Supporting Information

One-pot synthesis of pyrrolo[1,2-*a*]quinoxalines

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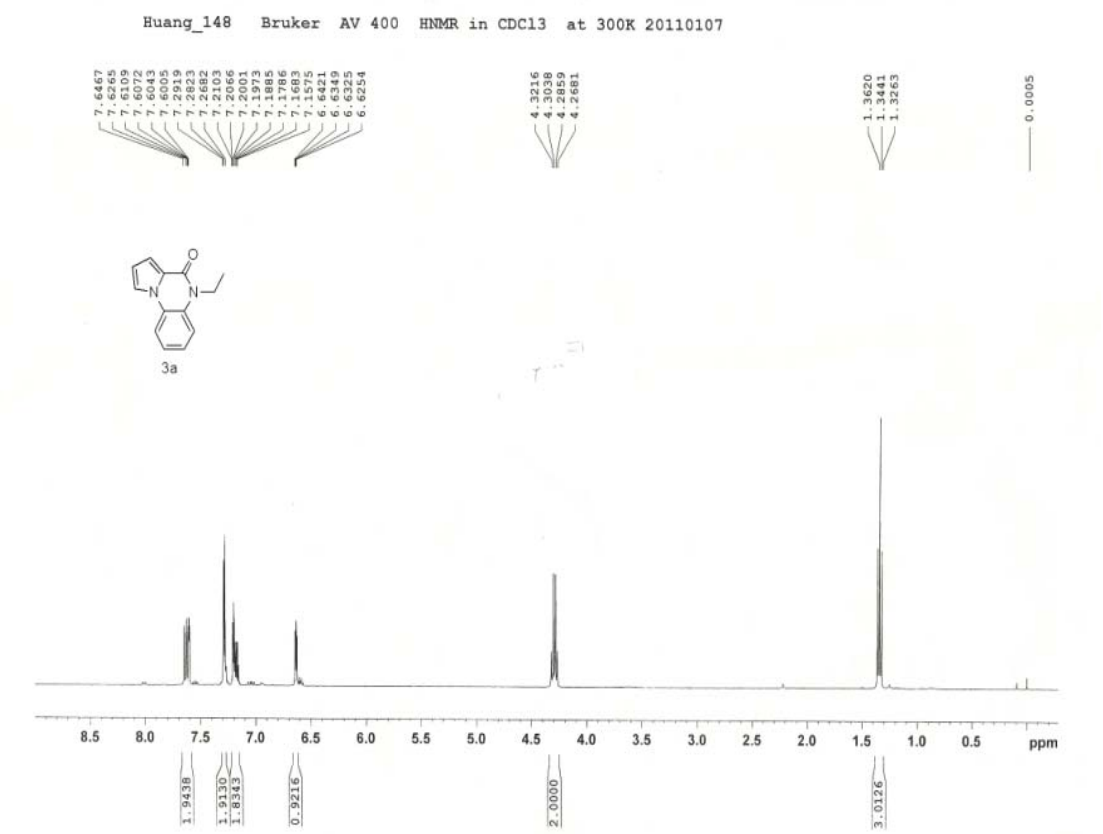
Single crystals of **5e** and **5g** suitable for X-ray crystal analysis were obtained by recrystallization from a hexane/CH_2Cl_2 mixed solvent. The diffraction data was collected with a Bruker SMART CCD diffractometer using a graphite monochromated Mo Kα radiation (λ= 0.71073 Å) at 298(2) or 293(2) K. The structure were solved by direct methods with SHELXS-97 program and refinements on F^2 were performed with SHELXL-97 program by full-matrix least-squares techniques with anisotropic thermal parameters for the non-hydrogen atoms.

Table S1 Crystal structure determination of 5e and 5g

Compound	**5e**	**5g**
Chemical formula	$C_{18}H_{13}FN_2O$	$C_{19}H_{16}N_2O$
Formula Mass	292.30	288.34
Crystal system	Monoclinic	Triclinic
a/Å	8.023	9.032(2)
b/Å	15.891	9.319(2)
c/Å	22.670	9.925(2)
α/°	90.00	88.946(2)
β/°	97.96	73.298(2)
γ/°	90.00	65.822(2)
Unit cell volume/Å^3	2862.5	725.2(3)
Temperature/K	298(2)	293(2)
Space group	*C*2/*c*	*P*-1
No. of formula units per unit cell, *Z*	8	2
No. of reflections measured	12000	6179
No. of independent reflections	3301	3244
R_{int}	0.0231	0.0201
Final R_1 values ($I > 2\sigma(I)$)	0.0495	0.0563
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1248	0.1758
Final R_1 values (all data)	0.0772	0.0787
Final $wR(F^2)$ values (all data)	0.1443	0.2001


Huang_148 Bruker AV 400 HNMR in CDCl3 at 300K 20110107
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7.6109
7.6072
7.6043
7.6005
7.2919
7.2823
7.2682
7.2103
7.2066
7.2001
7.1933
7.1885
7.1786
7.1683
7.1575
6.6421
6.6349
6.6325
6.6254
4.3216
4.3038
4.2859
4.2681
1.3620
1.3441
1.3263
0.0005
3a
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
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1.8343
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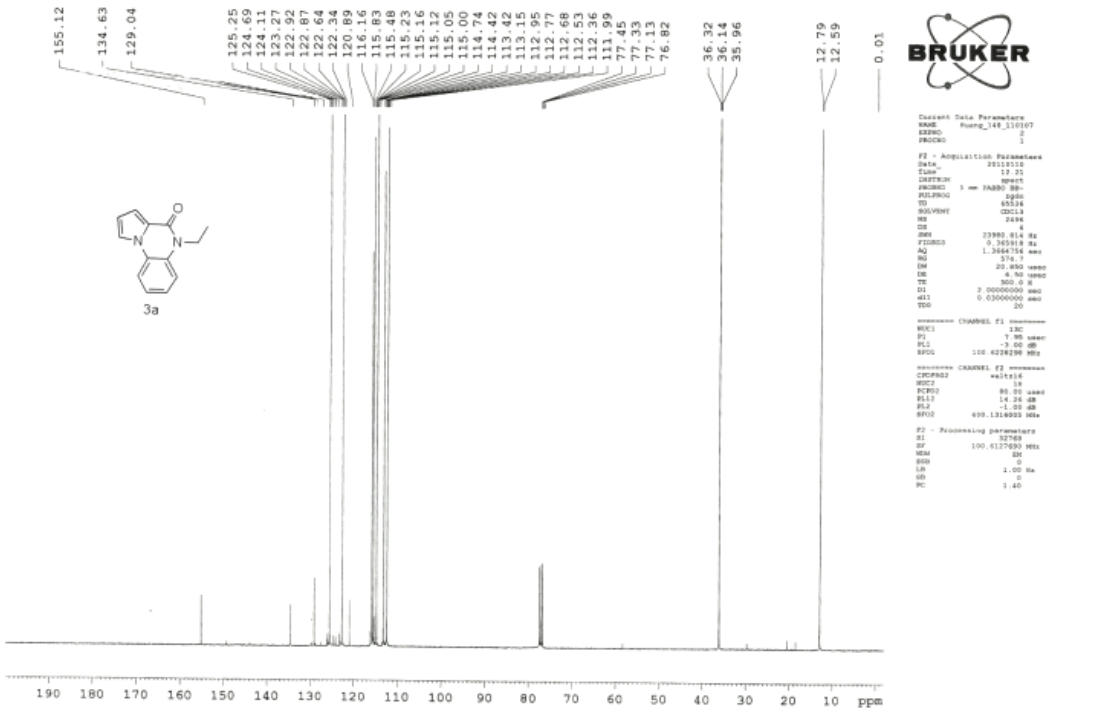
3.0126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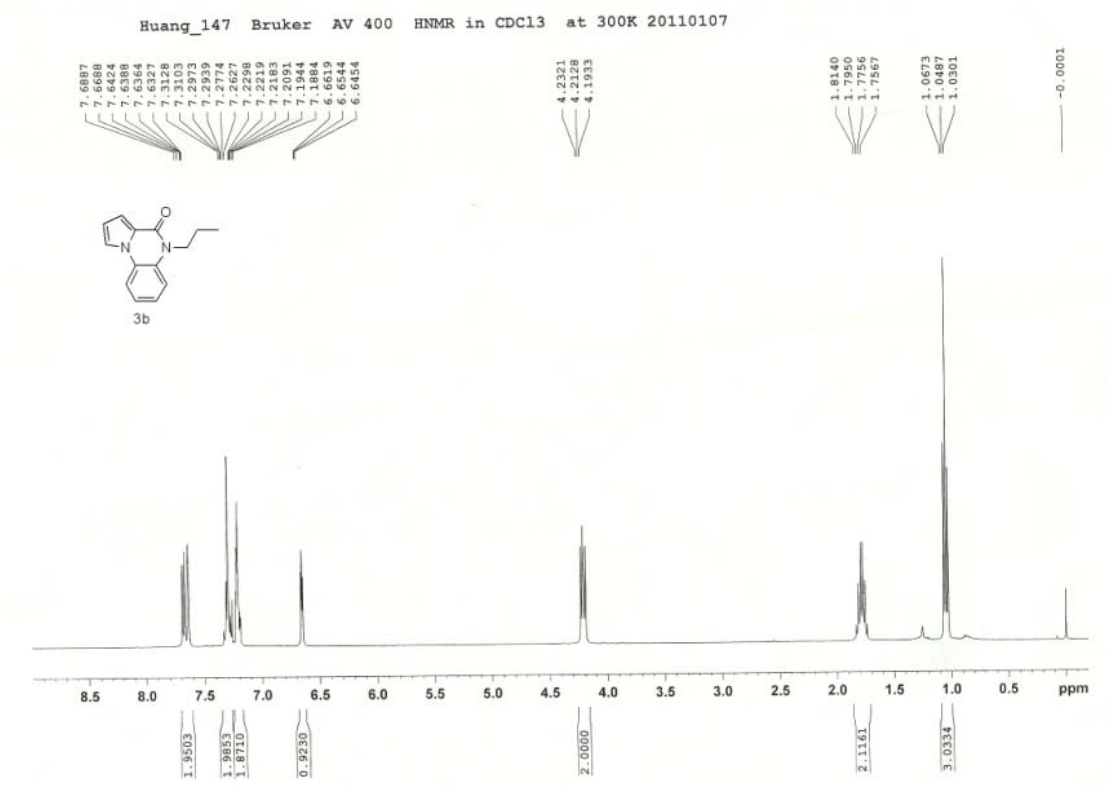
129.04
125.25
124.69
124.11
123.27
122.92
122.87
122.64
122.34
120.89
116.16
115.83
115.48
115.23
115.16
115.12
115.05
115.00
114.74
114.42
114.42
113.15
112.95
112.77
112.68
112.53
112.36
111.99
77.45
77.33
77.13
76.82
36.32
36.14
35.96
12.79
12.59
0.01
3a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER


