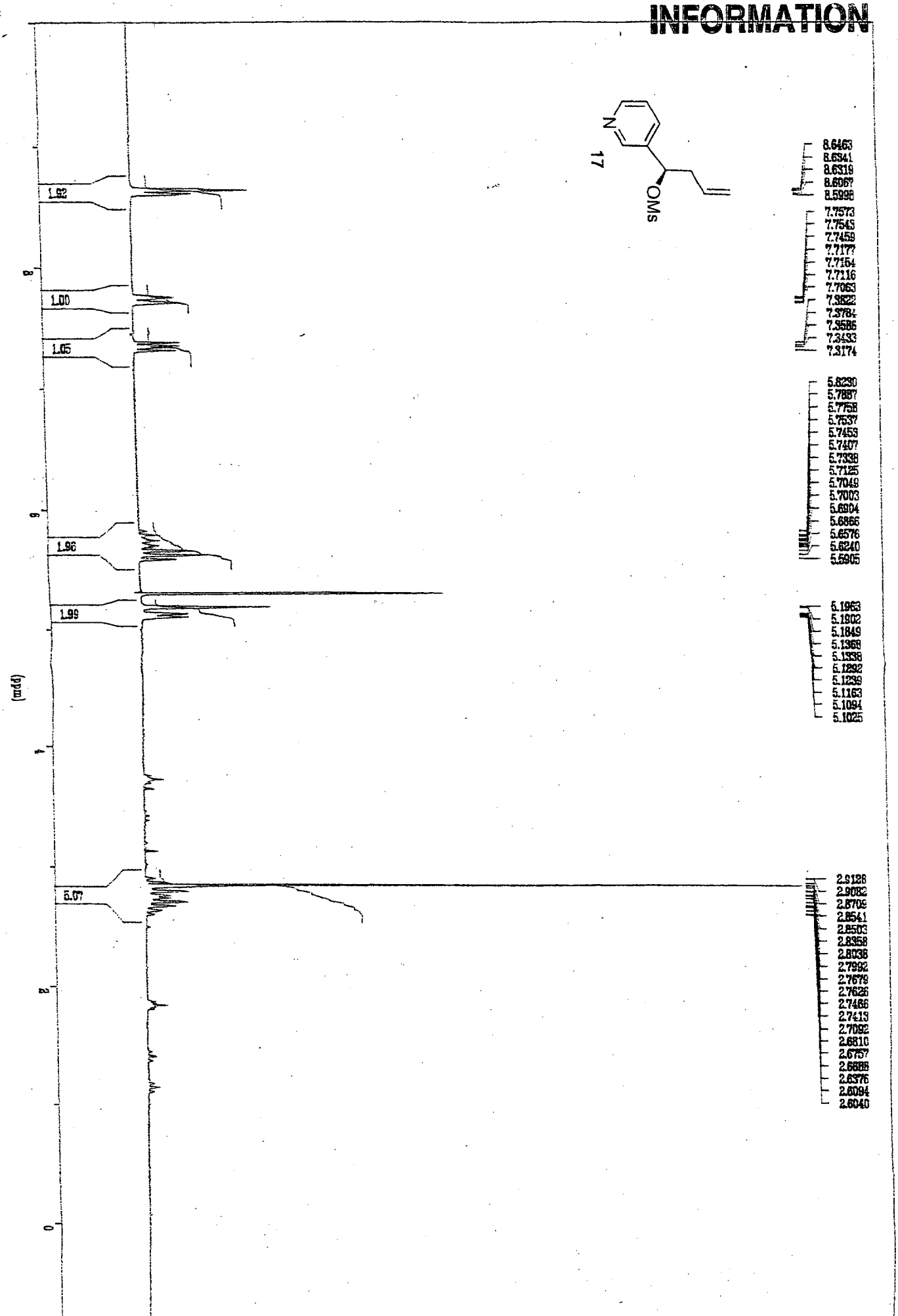
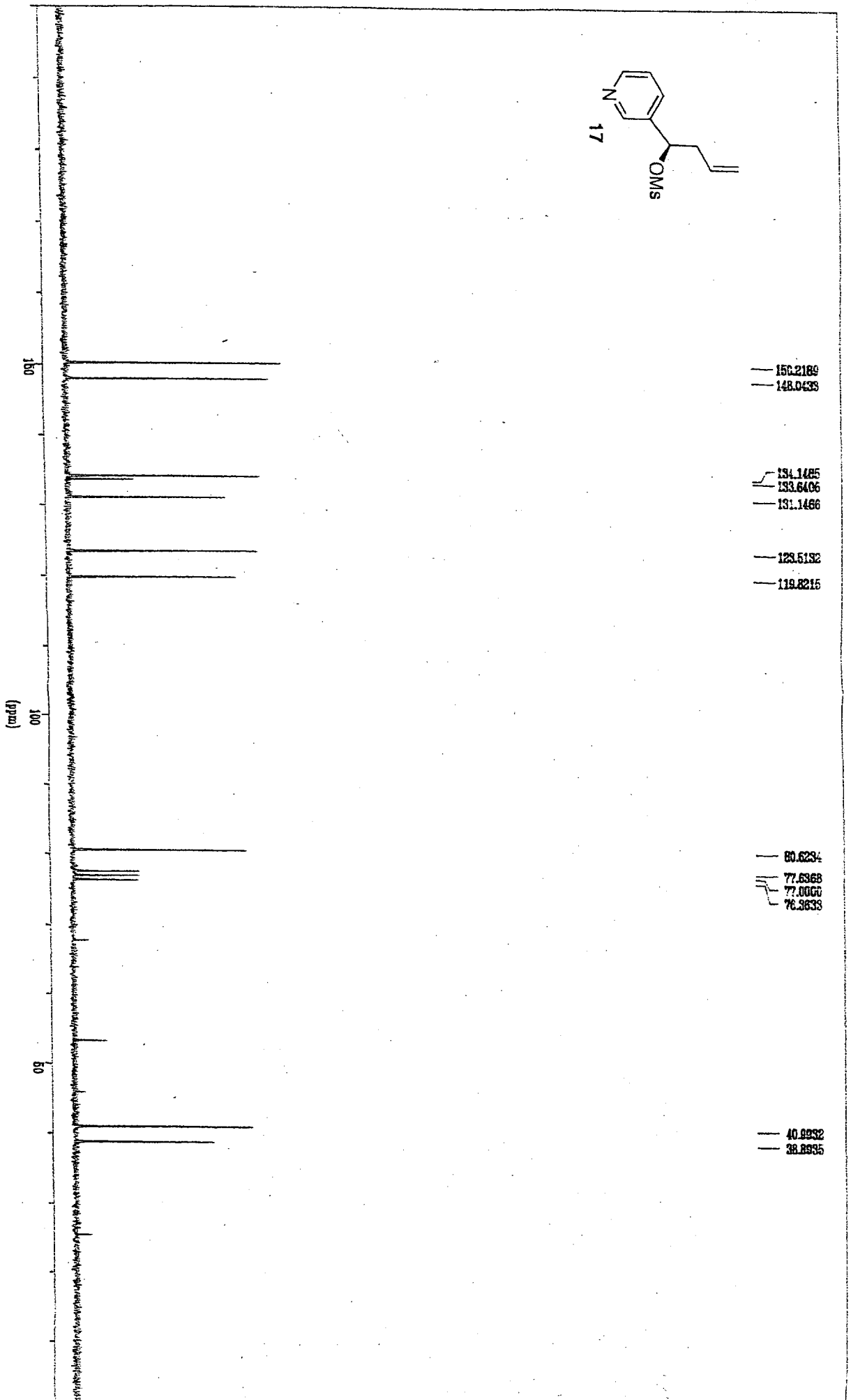
SUPPORTING INFORMATION

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131.1466
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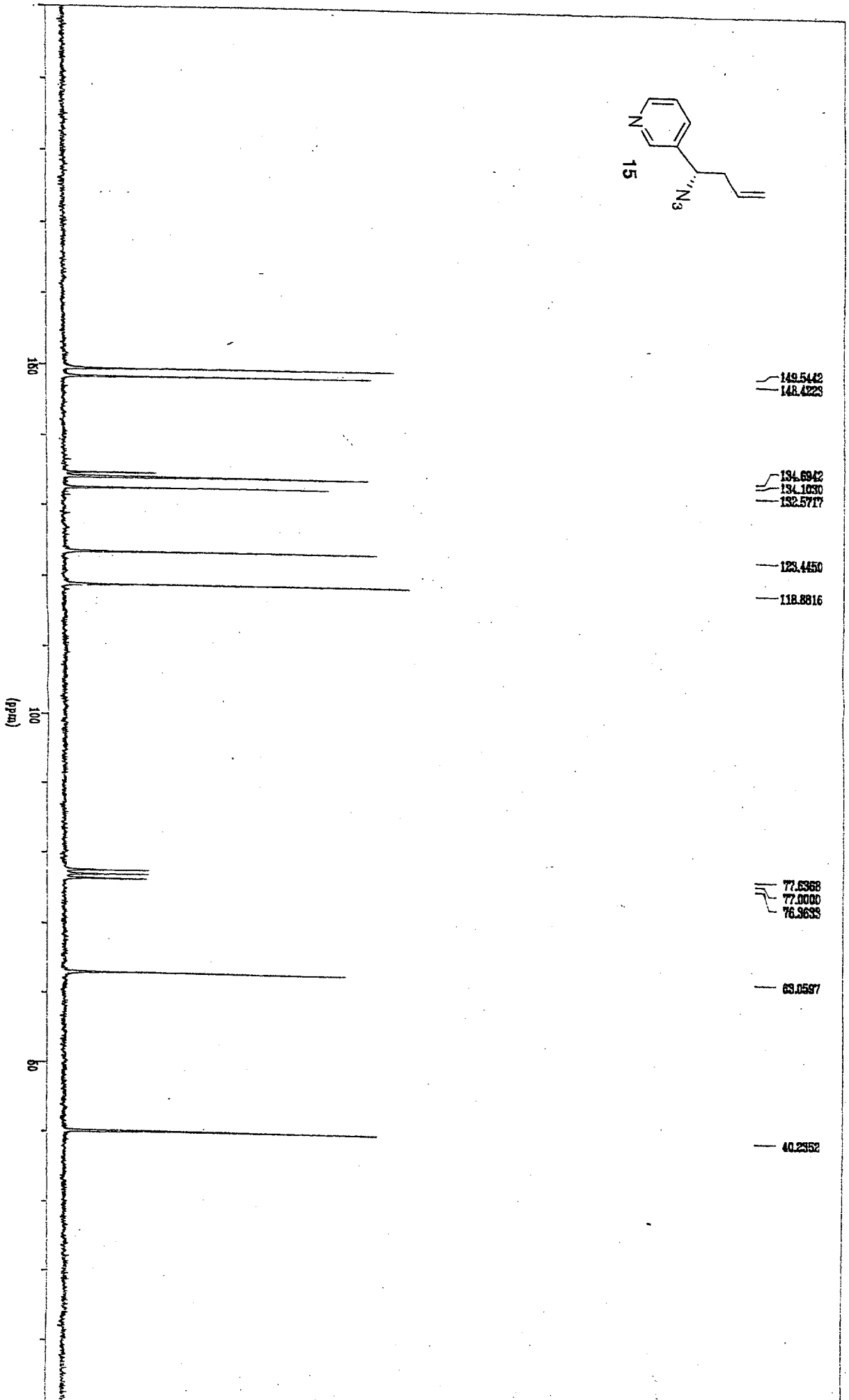
80.6234
77.6368
77.0000
76.3633
40.9932
38.8935
150
100
50
(ppm)


