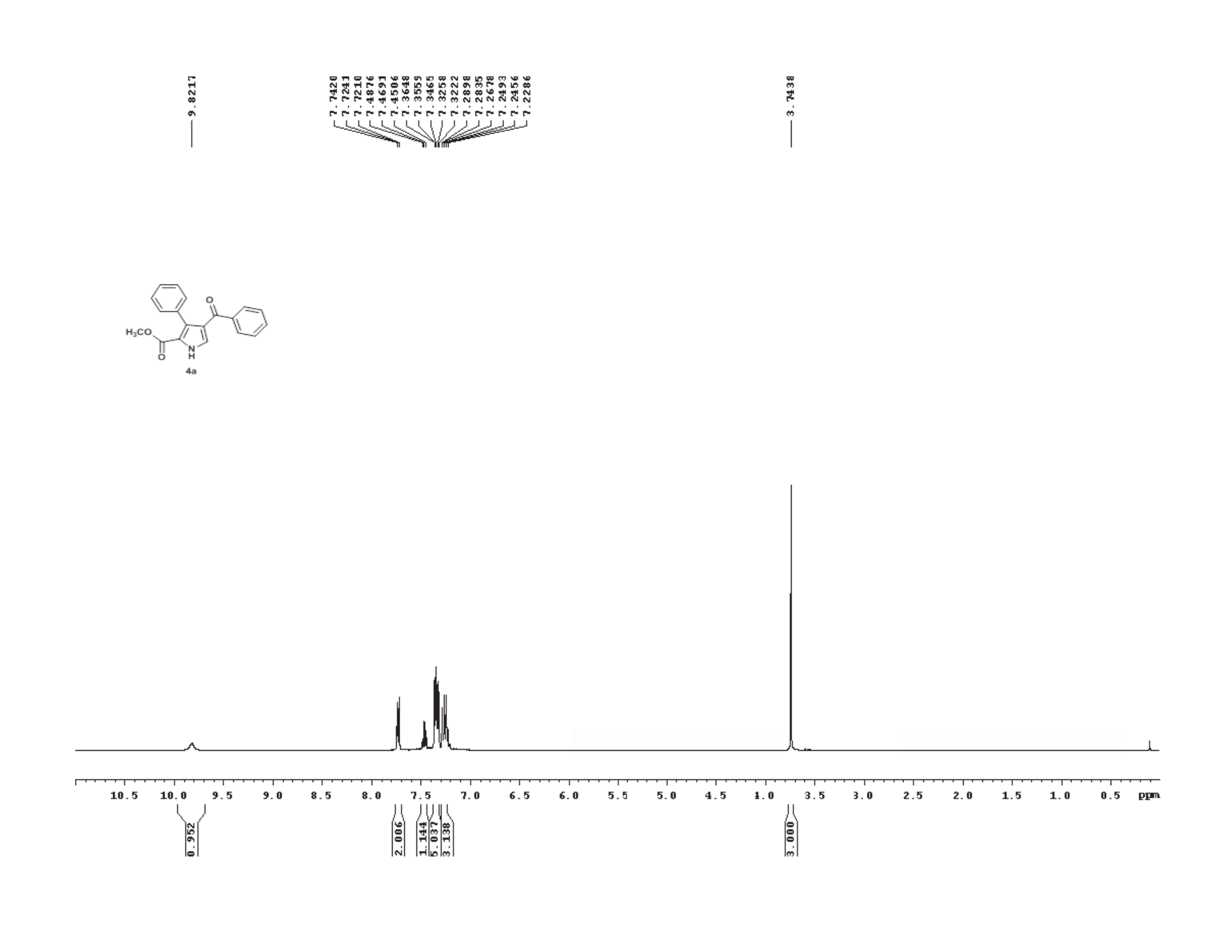
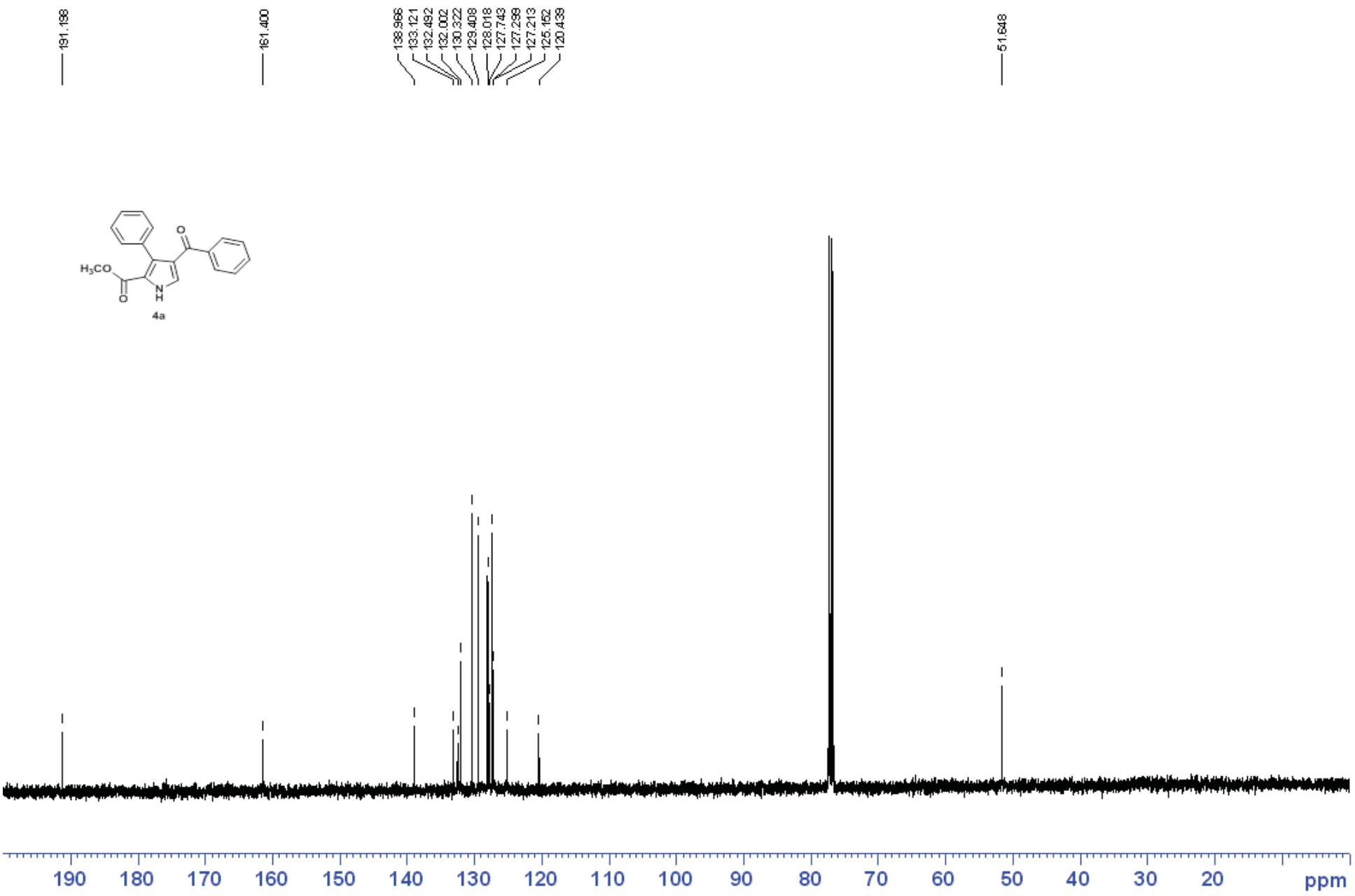
Multicomponent pathway inspired regioselective synthesis of 2,3,4-trisubstituted 1*H*-pyrroles *via* [3+2] cycloaddition reaction

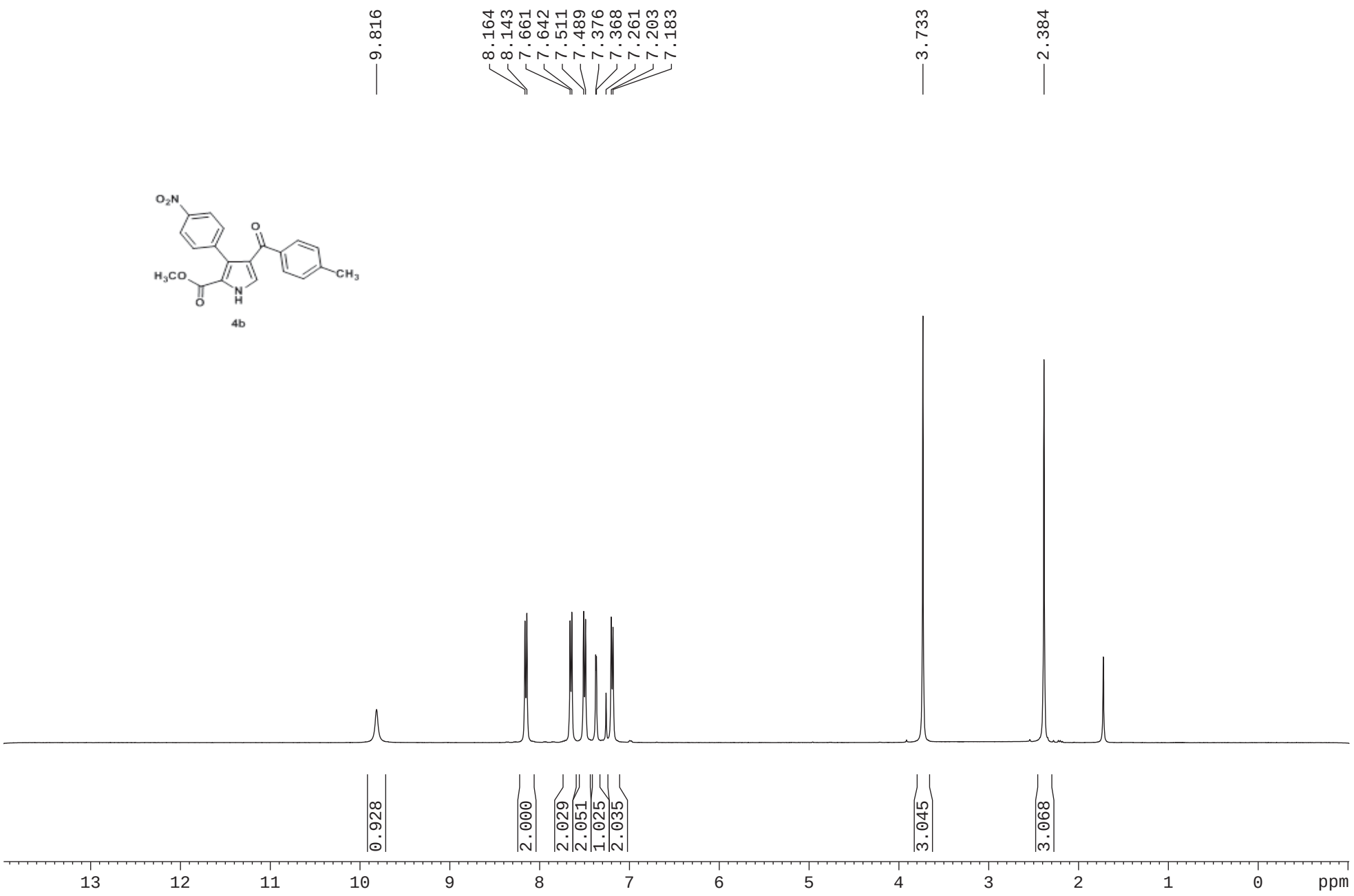
Hanuman P. Kalmode,[a] Kamlesh S. Vadagaonkar,[a] Kaliyappan Murugan*[b] and Atul C. Chaskar*[a,b,c]
[a]*Department of Dyestuff Technology, Institute of Chemical Technology, Mumbai 400019, India*
[b]*National Taiwan University, Taipei 10617, Taiwan*
[c]*National Centre for Nanosciences and Nanotechnology, University of Mumbai, Mumbai 400098, India*
Tel.: +91-22-3361 1111/ 2706; Fax: +91-22-3361 1020; E-mail: achaskar25@gmail.com.

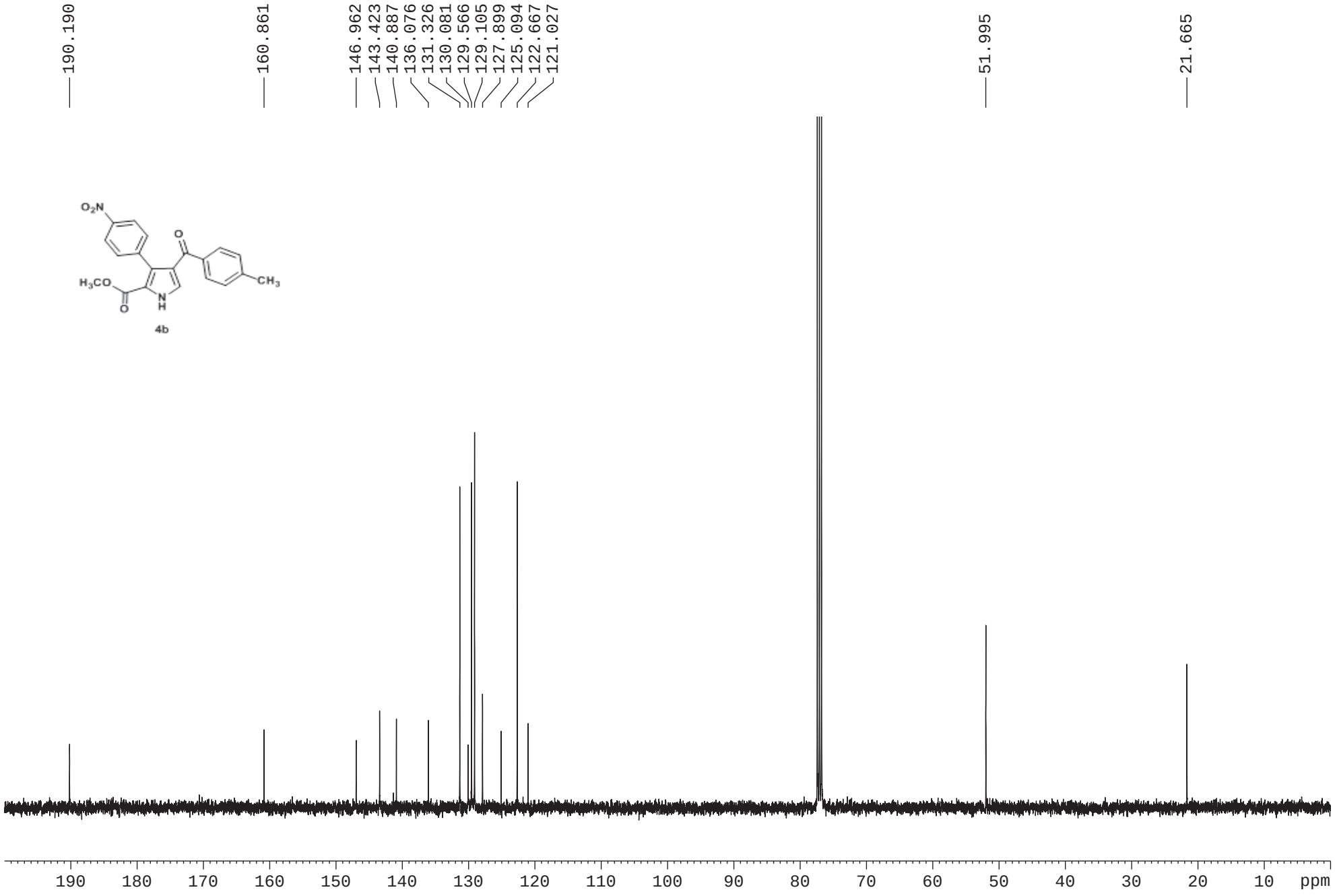
Supporting Information

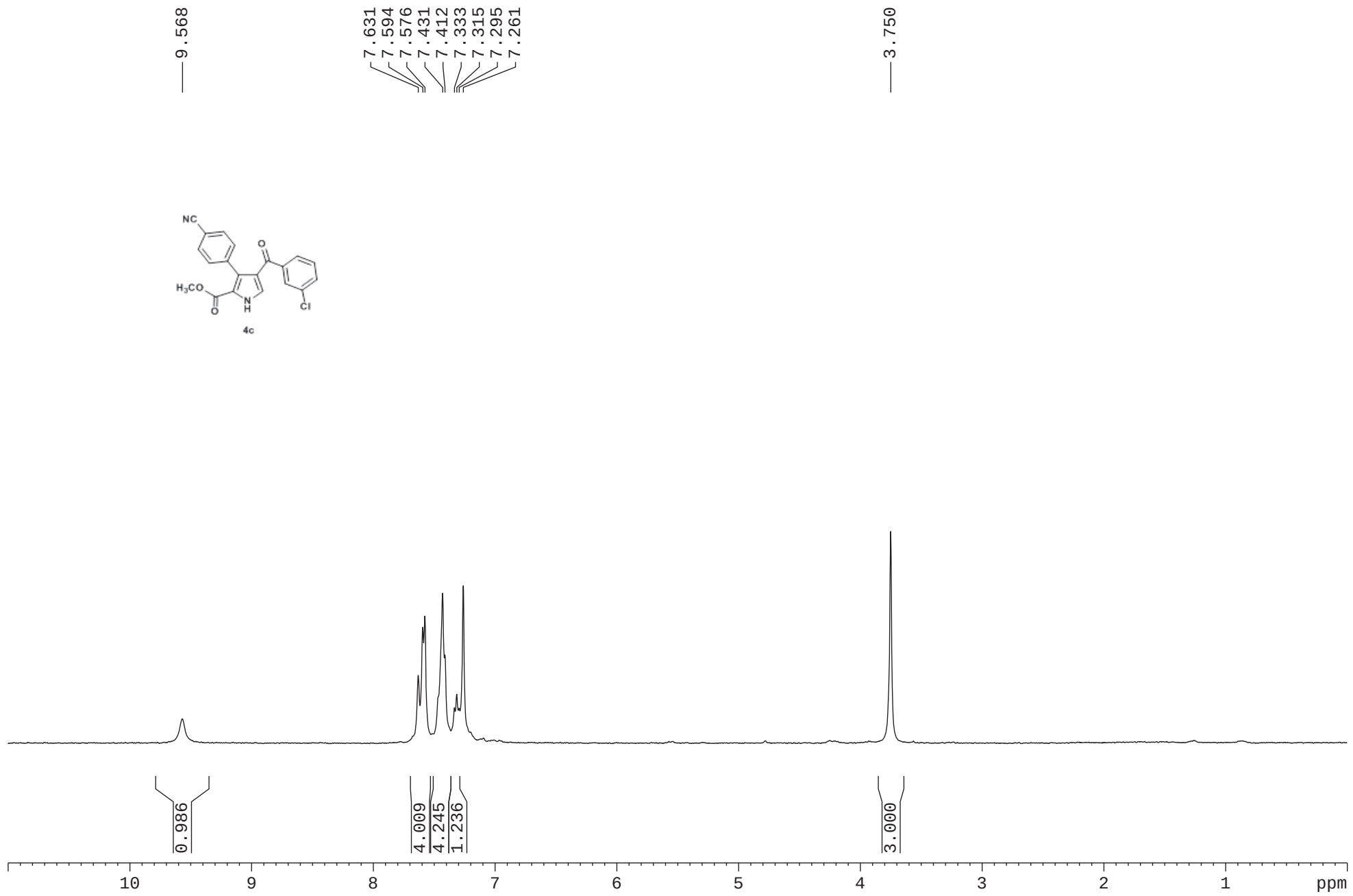
Contents

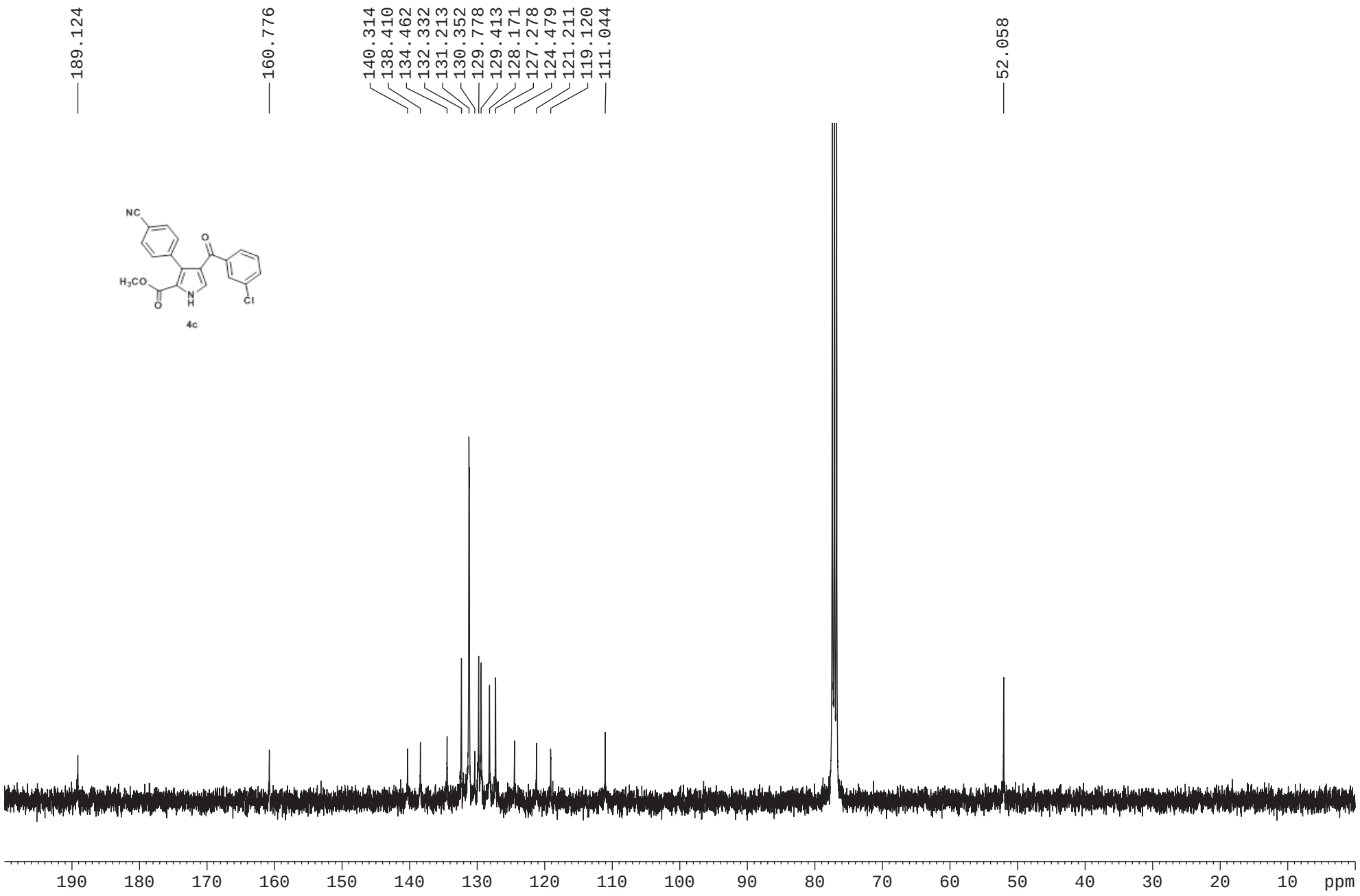

9.8217
7.7420
7.7241
7.7210
7.4876
7.4691
7.4506
7.3648
7.3559
7.3465
7.3258
7.3222
7.2898
7.2835
7.2678
7.2493
7.2456
7.2286
3.7438
H3CO
O
O
N
H
4a
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.952
2.006
1.144
5.037
3.138
3.000

