Supporting Information

for

Gold-catalyzed oxidation of arylallenes: Synthesis of quinoxalines and benzimidazoles

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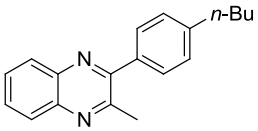
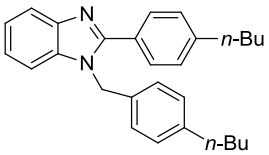
Analytical and spectroscopic data for new compounds



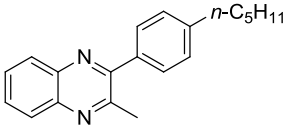
4a

2-(4-butylphenyl)-3-methylquinoxaline (4a): Orange oil; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.13-8.05 (m, 2H), 7.76-7.70 (m, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.81 (s, 3H), 2.72 (t, *J* = 7.5 Hz, 2H), 1.70-1.64 (m, 2H), 1.45-1.37 (m, 2H), 0.97 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.00, 152.63, 143.99, 141.09, 141.04, 136.31, 129.53, 029.17, 129.11, 128.86, 128.61, 128.24, 35.47, 33.50, 24.42, 22.30, 13.92; IR (cm^{-1}, KBr) 3421, 2955, 1634, 1384, 761. HRMS (EI) calcd for $C_{19}H_{20}N_2$ 276.1626, Found 276.1601.



5a

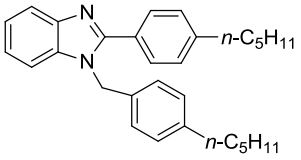
1-(4-butylbenzyl)-2-(4-butylphenyl)-1*H*-benzimidazole (5a): Yellow oil; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.86-7.84 (m, 1H), 7.62-7.61 (m, 2H), 7.30-7.20 (m, 5H), 7.13-7.12 (m, 2H), 7.02-7.00 (m, 2H), 5.42 (s, 2H), 2.67-2.57 (m, 4H), 1.63-1.56 (m, 4H), 1.38-1.24(m, 4H), 0.94-0.91 (m, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 154.39, 145.01, 143.13, 142.48, 136.10, 133.64, 129.17, 129.03, 128.82, 127.31, 125.91, 122.80, 122.53, 119.80, 110.56, 48.25, 35.50, 35.26, 33.56, 33.39, 22.38, 22.30, 13.95 (2C); IR (cm^{-1}, KBr) 3461, 2957, 1741, 1615, 1384, 1243, 745. HRMS (EI) calcd for $C_{28}H_{32}N_2$ 396.2565, Found 396.2569



4b

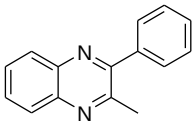
2-methyl-3-(4-pentylphenyl)quinoxaline (4b): Yellow oil; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.13-8.11 (m, 2H), 8.07-8.05 (m, 2H), 7.76-7.70 (m, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.81 (s, 3H), 2.70 (t, *J* = 7.5 Hz, 2H), 1.71-1.65 (m, 2H), 1.38-1.36 (m, 2H), 0.92 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 155.0, 152.6, 144.0, 141.1, 141.0, 136.3, 129.5, 129.2, 129.1, 128.9, 128.6,

128.3, 35.8, 31.5, 31.1, 24.5, 22.6, 14.0; IR (cm^{-1}, KBr) 3455, 2929, 2856, 1614, 1341, 910, 735. HRMS (EI) calcd for $C_{20}H_{22}N_2$ 290.1783, Found 290.1779



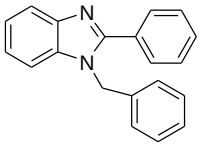
5b

1-(4-pentylbenzyl)-2-(4-pentylphenyl)-1*H*-benzimidazole (5b): Yellow oil; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.31-7.22 (m, 5H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 5.45 (s, 2H), 2.67 (t, *J* = 8.0 Hz, 2H), 2.60 (t, *J* = 8.0 Hz, 2H), 1.67-1.61 (m, 4H), 1.35-1.21 (m, 8H), 0.91 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 154.4, 145.0, 143.2, 142.5, 136.1, 133.7, 129.2, 129.0, 128.8, 127.4, 125.9, 122.8, 122.5, 119.8, 110.5, 48.3, 35.8, 35.5, 31.5, 31.4, 31.1, 30.9, 30.3, 29.7, 22.5, 14.0; IR (cm^{-1}, KBr) 3416, 2927, 1616, 1384, 912, 743. HRMS (EI) calcd for $C_{30}H_{36}N_2$ 424.2878, Found 424.2875



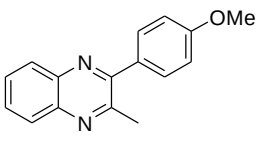
4c

2-methyl-3-phenylquinoxaline (4c) [1]: Yellow oil; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.13-8.10 (m, 1H), 8.07-8.05 (m, 1H), 7.75-7.71 (m, 2H), 7.67-7.64 (m, 2H), 7.55-7.49 (m, 3H), 2.81 (s, 3H).