15
149.5442
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134.1030
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76.3633
63.0597
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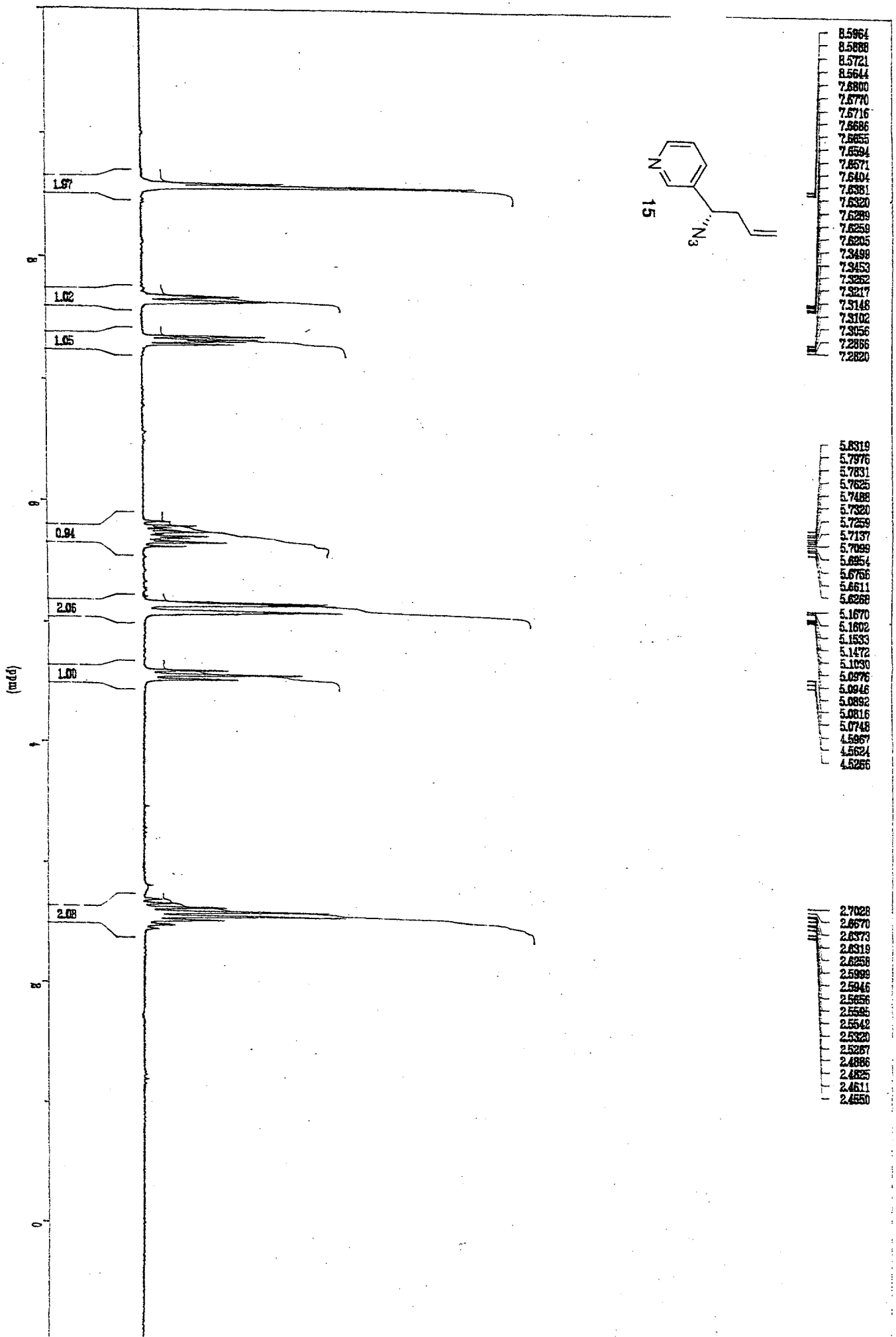
100
60
(ppm)


15
N
N3
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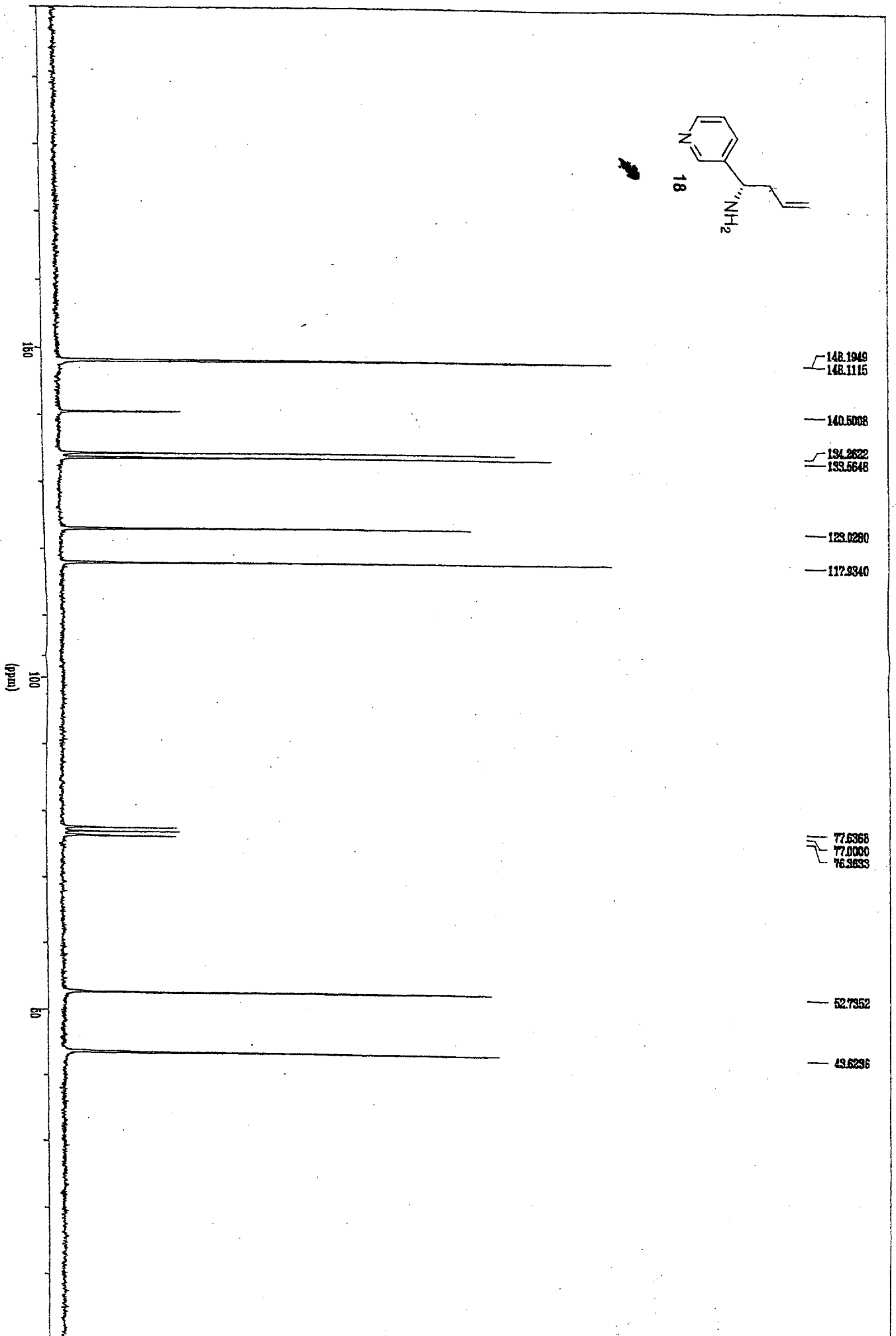
7.6655
7.6594
7.6571
7.6404
7.6381
7.6320
7.6289
7.6259
7.6205
7.3499
7.3453
7.3262
7.3217
7.3148
7.3102
7.3056
7.2866
7.2820
5.8319
5.7976
5.7831
5.7625
5.7488
5.7320
5.7259
5.7137
5.7099
5.6954
5.6766
5.6611
5.6268
5.1670
5.1602
5.1533
5.1472
5.1030
5.0976
5.0946
5.0892
5.0816
5.0748
4.5867
4.5624
4.5266
2.7028
2.6670
2.6373
2.6319
2.6258
2.5999
2.5946
2.5656
2.5595
2.5542
2.5320
2.5267
2.4866
2.4825
2.4611
2.4550
1.97
1.02
1.05
0.94
2.06
1.00
2.08
(ppm)
8
6
4
2
0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NH2
N
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140.5008
134.2622
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117.9340
77.6368
77.0000
76.3633
52.7352
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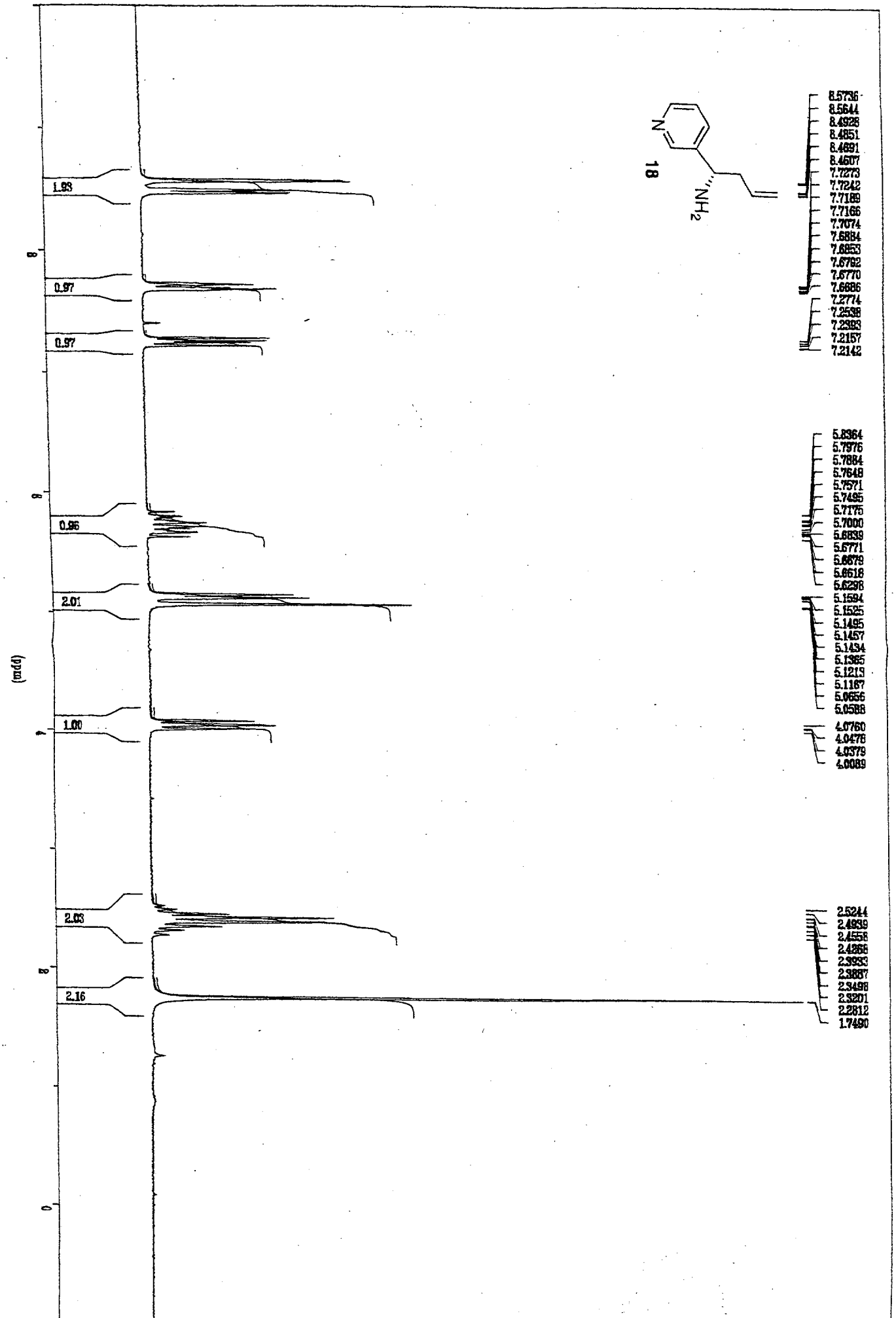
(ppm)
160
100
50


