Supporting Information for:

# Concise Asymmetric Synthesis of (+)-CP-99,994 and (+)-L-733,060 via Efficient Construction of Homochiral *syn*-1,2-Diamines and *syn*-1,2-Amino Alcohols.

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**General Information.** All $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded at ambient temperature in $CDCl_3$ (93.94 kG, $^{1}H$ 400 MHz). Chemical shifts are reported in parts per million as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), integration, and coupling constant. Optical rotations were recorded at 589 nm, and were reported as $[\alpha]_D$ (concentration in grams/100 mL solvent). Melting points were uncorrected.

Compound **10**:

To a cooled (0°C) solution of **9** (320 mg, 0.83 mmol) and $Et_3N$ (0.17 mL, 1.25 mmol) in $CH_2Cl_2$ (5 mL) was added dropwise MsCl (0.08 mL, 1.08 mmol), and the mixture was stirred at 0°C for 1h, diluted with $Et_2O$ (30 mL), and washed successively with 1M HCl, saturated aq. $NaHCO_3$ and brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was dissolved in DMF (3 mL) under Ar, to this was added $NaN_3$ (163 mg, 2.5 mmol) and the solution was stirred at 65°C overnight, cooled to rt, diluted with $Et_2O$ (30 mL), and washed successively with water and brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography (EtOAc/Hexanes=1/8) to afford **10** (280 mg, 83%) as a white solid.

Mp. 86–87 °C; $[\alpha]_D^{23}$ -19.9 (*c* 1.32, $CHCl_3$); $^{1}H$ NMR ($CDCl_3$) $\delta$ 7.419-7.25 (m, 5H), 5.26-5.17 (m, 1H), 4.87-4.75 (m, 1H), 4.07 (t, 2H, *J* = 6.0 Hz), 3.71-3.60 (m, 1H), 1.92-1.72 (m, 2H), 1.70-1.59 (m, 2H), 1.43 (br s, 9H), 1.17 (s, 9H); $^{13}C$ NMR ($CDCl_3$) $\delta$ 178.4, 155.3, 139.9, 128.8, 127.8, 126.4, 80.0, 67.3, 63.5, 57.1 (m), 38.7, 28.6, 28.3, 27.1, 25.5. ESI-MS *m/z* 427.3 ($M + Na^+$); HR-ESI-MS *m/z* Calcd for $C_{21}H_{32}N_4O_4Na$ 427.2321, Found 427.2349.

Compound **11**:

To a solution of **10** (234 mg, 0.58 mmol) in MeOH (5 mL) under Ar was added 30% NaOMe in MeOH (0.21 mL, 1.16 mmol), the solution was stirred at rt for 4h, quenched by water, and extracted with $Et_2O$ (3×15 mL). The combined organic phase was washed with brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure to afford the crude product which was used in the next step without further purifications.

To a cooled (0°C) solution of the crude alcohol (180 mg) and $Et_3N$ (0.11 mL, 0.84 mmol) in $CH_2Cl_2$ (5 mL) was added dropwise MsCl (0.05 mL, 0.68 mmol), and the mixture was stirred at 0°C for 30min, diluted with $Et_2O$ (30 mL), and washed successively with 1M HCl, saturated aq. $NaHCO_3$ and brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was dissolved in THF (5 mL) under Ar, NaH (66 mg, 60% dispersion in mineral oil, 1.65 mmol) was added and the mixture was stirred at rt for 6h, quenched by saturated aq. $NH_4Cl$, extracted with $Et_2O$ (3×15 mL), and washed with brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography (EtOAc/Hexanes=1/16) to afford **11** (139 mg, 80%) as a colorless oil.

$[\alpha]_D^{23}$ +50.1 (*c* 1.26, $CHCl_3$); $^{1}H$ NMR ($CDCl_3$) $\delta$ 7.45 (d, 2H, *J* = 7.9 Hz), 7.37-7.22 (m, 3H), 5.47 (d, 1H, *J* = 5.5 Hz), 3.99 (dd, 1H, *J* = 13.8, 3.6 Hz), 3.96-3.85 (m, 1H); 2.89 (td, 1H, *J* = 13.2, 3.3 Hz), 2.00-1.90 (m, 2H), 1.88-1.76 (m, 1H), 1.75-1.60 (m, 1H), 1.42 (s, 9H); $^{13}C$ NMR ($CDCl_3$) $\delta$ 154.9, 137.7, 128.4, 128.2, 127.3, 80.2, 60.6, 56.5, 39.1, 28.3, 24.7, 23.9. ESI-MS *m/z* 325.2 ($M + Na^+$); HR-ESI-MS *m/z* Calcd for $C_{16}H_{22}N_4O_2Na$ 325.1640, Found 325.1644.

Compound **14**:

To a solution of **5** (640 mg, 1.13 mmol) in MeOH (6 mL) was added a methanolic solution of HCl (2M, 3.4 mL) at rt, stirring was continued for 4h, and the solution was concentrated under reduced pressure. To a cooled (0$^{o}$C) solution of the residue, 4-methoxybenzoic anhydride (525 mg, 1.84 mmol) and DMAP (10 mg) in $CH_2Cl_2$ (15 mL) was added $Et_3N$ (0.76 mL, 5.2 mmol) dropwise over 10min, and the mixture was stirred at rt for 4h, diluted with $CH_2Cl_2$ (30 mL), washed with saturated aq. $NaHCO_3$ and brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography (EtOAc/Hexanes=1/2) to afford **14** (607 mg, 88%) as a white solid.

Mp. 112–113 $^{o}$C; $[\alpha]_D^{23}$ -41.3 (*c* 1.04, $CHCl_3$); $^{1}$H NMR ($CDCl_3$) $\delta$ 7.74 (d, 2H, *J* =8.9 Hz), 7.39-7.25 (m, 5H), 7.11 (d, 1H, *J* = 8.9 Hz), 6.90 (d, 2H, *J* = 8.9 Hz), 5.11 (dd, 1H, *J* = 7.9, 3.7 Hz), 4.06-3.95 (m, 3H), 3.83 (s, 3H), 2.56 (br s, 1H), 1.85-1.63 (m, 2H), 1.58-1.49 (m, 1H), 1.28-1.15 (m, 1H), 1.12 (s, 9H); $^{13}$C NMR ($CDCl_3$) $\delta$ 178.7, 166.5, 162.2, 138.0, 128.9, 128.6, 127.9, 127.8, 126.4, 113.7, 73.6, 63.8, 58.2, 55.4, 38.7, 30.2, 27.1, 25.2. ESI-MS *m/z* 414.2 (M + $H^+$); HR-ESI-MS *m/z* Calcd for $C_{24}H_{32}NO_5$ 414.2280, Found 414.2308.

Compound **19**:

A suspension of **16** (315 mg, 0.79 mmol) and 20% $Pd(OH)_2$/C (280 mg) in MeOH (5 mL) was stirred under $H_2$ atmosphere at rt for 2h, $Boc_2O$ (259 mg, 1.90 mmol) was then added, and the mixture was stirred for an additional 3h, filtered through celite, and concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography (EtOAc/Hexanes=1/4) to afford **19** (236 mg, 79%) as a white solid.

Mp. 68–69 $^{o}$C; $[\alpha]_D^{23}$ +7.8 (*c* 0.97, $CHCl_3$); $^{1}$H NMR ($CDCl_3$) $\delta$ 7.38-7.22 (m, 5H), 5.37 (br m, 1H), 4.64 (br m, 1H), 4.05 (t, 2H, *J* = 6.3 Hz), 3.84 (br m, 1H), 2.24 (br s, 1H), 1.90-1.48 (m, 4H), 1.42 (br s, 9H), 1.15 (s, 9H); $^{13}$C NMR ($CDCl_3$) $\delta$ 178.6, 156.1, 140.5, 128.8, 127.6, 126.5, 79.8, 74.8, 64.0, 58.9, 38.7, 30.2, 28.3, 27.1, 25.0. ESI-MS *m/z* 402.2 (M + $Na^+$); HR-ESI-MS *m/z* Calcd for $C_{21}H_{33}NO_5Na$ 402.2256, Found 402.2237.

Compound **20**:

To a cooled (0$^{o}$C) solution of **19** (180 mg, 0.47 mmol), 3,5-$(CF_3)_2C_6H_3CH_2Br$ (284 mg, 0.94 mmol) and TBAI (260 mg, 0.71 mmol) in dry DMF under Ar was added NaH (20 mg, 60% dispersion in mineral oil, 0.50 mmol) in two portions over 5 min, stirring was continued for 30min, and the reaction was quenched with aq. $NH_4Cl$ followed by extraction with ether (3×15 mL). The combined organic layer was washed with water and brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography (EtOAc/Hexanes=1/12) to afford **20** (238 mg, 83%) as a white solid.

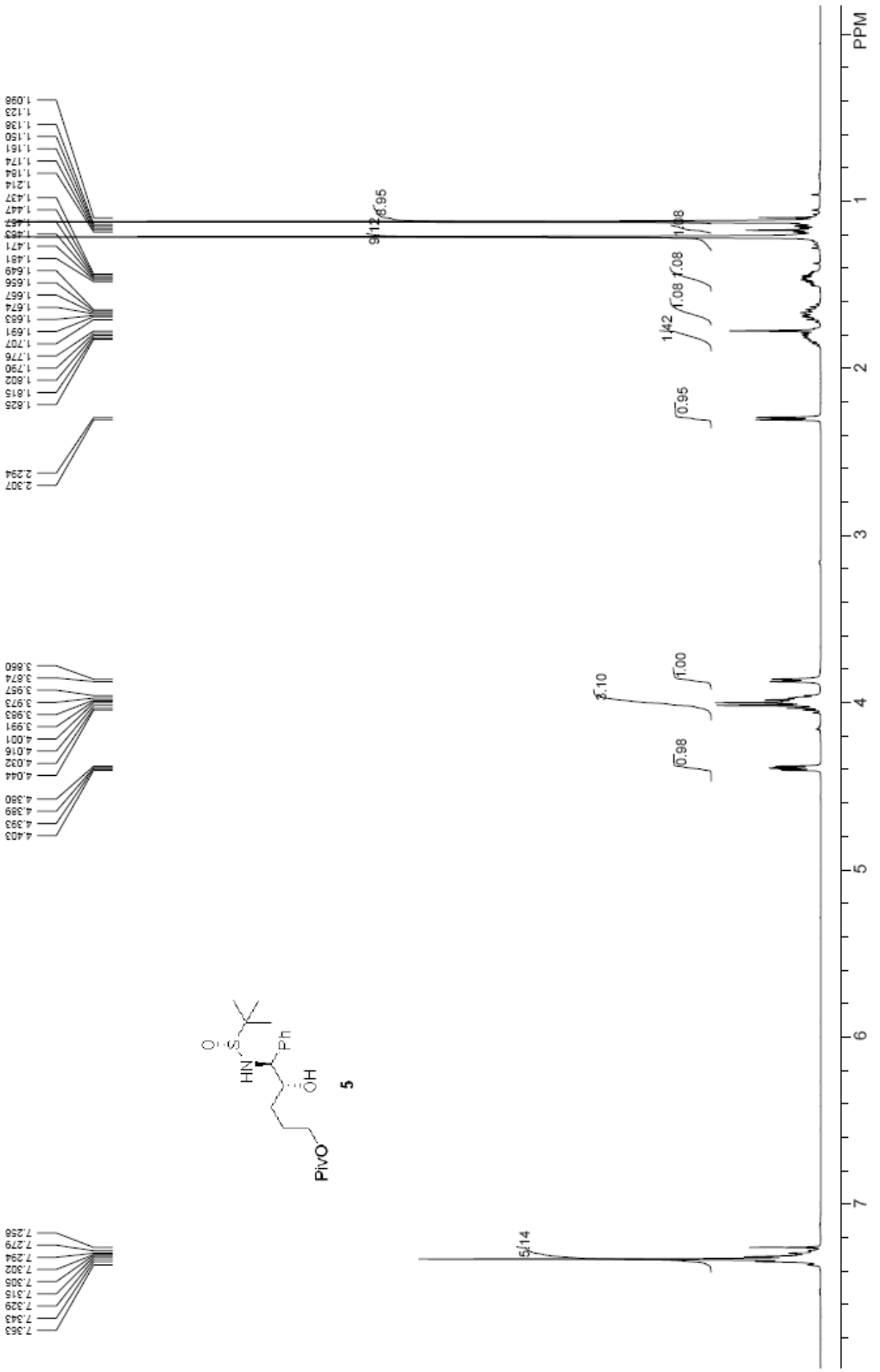
Mp. 61–62 $^{o}$C; $[\alpha]_D^{22}$ +14.1 (*c* 0.96, $CHCl_3$); $^{1}$H NMR ($CDCl_3$) $\delta$ 7.76 (br s, 1H), 7.52 (br s, 2H), 7.40-7.25 (m, 5H), 5.38 (br m, 1H), 4.86 (br m, 1H), 4.50-4.11 (AB, 2H, $J_{AB}$ = 11.7 Hz), 4.10 (t, 1H, *J* = 6.3 Hz), 3.71 (br m, 1H), 1.84-1.62 (m, 4H), 1.42 (br s, 9H), 1.20 (s, 9H); $^{13}$C NMR ($CDCl_3$) $\delta$ 178.5, 155.6, 140.9, 140.4, 131.6 (q, *J* = 32.9 Hz), 128.5, 127.6, 127.4, 126.2, 123.2 (q, *J* = 271 Hz), 121.6, 83.5, 79.8, 71.3, 63.8, 56.4, 38.7, 29.7, 28.3, 27.2, 25.1. ESI-MS *m/z* 628.3 (M + $Na^+$); HR-ESI-MS *m/z* Calcd for $C_{30}H_{37}F_6NO_5Na$ 628.2474, Found 628.2426.

Compound **21**:

To a solution of **20** (185 mg, 0.31 mmol) in MeOH (5 mL) under Ar was added 30% NaOMe in MeOH (0.11 mL, 0.62 mmol), the solution was stirred at rt for 4h, quenched by water, and extracted with $Et_2O$ (3×15 mL). The combined organic phase was washed with brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure to afford the crude product which was used in the next step without further purification.

To a cooled ($0^oC$) solution of the above crude alcohol and $Et_3N$ (0.07 mL, 0.5 mmol) in $CH_2Cl_2$ (10 mL) was added dropwise MsCl (0.03 mL, 0.45 mmol), and the mixture was stirred at $0^oC$ for 30min, diluted with $Et_2O$ (30 mL), and washed successively with 1M HCl, saturated aq. $NaHCO_3$ and brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was dissolved in THF (10 mL) under Ar, NaH (50 mg, 60% dispersion in mineral oil, 1.25 mmol) was added and the mixture was stirred at rt for 2 days, quenched by saturated aq. $NH_4Cl$, extracted with $Et_2O$ (3×15 mL), and washed with brine, dried ($Na_2SO_4$), filtered and concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography (EtOAc/Hexanes=1/16) to afford **21** (118 mg, 77%) as a colorless oil.