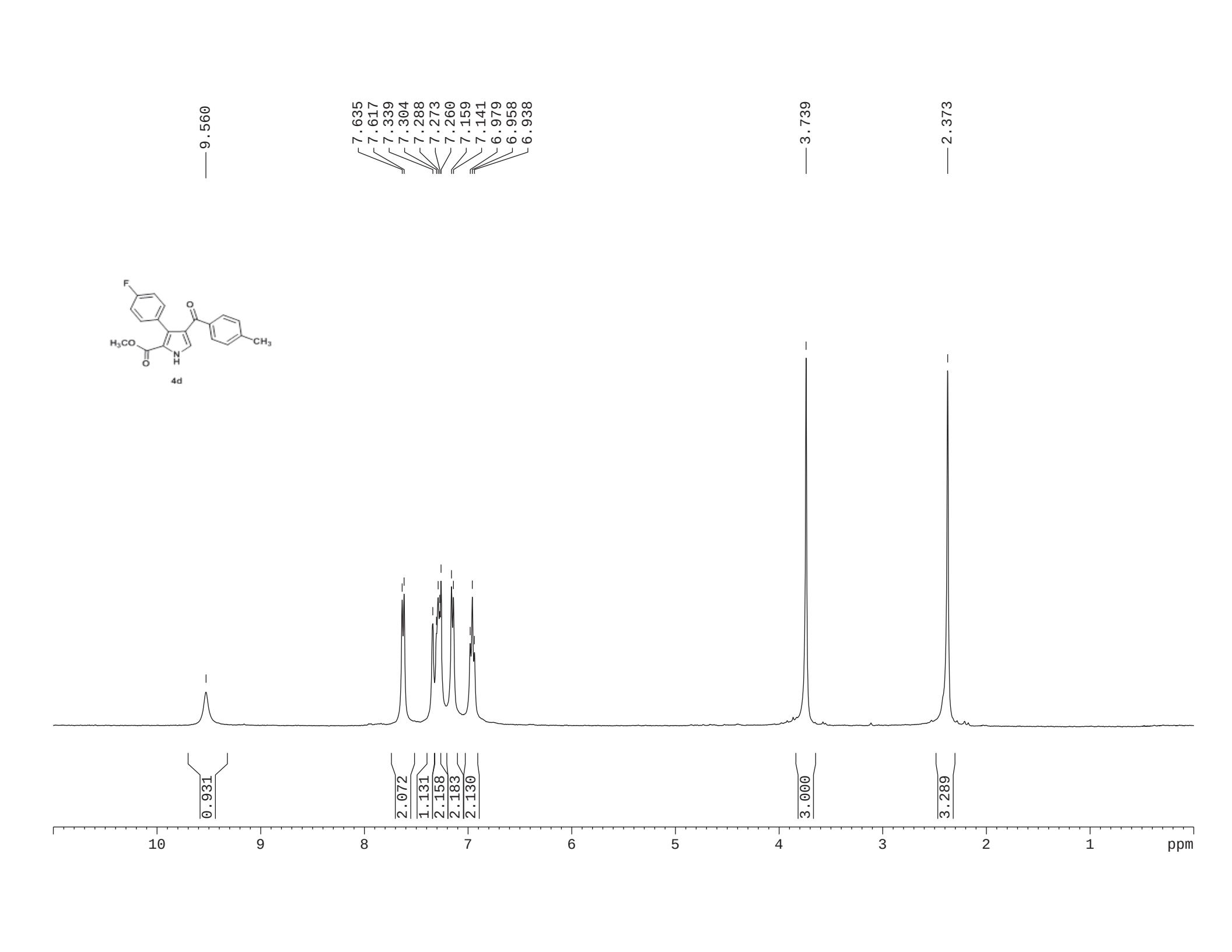

191.198
161.400
138.966
133.121
132.492
132.002
130.322
129.408
128.018
127.743
127.299
127.213
125.152
120.439
51.648
H3CO
O
O
N
H
4a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

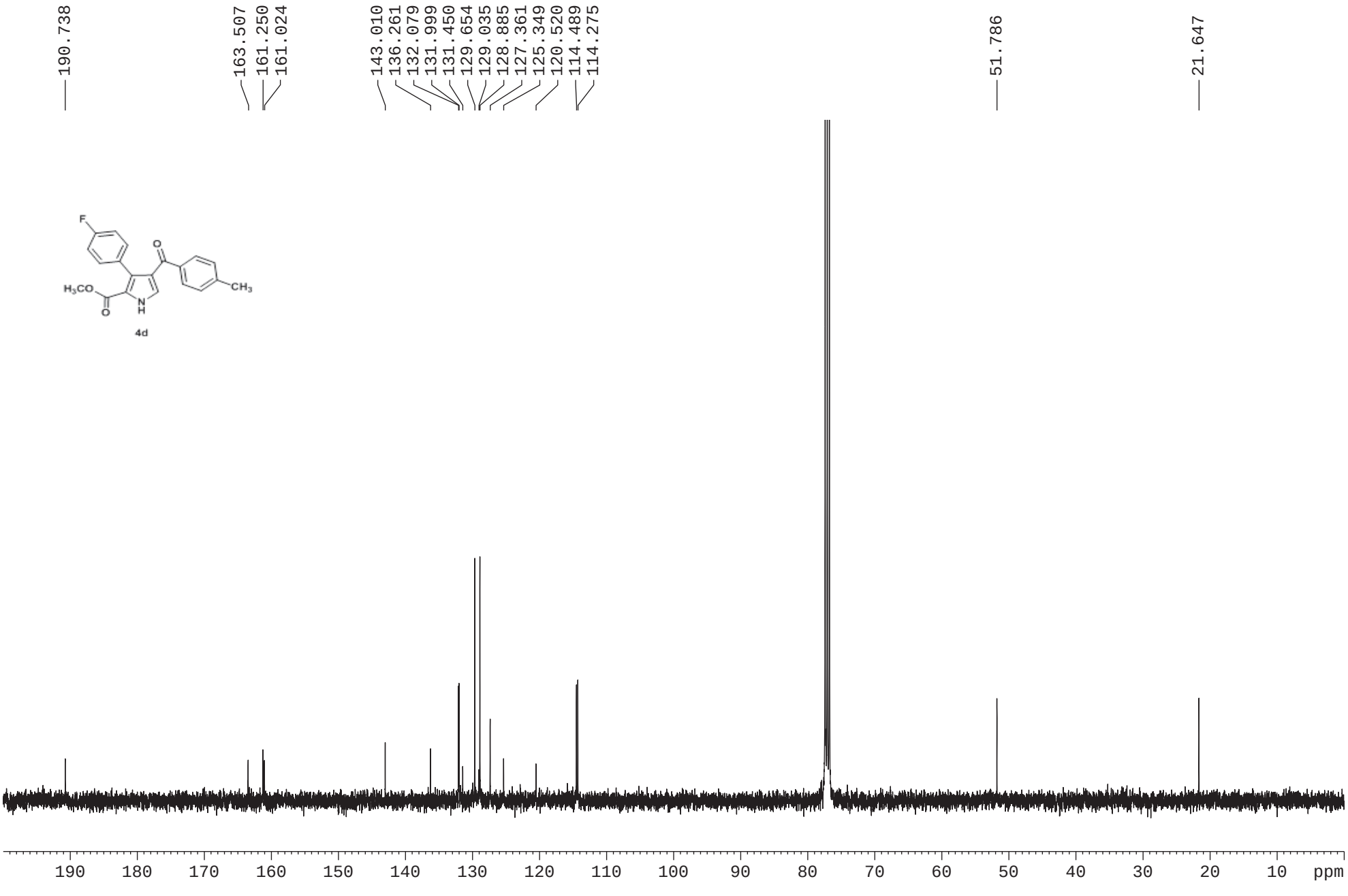

9.816
8.164
8.143
7.661
7.642
7.511
7.489
7.376
7.368
7.261
7.203
7.183
3.733
2.384
O2N
O
H3CO
O
N
H
CH3
4b
0.928
2.000
2.029
2.051
1.025
2.035
3.045
3.068
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

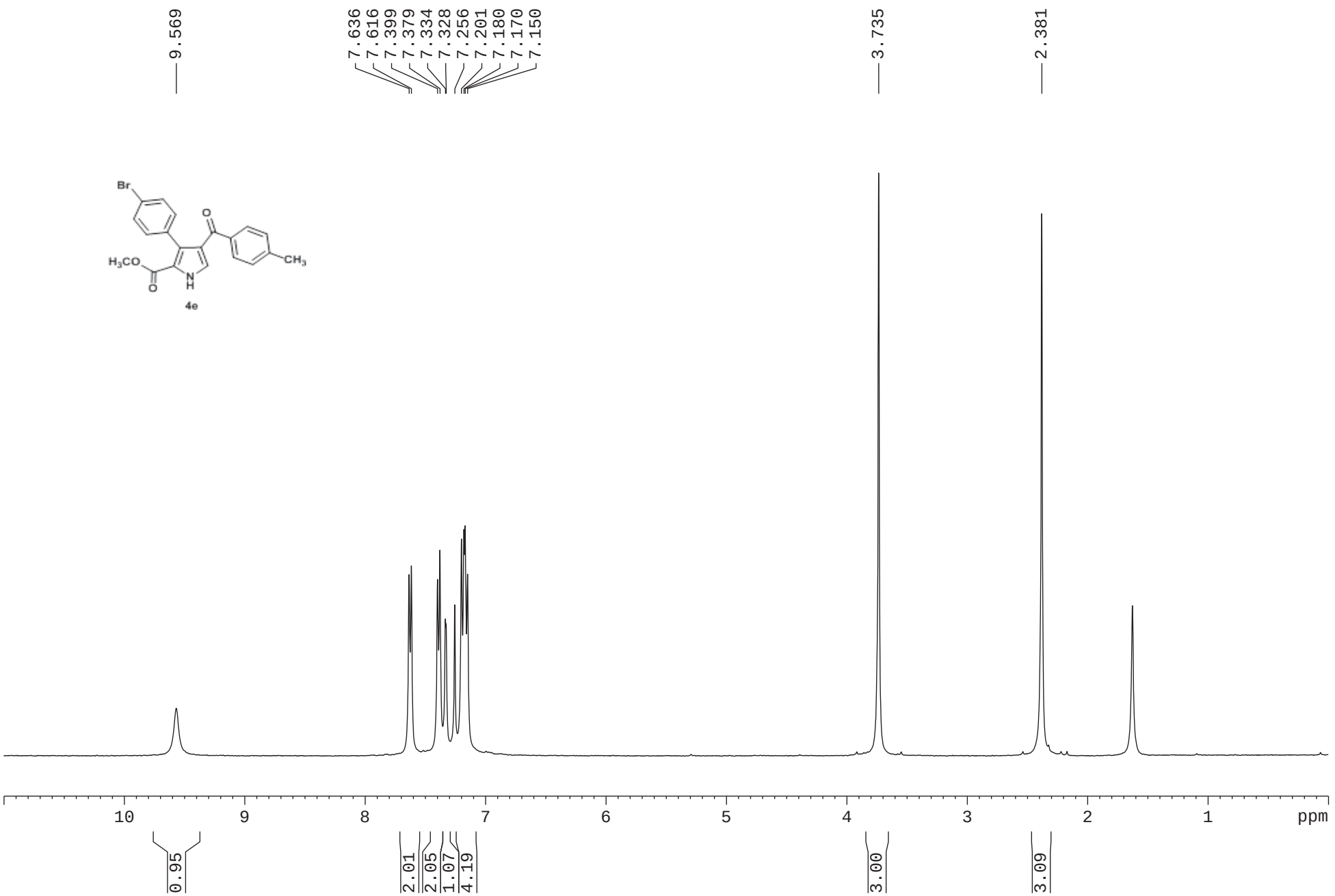

190.190
160.861
146.962
143.423
140.887
136.076
131.326
130.081
129.566
129.105
127.899
125.094
122.667
121.027
51.995
21.665
O2N
O
H3CO
O
N
H
CH3
4b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

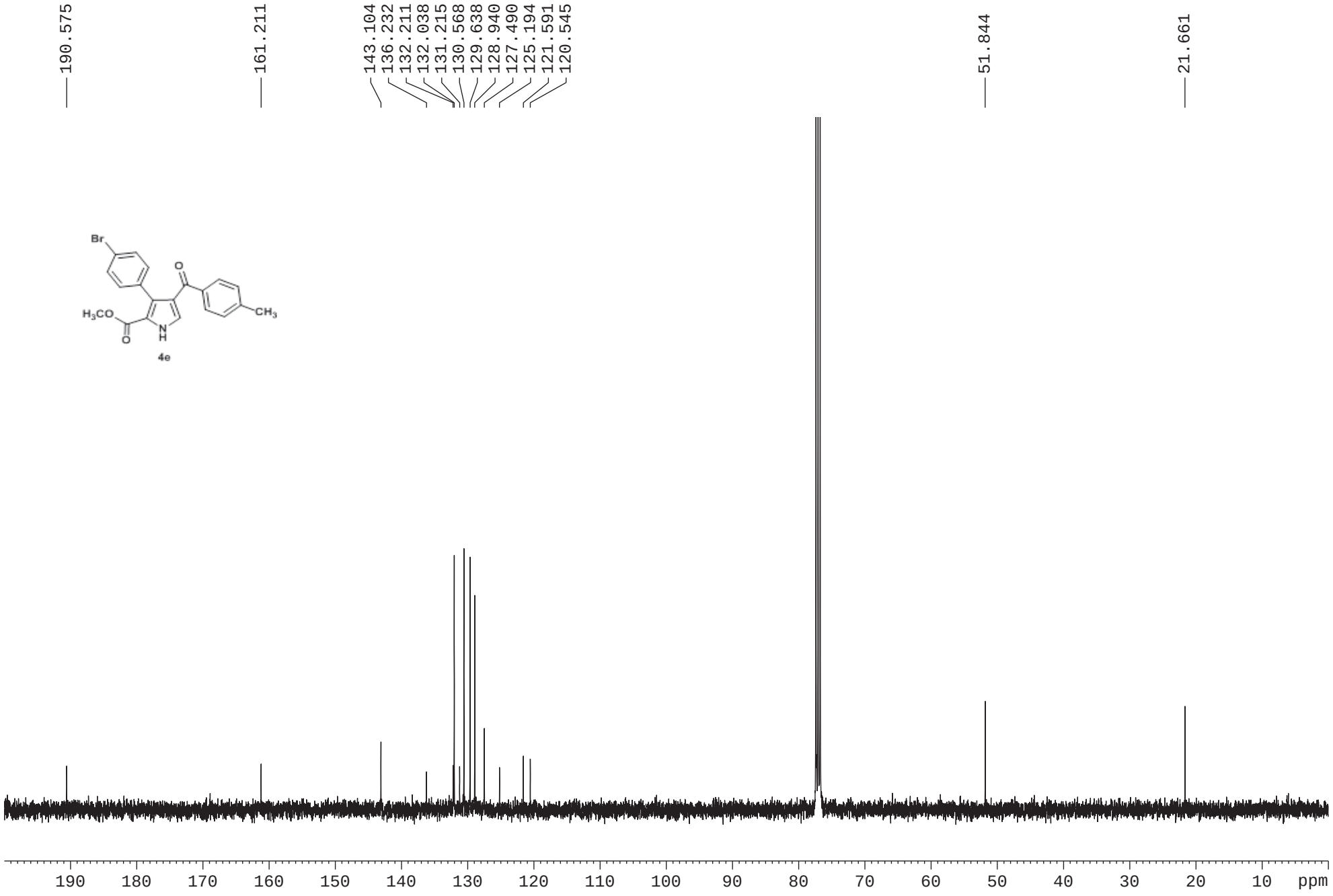

9.568
7.631
7.594
7.576
7.431
7.412
7.333
7.315
7.295
7.261
3.750
NC
O
H3CO
O
N
H
Cl
4c
0.986
4.009
4.245
1.236
3.000
10
9
8
7
6
5
4
3
2
1
ppm

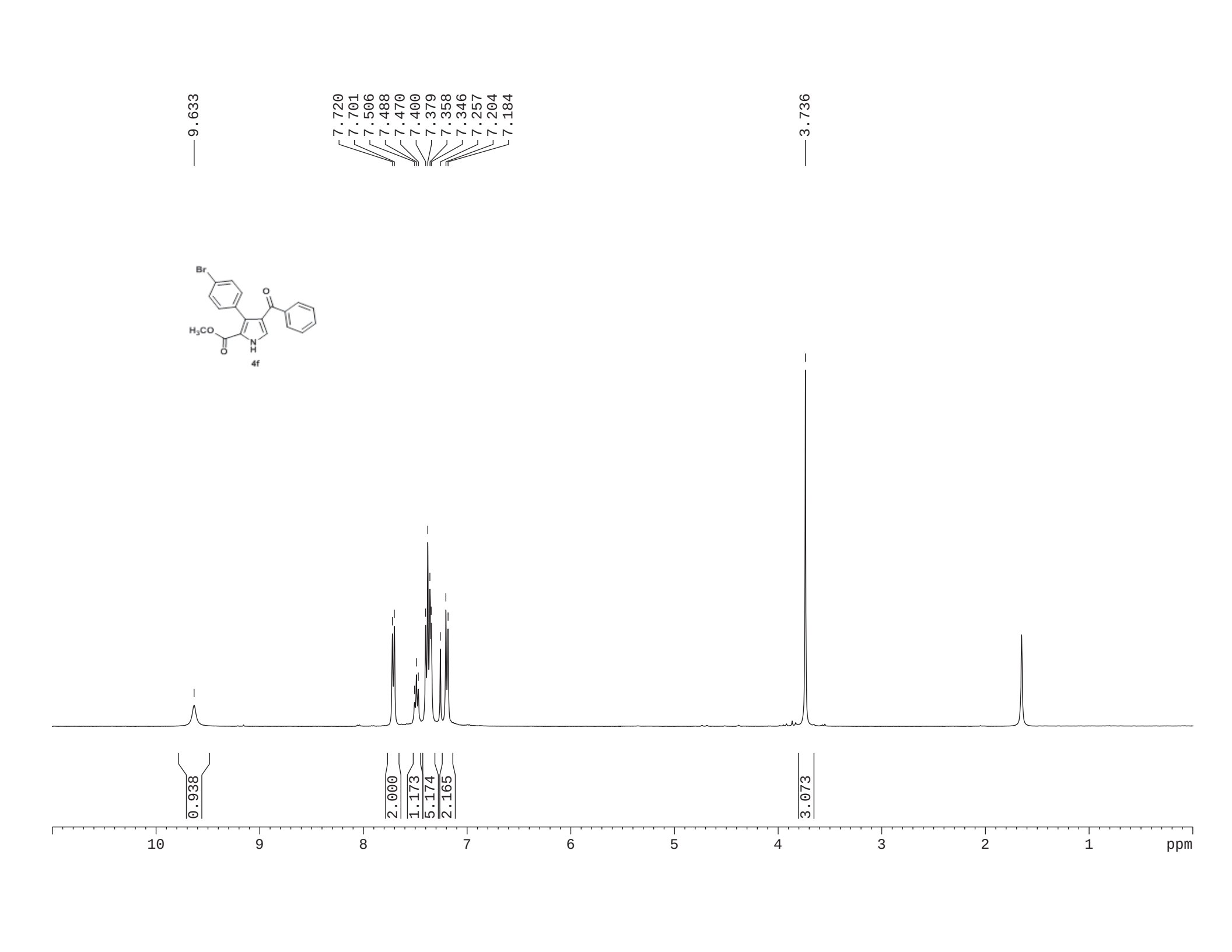

189.124
160.776
140.314
138.410
134.462
132.332
131.213
130.352
129.778
129.413
128.171
127.278
124.479
121.211
119.120
111.044
52.058
NC
O
H3CO
O
N
H
Cl
4c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

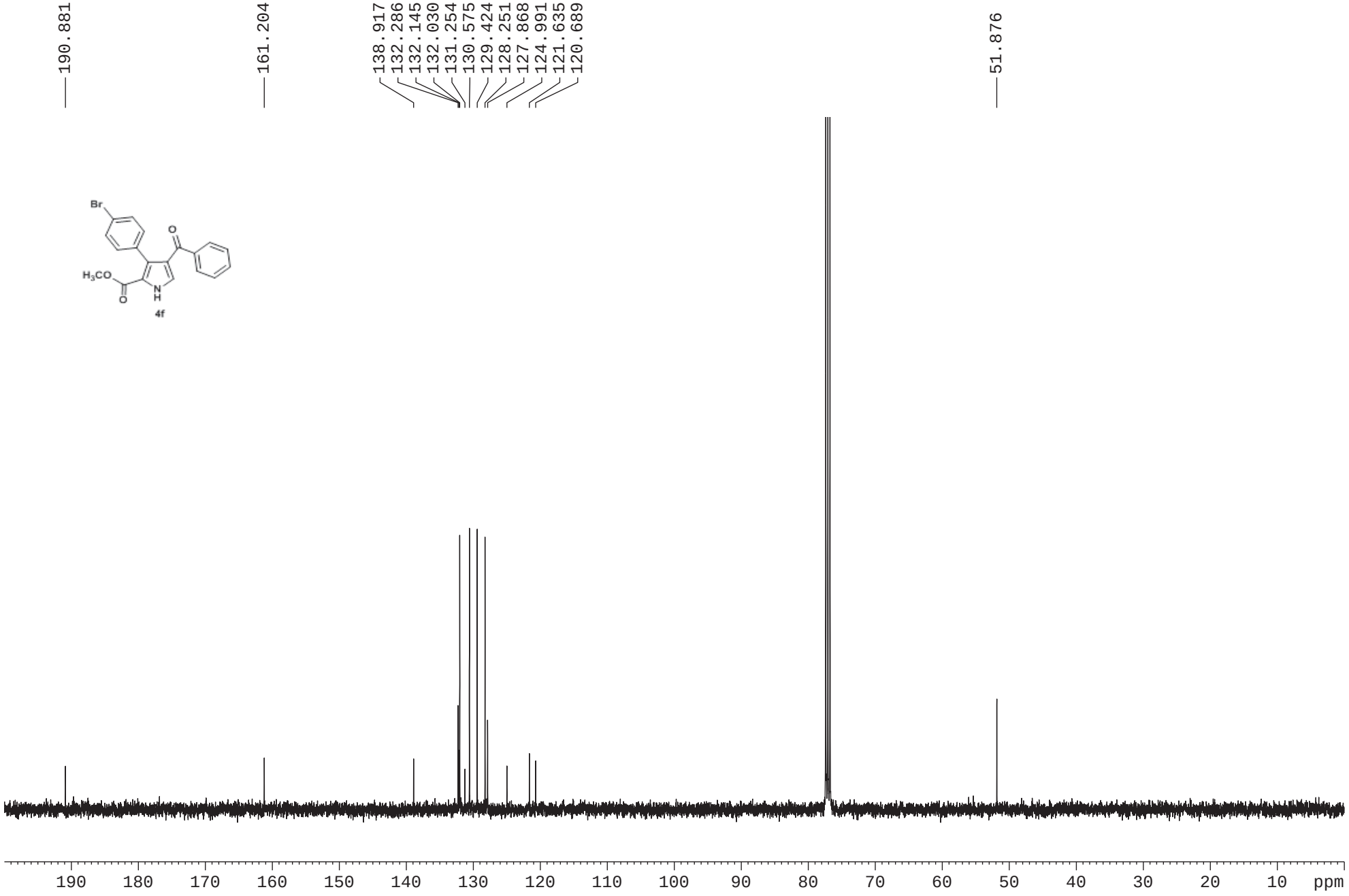

9.560
7.635
7.617
7.339
7.304
7.288
7.273
7.260
7.159
7.141
6.979
6.958
6.938
3.739
2.373
F
O
H3CO
O
N
H
CH3
4d
0.931
2.072
1.131
2.158
2.183
2.130
3.000
3.289
10
9
8
7
6
5
4
3
2
1
ppm