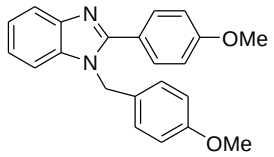
5c

1-benzyl-2-phenyl-1*H*-benzimidazole (5c) [2]: White solid; ^{1}H NMR ($CDCl_3$,500 MHz): δ 7.87 (d, *J* = 8.0, 1H), 7.70-7.68 (m, 2H), 7.48-7.43 (m, 3H), 7.35-7.28 (m, 4H), 7.26-7.22 (m, 2H), 7.21-7.10 (m, 2H), 5.46 (s, 2H).



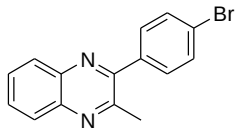
4d

2-(4-methoxyphenyl)-3-methylquinoxaline (4d) [3]: Yellow oil; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.11-8.07 (m, 1H), 8.05-8.02 (m, 1H), 7.72-7.71 (m, 2H), 7.65-7.62 (m, 2H), 7.07-7.03 (m, 2H), 3.89 (s, 3H), 2.80 (s, 3H).



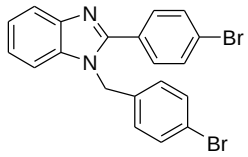
5d

1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-1*H*-benzimidazole (5d) [2]: Yellow solid; ^{1}H NMR ($CDCl_3$, 500 MHz):δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.70-7.68 (m, 2H), 7.48-7.43 (m, 3H), 7.35-7.28 (m, 2H), 7.26-7.22 (m, 2H), 7.21-7.10 (m, 2H), 5.46 (s, 2H), 3.89 (s, 3H), 3.66 (s, 3H).



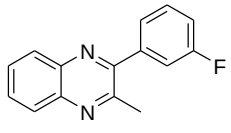
4e

2-(4-bromophenyl)-3-methylquinoxaline (4e) [4]: Orange oil; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.12-8.06 (m, 2H), 7.79-7.72 (m, 2H), 7.70-7.67 (m, 2H), 7.58-7.55 (m, 2H), 2.79 (s, 3H).



5e

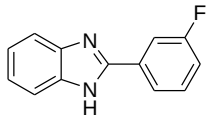
1-(4-bromobenzyl)-2-(4-bromophenyl)-1*H*-benzo[d]imidazole (5e) [2]: Yellow solid; mp 160^{o}C; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.70-7.68 (m, 2H), 7.48-7.43 (m, 3H), 7.35-7.28 (m, 2H), 7.26-7.22 (m, 2H), 7.21-7.10 (m, 2H), 5.46 (s, 2H).



4f

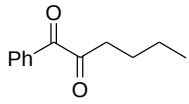
2-(3-fluorophenyl)-3-methylquinoxaline (4f): White solid, mp 85-87℃; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.13-8.06 (m, 2H), 7.79-7.73 (m, 2H), 7.54-7.38 (m, 3H), 7.23-7.19 (m, 1H), 2.80 (s, 3H); ^{13}C NMR

($CDCl_3$, 125 MHz): δ 162.79 (d, *J* = 246.25 Hz), 153.53, 153.51, 152.23, 141.45, 141.17 (d, *J* = 6.3 Hz), 140.92, 130.27 (d, *J* = 8.8 Hz), 130.13, 129.40 (d, *J* = 26.3 Hz), 128.42, 124.78 (d, *J* = 2.5 Hz), 116.35, 116.09 (d, *J* = 20.0 Hz), 24.31; IR (cm^{-1}, KBr) 3417, 2982, 1740, 1616, 1240, 1048, 762. HRMS (EI) calcd for $C_{15}H_{11}FN_2$ 238.0906, Found 238.0894.



5f

2-(3-fluorophenyl)-1*H*-benzimidazole (5f): White solid, mp 115-116℃; ^1H NMR ($CDCl_3$, 500 MHz): δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.81-7.78 (m, 1H), 7.67-7.65 (m, 2H), 7.46-7.42 (m, 1H), 7.32-7.29 (m, 2H), 7.17-7.14 (m, 1H); ^{13}C NMR (DMSO, 125 MHz): δ 162.92 (d, *J* = 241.3 Hz), 150.39, 144.08, 135.41, 132.93 (d, *J* = 7.5 Hz), 131.64 (d, *J* = 8.8 Hz), 123.41, 122.97 (d, *J* = 2.5 Hz), 122.39, 119.54, 117.08 (d, *J* = 20.0 Hz), 113.46 (d, *J* = 22.5 Hz), 111.96; IR (cm^{-1}, KBr) 3422, 2994, 1770, 1618, 1383, 1246, 1050. HRMS (EI) calcd for $C_{13}H_9FN_2$ 212.0750, Found 212.0764.



2g

1-phenylhexane-1,2-dione (2g) [5]: Yellow oil; ^1H NMR($CDCl_3$, 500 MHz):δ 7.57-7.53 (m, 2H), 7.40-7.25 (m,3H), 2.64 (t, *J* = 7.5 Hz, 3H), 1.73- 1.68 (m, 2H), 0.97 (t, *J* = 7.5 Hz, 3H).