$[\alpha]_D^{22}$ +45.1 (*c* 0.68, $CHCl_3$); $^1$H NMR ($CDCl_3$) $\delta$ 7.77 (br s, 1H), 7.71 (br s, 2H), 7.56 (br s, 1H), 7.54 (br s, 1H), 7.36-7.23 (m, 3H), 5.69 (br s, 1H), 4.73 (AB, 2H, $J_{AB}$= 12.9 Hz), 3.95 (dd, 1H, *J* = 12.9, 3.6 Hz), 3.94-3.84 (m, 1H), 2.76 (ddd, 1H, *J* = 12.6, 12.6, 3.5 Hz), 2.04-1.94 (m, 2H), 1.78-1.58 (m, 2H), 1.46 (s, 9H); $^{13}$C NMR ($CDCl_3$) $\delta$ 155.2, 141.0, 138.0, 131.6 (q, *J* = 32.8 Hz), 128.3, 127.2, 127.0, 123.2 (q, *J* = 271 Hz), 121.4 (m), 80.1, 78.7, 69.1, 55.5, 39.2, 28.4, 25.8, 24.1. ESI-MS *m/z* 526.1 (M + $Na^+$); HR-ESI-MS *m/z* Calcd for $C_{25}H_{28}F_6NO_3$ (M + $H^+$) 504.1973, Found 504.1949.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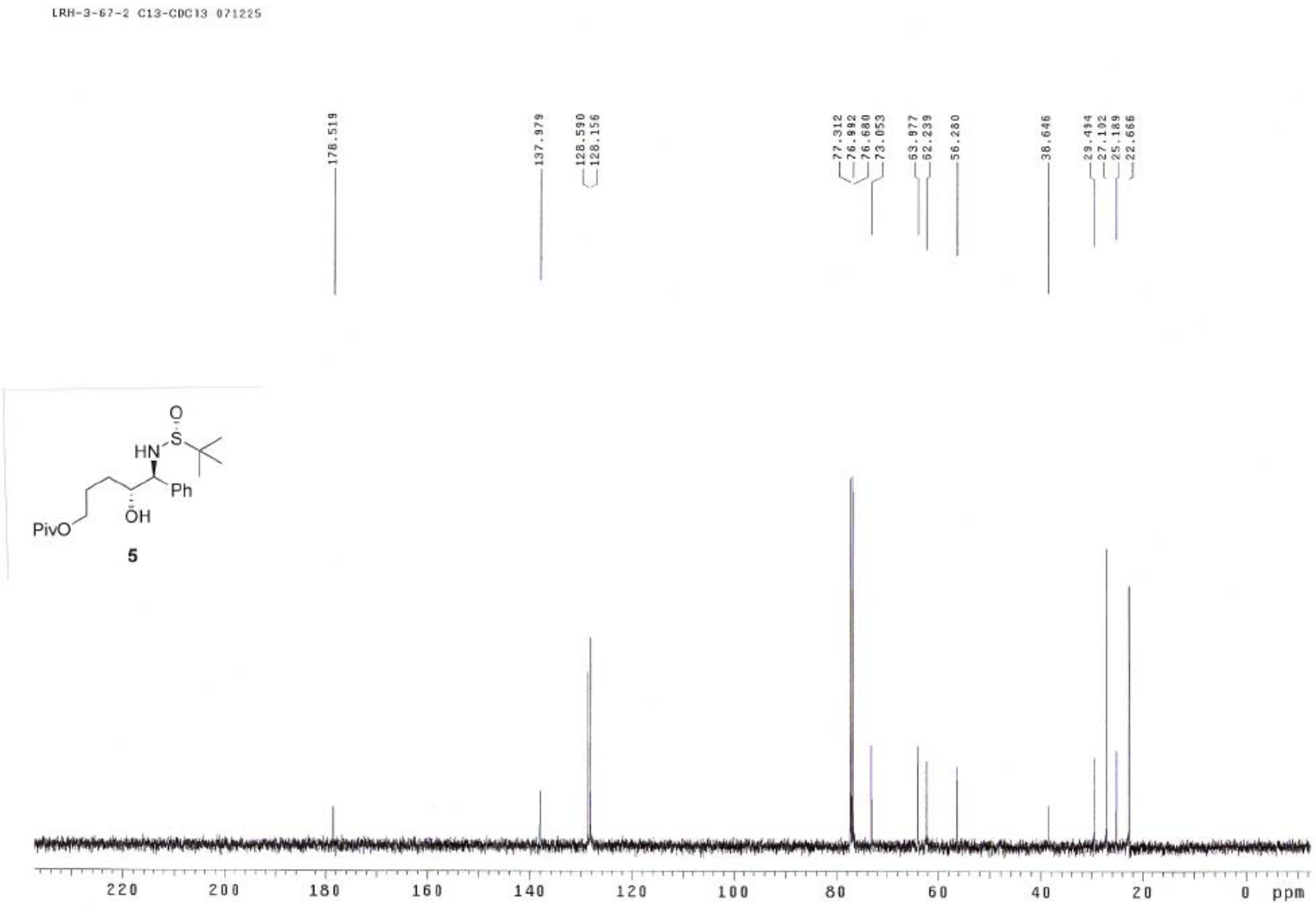
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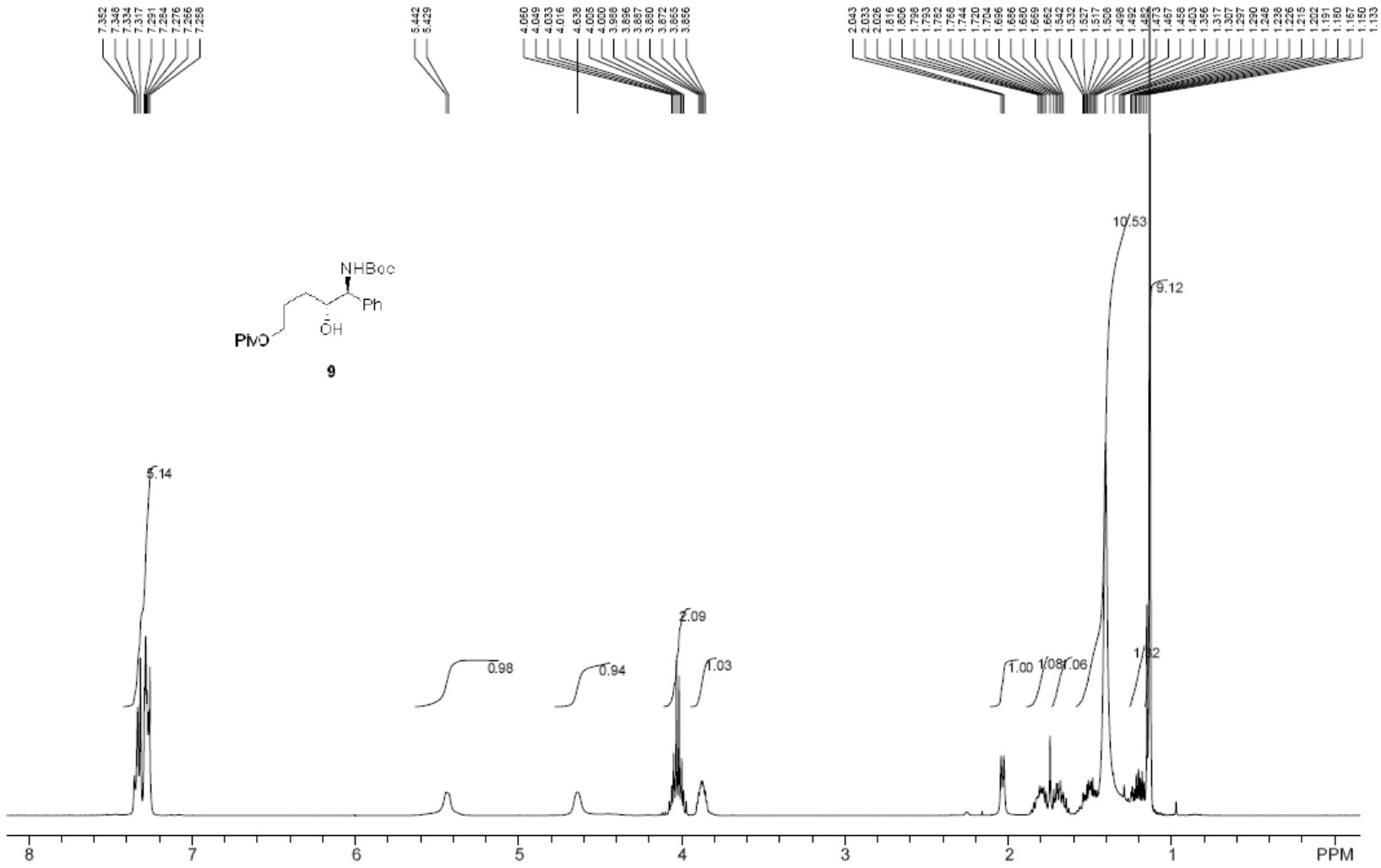
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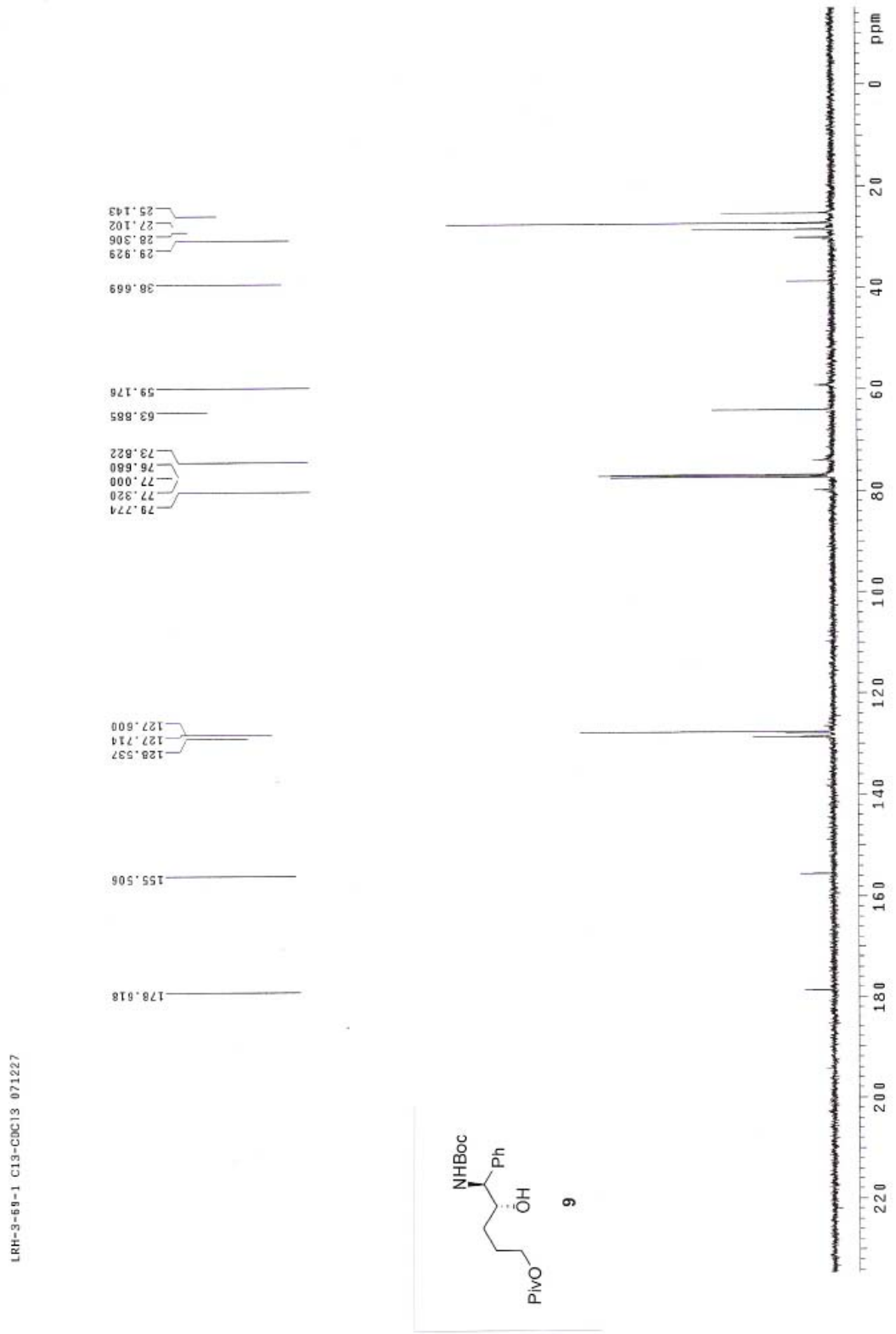
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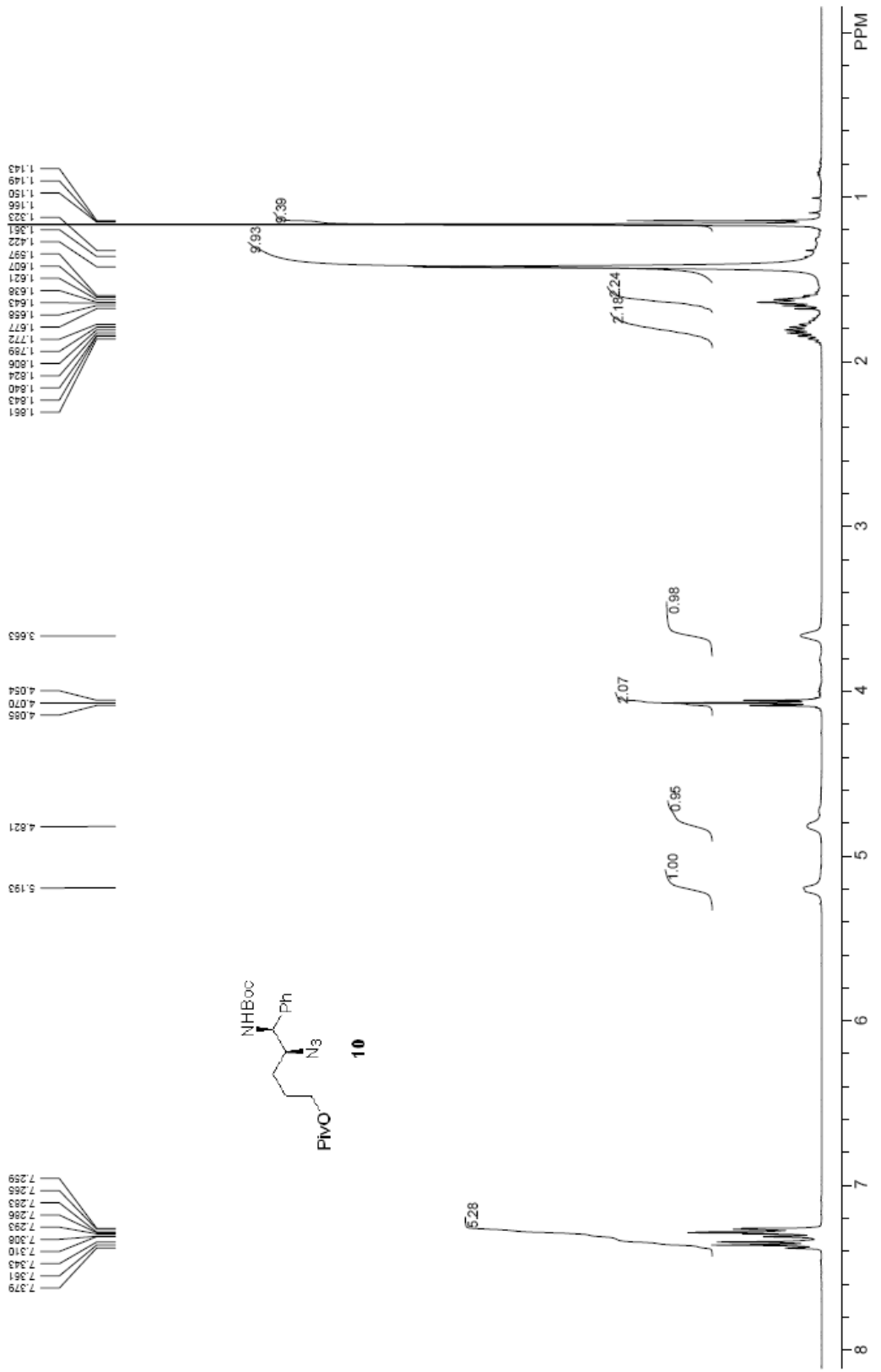