Huang_147 Bruker AV 400 HNMR in CDCl3 at 300K 20110107
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7.6688
7.6424
7.6388
7.6364
7.6327
7.3128
7.3103
7.2973
7.2939
7.2774
7.2627
7.2298
7.2219
7.2183
7.2091
7.1944
7.1884
6.6619
6.6544
6.6454
4.2321
4.2128
4.1933
1.8140
1.7950
1.7756
1.7567
1.0673
1.0487
1.0301
-0.0001
3b
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
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0.9230
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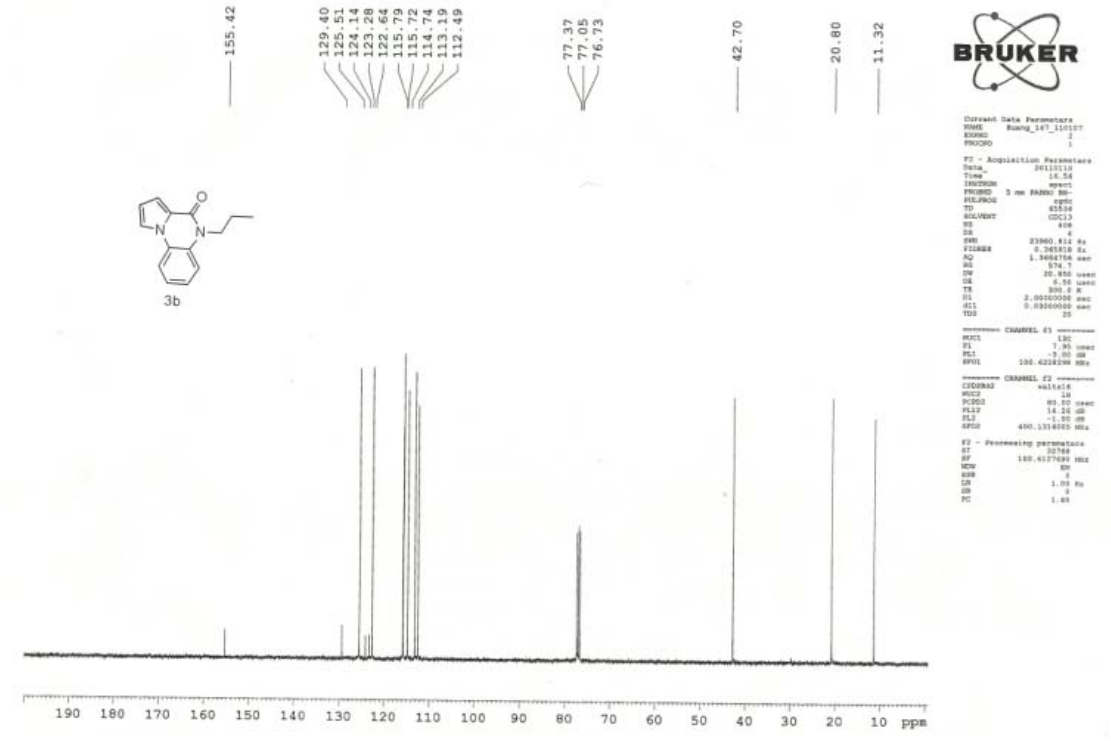
2.1161
3.0334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113.19
112.49
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20.80
11.32
BRUKER
3b
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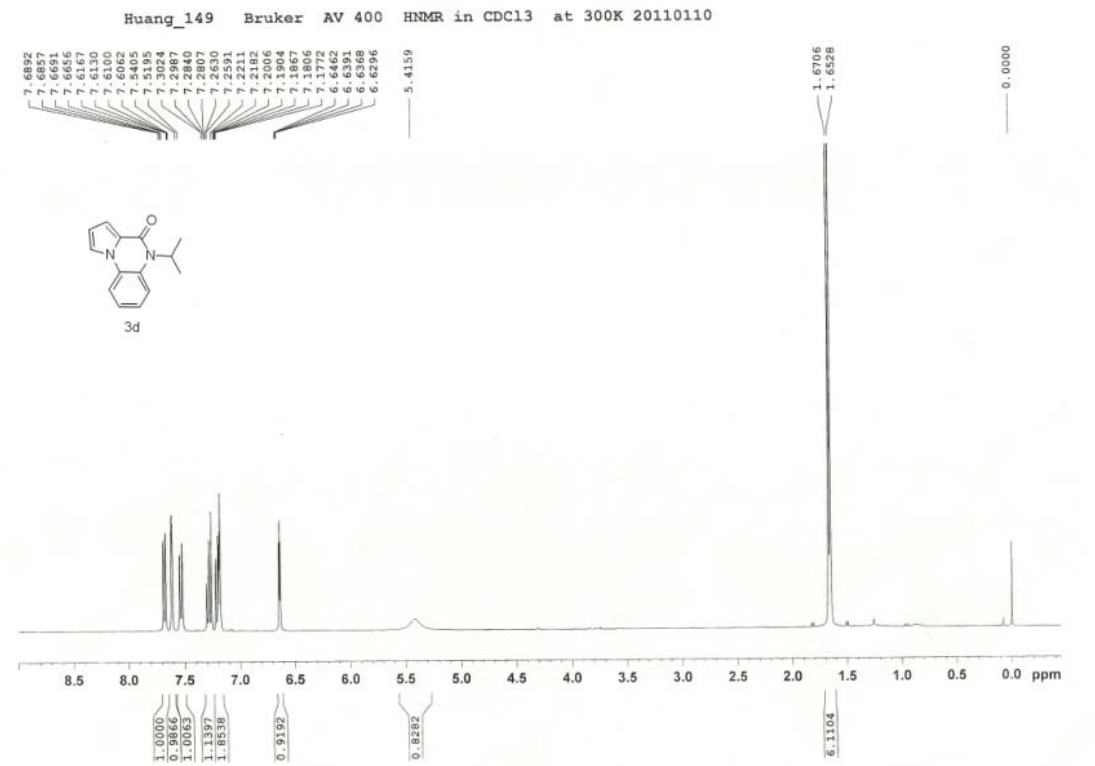
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7.6100
7.6062
7.5405
7.5195
7.3024
7.2987
7.2840
7.2807
7.2630
7.2591
7.2211
7.2182
7.2006
7.1904
7.1867
7.1806
7.1772
7.1468
6.6462
6.6391
6.6368
6.6296
5.4159
1.6706
1.6528
0.0000
3d
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
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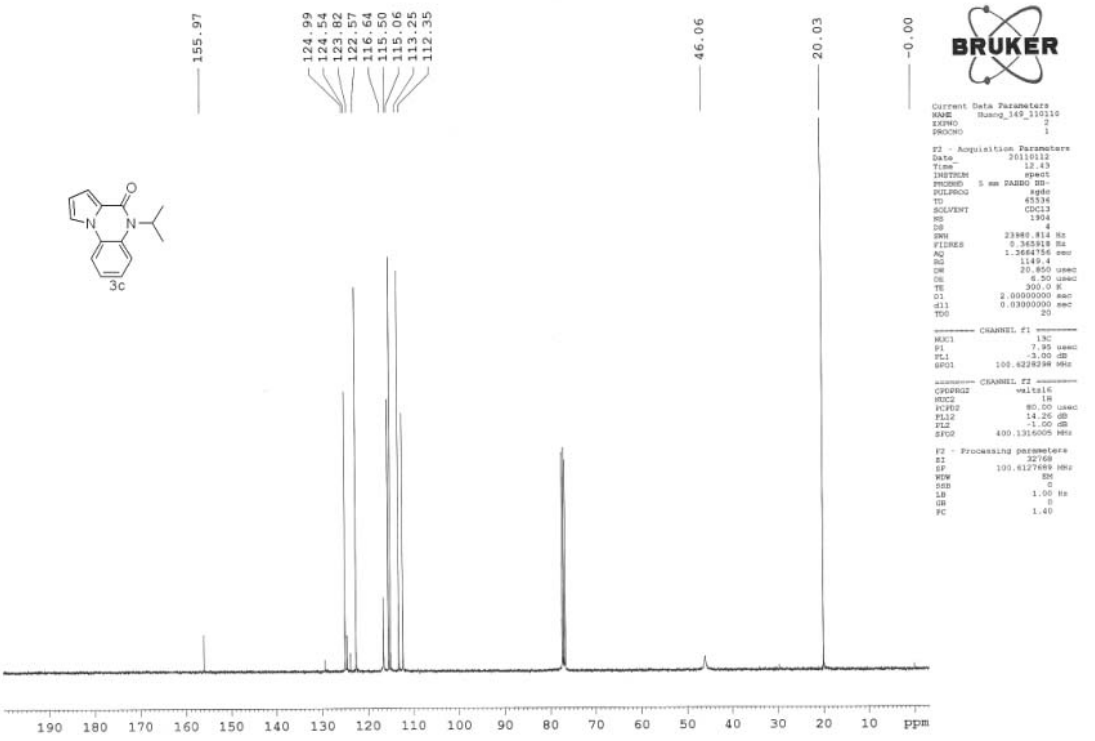
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124.99
124.54
123.82
122.57
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112.35
46.06
20.03
-0.00
3c
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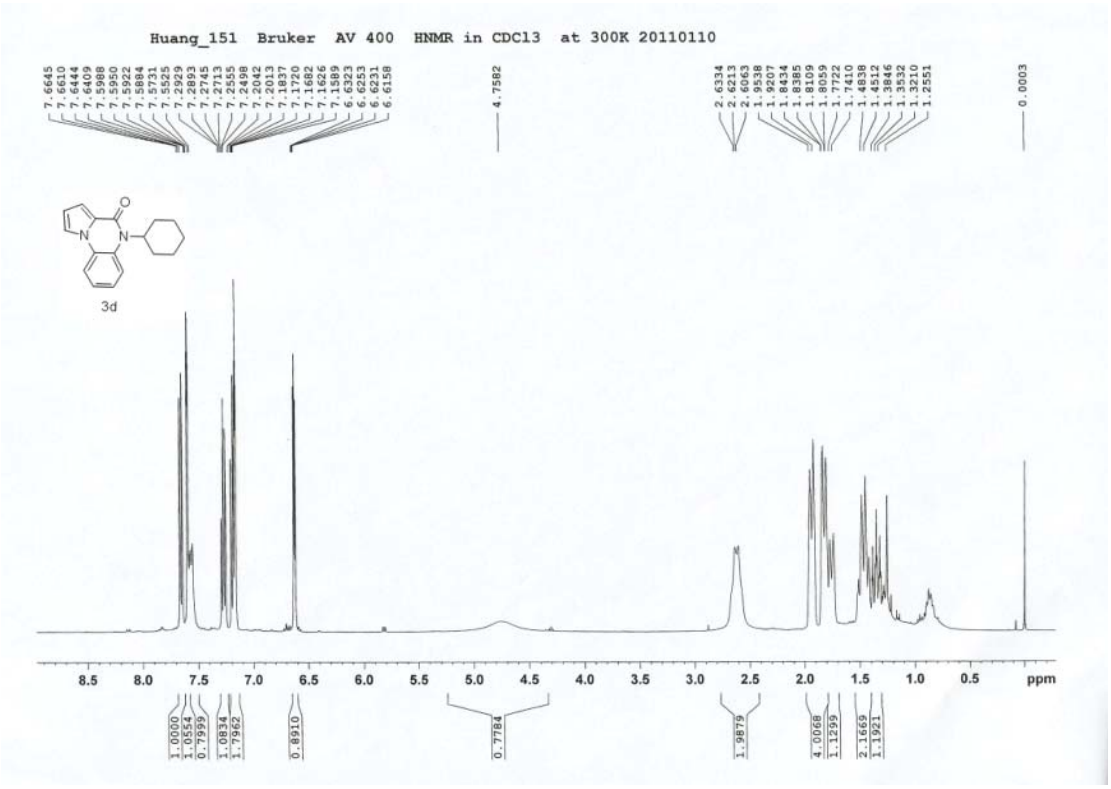
Huang_151 Bruker AV 400 HNMR in CDCl3 at 300K 20110110
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7.6610
7.6444
7.6409
7.5988
7.5950
7.5922
7.5884
7.5731
7.5521
7.2929
7.2893
7.2745
7.2713
7.2555
7.2498
7.2042
7.2013
7.1837
7.1720
7.1682
7.1626
7.1389
7.1353
6.6253
6.6231
6.6158
4.7582
2.6334
2.6213
2.6063
1.9538
1.9207
1.8434
1.8185
1.8109
1.8059
1.7722
1.7410
1.4838
1.4512
1.3846
1.3532
1.3210
1.2551
0.0003
3d
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
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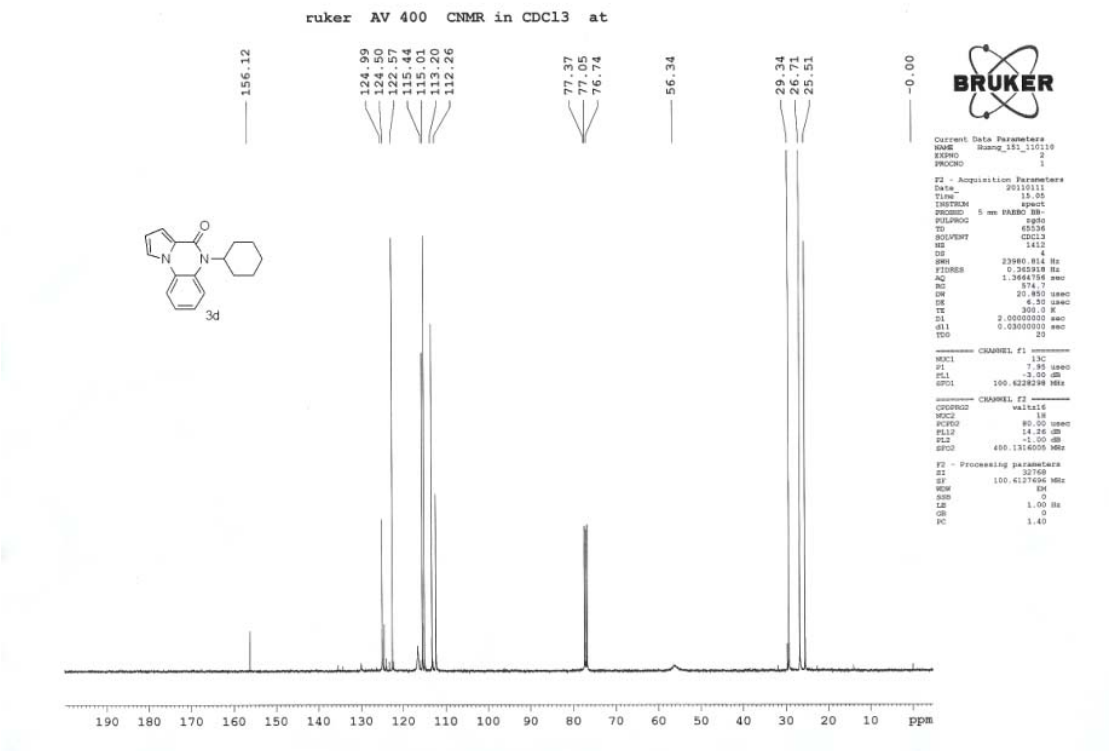
ruker AV 400 CNMR in CDCl3 at
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124.99
124.50
122.57
115.44
115.01
113.20
112.26
77.37
77.05
76.74
56.34
29.34
26.71
25.51
-0.00
3d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
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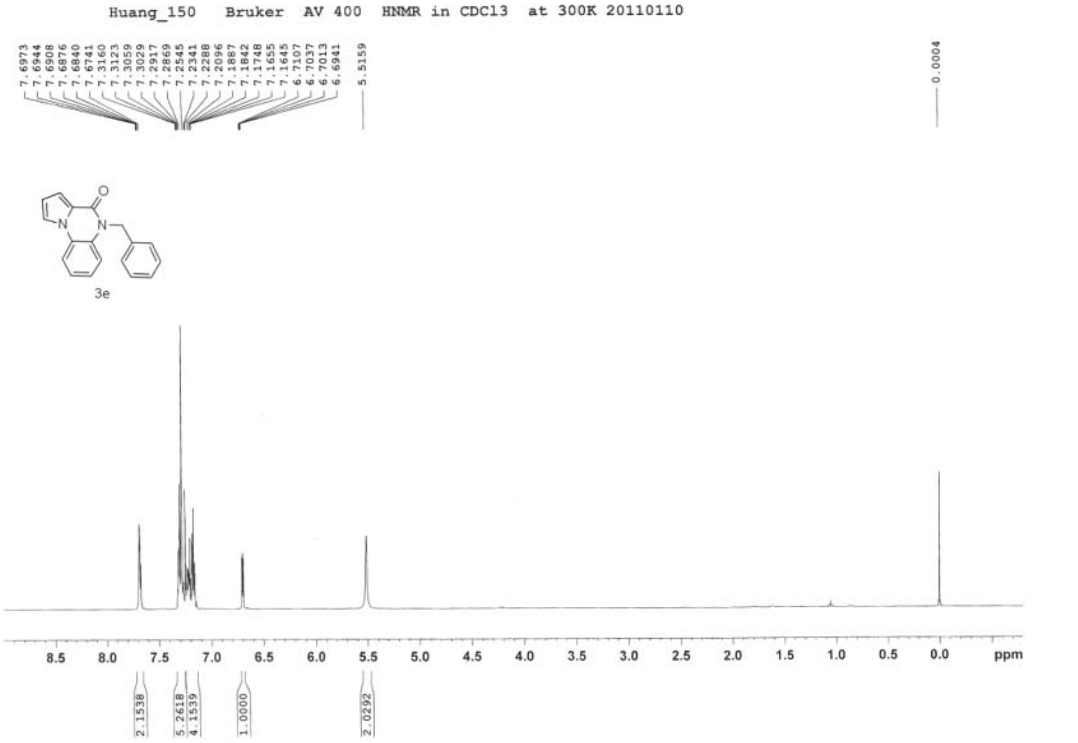
40
30
20
10
ppm