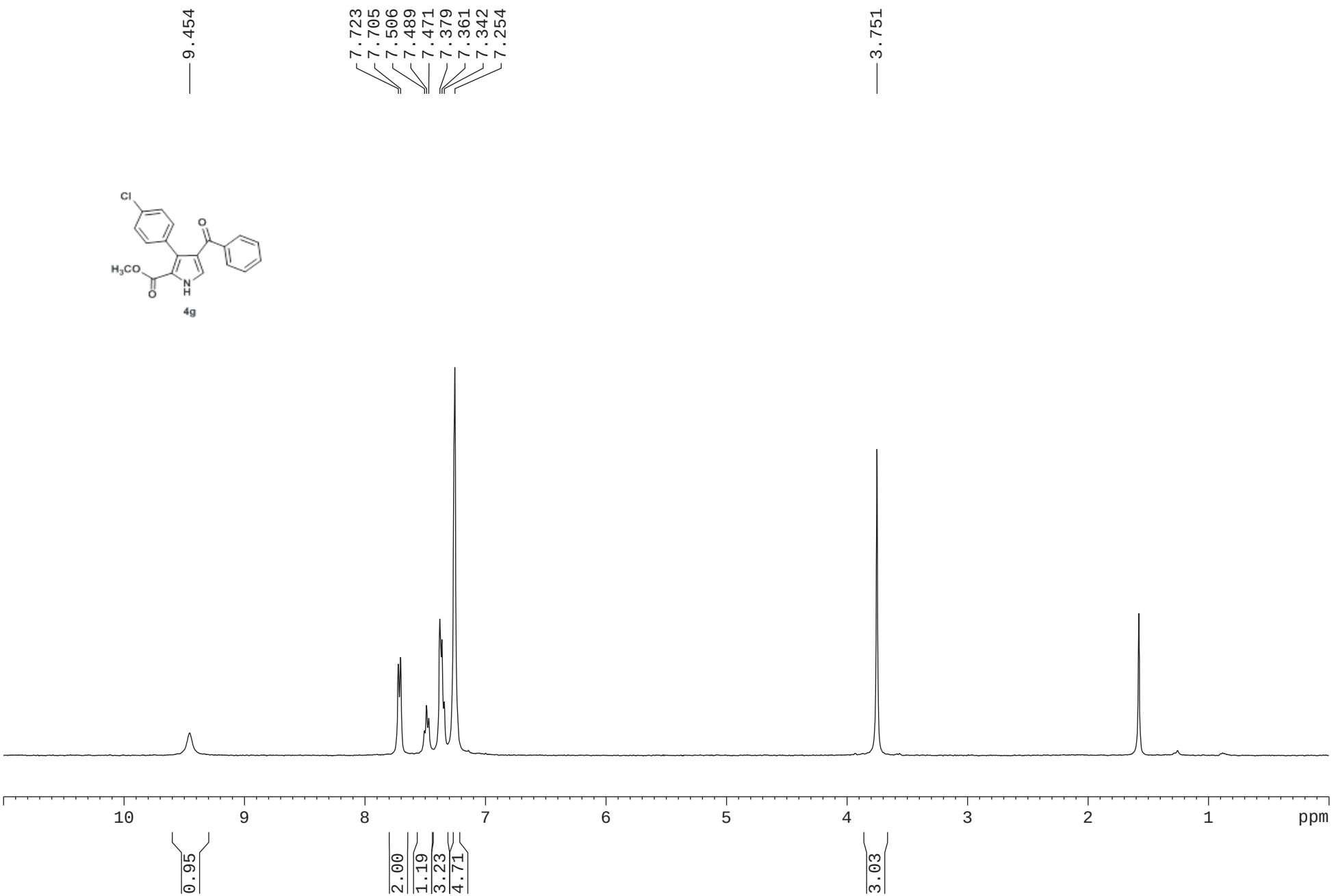

190.738
163.507
161.250
161.024
143.010
136.261
132.079
131.999
131.450
129.654
129.035
128.885
127.361
125.349
120.520
114.489
114.275
51.786
21.647
F
O
H3CO
O
N
H
CH3
4d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

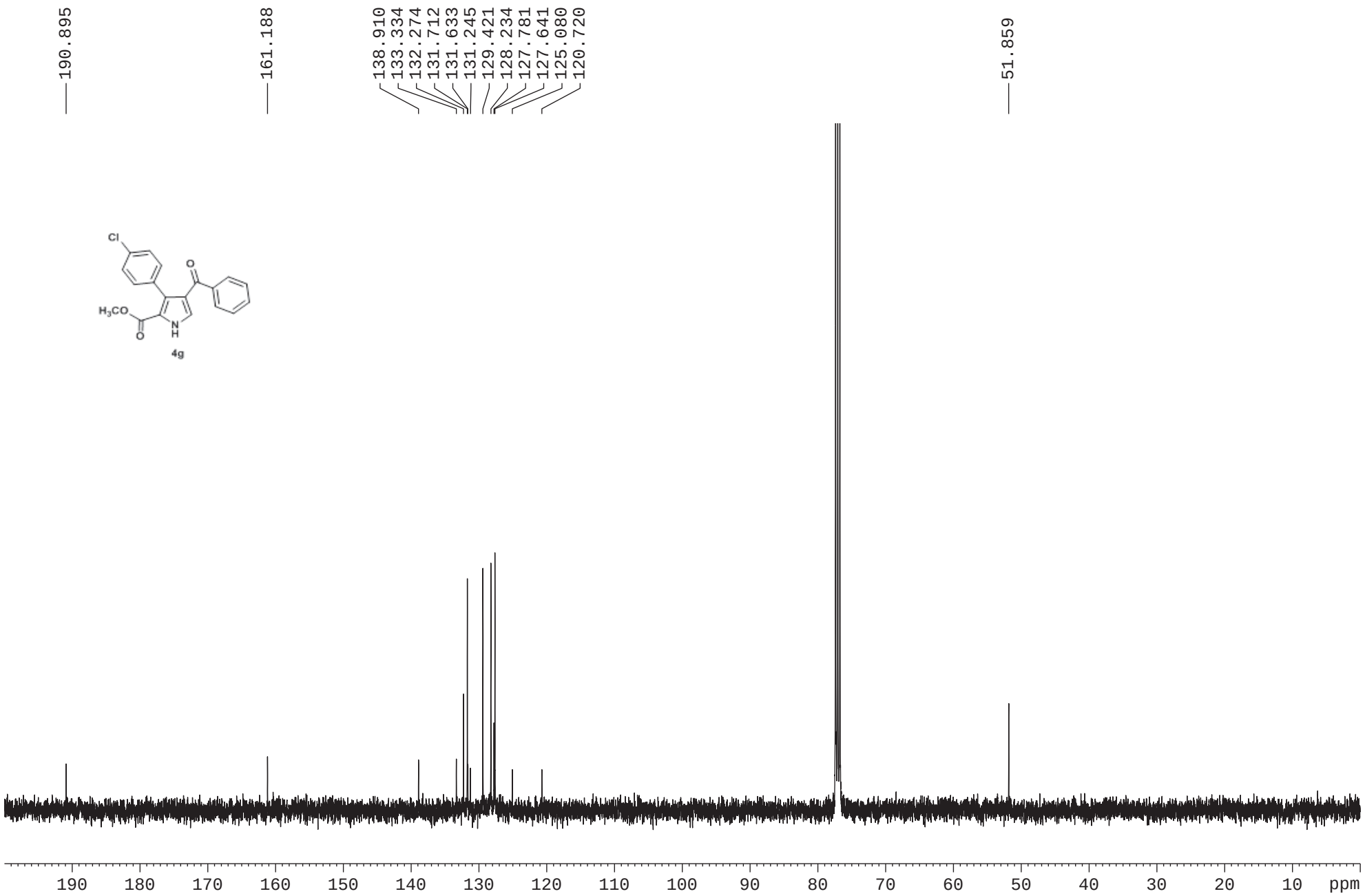

9.569
7.636
7.616
7.399
7.379
7.334
7.328
7.256
7.201
7.180
7.170
7.150
3.735
2.381
Br
O
H3CO
O
N
H
CH3
4e
10
9
8
7
6
5
4
3
2
1
ppm
0.95
2.01
2.05
1.07
4.19
3.00
3.09

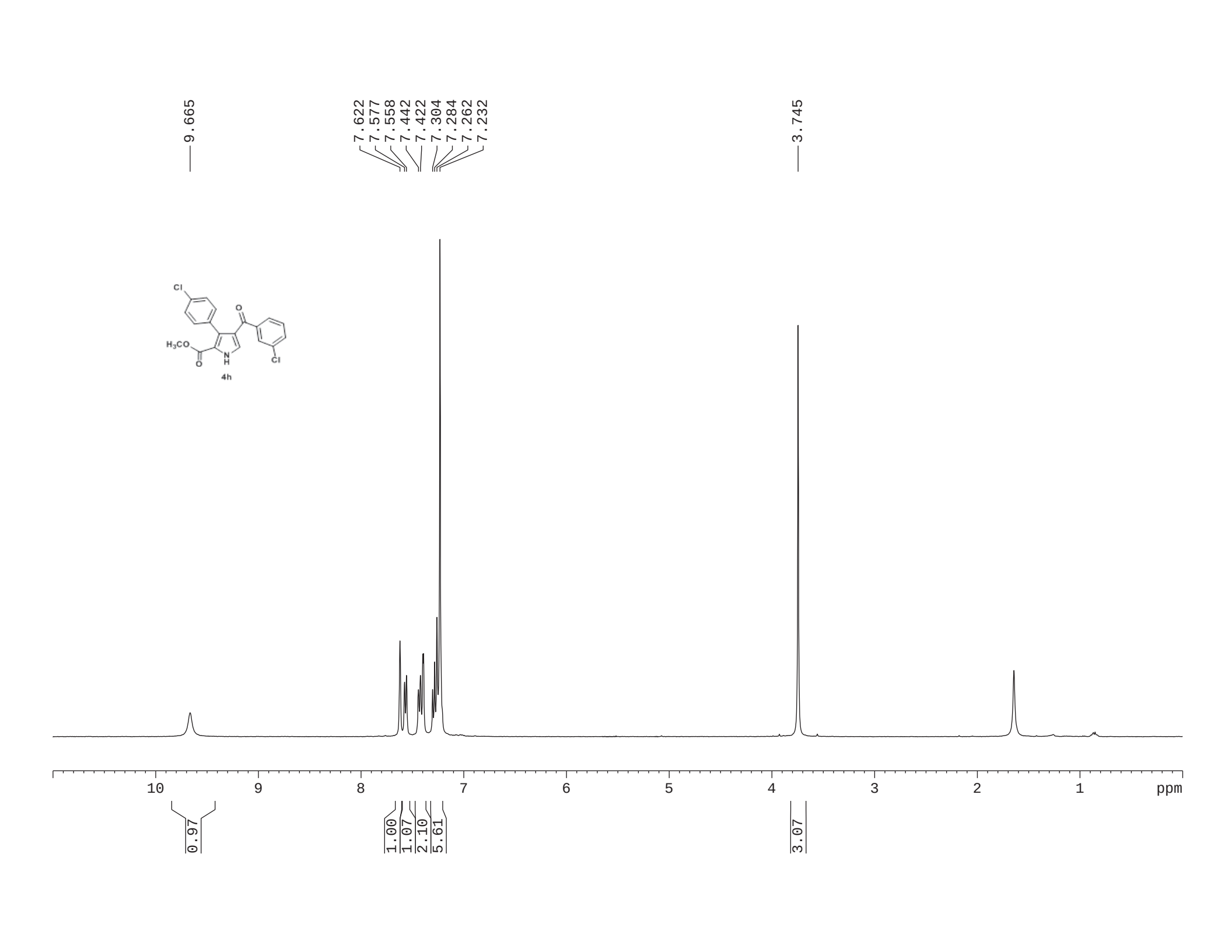

190.575
161.211
143.104
136.232
132.211
132.038
131.215
130.568
129.638
128.940
127.490
125.194
121.591
120.545
51.844
21.661
Br
O
H3CO
O
N
H
CH3
4e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

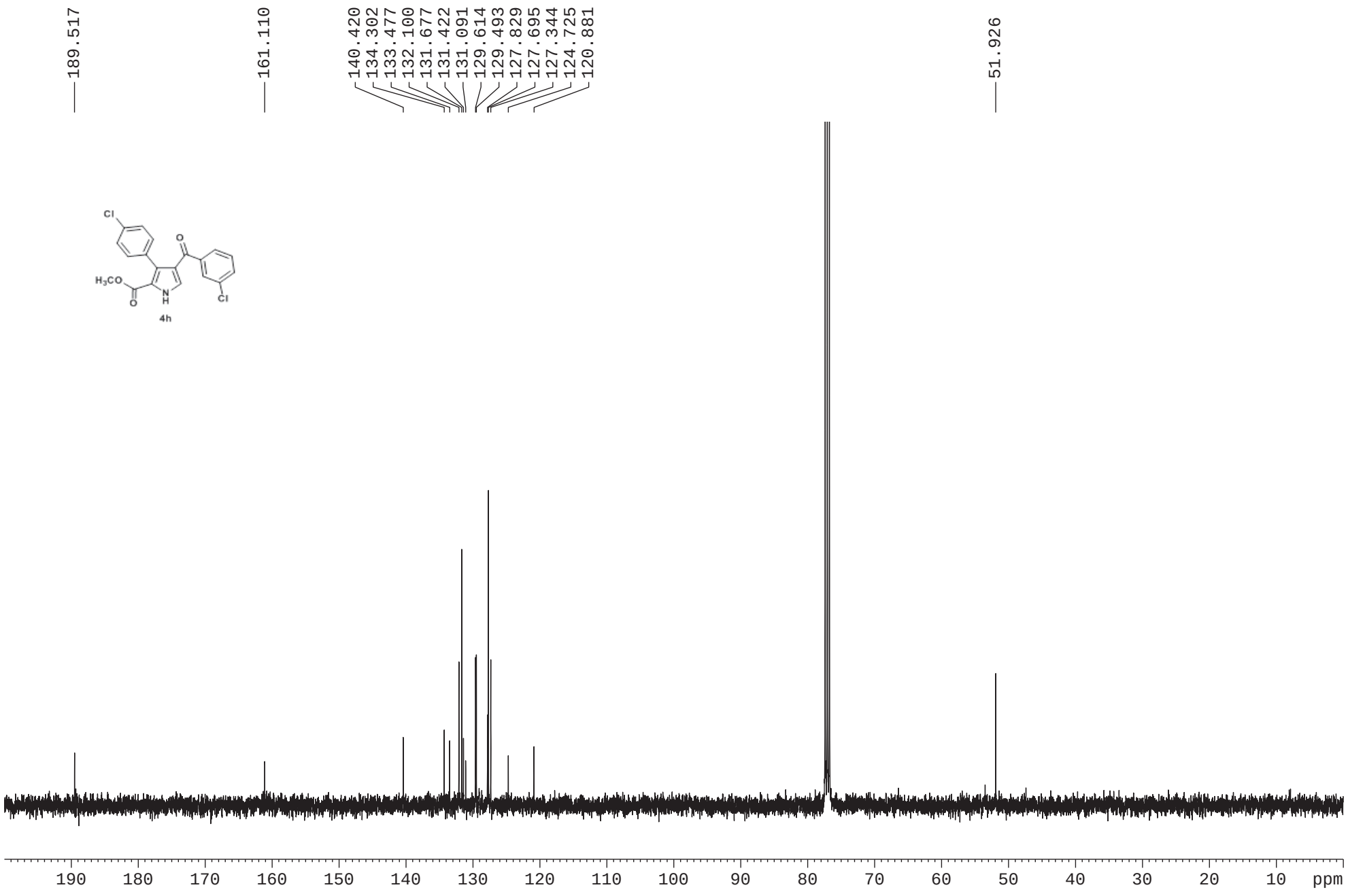

9.633
7.720
7.701
7.506
7.488
7.470
7.400
7.379
7.358
7.346
7.257
7.204
7.184
3.736
Br
O
H3CO
O
N
H
4f
0.938
2.000
1.173
5.174
2.165
3.073
10
9
8
7
6
5
4
3
2
1
ppm

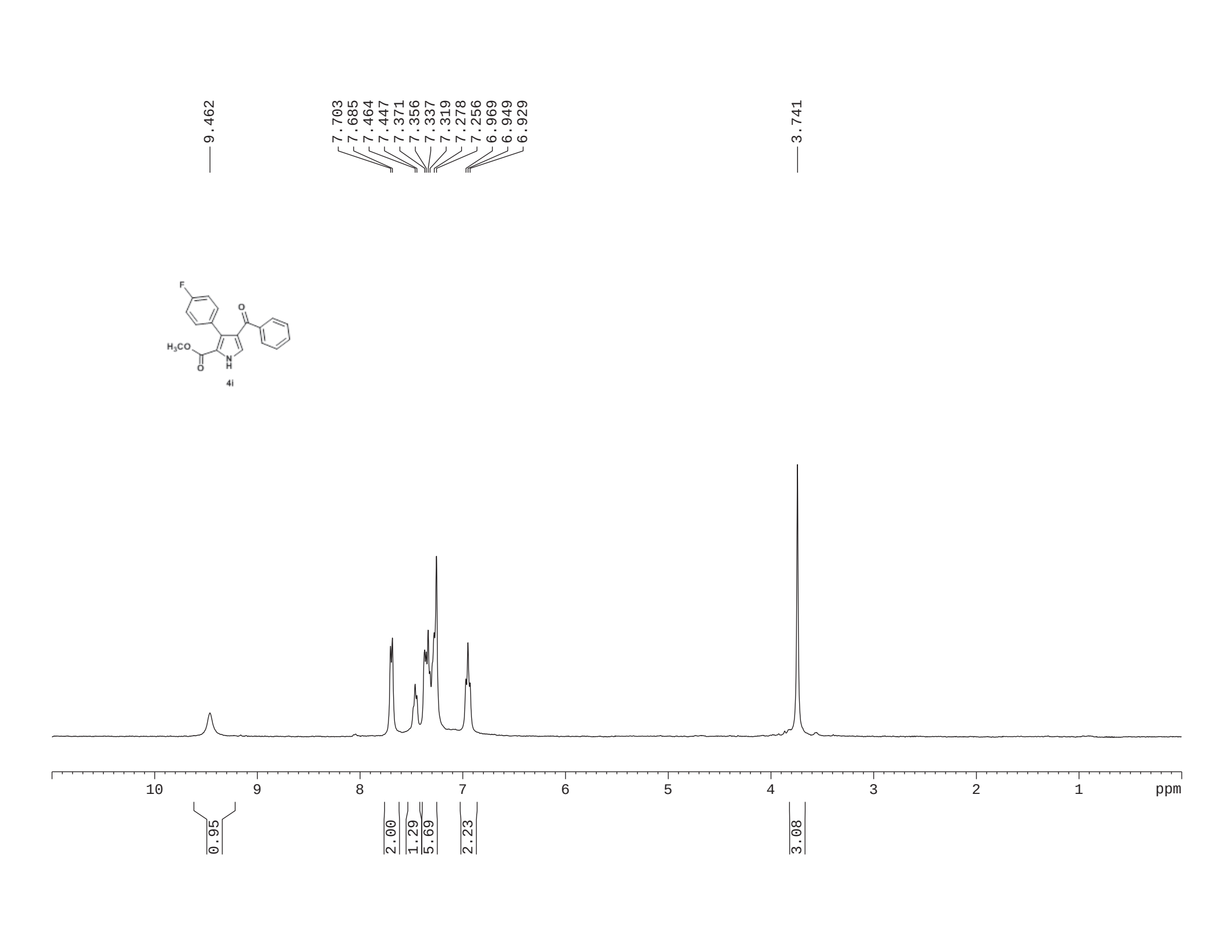

190.881
161.204
138.917
132.286
132.145
132.030
131.254
130.575
129.424
128.251
127.868
124.991
121.635
120.689
51.876
Br
O
H3CO
O
N
H
4f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

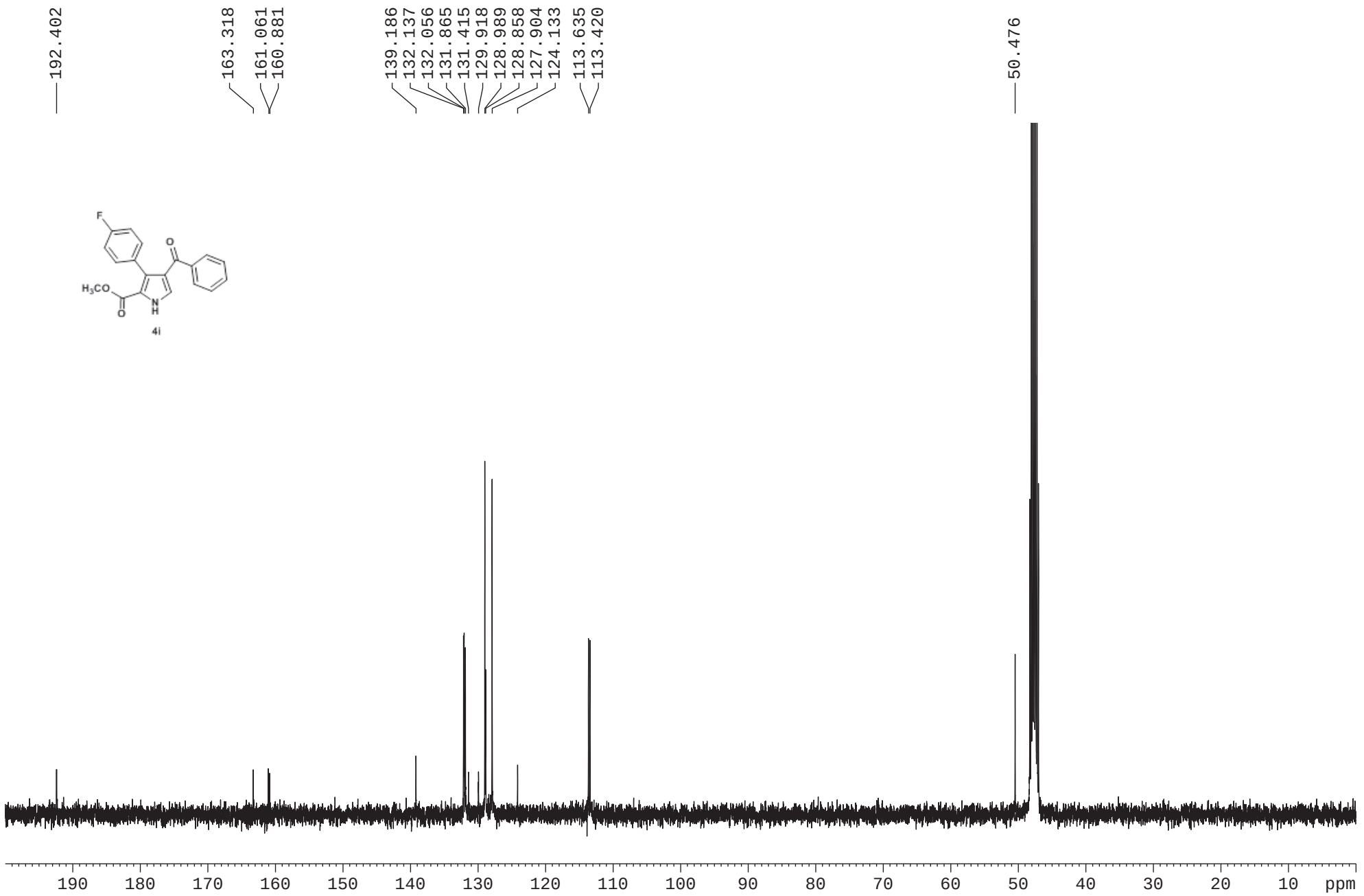

9.454
7.723
7.705
7.506
7.489
7.471
7.379
7.361
7.342
7.254
3.751
Cl
O
H3CO
O
N
H
4g
10
9
8
7
6
5
4
3
2
1
ppm
0.95
2.00
1.19
3.23
4.71
3.03