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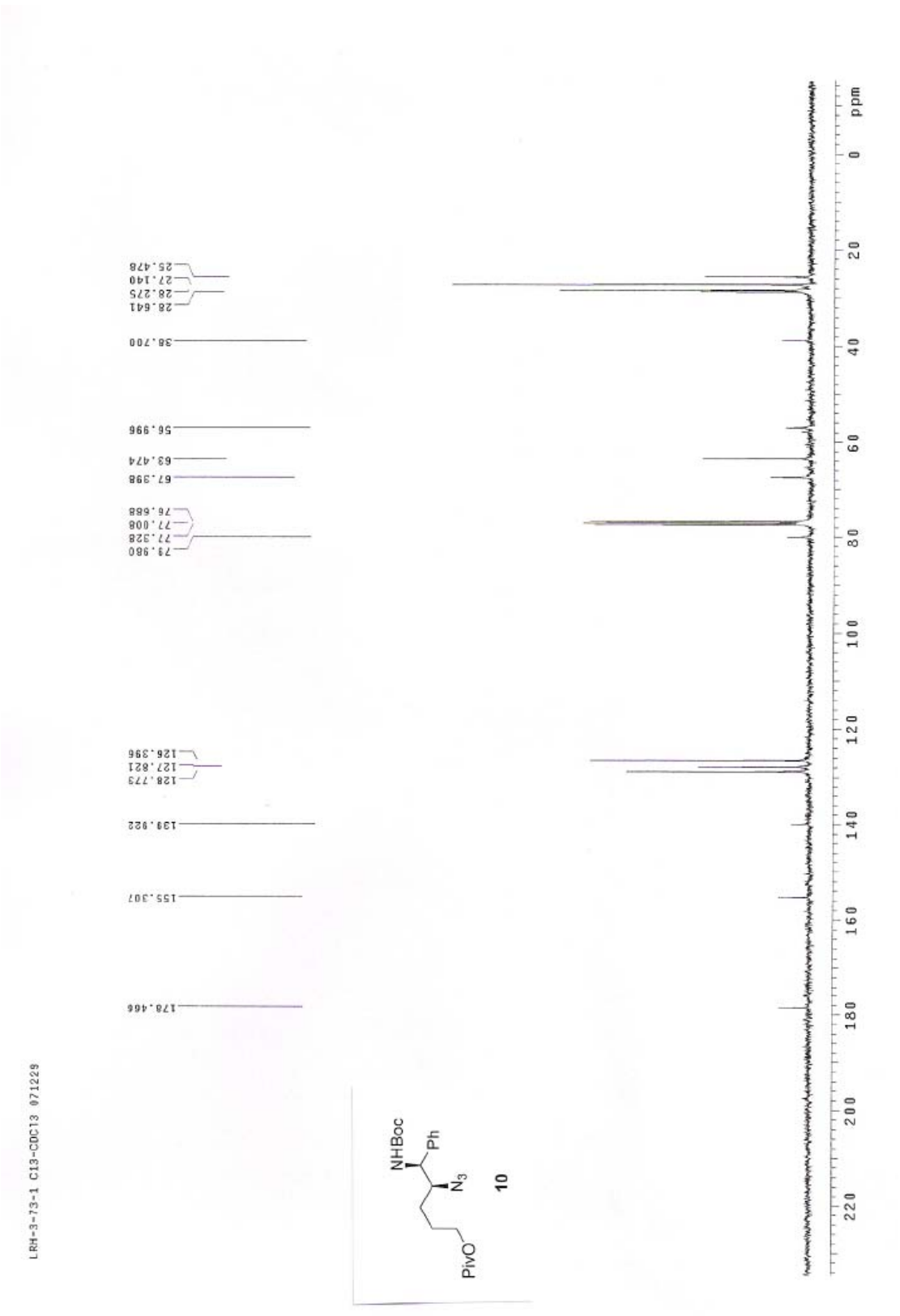
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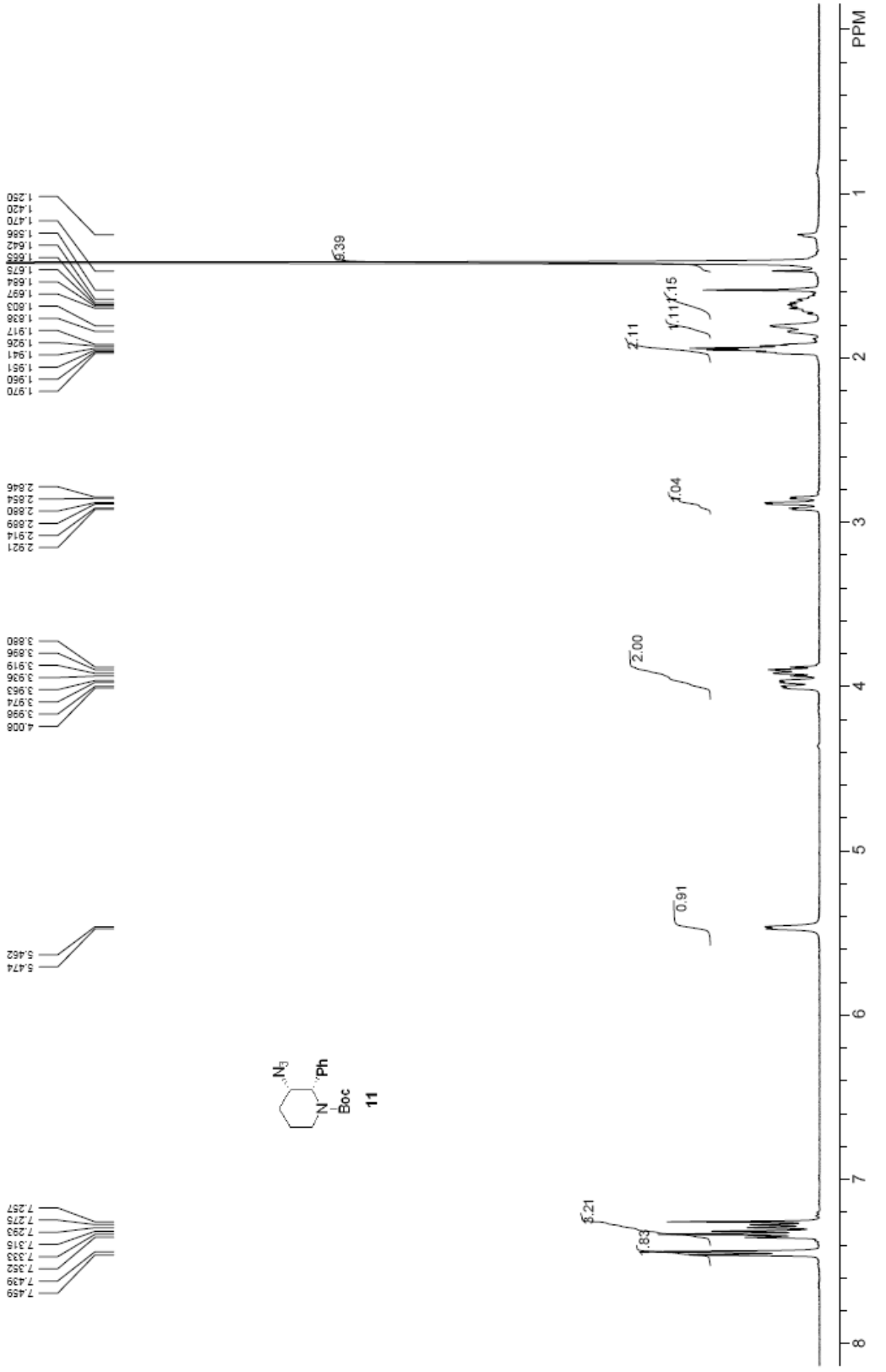
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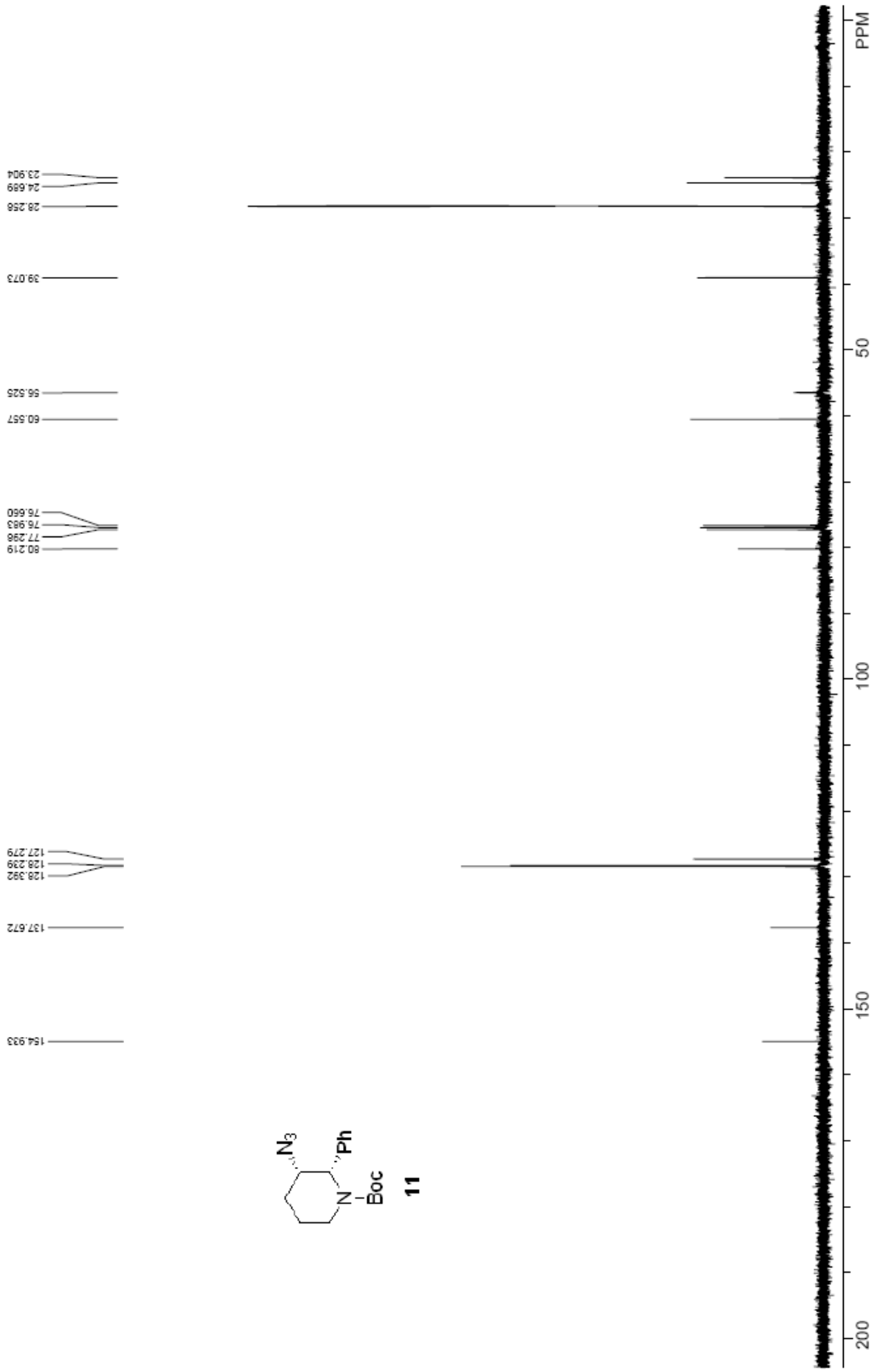
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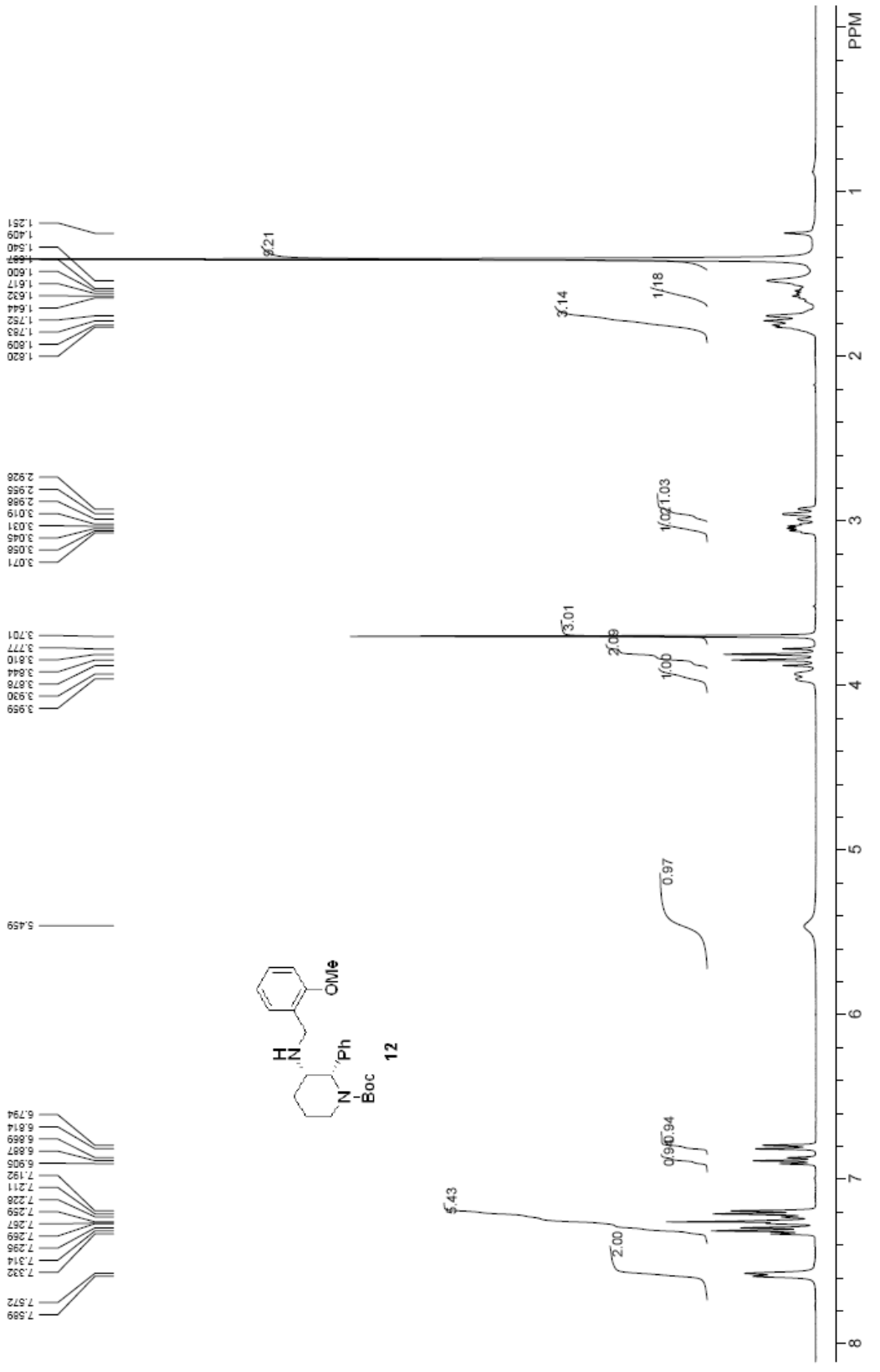
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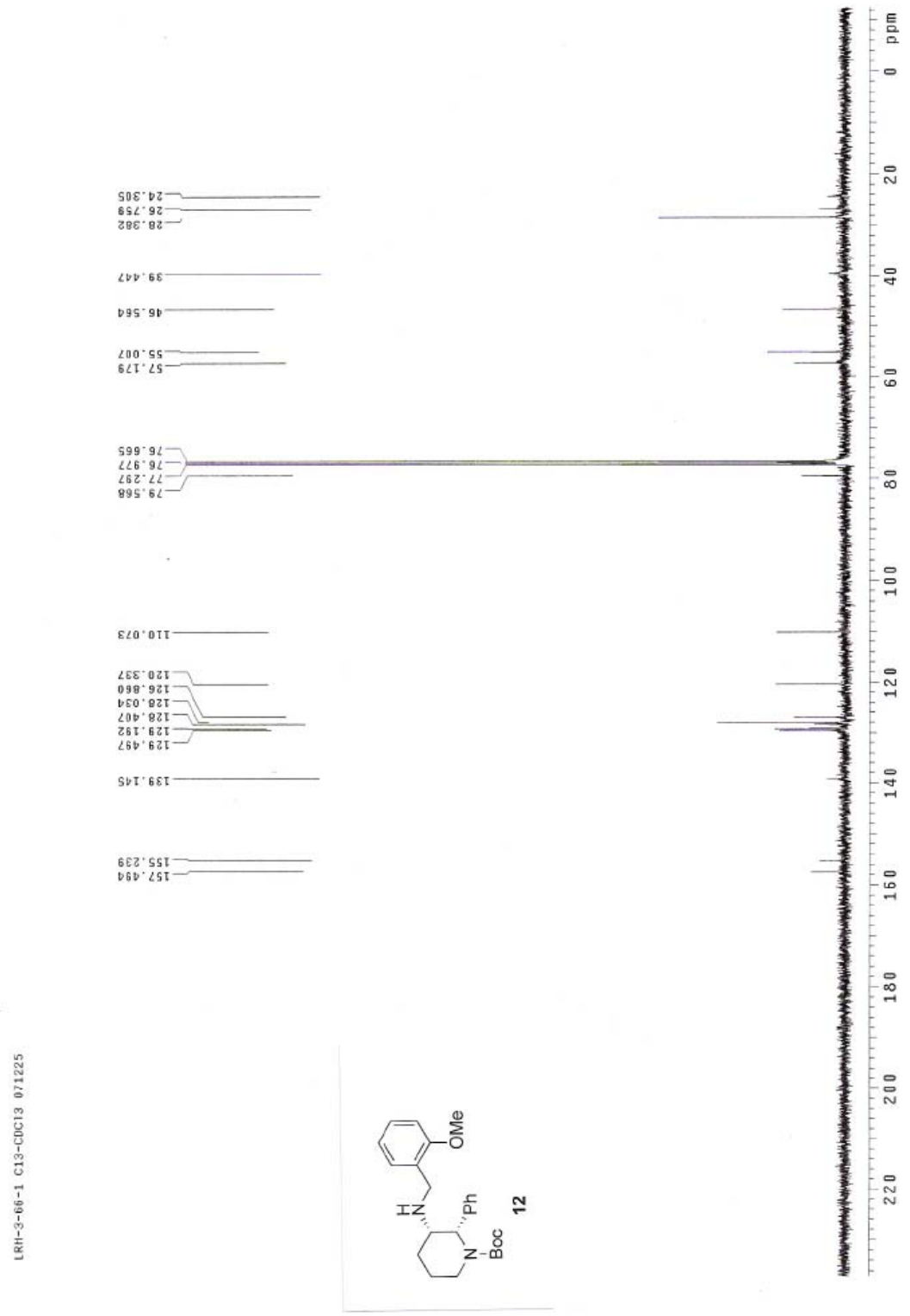