Huang_150 Bruker AV 400 HNMR in CDCl3 at 300K 20110110
7.6973
7.6944
7.6908
7.6876
7.6840
7.6741
7.3160
7.3123
7.3059
7.3029
7.2917
7.2869
7.2545
7.2341
7.2288
7.2096
7.1882
7.1842
7.1748
7.1655
7.1645
6.7107
6.7037
6.7013
6.6941
5.5159
0.0004
3e
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 ppm
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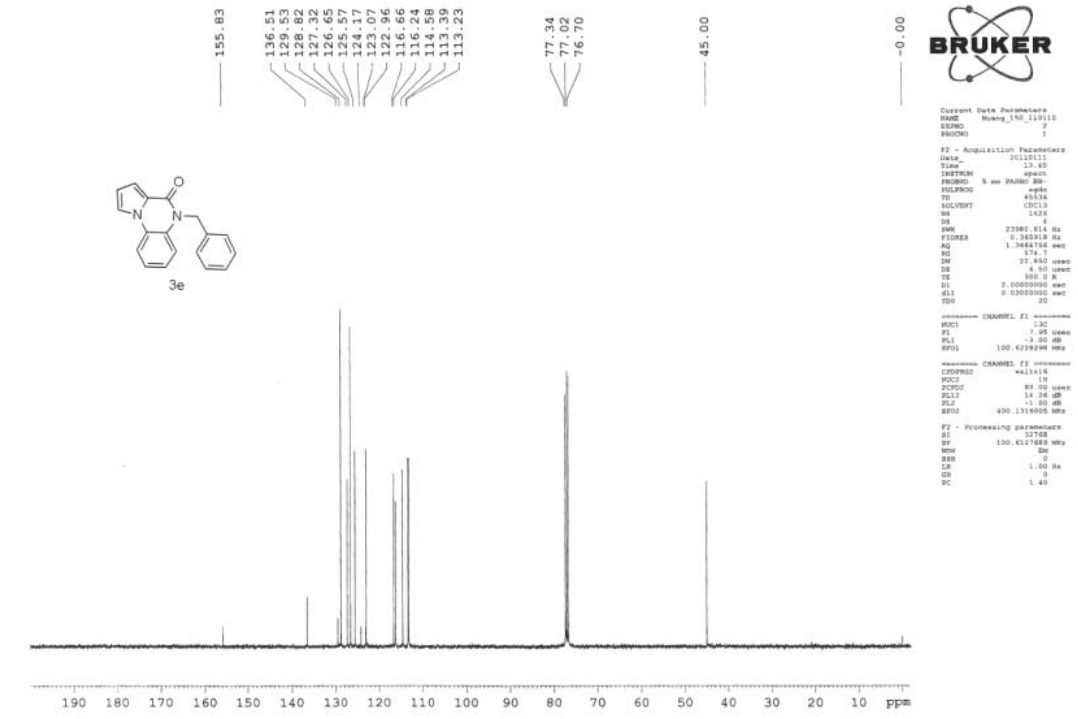
5.2618
4.1539
1.0000
2.0292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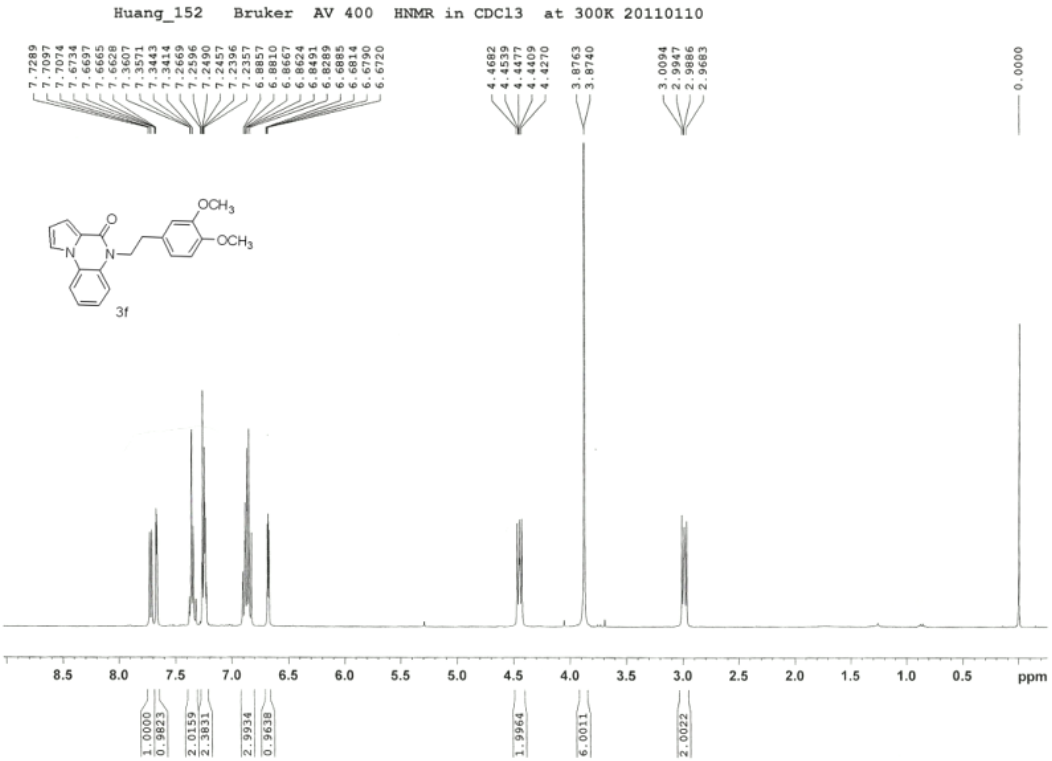
123.07
122.96
116.66
116.24
114.58
113.39
113.23
77.34
77.02
76.70
45.00
-0.00
BRUKER
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Huang_152 Bruker AV 400 HNMR in CDCl3 at 300K 20110110
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7.7097
7.7074
7.6734
7.6697
7.6665
7.6628
7.3607
7.3571
7.3443
7.3414
7.2669
7.2596
7.2490
7.2457
7.2396
7.2357
6.8857
6.8810
6.6667
6.6634
6.6491
6.6289
6.6885
6.6814
6.6790
6.6720
4.4682
4.4539
4.4477
4.4409
4.4270
3.8763
3.8740
3.0094
2.9947
2.9886
2.9683
0.0000
OCH3
OCH3
O
N
N
3f
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
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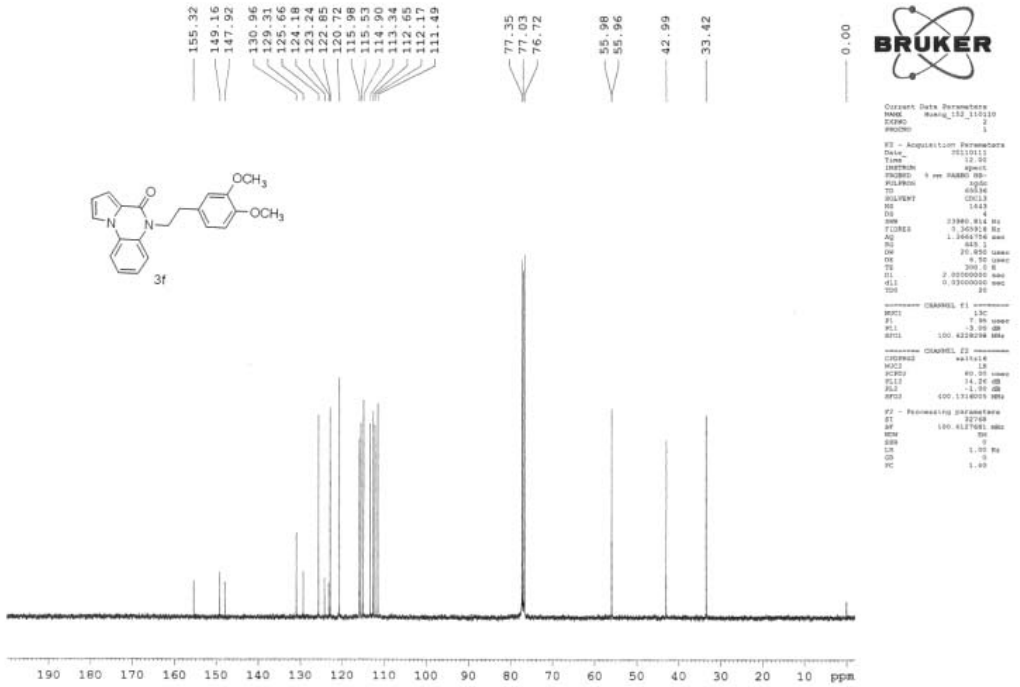
0.9638
1.9964
6.0011
2.0022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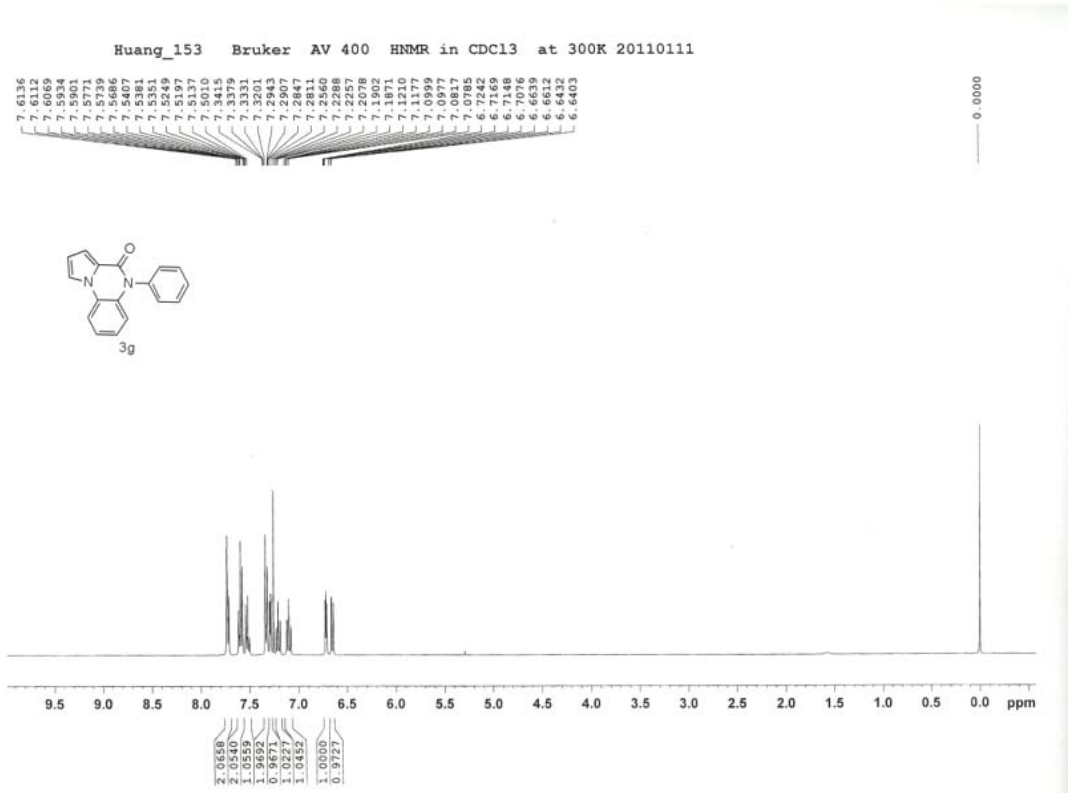
147.92
130.96
129.31
125.66
124.18
123.24
122.85
120.72
115.98
115.53
114.90
113.34
112.65
112.17
111.49
77.35
77.03
76.72
55.98
55.96
42.99
33.42
0.00
OCH3
OCH3
O
N
N
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Huang_153 Bruker AV 400 HNMR in CDCl3 at 300K 20110111
7.6136
7.6112
7.6069
7.5934
7.5901
7.5771
7.5739
7.5606
7.5467
7.5381
7.5351
7.5249
7.5197
7.5137
7.5010
7.3415
7.3379
7.3331
7.3201
7.2943
7.2907
7.2847
7.2811
7.2660
7.2588
7.2257
7.2078
7.1902
7.1671
7.1210
7.1177
7.0999
7.0977
7.0817
7.0785
6.7242
6.7169
6.7148
6.7076
6.6659
6.6632
6.6512
6.6403
0.0000
3g
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 ppm
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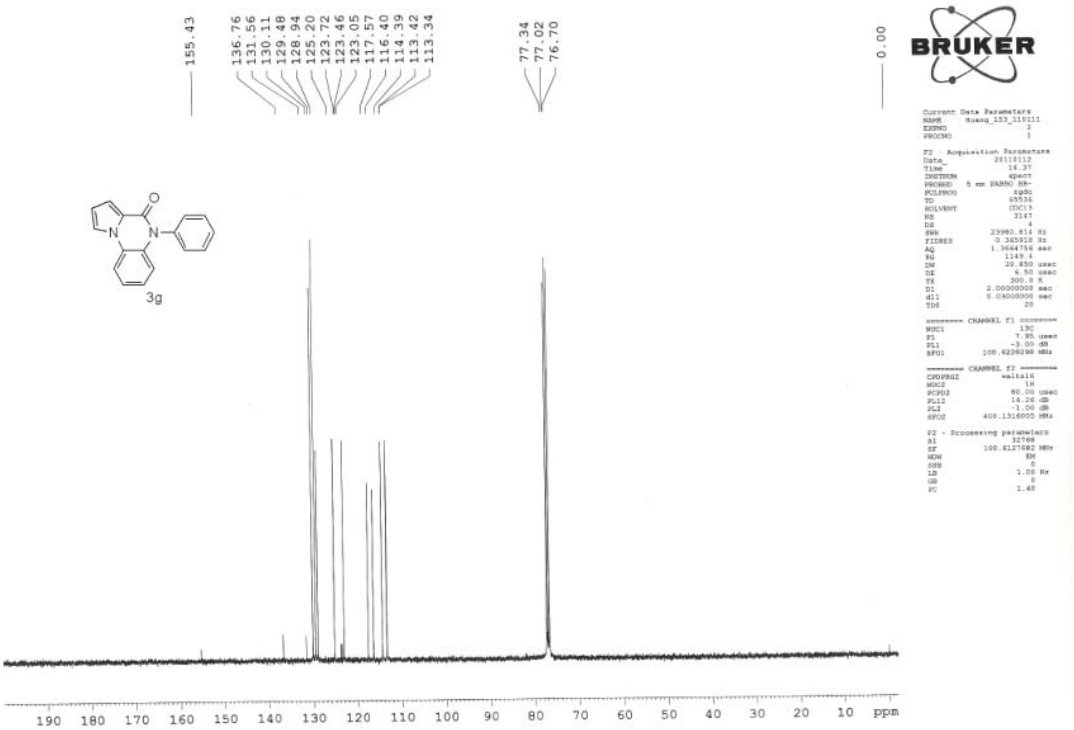
2.0540
1.0559
1.9692
0.9671
1.0227
1.0452
1.0000
0.9727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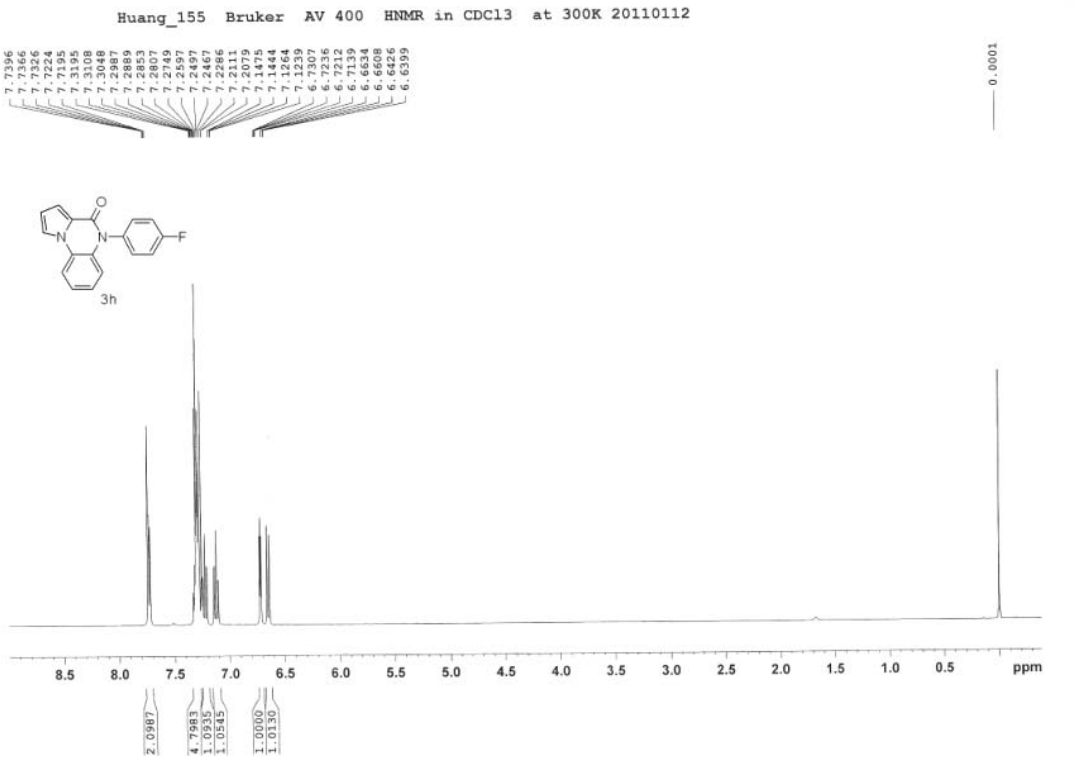
125.20
123.72
123.46
123.05
117.57
116.40
114.39
113.42
113.34
77.34
77.02
76.70
0.00
BRUKER
3g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Huang_155 Bruker AV 400 HNMR in CDCl3 at 300K 20110112
7.7396
7.7366
7.7326
7.7224
7.7195
7.3195
7.3108
7.3048
7.2987
7.2889
7.2853
7.2807
7.2749
7.2597
7.2497
7.2466
7.2211
7.2079
7.1475
7.1444
7.1264
7.1239
6.7307
6.7236
6.7212
6.7139
6.6634
6.6608
6.6426
6.6399
0.0001
3h
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
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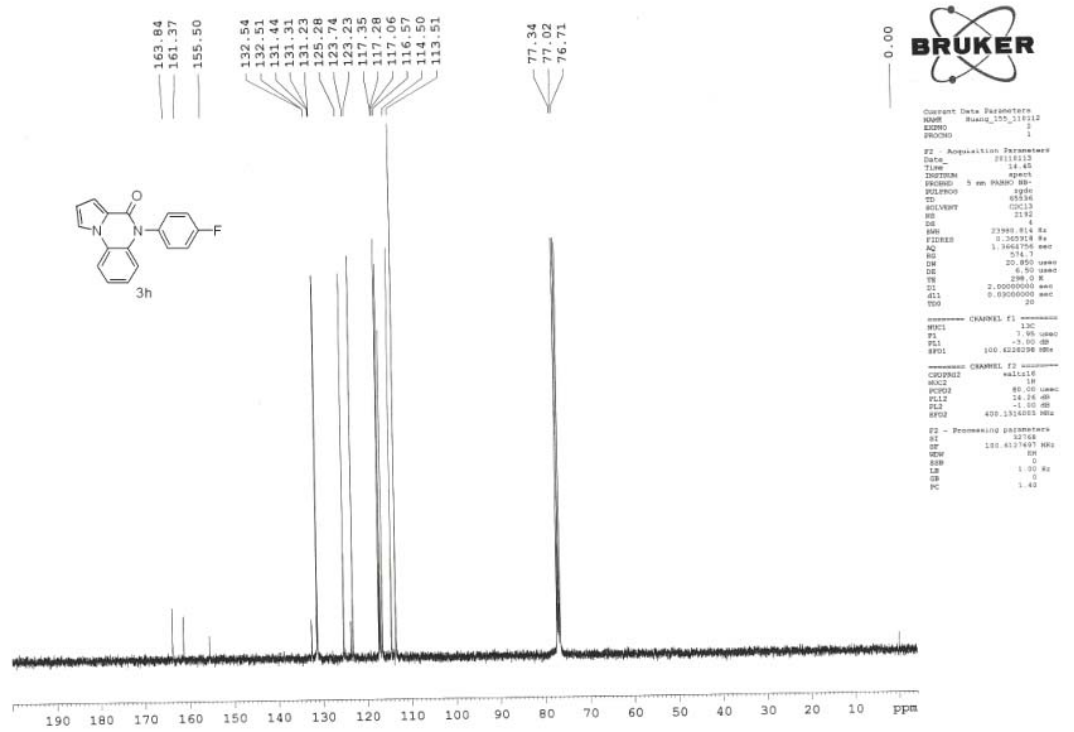
1.0925
1.0545
1.0000
1.0130