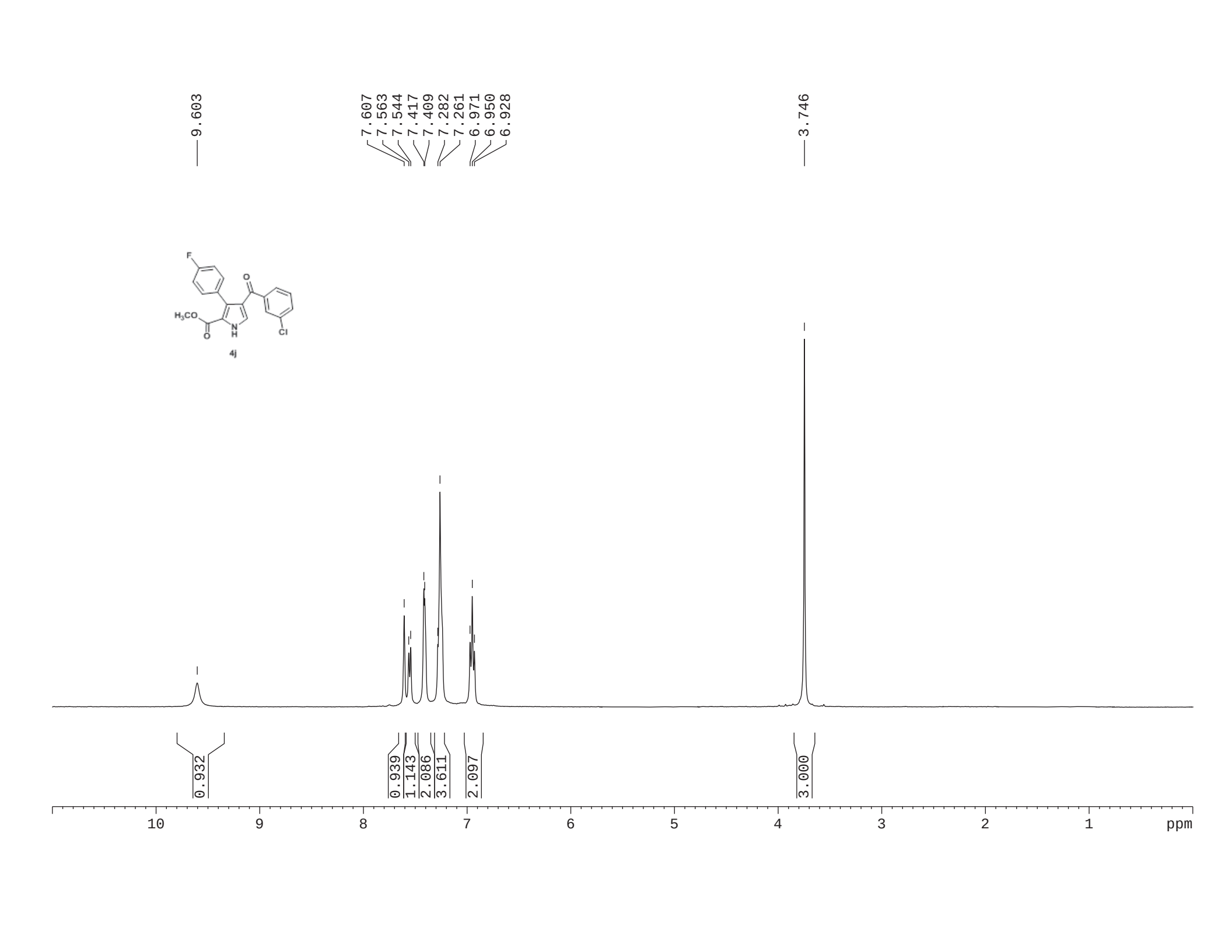

190.895
161.188
138.910
133.334
132.274
131.712
131.633
131.245
129.421
128.234
127.781
127.641
125.080
120.720
51.859
Cl
O
H3CO
O
N
H
4g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

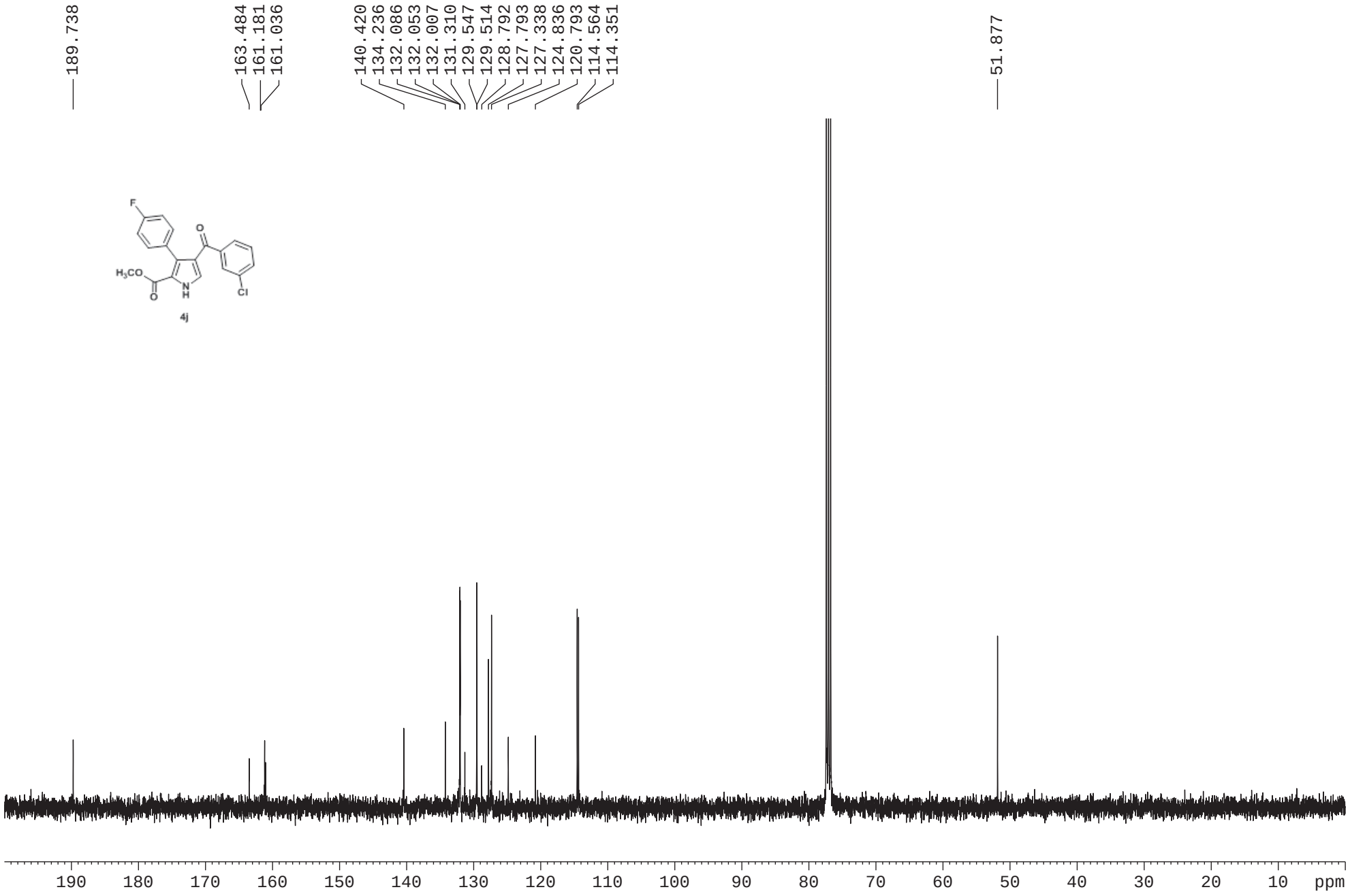

9.665
7.622
7.577
7.558
7.442
7.422
7.304
7.284
7.262
7.232
3.745
Cl
O
H3CO
O
N
H
Cl
4h
10
9
8
7
6
5
4
3
2
1
ppm
0.97
1.00
1.07
2.10
5.61
3.07

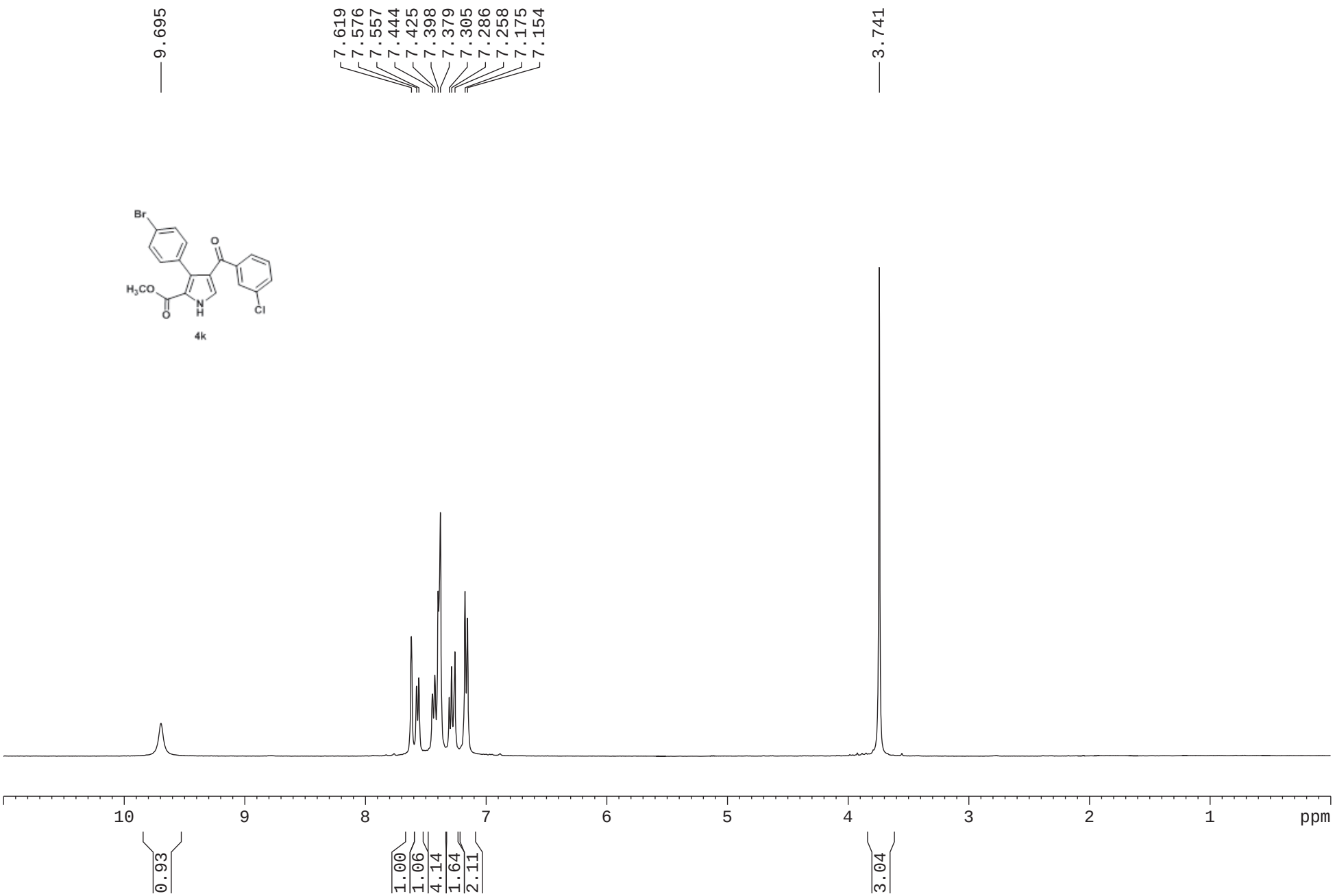

189.517
161.110
140.420
134.302
133.477
132.100
131.677
131.422
131.091
129.614
129.493
127.829
127.695
127.344
124.725
120.881
51.926
Cl
O
H3CO
N
H
O
Cl
4h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

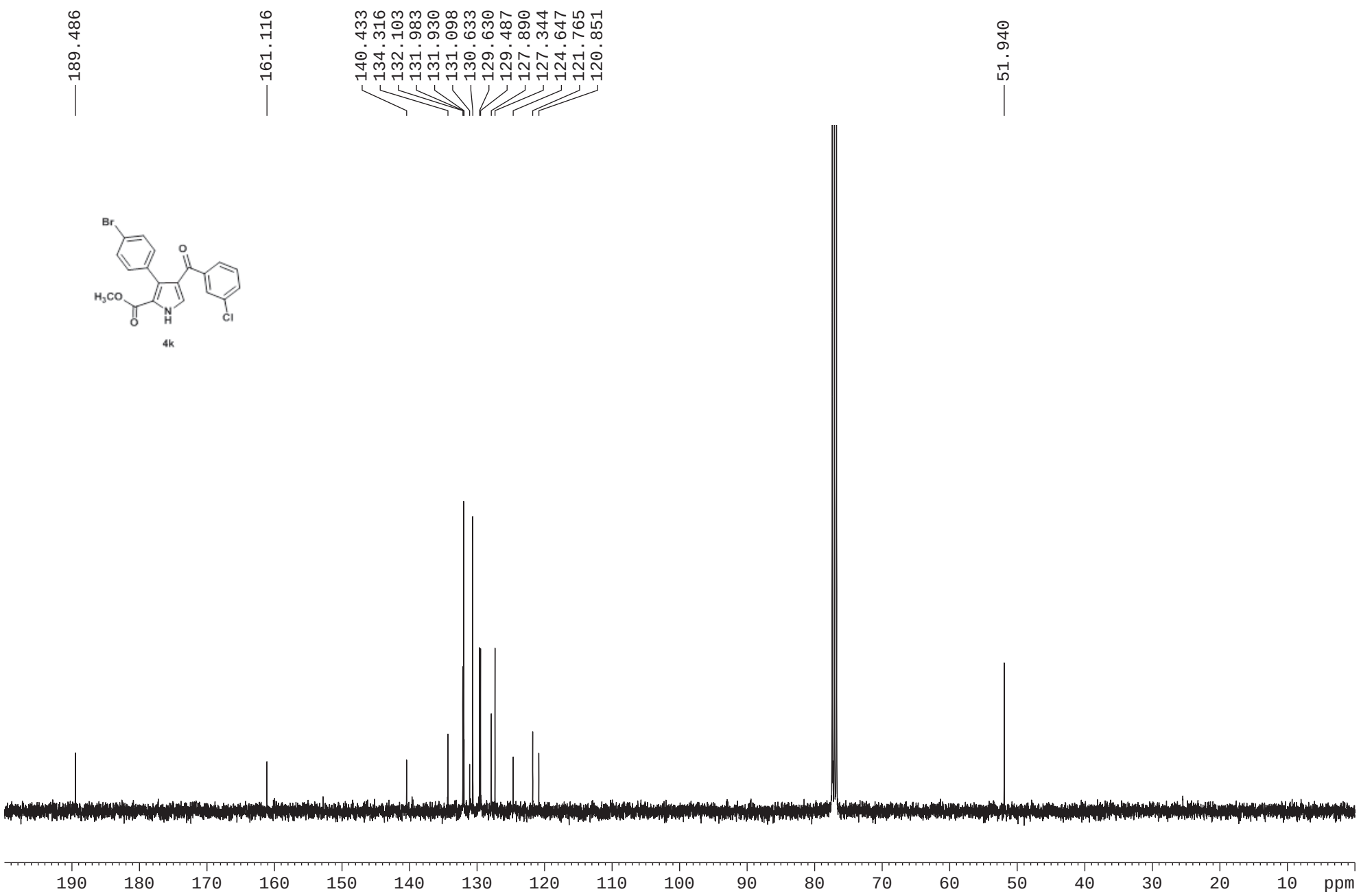

9.462
7.703
7.685
7.464
7.447
7.371
7.356
7.337
7.319
7.278
7.256
6.969
6.949
6.929
3.741
F
O
H3CO
O
N
H
4i
10
9
8
7
6
5
4
3
2
1
ppm
0.95
2.00
1.29
5.69
2.23
3.08

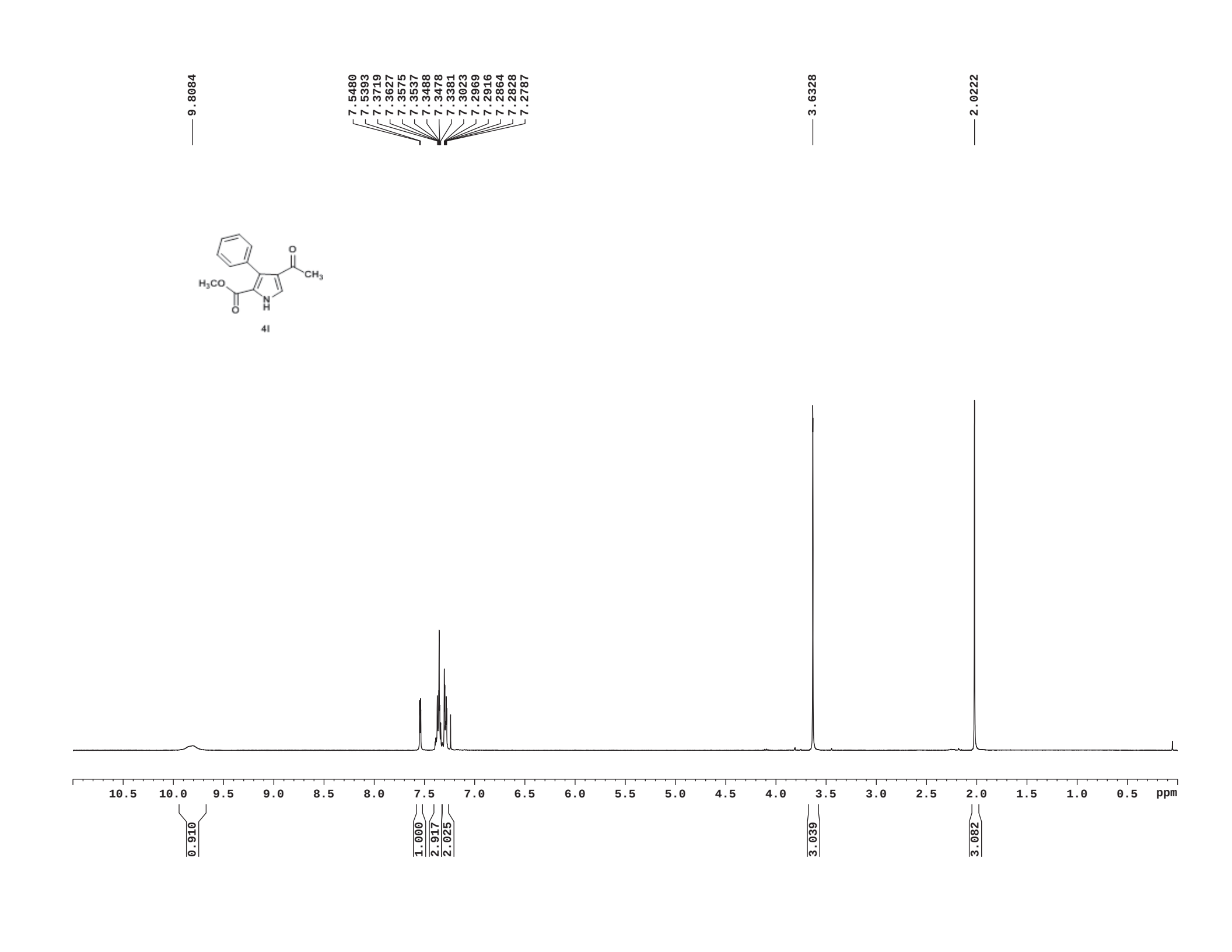

192.402
163.318
161.061
160.881
139.186
132.137
132.056
131.865
131.415
129.918
128.989
128.858
127.904
124.133
113.635
113.420
50.476
F
O
H3CO
O
N
H
4i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

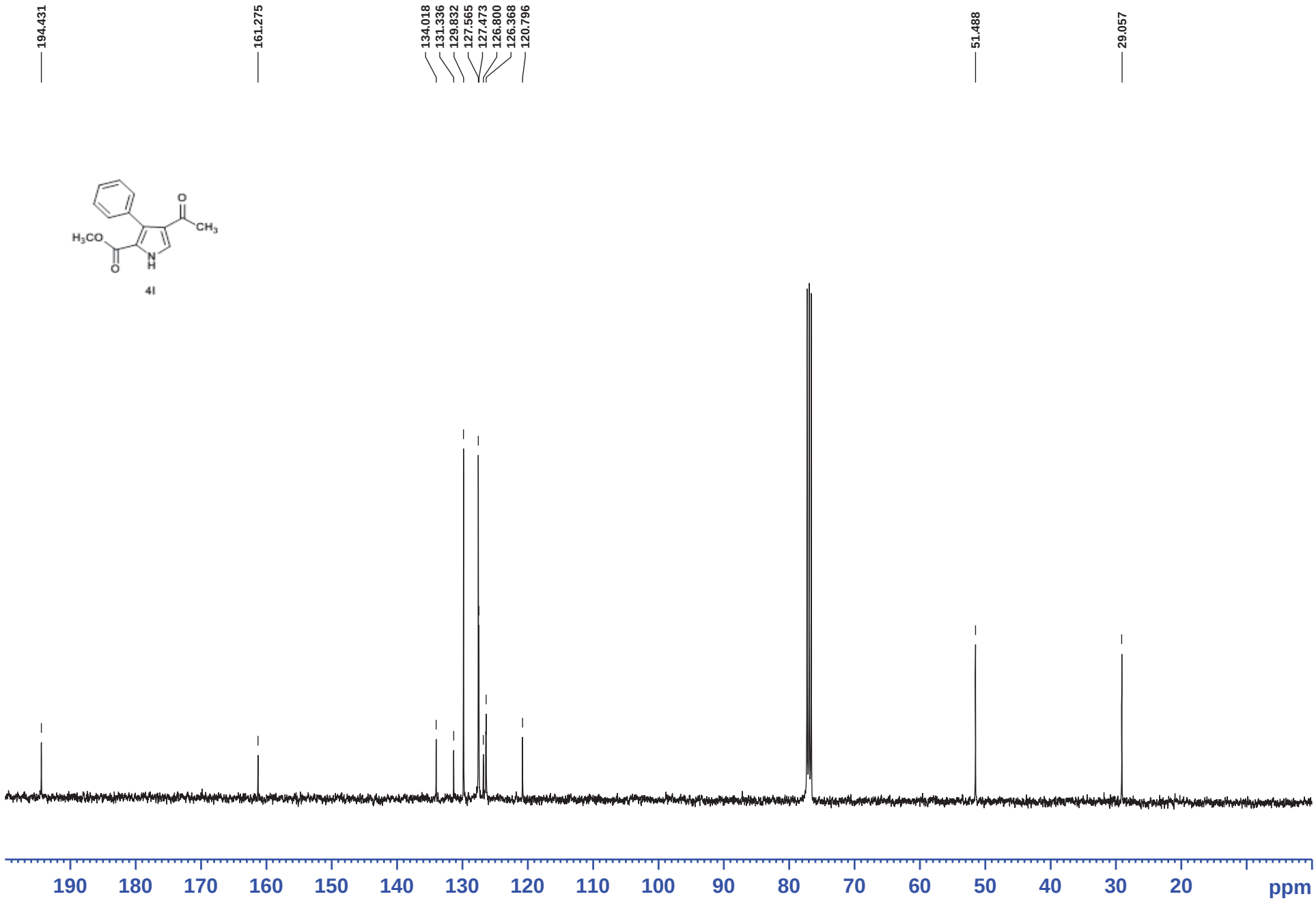

9.603
7.607
7.563
7.544
7.417
7.409
7.282
7.261
6.971
6.950
6.928
3.746
F
O
H3CO
N
H
O
Cl
4j
0.932
0.939
1.143
2.086
3.611
2.097
3.000
10
9
8
7
6
5
4
3
2
1
ppm

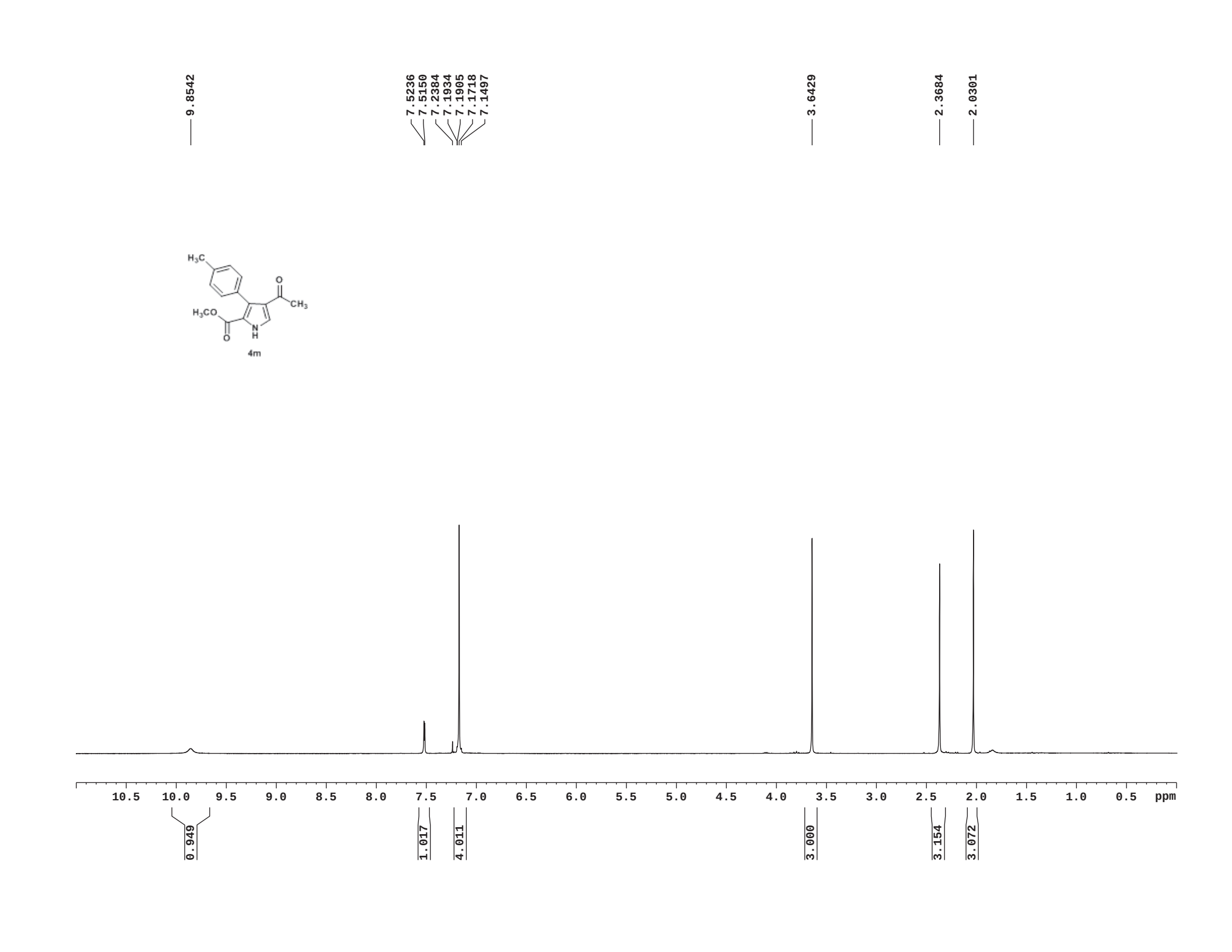

189.738
163.484
161.181
161.036
140.420
134.236
132.086
132.053
132.007
131.310
129.547
129.514
128.792
127.793
127.338
124.836
120.793
114.564
114.351
51.877
F
O
H3CO
N
H
O
Cl
4j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