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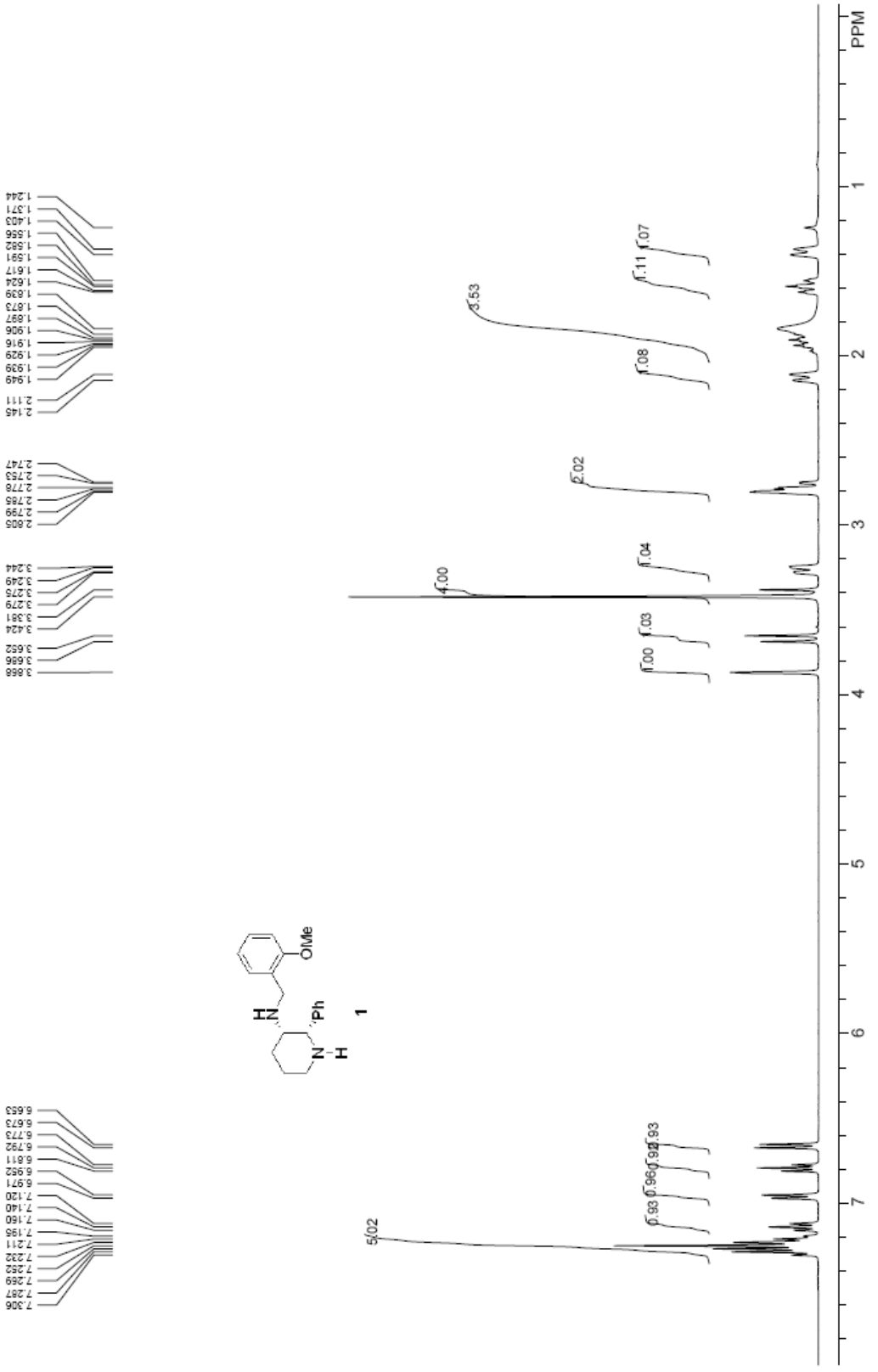
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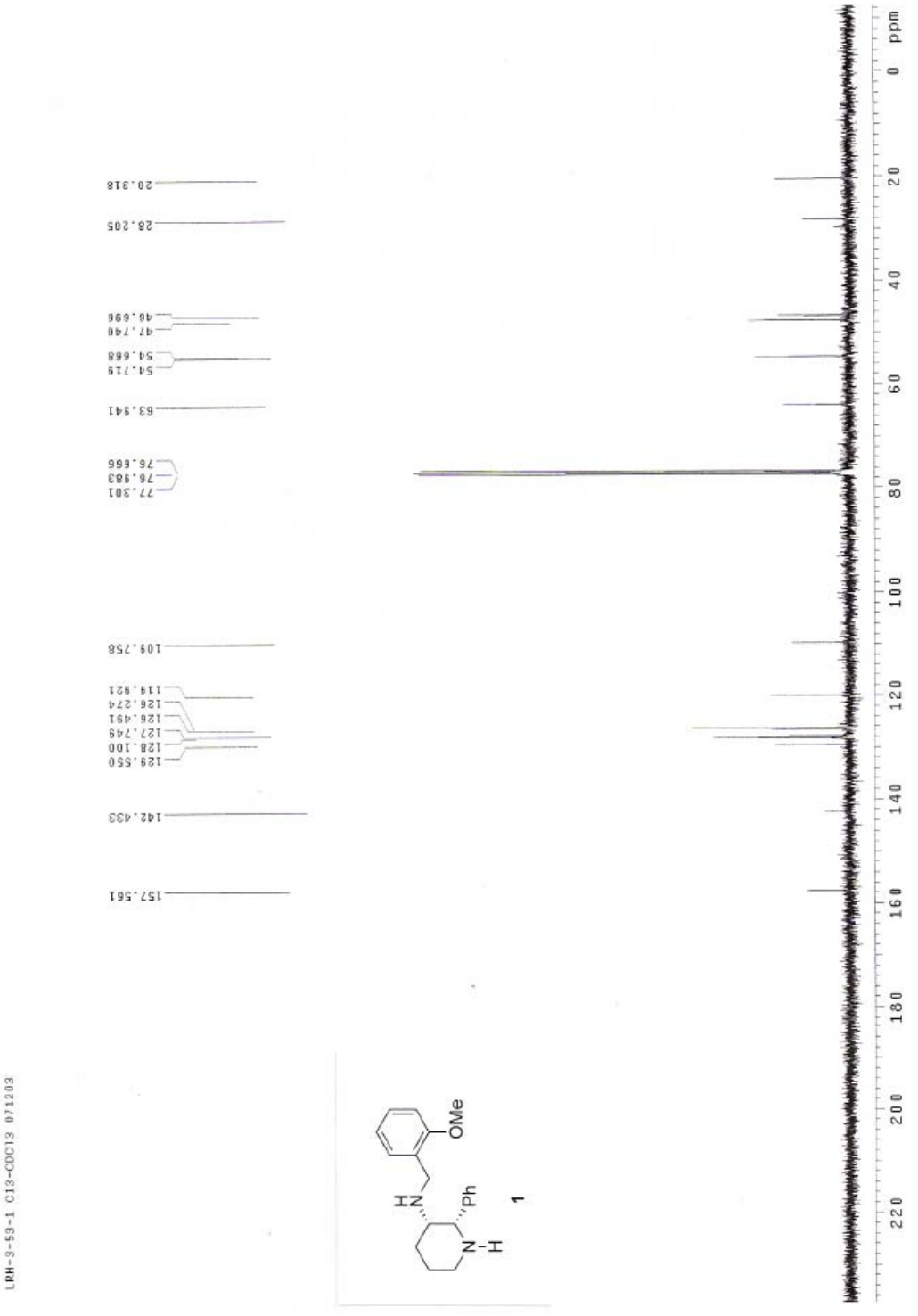
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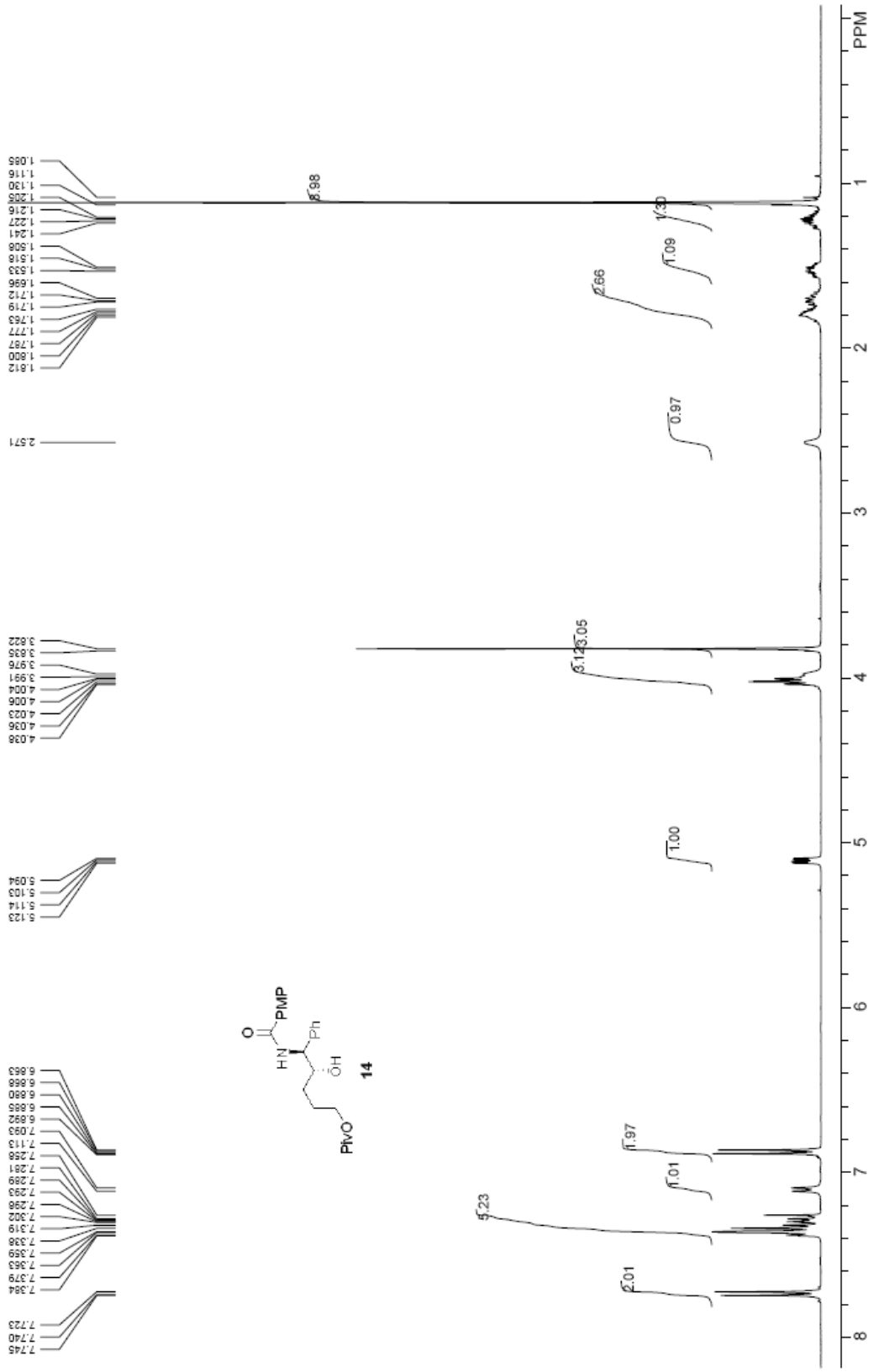
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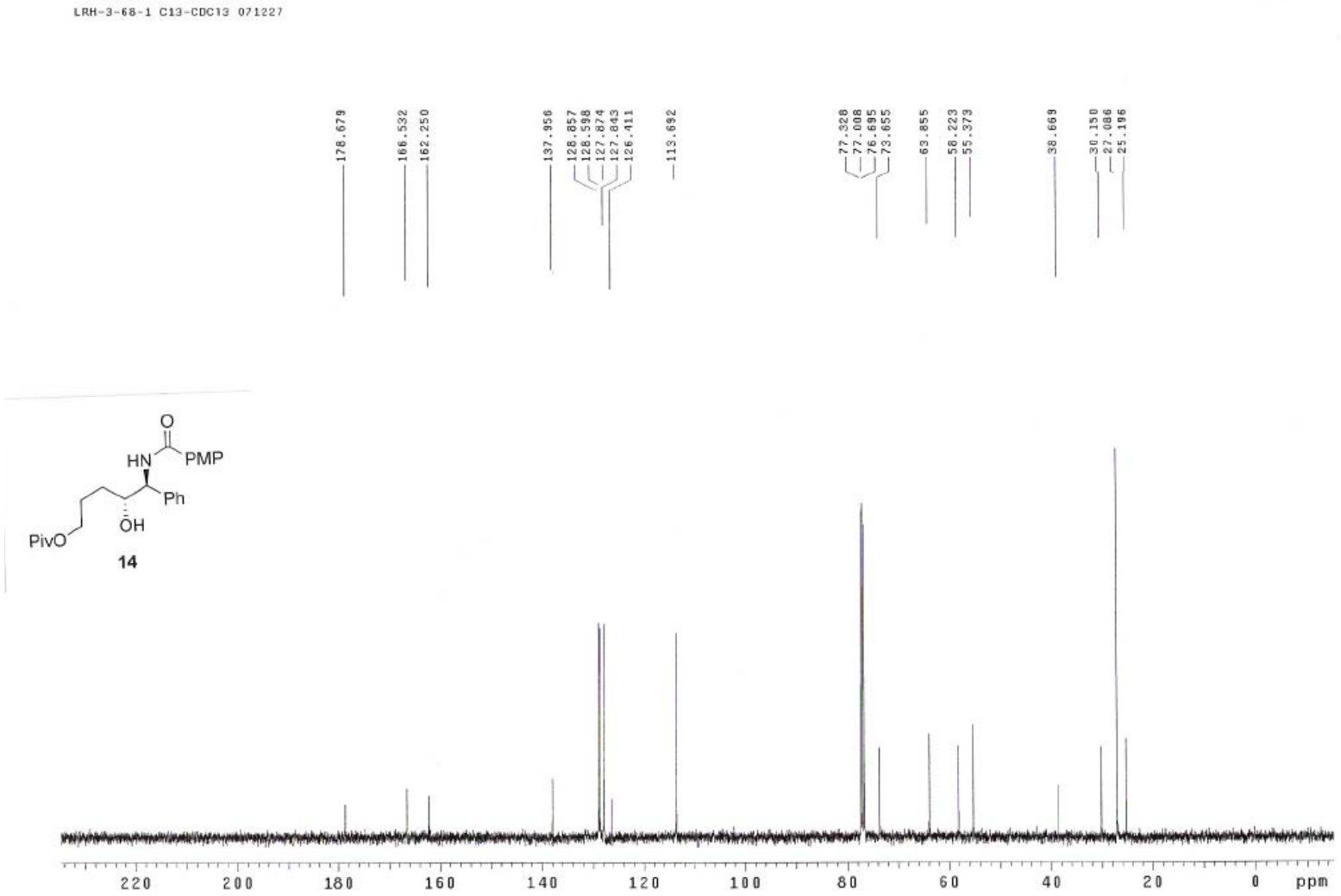
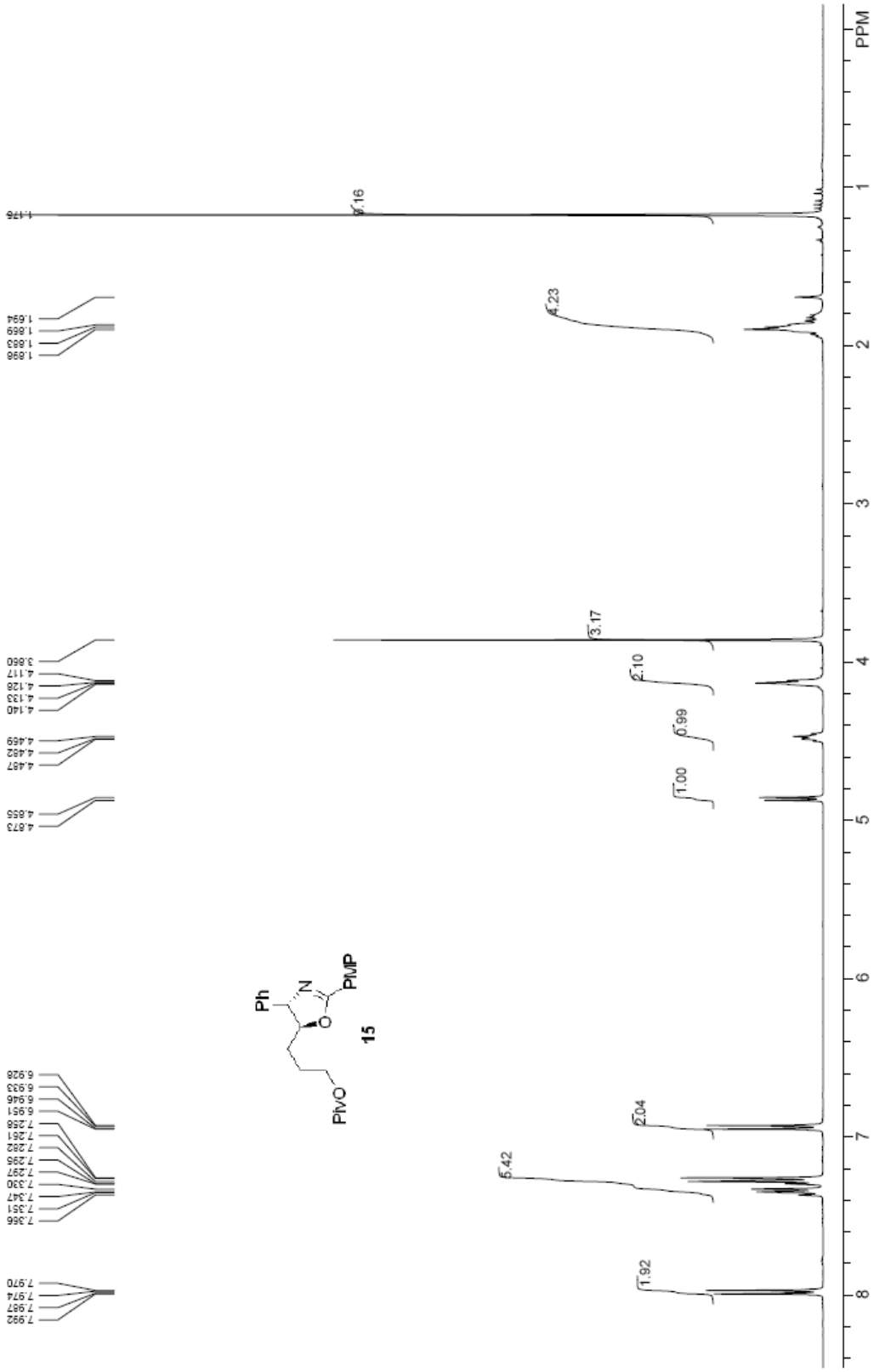
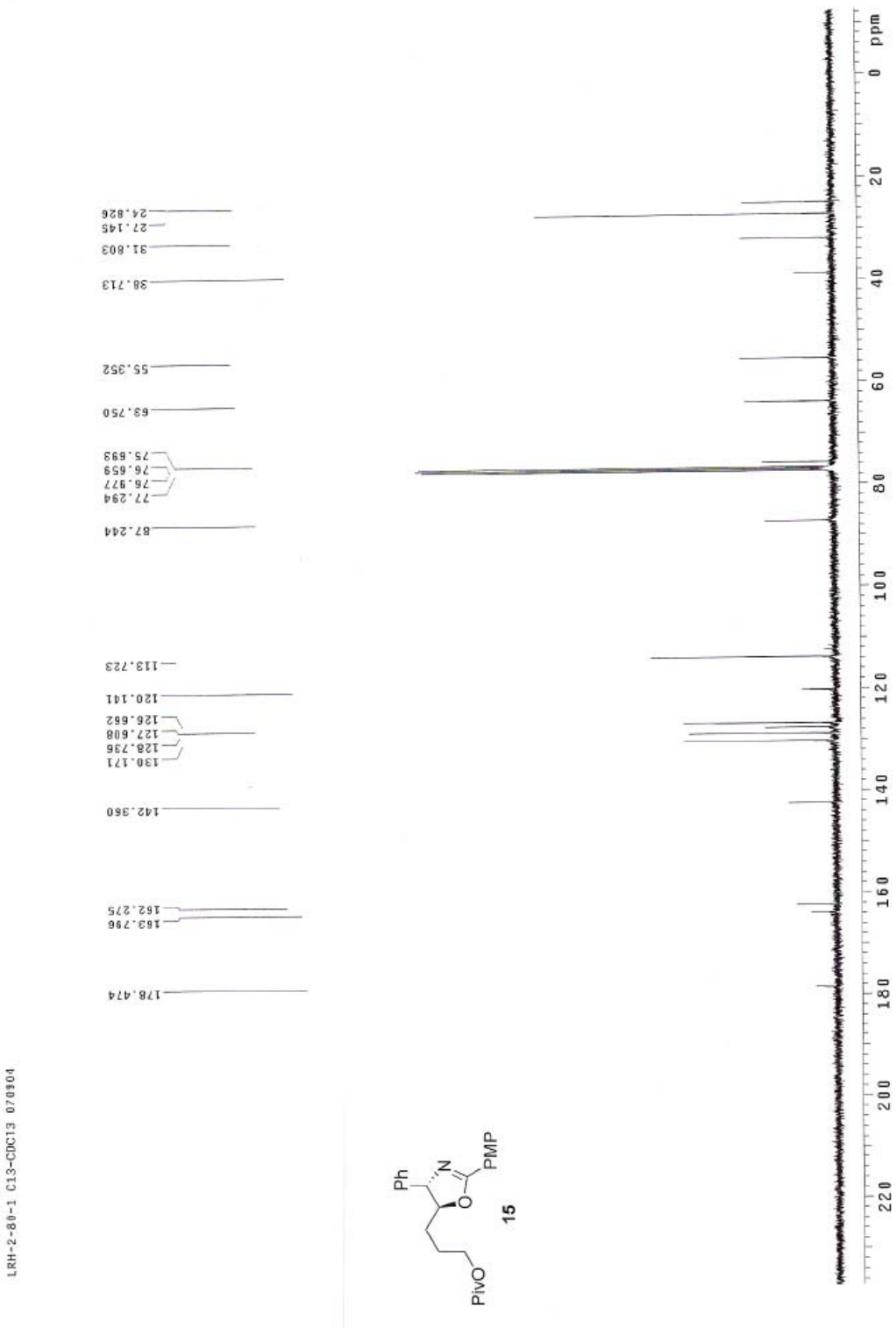
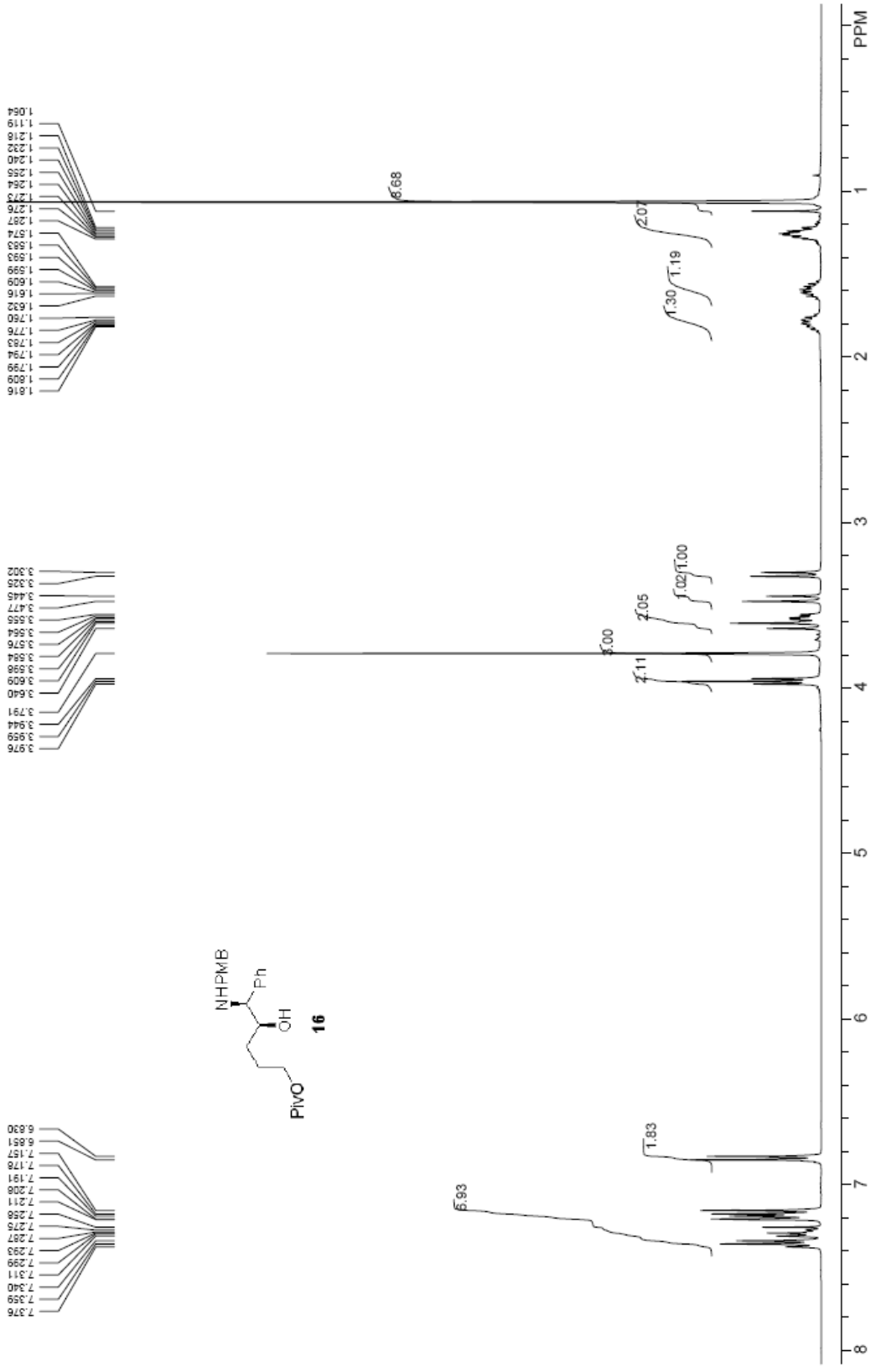
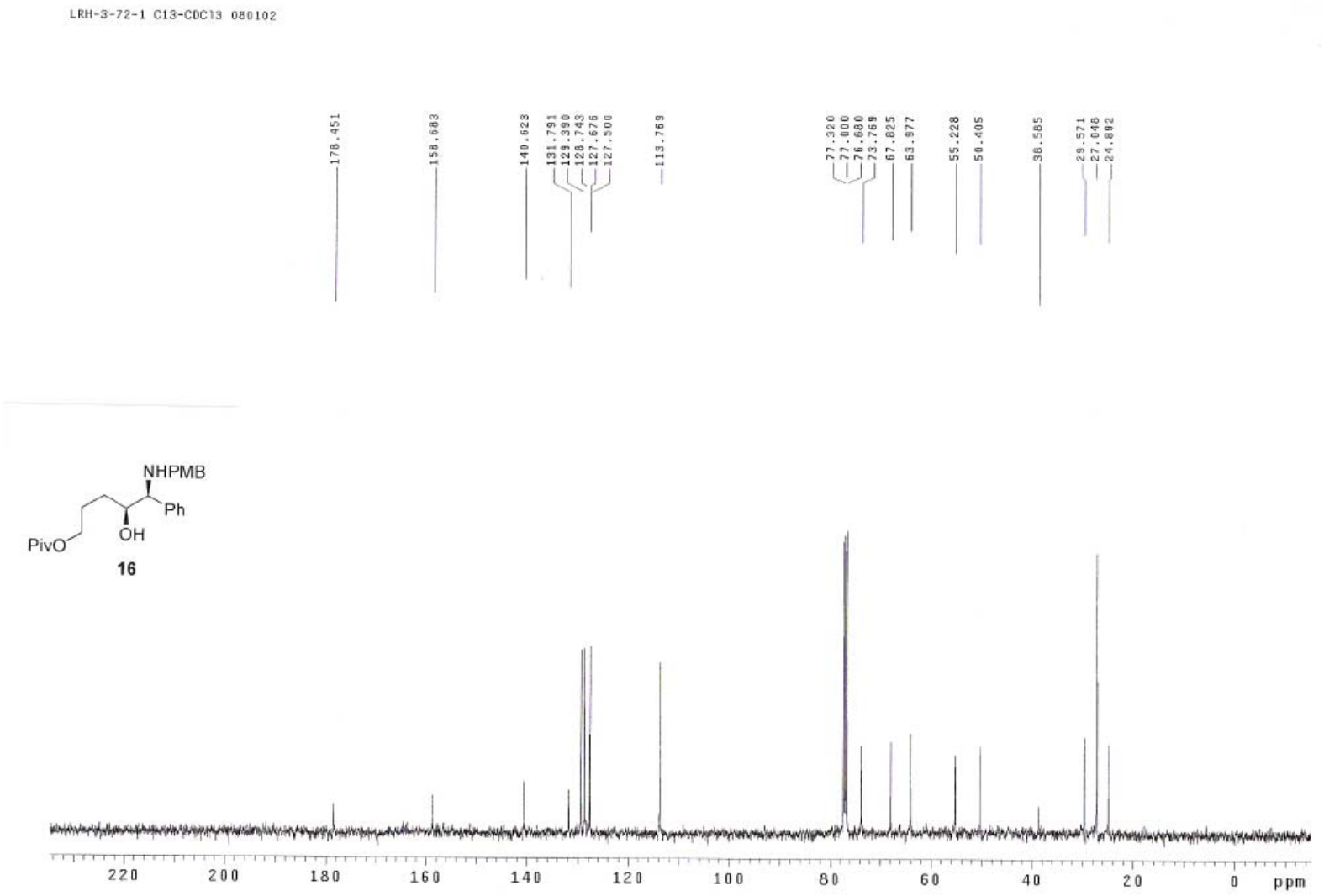
14
PPM

