SUPPORTING INFORMATION

for

Palladium-Catalyzed Direct C–H Arylation of Cyclic Enaminones with Aryl Iodides

Yi-Yun Yu, Lei Bi, and Gunda I. Georg*

Department of Chemistry and Department of Medicinal Chemistry and

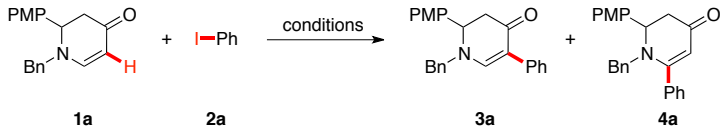
the Institute for Therapeutics Discovery and Development, University of Minnesota

717 Delaware Street SE, Minneapolis, Minnesota 55414 USA

Table of Contents

1. Initial screen of catalytic conditions

Table S1. Condition Screening of Direct C–H Arylation of Cyclic Enaminones



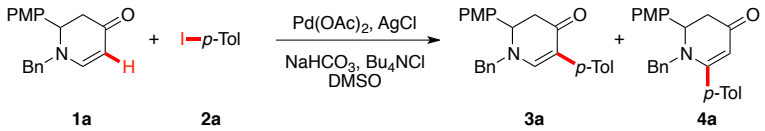
1a **2a** **3a** **4a**

Entry	Catalytic Conditions	**3a** (%)	**4a** (%)
1	$Pd(PPh_3)_4$ (10 mol %), TEA (2.0 equiv), CH_3CN, 80 °C, 18 h	0	1
2	$Pd_2(dba)_3$ (10 mol %), Bu_4NCl (2.0 equiv), NMP, 100 °C, 18 h	8	1
3	$Pd(dba)_2$ (10 mol %), Bu_4NCl (1.0 equiv), $NaHCO_3$ (2 equiv), DMF, 80 °C, 18 h	11	2
4	$PdCl_2(PPh_3)_2$ (10 mol %), $AgNO_3$ (1.0 equiv), KF (2.0 equiv), DMSO, 100 °C, 24 h	16	4
5	$[Pd(dppf)Cl_2]CH_2Cl_2$ (10 mol%), Ag_2CO_3 (2.0 equiv), DMSO, 80 °C, 24 h	0	0
6	$Pd(OAc)_2$ (10 mol%), PPh_3 (40 mol %), TEA (2.0 equiv), $AgNO_3$ (1.5 equiv), CH_3CN, 80 °C, 18 h	0	1
7	$Pd(OAc)_2$ (10 mol%), $NaHCO_3$ (3.0 equiv), Bu_4NCl (1.0 equiv), DMF, 80 °C, 18 h	30	2
8	CuCl (10 mol %), Li*O*t*Bu (2.0 equiv), DMF, 140 °C, 22 h	0	0
9	DMEDA (20 mol%), K*O*t*Bu (3.0 equiv), dioxane, 80 °C, 23 h	0	0
10	K*O*t*Bu (2.5 equiv), dioxane, 140 °C, 23 h	0	0

[a] NMR yields with Ph_3SiMe (1.0 equiv) as the internal standard.

2. Additional optimization data

Table S2. Optimization of reaction stoichiometry and time

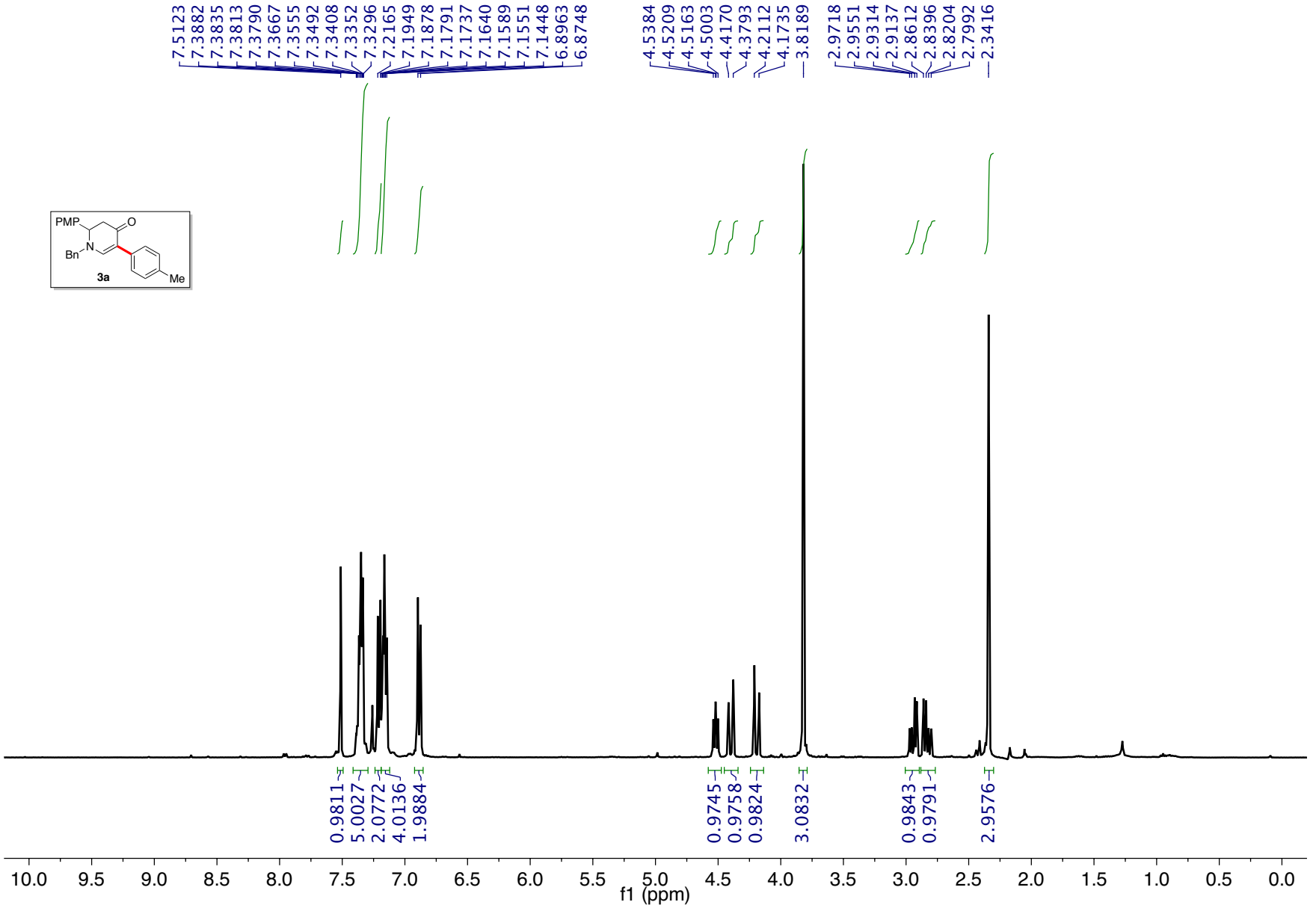


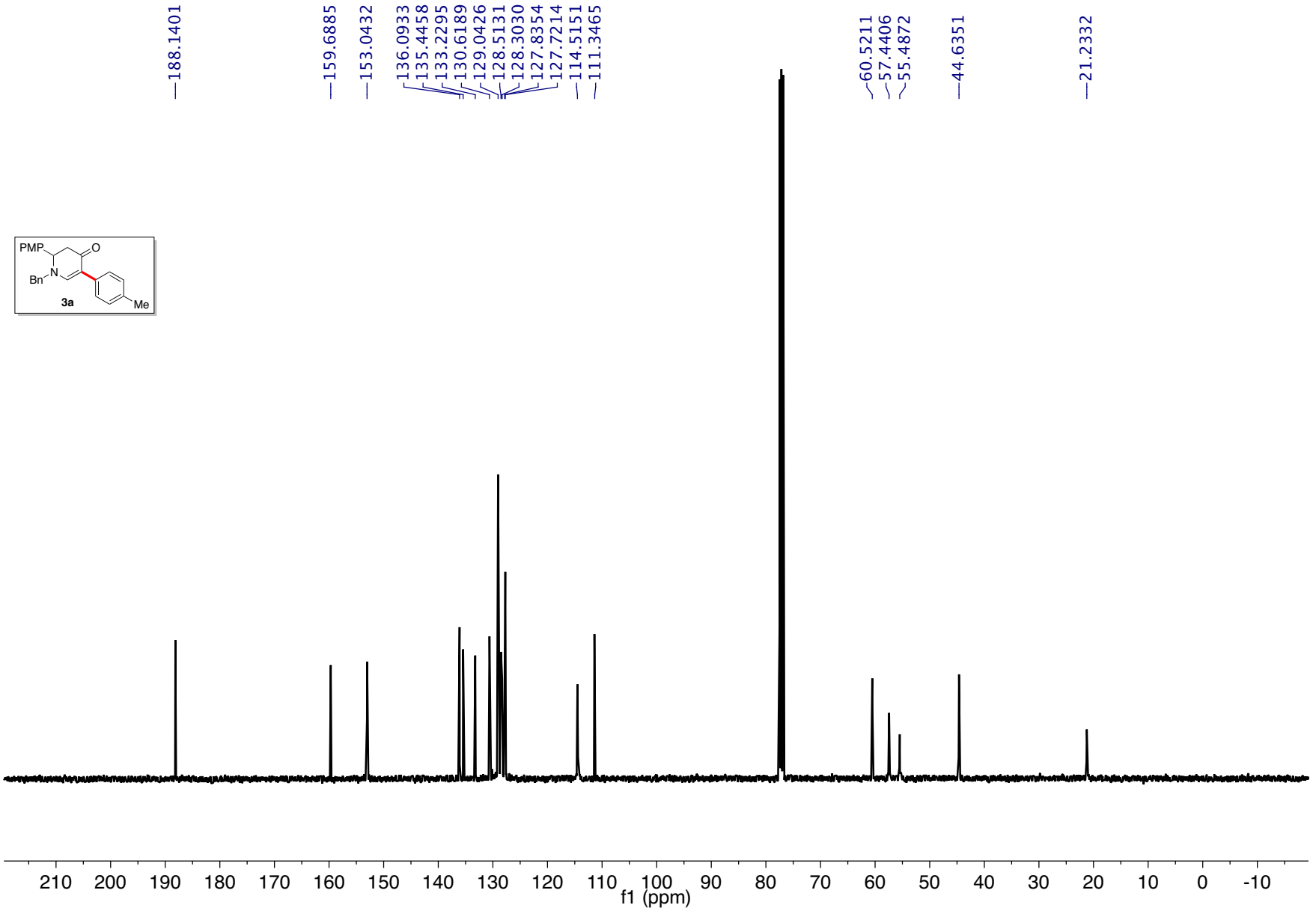
Entry	**1a** (mmol)	**2a** (equiv)	$Pd(OAc)_2$ (mol %)	AgCl (equiv)	$NaHCO_3$ (equiv)	Bu_4NCl (equiv)	DMSO (mL)	*t* (h)	**3a** (%)	**4a** (%)
1	0.2	3.0	20	1.2	3.0	**0.1**	1.0	24	48	0
2	0.2	3.0	20	1.2	3.0	**0.5**	1.0	24	64	0
3	0.2	3.0	20	1.2	3.0	**1.0**	1.0	24	65	0
4	0.2	3.0	20	1.2	3.0	**2.0**	1.0	24	36	0
5	0.2	3.0	20	1.2	3.0	**3.0**	1.0	24	19	0
6	0.2	3.0	20	**0.1**	3.0	0.5	1.0	24	57	3
7	0.2	3.0	20	**0.5**	3.0	0.5	1.0	24	58	1
8	0.2	3.0	20	**2.0**	3.0	0.5	1.0	24	54	0
9	0.2	3.0	20	**3.0**	3.0	0.5	1.0	24	55	0
10	0.2	**1.1**	20	1.2	3.0	0.5	1.0	24	52	0
11	0.2	**1.5**	20	1.2	3.0	0.5	1.0	24	60	0
12	0.2	**2.0**	20	1.2	3.0	0.5	1.0	24	63	0
13	0.2	**4.0**	20	1.2	3.0	0.5	1.0	24	64	0
14	0.2	**6.0**	20	1.2	3.0	0.5	1.0	24	68	0
15	0.2	**15.0**	20	1.2	3.0	0.5	1.0	24	63	0
16	0.2	3.0	20	1.2	**1.0**	0.5	1.0	24	64	0

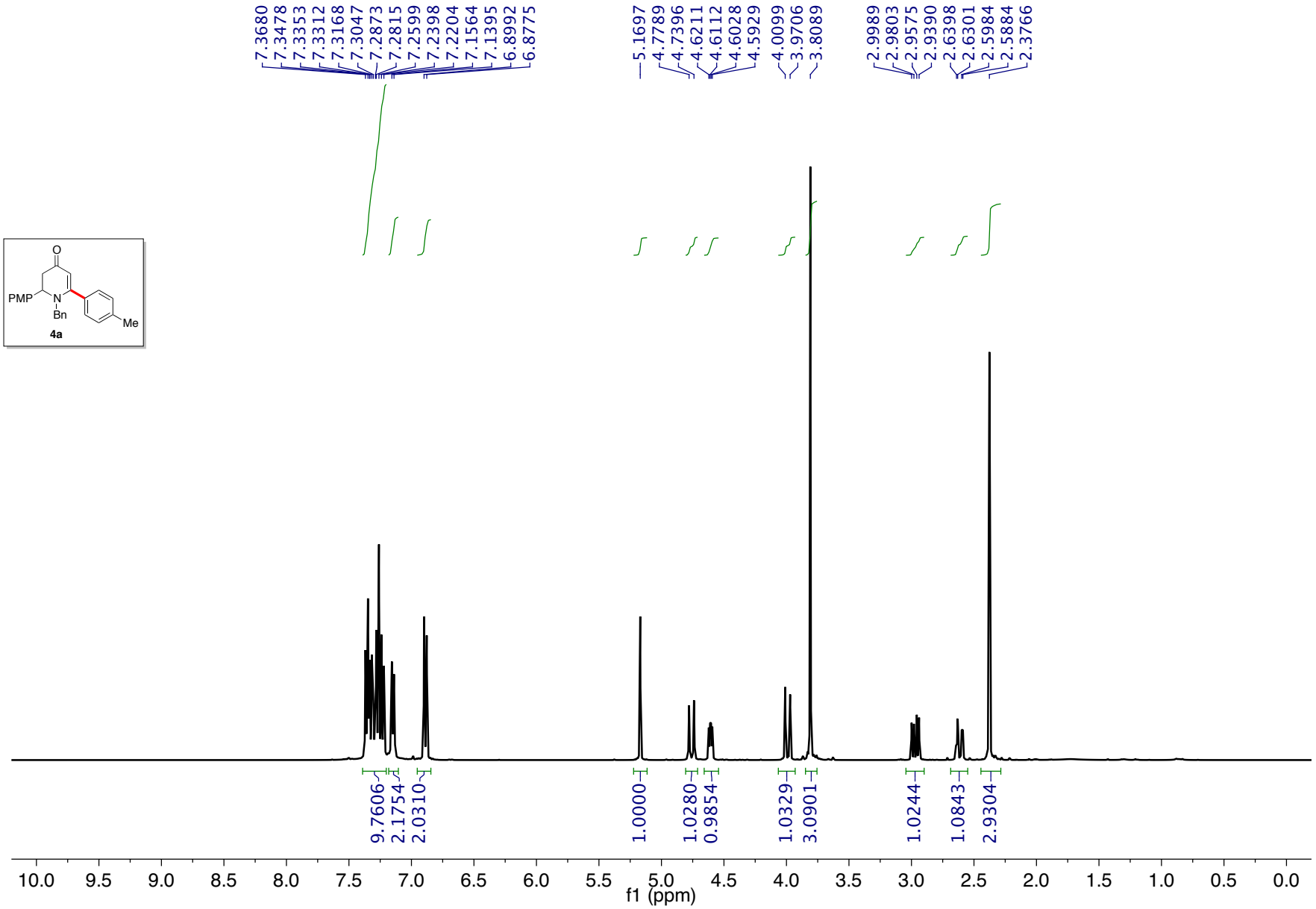
17	0.2	3.0	20	1.2	**2.0**	0.5	1.0	24	61	0
18	0.2	3.0	20	1.2	**5.0**	0.5	1.0	24	59	0
19	0.2	3.0	20	1.2	**10.0**	0.5	1.0	24	59	0
20	0.2	3.0	**0.1**	1.2	1.0	0.5	1.0	24	0	0
21	0.2	3.0	**5**	1.2	1.0	0.5	1.0	24	46	0
22	0.2	3.0	**10**	1.2	1.0	0.5	1.0	24	56	0
23	0.2	3.0	**15**	1.2	1.0	0.5	1.0	24	61	0
24	0.2	3.0	**30**	1.2	1.0	0.5	1.0	24	60	0
25	0.2	3.0	20	1.2	1.0	0.5	1.0	**0.5**	34	0
26	0.2	3.0	20	1.2	1.0	0.5	1.0	**1**	47	0
27	0.2	3.0	20	1.2	1.0	0.5	1.0	**2**	57	<1
28	0.2	3.0	20	1.2	1.0	0.5	1.0	**4**	58	<1
29	0.2	3.0	20	1.2	1.0	0.5	1.0	**8**	62	<1
30	0.2	3.0	20	1.2	1.0	0.5	1.0	**12**	64	<1
31	0.2	3.0	20	1.2	1.0	0.5	**0.5**	24	64	0
32	0.2	3.0	20	1.2	1.0	0.5	**2.0**	24	55	0
33	0.2	3.0	20	1.2	1.0	0.5	**3.0**	24	52	0
34	0.1	3.0	20	1.2	1.0	–	0.5	24	63	3
35	0.1	3.0	20	1.2	1.0	0.5	0.5	24	**75 (72[c])**	**<1**
36[b]	0.1	3.0	20	1.2	1.0	0.5	0.5	24	74	<1

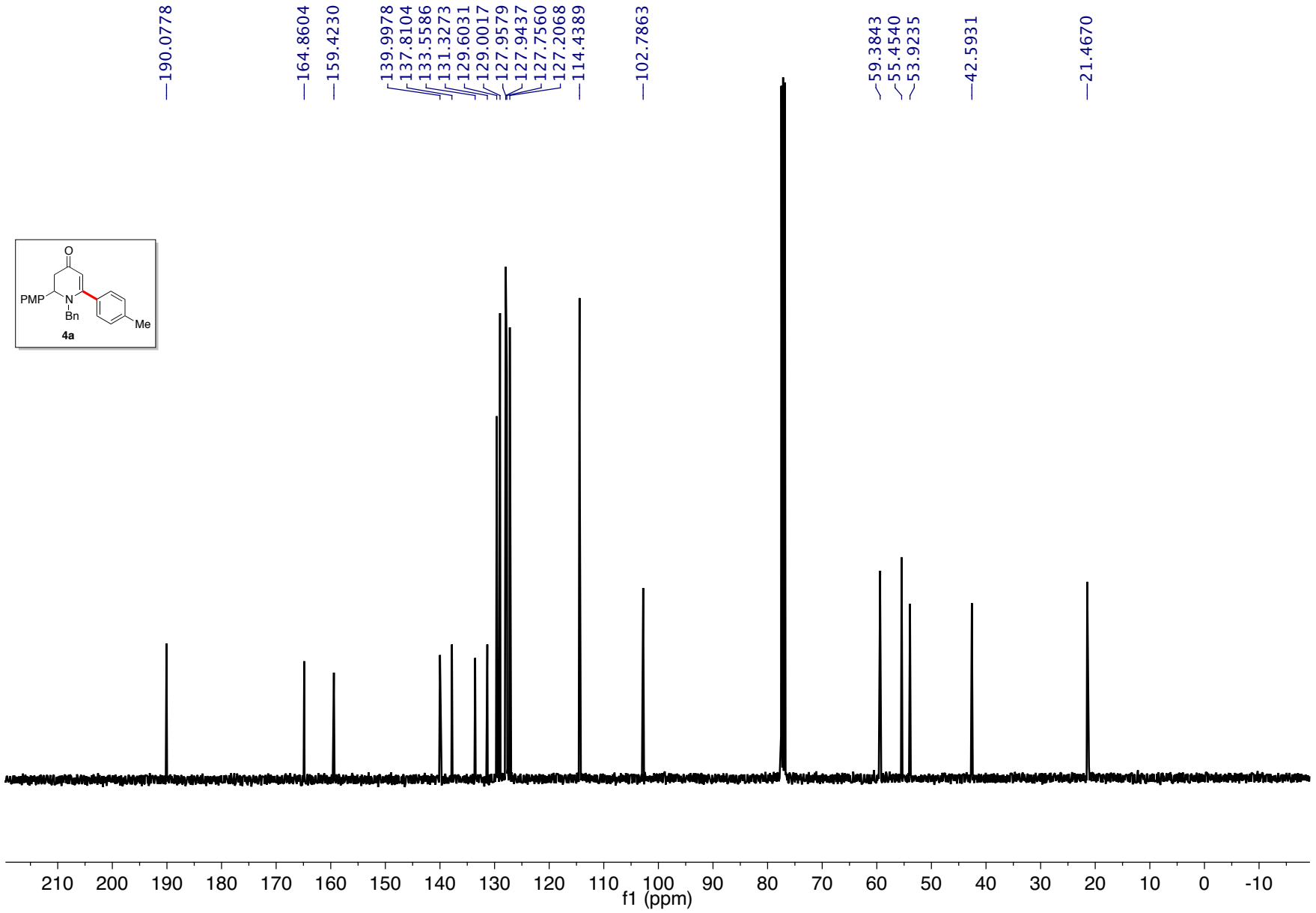
[a] NMR yields with Ph_3SiMe (1.0 equiv) as the internal standard. (*p*-Tol = *para*-tolyl) [b] With 4Å MS. [c] Isolated yield.

