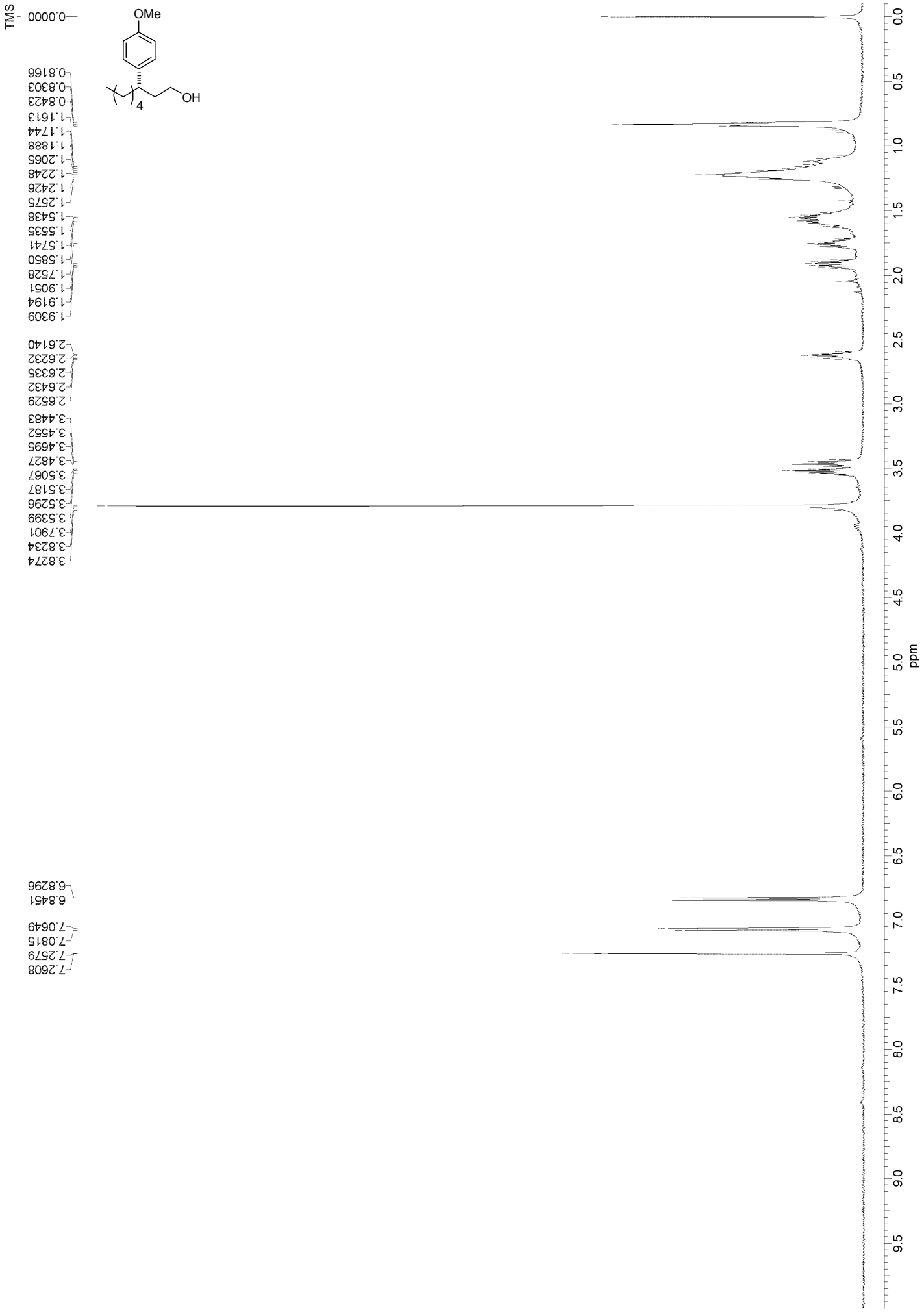
^{1}H-NMR of **5**


TMS
0.0000
Me
OH
4
0.8143
0.8274
0.8412
1.1000
1.1779
1.1888
1.1933
1.2111
1.2220
1.2340
1.2535
1.5627
1.5735
1.5798
1.5913
1.9108
1.9148
1.9383
2.3197
2.6214
2.6312
2.6403
2.6495
2.6604
3.4500
3.4563
3.4706
3.4844
3.5038
3.5176
3.5285
3.5359
7.0397
7.0558
7.0930
7.1090
7.2591
ppm