References

1. More, S. V.; Sastry, M. N. V.; Yao, C.-F. *Green Chem.* **2006**, *8*, 91. doi:10.1039/b510677j

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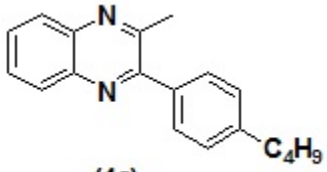
3. Hahn, W. E.; Lesiak, J. *Pol. J. Chem.* **1985**, *59*, 627.

4. Lee, D. G.; Chang, V. S. *Synthesis* **1978,** 462. doi:10.1055/s-1978-24783

5. Ren, W.; Liu, J.-F.; Chen, L.; Wan, X.-B. *Adv. Synth. Catal*. **2010**, *352*, 1424. doi:10.1002/adsc.201000250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3.00
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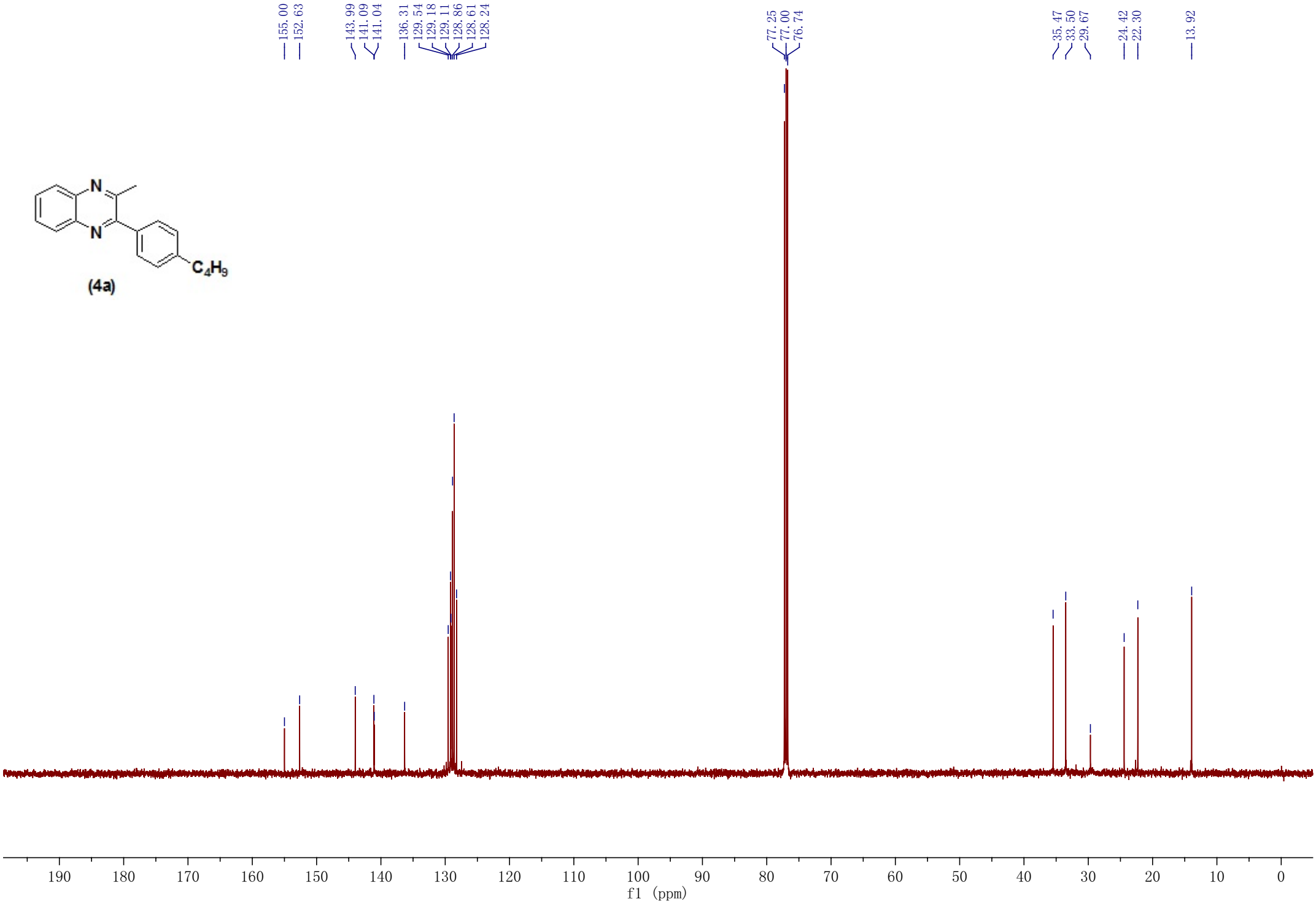
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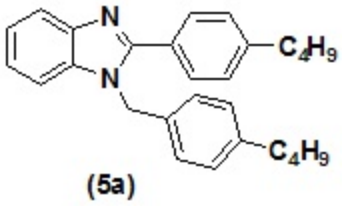
f1 (ppm)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(5a)