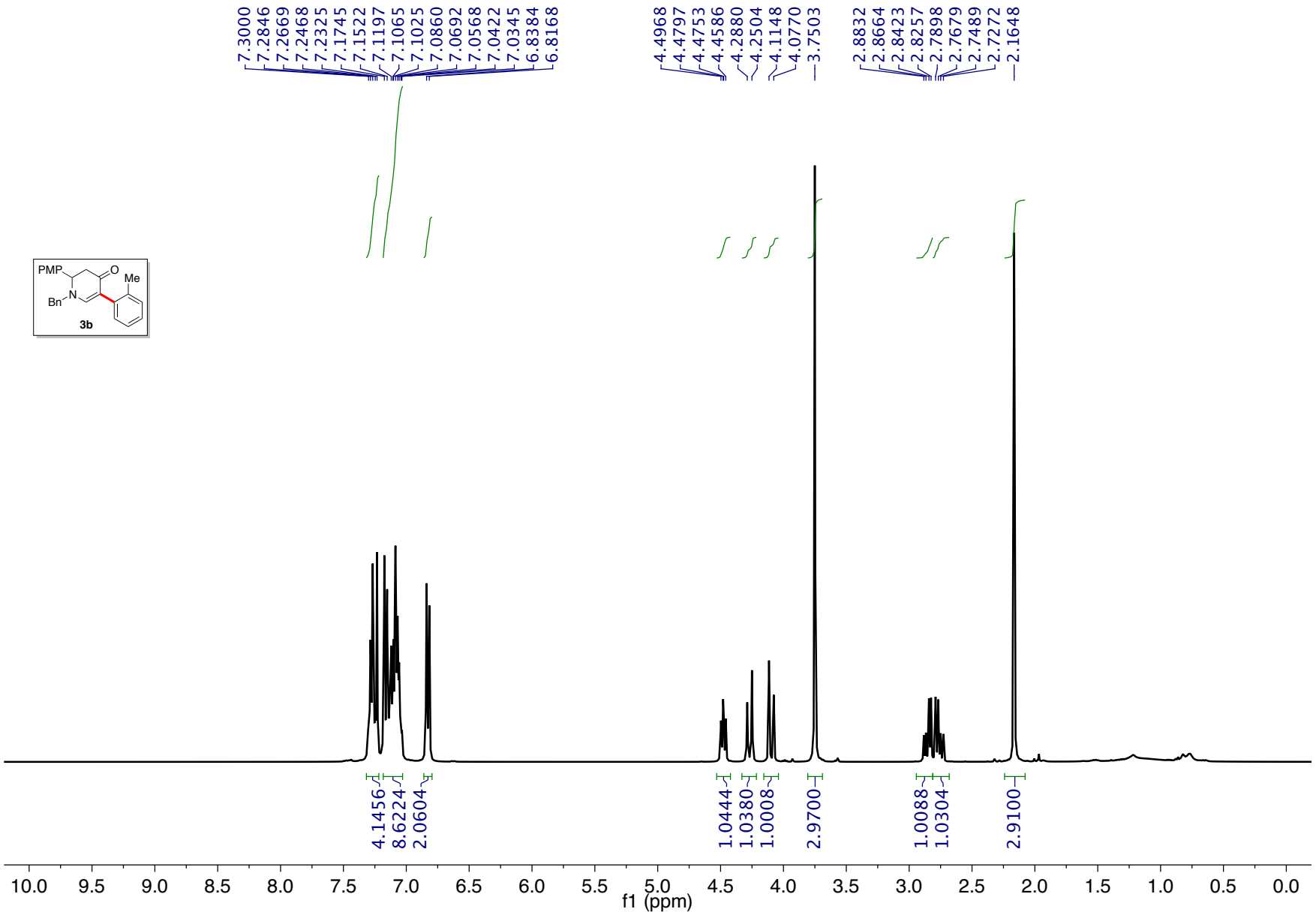
3. ^{1}H NMR and ^{13}C NMR spectra for compounds **3a, 4a, 3b–3v**

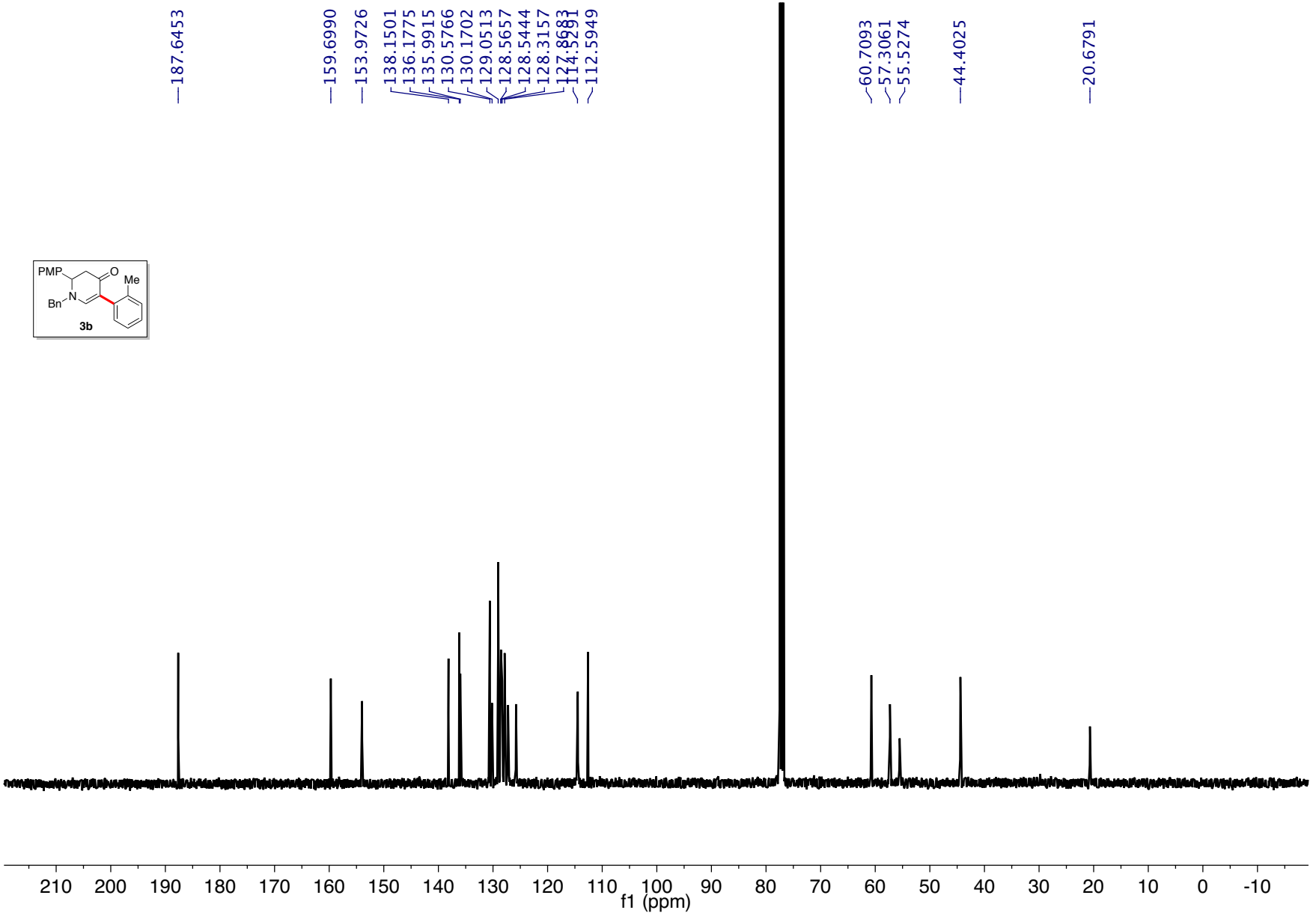


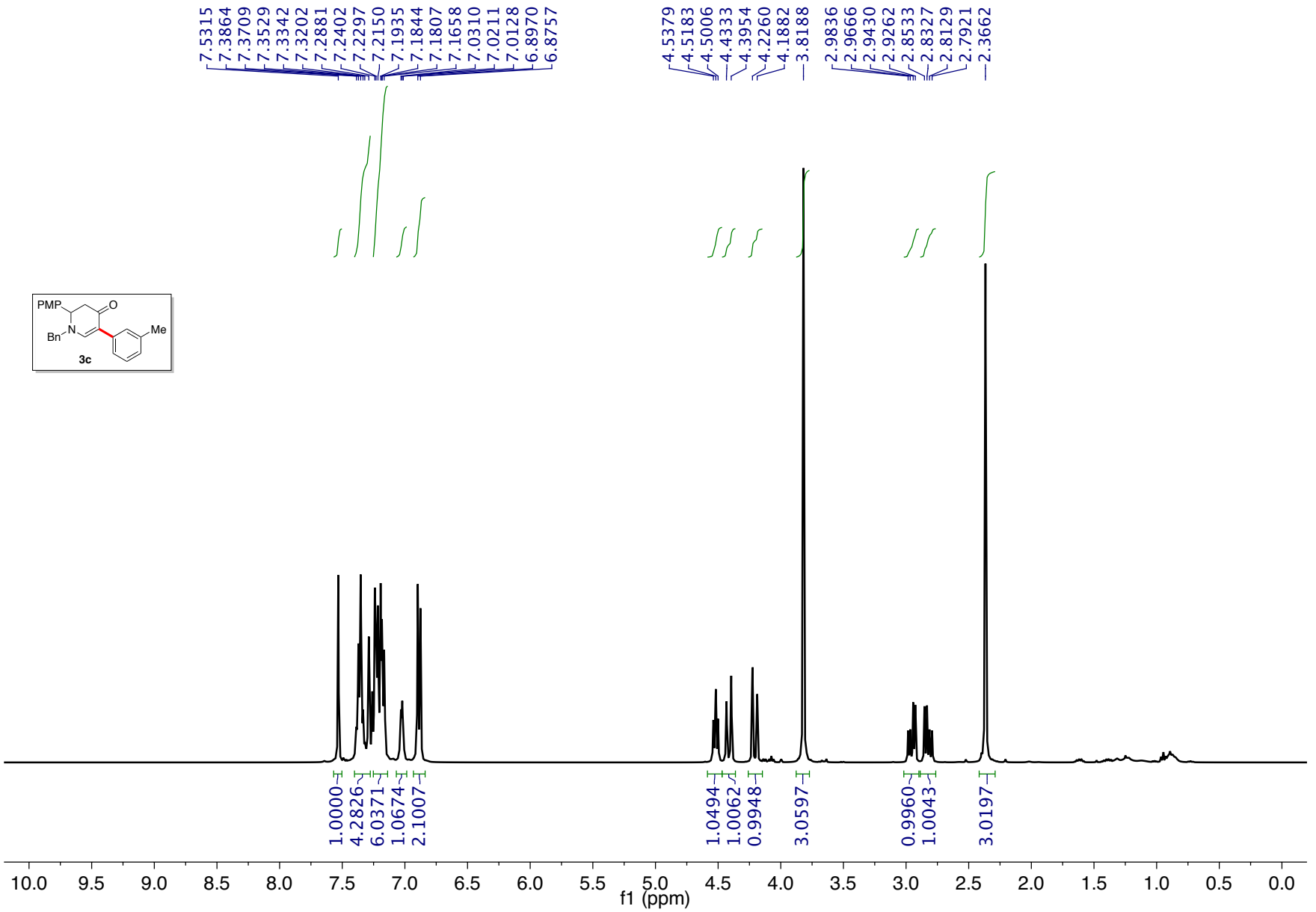

188.1401
159.6885
153.0432
136.0933
135.4458
133.2295
130.6189
129.0426
128.5131
128.3030
127.8354
127.7214
114.5151
111.3465
60.5211
57.4406
55.4872
44.6351
21.2332
PMP
Bn
N
O
Me
3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

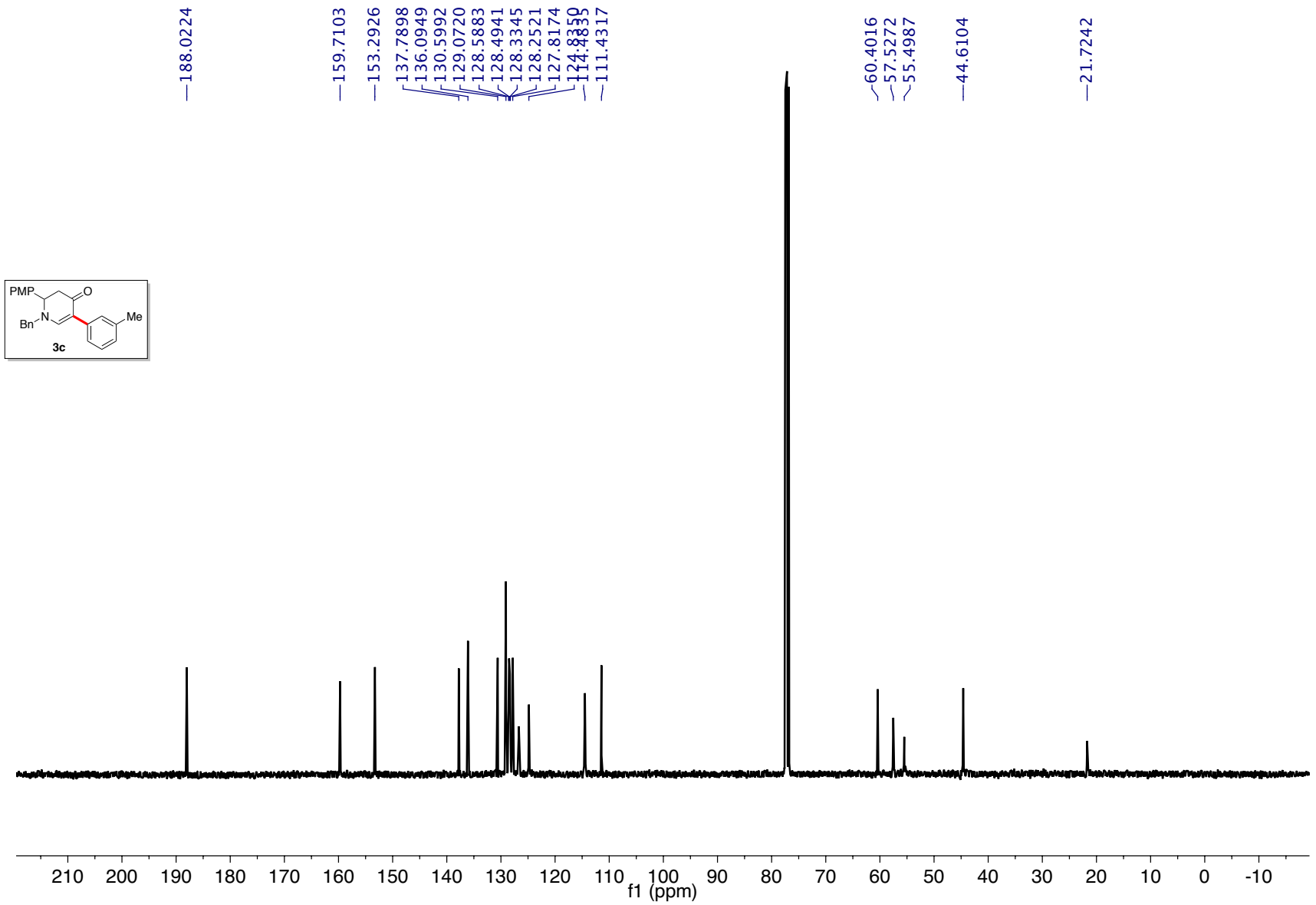

7.3680
7.3478
7.3353
7.3312
7.3168
7.3047
7.2873
7.2815
7.2599
7.2398
7.2204
7.1564
7.1395
6.8992
6.8775
5.1697
4.7789
4.7396
4.6211
4.6112
4.6028
4.5929
4.0099
3.9706
3.8089
2.9989
2.9803
2.9575
2.9390
2.6398
2.6301
2.5984
2.5884
2.3766
O
PMP
N
Bn
Me
4a
9.7606
2.1754
2.0310
1.0000
1.0280
0.9854
1.0329
3.0901
1.0244
1.0843
2.9304
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
f1 (ppm)

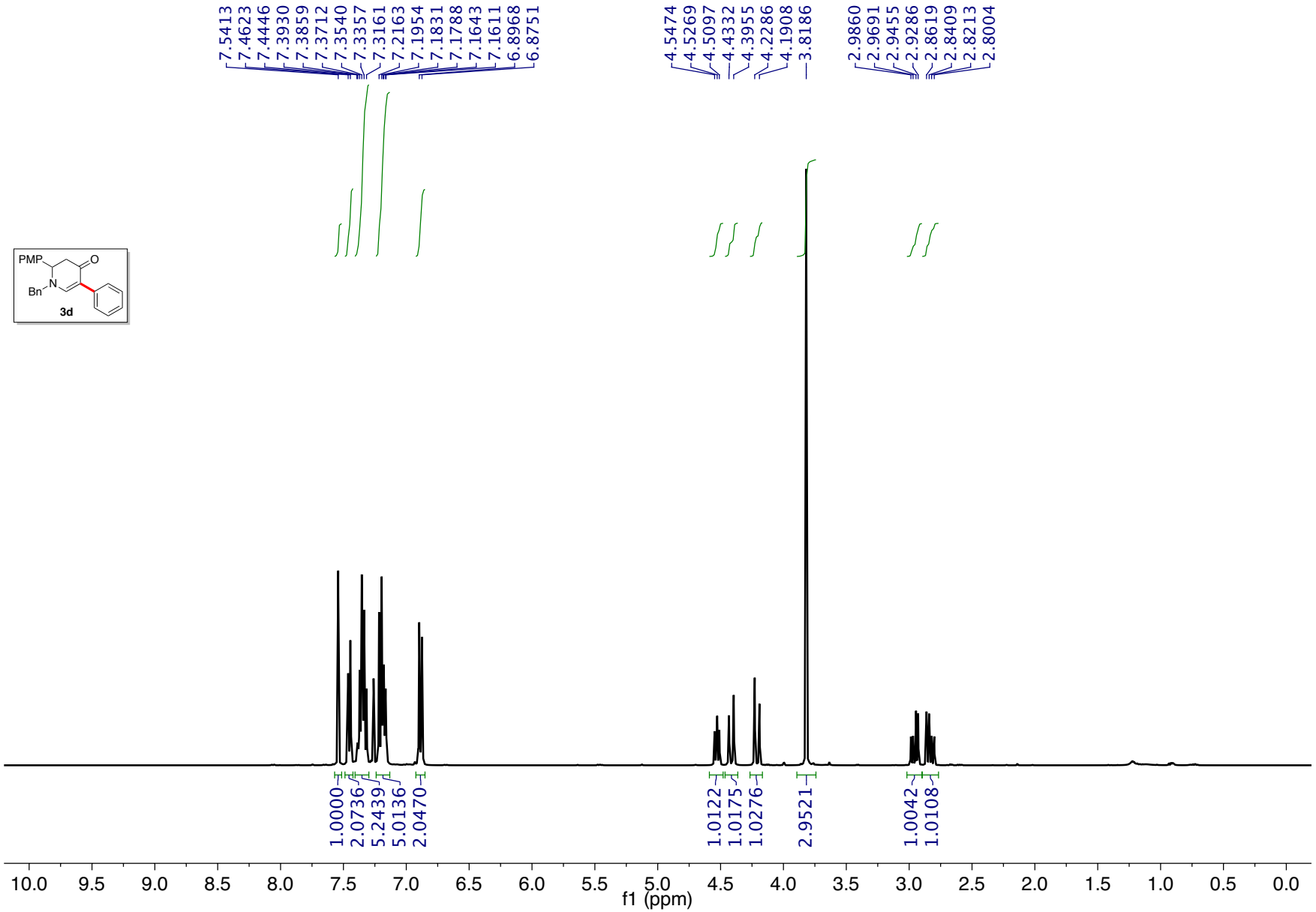

190.0778
164.8604
159.4230
139.9978
137.8104
133.5586
131.3273
129.6031
129.0017
127.9579
127.9437
127.7560
127.2068
114.4389
102.7863
59.3843
55.4540
53.9235
42.5931
21.4670
O
PMP
N
Bn
Me
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

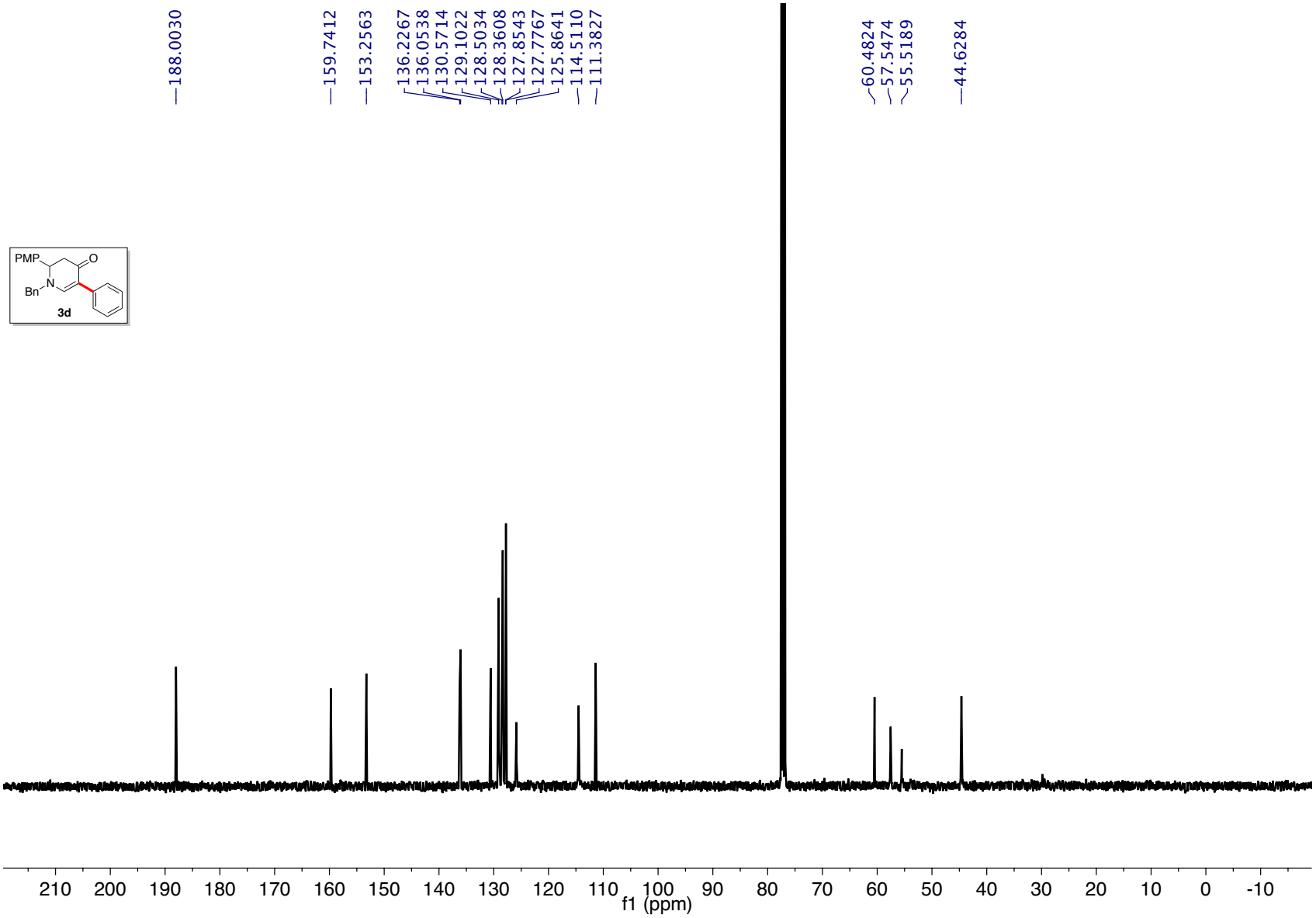

7.3000
7.2846
7.2669
7.2468
7.2325
7.1745
7.1522
7.1197
7.1065
7.1025
7.0860
7.0692
7.0568
7.0422
7.0345
6.8384
6.8168
4.4968
4.4797
4.4753
4.4586
4.2880
4.2504
4.1148
4.0770
3.7503
2.8832
2.8664
2.8423
2.8257
2.7898
2.7679
2.7489
2.7272
2.1648
PMP
O
Me
N
Bn
3b
4.1456
8.6224
2.0604
1.0444
1.0380
1.0008
2.9700
1.0088
1.0304
2.9100
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
f1 (ppm)

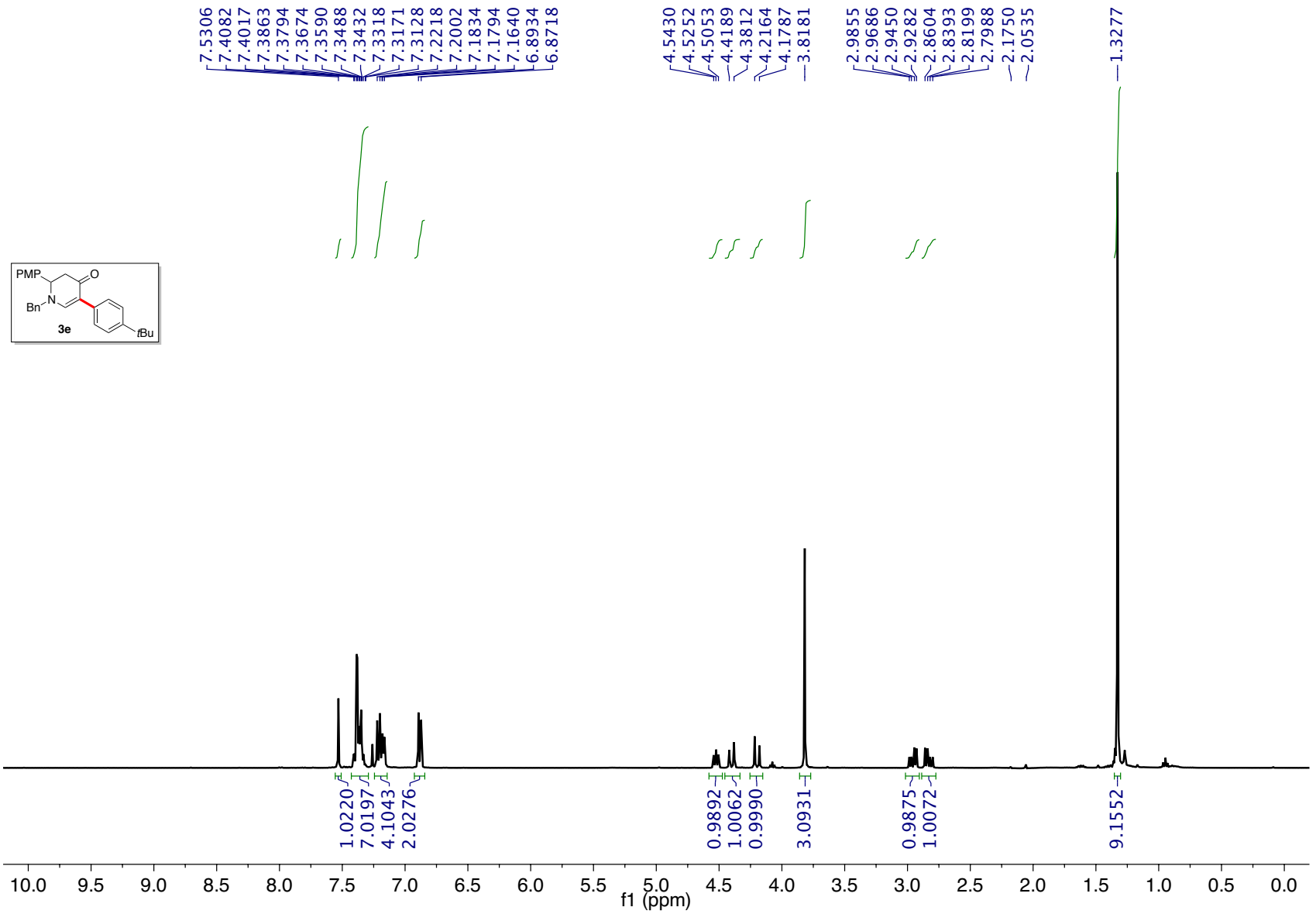

187.6453
159.6990
153.9726
138.1501
136.1775
135.9915
130.5766
130.1702
129.0513
128.5657
128.5444
128.3157
127.8683
114.5281
112.5949
60.7093
57.3061
55.5274
44.4025
20.6791
PMP
O
Me
N
Bn
3b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