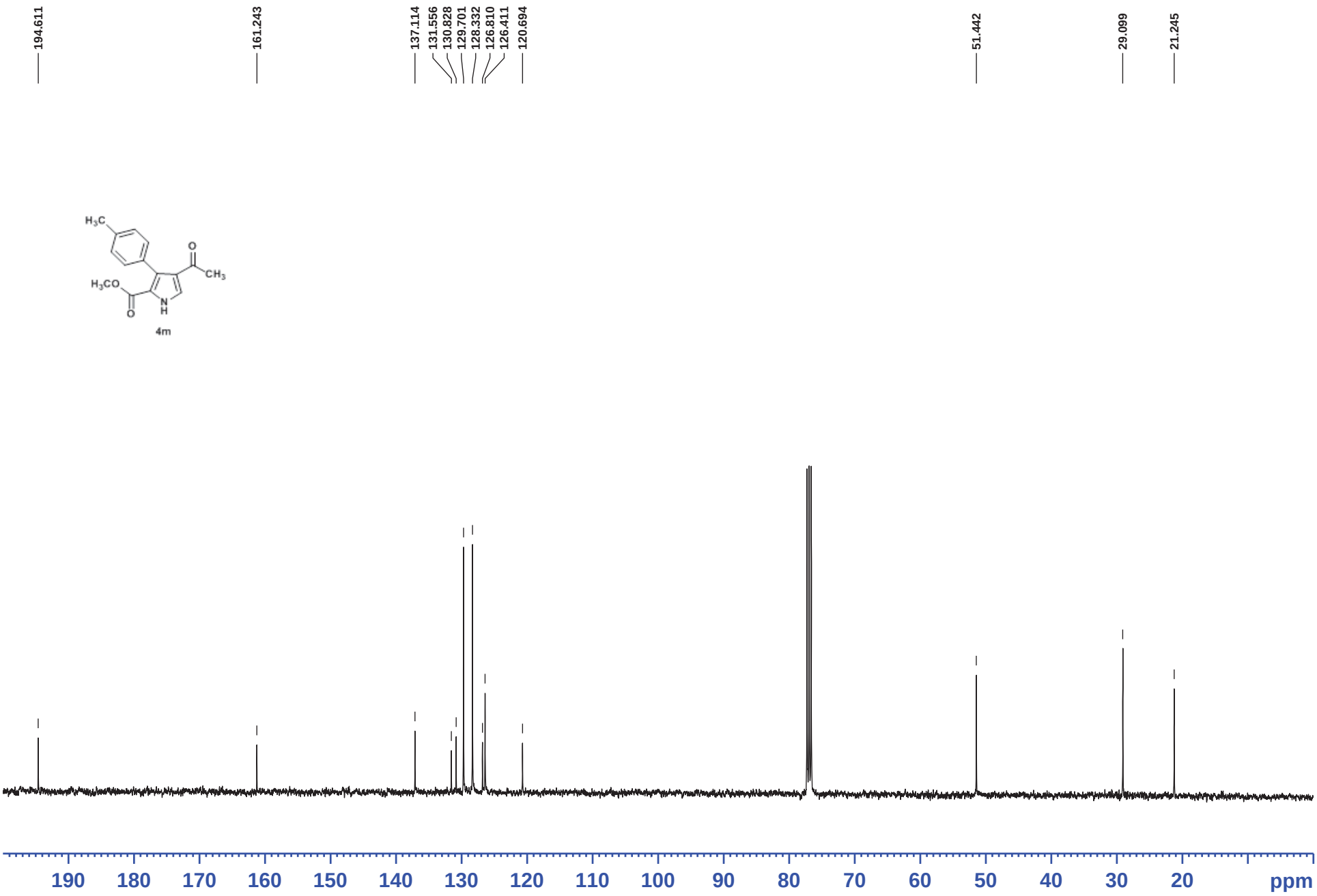

9.695
7.619
7.576
7.557
7.444
7.425
7.398
7.379
7.305
7.286
7.258
7.175
7.154
3.741
Br
O
H3CO
N
H
O
Cl
4k
10
9
8
7
6
5
4
3
2
1
ppm
0.93
1.00
1.06
4.14
1.64
2.11
3.04

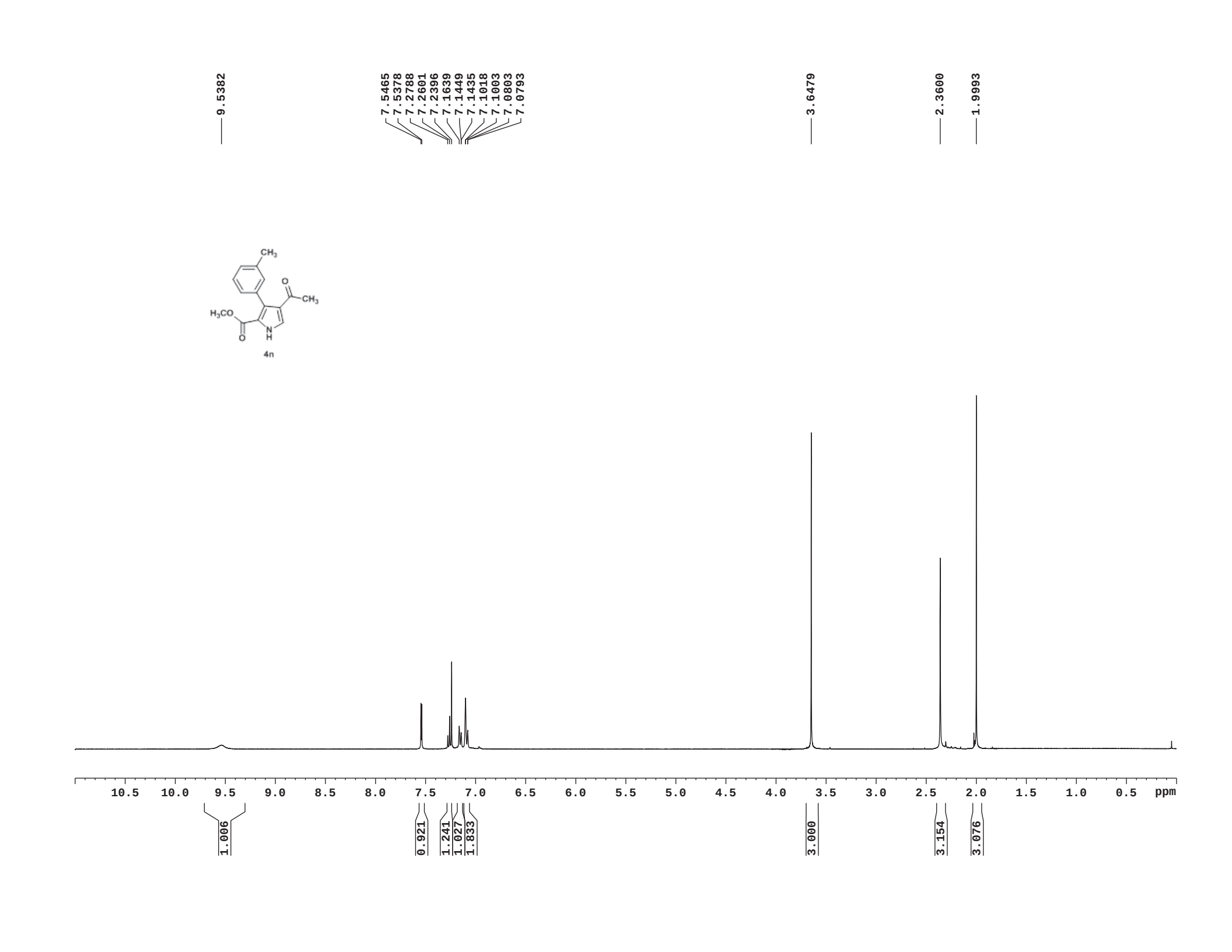

189.486
161.116
140.433
134.316
132.103
131.983
131.930
131.098
130.633
129.630
129.487
127.890
127.344
124.647
121.765
120.851
51.940
Br
O
H3CO
O
N
H
Cl
4k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

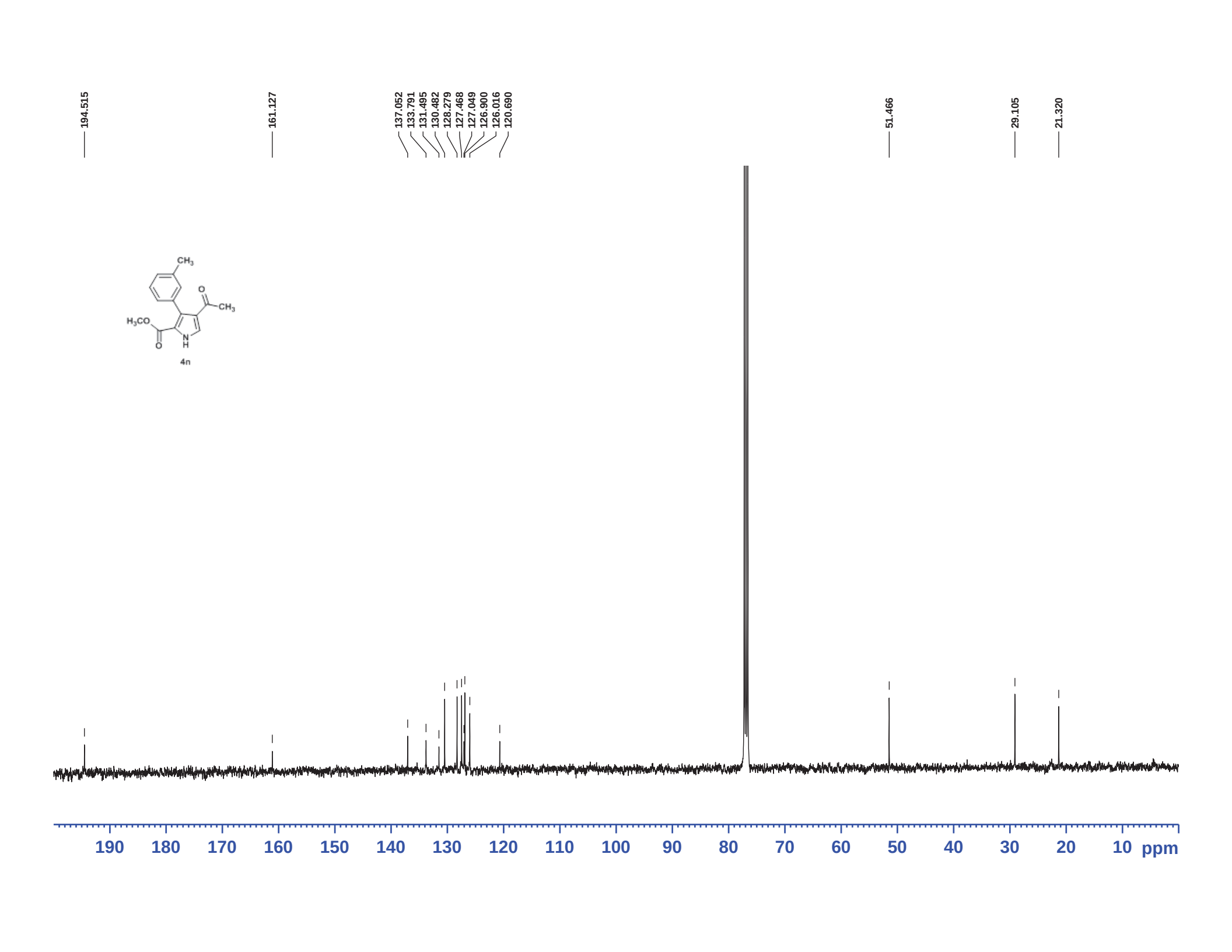

9.8084
7.5480
7.5393
7.3719
7.3627
7.3575
7.3537
7.3488
7.3478
7.3381
7.3023
7.2969
7.2916
7.2864
7.2828
7.2787
3.6328
2.0222
H3CO
O
CH3
N
H
O
4l
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.910
1.000
2.917
2.025
3.039
3.082

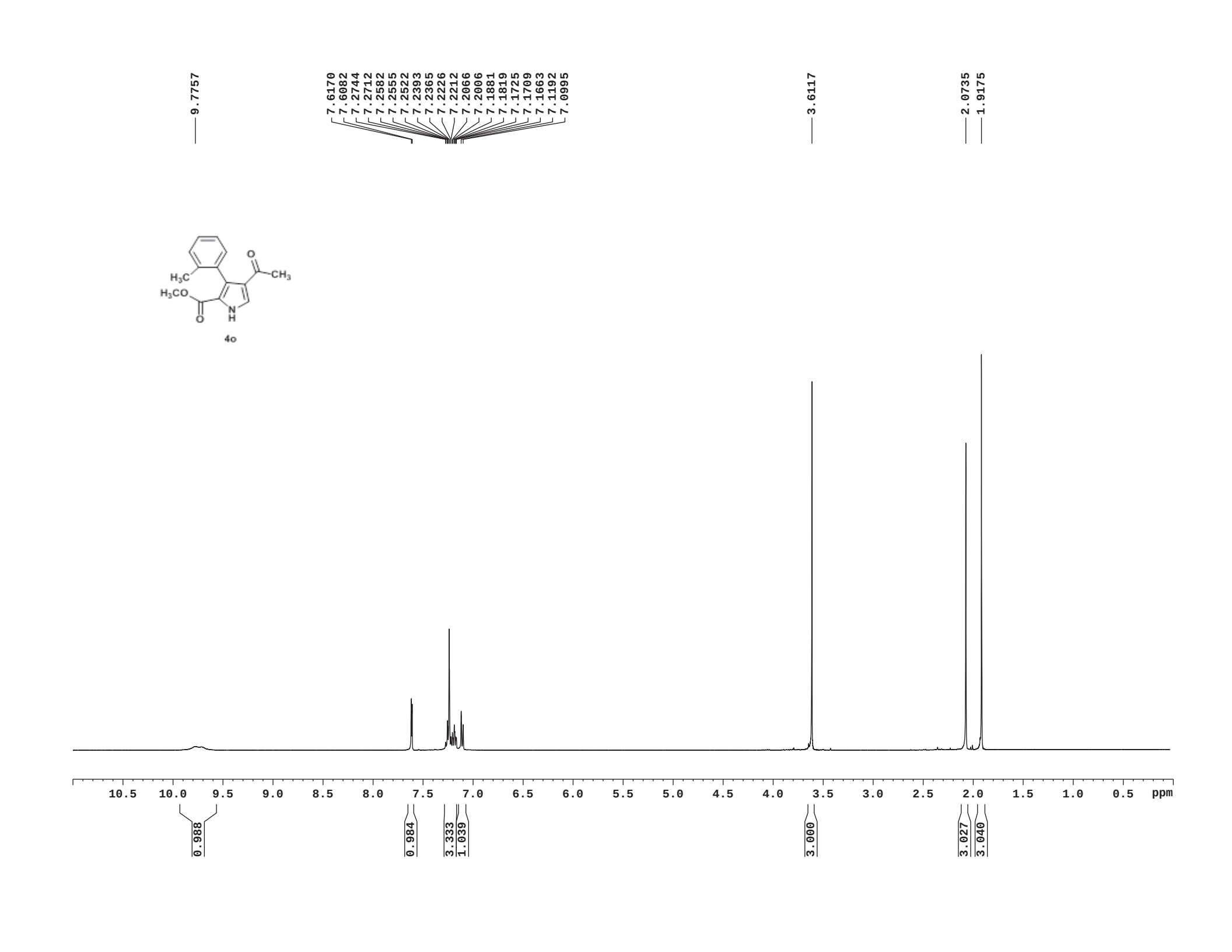

194.431
161.275
134.018
131.336
129.832
127.565
127.473
126.800
126.368
120.796
51.488
29.057
O
CH3
H3CO
O
N
H
4l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

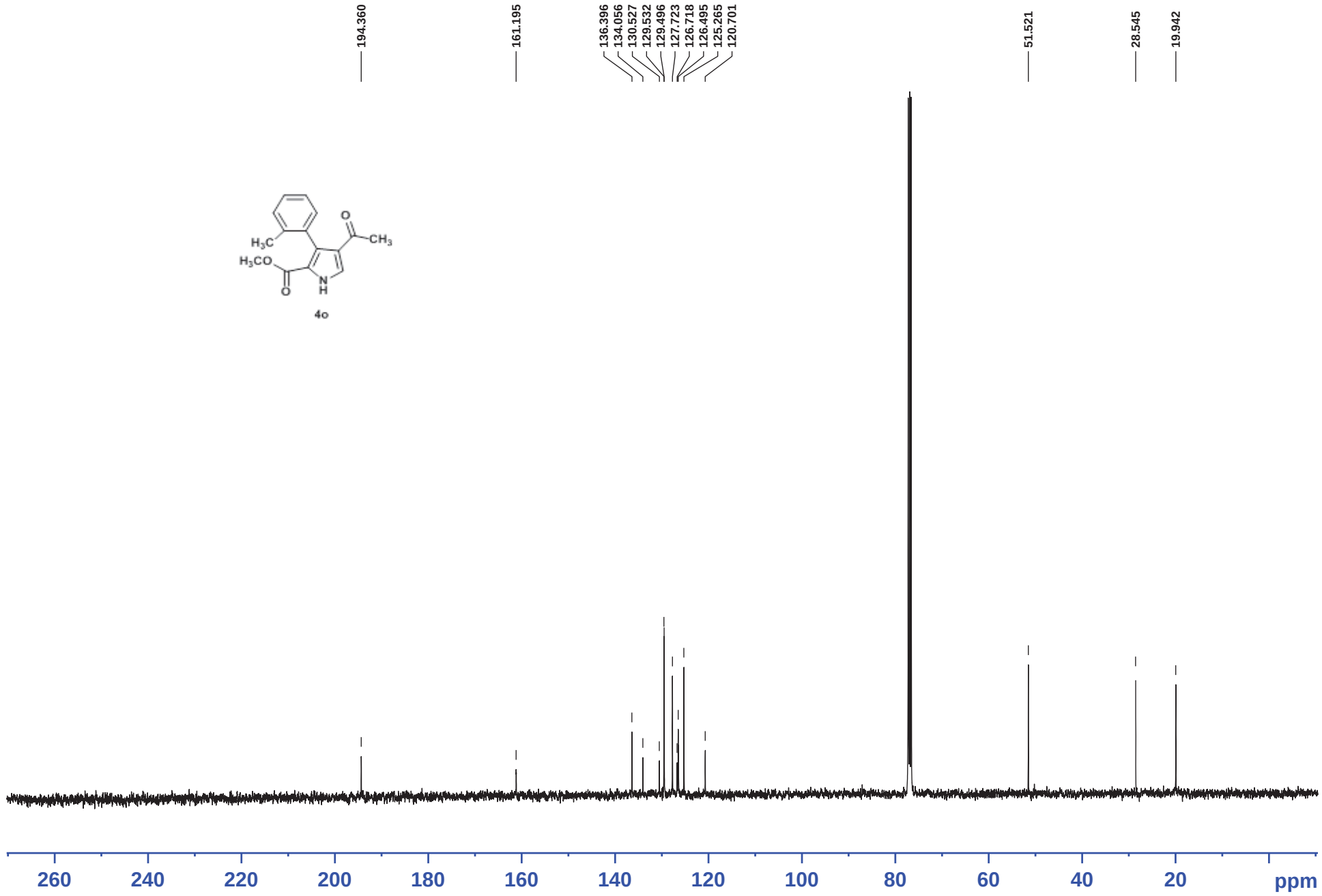

9.8542
7.5236
7.5150
7.2384
7.1934
7.1905
7.1718
7.1497
3.6429
2.3684
2.0301
H3C
O
CH3
H3CO
O
N
H
4m
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.949
1.017
4.011
3.000
3.154
3.072

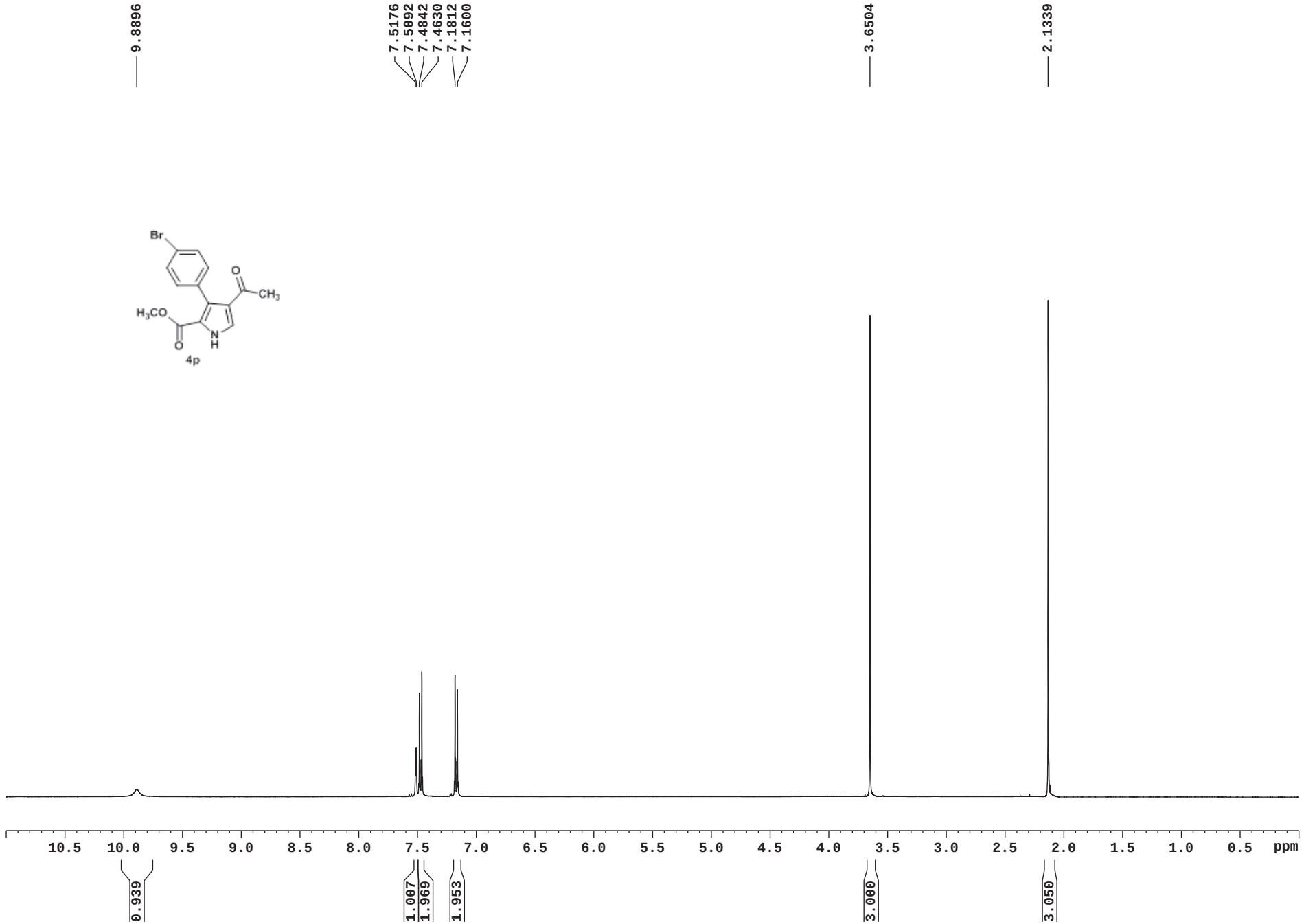

194.611
161.243
137.114
131.556
130.828
129.701
128.332
126.810
126.411
120.694
51.442
29.099
21.245
H3C
O
CH3
H3CO
O
N
H
4m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