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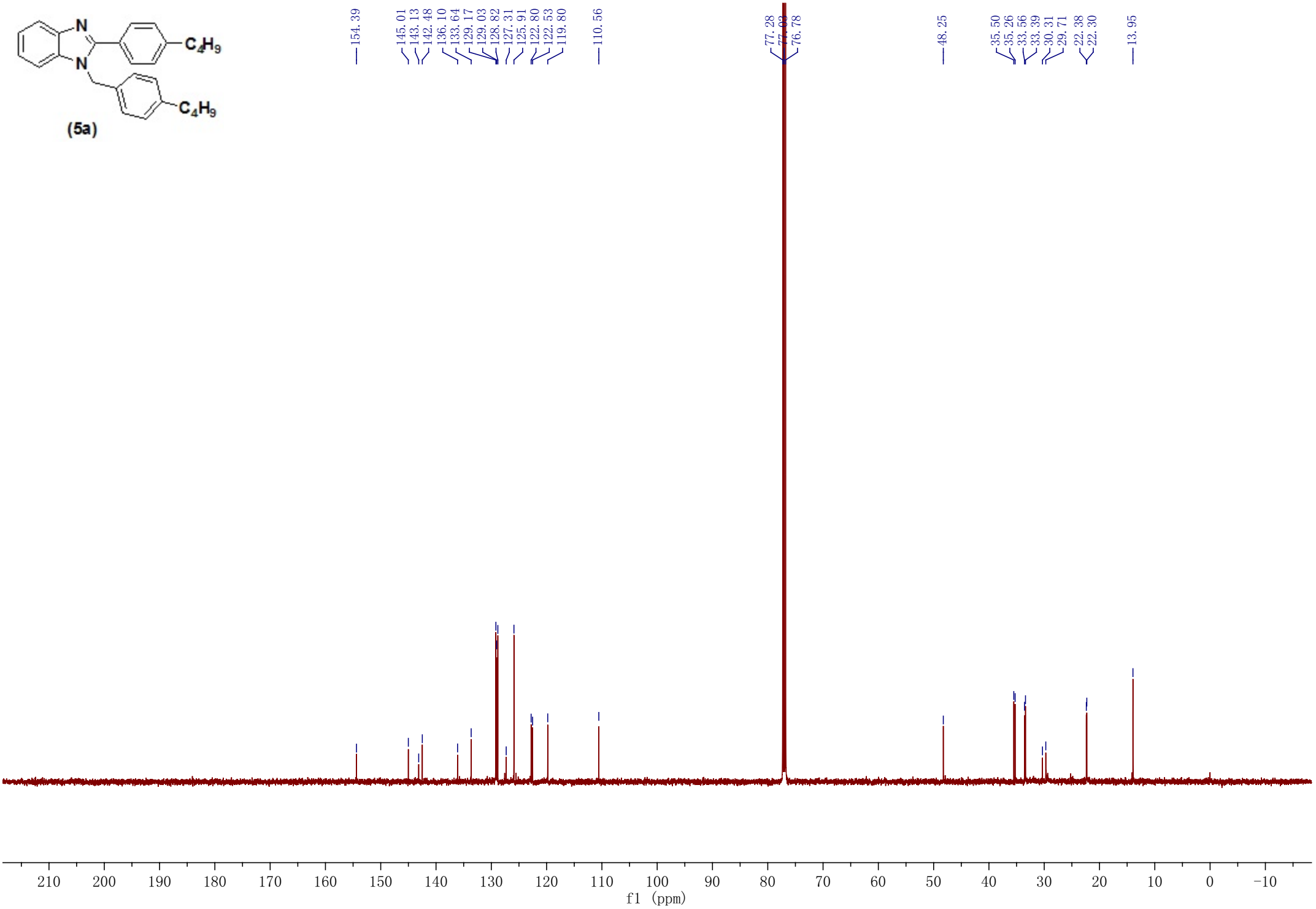
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C4H9
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22.38
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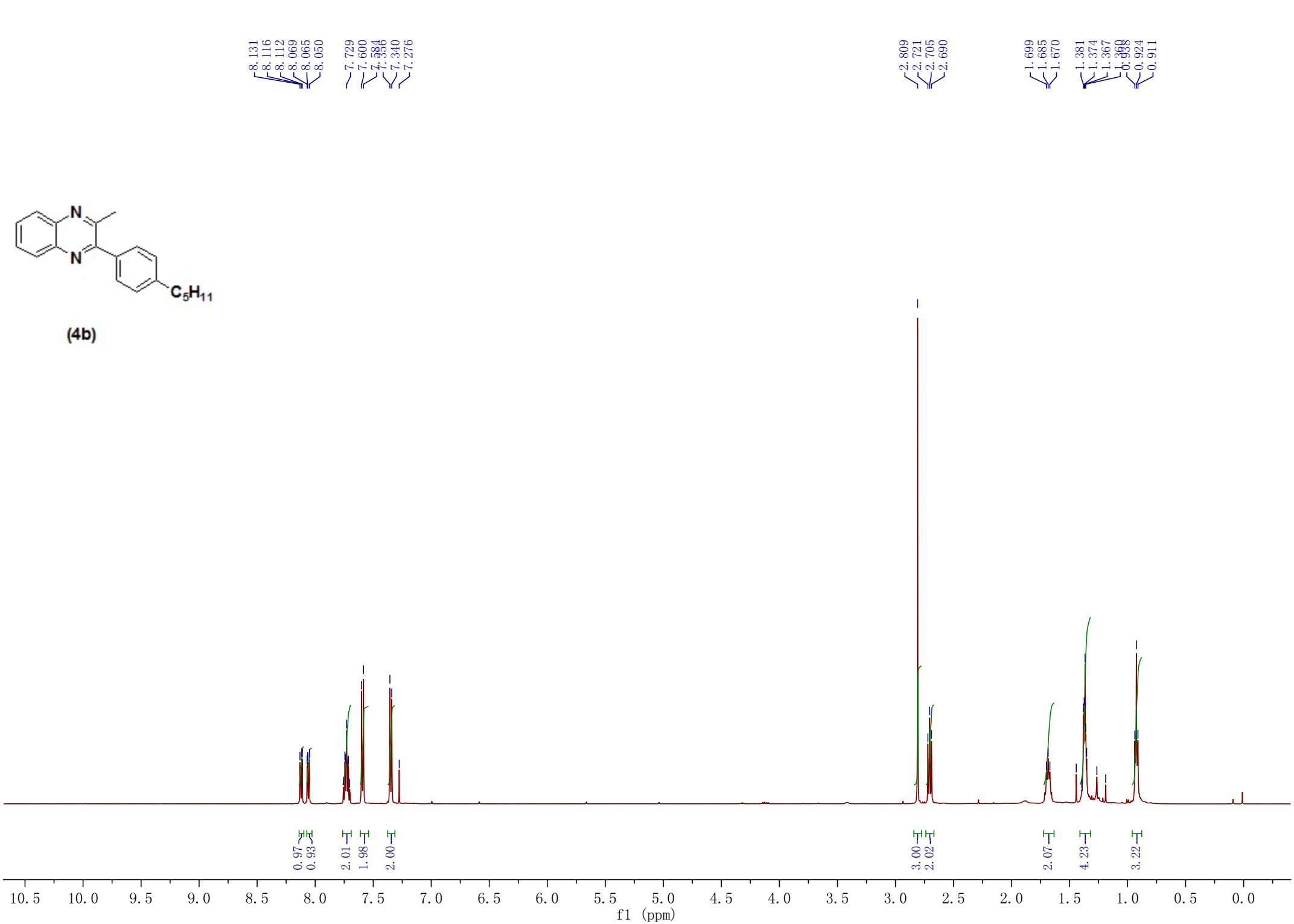