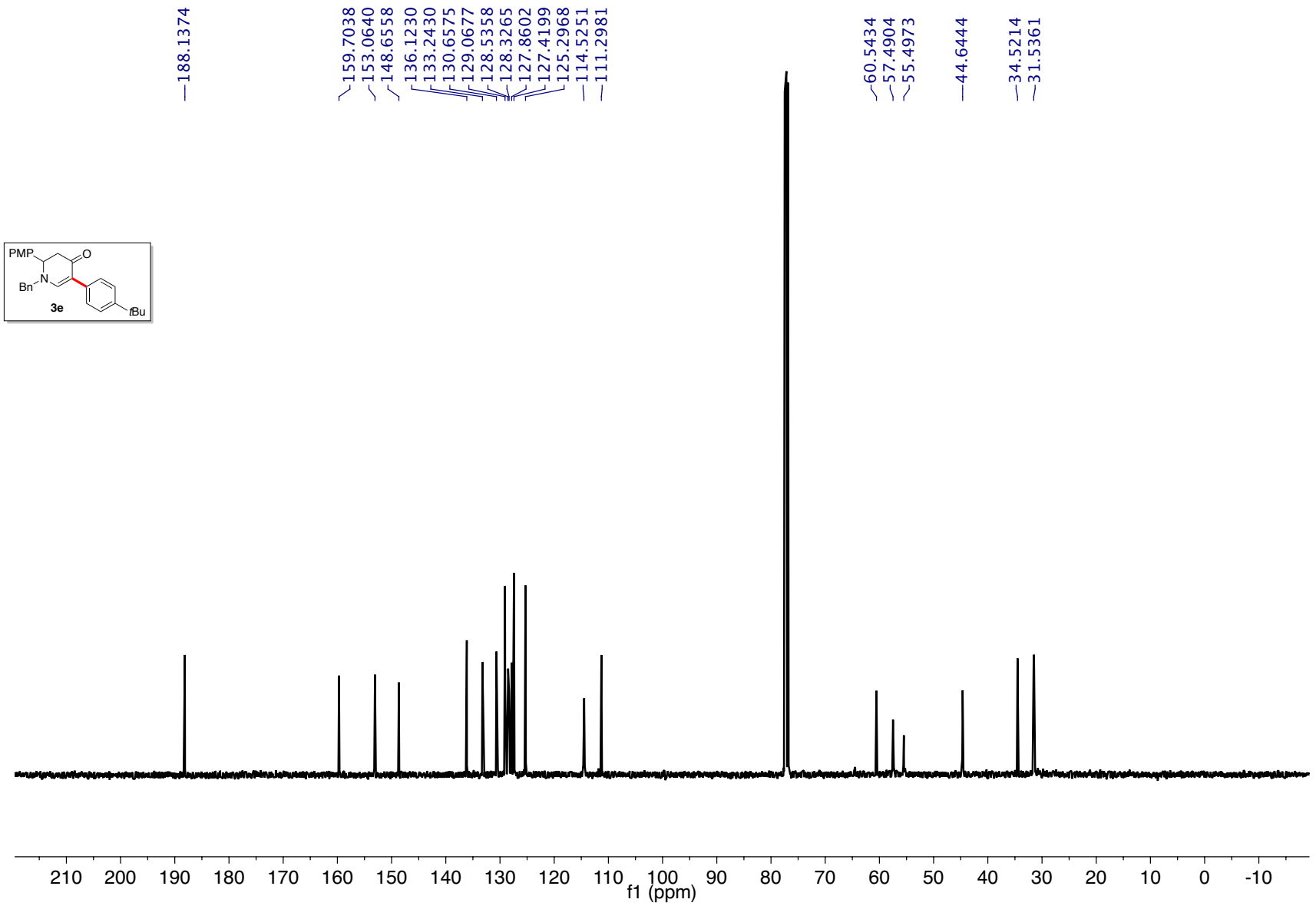

7.5315
7.3864
7.3709
7.3529
7.3342
7.3202
7.2881
7.2402
7.2297
7.2150
7.1935
7.1844
7.1807
7.1658
7.0310
7.0211
7.0128
6.8970
6.8757
4.5379
4.5183
4.5006
4.4333
4.3954
4.2260
4.1882
3.8188
2.9836
2.9666
2.9430
2.9262
2.8533
2.8327
2.8129
2.7921
2.3662
PMP
Bn
N
O
Me
3c
1.0000
4.2826
6.0371
1.0674
2.1007
1.0494
1.0062
0.9948
3.0597
0.9960
1.0043
3.0197
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
f1 (ppm)

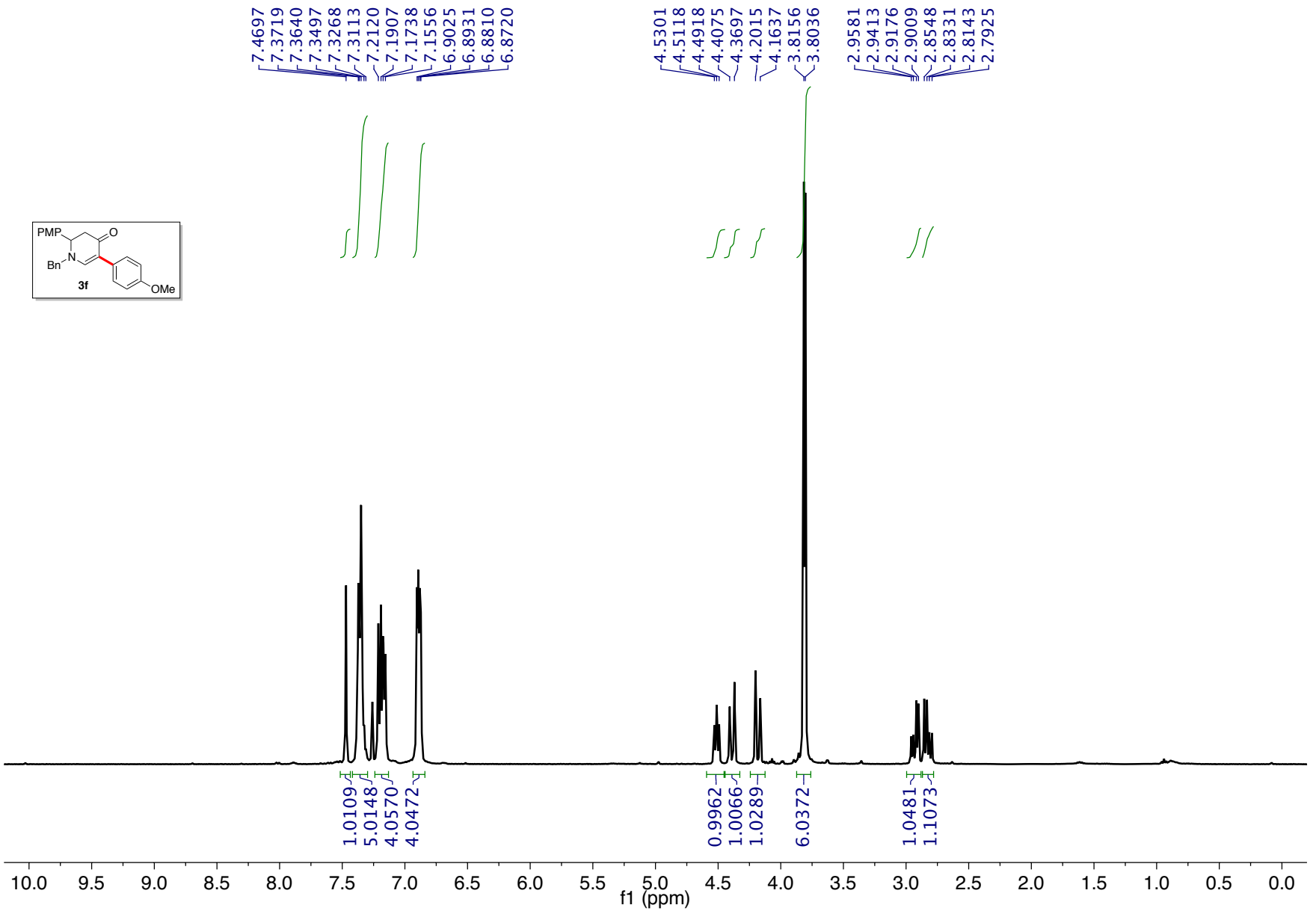

188.0224
159.7103
153.2926
137.7898
136.0949
130.5992
129.0720
128.5883
128.4941
128.3345
128.2521
127.8174
124.8350
114.4835
111.4317
60.4016
57.5272
55.4987
44.6104
21.7242
PMP
O
N
Bn
Me
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

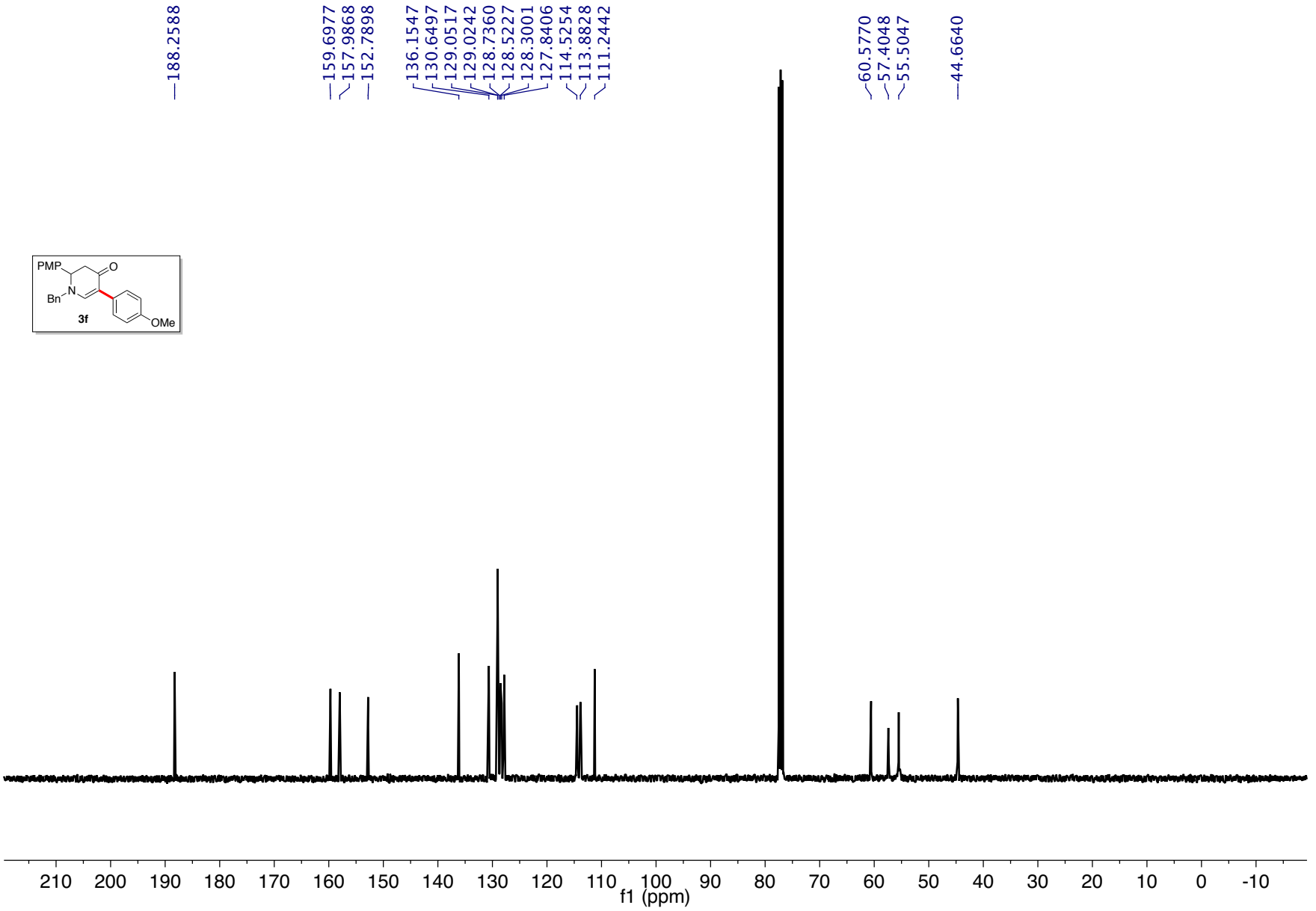

7.5413
7.4623
7.4446
7.3930
7.3859
7.3712
7.3540
7.3357
7.3161
7.2163
7.1954
7.1831
7.1788
7.1643
7.1611
6.8968
6.8751
4.5474
4.5269
4.5097
4.4332
4.3955
4.2286
4.1908
3.8186
2.9860
2.9691
2.9455
2.9286
2.8619
2.8409
2.8213
2.8004
PMP
O
N
Bn
3d
1.0000
2.0736
5.2439
5.0136
2.0470
1.0122
1.0175
1.0276
2.9521
1.0042
1.0108
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
f1 (ppm)

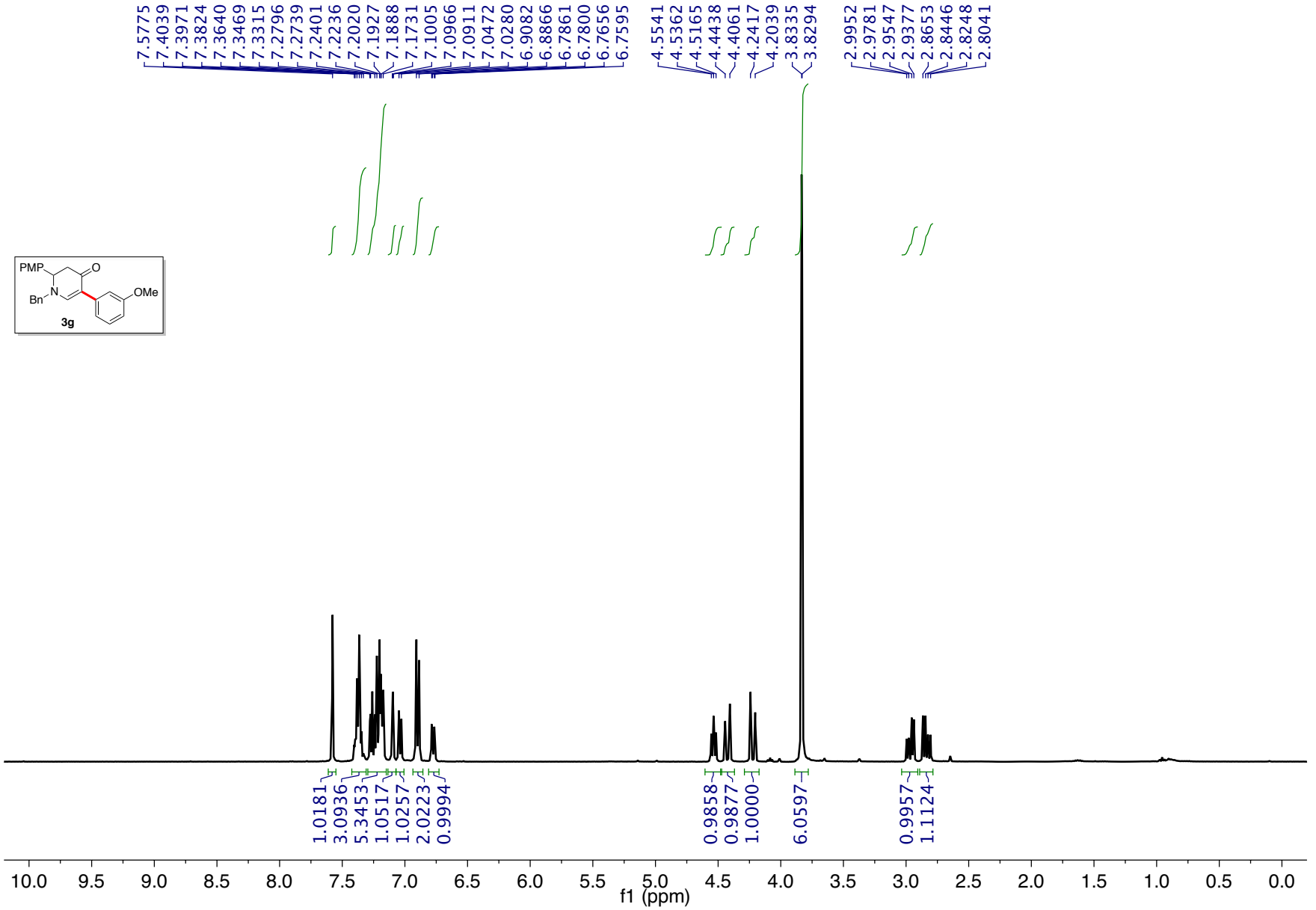

188.0030
159.7412
153.2563
136.2267
136.0538
130.5714
129.1022
128.5034
128.3608
127.8543
127.7767
125.8641
114.5110
111.3827
60.4824
57.5474
55.5189
44.6284
PMP
Bn
N
O
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

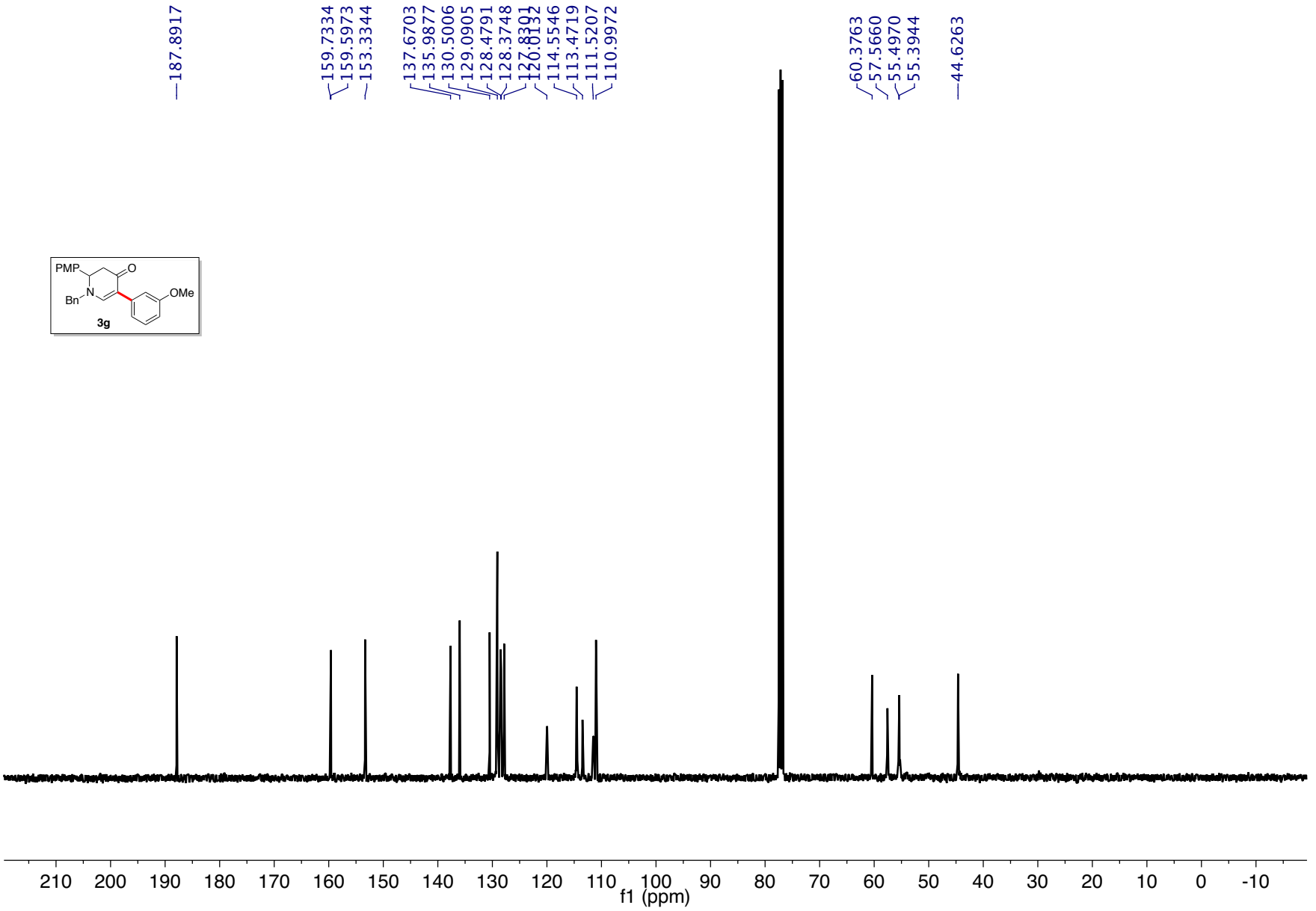

7.5306
7.4082
7.4017
7.3863
7.3794
7.3674
7.3590
7.3488
7.3432
7.3318
7.3171
7.3128
7.2218
7.2002
7.1834
7.1794
7.1640
6.8934
6.8718
4.5430
4.5252
4.5053
4.4189
4.3812
4.2164
4.1787
3.8181
2.9855
2.9686
2.9450
2.9282
2.8604
2.8393
2.8199
2.7988
2.1750
2.0535
1.3277
PMP
Bn
N
O
3e
tBu
1.0220
7.0197
4.1043
2.0276
0.9892
1.0062
0.9990
3.0931
0.9875
1.0072
9.1552
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
f1 (ppm)

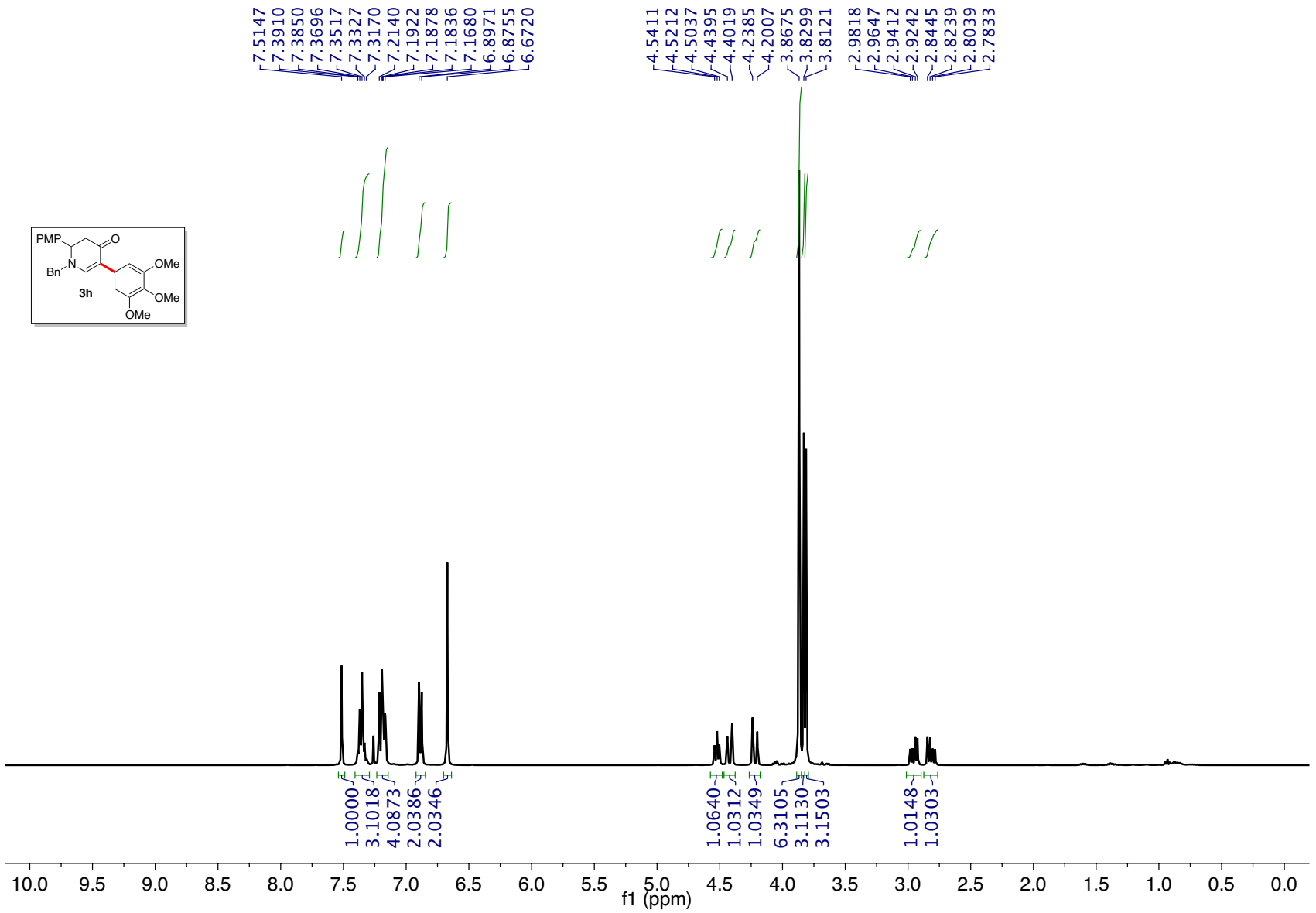

188.1374
159.7038
153.0640
148.6558
136.1230
133.2430
130.6575
129.0677
128.5358
128.3265
127.8602
127.4199
125.2968
114.5251
111.2981
60.5434
57.4904
55.4973
44.6444
34.5214
31.5361
PMP
O
N
Bn
3e
tBu
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