163.84
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132.51
131.44
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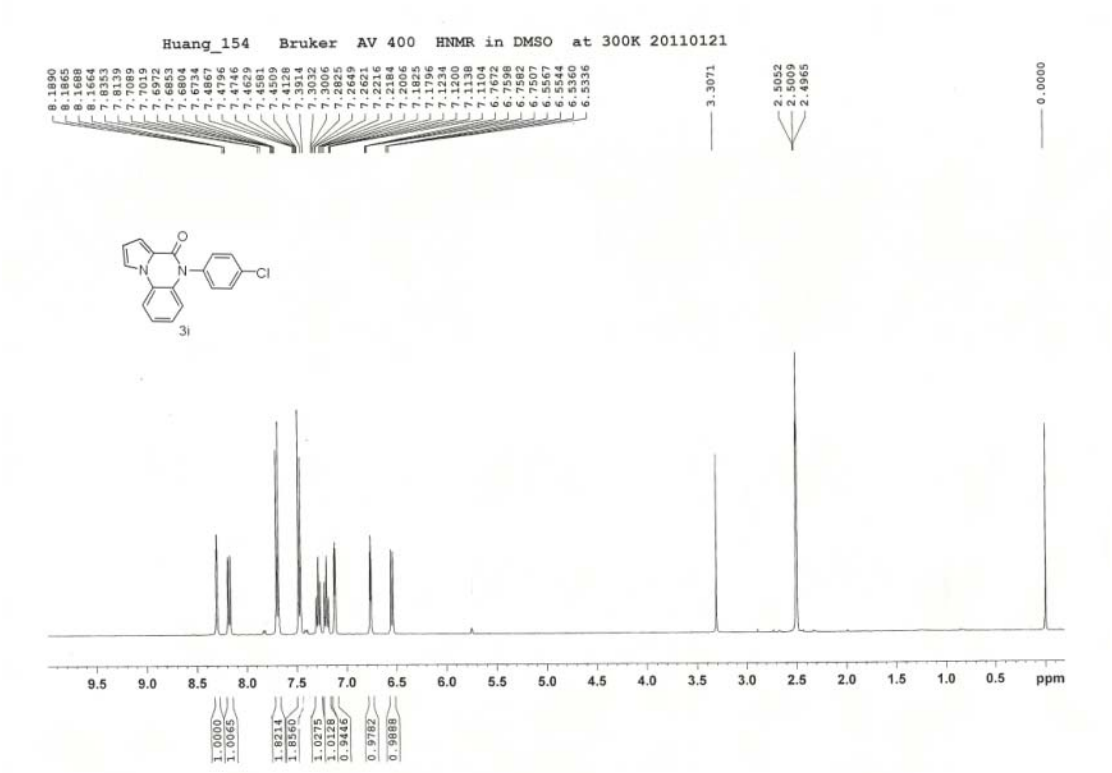
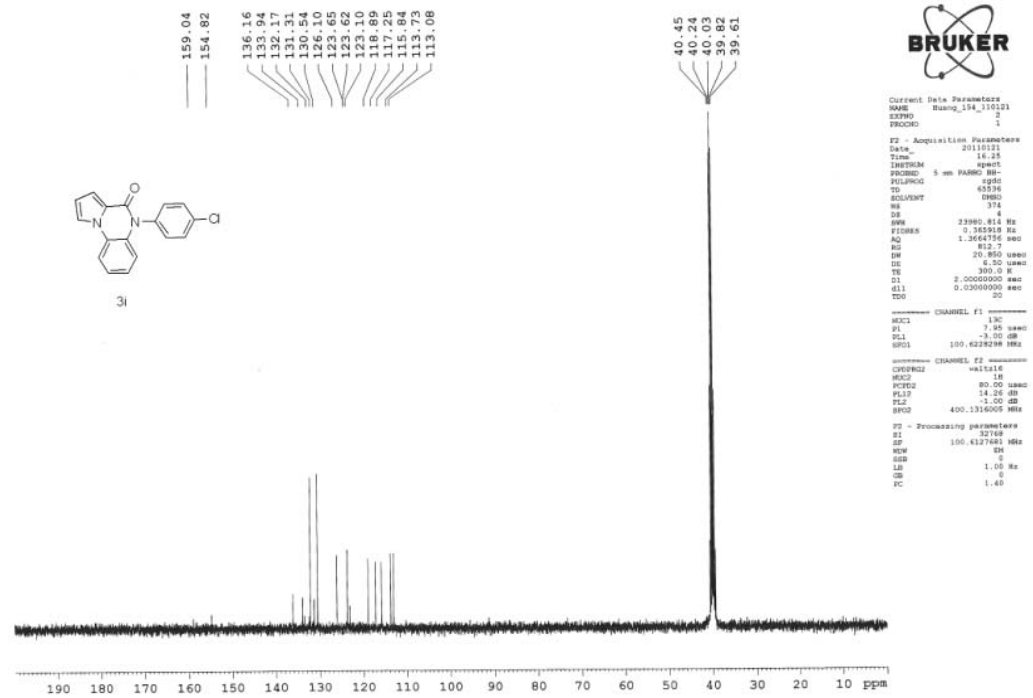
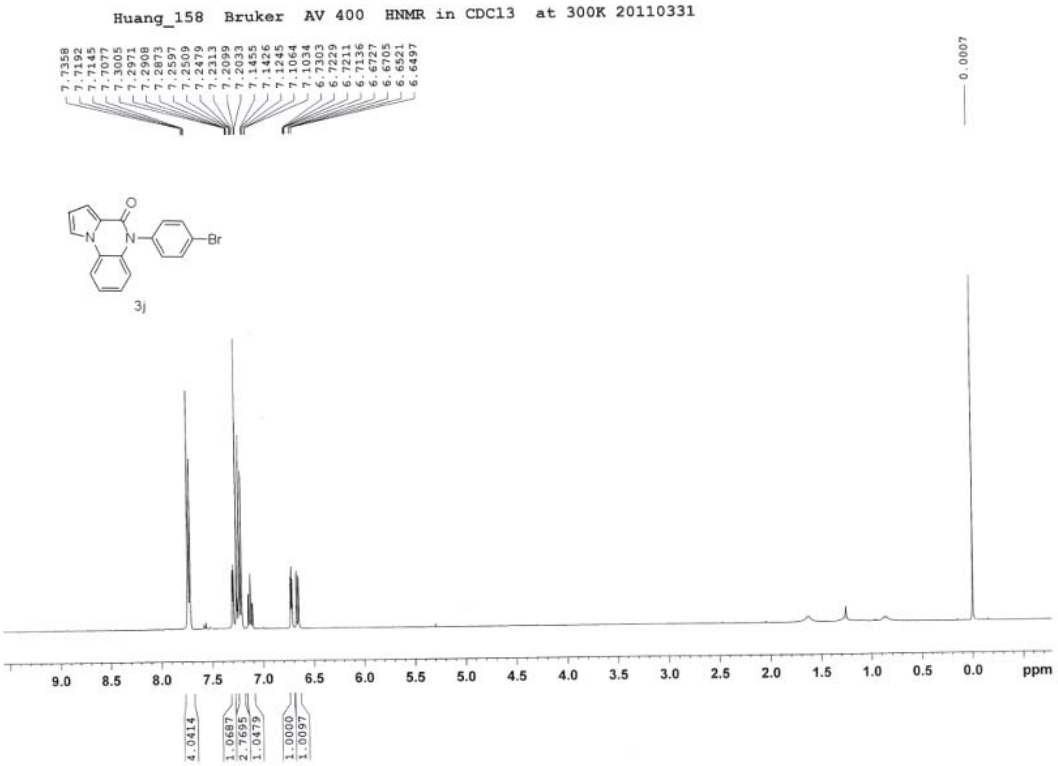
131.23
125.28
123.74
123.23
117.35
117.28
117.06
116.57
114.50
113.51
77.34
77.02
76.71
0.00
BRUKER
3h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Huang_154 Bruker AV 400 HNMR in DMSO at 300K 20110121
3i
ppm


3i
ppm


Huang_158 Bruker AV 400 HNMR in CDCl3 at 300K 20110331
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7.3005
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7.2908
7.2873
7.2597
7.2509
7.2479
7.2313
7.2099
7.2033
7.1455
7.1426
7.1245
7.1064
7.1034
7.1003
6.7229
6.7211
6.7136
6.6727
6.6705
6.6521
6.6497
0.0007
Br
3j
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 ppm
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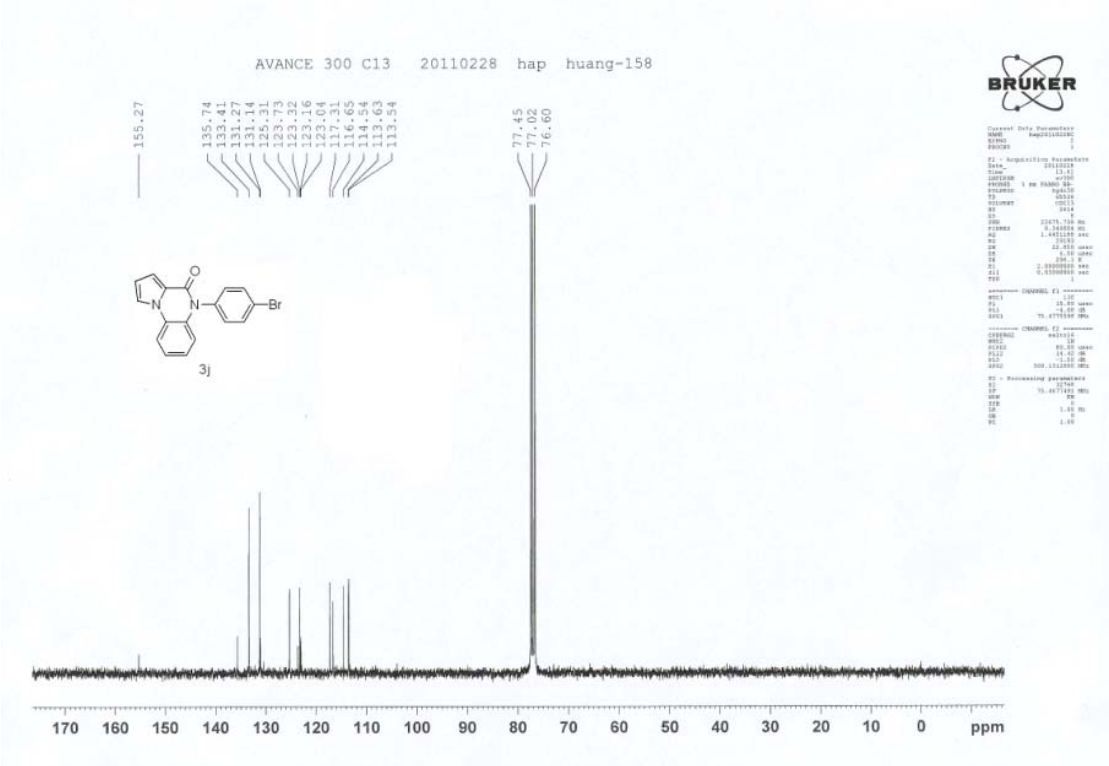
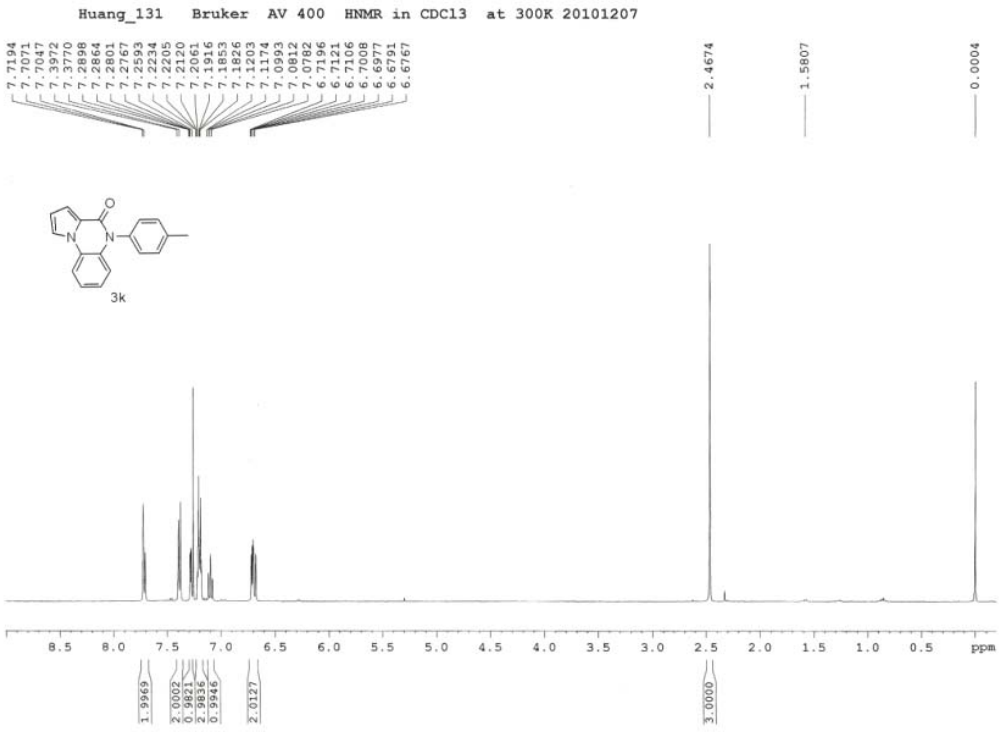
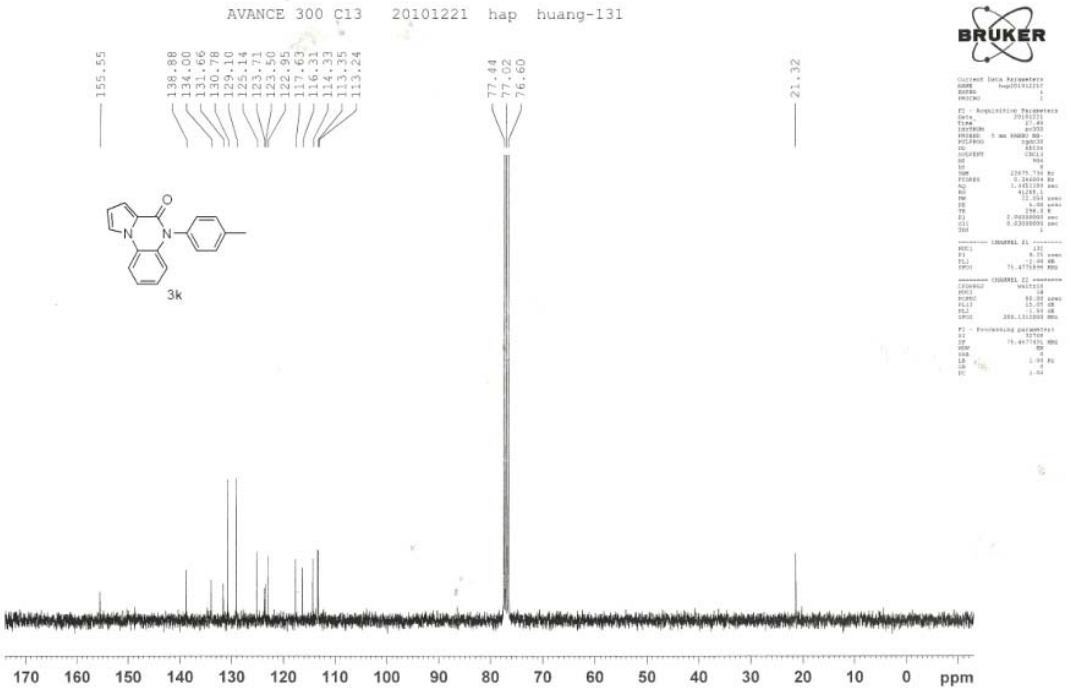
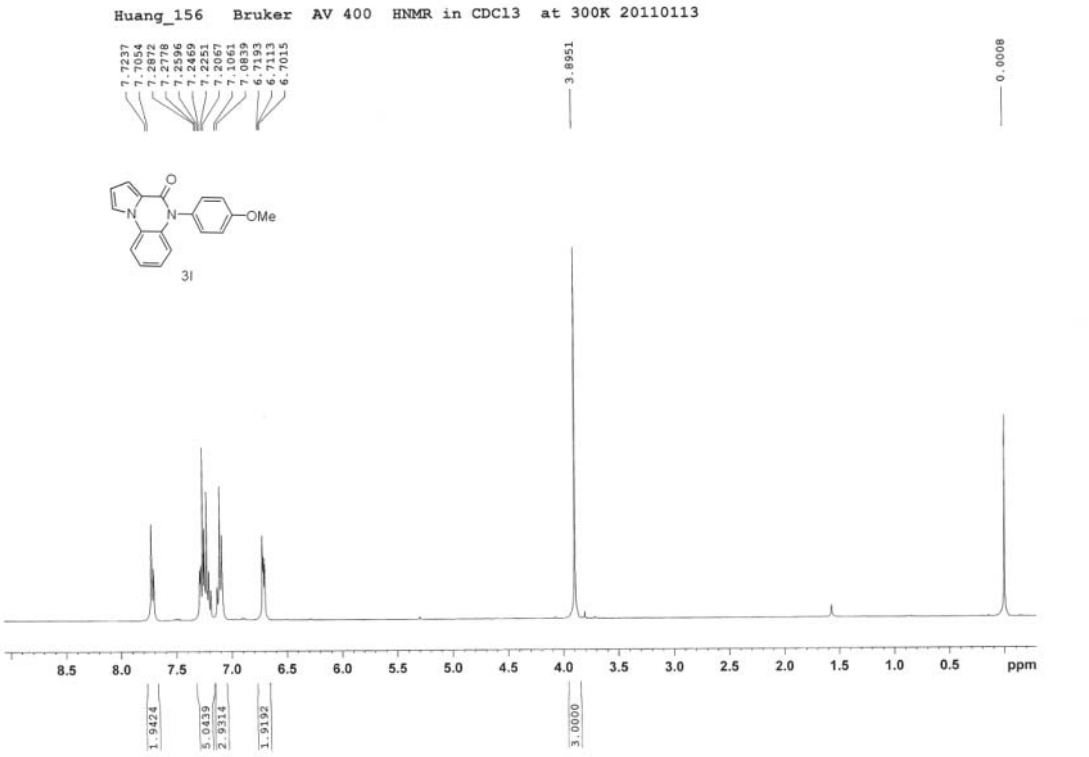
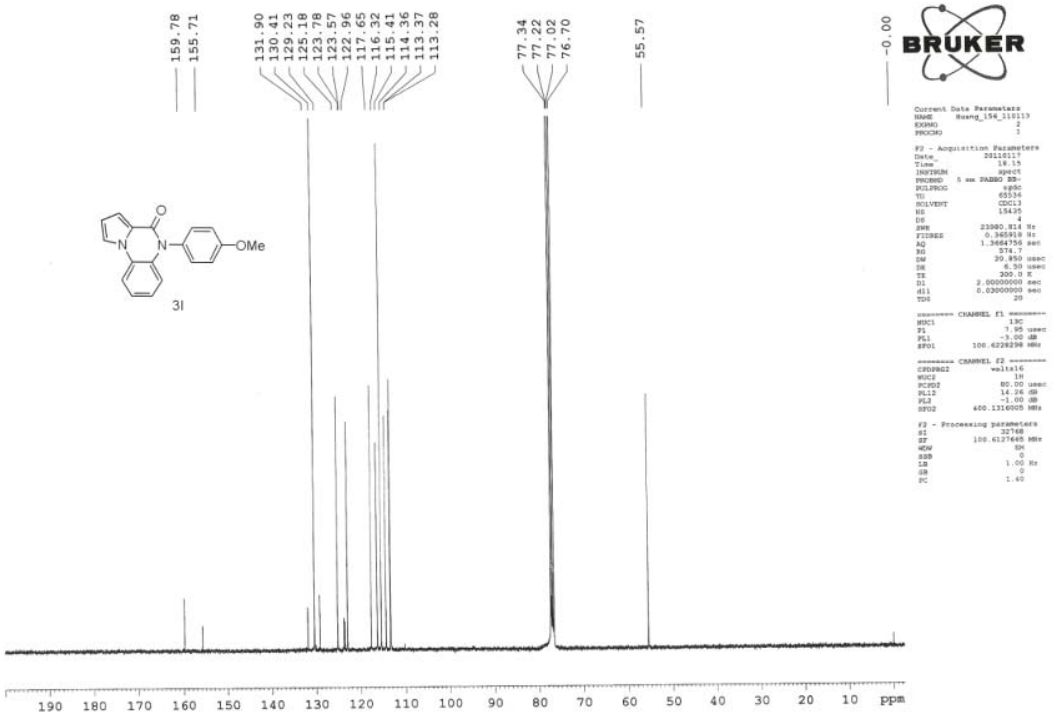
2.7695
1.0479
1.0000
1.0097