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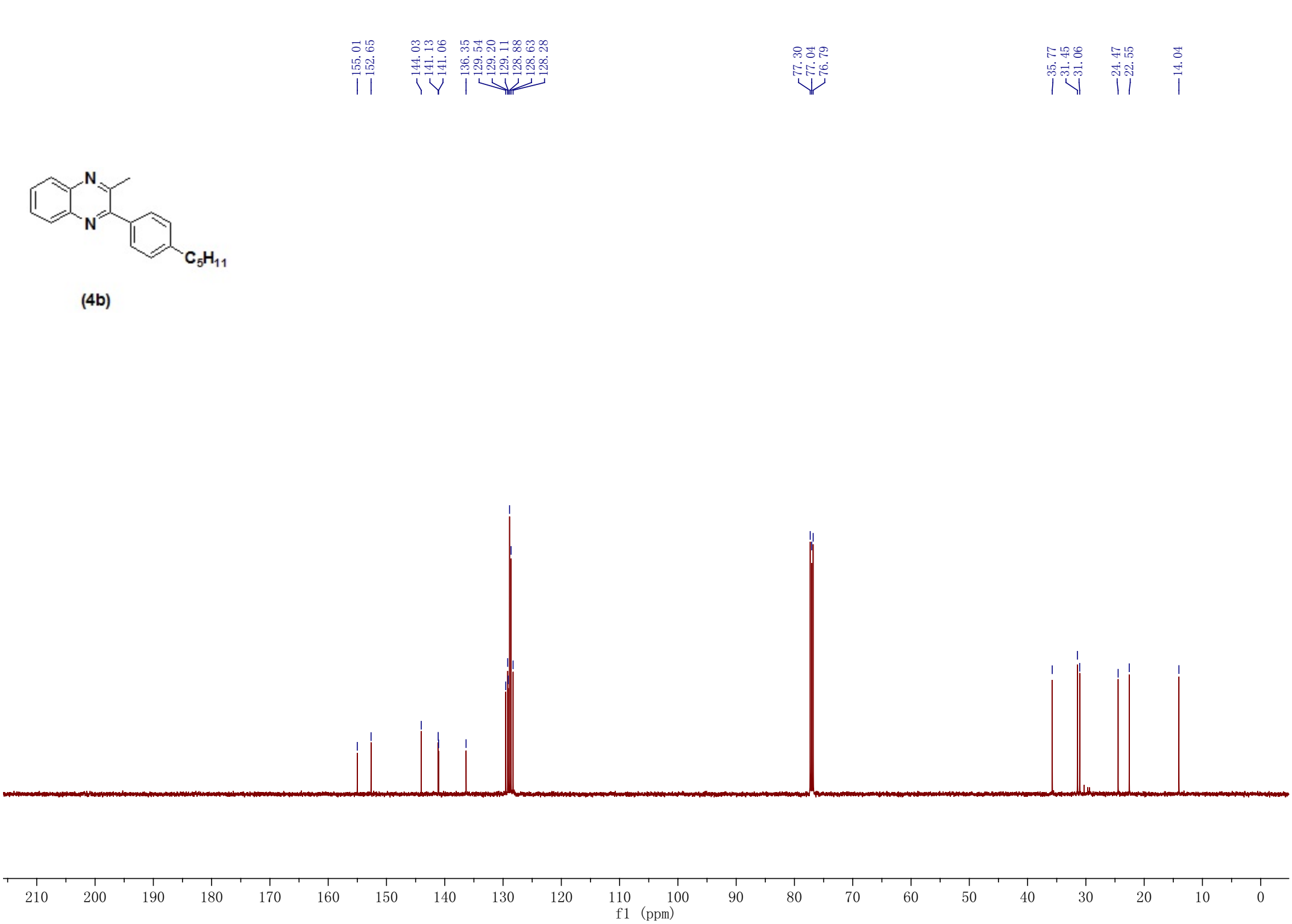
f1 (ppm)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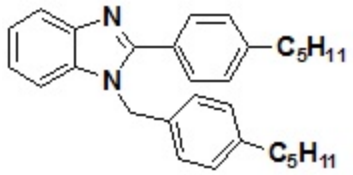
f1 (ppm)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N
C_5H_{11}
C_5H_{11}