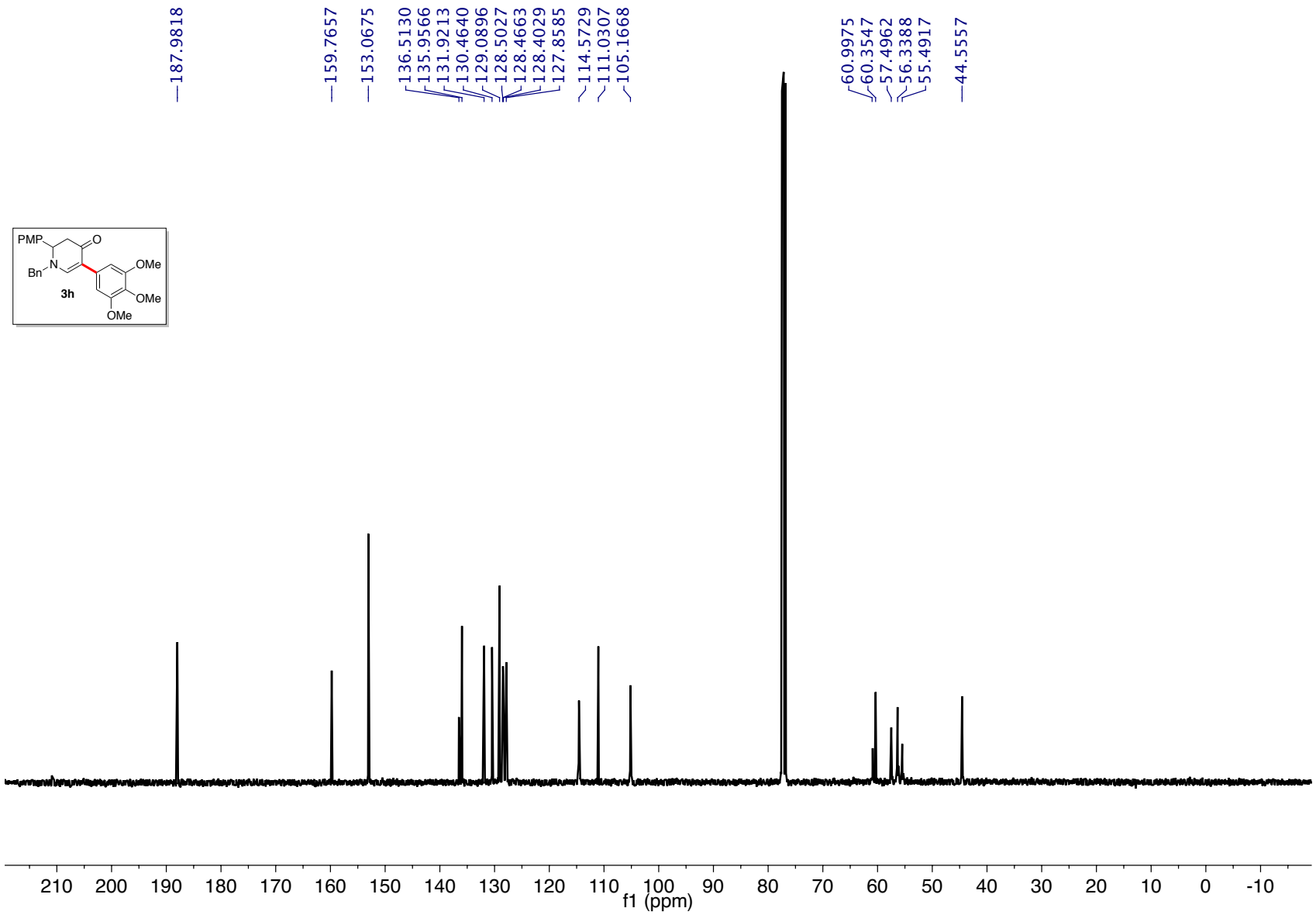

7.4697
7.3719
7.3640
7.3497
7.3268
7.3113
7.2120
7.1907
7.1738
7.1556
6.9025
6.8931
6.8810
6.8720
4.5301
4.5118
4.4918
4.4075
4.3697
4.2015
4.1637
3.8156
3.8036
2.9581
2.9413
2.9176
2.9009
2.8548
2.8331
2.8143
2.7925
PMP
O
Bn
N
3f
OMe
1.0109
5.0148
4.0570
4.0472
0.9962
1.0066
1.0289
6.0372
1.0481
1.1073
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
f1 (ppm)

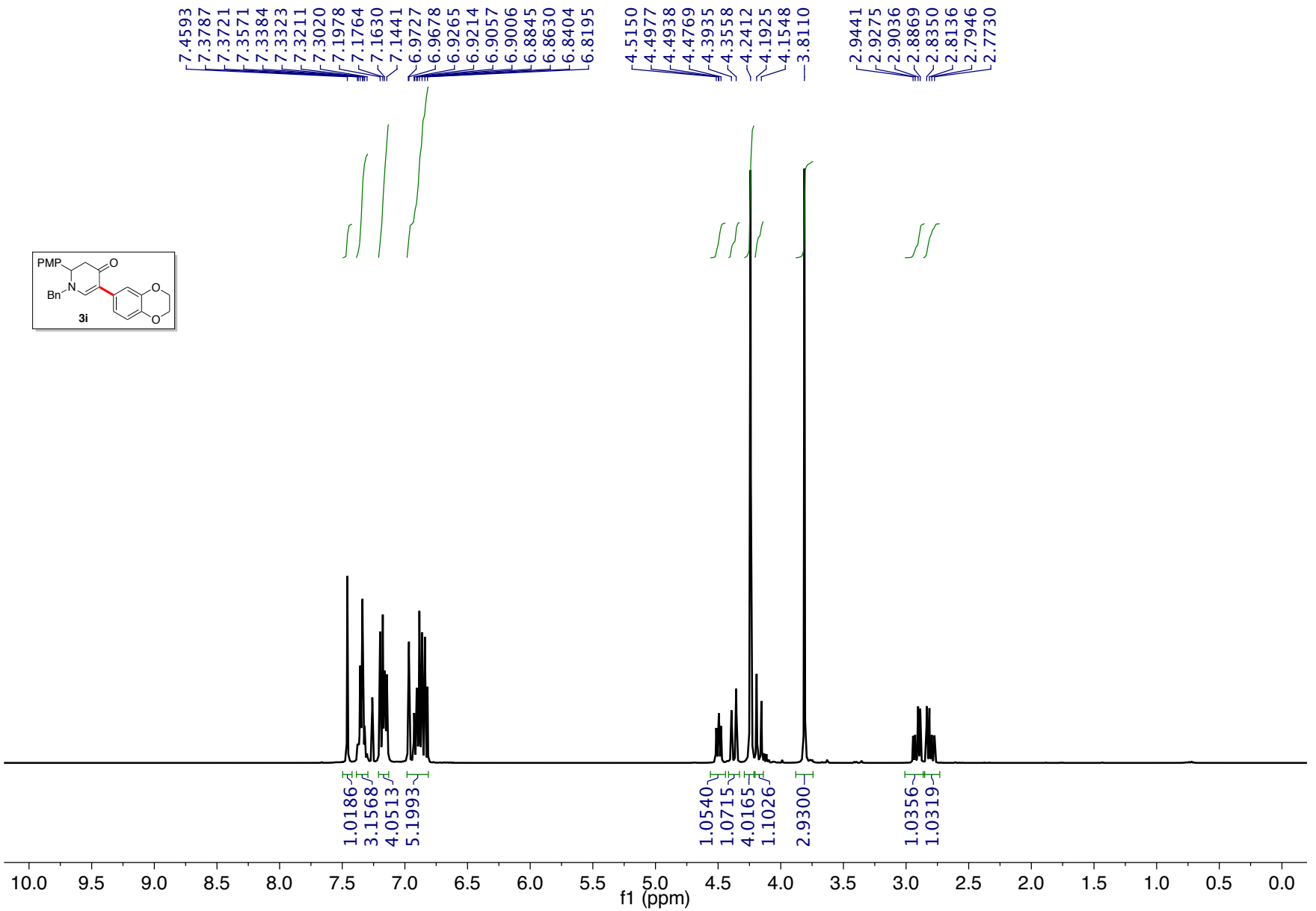

188.2588
159.6977
157.9868
152.7898
136.1547
130.6497
129.0517
129.0242
128.7360
128.5227
128.3001
127.8406
114.5254
113.8828
111.2442
60.5770
57.4048
55.5047
44.6640
PMP
Bn
N
O
OMe
3f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

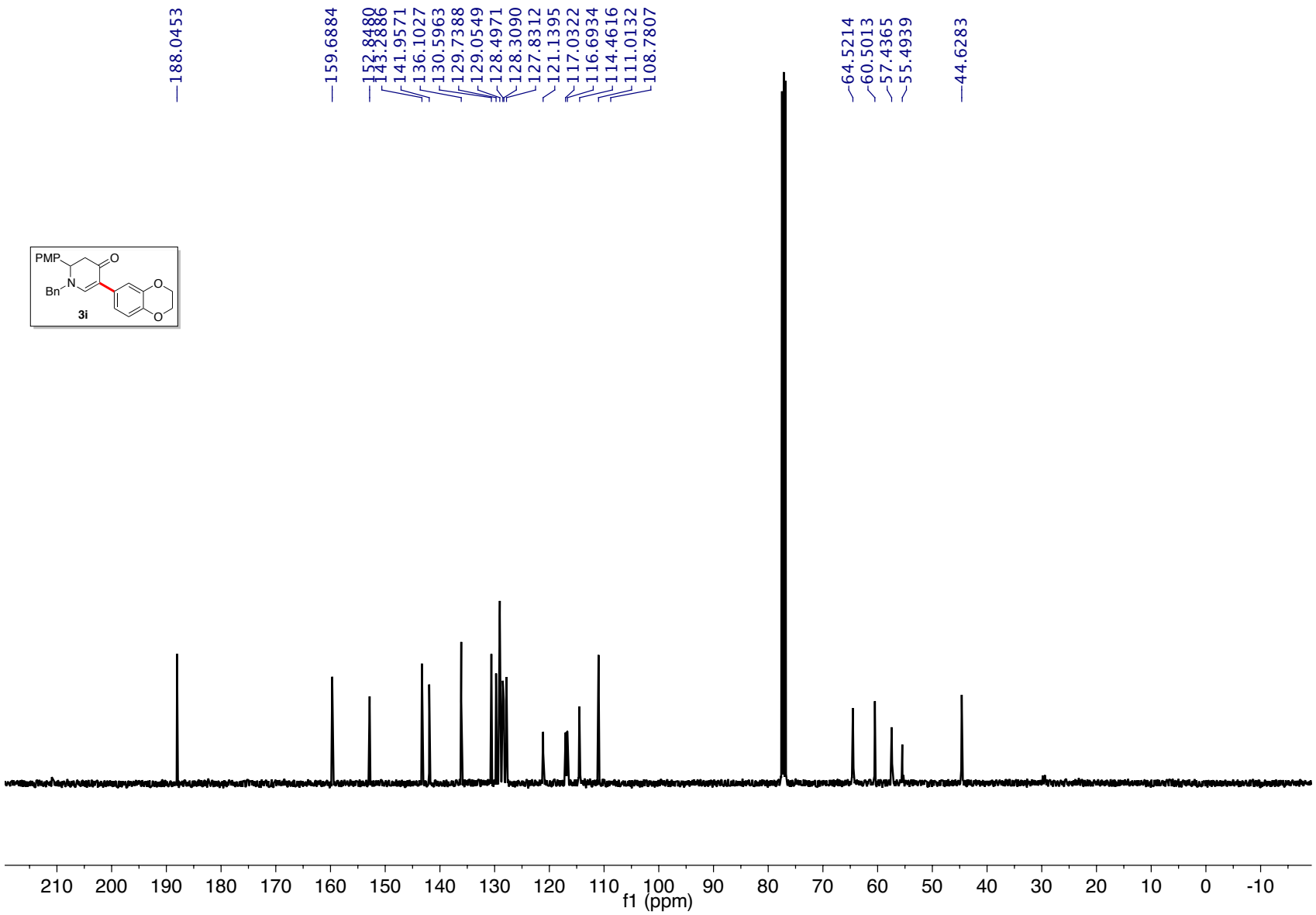

7.5775
7.4039
7.3971
7.3824
7.3640
7.3469
7.3315
7.2796
7.2739
7.2401
7.2236
7.2020
7.1927
7.1888
7.1731
7.1005
7.0966
7.0911
7.0472
7.0280
6.9082
6.8866
6.7861
6.7800
6.7656
6.7595
4.5541
4.5362
4.5165
4.4438
4.4061
4.2417
4.2039
3.8335
3.8294
2.9952
2.9781
2.9547
2.9377
2.8653
2.8446
2.8248
2.8041
PMP
O
N
Bn
OMe
3g
1.0181
3.0936
5.3453
1.0517
1.0257
2.0223
0.9994
0.9858
0.9877
1.0000
6.0597
0.9957
1.1124
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
f1 (ppm)

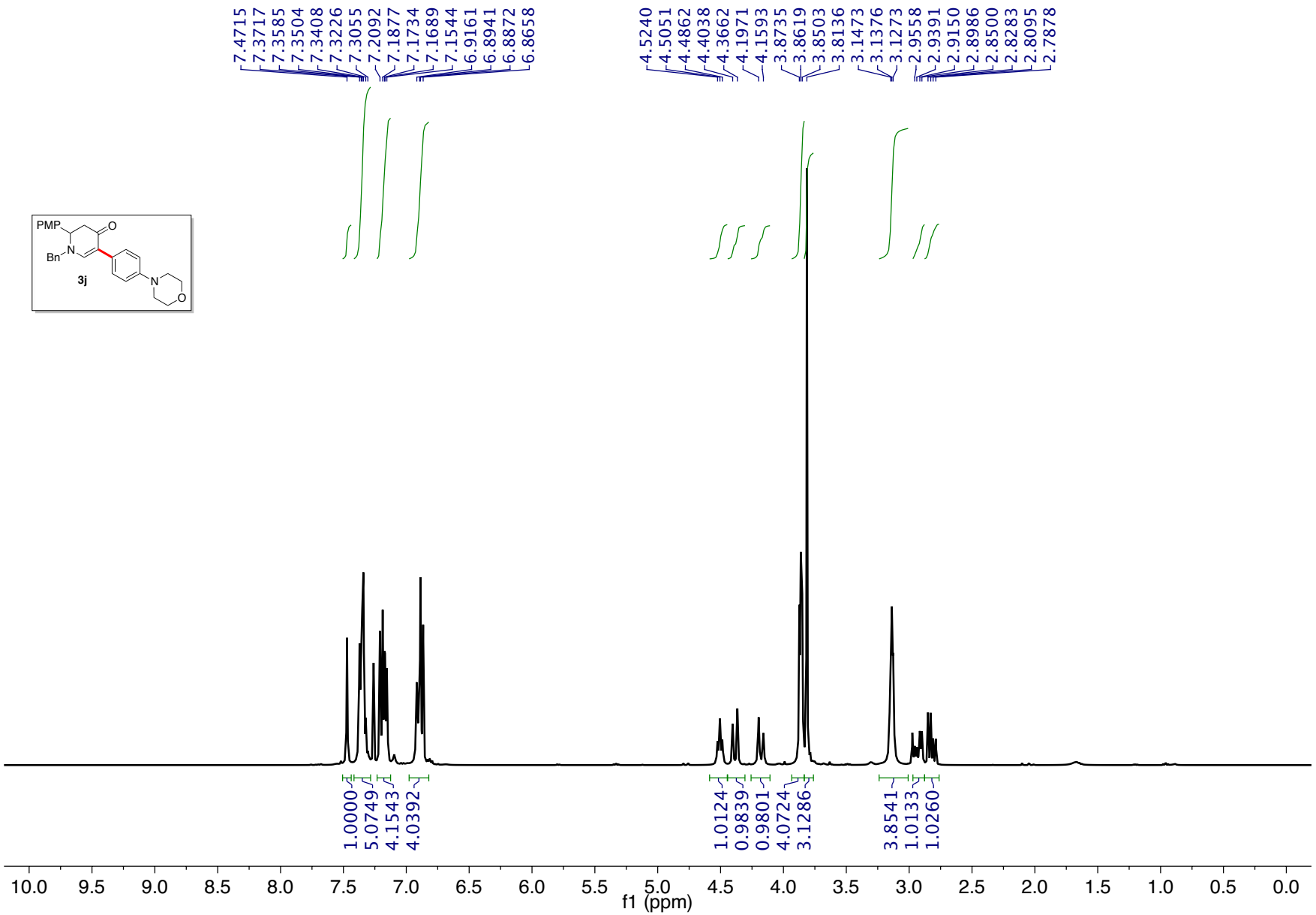

187.8917
159.7334
159.5973
153.3344
137.6703
135.9877
130.5006
129.0905
128.4791
128.3748
127.8391
120.0132
114.5546
113.4719
111.5207
110.9972
60.3763
57.5660
55.4970
55.3944
44.6263
PMP
O
N
Bn
OMe
3g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

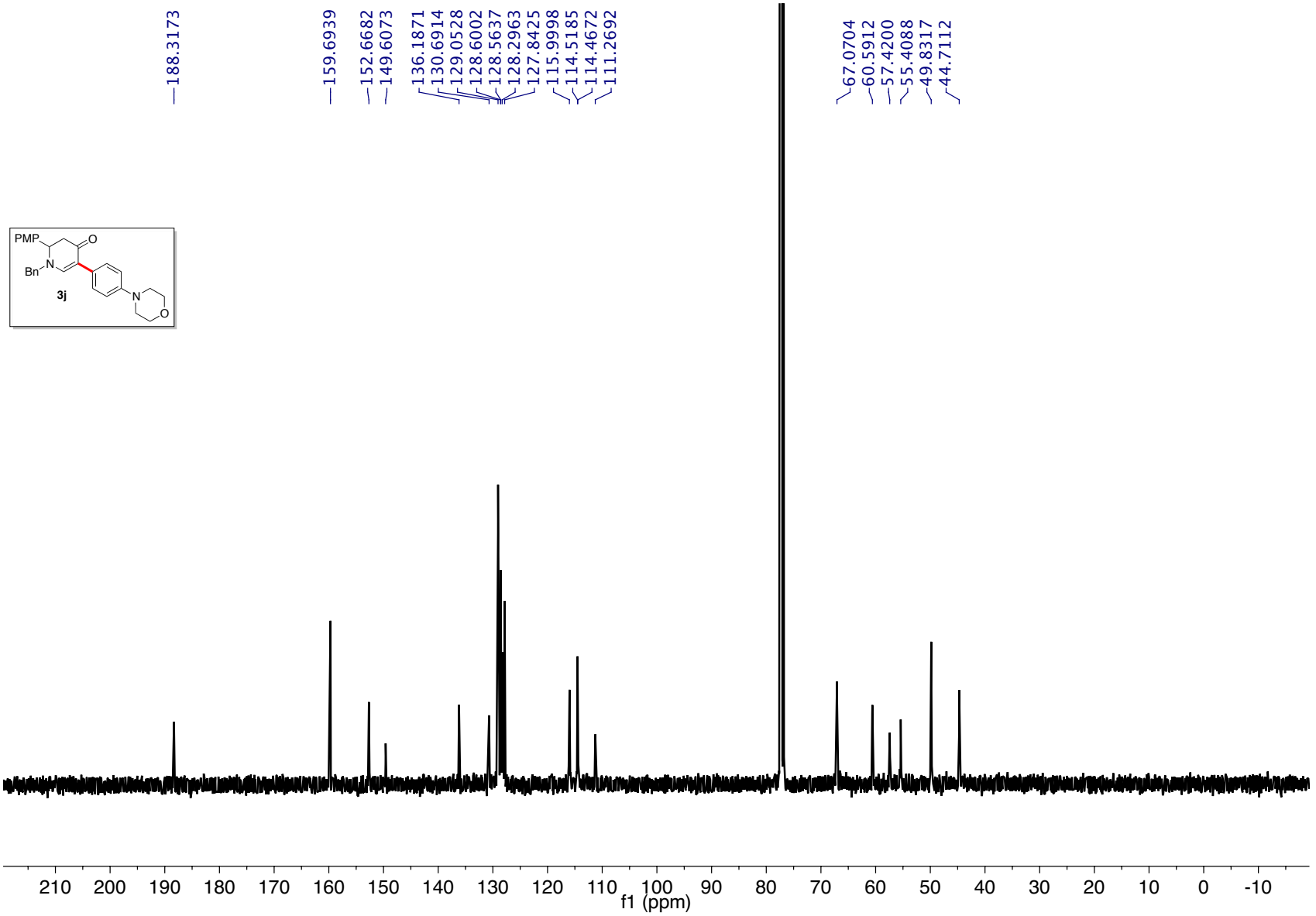

7.5147
7.3910
7.3850
7.3696
7.3517
7.3327
7.3170
7.2140
7.1922
7.1878
7.1836
7.1680
6.8971
6.8755
6.6720
4.5411
4.5212
4.5037
4.4395
4.4019
4.2385
4.2007
3.8675
3.8299
3.8121
2.9818
2.9647
2.9412
2.9242
2.8445
2.8239
2.8039
2.7833
PMP
O
N
Bn
OMe
OMe
OMe
3h
1.0000
3.1018
4.0873
2.0386
2.0346
1.0640
1.0312
1.0349
6.3105
3.1130
3.1503
1.0148
1.0303
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
f1 (ppm)

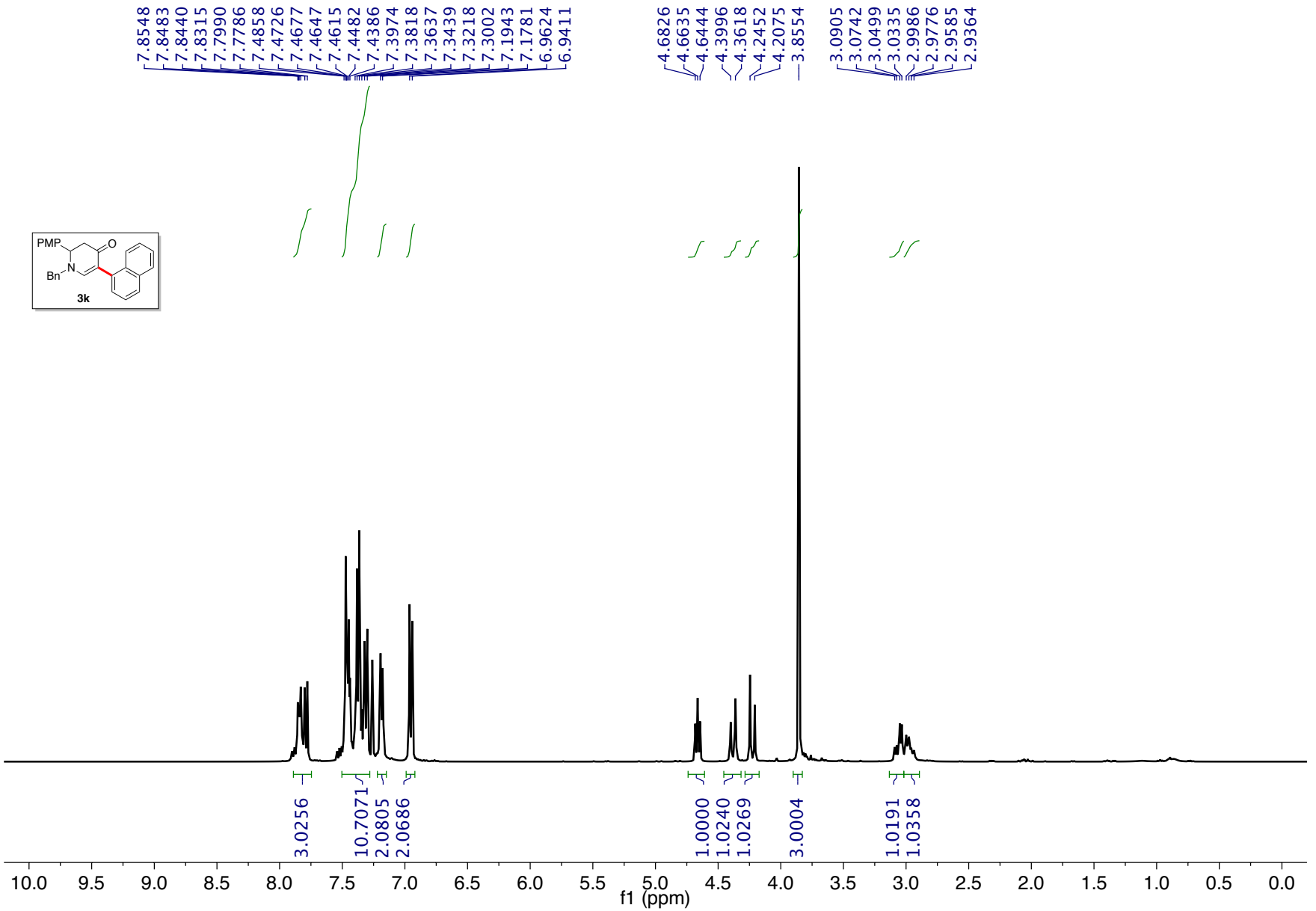

187.9818
159.7657
153.0675
136.5130
135.9566
131.9213
130.4640
129.0896
128.5027
128.4663
128.4029
127.8585
114.5729
111.0307
105.1668
60.9975
60.3547
57.4962
56.3388
55.4917
44.5557
PMP
Bn
N
O
OMe
OMe
OMe
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