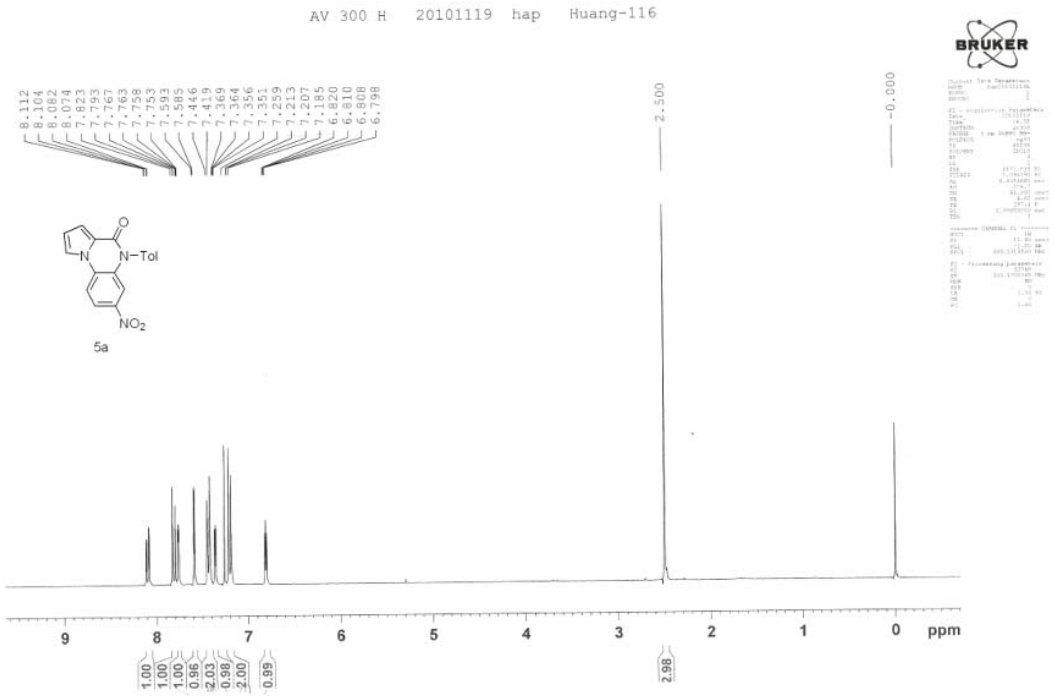

AVANCE 300 C13 20110228 hap huang-158
BRUKER
155.27
135.74
133.41
131.27
131.14
125.31
123.73
123.72
123.16
123.04
117.31
116.65
114.54
113.63
113.54
77.45
77.02
76.60
Br
3j
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