18
NH2
N
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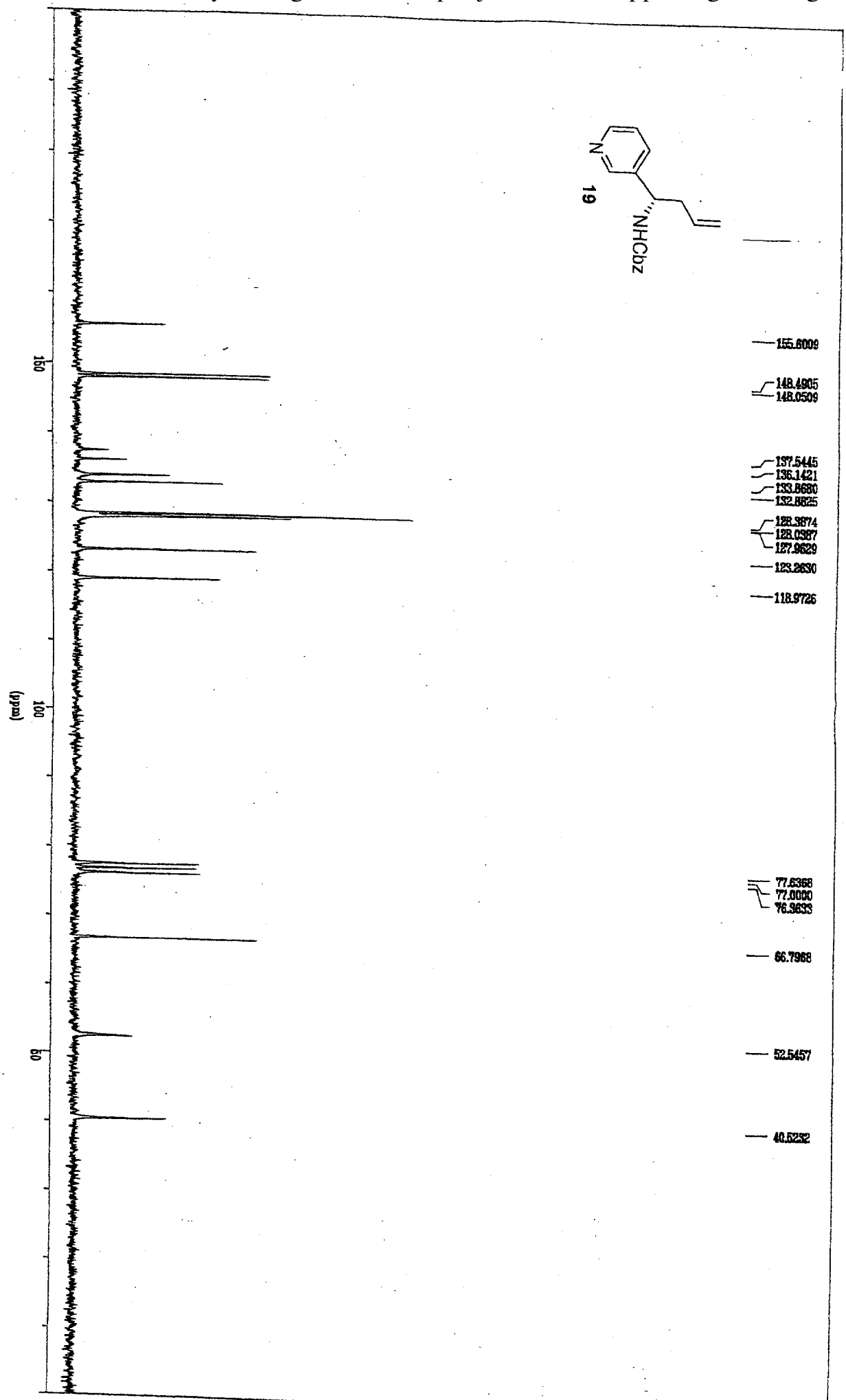
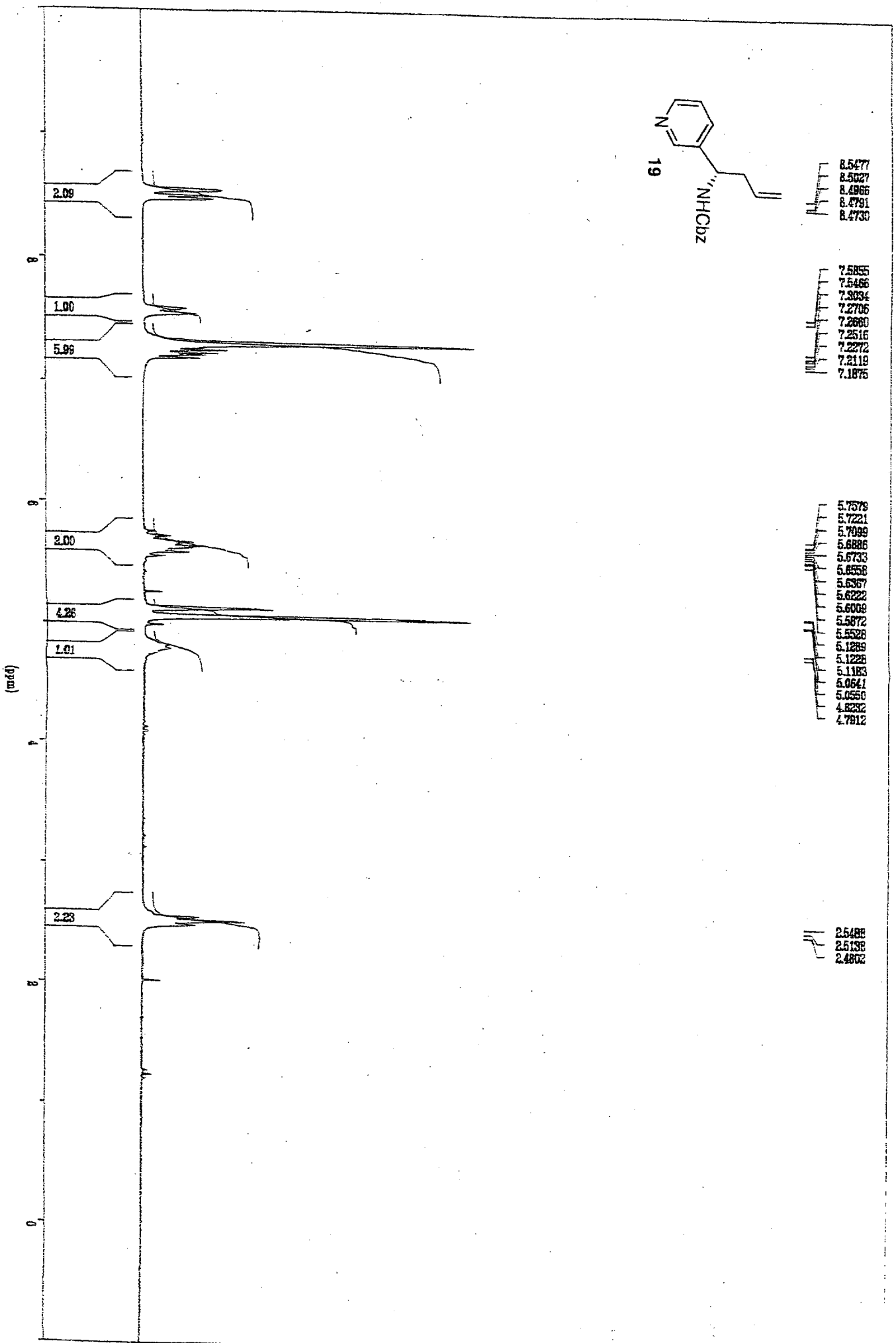
8.4928
8.4851
8.4691
8.4607
7.7273
7.7242
7.7189
7.7166
7.7074
7.6884
7.6853
7.6792
7.6770
7.6686
7.2774
7.2538
7.2393
7.2157
7.2142
5.8364
5.7976
5.7884
5.7648
5.7571
5.7495
5.7175
5.7000
5.6839
5.6771
5.6679
5.6618
5.6298
5.1594
5.1525
5.1495
5.1457
5.1434
5.1365
5.1213
5.1167
5.0656
5.0588
4.0760
4.0478
4.0379
4.0089
2.5244
2.4939
2.4558
2.4268
2.3933
2.3887
2.3498
2.3201
2.2812
1.7490
1.93
0.97
0.97
0.96
2.01
1.00
2.03
2.16
(ppm)