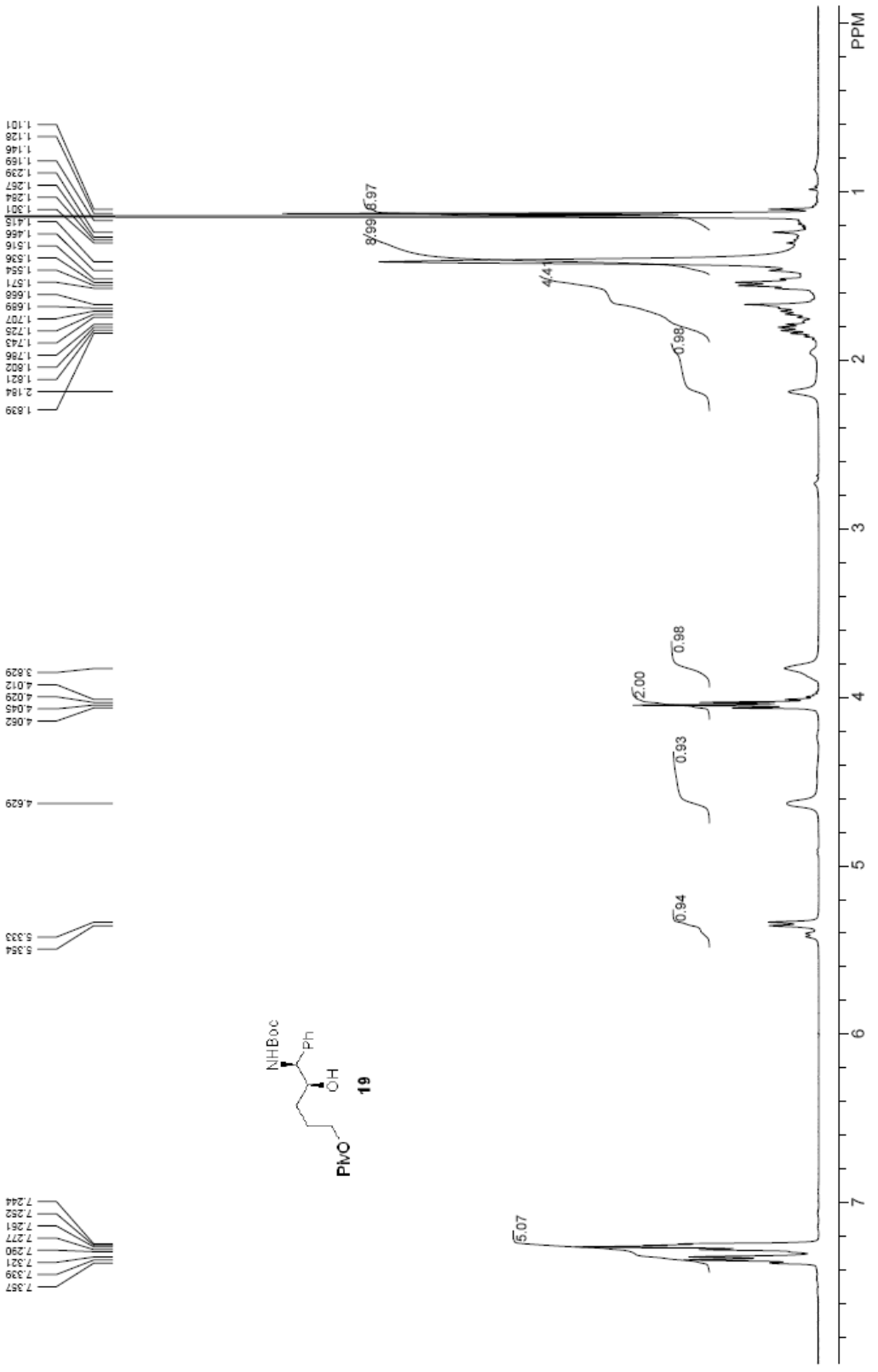

LRH-3-68-1 C13-CDCl3 071227
178.679
166.532
162.250
137.956
128.857
128.598
127.874
127.843
126.411
113.682
77.328
77.008
76.695
73.655
63.855
58.223
55.373
38.669
30.150
27.086
25.196
O
HN
PMP
Ph
OH
PivO
14
220
200
180
160
140
120
100
80
60
40
20
0
ppm

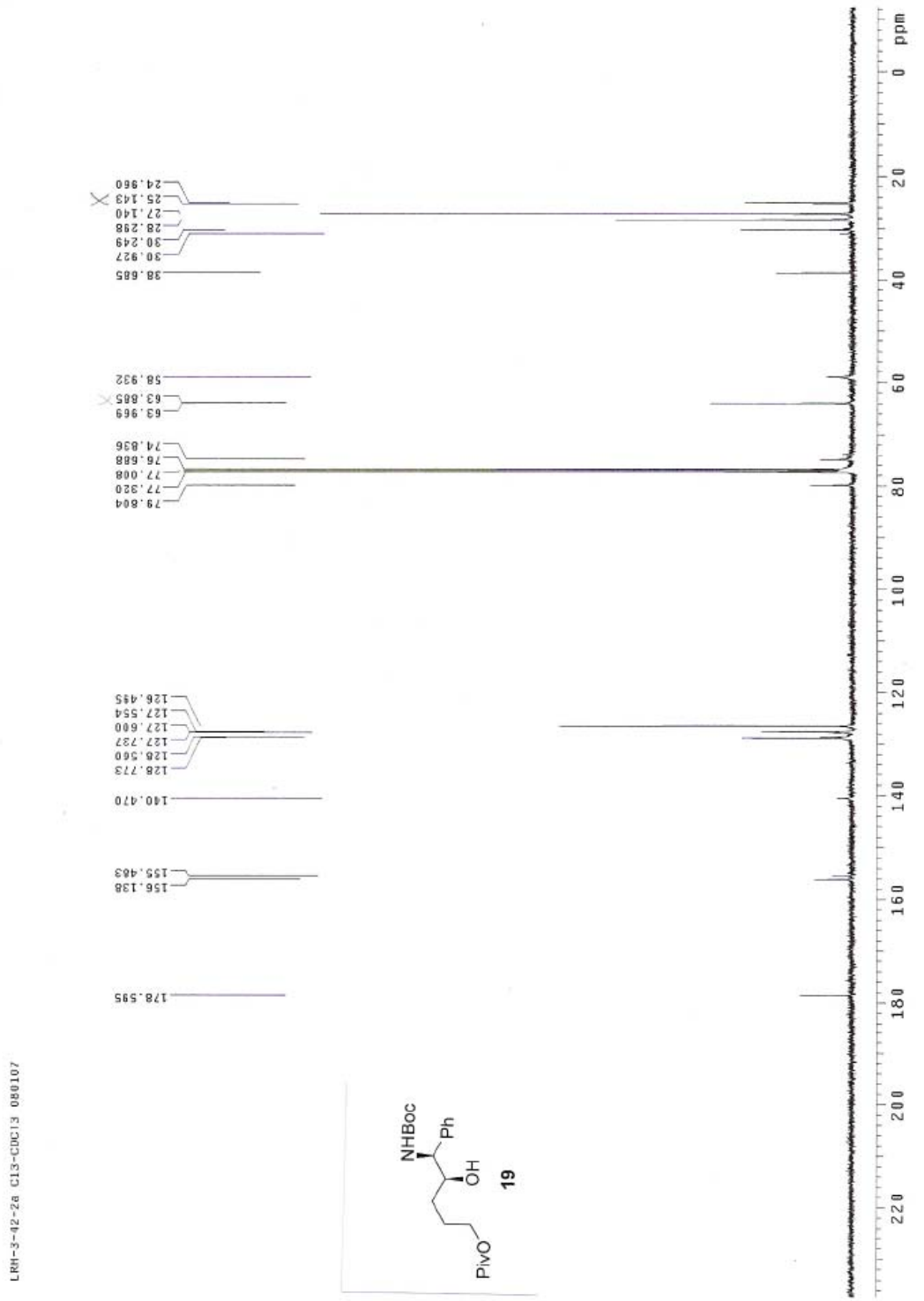

PPM
1
2
3
4
5
6
7
8
9.16
4.23
3.17
2.10
0.99
1.00
2.04
5.42
1.92
1.726
1.896
1.883
1.869
1.694
3.860
4.117
4.126
4.133
4.140
4.487
4.482
4.469
4.873
4.855
7.992
7.987
7.974
7.970
7.366
7.351
7.347
7.330
7.297
7.296
7.282
7.261
7.256
6.951
6.946
6.933
6.928
Ph
N
O
PMP
PivO
15