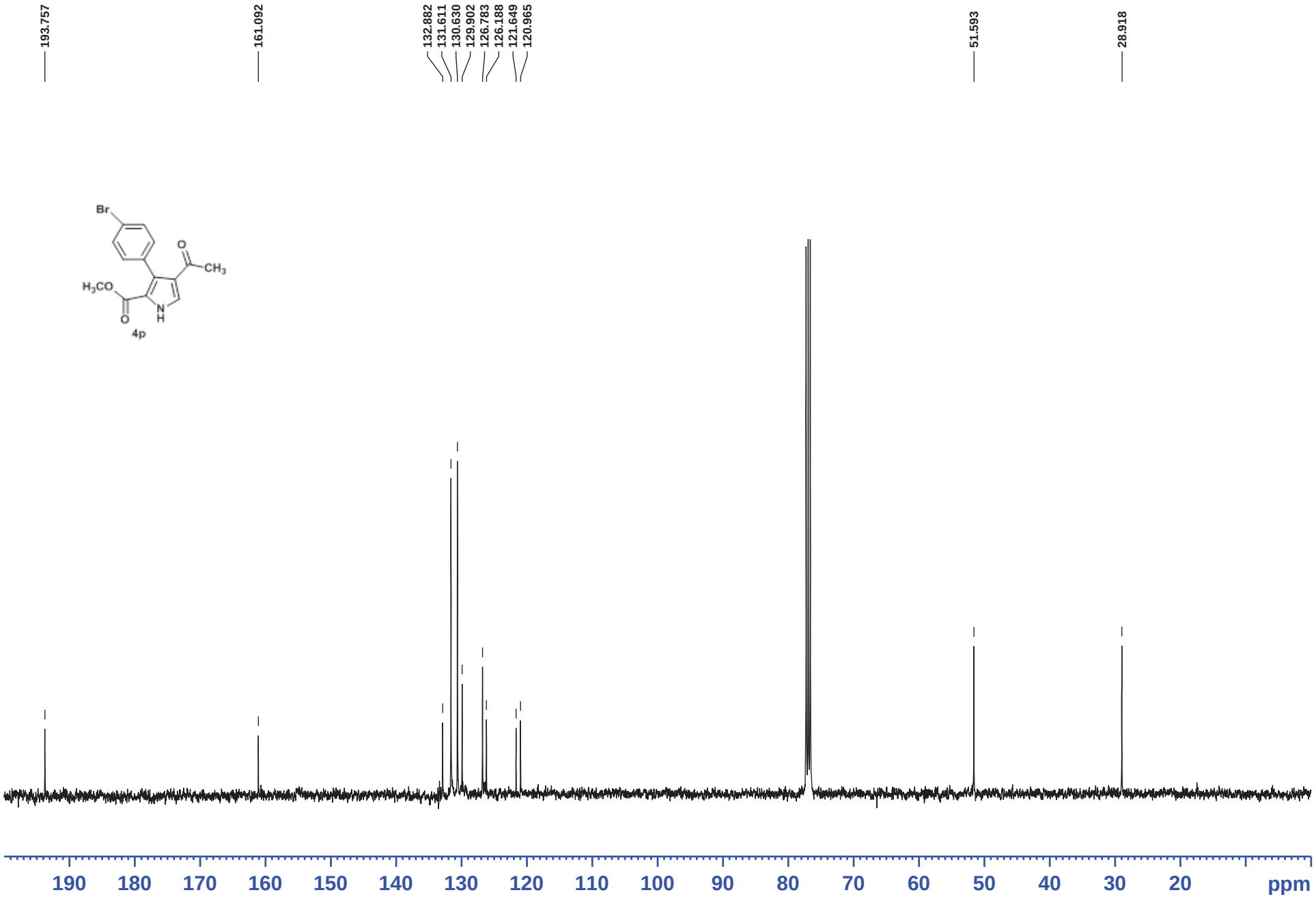

9.5382
7.5465
7.5378
7.2788
7.2601
7.2396
7.1639
7.1449
7.1435
7.1018
7.1003
7.0803
7.0793
3.6479
2.3600
1.9993
CH3
O
CH3
H3CO
O
N
H
4n
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.006
0.921
1.241
1.027
1.833
3.000
3.154
3.076

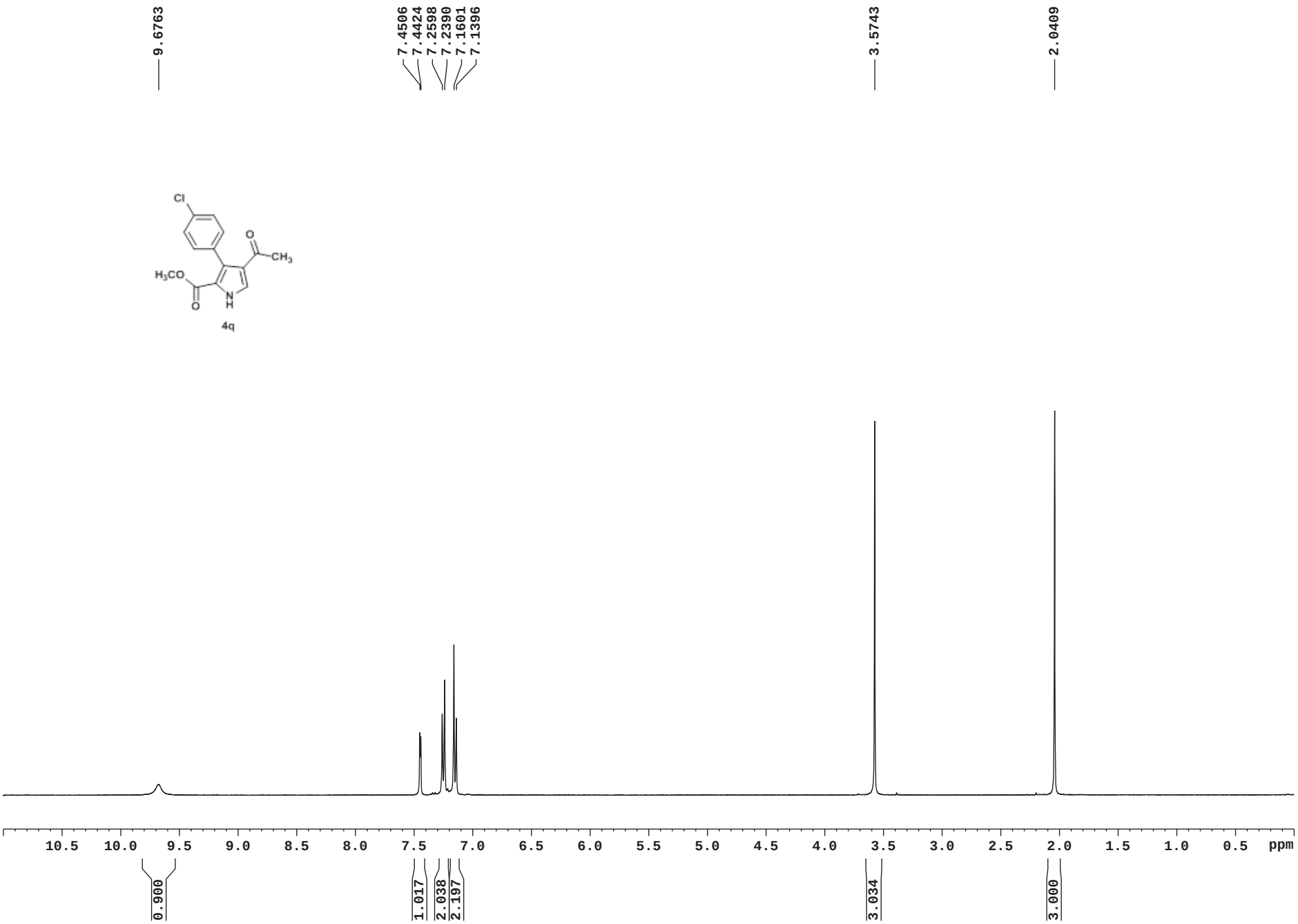

194.515
161.127
137.052
133.791
131.495
130.482
128.279
127.468
127.049
126.900
126.016
120.690
51.466
29.105
21.320
CH3
O
CH3
H3CO
O
N
H
4n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

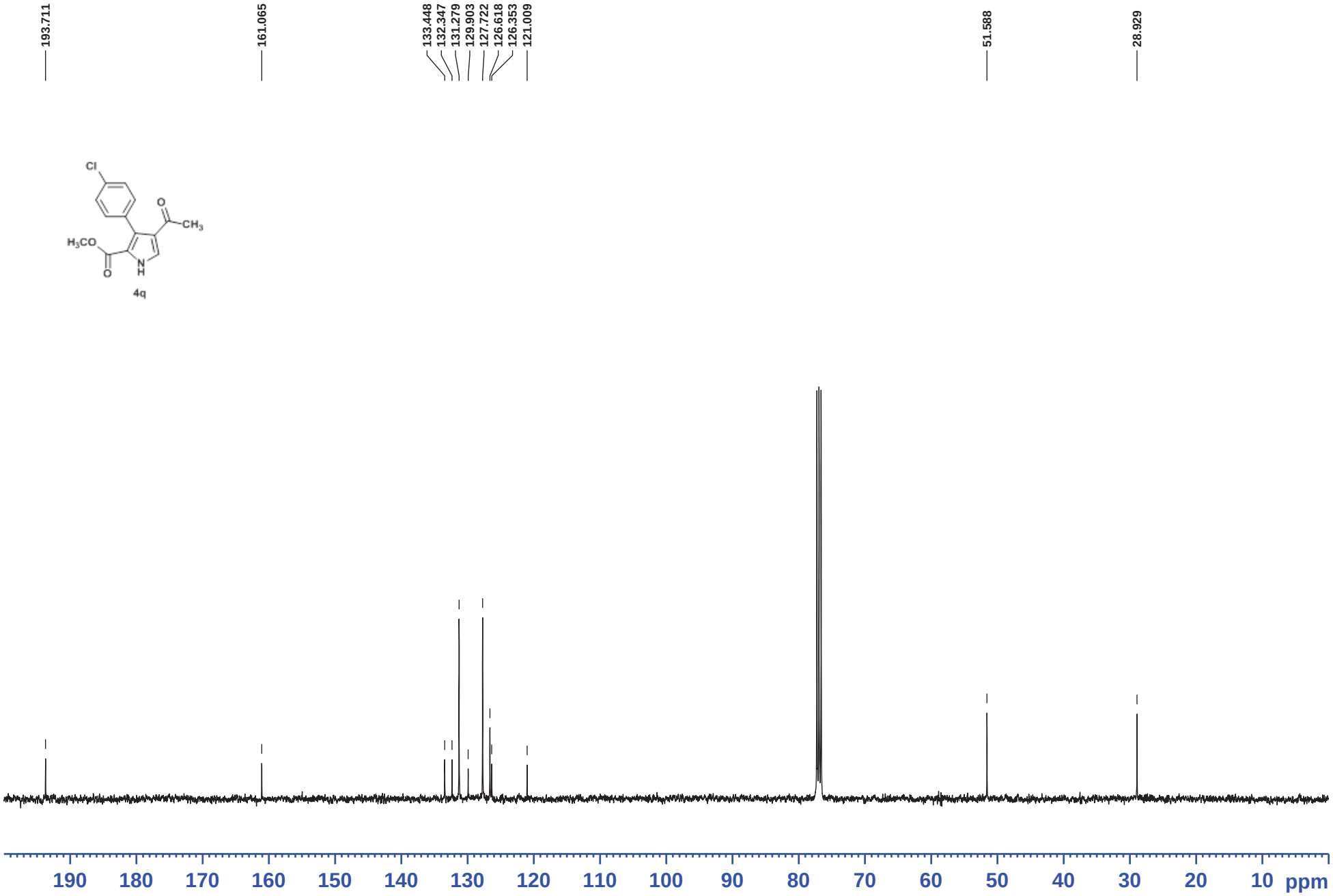

9.7757
7.6170
7.6082
7.2744
7.2712
7.2582
7.2555
7.2522
7.2393
7.2365
7.2226
7.2212
7.2066
7.2006
7.1881
7.1819
7.1725
7.1709
7.1663
7.1192
7.0995
3.6117
2.0735
1.9175
4o
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.988
0.984
3.333
1.039
3.000
3.027
3.040

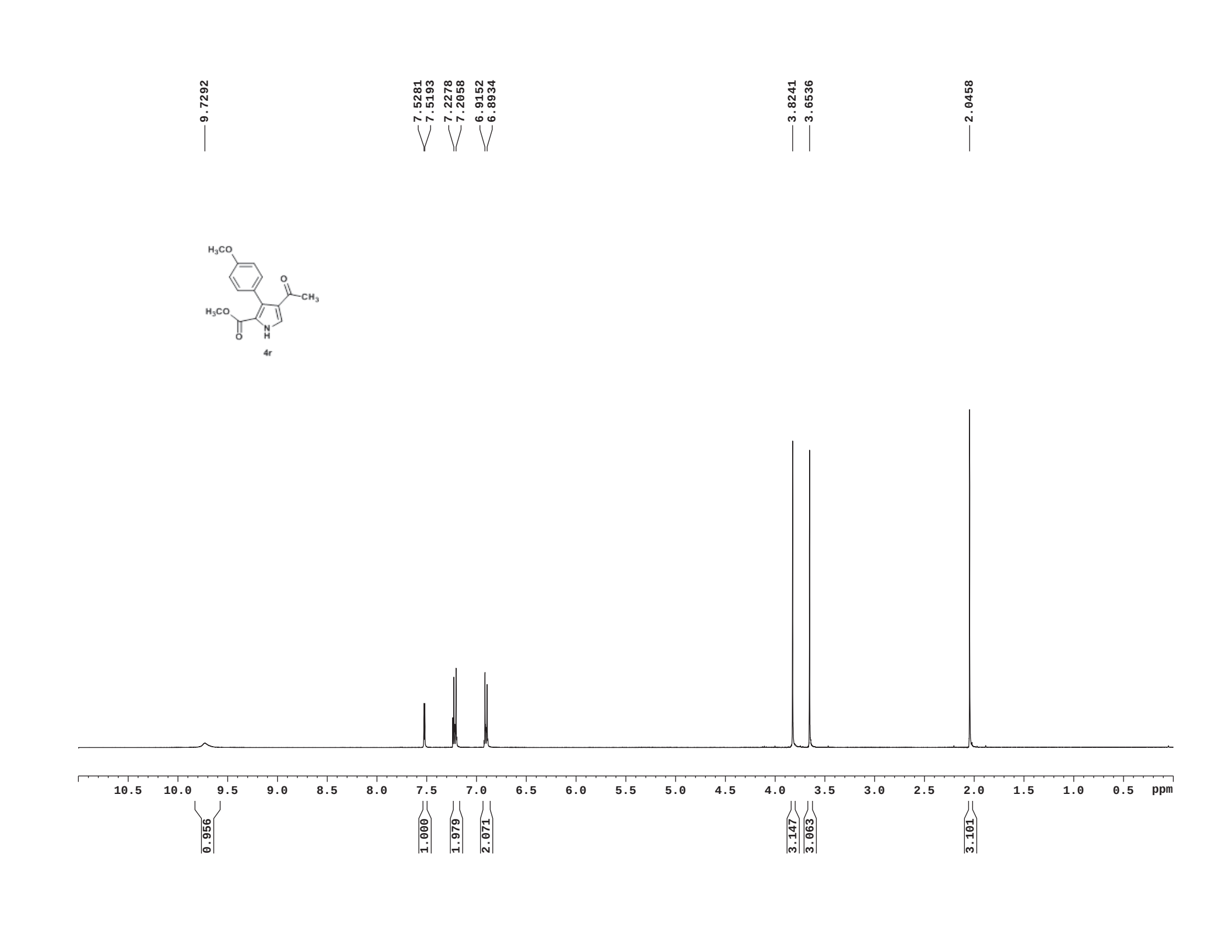

194.360
161.195
136.396
134.056
130.527
129.532
129.496
127.723
126.718
126.495
125.265
120.701
51.521
28.545
19.942
O
CH3
H3C
H3CO
O
N
H
4o
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm

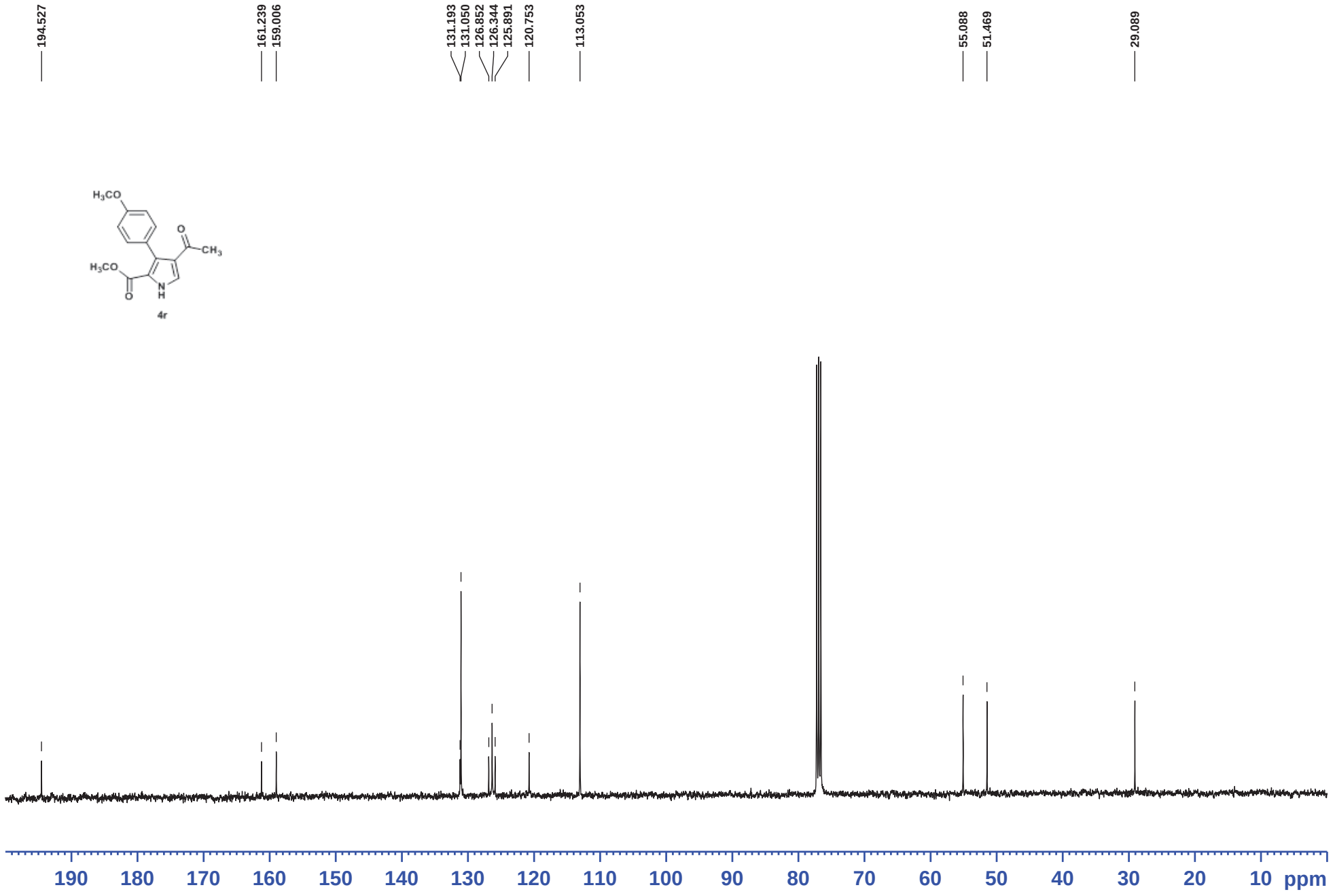

9.8896
7.5176
7.5092
7.4842
7.4630
7.1812
7.1600
3.6504
2.1339
Br
O
CH3
H3CO
O
N
H
4p
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.939
1.007
1.969
1.953
3.000
3.050

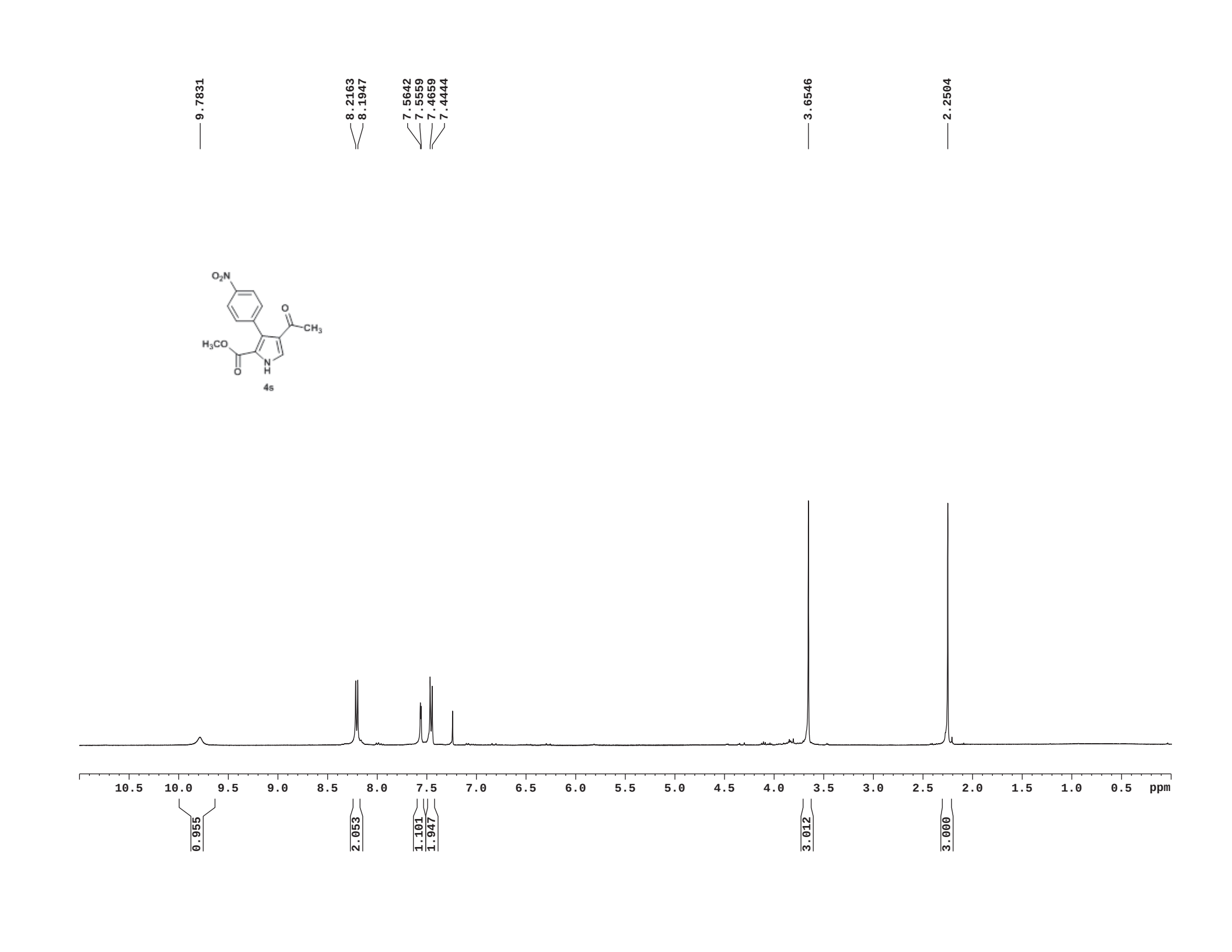

193.757
161.092
132.882
131.611
130.630
129.902
126.783
126.188
121.649
120.965
51.593
28.918
Br
O
CH3
H3CO
O
N
H
4p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