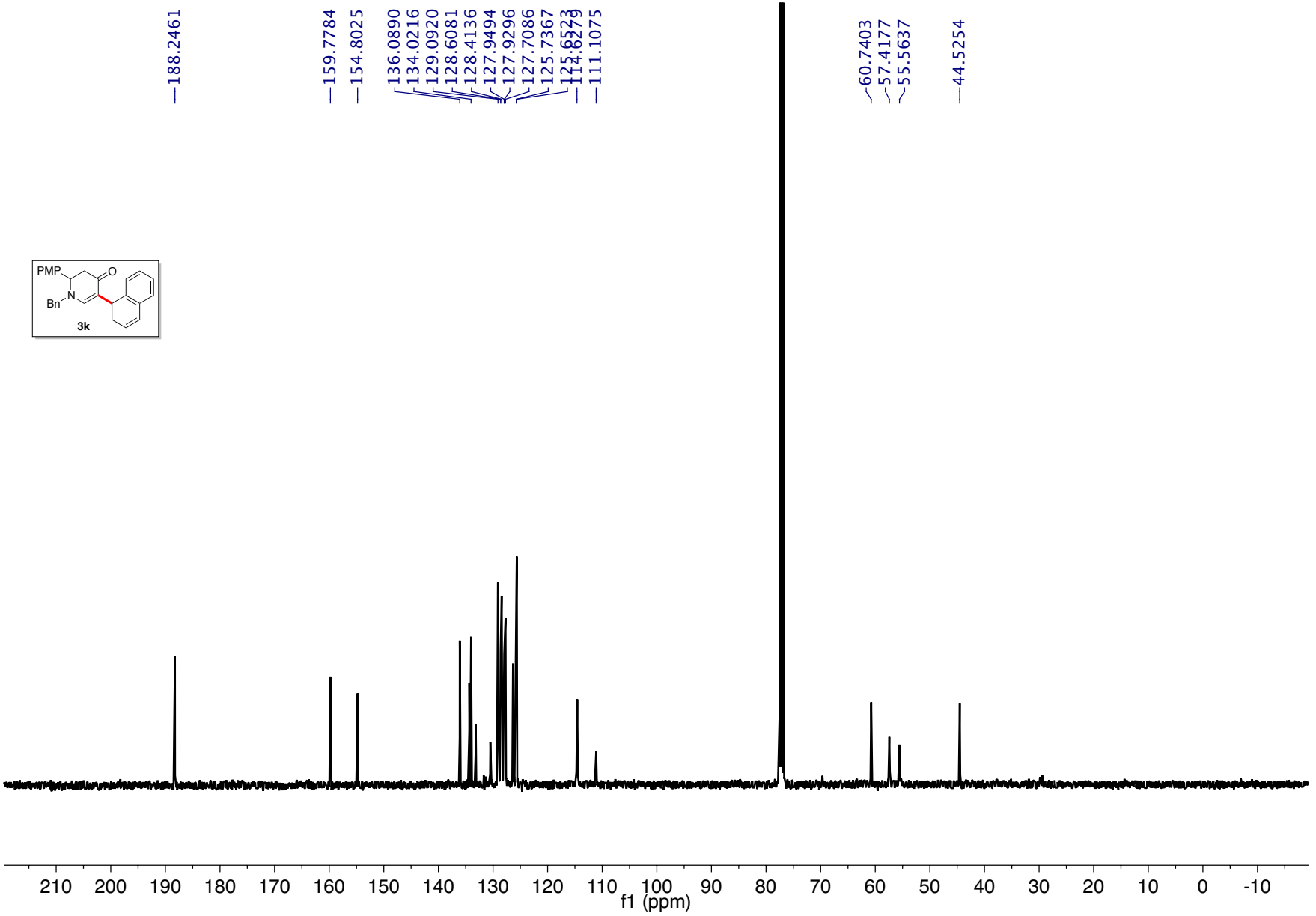

7.4593
7.3787
7.3721
7.3571
7.3384
7.3323
7.3211
7.3020
7.1978
7.1764
7.1630
7.1441
6.9727
6.9678
6.9265
6.9214
6.9057
6.9006
6.8845
6.8630
6.8404
6.8195
4.5150
4.4977
4.4938
4.4769
4.3935
4.3558
4.2412
4.1925
4.1548
3.8110
2.9441
2.9275
2.9036
2.8869
2.8350
2.8136
2.7946
2.7730
PMP
Bn
N
O
O
O
3i
1.0186
3.1568
4.0513
5.1993
1.0540
1.0715
4.0165
1.1026
2.9300
1.0356
1.0319
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
f1 (ppm)

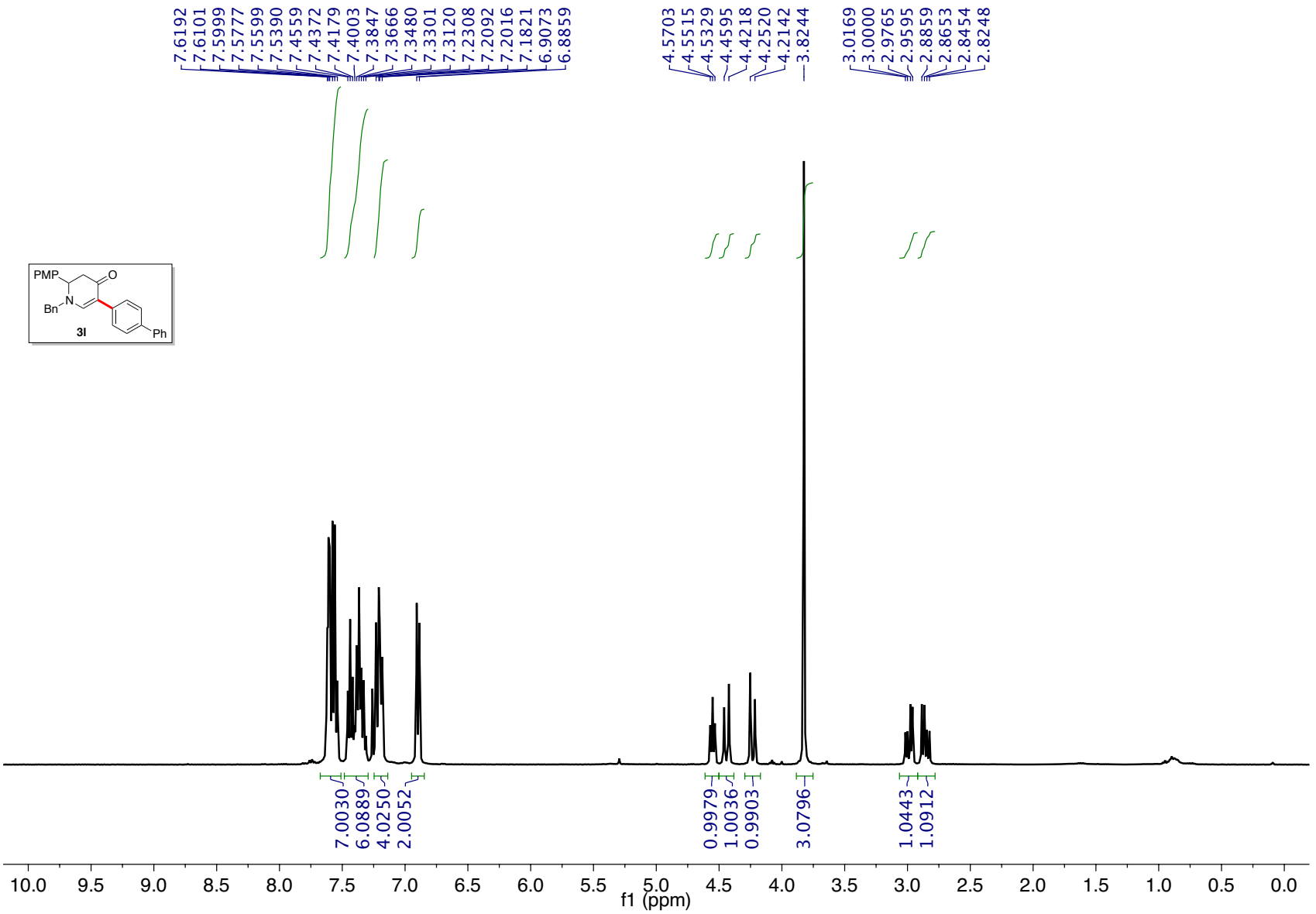

188.0453
159.6884
152.8480
143.2886
141.9571
136.1027
130.5963
129.7388
129.0549
128.4971
128.3090
127.8312
121.1395
117.0322
116.6934
114.4616
111.0132
108.7807
64.5214
60.5013
57.4365
55.4939
44.6283
PMP
Bn
N
O
O
O
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

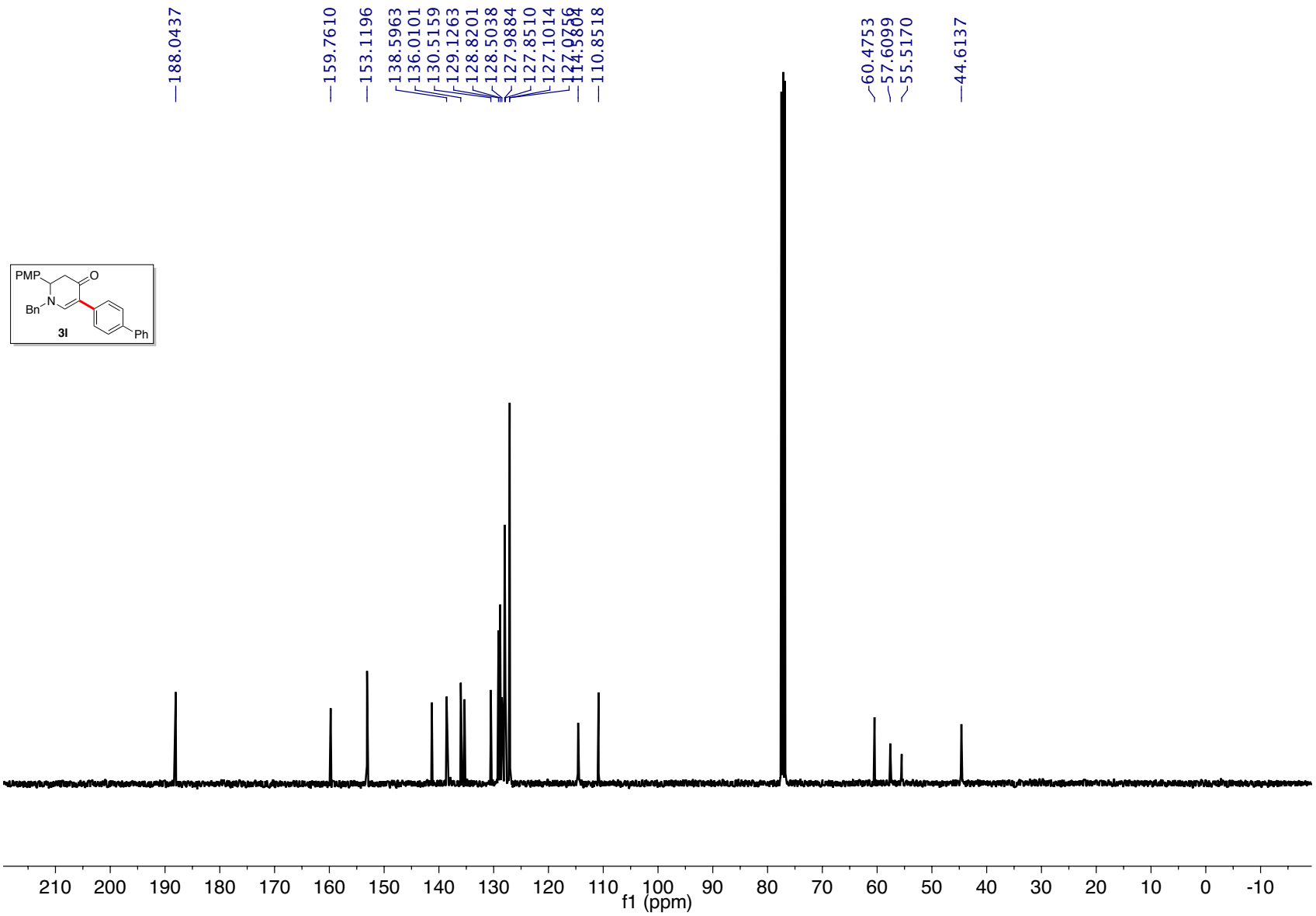

7.4715
7.3717
7.3585
7.3504
7.3408
7.3226
7.3055
7.2092
7.1877
7.1734
7.1689
7.1544
6.9161
6.8941
6.8872
6.8658
4.5240
4.5051
4.4862
4.4038
4.3662
4.1971
4.1593
3.8735
3.8619
3.8503
3.8136
3.1473
3.1376
3.1273
2.9558
2.9391
2.9150
2.8986
2.8500
2.8283
2.8095
2.7878
PMP
O
N
Bn
3j
N
O
1.0000
5.0749
4.1543
4.0392
1.0124
0.9839
0.9801
4.0724
3.1286
3.8541
1.0133
1.0260
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
f1 (ppm)

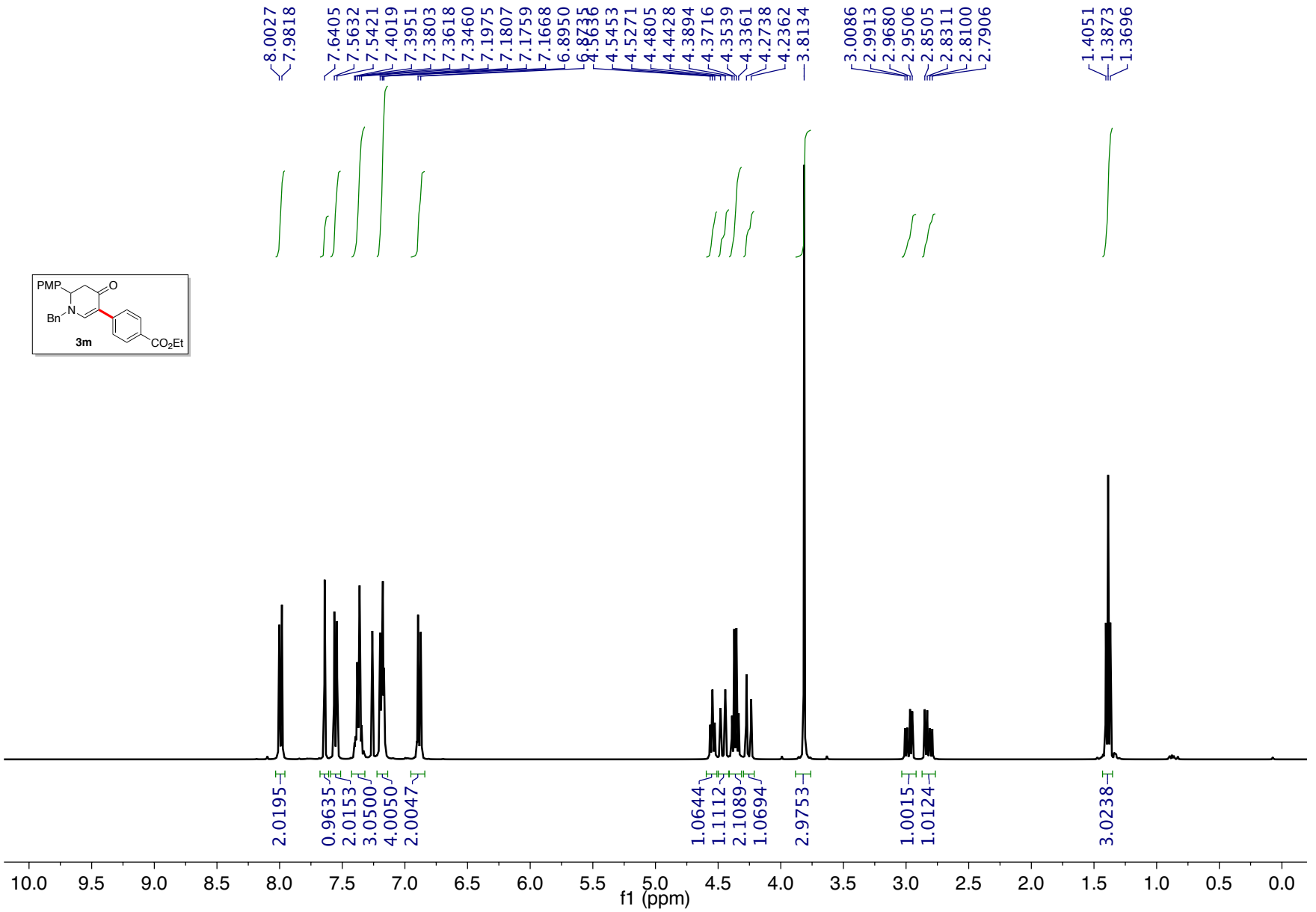

188.3173
159.6939
152.6682
149.6073
136.1871
130.6914
129.0528
128.6002
128.5637
128.2963
127.8425
115.9998
114.5185
114.4672
111.2692
67.0704
60.5912
57.4200
55.4088
49.8317
44.7112
PMP
Bn
N
O
3j
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

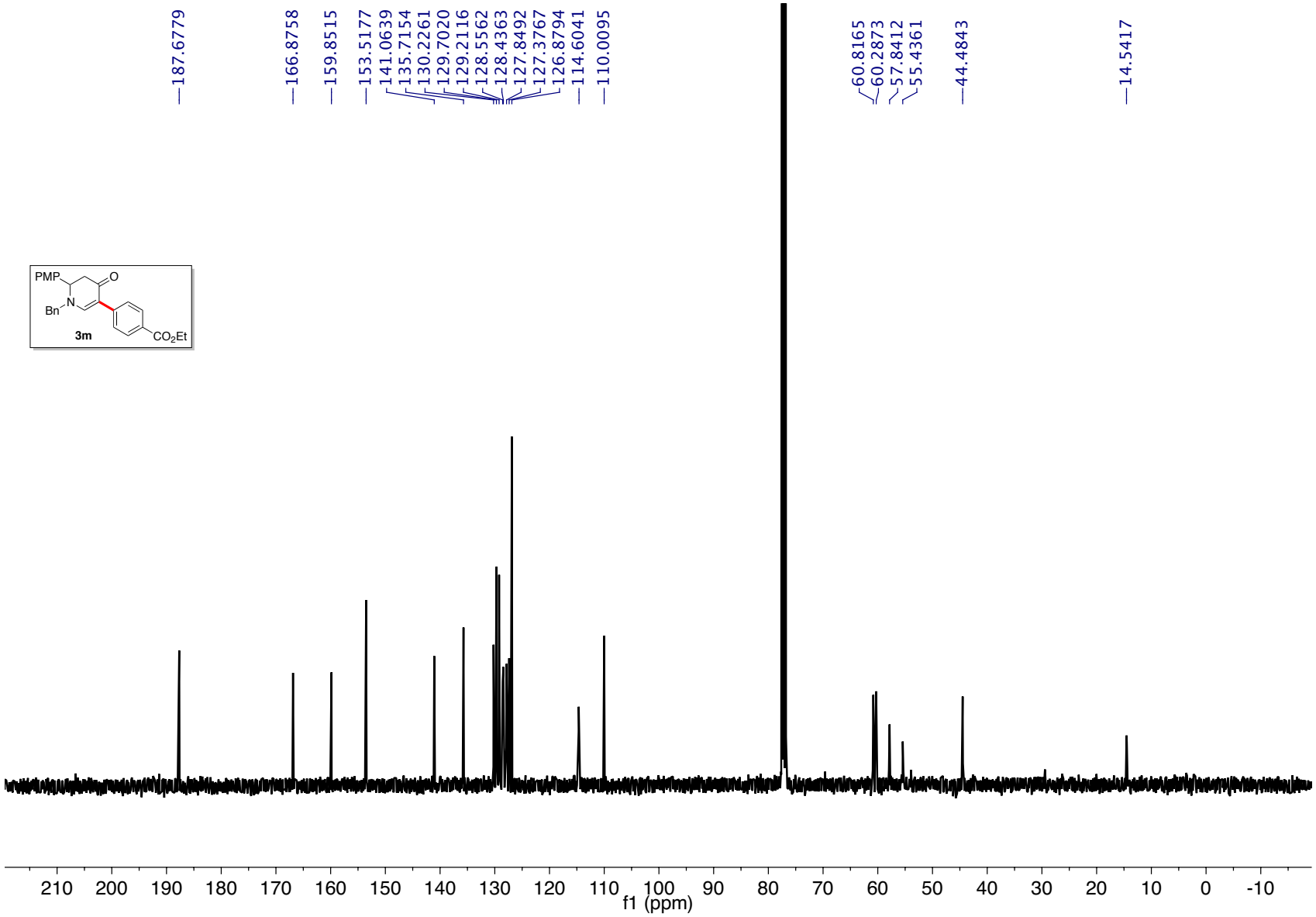

7.8548
7.8483
7.8440
7.8315
7.7990
7.7786
7.4858
7.4726
7.4677
7.4647
7.4615
7.4482
7.4386
7.3974
7.3818
7.3637
7.3439
7.3218
7.3002
7.1943
7.1781
6.9624
6.9411
4.6826
4.6635
4.6444
4.3996
4.3618
4.2452
4.2075
3.8554
3.0905
3.0742
3.0499
3.0335
2.9986
2.9776
2.9585
2.9364
PMP
O
N
Bn
3k
3.0256
10.7071
2.0805
2.0686
1.0000
1.0240
1.0269
3.0004
1.0191
1.0358
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
f1 (ppm)

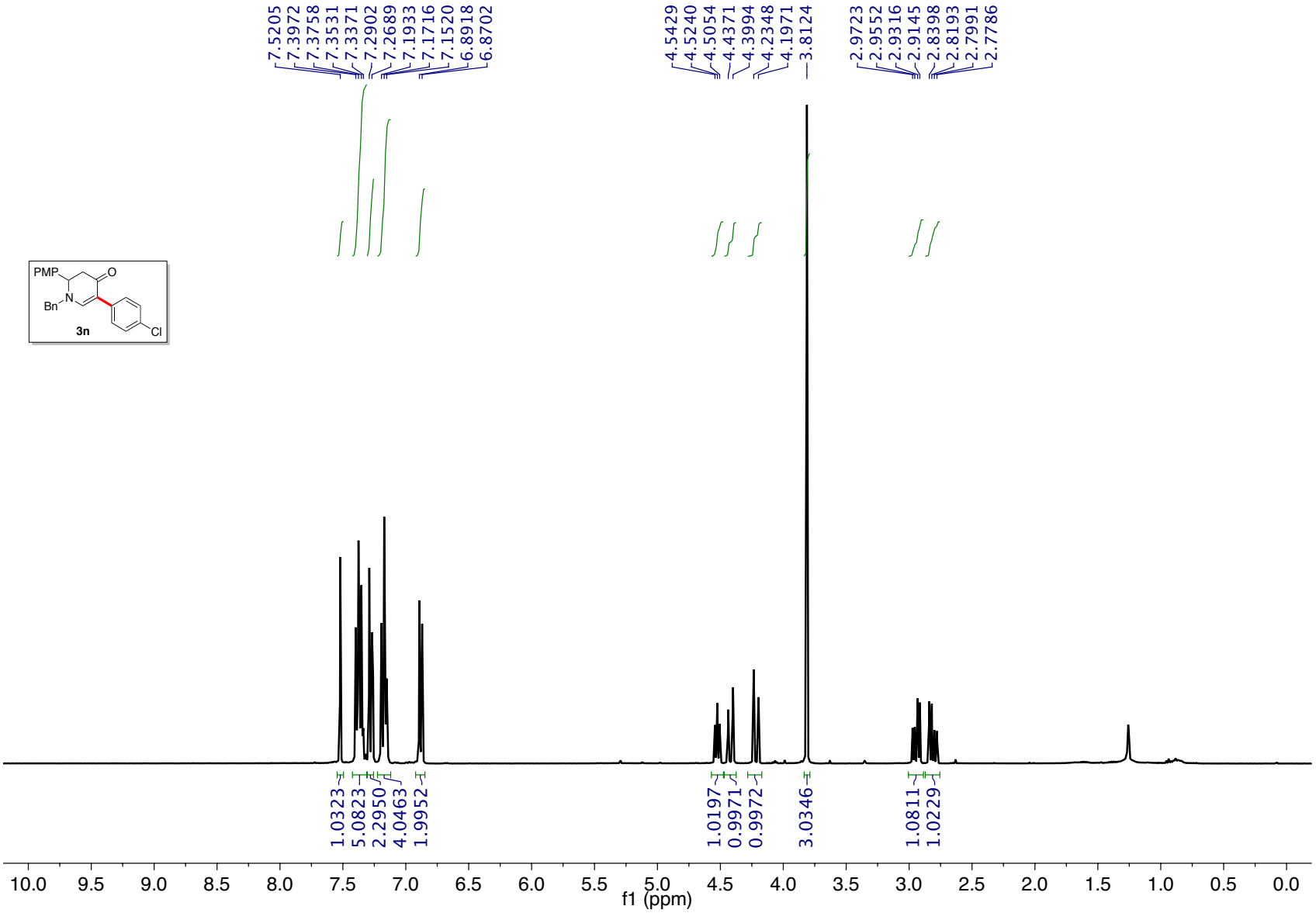

188.2461
159.7784
154.8025
136.0890
134.0216
129.0920
128.6081
128.4136
127.9494
127.9296
127.7086
125.7367
125.6523
114.8279
111.1075
60.7403
57.4177
55.5637
44.5254
PMP
Bn
N
O
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