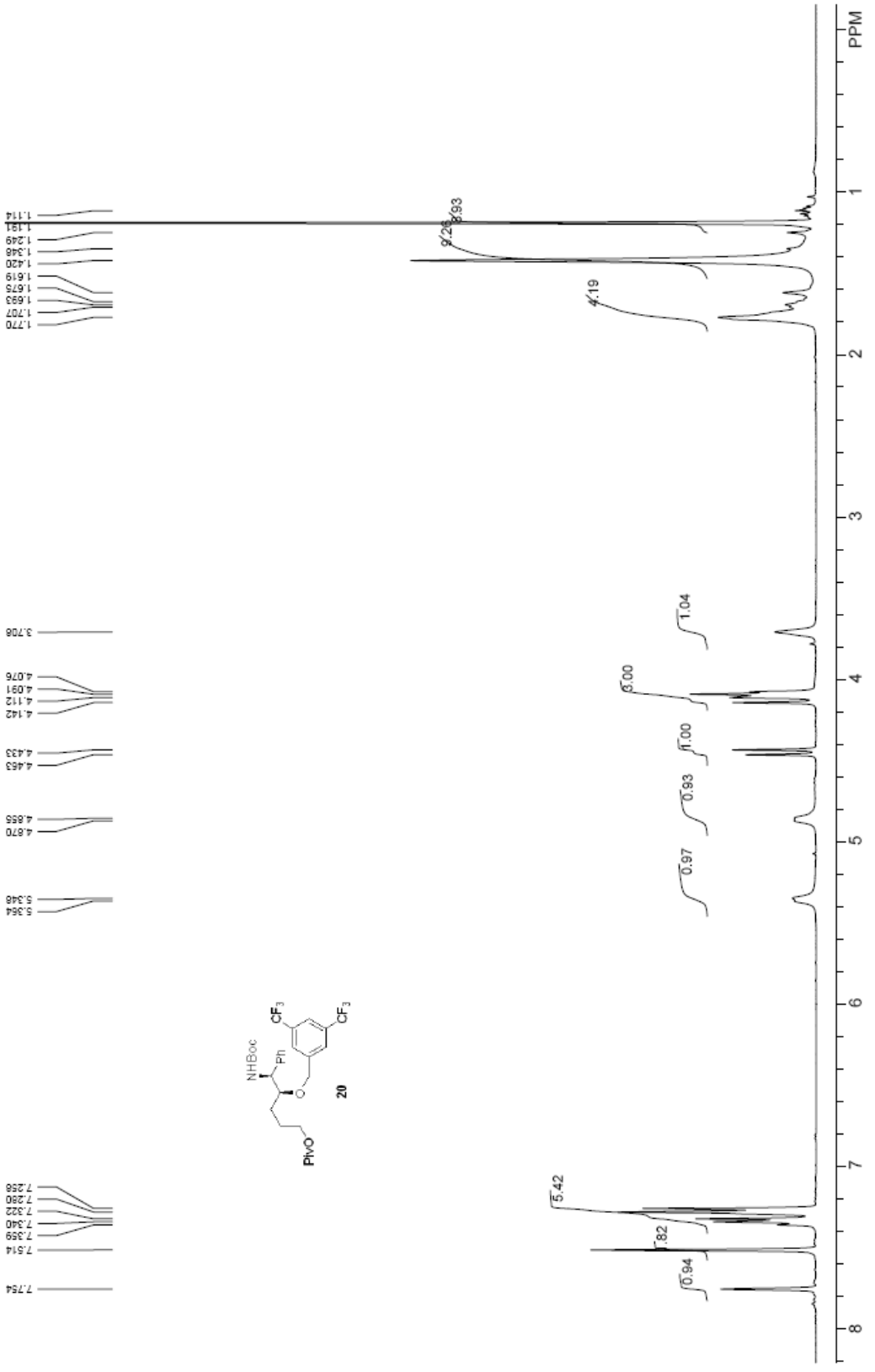

LRH-2-80-1 C13-CDCl3 070304
178.474
163.796
162.275
142.360
130.171
128.736
127.608
126.662
120.141
113.723
87.244
77.294
76.977
76.659
75.693
63.750
55.352
38.713
31.803
27.145
24.828
0 ppm
Ph
N
O
PMP
PivO
15

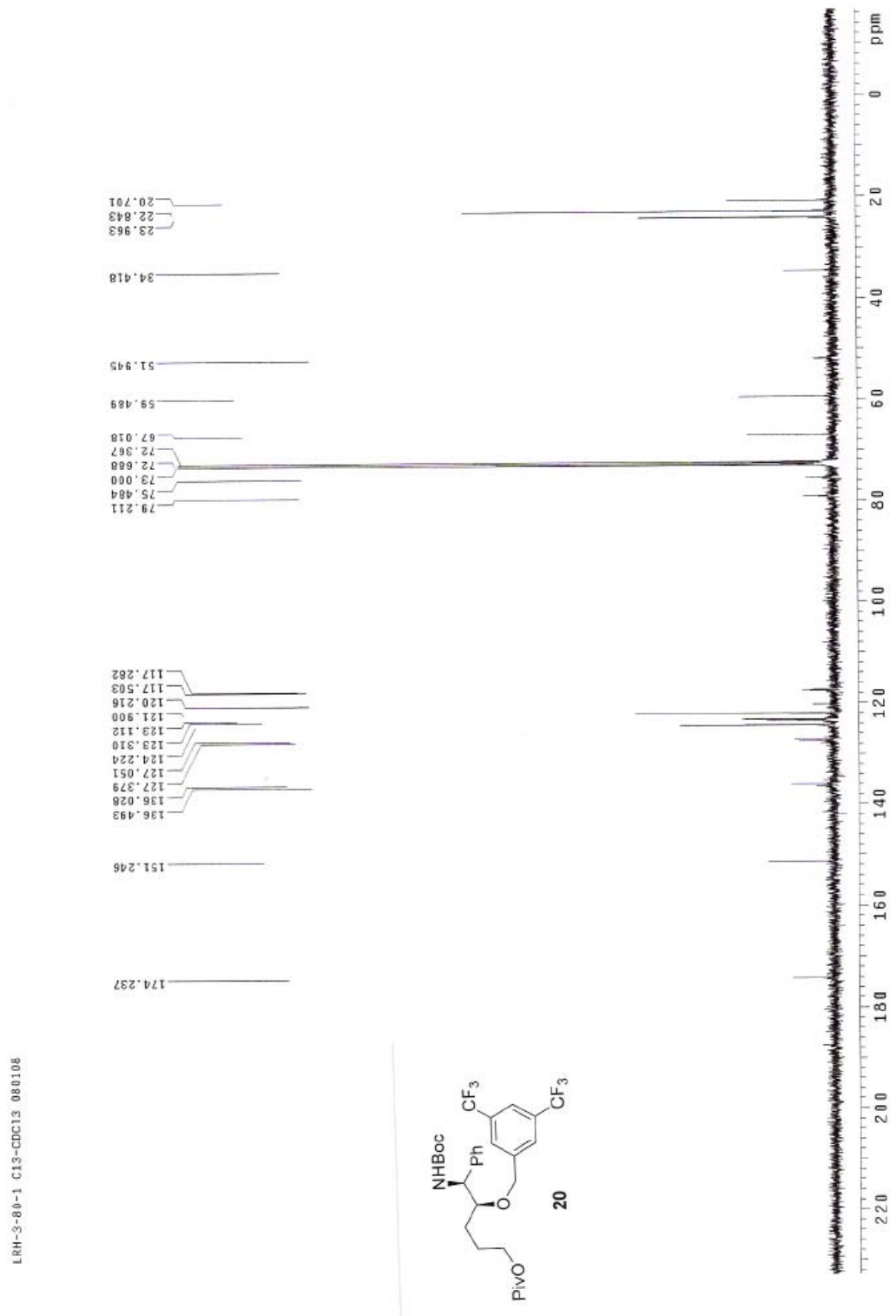

NHPMB
Ph
OH
PivO
16
PPM
6.68
2.07
1.19
1.30
3.00
2.05
1.02
1.00
2.11
1.83
6.93

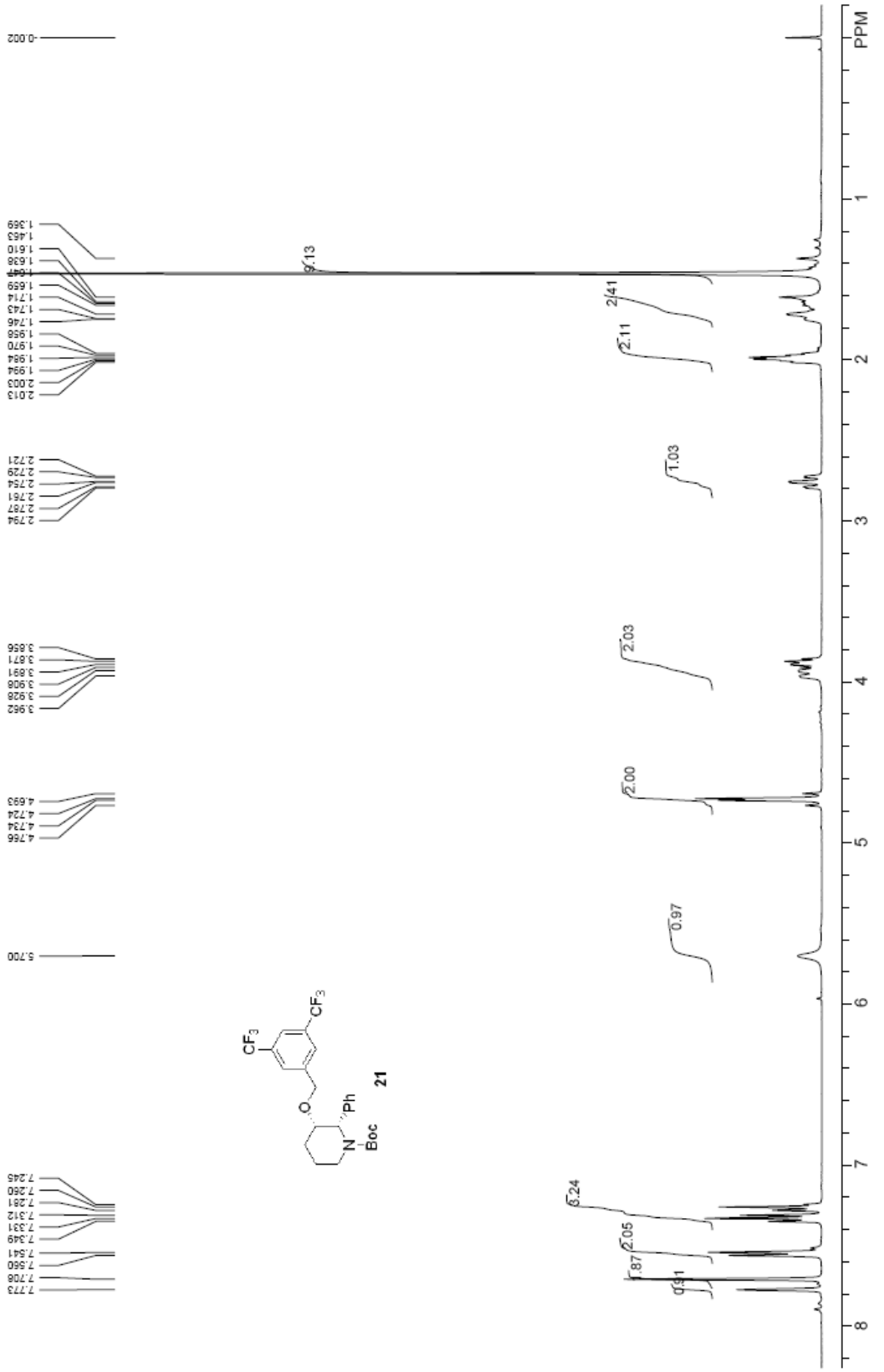

LRH-3-72-1 C13-CDCl3 080102
178.451
158.683
140.623
131.791
129.390
128.743
127.676
127.500
113.769
77.320
77.000
76.680
73.769
67.825
63.977
55.228
50.405
36.585
29.571
27.048
24.892
NHPMB
Ph
OH
PivO
16
220
200
180
160
140
120
100
80
60
40
20
0
ppm