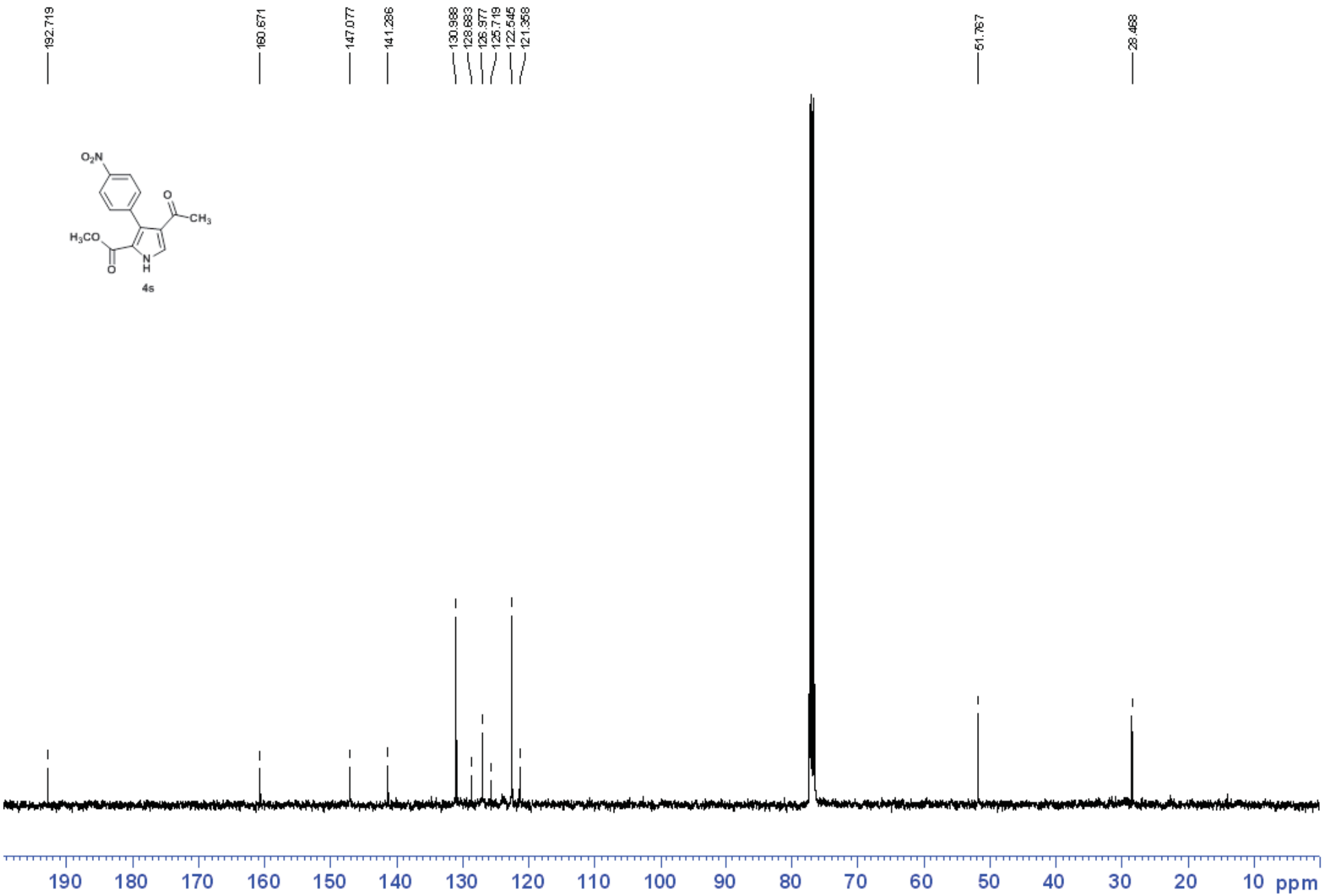

9.6763
7.4506
7.4424
7.2598
7.2390
7.1601
7.1396
3.5743
2.0409
Cl
O
CH3
H3CO
O
N
H
4q
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.900
1.017
2.038
2.197
3.034
3.000


193.711
161.065
133.448
132.347
131.279
129.903
127.722
126.618
126.353
121.009
51.588
28.929
Cl
O
CH3
H3CO
O
N
H
4q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

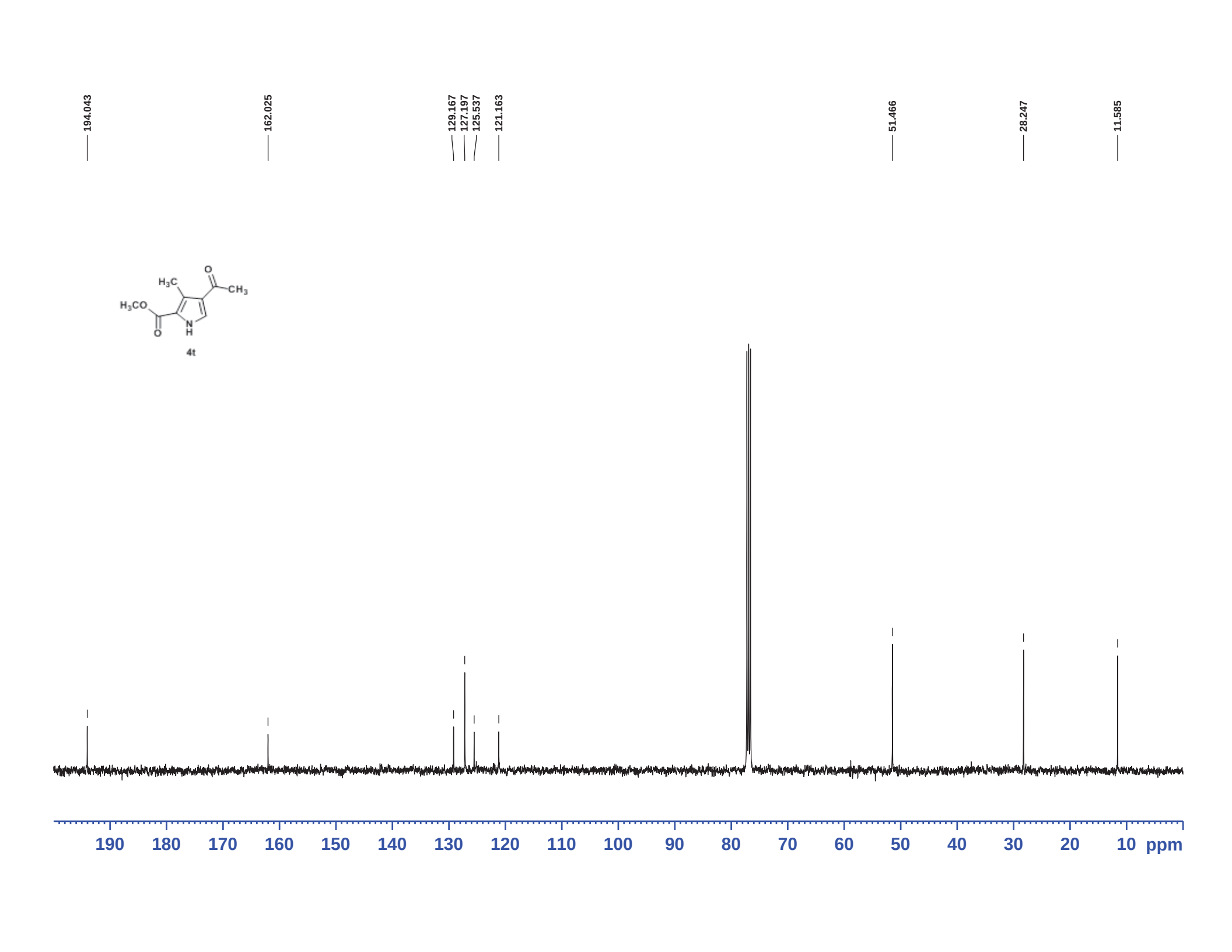

9.7292
7.5281
7.5193
7.2278
7.2058
6.9152
6.8934
3.8241
3.6536
2.0458
H3CO
O
CH3
H3CO
O
N
H
4r
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.956
1.000
1.979
2.071
3.147
3.063
3.101

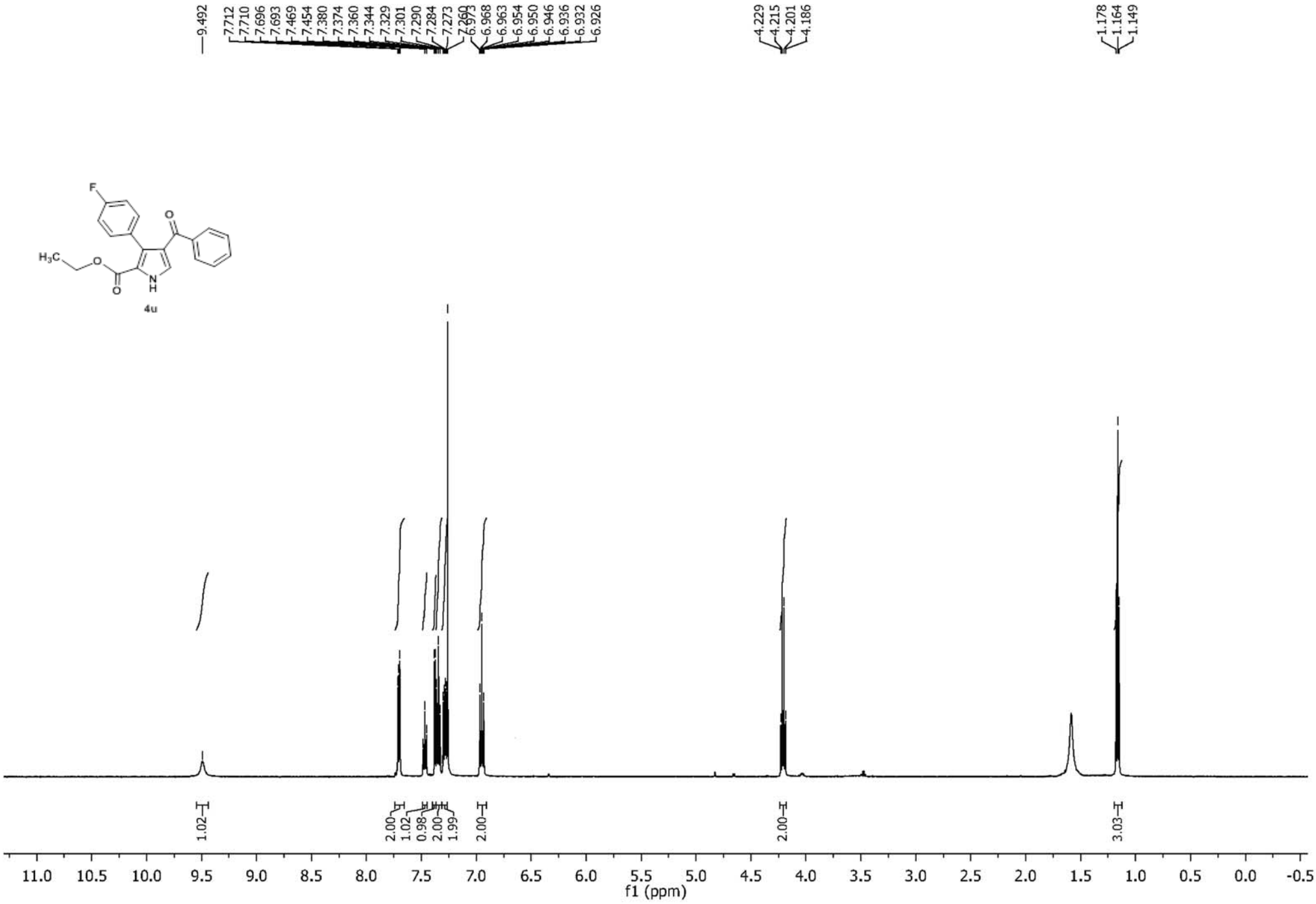

194.527
161.239
159.006
131.193
131.050
126.852
126.344
125.891
120.753
113.053
55.088
51.469
29.089
H3CO
O
CH3
H3CO
O
N
H
4r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

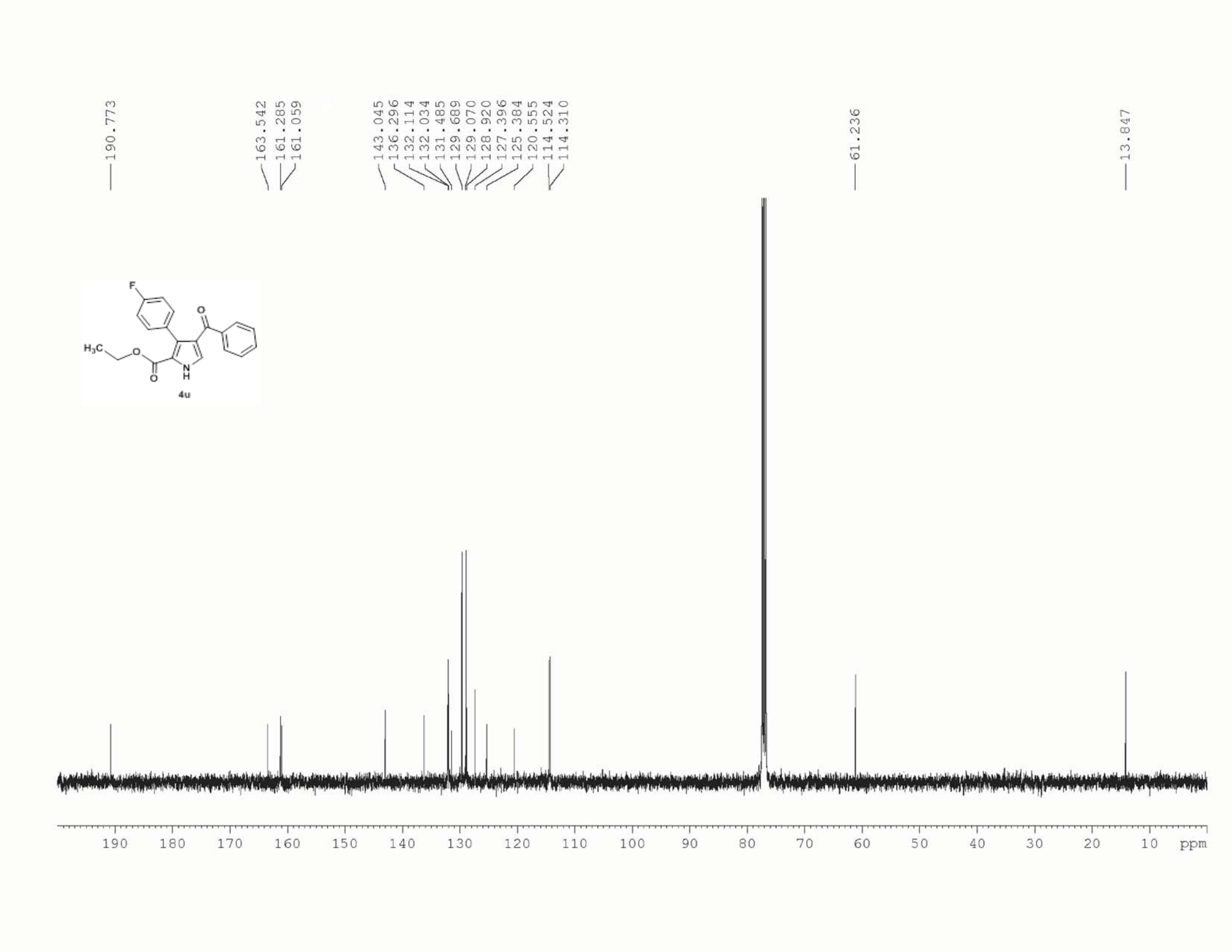

9.7831
8.2163
8.1947
7.5642
7.5559
7.4659
7.4444
3.6546
2.2504
O2N
O
CH3
H3CO
O
N
H
4s
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.955
2.053
1.101
1.947
3.012
3.000

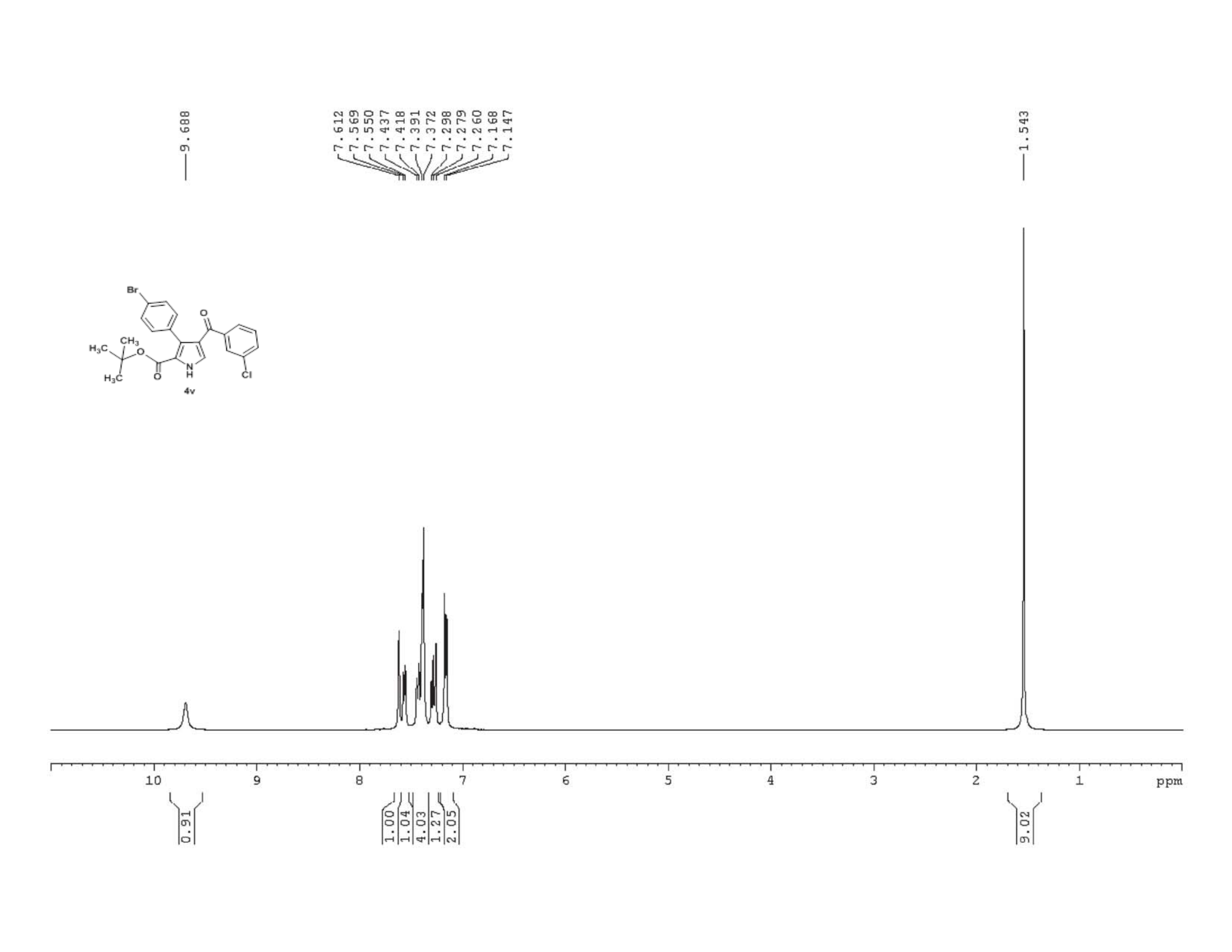

192.719
160.671
147.077
141.286
130.988
128.683
126.977
125.719
122.545
121.358
51.767
28.468
O2N
O
CH3
H3CO
O
N
H
4s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

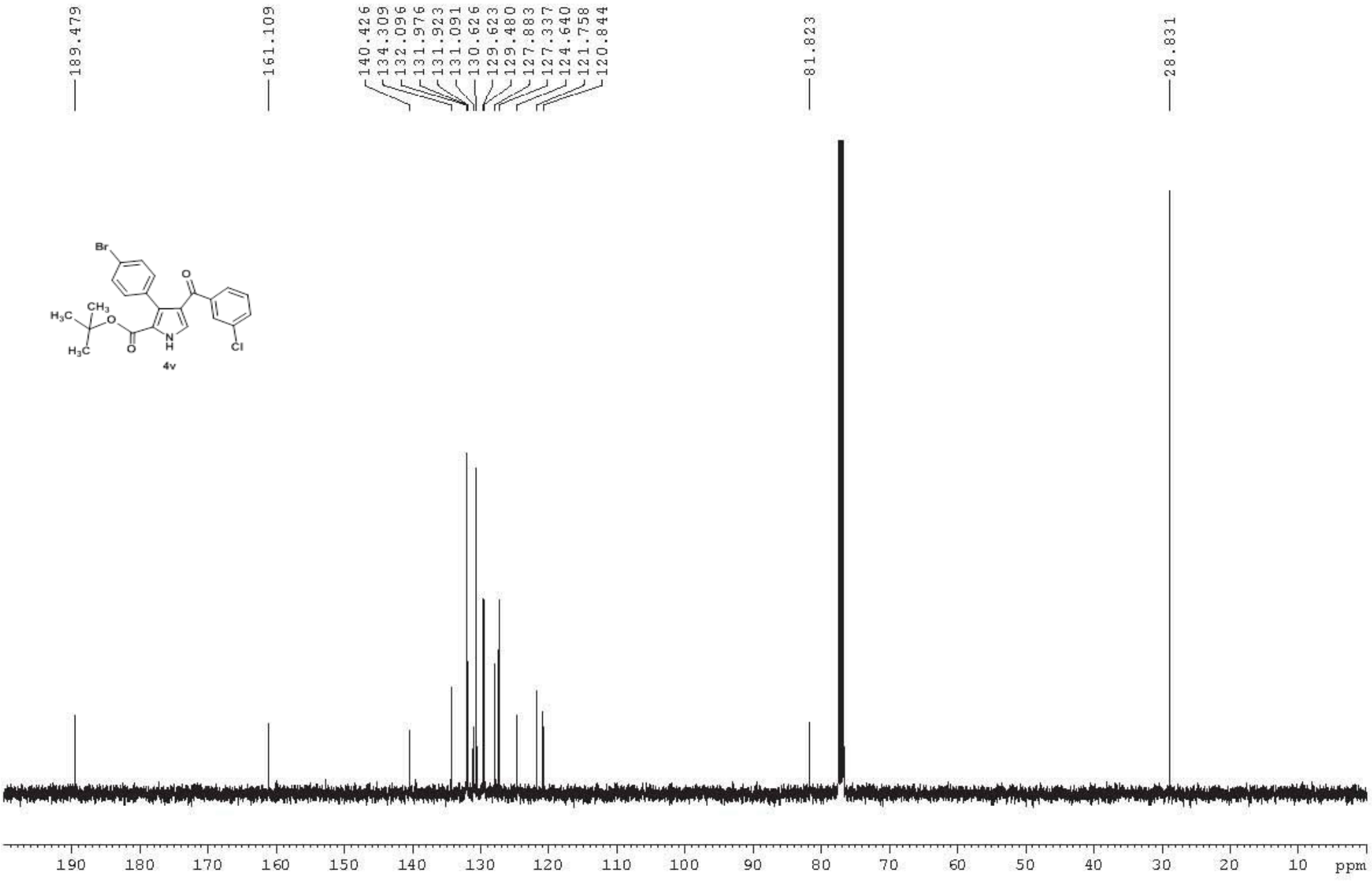

9.4716
7.4356
7.4270
3.8568
2.5929
2.3944
H3C
O
CH3
H3CO
O
N
H
4t
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.937
1.000
3.137
3.011
3.078