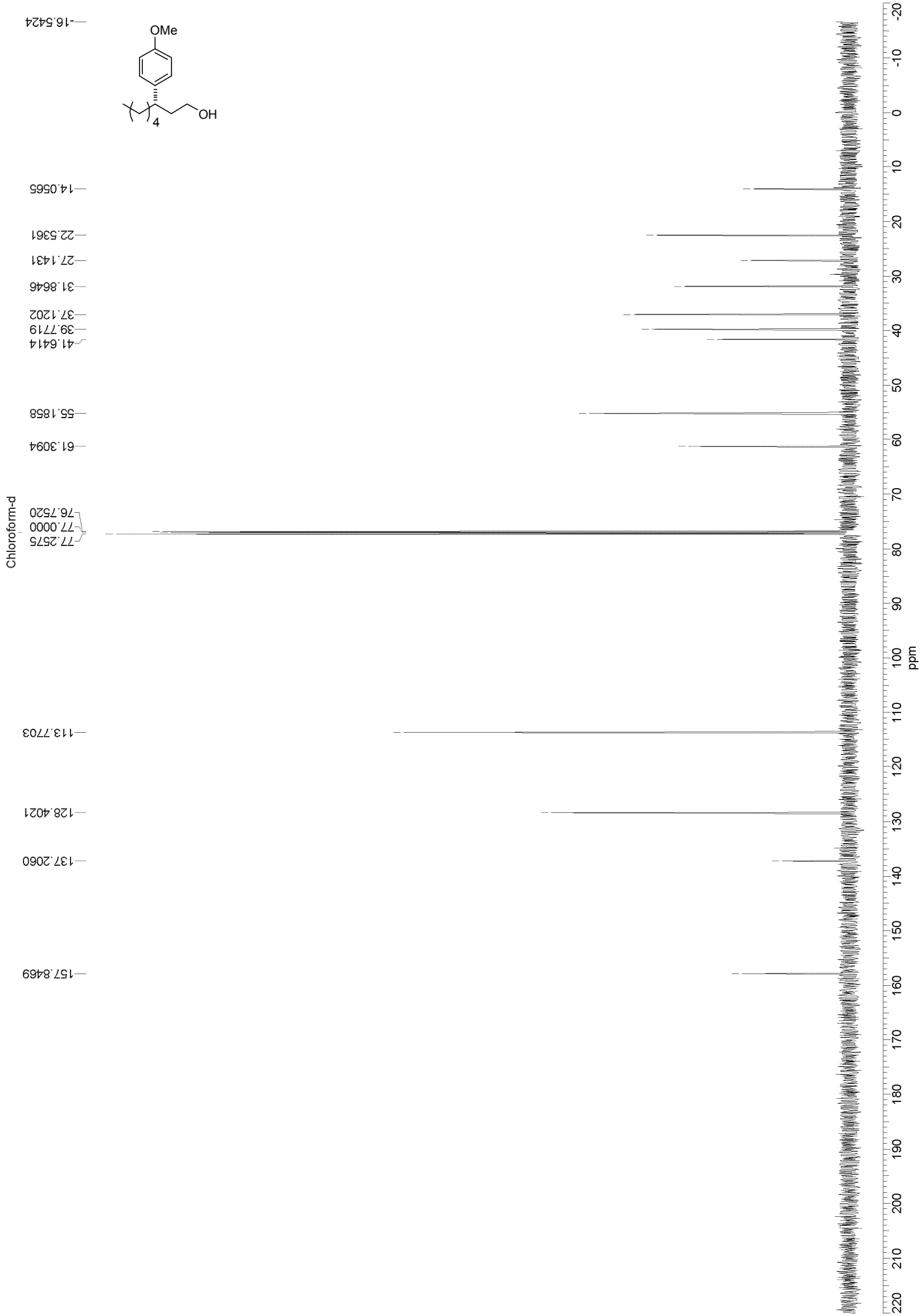
^{13}C-NMR of **5**


Me
OH
4
14.0565
21.0100
22.5266
27.1622
31.8837
37.0153
39.6765
42.0802
61.3381
Chloroform-d
76.7425
77.0000
77.2575
127.4292
129.0984
135.5081
142.1277
ppm