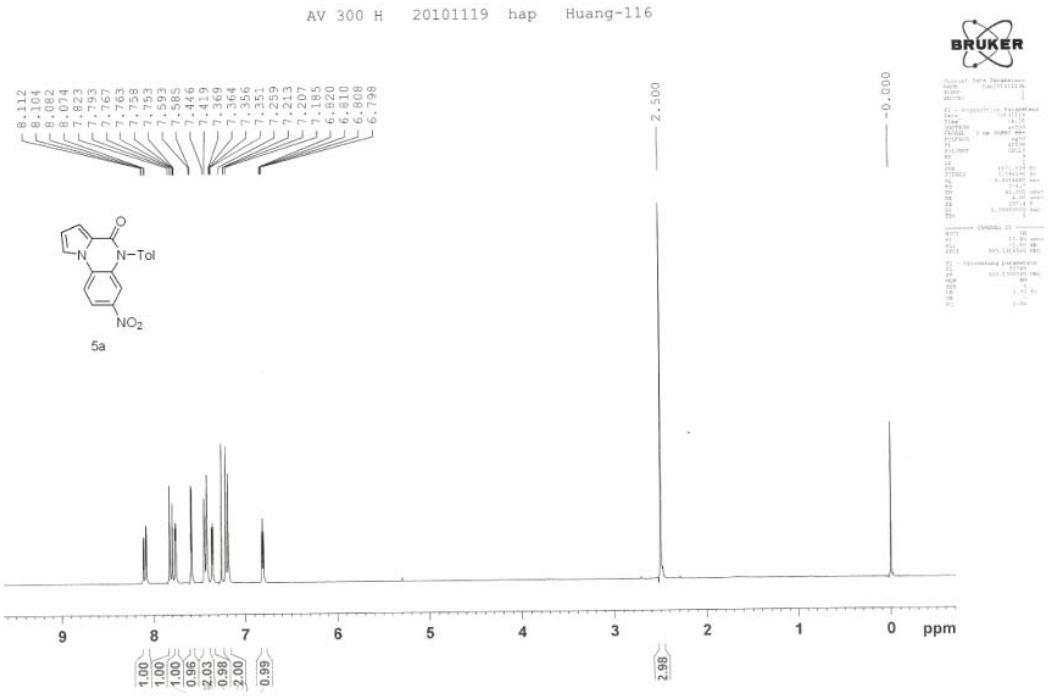


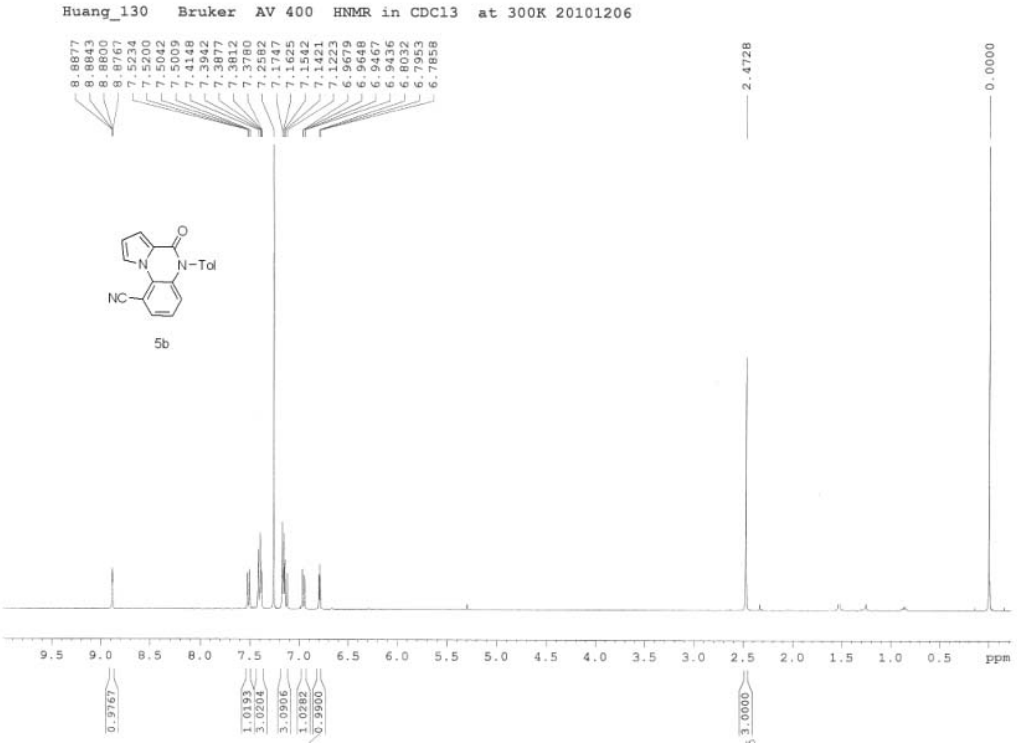


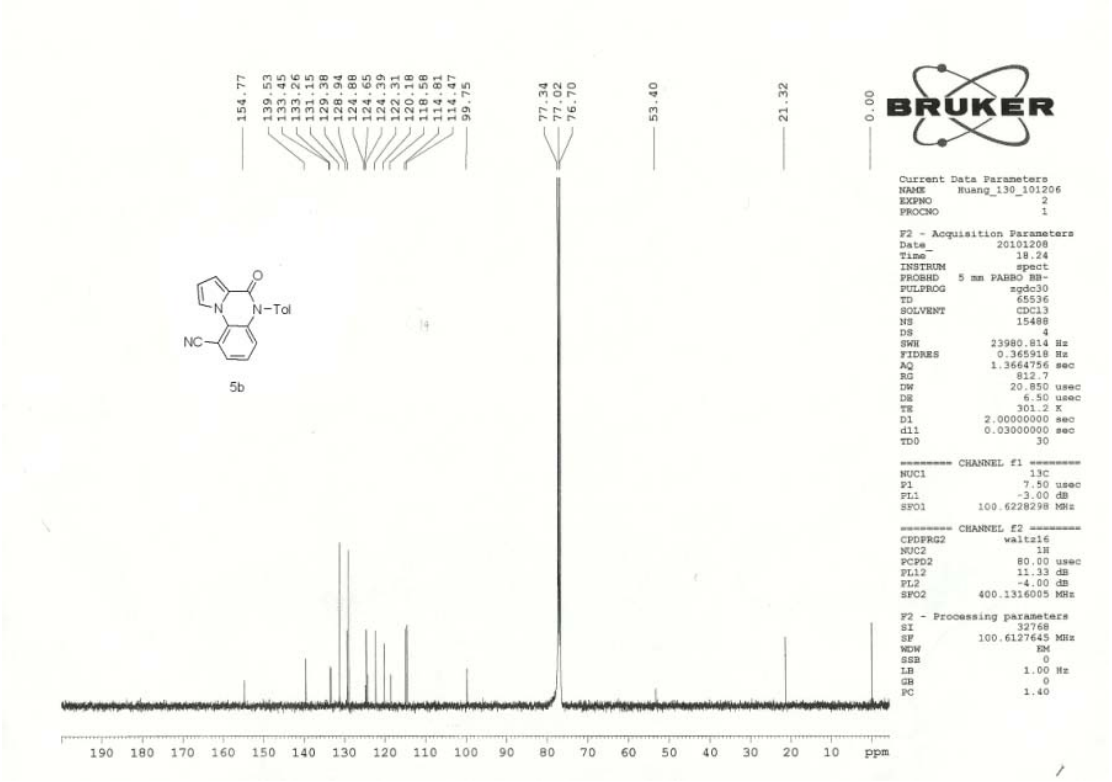


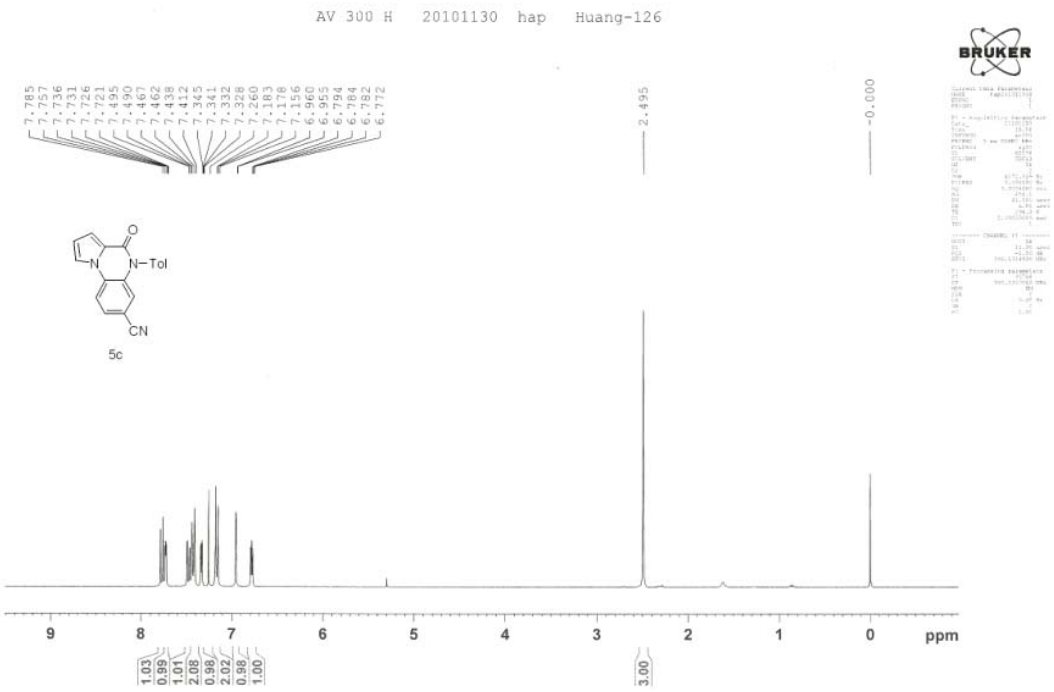


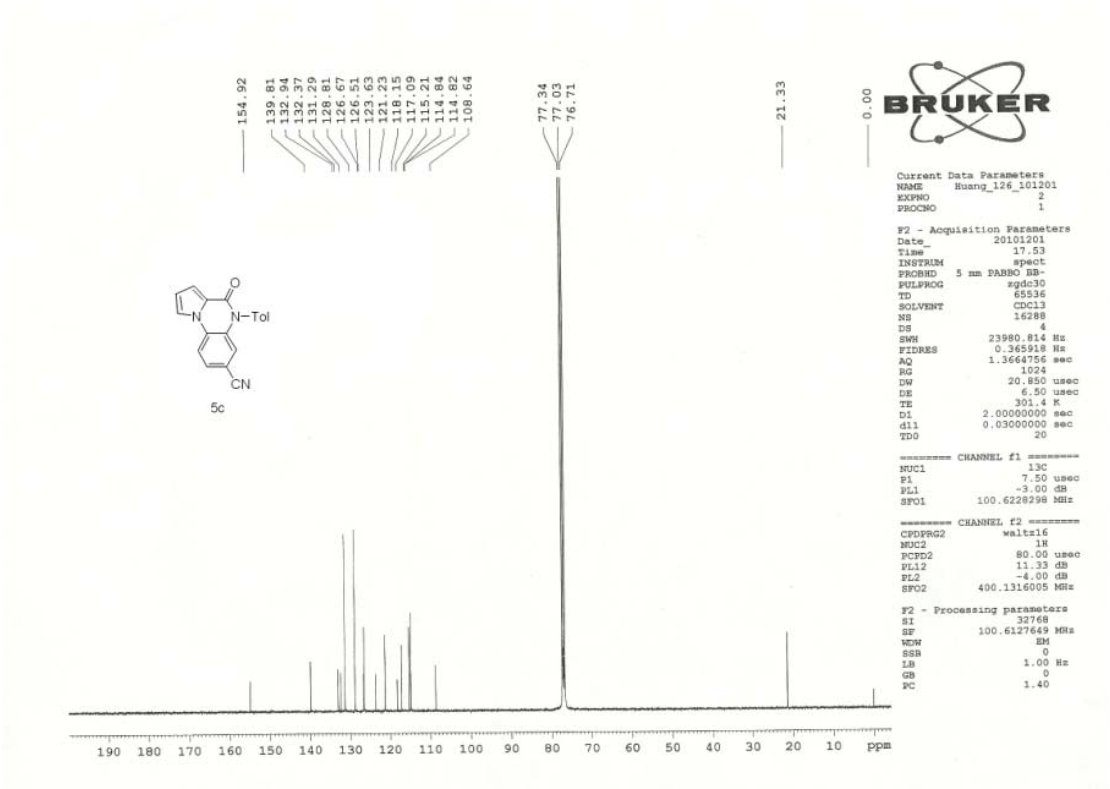

AV 300 H 20101119 hap Huang-116
BRUKER
8.112
8.104
8.082
8.074
7.823
7.793
7.767
7.763
7.758
7.753
7.593
7.585
7.446
7.419
7.369
7.364
7.356
7.351
7.259
7.213
7.207
7.185
6.820
6.810
6.808
6.798
2.500
-0.000
N
N–Tol
O
NO2
5a
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
0.96
2.03
0.98
2.00
0.99
2.98

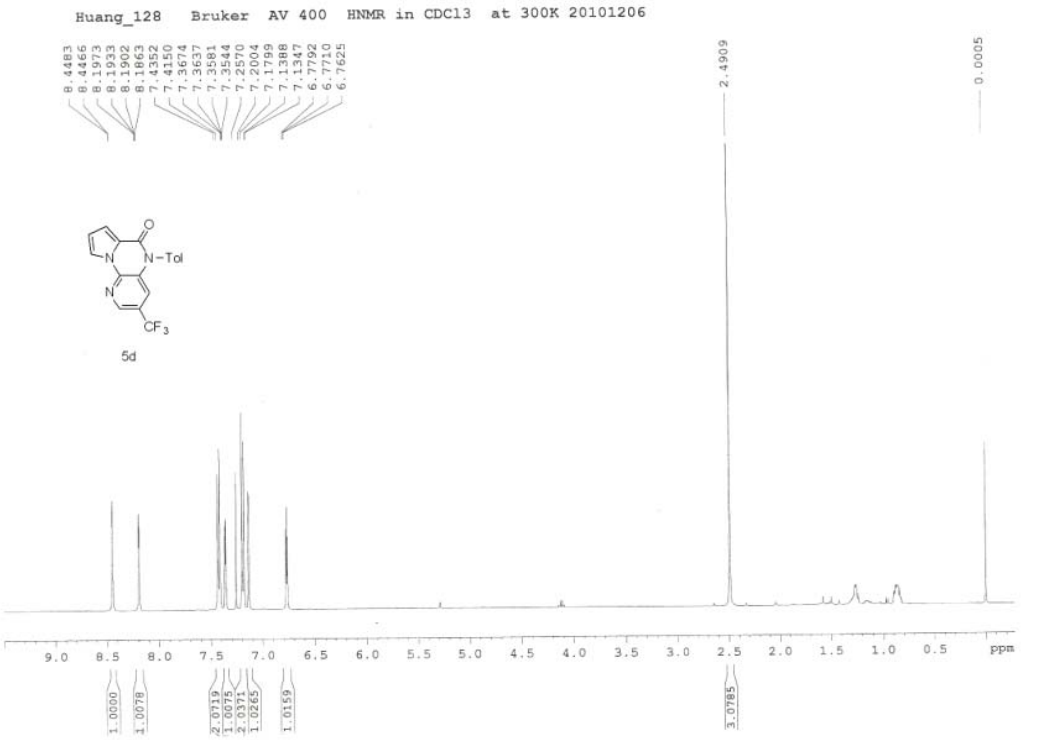

AV 300 H 20101119 hap Huang-116
BRUKER
8.112
8.104
8.082
8.074
7.823
7.793
7.767
7.763
7.758
7.753
7.593
7.585
7.446
7.419
7.369
7.364
7.356
7.351
7.259
7.213
7.207
7.185
6.820
6.810
6.808
6.798
2.500
-0.000
N
N–Tol
O
NO2
5a
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
0.96
2.03
0.98
2.00
0.99
2.98

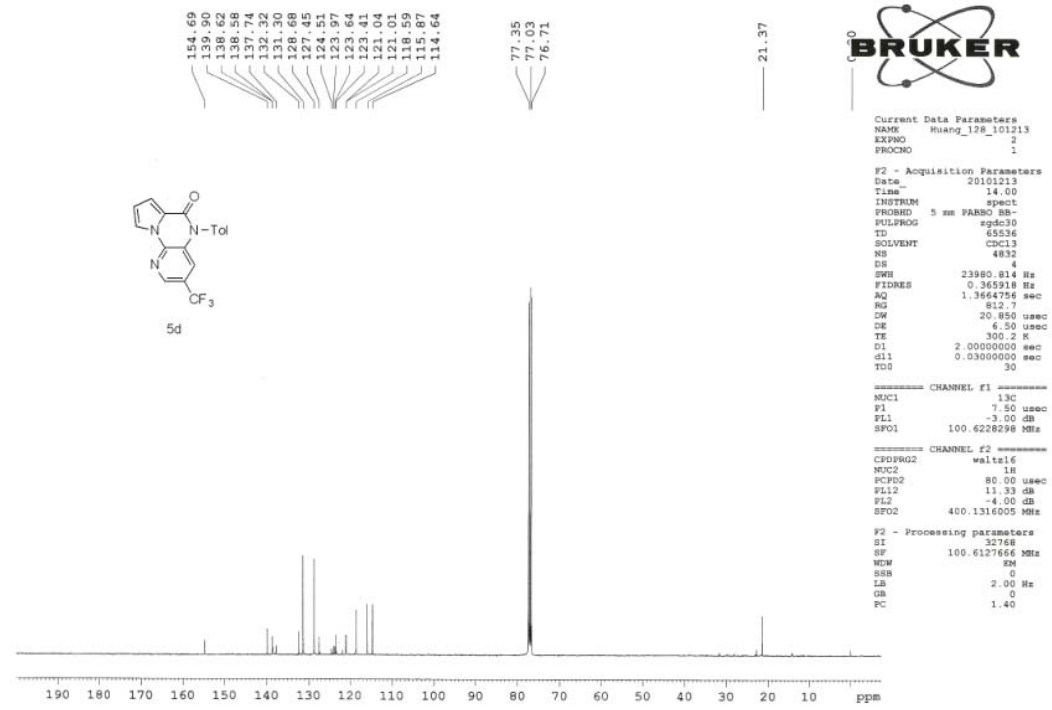




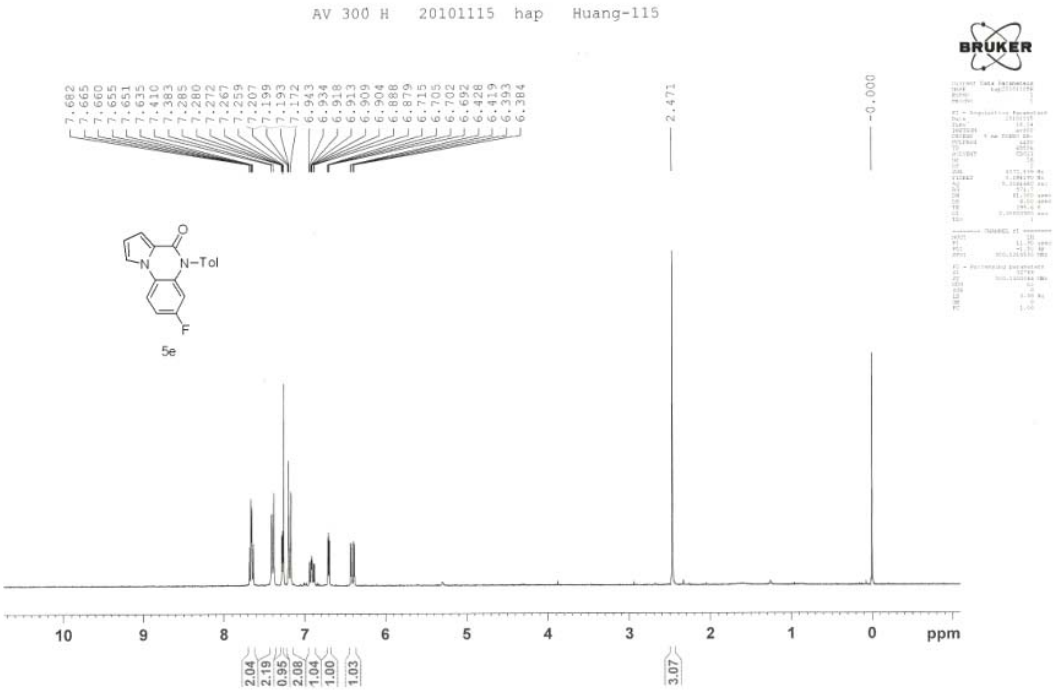

AV 300 H 20101130 hap Huang-126
BRUKER
7.785
7.757
7.736
7.731
7.726
7.721
7.495
7.490
7.467
7.462
7.438
7.412
7.345
7.341
7.332
7.328
7.260
7.183
7.178
7.156
6.960
6.955
6.794
6.784
6.782
6.772
2.495
-0.000
N-Tol
CN
5c
9
8
7
6
5
4
3
2
1
0
ppm
1.03
0.99
1.01
2.08
0.98
2.02
0.98
1.00
3.00

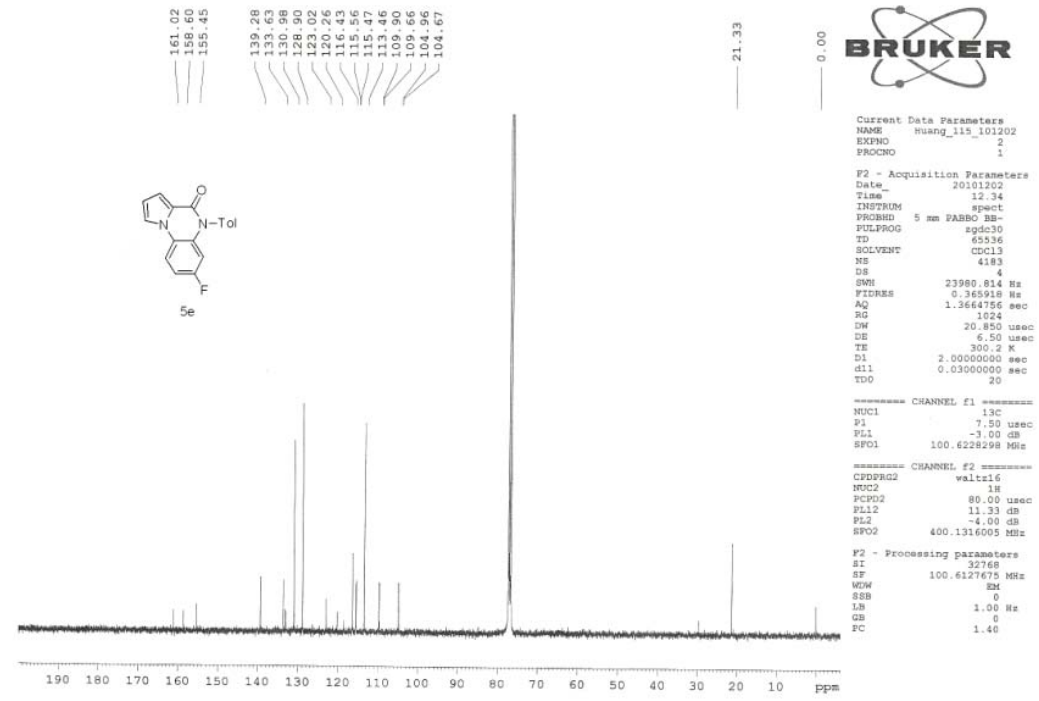

154.92
139.81
132.94
132.37
131.29
128.81
126.67
126.51
123.63
121.23
118.15
117.09
115.21
114.84
114.82
108.64
77.34
77.03
76.71
21.33
0.00
BRUKER
N-Tol
CN
5c
Current Data Parameters
NAME Huang_126_101201
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101201
Time 17.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 16288
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.36647568 sec
RG 1024
DW 20.850 usec
DE 6.50 usec
TE 301.4 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 11.33 dB
PL2 -4.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127649 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