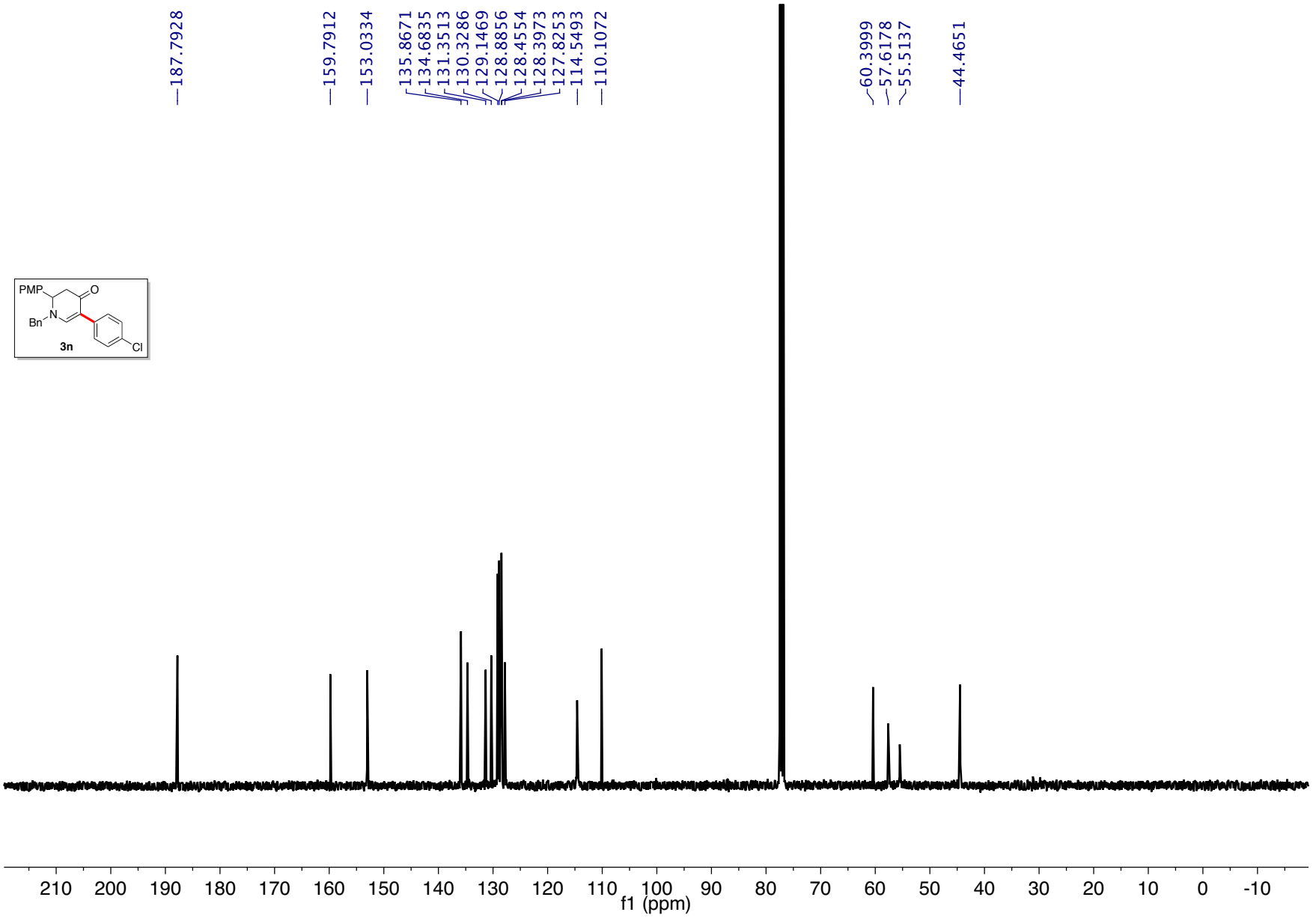

7.6192
7.6101
7.5999
7.5777
7.5599
7.5390
7.4559
7.4372
7.4179
7.4003
7.3847
7.3666
7.3480
7.3301
7.3120
7.2308
7.2092
7.2016
7.1821
6.9073
6.8859
4.5703
4.5515
4.5329
4.4595
4.4218
4.2520
4.2142
3.8244
3.0169
3.0000
2.9765
2.9595
2.8859
2.8653
2.8454
2.8248
PMP
O
N
Bn
3l
Ph
7.0030
6.0889
4.0250
2.0052
0.9979
1.0036
0.9903
3.0796
1.0443
1.0912
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
f1 (ppm)

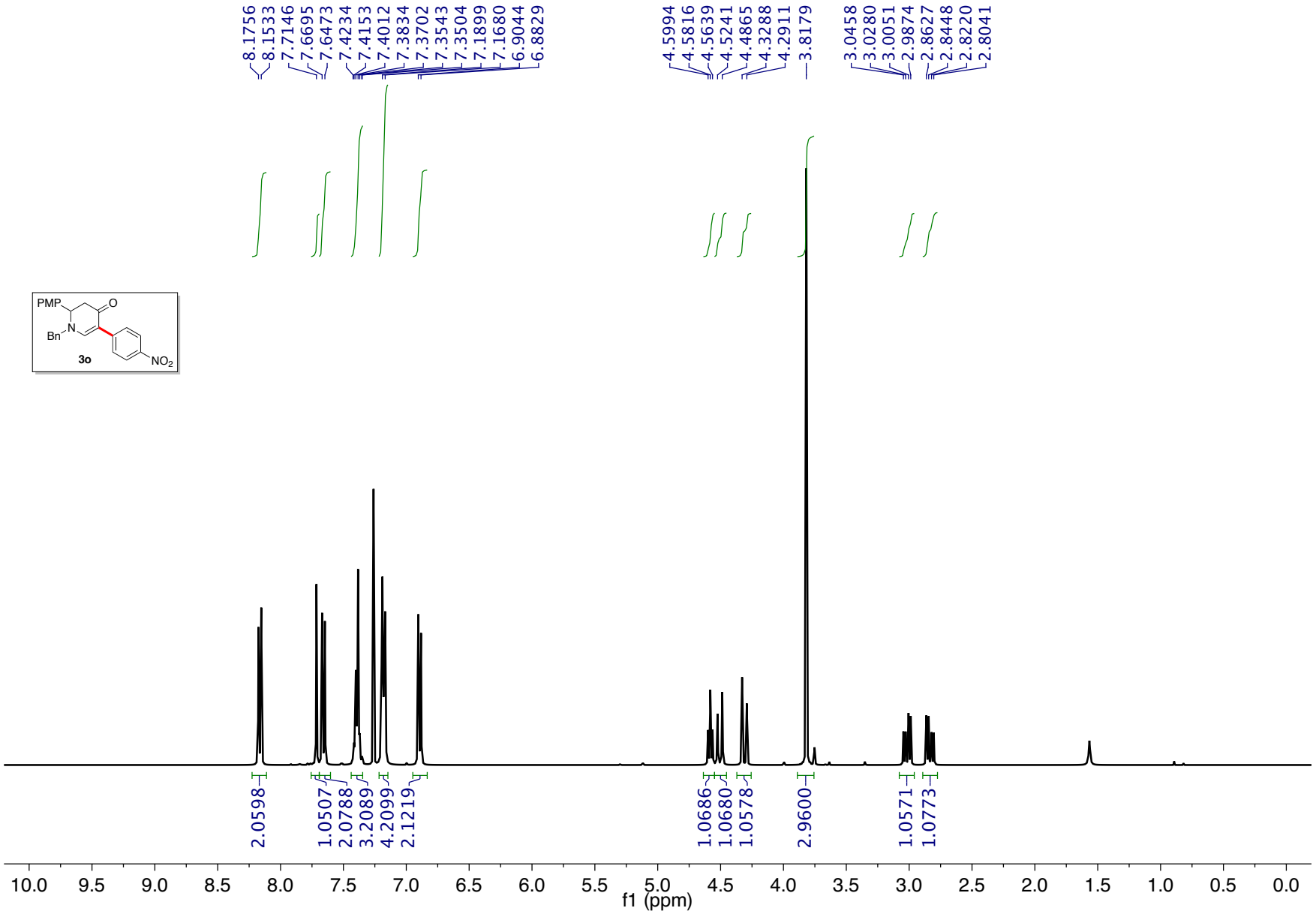

188.0437
159.7610
153.1196
138.5963
136.0101
130.5159
129.1263
128.8201
128.5038
127.9884
127.8510
127.1014
114.3804
110.8518
60.4753
57.6099
55.5170
44.6137
PMP
O
N
Bn
Ph
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

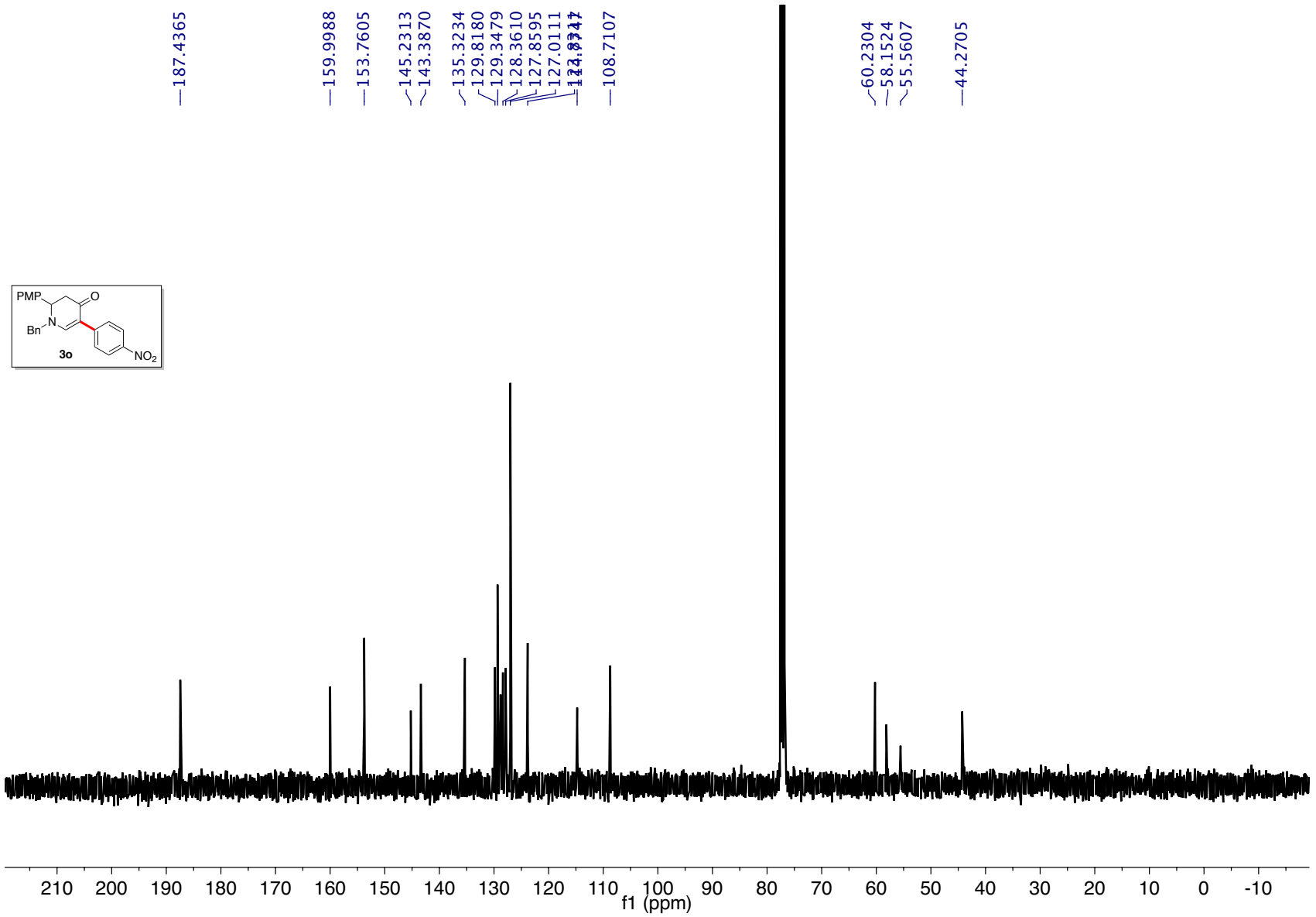

8.0027
7.9818
7.6405
7.5632
7.5421
7.4019
7.3951
7.3803
7.3618
7.3460
7.1975
7.1807
7.1759
7.1668
6.8950
4.5453
4.5271
4.4805
4.4428
4.3894
4.3716
4.3539
4.3361
4.2738
4.2362
3.8134
3.0086
2.9913
2.9680
2.9506
2.8505
2.8311
2.8100
2.7906
1.4051
1.3873
1.3696
PMP
Bn
N
O
CO2Et
3m
2.0195
0.9635
2.0153
3.0500
4.0050
2.0047
1.0644
1.1112
2.1089
1.0694
2.9753
1.0015
1.0124
3.0238
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
f1 (ppm)

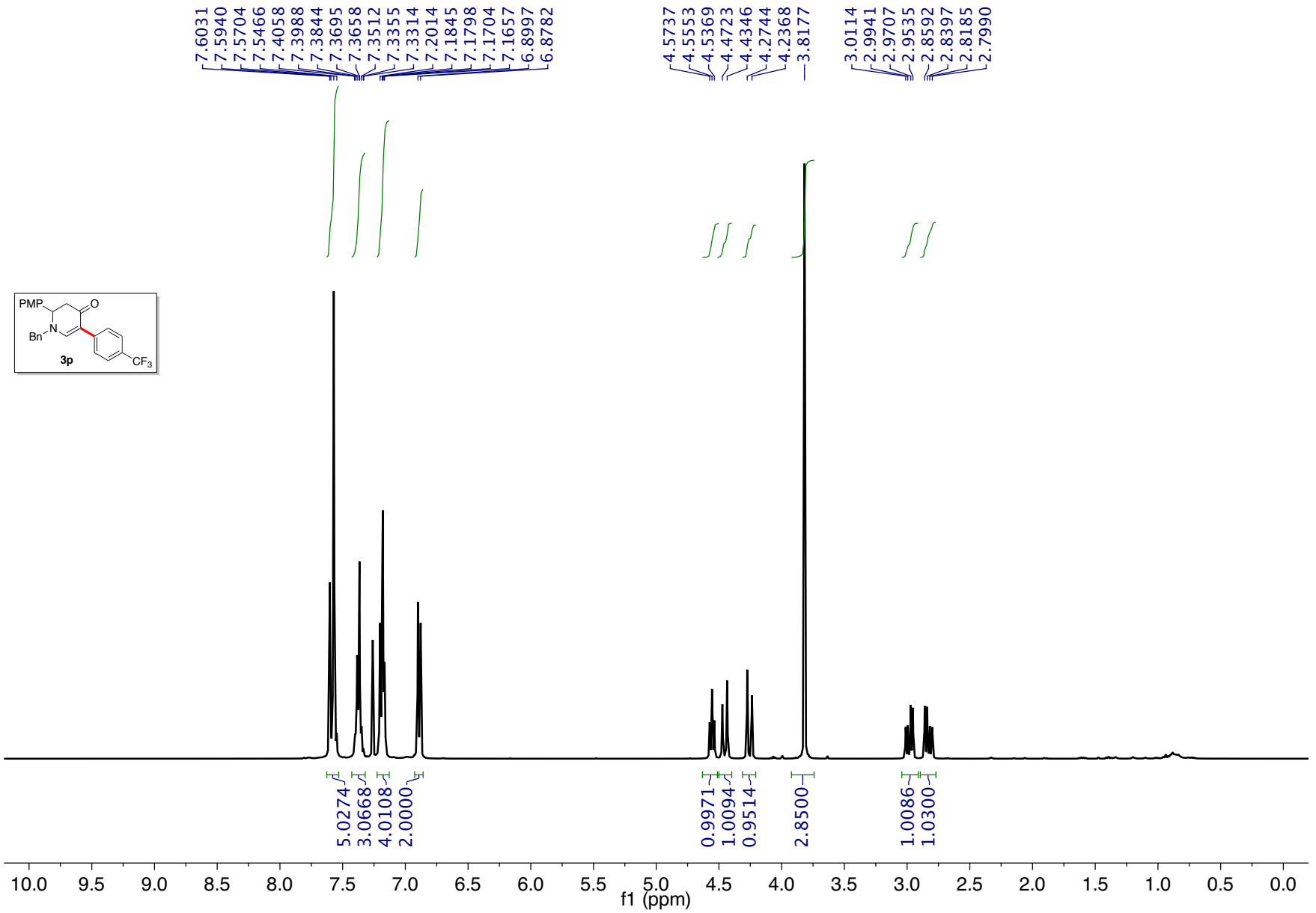

187.6779
166.8758
159.8515
153.5177
141.0639
135.7154
130.2261
129.7020
129.2116
128.5562
128.4363
127.8492
127.3767
126.8794
114.6041
110.0095
60.8165
60.2873
57.8412
55.4361
44.4843
14.5417
PMP
O
N
Bn
3m
CO2Et
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

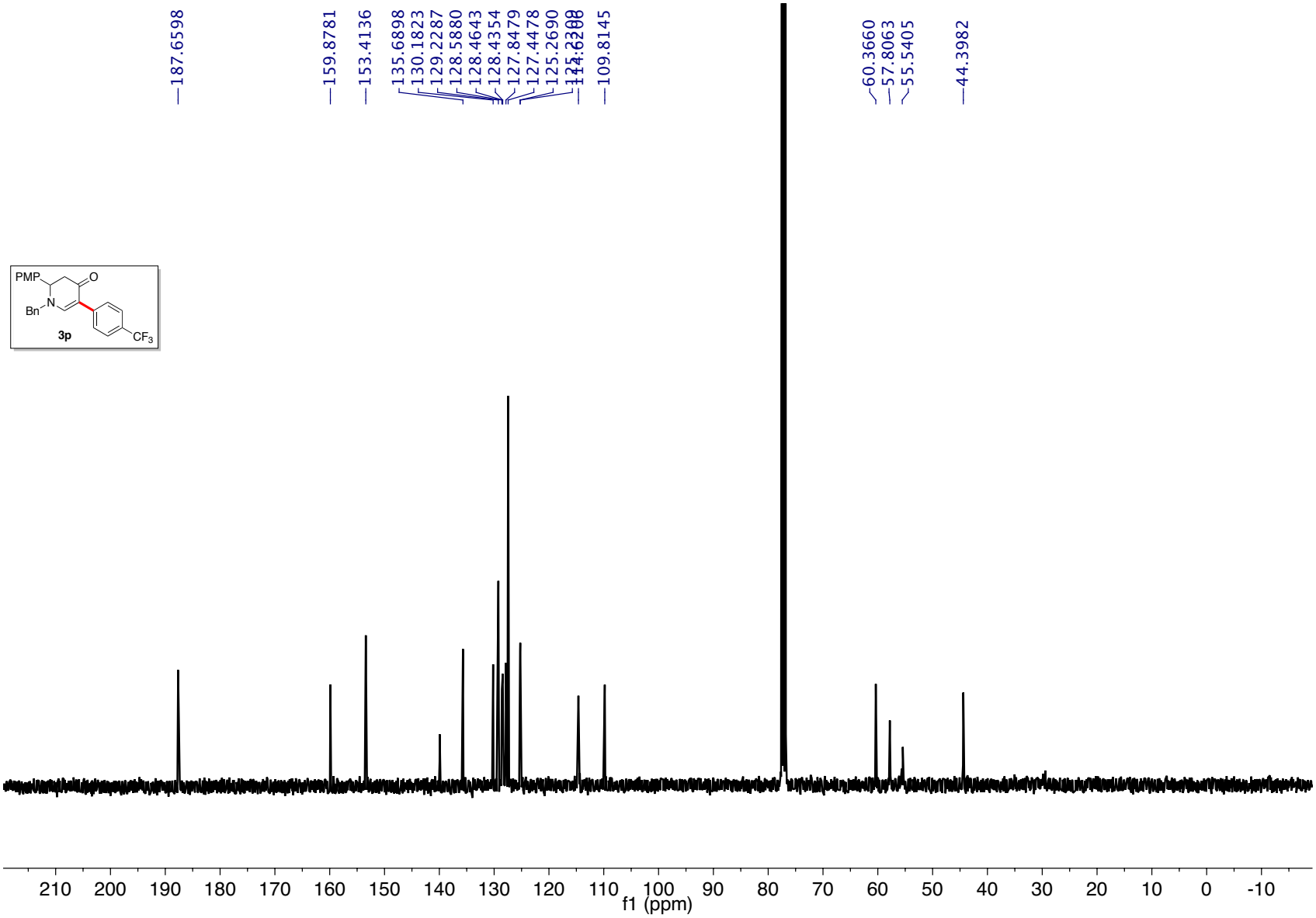

7.5205
7.3972
7.3758
7.3531
7.3371
7.2902
7.2689
7.1933
7.1716
7.1520
6.8918
6.8702
4.5429
4.5240
4.5054
4.4371
4.3994
4.2348
4.1971
3.8124
2.9723
2.9552
2.9316
2.9145
2.8398
2.8193
2.7991
2.7786
PMP
O
N
Bn
Cl
3n
1.0323
5.0823
2.2950
4.0463
1.9952
1.0197
0.9971
0.9972
3.0346
1.0811
1.0229
10.0 9.5 9.0 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
f1 (ppm)

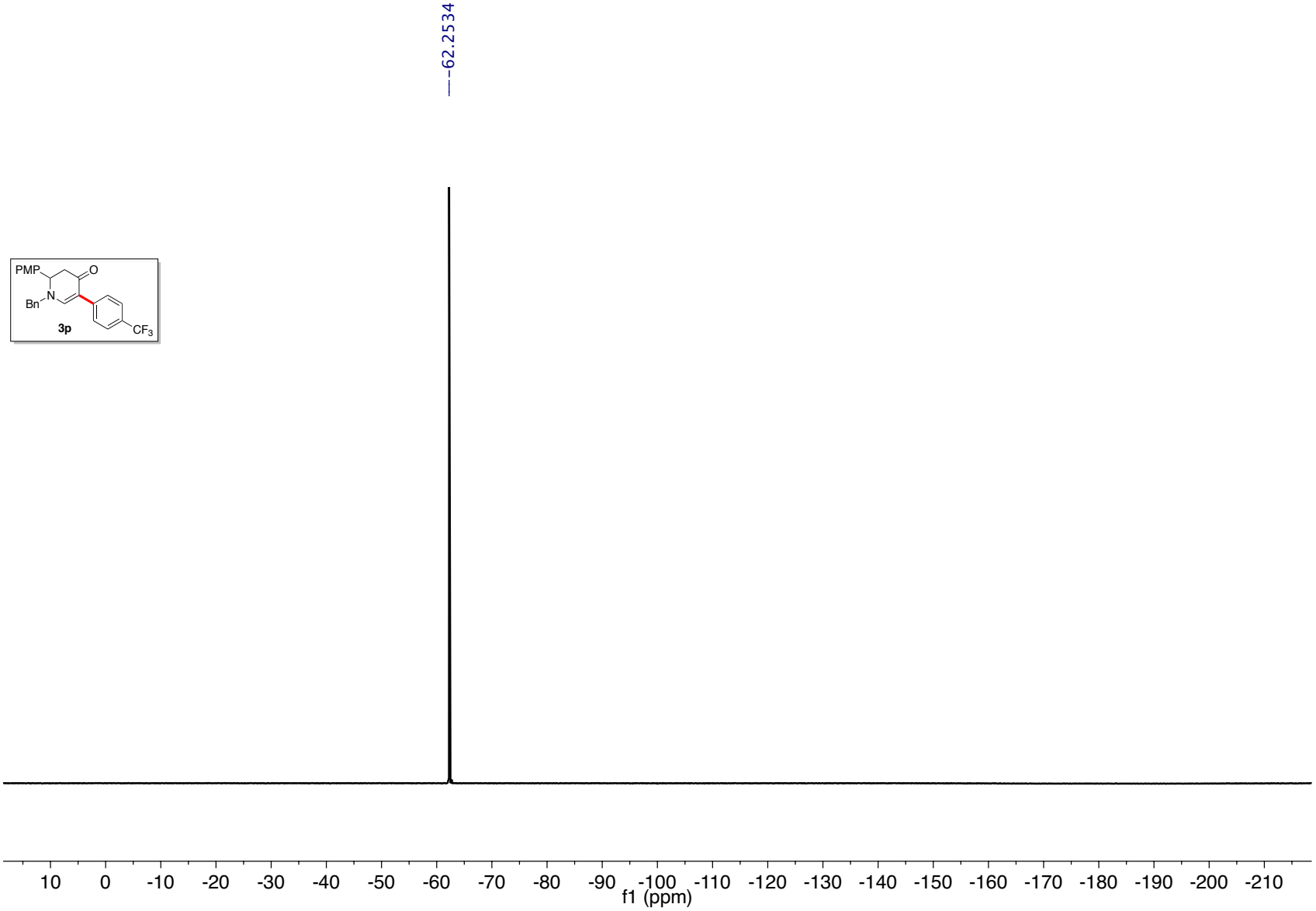

187.7928
159.7912
153.0334
135.8671
134.6835
131.3513
130.3286
129.1469
128.8856
128.4554
128.3973
127.8253
114.5493
110.1072
60.3999
57.6178
55.5137
44.4651
PMP
Bn
N
O
Cl
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