19
NHCbz
N
155.6009
148.4905
148.0509
137.5445
136.1421
133.8680
132.8825
128.3874
128.0387
127.9629
123.2630
118.9726
77.6368
77.0000
76.3633
66.7968
52.5457
40.5232
(ppm)
150
100
50


19
NHCbz
N
8.5477
8.5027
8.4966
8.4791
8.4730
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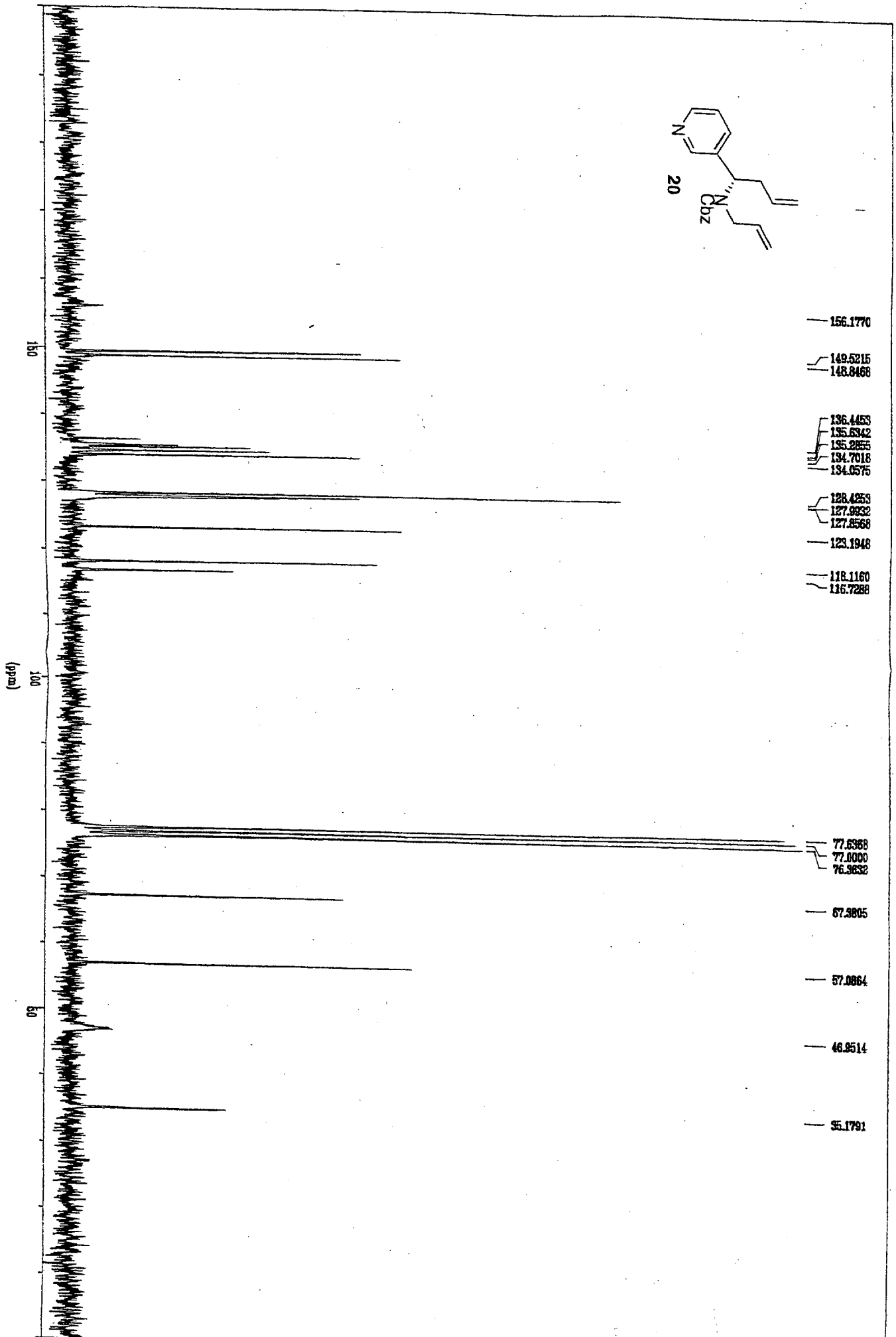
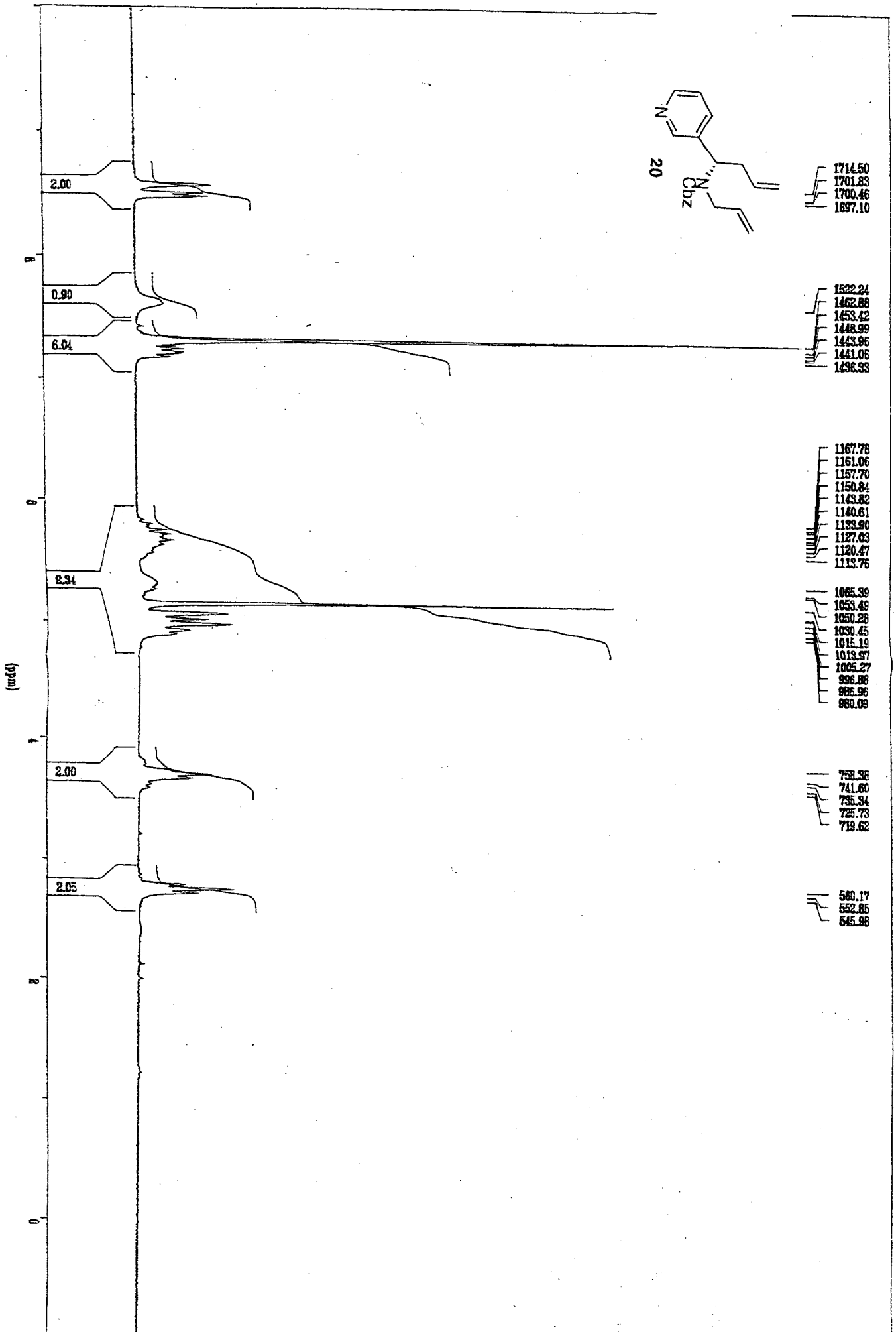