(5b)

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7.303
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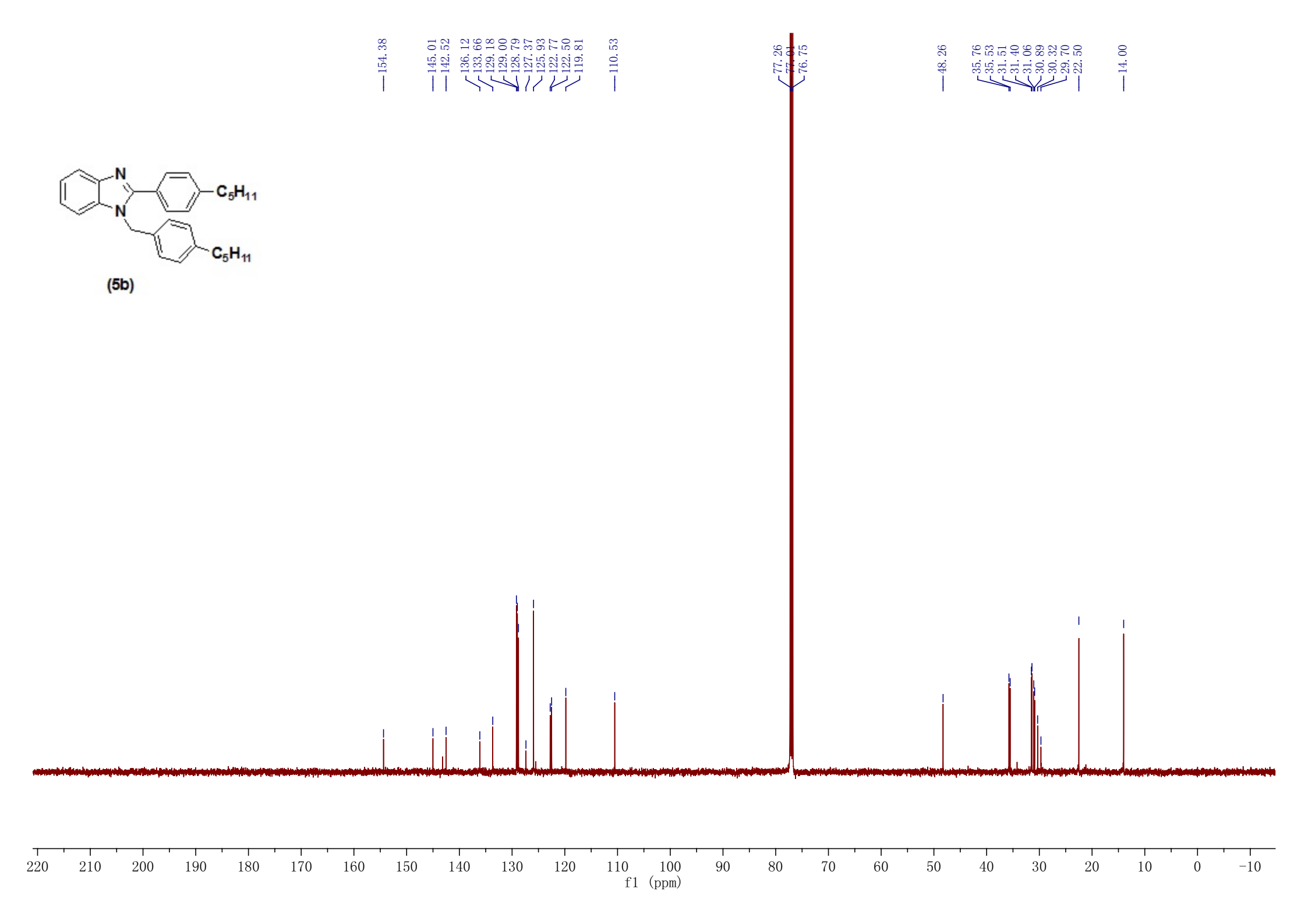