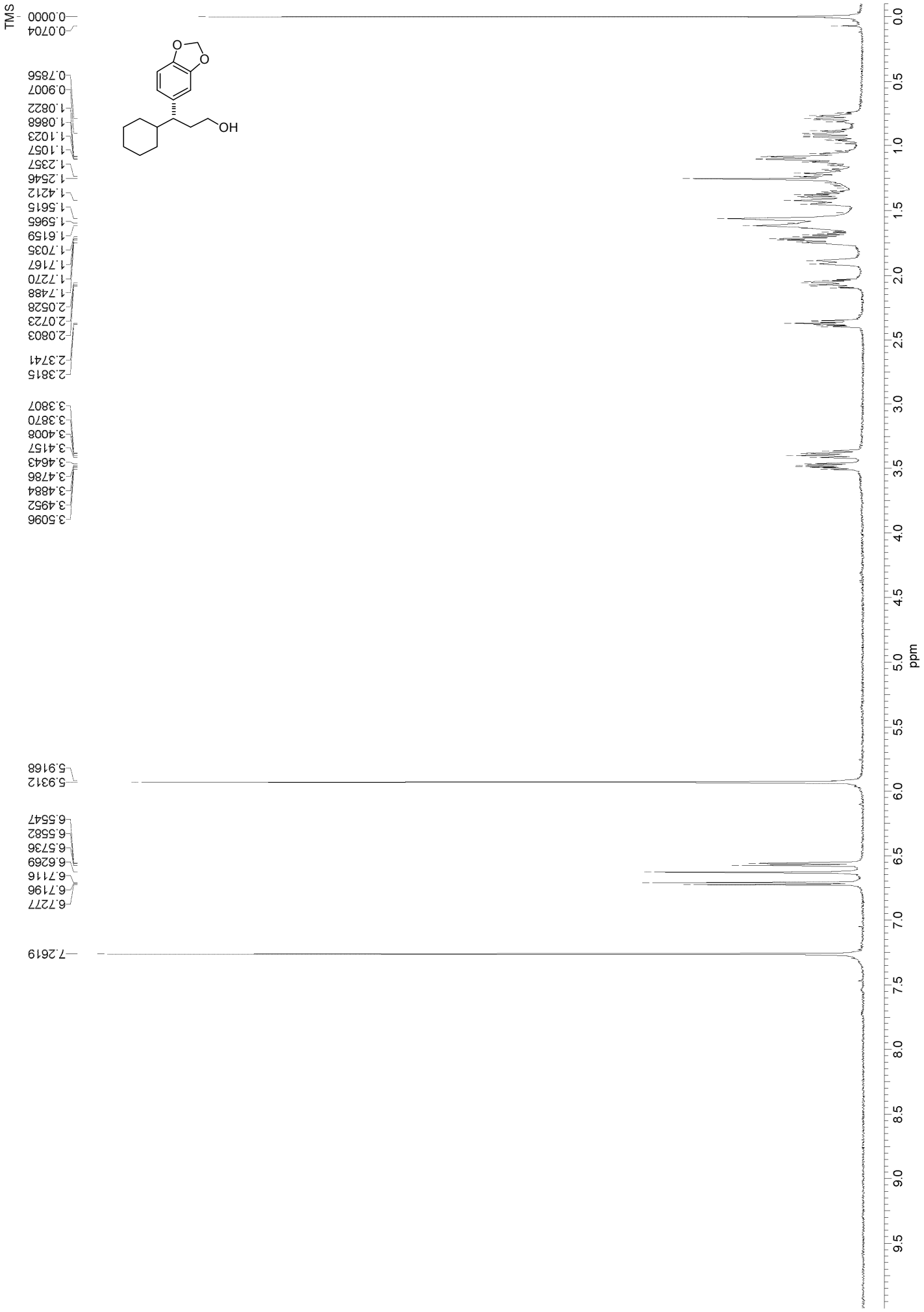
^{1}H-NMR of **6**


TMS
0.0000
OMe
OH
4
0.8166
0.8303
0.8423
1.1613
1.1744
1.1888
1.2065
1.2248
1.2426
1.2575
1.5438
1.5535
1.5741
1.5850
1.7528
1.9051
1.9194
1.9309
2.6140
2.6232
2.6335
2.6432
2.6529
3.4483
3.4552
3.4695
3.4827
3.5067
3.5187
3.5296
3.5399
3.7901
3.8234
3.8274
6.8296
6.8451
7.0649
7.0815
7.2579
7.2608
ppm

^{13}C-NMR of **6**


OMe
OH
4
-16.5424
14.0565
22.5361
27.1431
31.8646
37.1202
39.7719
41.6414
55.1858
61.3094
Chloroform-d
76.7520
77.0000
77.2575
113.7703
128.4021
137.2060
157.8469
ppm