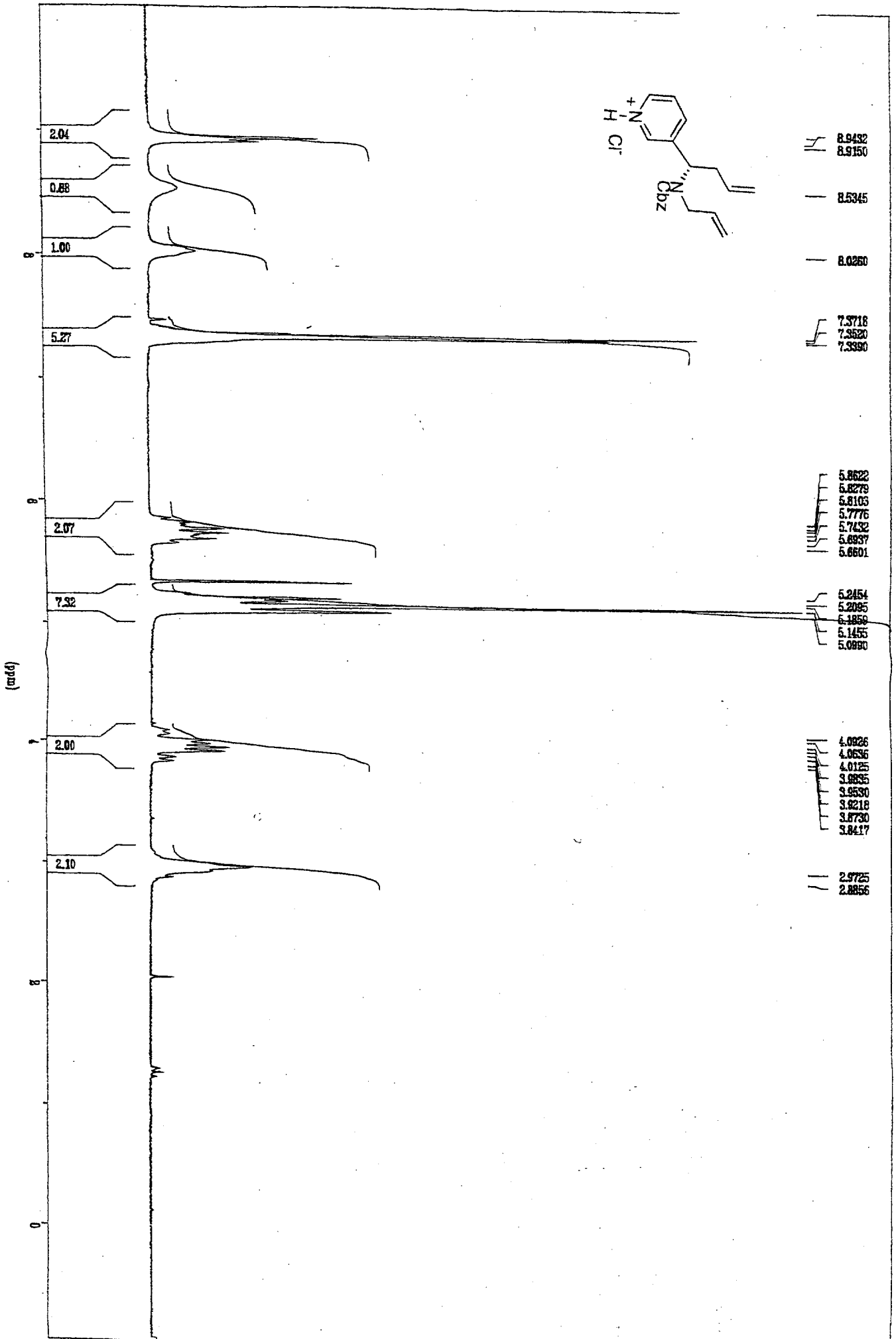
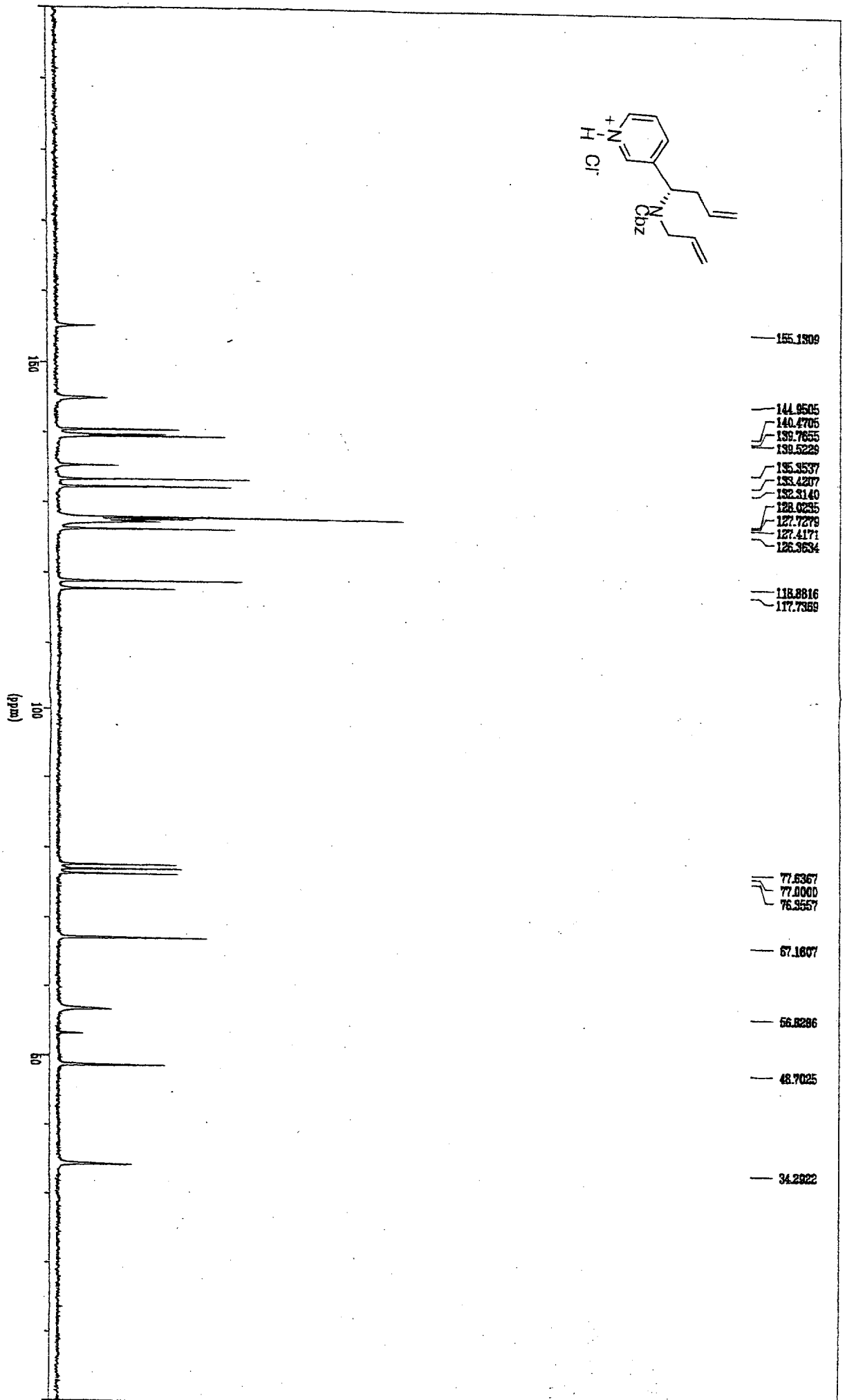
7.5466
7.3034
7.2706
7.2660
7.2516
7.2272
7.2119
7.1875
5.7579
5.7221
5.7099
5.6886
5.6733
5.6558
5.6367
5.6222
5.6009
5.5872
5.5528
5.1289
5.1226
5.1183
5.0641
5.0550
4.8232
4.7912
2.5488
2.5138
2.4802
2.09
1.00
5.96
2.00
4.26
1.01
2.23
(ppm)