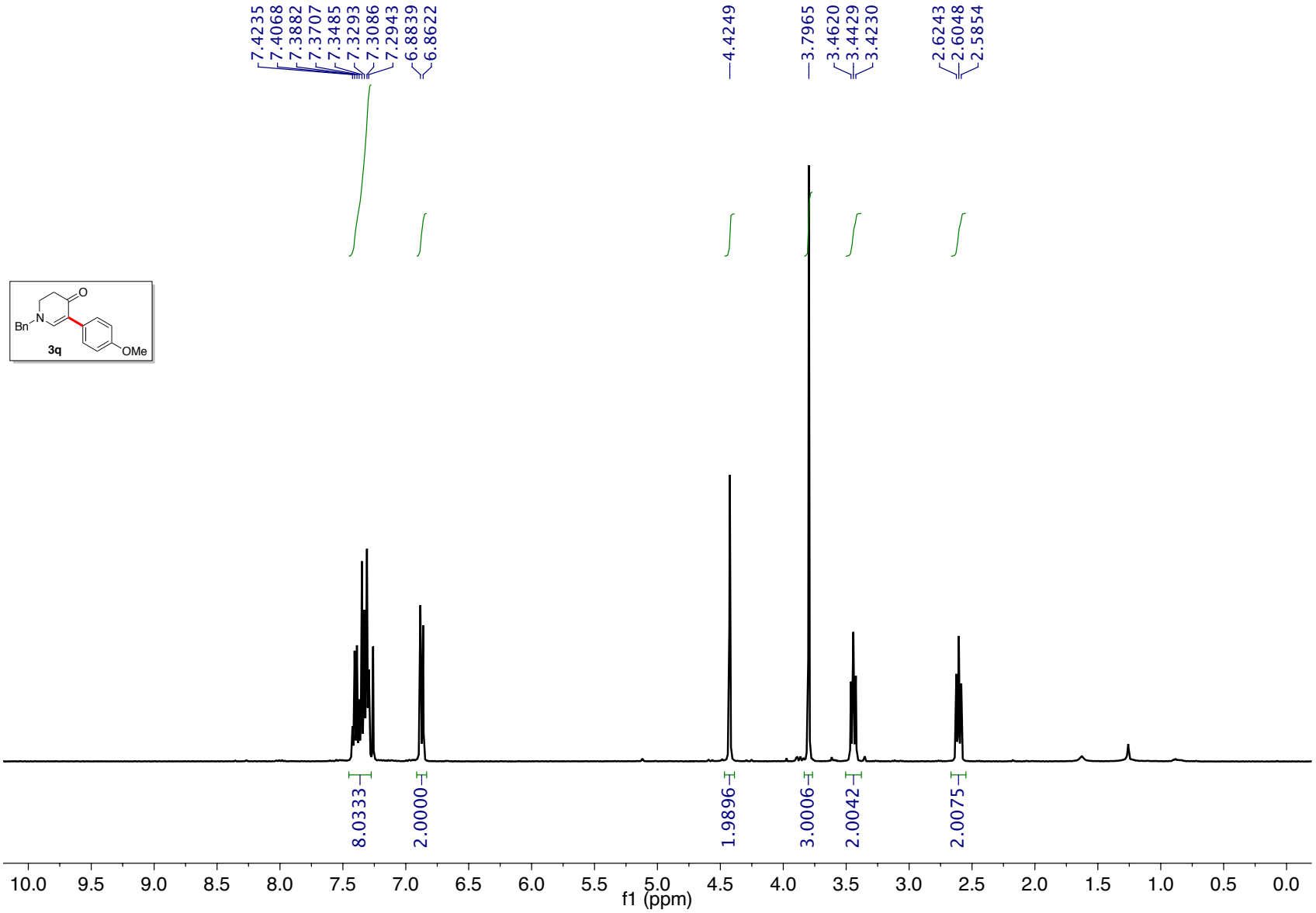

8.1756
8.1533
7.7146
7.6695
7.6473
7.4234
7.4153
7.4012
7.3834
7.3702
7.3543
7.3504
7.1899
7.1680
6.9044
6.8829
4.5994
4.5816
4.5639
4.5241
4.4865
4.3288
4.2911
3.8179
3.0458
3.0280
3.0051
2.9874
2.8627
2.8448
2.8220
2.8041
PMP
O
Bn
N
3o
NO2
2.0598
1.0507
2.0788
3.2089
4.2099
2.1219
1.0686
1.0680
1.0578
2.9600
1.0571
1.0773
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
f1 (ppm)

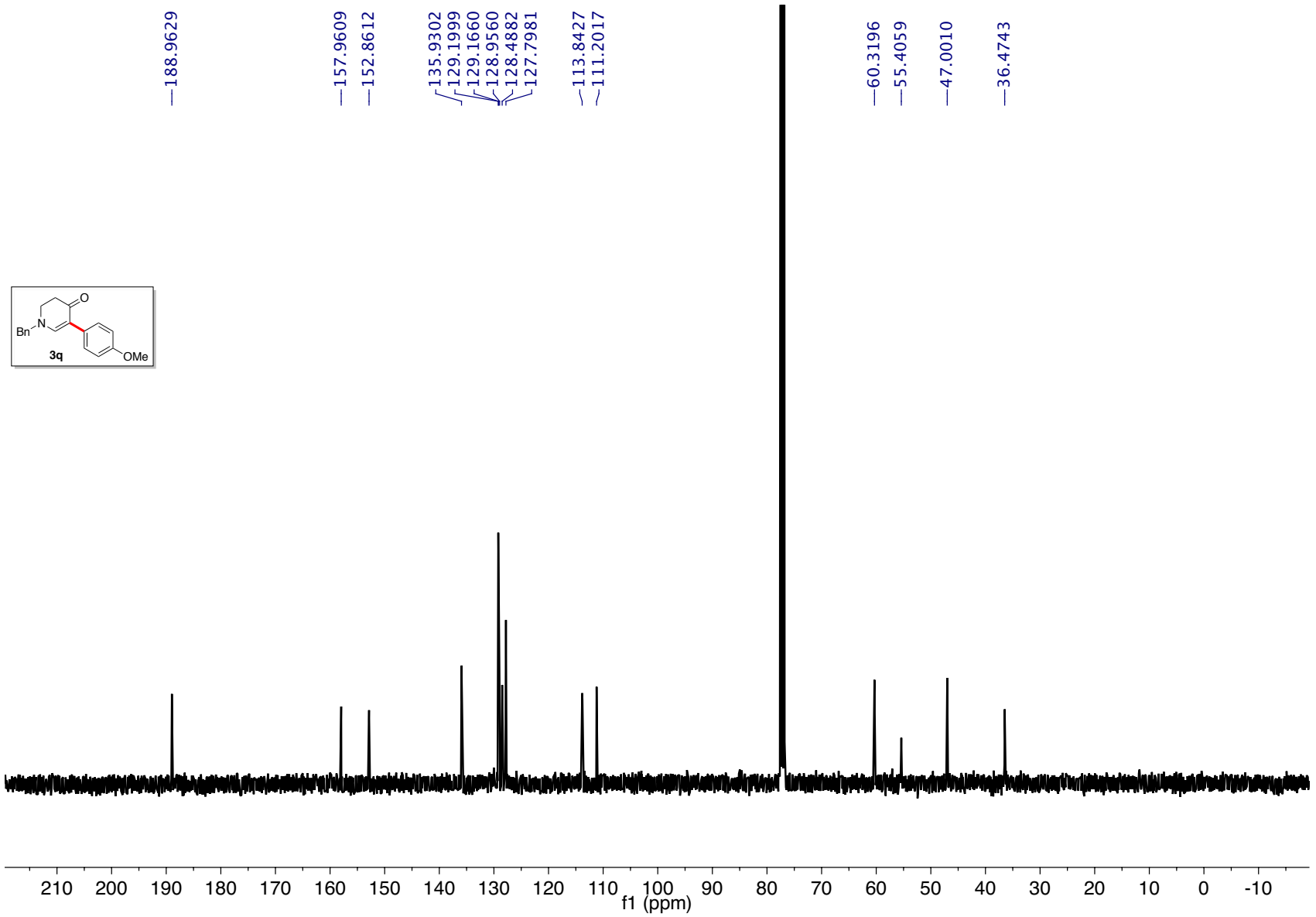

187.4365
159.9988
153.7605
145.2313
143.3870
135.3234
129.8180
129.3479
128.3610
127.8595
127.0111
108.7107
60.2304
58.1524
55.5607
44.2705
PMP
O
N
Bn
3o
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

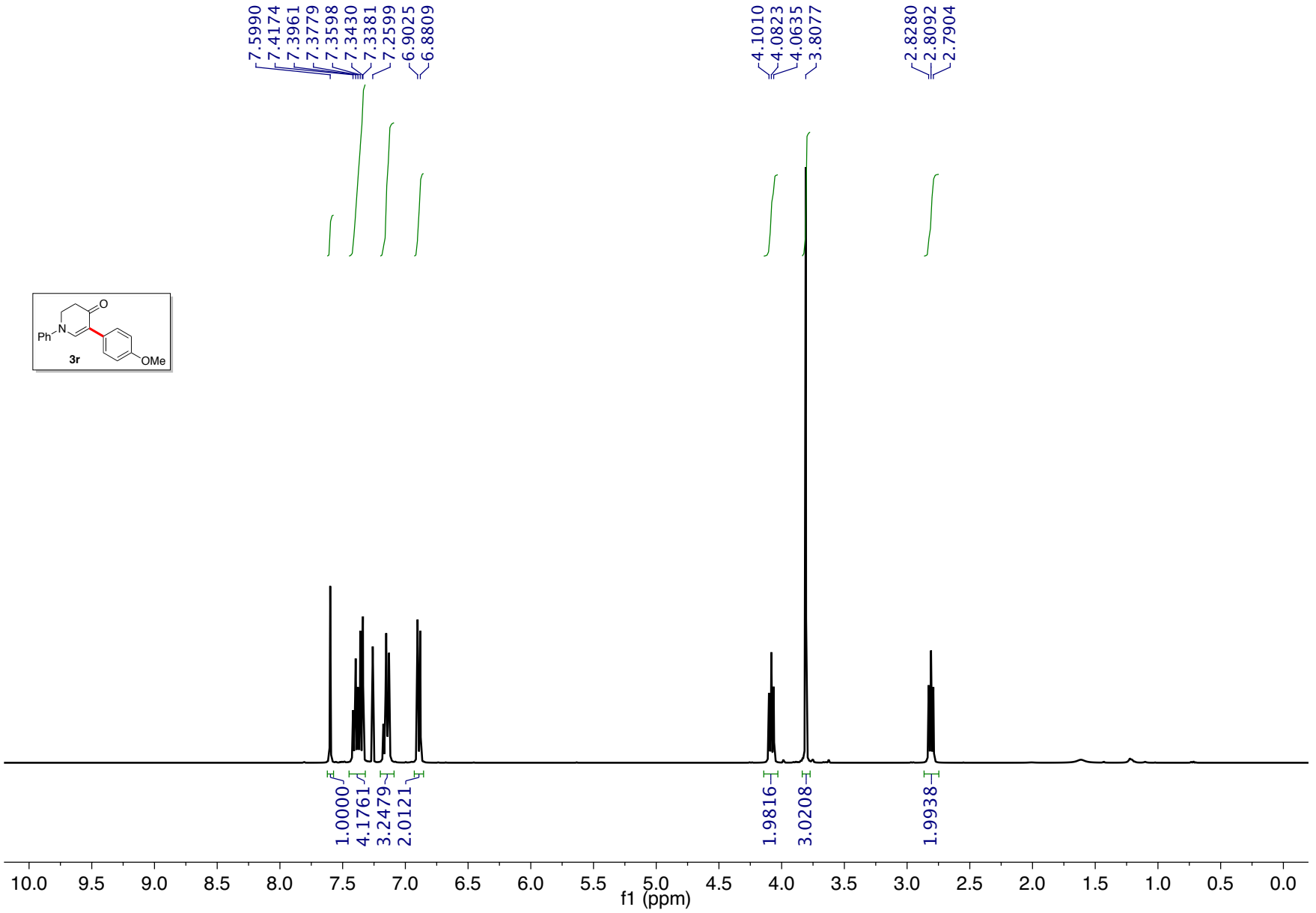

7.6031
7.5940
7.5704
7.5466
7.4058
7.3988
7.3844
7.3695
7.3658
7.3512
7.3355
7.3314
7.2014
7.1845
7.1798
7.1704
7.1657
6.8997
6.8782
4.5737
4.5553
4.5369
4.4723
4.4346
4.2744
4.2368
3.8177
3.0114
2.9941
2.9707
2.9535
2.8592
2.8397
2.8185
2.7990
PMP
O
N
Bn
3p
CF3
5.0274
3.0668
4.0108
2.0000
0.9971
1.0094
0.9514
2.8500
1.0086
1.0300
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
f1 (ppm)

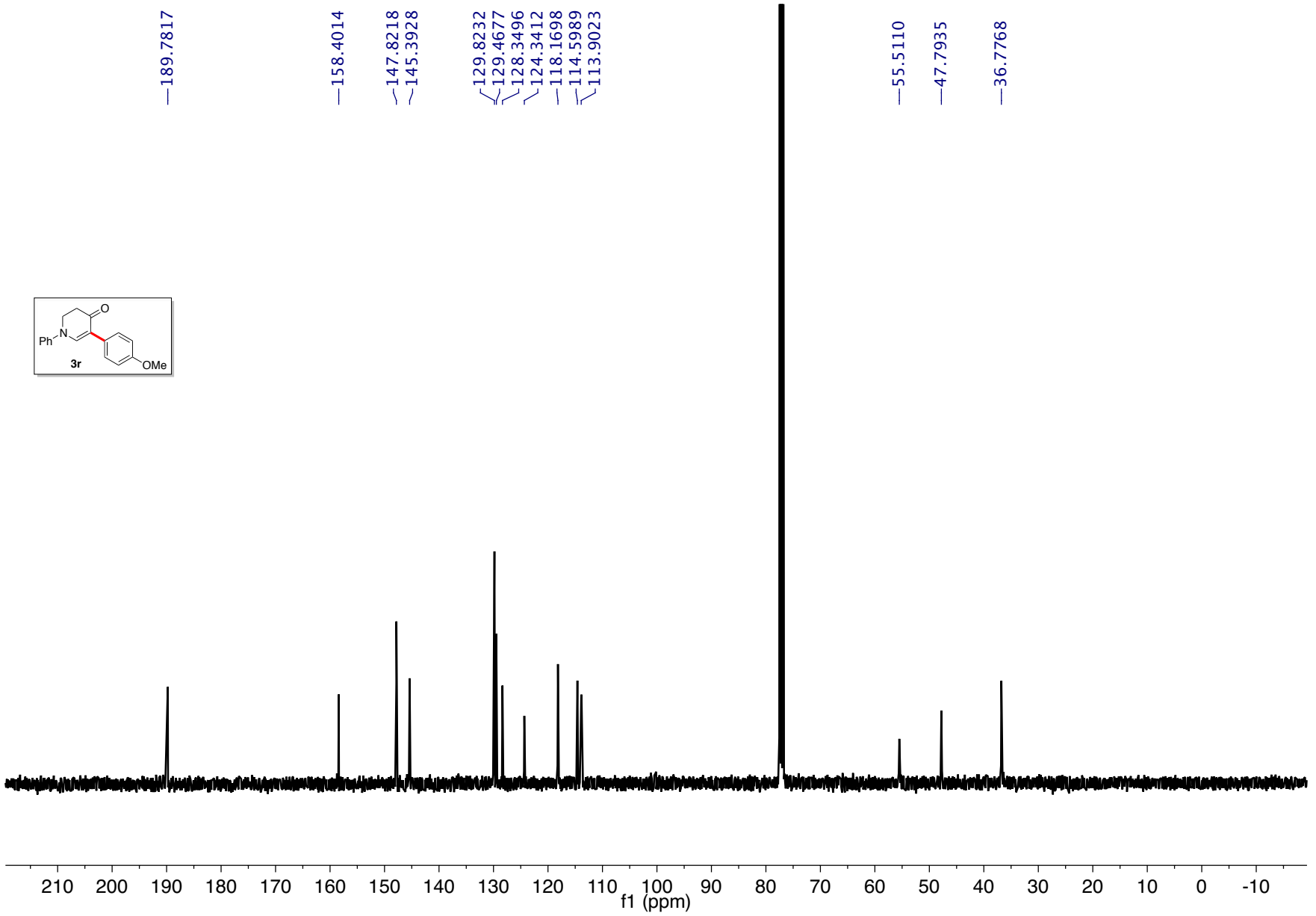

187.6598
159.8781
153.4136
135.6898
130.1823
129.2287
128.5880
128.4643
128.4354
127.8479
127.4478
125.2690
109.8145
60.3660
57.8063
55.5405
44.3982
PMP
Bn
N
O
CF3
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

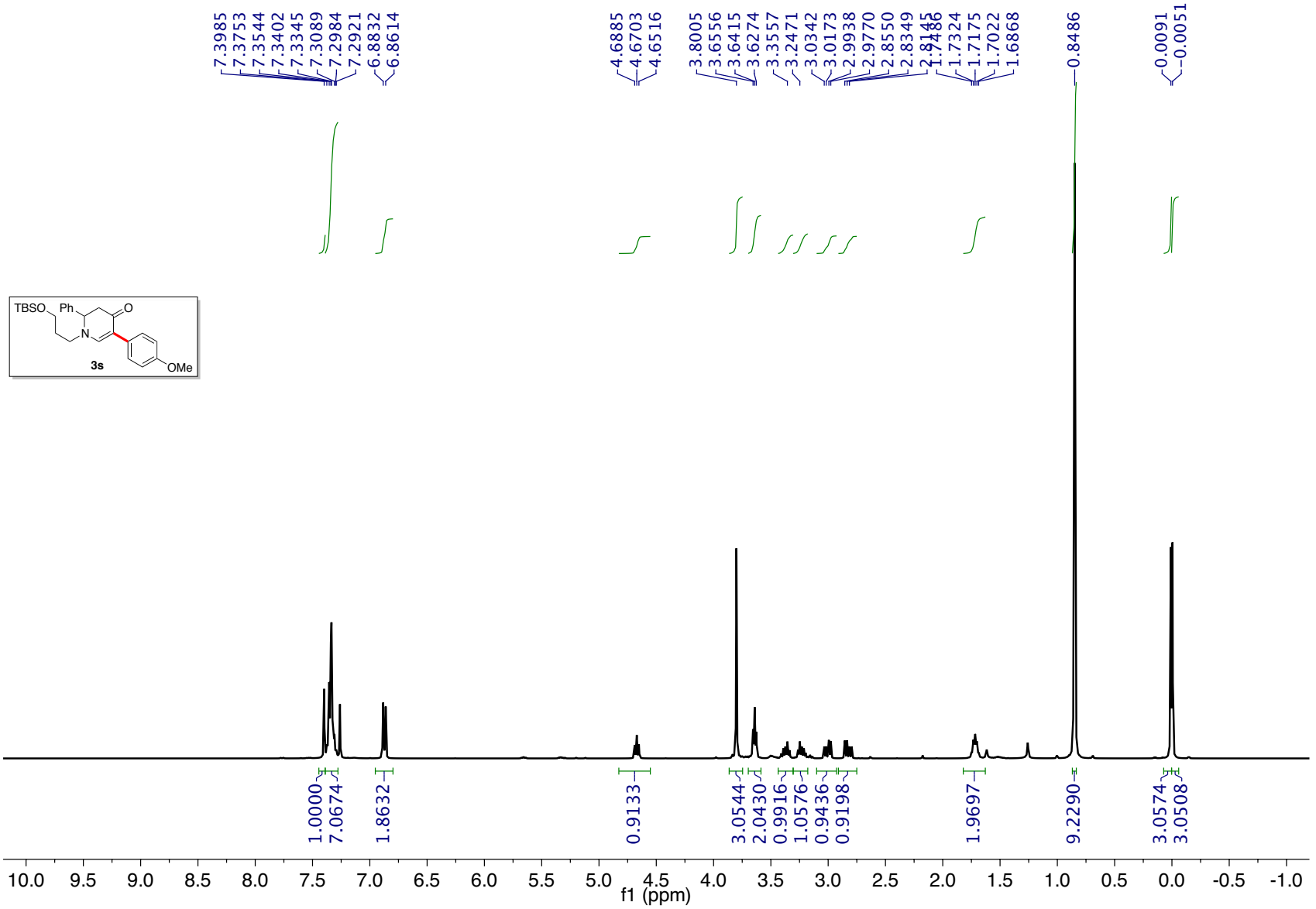

−62.2534
PMP
O
N
Bn
3p
CF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

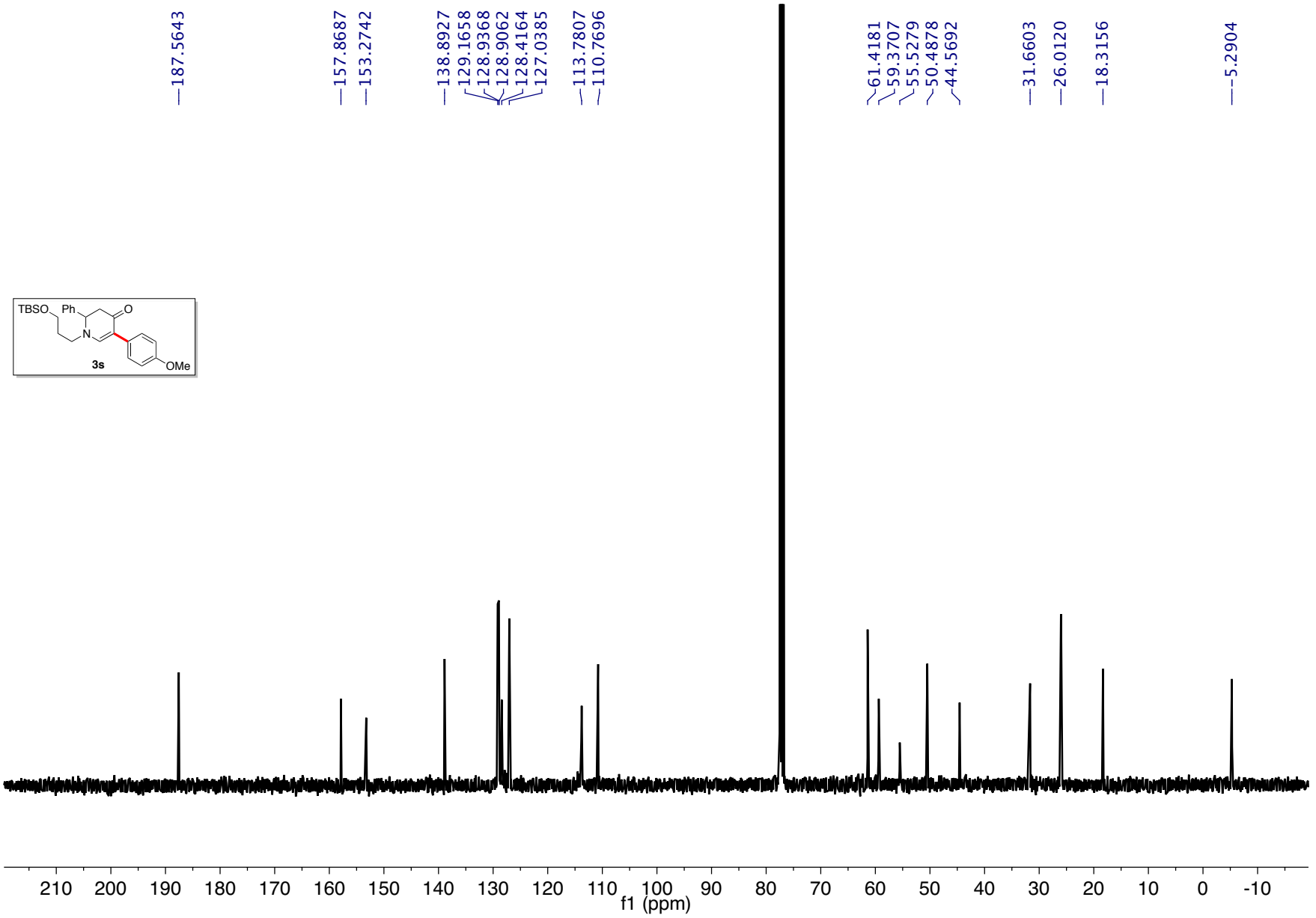

7.4235
7.4068
7.3882
7.3707
7.3485
7.3293
7.3086
7.2943
6.8839
6.8622
4.4249
3.7965
3.4620
3.4429
3.4230
2.6243
2.6048
2.5854
Bn
N
O
OMe
3q
8.0333
2.0000
1.9896
3.0006
2.0042
2.0075
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

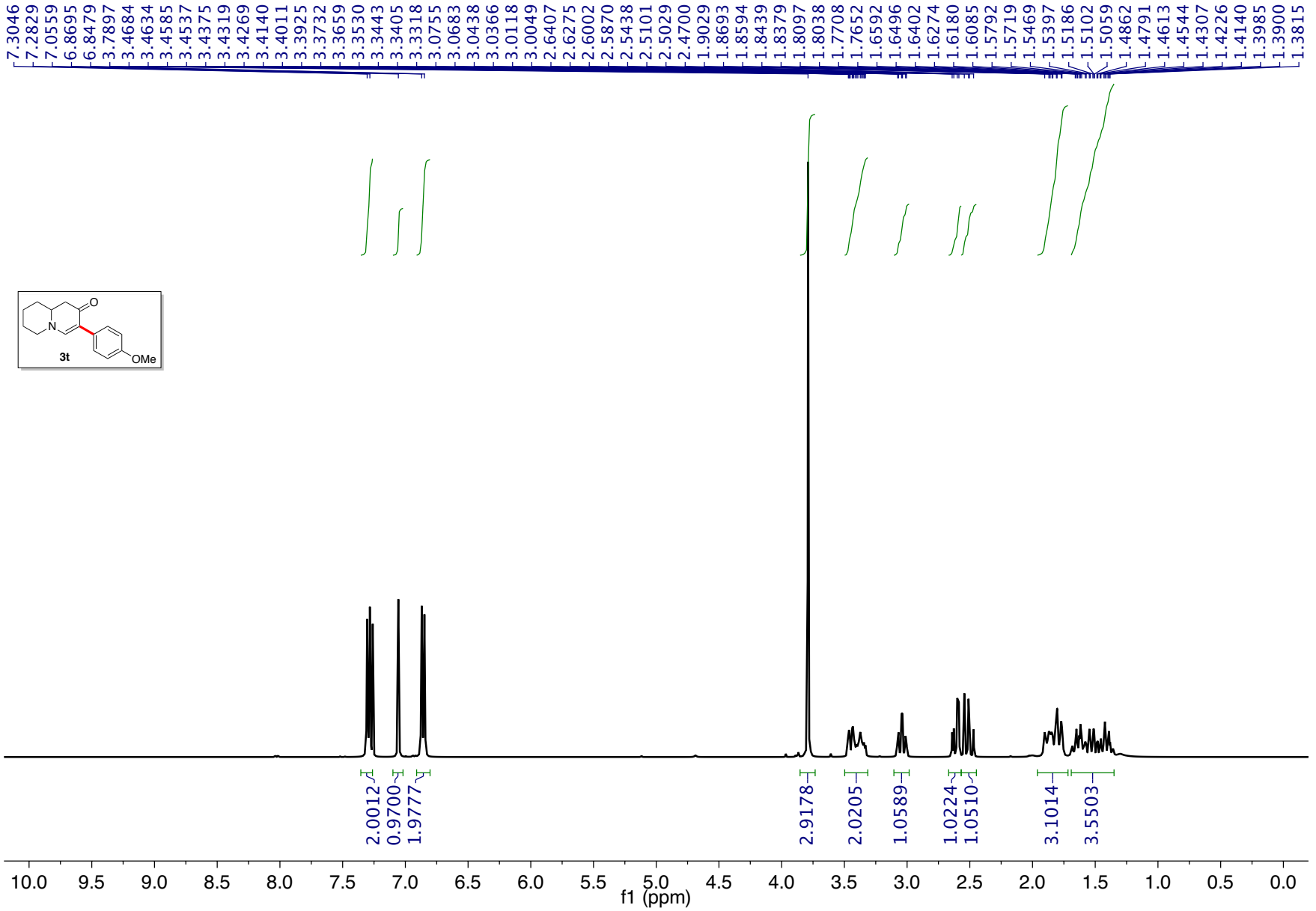

188.9629
157.9609
152.8612
135.9302
129.1999
129.1660
128.9560
128.4882
127.7981
113.8427
111.2017
60.3196
55.4059
47.0010
36.4743
Bn
N
O
OMe
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