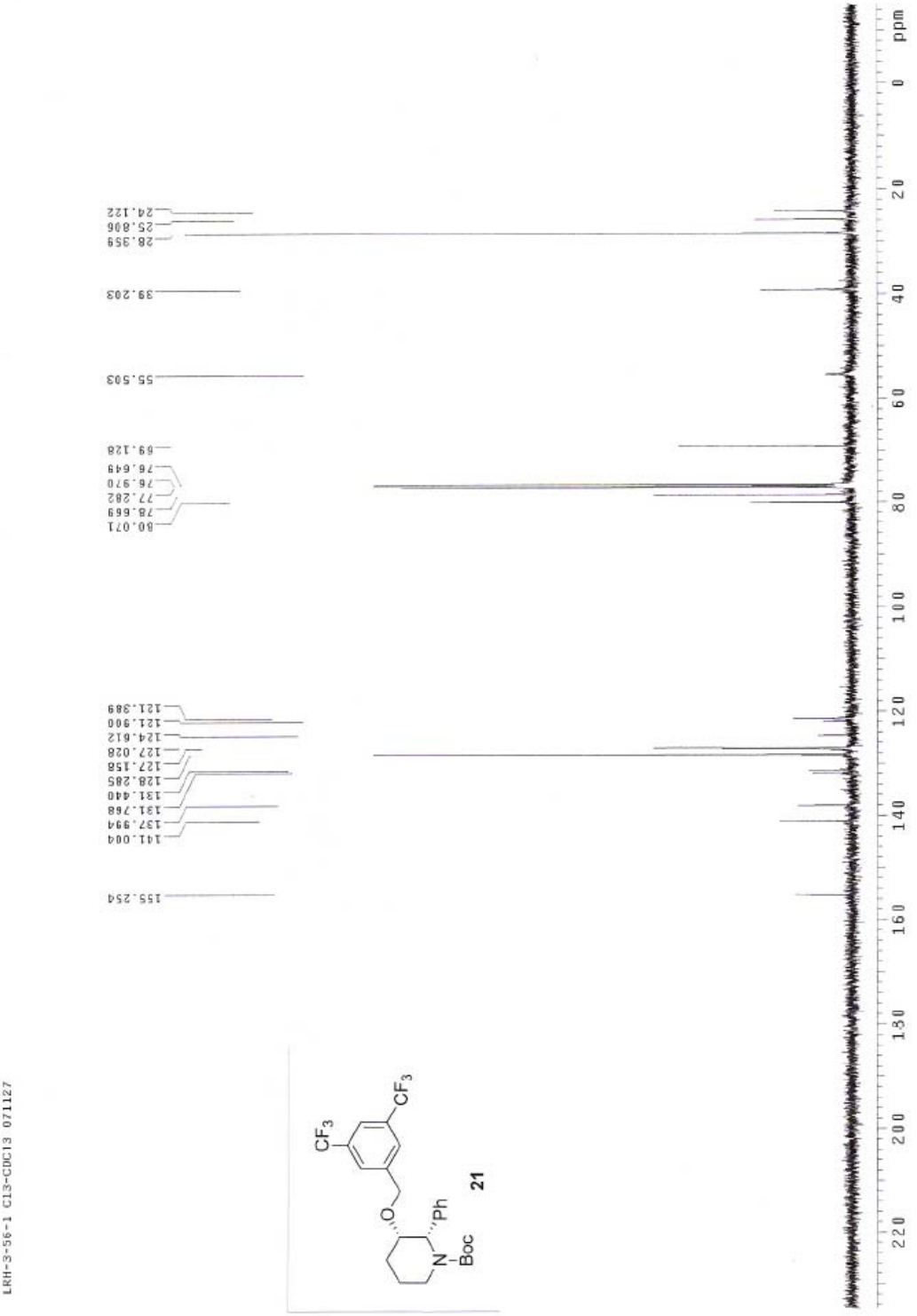

PPM
1 2 3 4 5 6 7
6.07
0.94
0.93
2.00
0.98
0.98
4.41
8.99
6.97
NHBoc
Ph
OH
PMO
19
7.357
7.339
7.321
7.290
7.277
7.261
7.252
7.244
5.354
5.333
4.629
4.062
4.045
4.029
4.012
3.829
1.839
2.184
1.821
1.802
1.786
1.743
1.725
1.707
1.689
1.668
1.571
1.554
1.536
1.516
1.466
1.415
1.301
1.284
1.267
1.239
1.169
1.146
1.128
1.101

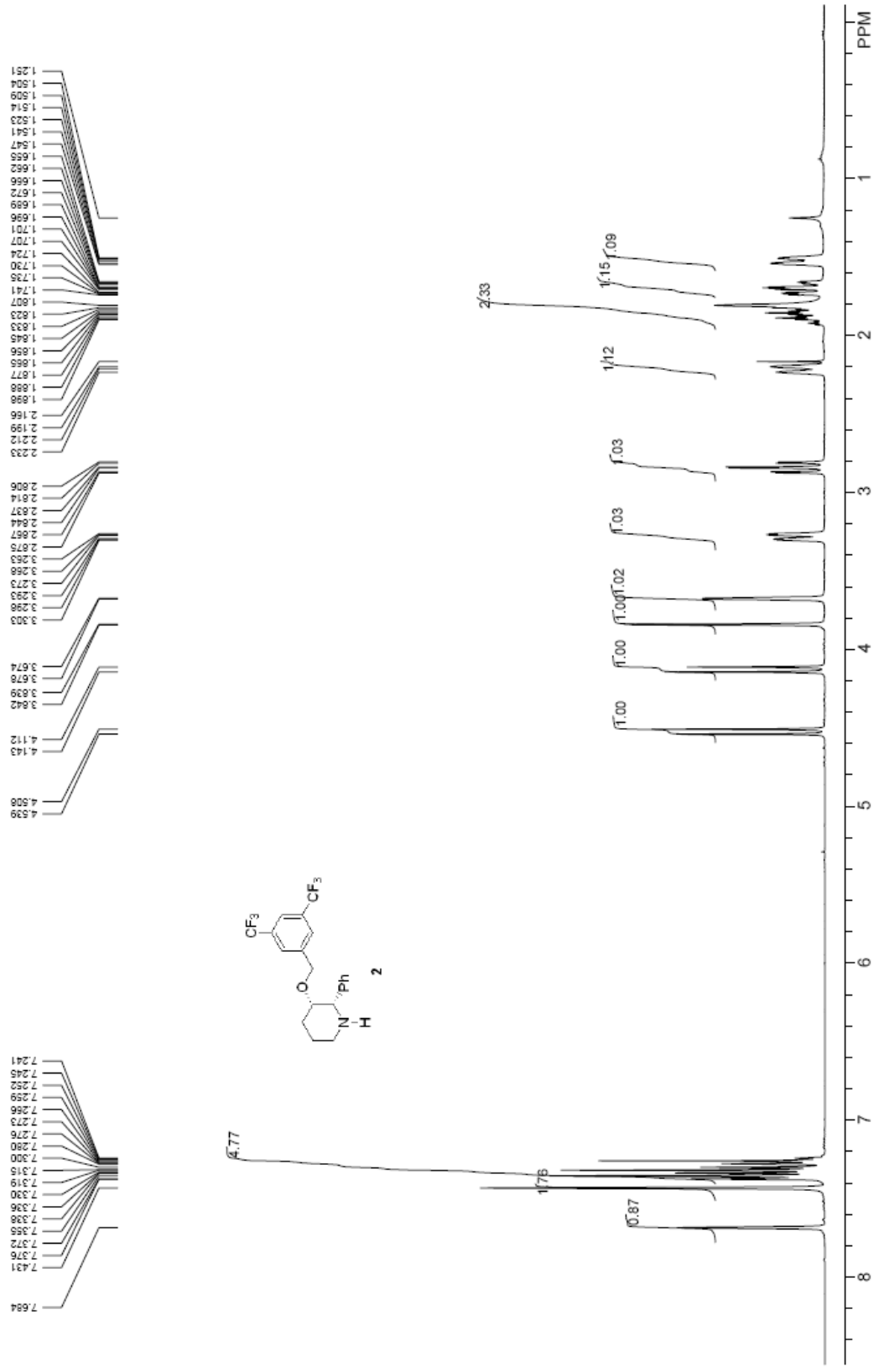

LRM-3-42-2a C13-CDCl3 080107
178.595
156.138
155.463
140.470
128.773
128.560
127.737
127.600
127.554
126.485
79.804
77.320
77.008
76.688
74.836
63.969
63.885
58.932
38.685
30.927
30.249
28.298
27.140
25.143
24.960
NHBoc
Ph
OH
PivO
19
ppm

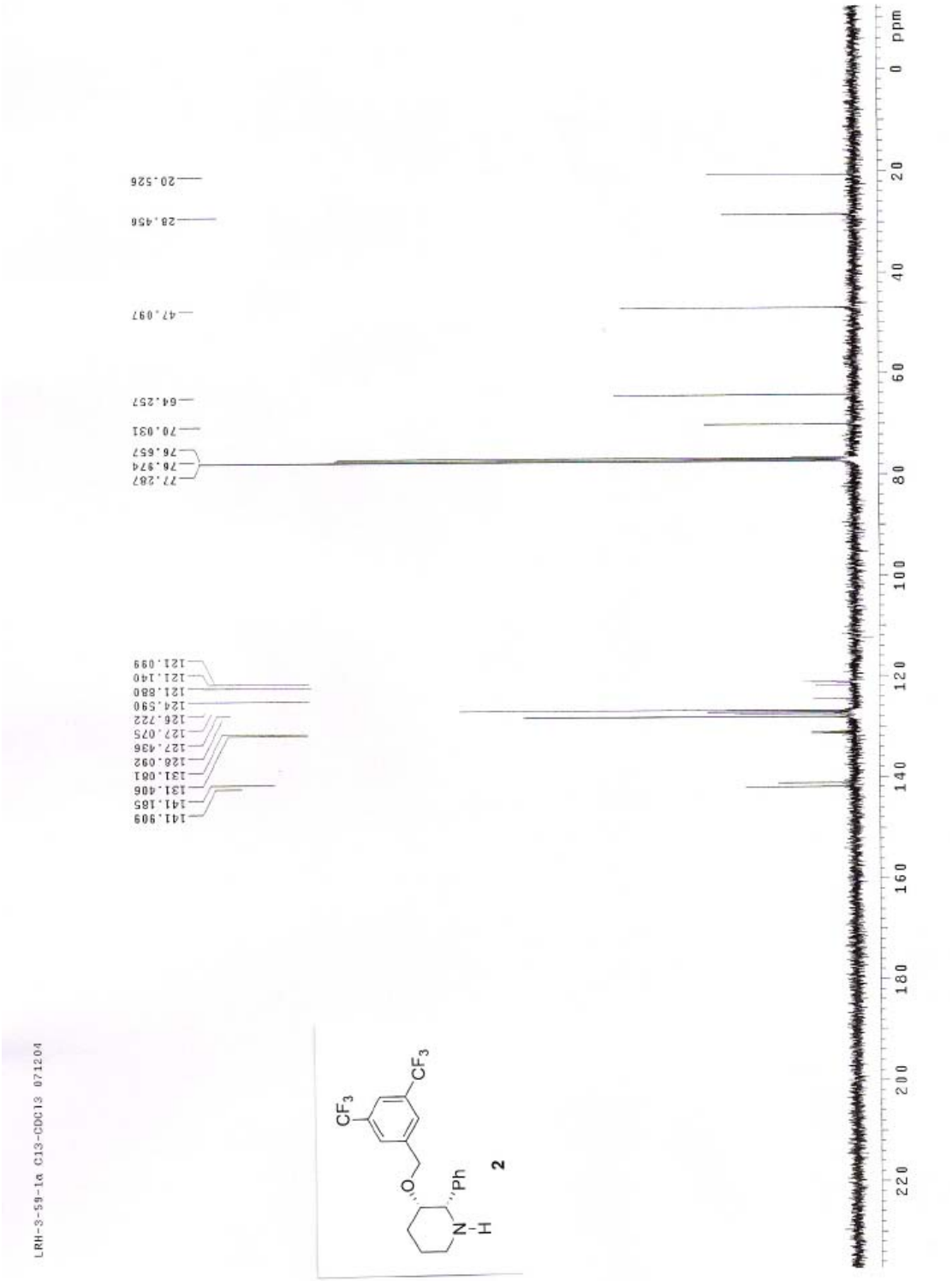

PPM
1 2 3 4 5 6 7 8
1.14
1.91
9.26
8.93
4.19
1.04
3.00
1.00
0.93
0.97
5.42
1.82
0.94
1.770
1.707
1.693
1.675
1.619
1.420
1.346
1.249
1.191
1.114
3.708
4.076
4.091
4.112
4.142
4.433
4.463
4.856
4.870
5.346
5.364
7.754
7.514
7.359
7.340
7.322
7.280
7.256
NHBoc
Ph
O
PivO
CF3
CF3
20


LRH-3-80-1 C13-CDCl3 080108
20.701
22.843
23.963
34.418
51.945
59.489
67.018
72.367
72.686
73.000
75.484
79.211
117.282
117.503
120.216
121.900
123.112
123.310
124.224
127.051
127.379
136.028
136.493
151.246
174.237
NHBoc
Ph
O
PivO
CF3
CF3
20
ppm


-0.002
1.369
1.463
1.526
1.610
1.647
1.659
1.714
1.743
1.746
1.956
1.970
1.984
1.994
2.003
2.013
2.721
2.729
2.754
2.761
2.787
2.794
3.656
3.671
3.891
3.908
3.928
3.962
4.693
4.724
4.734
4.766
5.700
7.245
7.260
7.281
7.312
7.331
7.349
7.541
7.560
7.708
7.773
9.13
2.41
2.11
1.03
2.03
2.00
0.97
6.24
2.05
1.87
1.91
CF3
CF3
O
Ph
N
Boc
21
PPM
1
2
3
4
5
6
7
8


LRH-3-56-1 C13-CDC13 071127
155.254
141.004
137.994
131.768
131.440
128.285
127.158
127.028
124.612
121.900
121.389
80.071
78.669
77.282
76.970
76.649
69.128
55.503
39.203
28.359
25.006
24.122
CF3
CF3
O
Ph
N
Boc
21
ppm


7.684
7.431
7.376
7.372
7.355
7.338
7.336
7.330
7.319
7.315
7.300
7.280
7.276
7.273
7.266
7.259
7.252
7.245
7.241
4.539
4.508
4.143
4.112
3.842
3.839
3.678
3.674
3.303
3.296
3.293
3.273
3.266
3.263
2.875
2.867
2.844
2.837
2.814
2.806
2.233
2.212
2.199
2.166
1.898
1.888
1.877
1.865
1.856
1.845
1.833
1.823
1.807
1.741
1.735
1.730
1.724
1.707
1.701
1.696
1.689
1.672
1.666
1.662
1.655
1.547
1.541
1.523
1.514
1.509
1.504
1.251
CF3
CF3
O
Ph
N
H
2
4.77
1.76
0.87
2.33
1.15
1.09
1.12
1.03
1.03
1.02
1.00
1.00
1.00
PPM


LRH-3-59-1a C13-CDCl3 071204
20.526
28.456
47.097
64.257
70.031
76.657
76.974
77.287
121.099
121.140
121.880
124.590
126.722
127.075
127.436
128.092
131.061
131.406
141.185
141.909
CF3
CF3
O
Ph
N
H
2
0 ppm
20
40
60
80
100
120
140
160
180
200
220