20
N
N
Cbz
156.1770
149.5215
148.8468
136.4453
135.6342
135.2855
134.7018
134.0575
128.4253
127.9932
127.8568
123.1948
118.1160
116.7288
77.6368
77.0000
76.3632
67.3805
57.0864
46.9514
35.1791
150
100
50
(ppm)


20
Cbz
N
2.00
0.90
6.04
2.34
2.00
2.05
8
6
4
2
0
(ppm)
1714.50
1701.83
1700.46
1697.10
1522.24
1462.88
1453.42
1448.99
1443.96
1441.06
1436.33
1167.78
1161.06
1157.70
1150.84
1143.82
1140.61
1133.90
1127.03
1120.47
1113.76
1065.39
1053.49
1050.28
1030.45
1015.19
1013.97
1005.27
996.88
986.96
980.09
758.38
741.60
735.34
725.73
719.62
560.17
552.85
545.98


2.04
0.88
1.00
5.27
2.07
7.32
2.00
2.10
(ppm)
8.9432
8.9150
8.5345
8.0260
7.3718
7.3520
7.3390
5.8622
5.8279
5.8103
5.7776
5.7432
5.6937
5.6601
5.2454
5.2095
5.1455
5.0990
4.0926
4.0636
4.0125
3.9835
3.9530
3.9218
3.8730
3.8417
2.9725
2.8856
Cl
H
N
Cbz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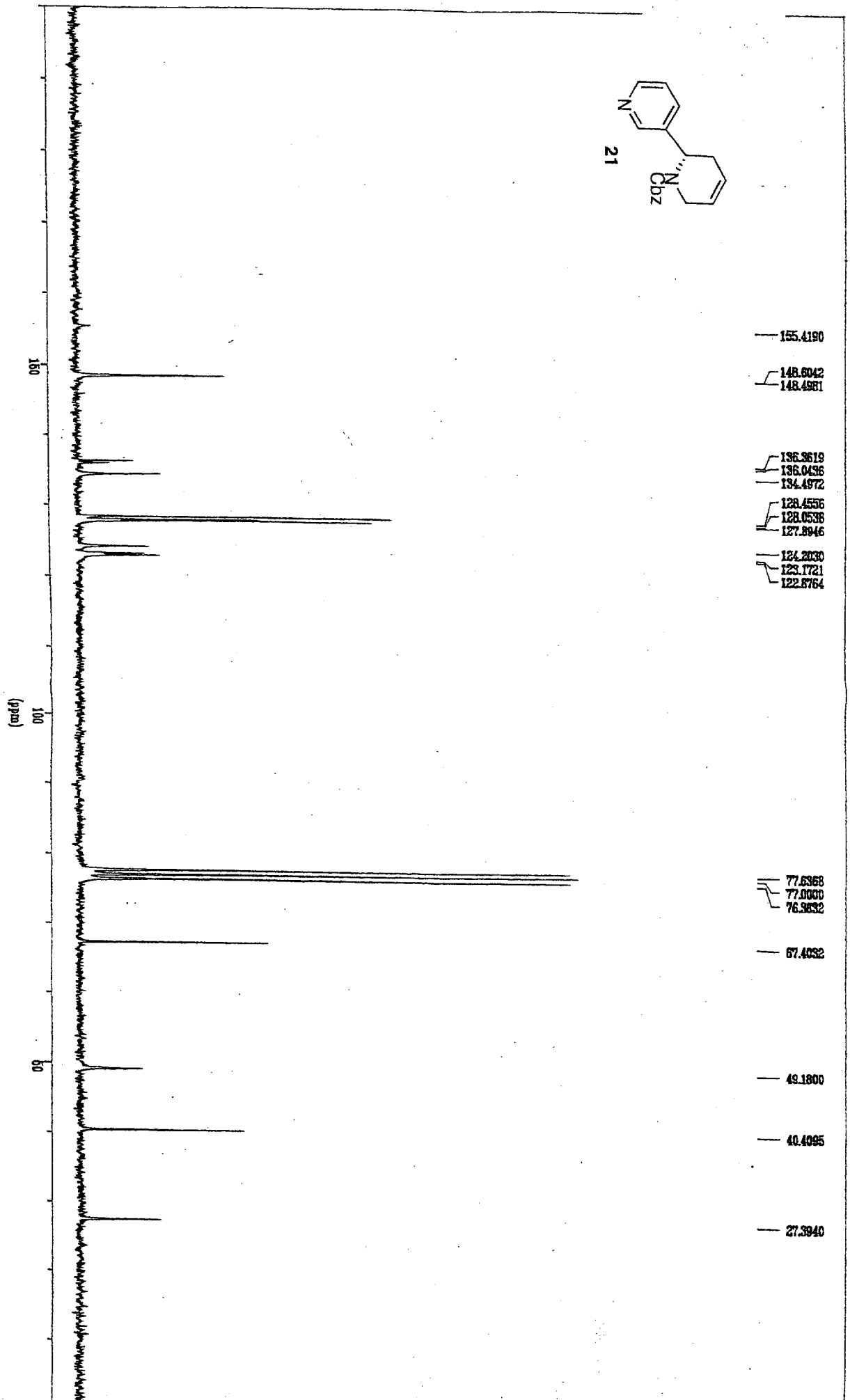
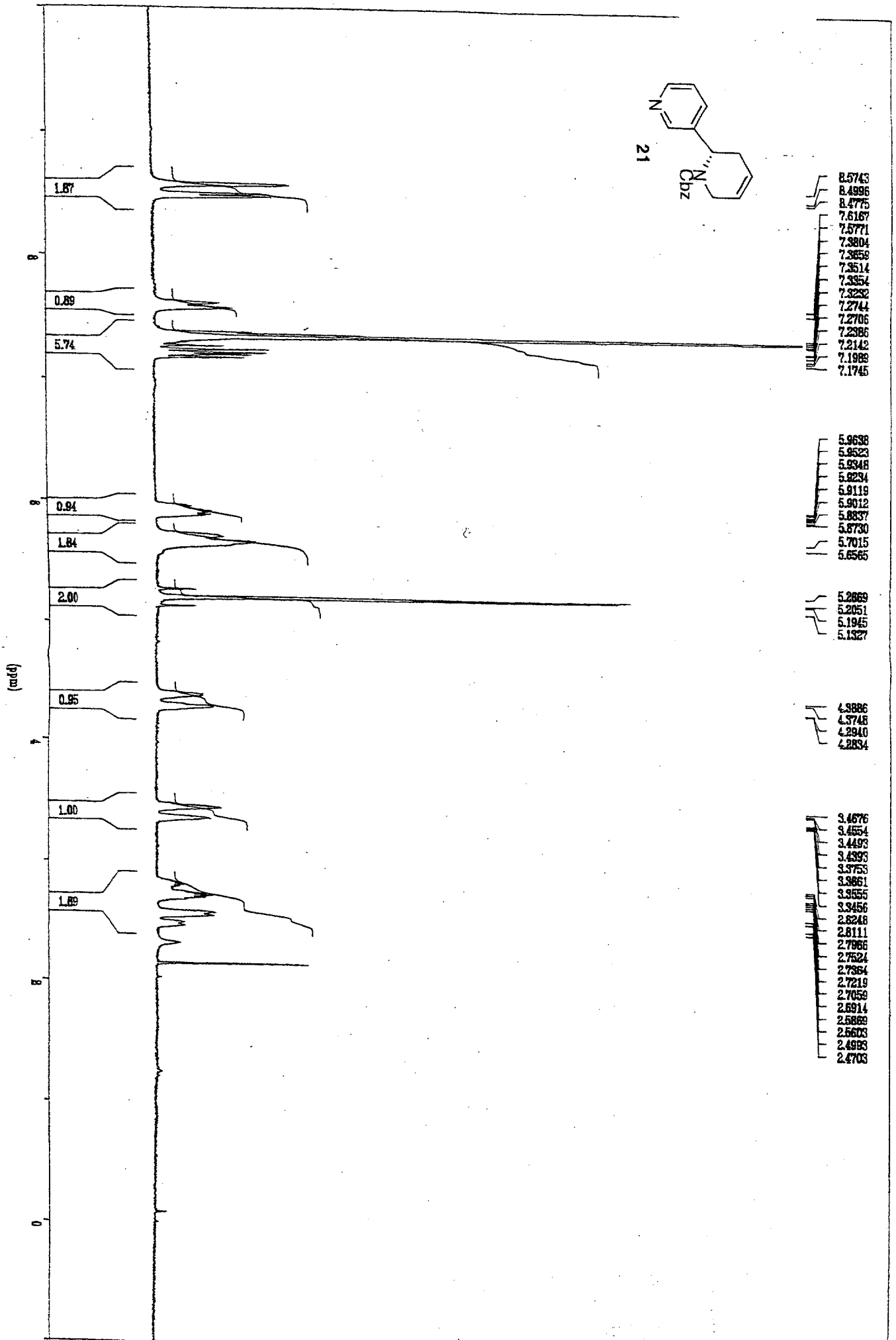
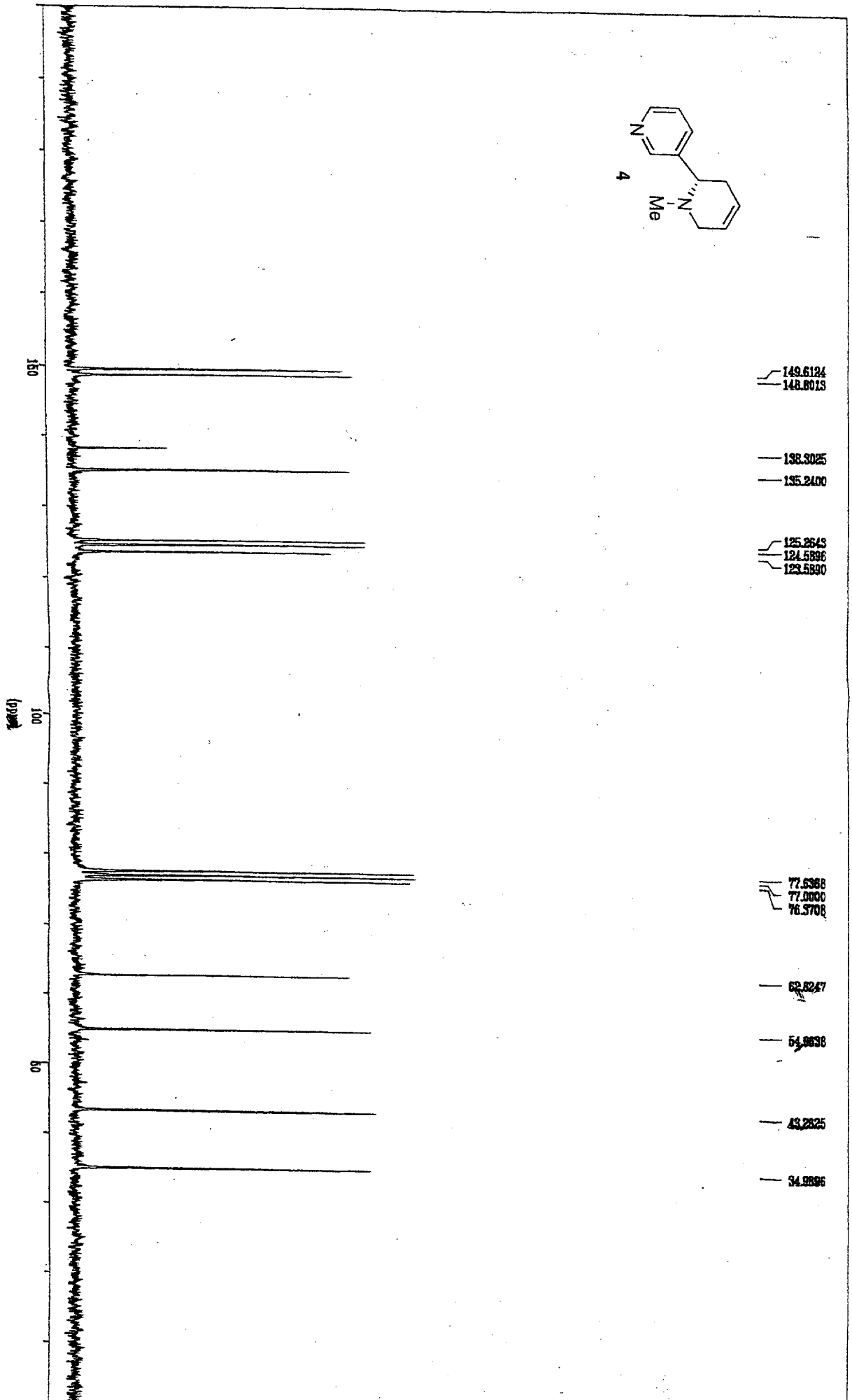
140.4705
139.7655
139.5229
135.3537
133.4207
132.3140
128.0235
127.7279
127.4171
126.3634
118.8816
117.7369
77.6367
77.0000
76.3557
67.1607
56.8286
48.7025
34.2922
160
100
60
(ppm)
Cl⁻
H
N
CbZ


21
N
N
Cbz
155.4190
148.6042
148.4981
136.3619
136.0436
134.4972
128.4556
128.0538
127.8946
124.2030
123.1721
122.8764
77.6368
77.0000
76.3632
67.4032
49.1800
40.4095
27.3940
160
100
60
(ppm)


21
Cbz
N
N
8.5743
8.4996
8.4775
7.6167
7.5771
7.3804
7.3659
7.3514
7.3354
7.3232
7.2744
7.2706
7.2386
7.2142
7.1989
7.1745
5.9638
5.9523
5.9348
5.9234
5.9119
5.9012
5.8837
5.8730
5.7015
5.6565
5.2869
5.2051
5.1945
5.1327
4.3886
4.3746
4.2940
4.2834
3.4676
3.4554
3.4493
3.4393
3.3753
3.3661
3.3555
3.3456
2.8248
2.8111
2.7966
2.7524
2.7364
2.7219
2.7059
2.6914
2.5869
2.5603
2.4993
2.4703
1.87
0.89
5.74
0.94
1.84
2.00
0.95
1.00
1.89
(ppm)