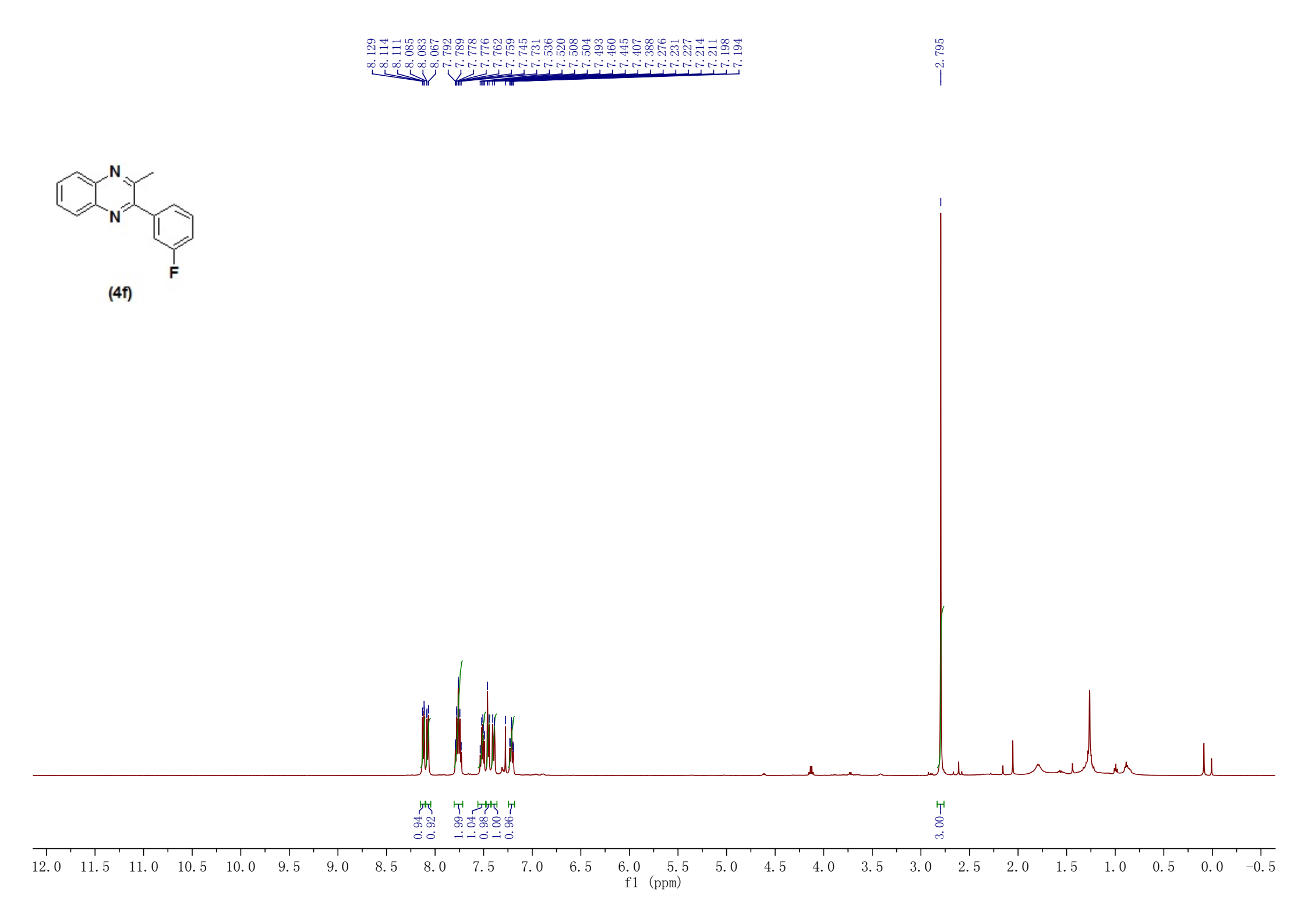
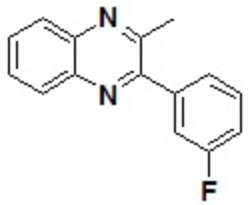
6.53
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