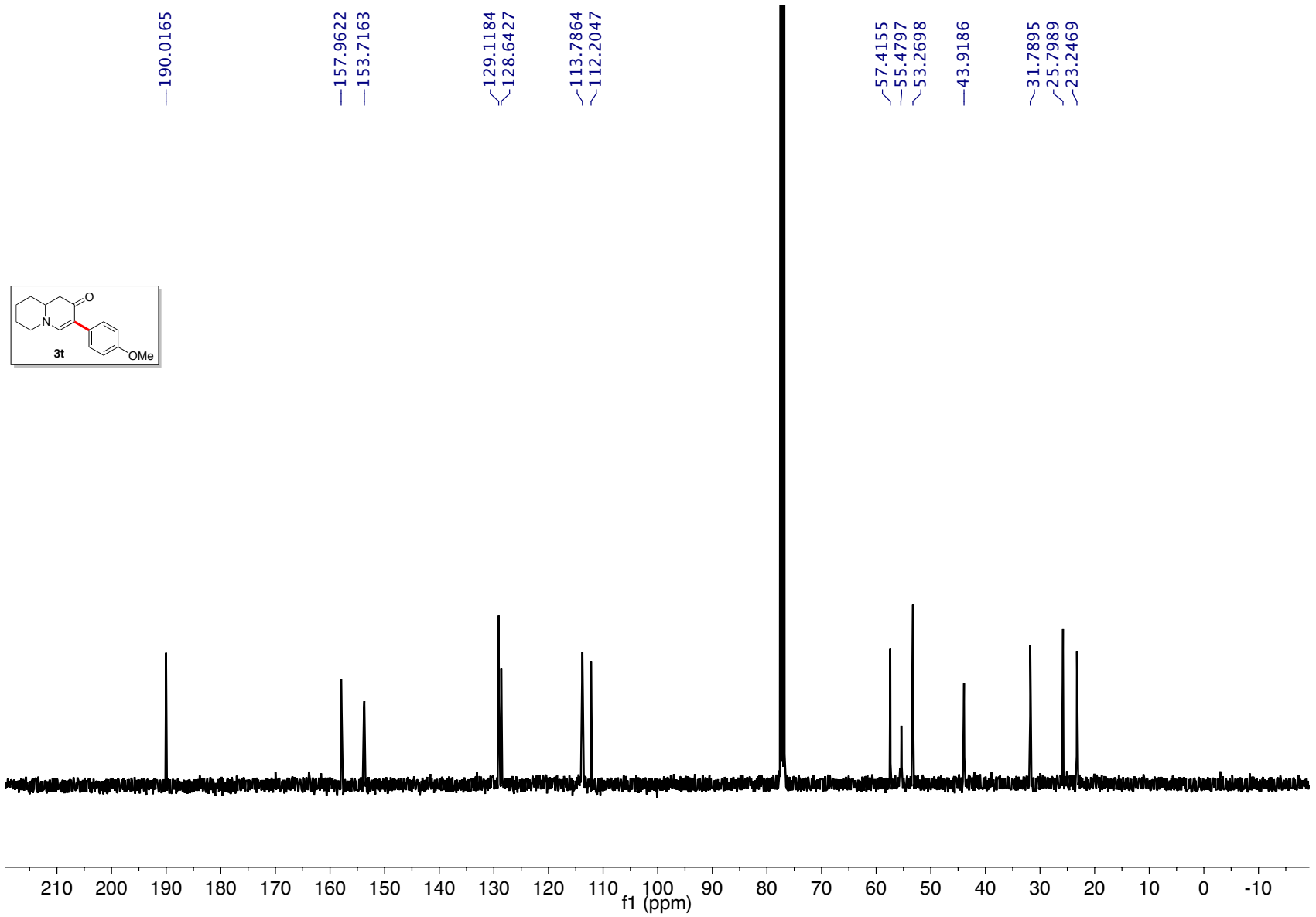

7.5990
7.4174
7.3961
7.3779
7.3598
7.3430
7.3381
7.2599
6.9025
6.8809
4.1010
4.0823
4.0635
3.8077
2.8280
2.8092
2.7904
Ph
N
O
3r
OMe
1.0000
4.1761
3.2479
2.0121
1.9816
3.0208
1.9938
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

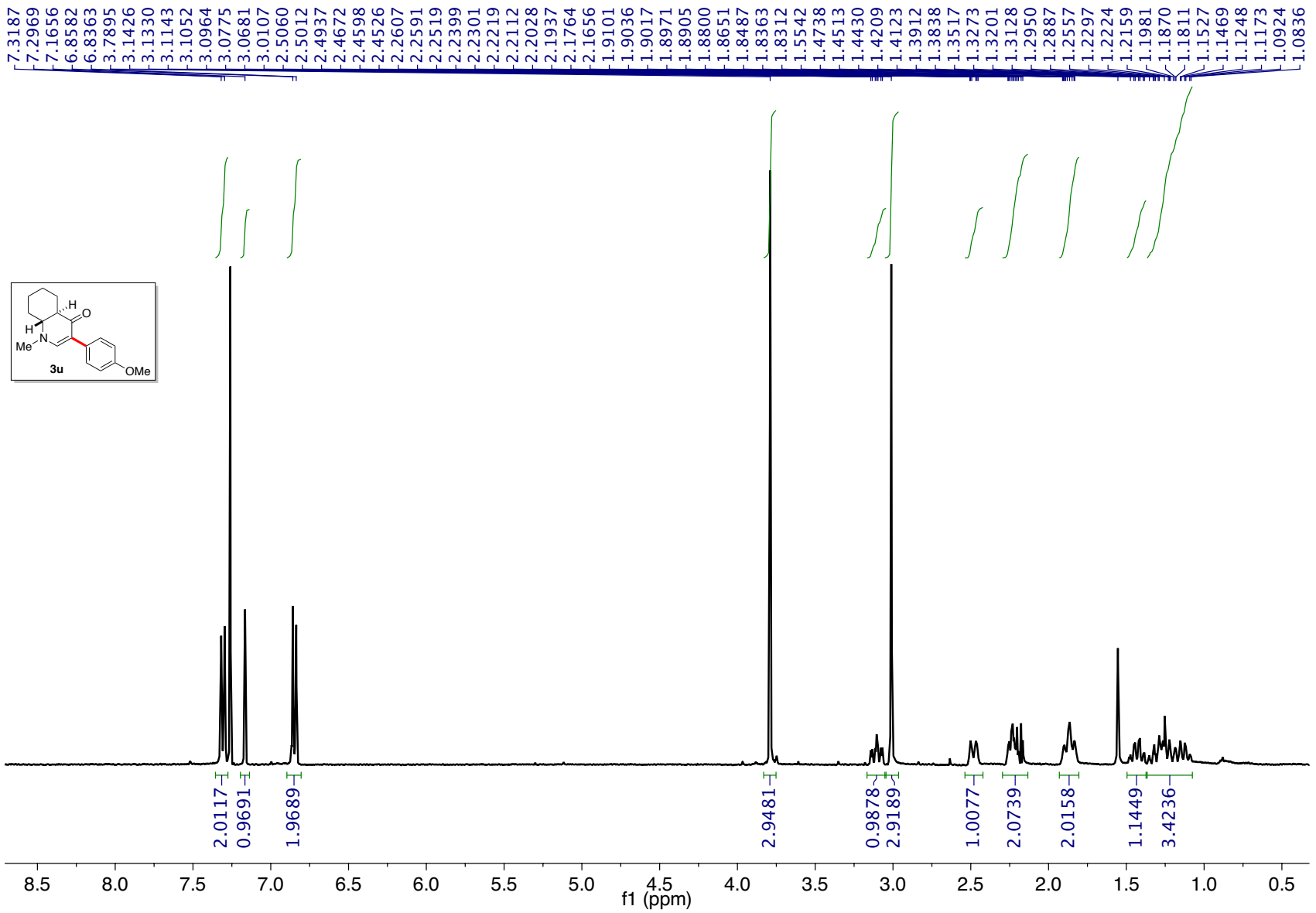

189.7817
158.4014
147.8218
145.3928
129.8232
129.4677
128.3496
124.3412
118.1698
114.5989
113.9023
55.5110
47.7935
36.7768
Ph
N
O
OMe
3r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

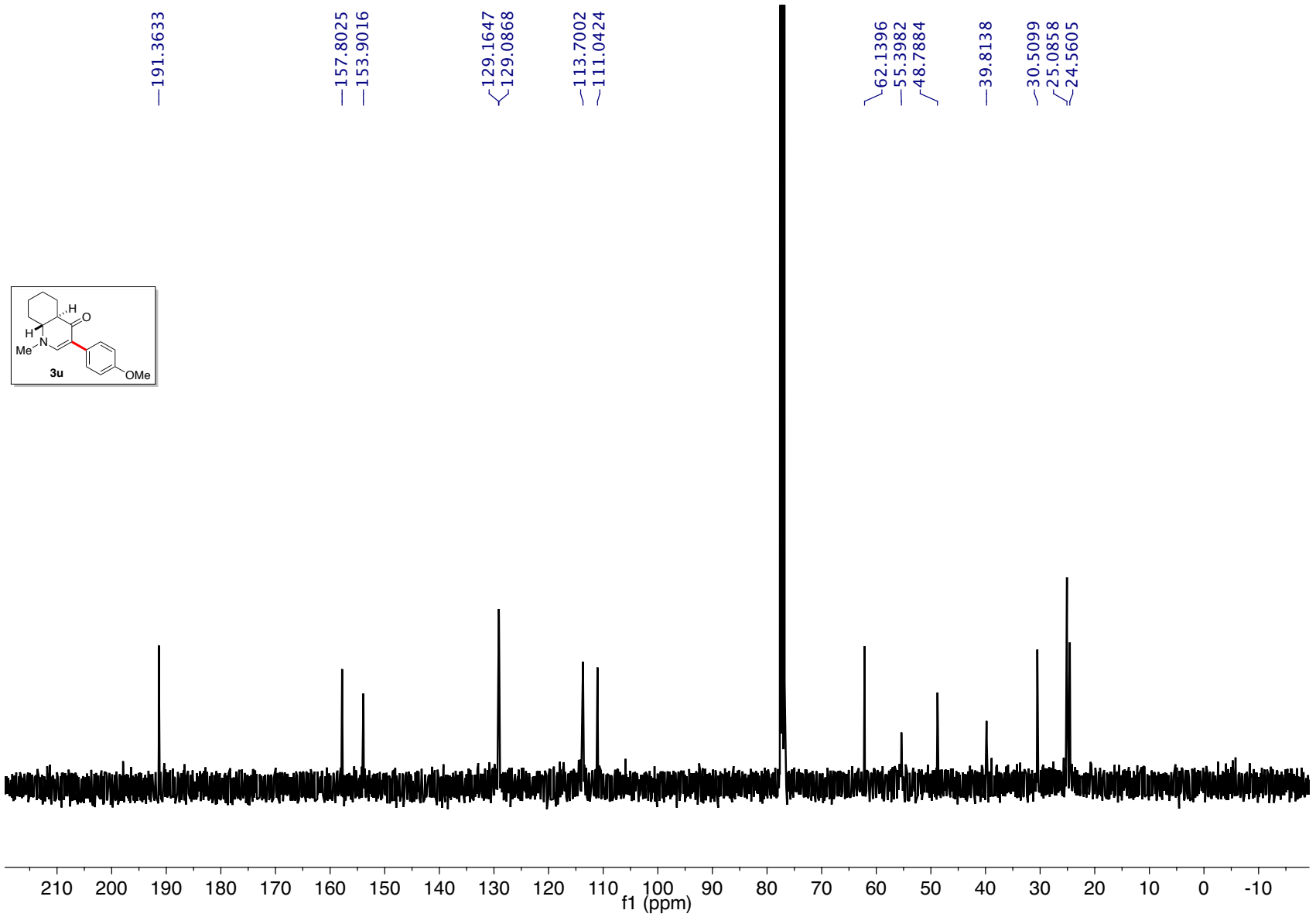

7.3985
7.3753
7.3544
7.3402
7.3345
7.3089
7.2984
7.2921
6.8832
6.8614
4.6885
4.6703
4.6516
3.8005
3.6556
3.6415
3.6274
3.3557
3.2471
3.0342
3.0173
2.9938
2.9770
2.8550
2.8349
1.7324
1.7175
1.7022
1.6868
0.8486
0.0091
-0.0051
TBSO
Ph
O
N
OMe
3s
1.0000
7.0674
1.8632
0.9133
3.0544
2.0430
0.9916
1.0576
0.9436
0.9198
1.9697
9.2290
3.0574
3.0508
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 -1.0
f1 (ppm)

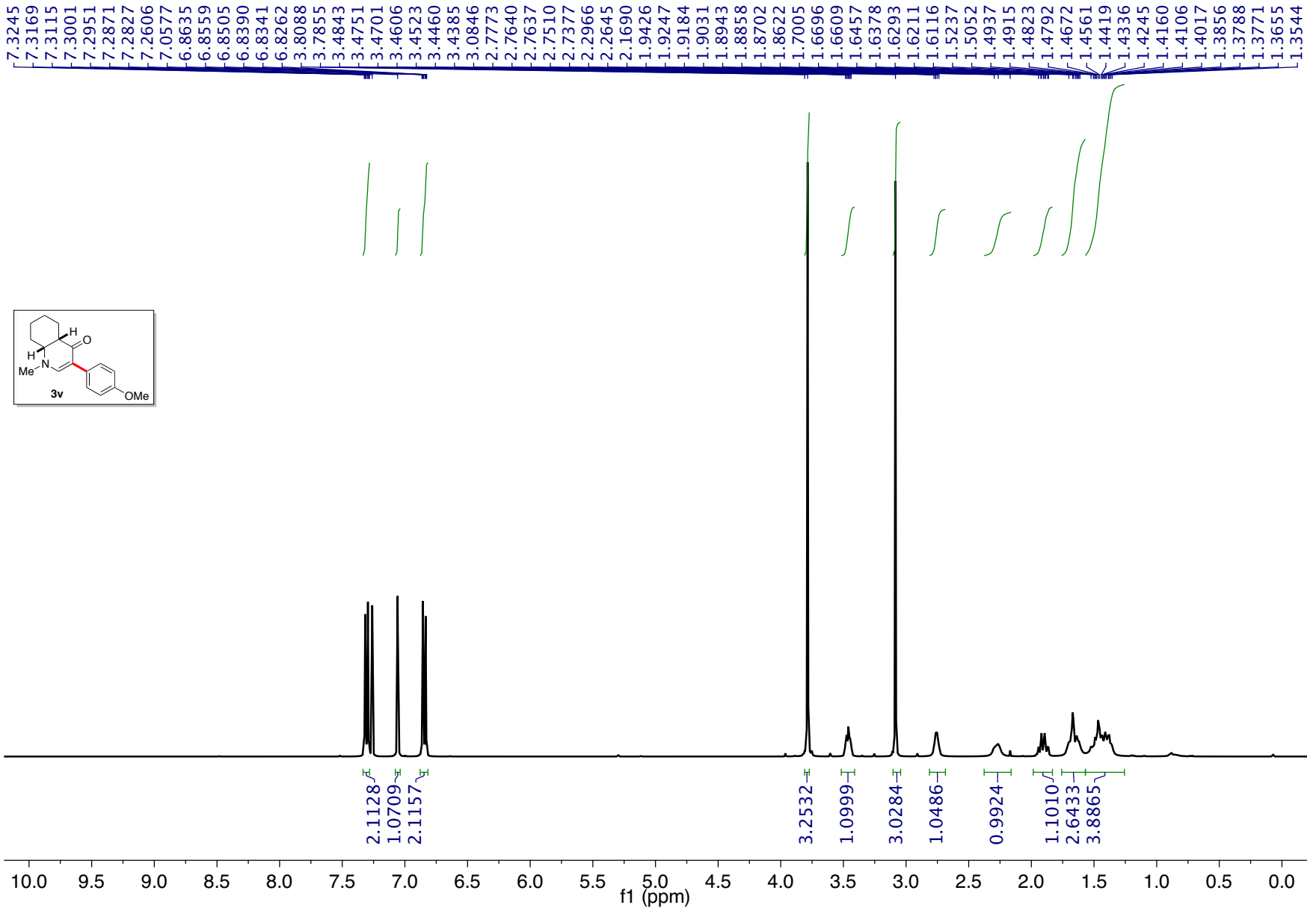

187.5643
157.8687
153.2742
138.8927
129.1658
128.9368
128.9062
128.4164
127.0385
113.7807
110.7696
61.4181
59.3707
55.5279
50.4878
44.5692
31.6603
26.0120
18.3156
-5.2904
TBSO
Ph
O
N
OMe
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

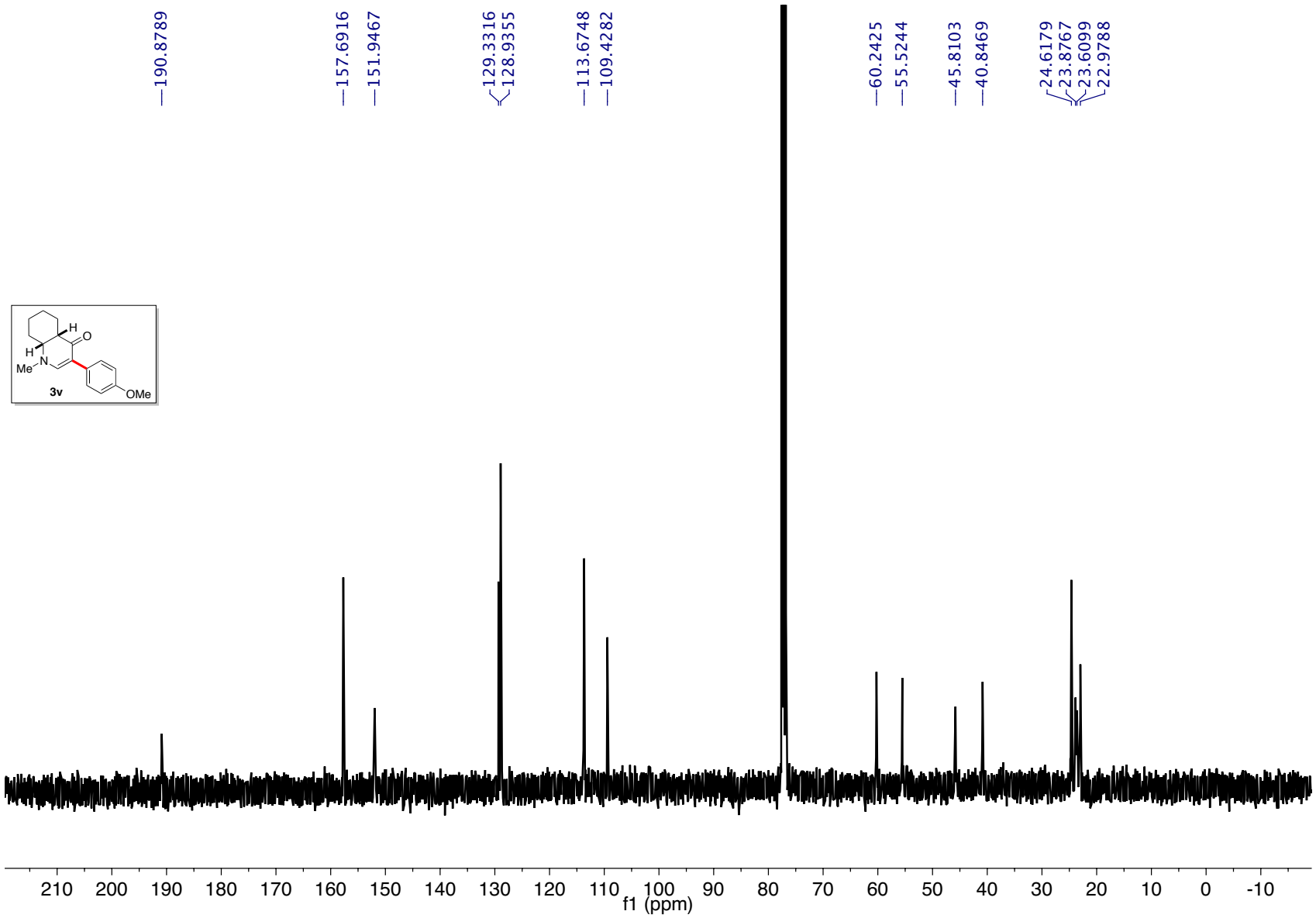

7.3046
7.2829
7.0559
6.8695
6.8479
3.7897
3.4684
3.4634
3.4585
3.4537
3.4375
3.4319
3.4269
3.4140
3.4011
3.3925
3.3732
3.3659
3.3530
3.3443
3.3405
3.3318
3.0755
3.0683
3.0438
3.0366
3.0118
3.0049
2.6407
2.6275
2.6002
2.5870
2.5438
2.5101
2.5029
2.4700
1.9029
1.8693
1.8594
1.8439
1.8379
1.8097
1.8038
1.7708
1.7652
1.6592
1.6496
1.6402
1.6274
1.6180
1.6085
1.5792
1.5719
1.5469
1.5397
1.5186
1.5102
1.5059
1.4862
1.4791
1.4613
1.4544
1.4307
1.4226
1.4140
1.3985
1.3900
1.3815
O
N
3t
OMe
2.0012
0.9700
1.9777
2.9178
2.0205
1.0589
1.0224
1.0510
3.1014
3.5503
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
f1 (ppm)


190.0165
157.9622
153.7163
129.1184
128.6427
113.7864
112.2047
57.4155
55.4797
53.2698
43.9186
31.7895
25.7989
23.2469
O
N
3t
OMe
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)


7.3187
7.2969
7.1656
6.8582
6.8363
3.7895
3.1426
3.1330
3.1143
3.1052
3.0964
3.0775
3.0681
3.0107
2.5060
2.5012
2.4937
2.4672
2.4598
2.4526
2.2607
2.2591
2.2519
2.2399
2.2301
2.2219
2.2112
2.2028
2.1937
2.1764
2.1656
1.9101
1.9036
1.9017
1.8971
1.8905
1.8800
1.8651
1.8487
1.8363
1.8312
1.5542
1.4738
1.4513
1.4430
1.4209
1.4123
1.3912
1.3838
1.3517
1.3273
1.3201
1.3128
1.2950
1.2887
1.2557
1.2297
1.2224
1.2159
1.1981
1.1870
1.1811
1.1527
1.1469
1.1248
1.1173
1.0924
1.0836
H
O
H
N
Me
3u
OMe
2.0117
0.9691
1.9689
2.9481
0.9878
2.9189
1.0077
2.0739
2.0158
1.1449
3.4236
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
f1 (ppm)


191.3633
157.8025
153.9016
129.1647
129.0868
113.7002
111.0424
62.1396
55.3982
48.7884
39.8138
30.5099
25.0858
24.5605
H
O
H
N
Me
3u
OMe
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)


7.3245
7.3169
7.3115
7.3001
7.2951
7.2871
7.2827
7.2606
7.0577
6.8635
6.8559
6.8505
6.8390
6.8341
6.8262
3.8088
3.7855
3.4843
3.4751
3.4701
3.4606
3.4523
3.4460
3.4385
3.0846
2.7773
2.7640
2.7637
2.7510
2.7377
2.2966
2.2645
2.1690
1.9426
1.9247
1.9184
1.9031
1.8943
1.8858
1.8702
1.8622
1.7005
1.6696
1.6609
1.6457
1.6378
1.6293
1.6211
1.6116
1.5237
1.5052
1.4937
1.4915
1.4823
1.4792
1.4672
1.4561
1.4419
1.4336
1.4245
1.4160
1.4106
1.4017
1.3856
1.3788
1.3771
1.3655
1.3544
H
O
H
Me
N
3v
OMe
2.1128
1.0709
2.1157
3.2532
1.0999
3.0284
1.0486
0.9924
1.1010
2.6433
3.8865
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
f1 (ppm)


190.8789
157.6916
151.9467
129.3316
128.9355
113.6748
109.4282
60.2425
55.5244
45.8103
40.8469
24.6179
23.8767
23.6099
22.9788
H
O
H
Me
N
3v
OMe
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)