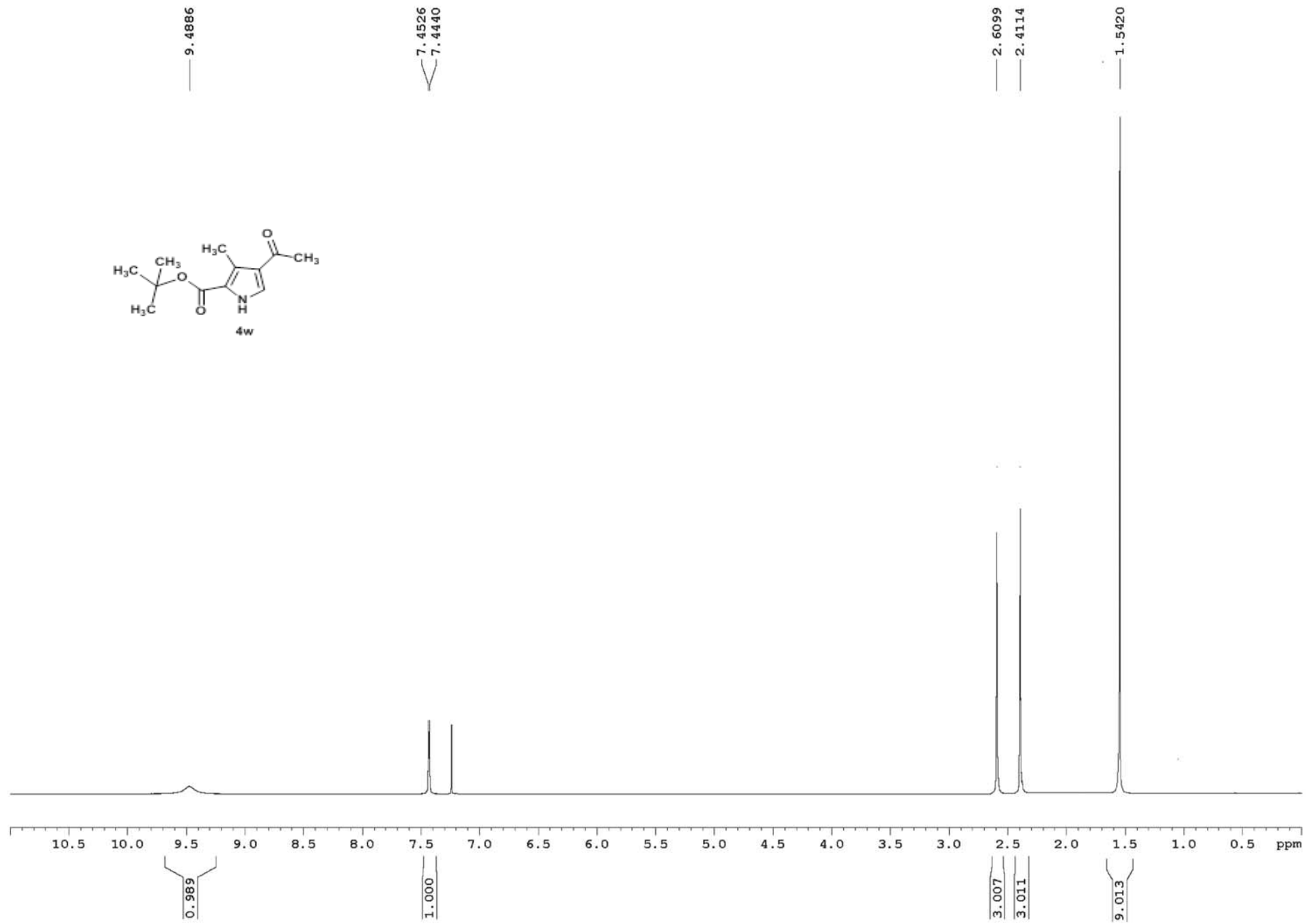

194.043
162.025
129.167
127.197
125.537
121.163
51.466
28.247
11.585
H3C
O
CH3
H3CO
O
N
H
4t
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

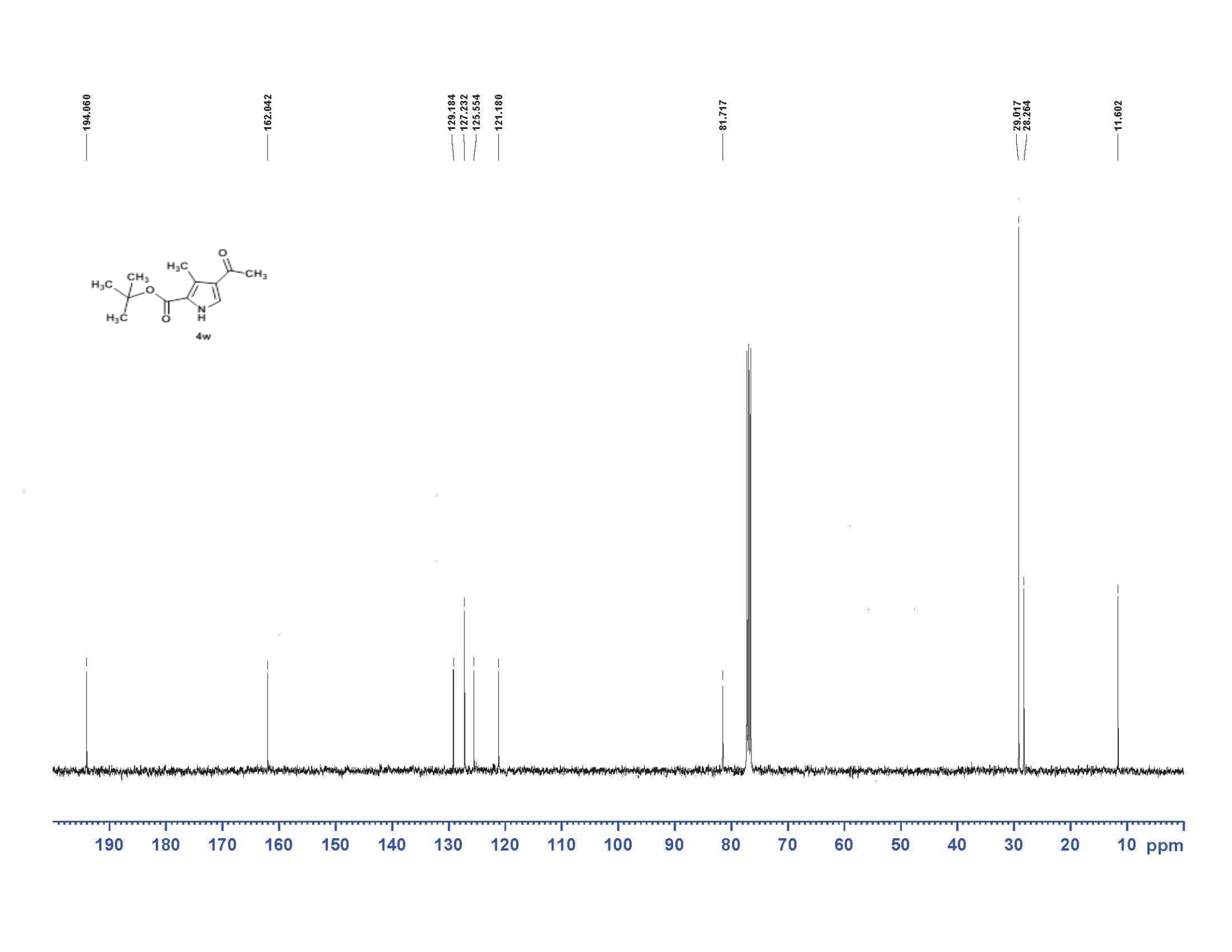

9.492
7.712
7.710
7.696
7.693
7.469
7.454
7.380
7.374
7.360
7.344
7.329
7.301
7.290
7.284
7.273
7.260
6.973
6.968
6.963
6.954
6.950
6.946
6.936
6.932
6.926
4.229
4.215
4.201
4.186
1.178
1.164
1.149
F
O
O
H3C
O
O
N
H
4u
1.02
2.00
1.02
0.98
2.00
1.99
2.00
2.00
3.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

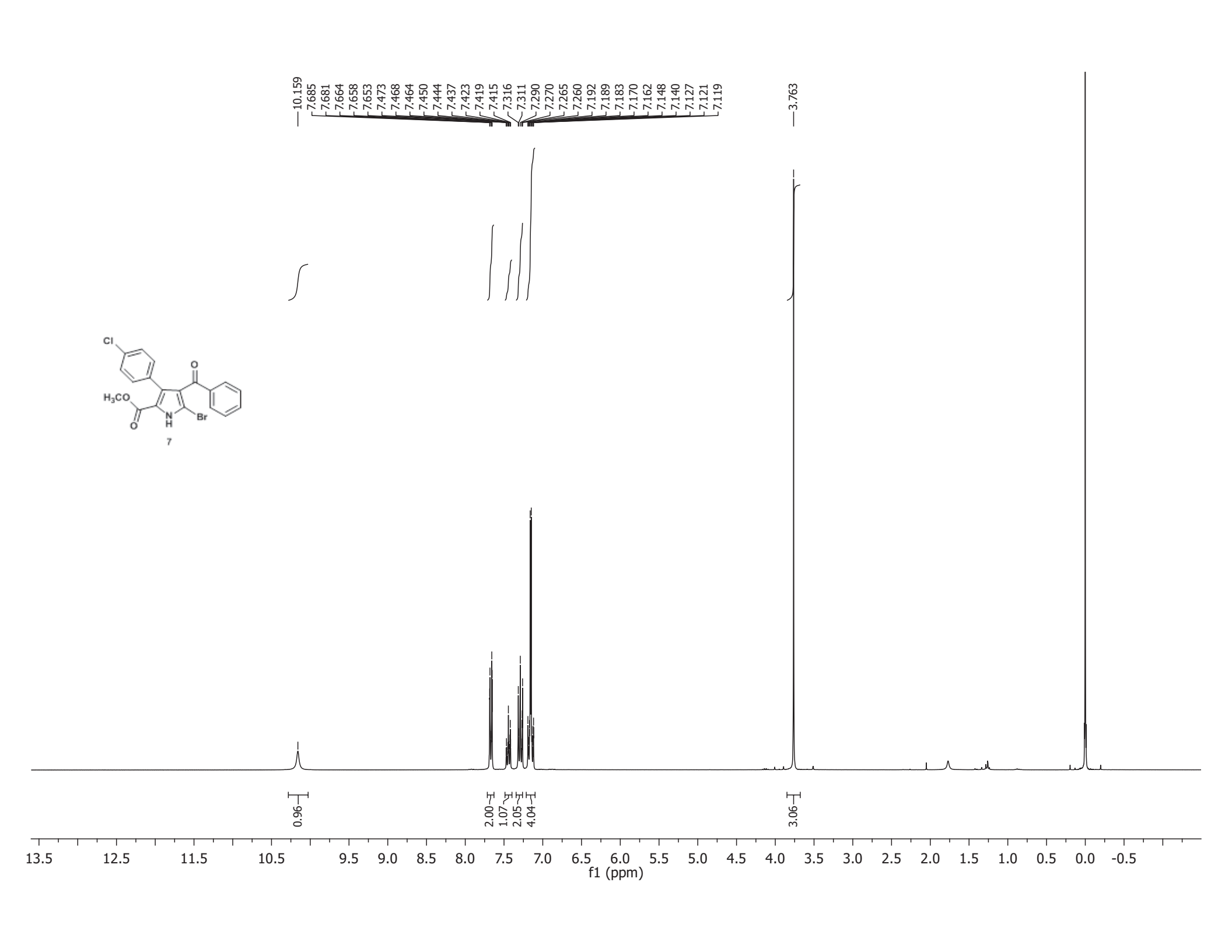

190.773
163.542
161.285
161.059
143.045
136.296
132.114
132.034
131.485
129.689
129.070
128.920
127.396
125.384
120.555
114.524
114.310
61.236
13.847
F
O
H3C
O
O
N
H
4u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

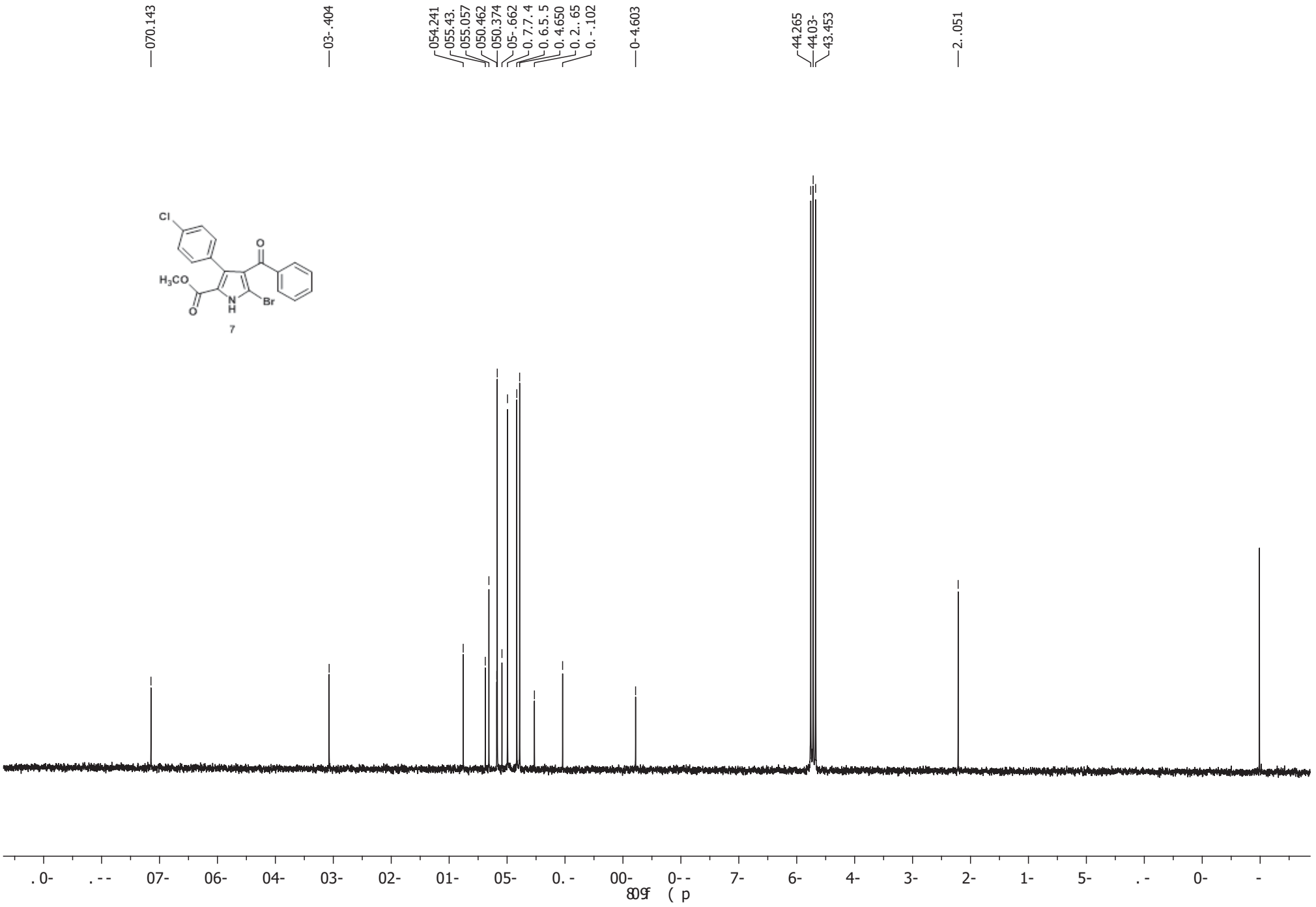

9.688
7.612
7.569
7.550
7.437
7.418
7.391
7.372
7.298
7.279
7.260
7.168
7.147
1.543
Br
O
CH3
H3C
O
O
N
H
H3C
O
Cl
4v
10
9
8
7
6
5
4
3
2
1
ppm
0.91
1.00
1.04
4.03
1.27
2.05
9.02

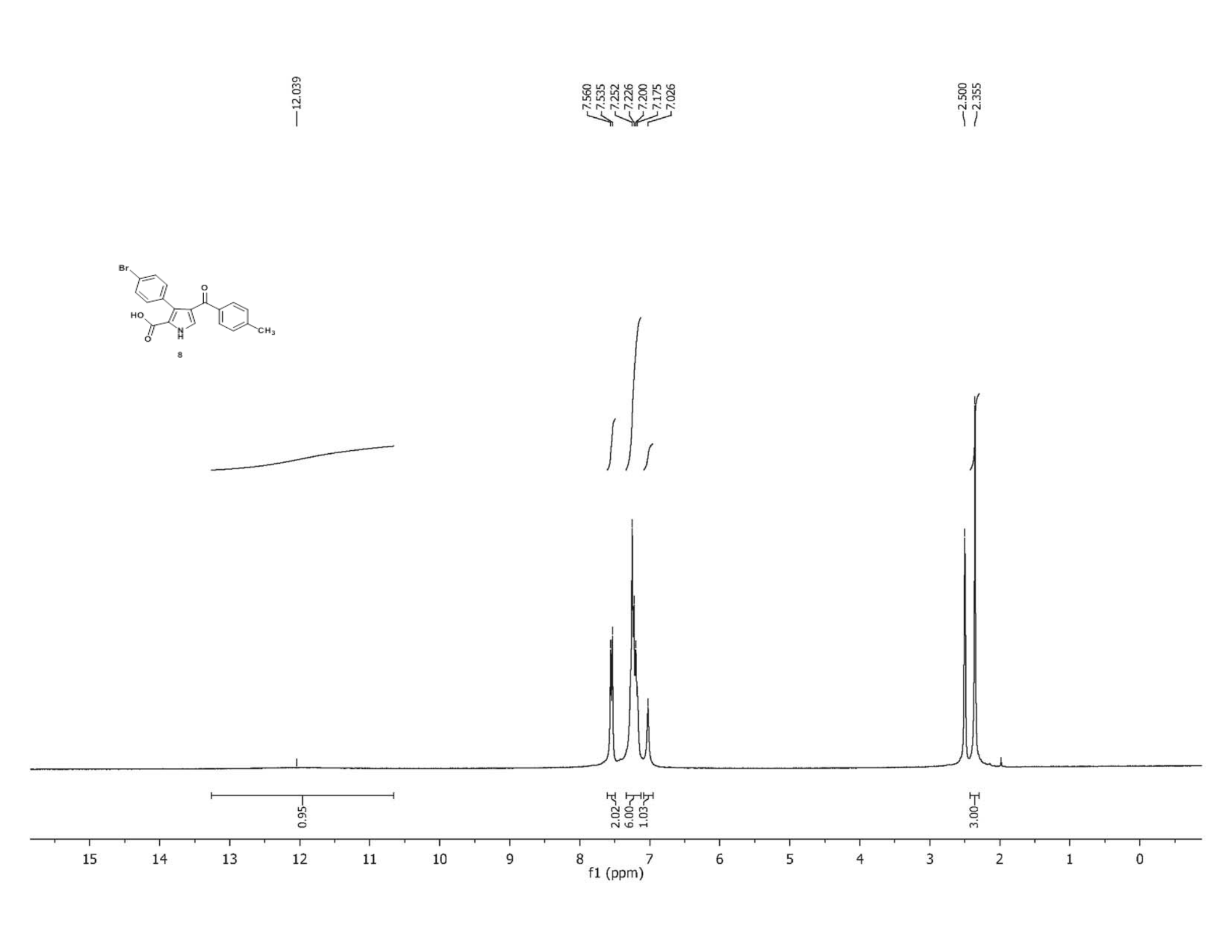

189.479
161.109
140.426
134.309
132.096
131.976
131.923
131.091
130.626
129.623
129.480
127.883
127.337
124.640
121.758
120.844
81.823
28.831
Br
O
CH3
H3C
O
H3C
O
N
H
Cl
4v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

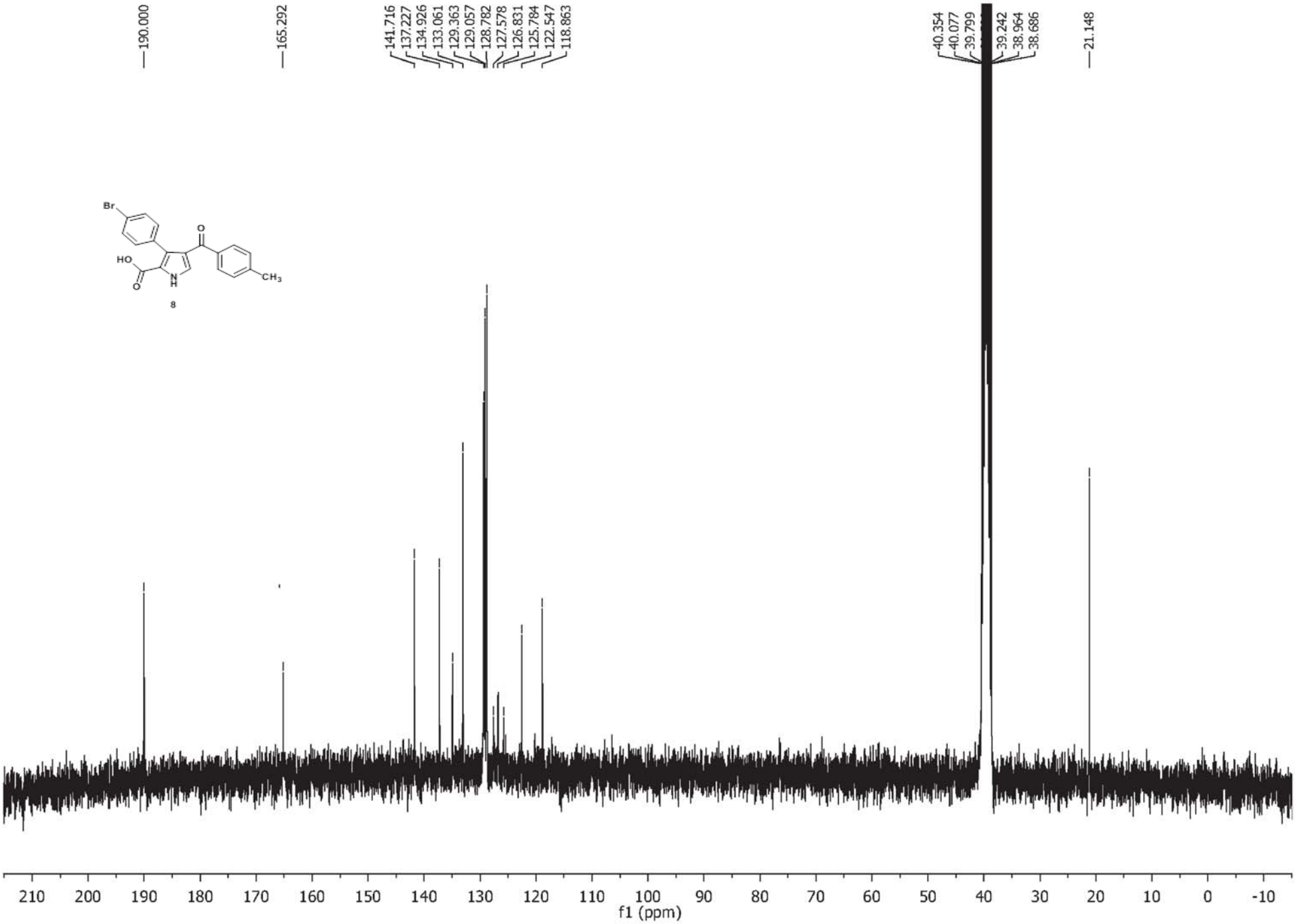

9.4886
7.4526
7.4440
2.6099
2.4114
1.5420
4w
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.989
1.000
3.007
3.011
9.013


194.060
162.042
129.184
127.232
125.554
121.180
81.717
29.017
28.264
11.602
4w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


10.159
7.685
7.681
7.664
7.658
7.653
7.473
7.468
7.464
7.450
7.444
7.437
7.423
7.419
7.415
7.316
7.311
7.290
7.270
7.265
7.260
7.192
7.189
7.183
7.170
7.162
7.148
7.140
7.127
7.121
7.119
3.763
Cl
O
H3CO
N
H
Br
O
7
0.96
2.00
1.07
2.05
4.04
3.06
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


070.143
03-.404
054.241
055.43.
055.057
050.462
050.374
05-.662
0.7.7.4
0.6.5.5
0.4.650
0.2..65
0.-.102
0-4.603
44.265
44.03-
43.453
2..051
Cl
O
H3CO
N
H
Br
O
7
809f (p


12.039
7.560
7.535
7.252
7.226
7.200
7.175
7.026
2.500
2.355
Br
HO
O
O
N
H
CH3
8
0.95
2.02
6.00
1.03
3.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


190.000
165.292
141.716
137.227
134.926
133.061
129.363
129.057
128.782
127.578
126.831
125.784
122.547
118.863
40.354
40.077
39.799
39.242
38.964
38.686
21.148
Br
HO
O
O
N
H
CH3
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)