154.38
145.01
142.52
136.12
133.66
129.18
129.00
128.79
127.37
125.93
122.77
122.50
119.81
110.53
77.26
77.01
76.75
48.26
35.76
35.53
31.51
31.40
31.06
30.89
30.32
29.70
22.50
14.00
N
N
C5H11
C5H11
(5b)
220
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)

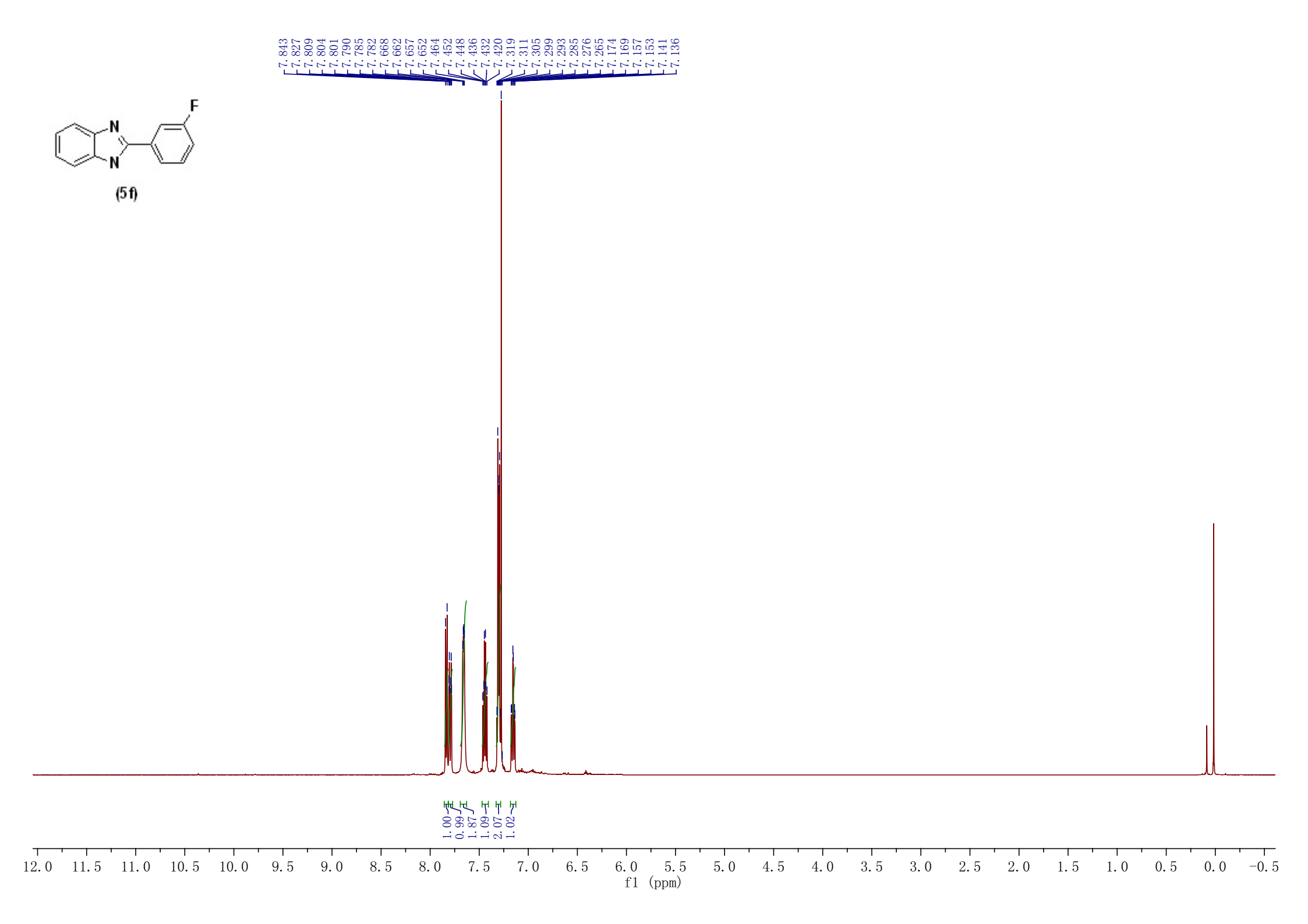

8.129
8.114
8.111
8.085
8.083
8.067
7.792
7.789
7.778
7.776
7.762
7.759
7.745
7.731
7.536
7.520
7.508
7.504
7.493
7.460
7.445
7.407
7.388
7.276
7.231
7.227
7.214
7.211
7.198
7.194
2.795
N
N
F
(4f)
0.94
0.92
1.99
1.04
0.98
1.00
0.96
3.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

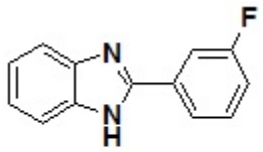


(4f)

163.77
161.80
153.53
152.23
141.45
141.20
141.14
140.93
130.13
129.50
129.29
128.42
116.35
116.17
116.01
77.34
77.08
76.83
29.74
24.31

f1 (ppm)


7.843
7.827
7.809
7.804
7.801
7.790
7.785
7.782
7.668
7.662
7.657
7.652
7.464
7.452
7.448
7.436
7.432
7.420
7.319
7.311
7.305
7.299
7.293
7.285
7.276
7.265
7.174
7.169
7.157
7.153
7.141
7.136
F
N
N
(5f)
1.00
0.99
1.87
1.09
2.07
1.02
12.0
11.5
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)


F
N
N
H

(5f)

163.88
161.95
150.39
144.08
135.41
132.96
132.90
131.67
131.60
123.41
122.98
122.96
122.39
119.54
117.16
117.00
113.55
113.37
111.96
40.45
40.37
40.28
40.21
40.12
39.95
39.78
39.62
39.45
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)