4
Me
N
N
149.6124
148.8013
138.3025
135.2400
125.2643
124.5896
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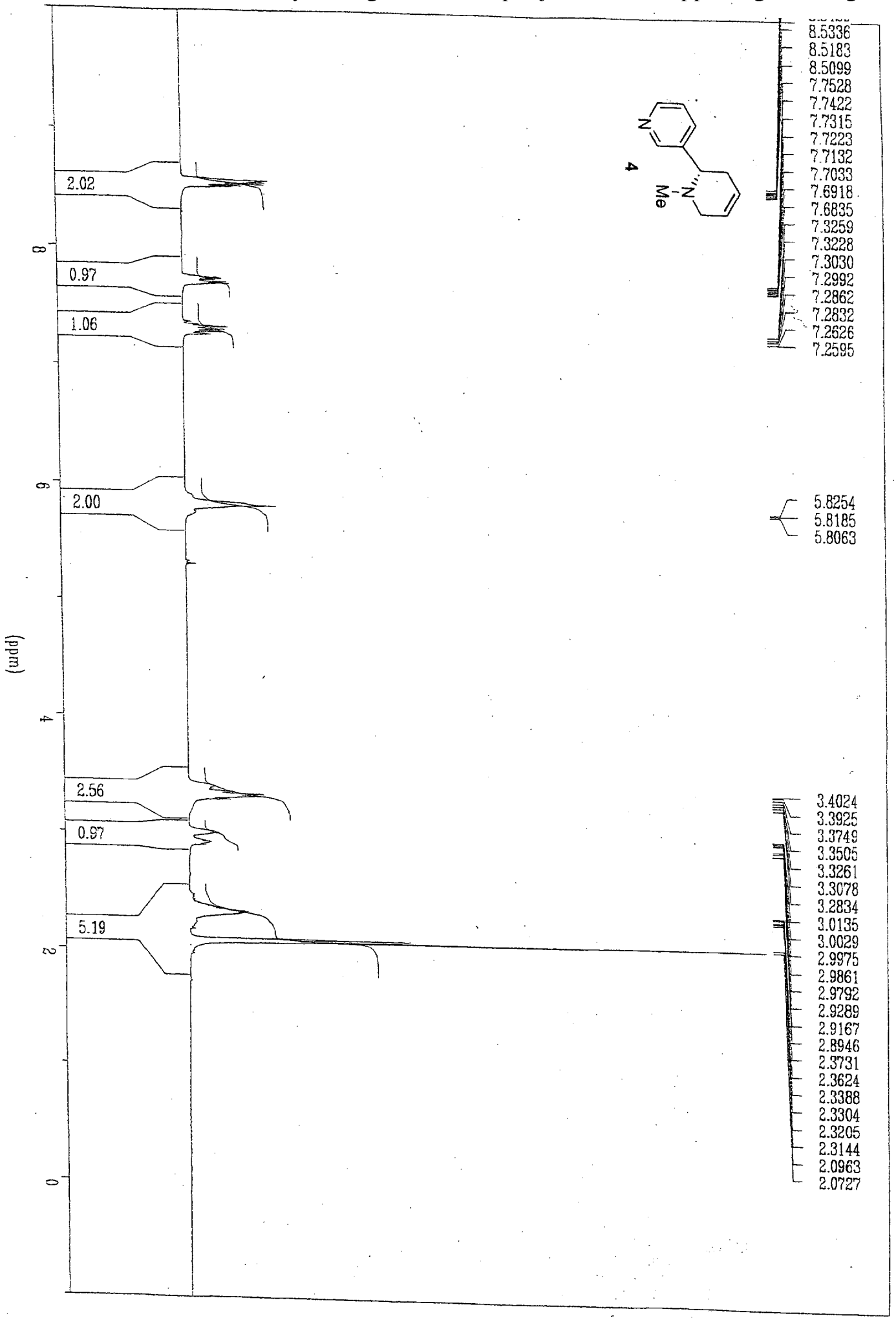
77.5368
77.0000
76.3708
62.8247
54.9638
43.2825
34.9896
150
100
50
(ppm)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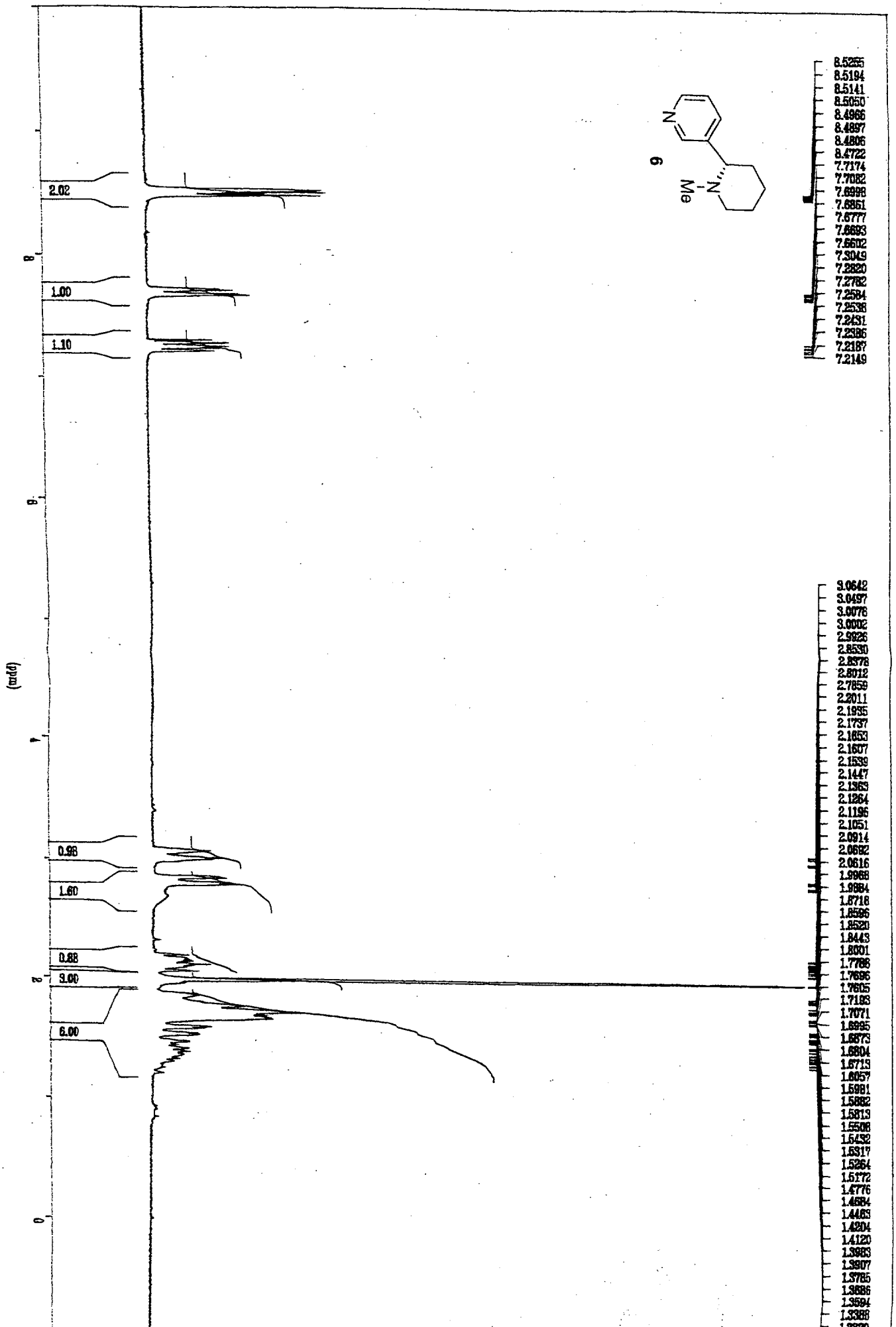
8.5183
8.5099
7.7528
7.7422
7.7315
7.7223
7.7132
7.7033
7.6918
7.6835
7.3259
7.3228
7.3030
7.2992
7.2862
7.2832
7.2626
7.2595
5.8254
5.8185
5.8063
3.4024
3.3925
3.3749
3.3505
3.3261
3.3078
3.2834
3.0135
3.0029
2.9975
2.9861
2.9792
2.9289
2.9167
2.8946
2.3731
2.3624
2.3388
2.3304
2.3205
2.3144
2.0963
2.0727
N
N
Me
4
2.02
0.97
1.06
2.00
2.56
0.97
5.19
8
6
4
2
0
(ppm)


(ppm)
2.02
1.00
1.10
0.98
1.60
0.88
3.00
6.00
6
Me
N
N
8.5255
8.5194
8.5141
8.5050
8.4966
8.4897
8.4806
8.4722
7.7174
7.7082
7.6998
7.6851
7.6777
7.6693
7.6602
7.3049
7.2820
7.2782
7.2584
7.2538
7.2431
7.2386
7.2187
7.2149
3.0642
3.0497
3.0076
3.0002
2.9926
2.8530
2.8378
2.8012
2.7859
2.2011
2.1955
2.1737
2.1653
2.1607
2.1539
2.1447
2.1363
2.1264
2.1196
2.1051
2.0914
2.0692
2.0616
1.9968
1.9884
1.8718
1.8596
1.8520
1.8443
1.8001
1.7786
1.7696
1.7605
1.7183
1.7071
1.6995
1.6873
1.6804
1.6713
1.6057
1.5981
1.5882
1.5813
1.5508
1.5432
1.5317
1.5264
1.5172
1.4776
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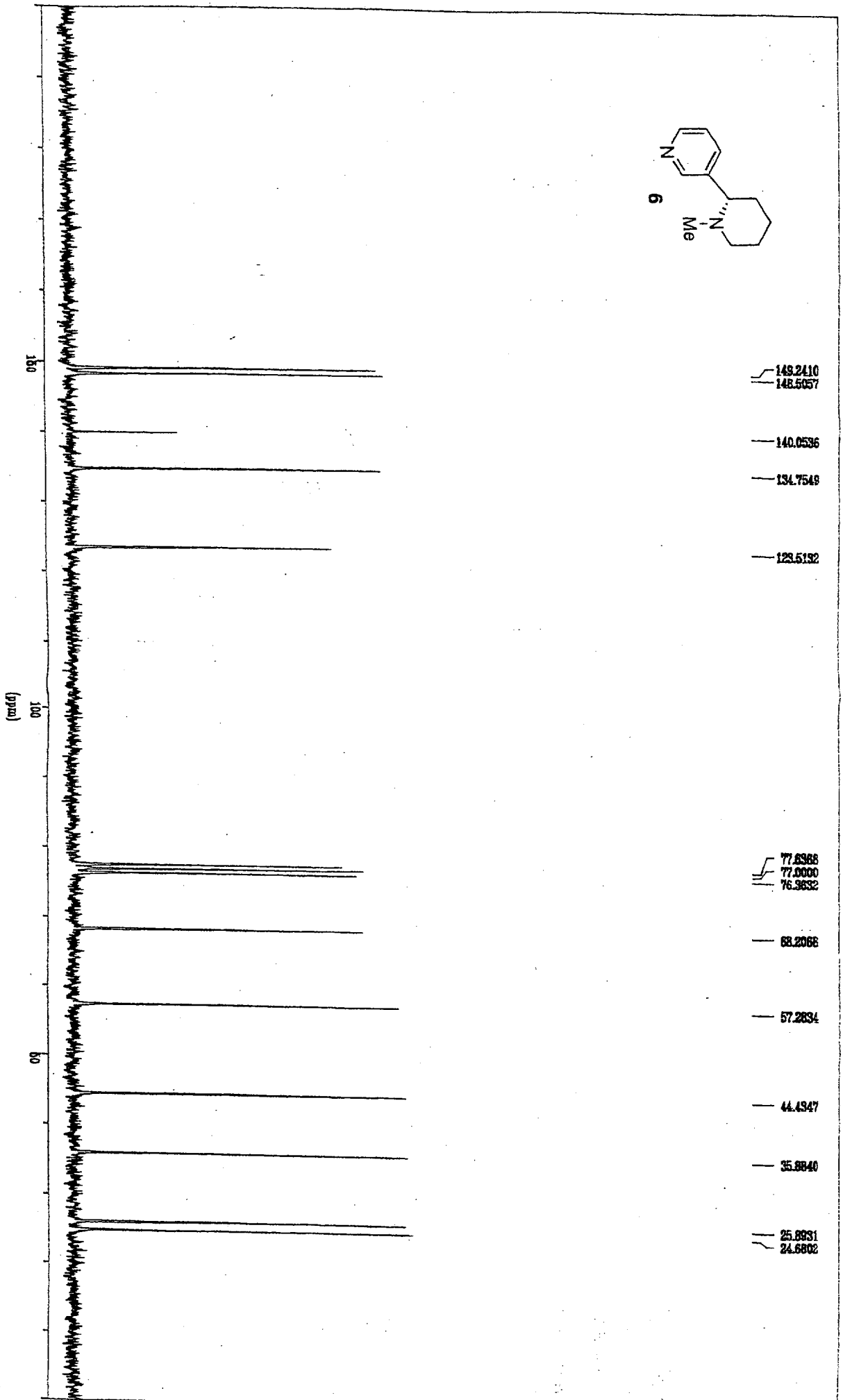
1.4204
1.4120
1.3983
1.3907
1.3785
1.3686
1.3594
1.3388