^{1}H-NMR of **7**


TMS
0.0000
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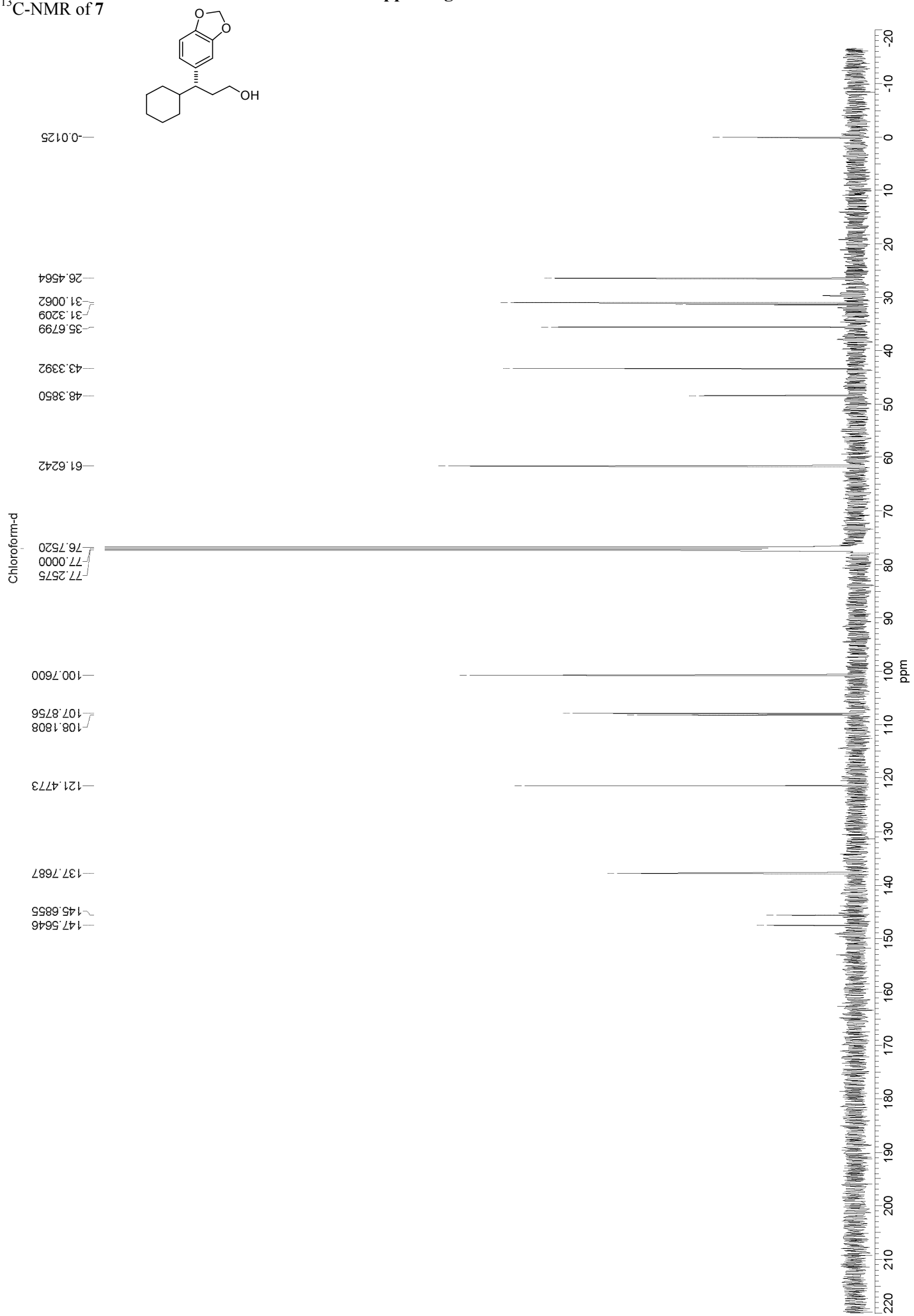
0.7856
0.9007
1.0822
1.0868
1.1023
1.1057
1.2357
1.2546
1.4212
1.5615
1.5965
1.6159
1.7035
1.7167
1.7270
1.7488
2.0528
2.0723
2.0803
2.3741
2.3815
3.3807
3.3870
3.4008
3.4157
3.4643
3.4786
3.4884
3.4952
3.5096
5.9168
5.9312
6.5547
6.5582
6.5736
6.6269
6.7116
6.7196
6.7277
7.2619
O
O
O
OH
ppm

^{13}C-NMR of **7**


O
O
OH
-0.0125
26.4564
31.0062
31.3209
35.6799
43.3392
48.3850
61.6242
Chloroform-d
76.7520
77.0000
77.2575
100.7600
107.8756
108.1808
121.4773
137.7687
145.6855
147.5646
ppm