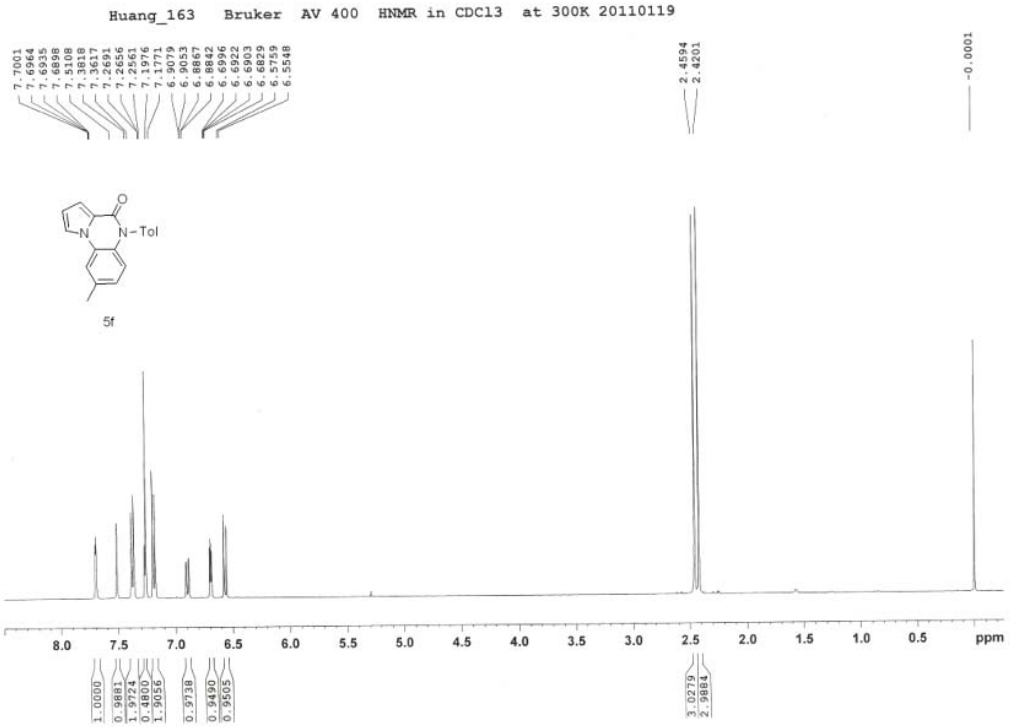

Huang_128 Bruker AV 400 HNMR in CDCl3 at 300K 20101206
8.4483
8.4466
8.1973
8.1933
8.1902
8.1863
7.4352
7.4150
7.3674
7.3637
7.3581
7.3544
7.2570
7.2004
7.1799
7.1388
7.1347
6.7792
6.7710
6.7625
2.4909
0.0005
N-Tol
CF3
5d
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.0000
1.0078
2.0719
1.0075
2.0371
1.0265
1.0159
3.0785

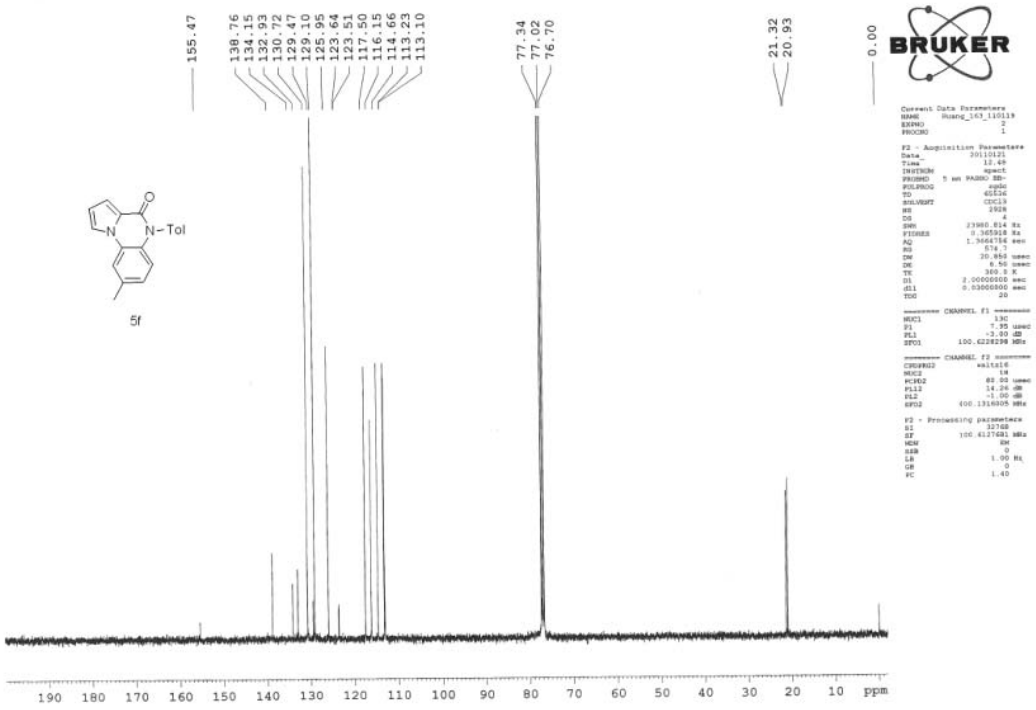

154.69
139.90
138.62
138.58
137.74
132.32
131.30
128.68
127.45
124.51
123.97
123.64
123.41
121.04
121.01
118.59
115.87
114.64
77.35
77.03
76.71
21.37
N-Tol
CF3
5d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

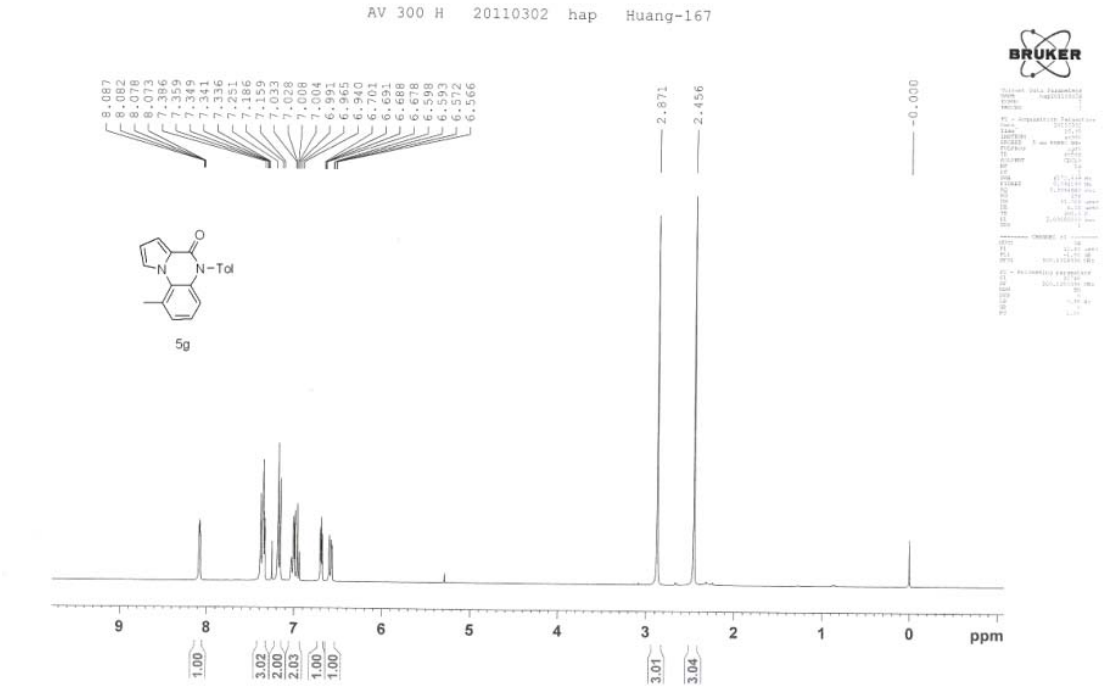
BRUKER
Current Data Parameters
NAME Huang_128_101213
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101213
Time 14.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 4832
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 812.7
DW 20.850 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 30
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 11.33 dB
PL2 -4.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127666 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

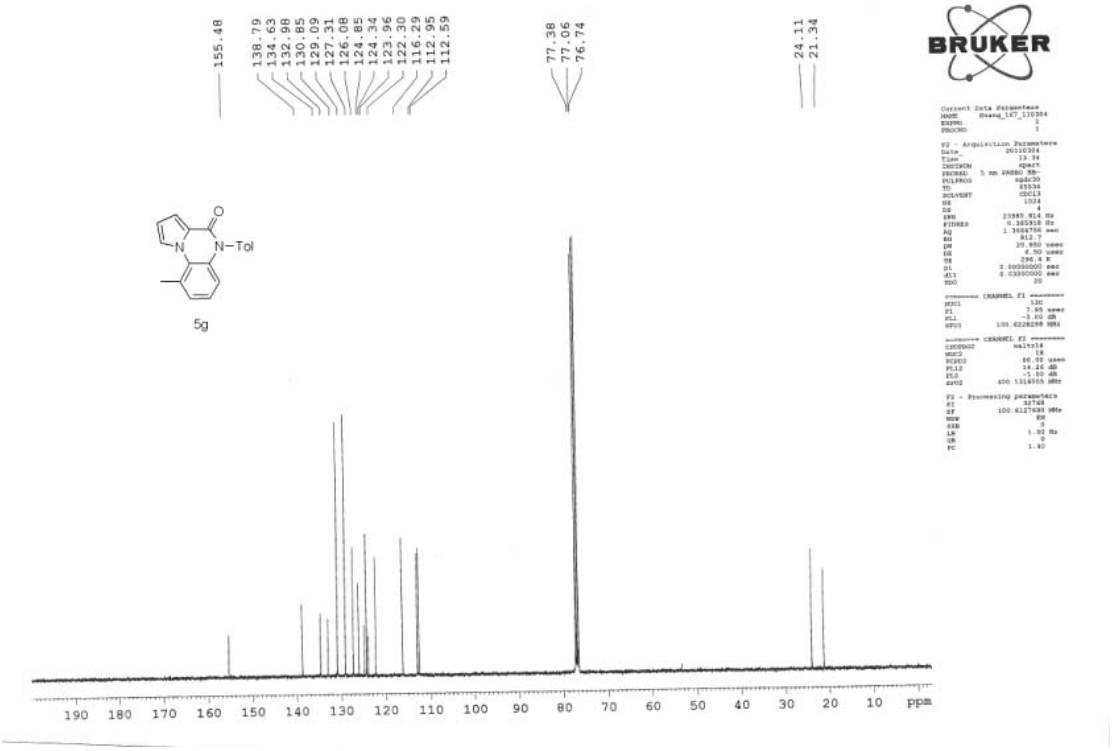

AV 300 H 20101115 hap Huang-115
BRUKER
7.682
7.665
7.660
7.655
7.651
7.635
7.410
7.383
7.285
7.280
7.272
7.267
7.259
7.207
7.199
7.193
7.172
6.943
6.934
6.918
6.913
6.909
6.904
6.888
6.879
6.715
6.705
6.702
6.692
6.428
6.419
6.393
6.384
2.471
0.000
N-Tol
F
5e
10 9 8 7 6 5 4 3 2 1 0 ppm
2.04 2.19 0.95 2.08 1.04 1.00 1.03
3.07

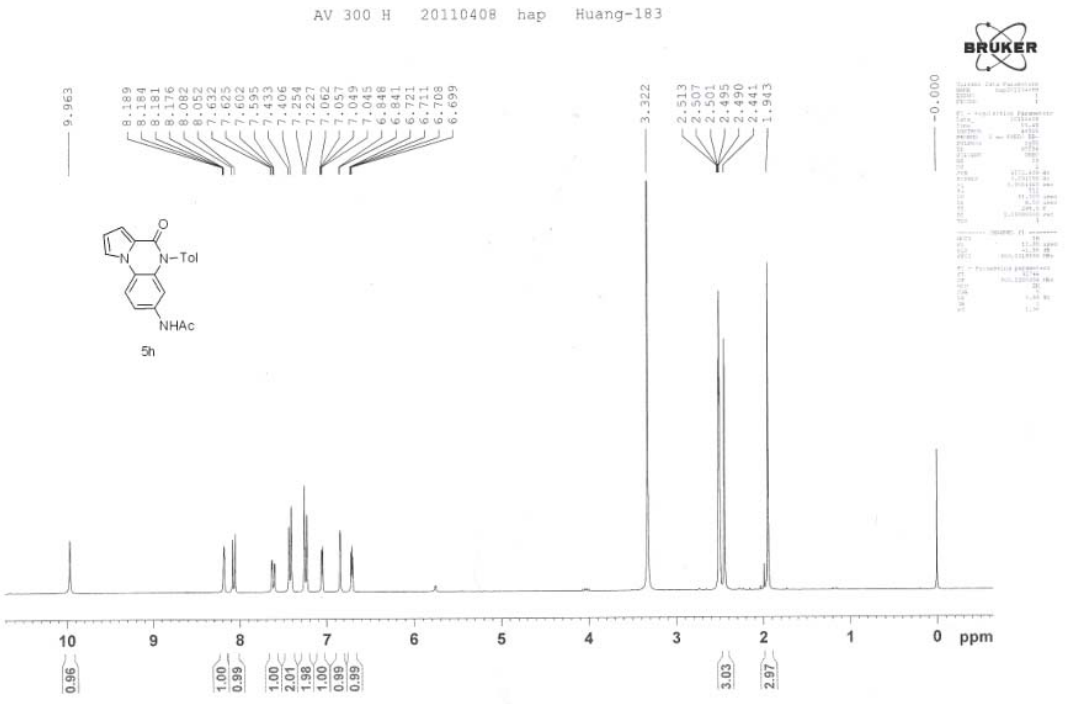

161.02
158.60
155.45
139.28
133.63
130.98
128.90
123.02
120.26
116.43
115.56
115.47
113.46
109.90
109.66
104.96
104.67
21.33
0.00
BRUKER
N-Tol
F
5e
Current Data Parameters
NAME Huang_115_101202
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101202
Time 12.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 4183
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1024
DW 20.850 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 11.33 dB
PL2 -4.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127675 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