6
Me
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149.2410
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140.0536
134.7549
123.5132
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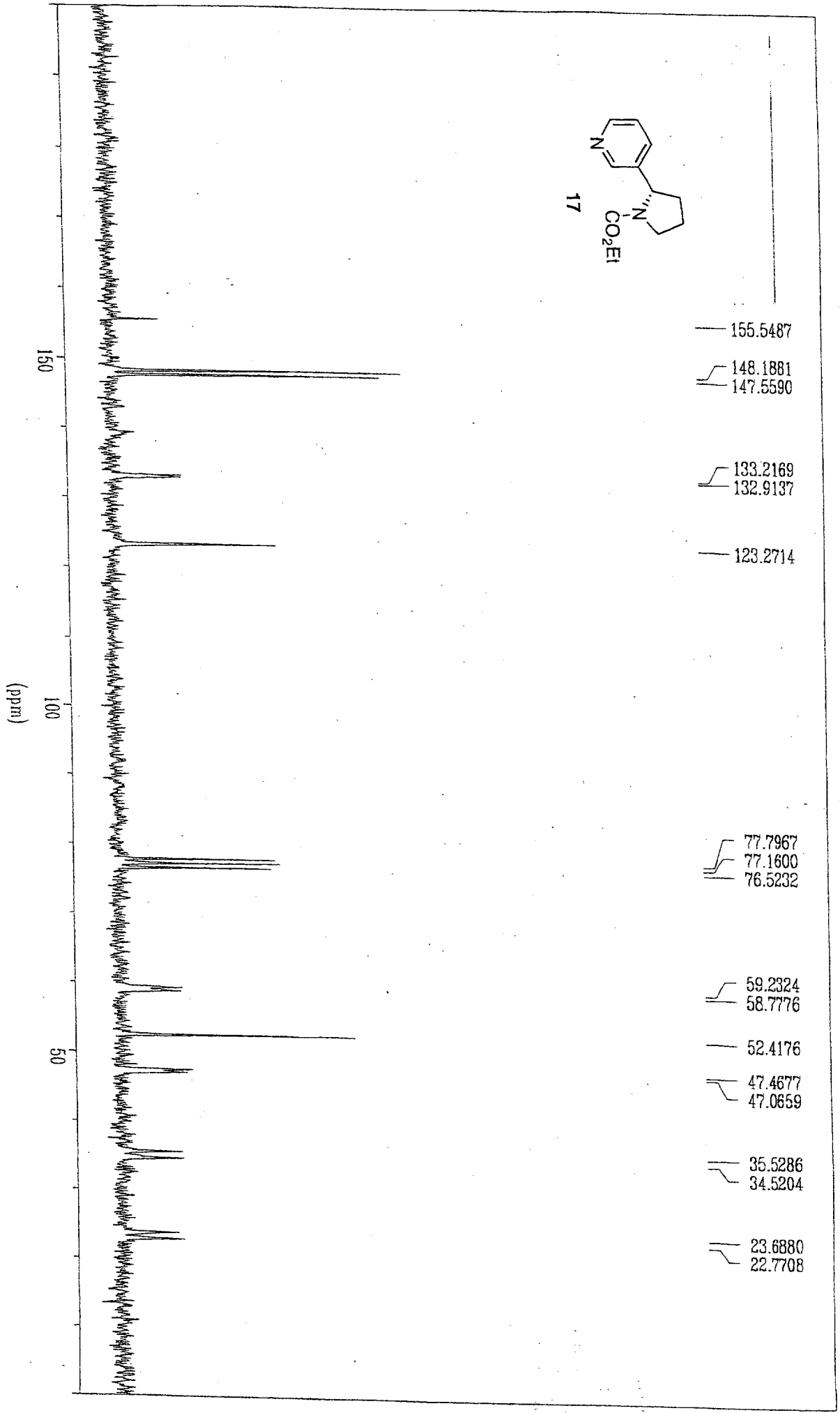
68.2068
57.2834
44.4347
35.8840
25.8931
24.6802
(ppm)
150
100
50


17
155.5487
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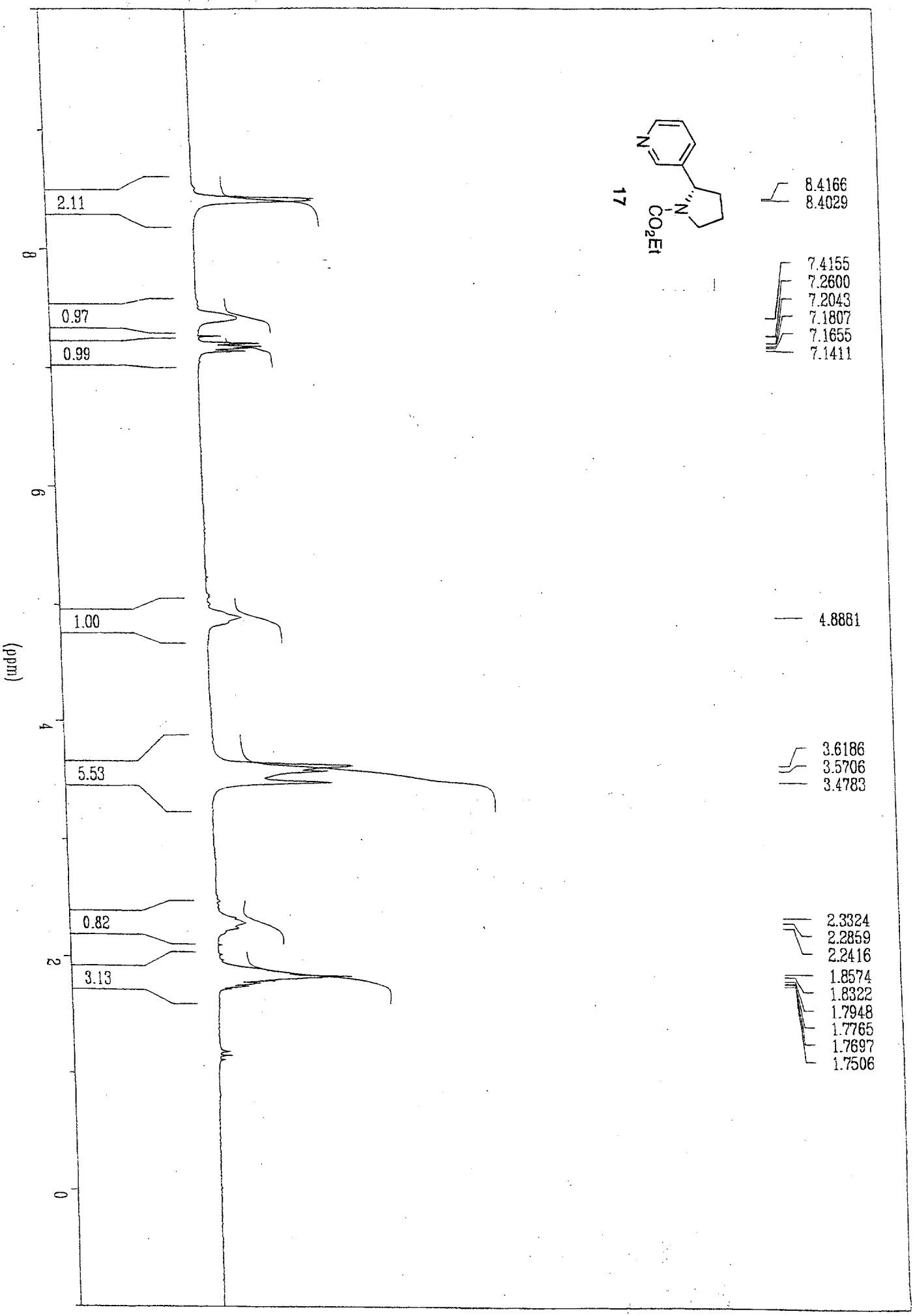
147.5590
133.2169
132.9137
123.2714
77.7967
77.1600
76.5232
59.2324
58.7776
52.4176
47.4677
47.0659
35.5286
34.5204
23.6880
22.7708
150
100
50
(ppm)


17
N
N
CO2Et
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8.4029
7.4155
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7.1807
7.1655
7.1411
4.8881
3.6186
3.5706
3.4783
2.3324
2.2859
2.2416
1.8574
1.8322
1.7948
1.7765
1.7697
1.7506
2.11
0.97
0.99
1.00
5.53
0.82
3.13
8
6
4
2
0
(ppm)