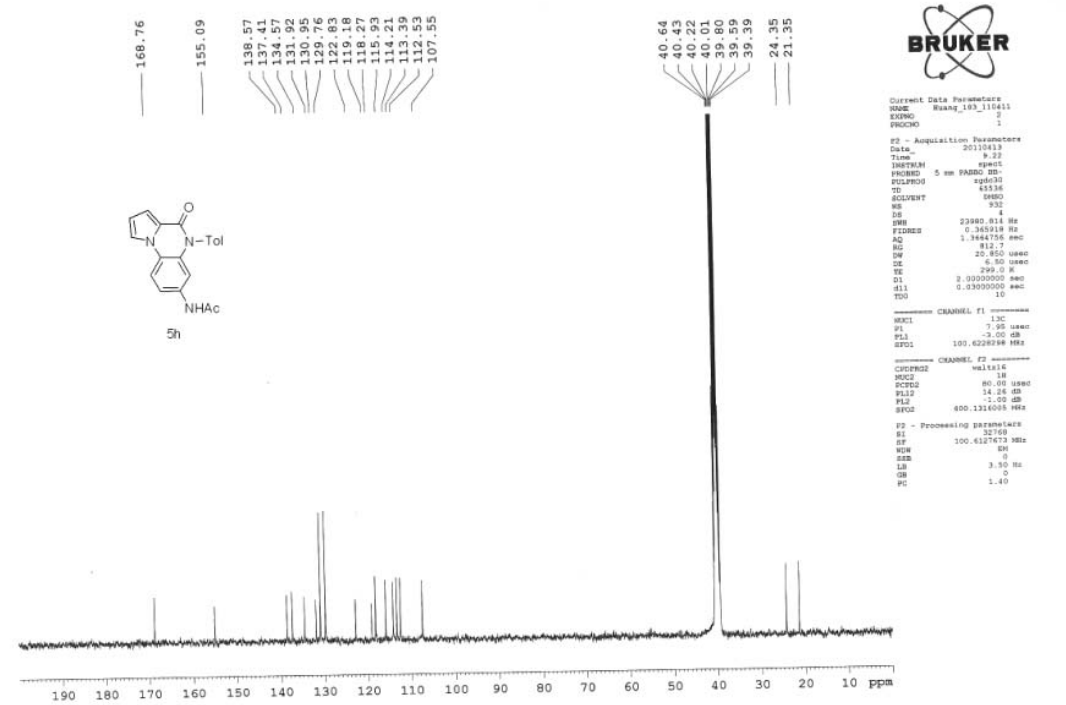


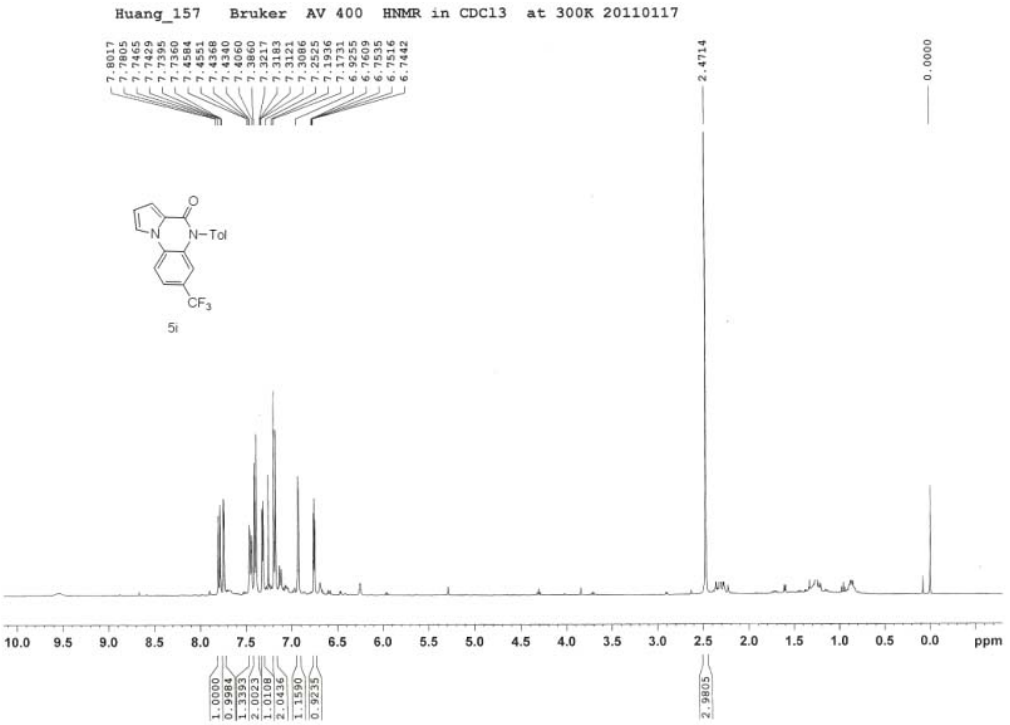


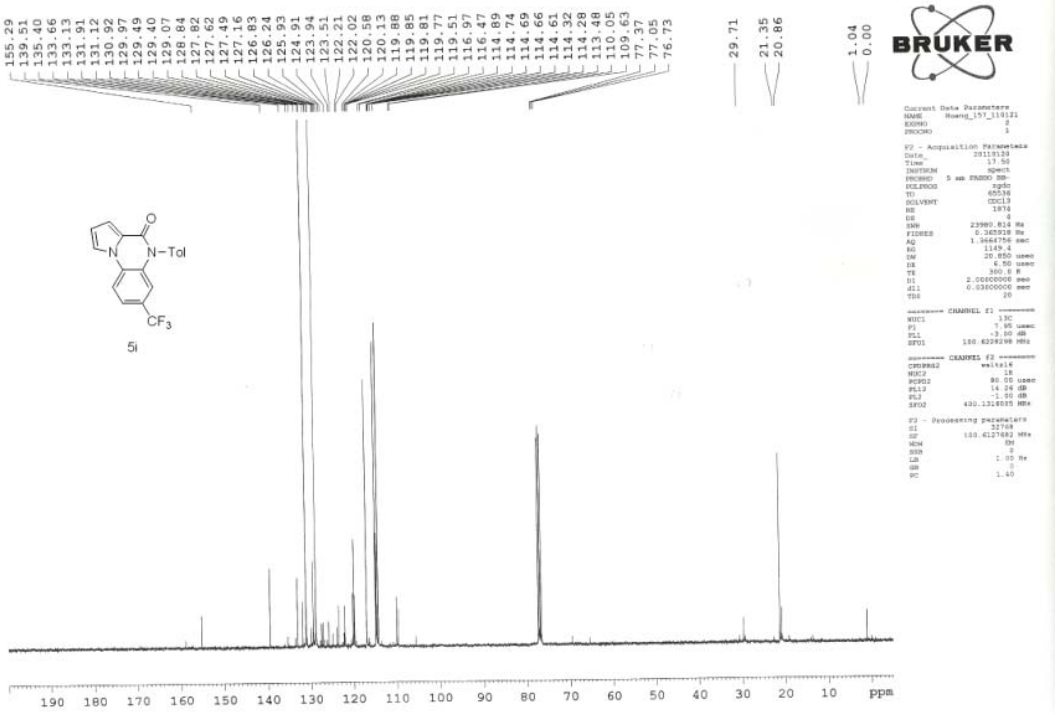

AV 300 H 20110302 hap Huang-167
BRUKER
8.087
8.082
8.078
8.073
7.386
7.359
7.349
7.341
7.336
7.251
7.186
7.159
7.033
7.028
7.008
7.004
6.991
6.965
6.940
6.701
6.691
6.688
6.678
6.598
6.593
6.572
6.566
2.871
2.456
-0.000
N-Tol
5g
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.02
2.00
2.03
1.00
1.00
3.01
3.04

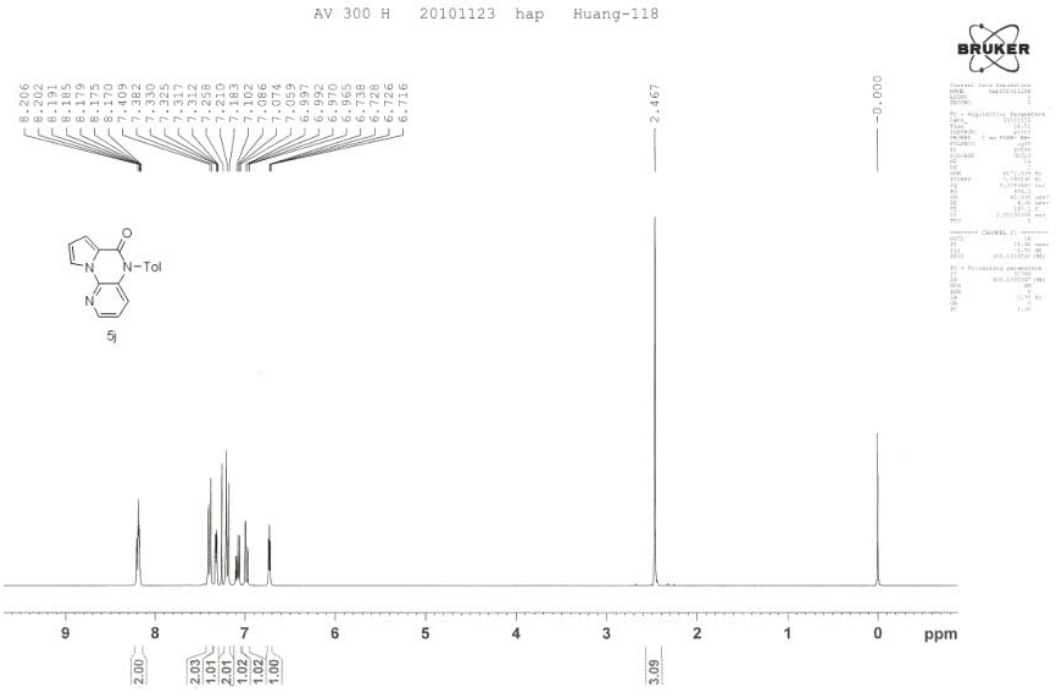

155.48
138.79
134.63
132.98
130.85
129.09
127.31
126.08
124.85
124.34
123.96
122.30
116.29
112.95
112.59
77.38
77.06
76.74
24.11
21.34
BRUKER
N-Tol
5g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

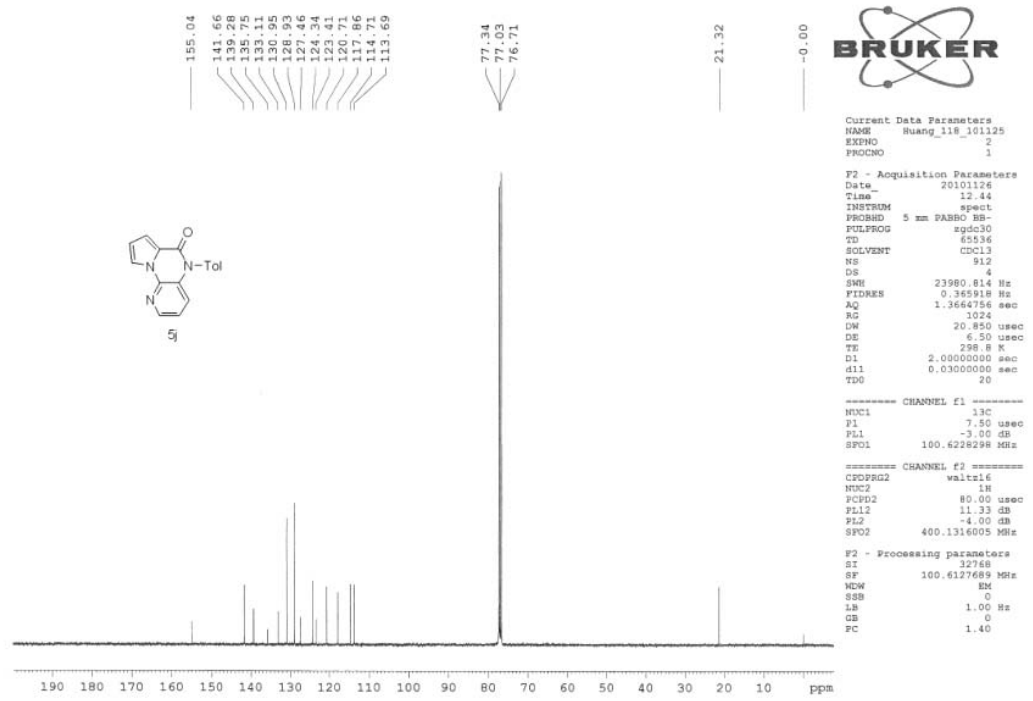

AV 300 H 20110408 hap Huang-183
BRUKER
9.963
8.189
8.184
8.181
8.176
8.082
8.052
7.632
7.625
7.602
7.595
7.433
7.406
7.234
7.227
7.062
7.057
7.049
7.045
6.848
6.841
6.721
6.711
6.708
6.699
3.322
2.513
2.507
2.501
2.495
2.490
2.441
1.943
-0.000
N–Tol
NHAc
5h
10 9 8 7 6 5 4 3 2 1 0 ppm
0.96
1.00
0.99
1.00
2.01
1.98
1.00
0.99
0.99
3.03
2.97

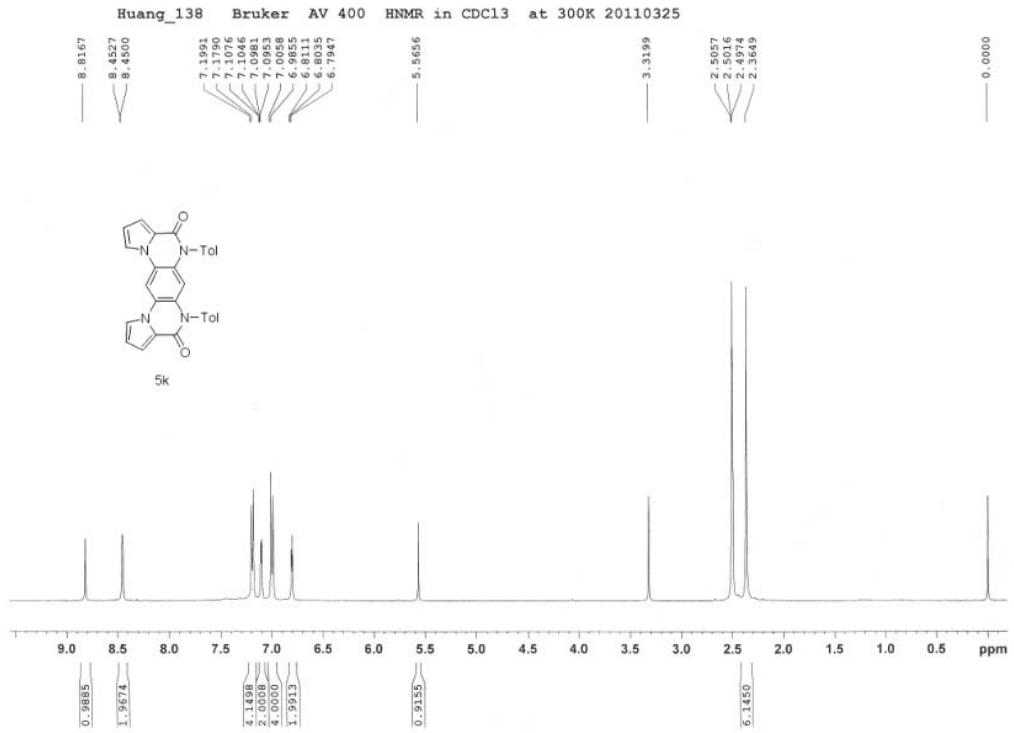

168.76
155.09
138.57
137.41
134.57
131.92
130.95
129.76
122.83
119.18
118.27
115.93
114.21
113.39
112.53
107.55
40.64
40.43
40.22
40.01
39.80
39.59
39.39
24.35
21.35
BRUKER
N–Tol
NHAc
5h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

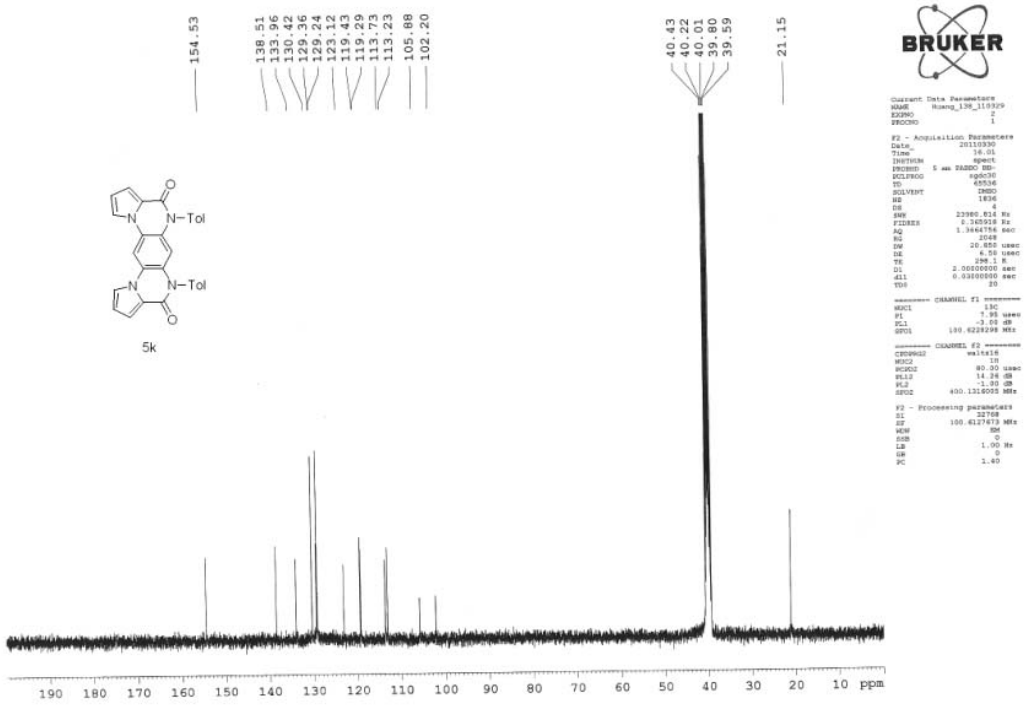

Huang_157 Bruker AV 400 HNMR in CDCl3 at 300K 20110117
7.8017
7.7805
7.7465
7.7429
7.7395
7.7360
7.4584
7.4551
7.4368
7.4340
7.4060
7.3860
7.3217
7.3183
7.3121
7.3086
7.2525
7.1936
7.1731
6.9255
6.7659
6.7535
6.7516
6.7442
2.4714
0.0000
N-Tol
CF3
5i
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.0000
0.9984
1.3393
2.0023
1.0198
2.0436
1.1590
0.9235
2.9805

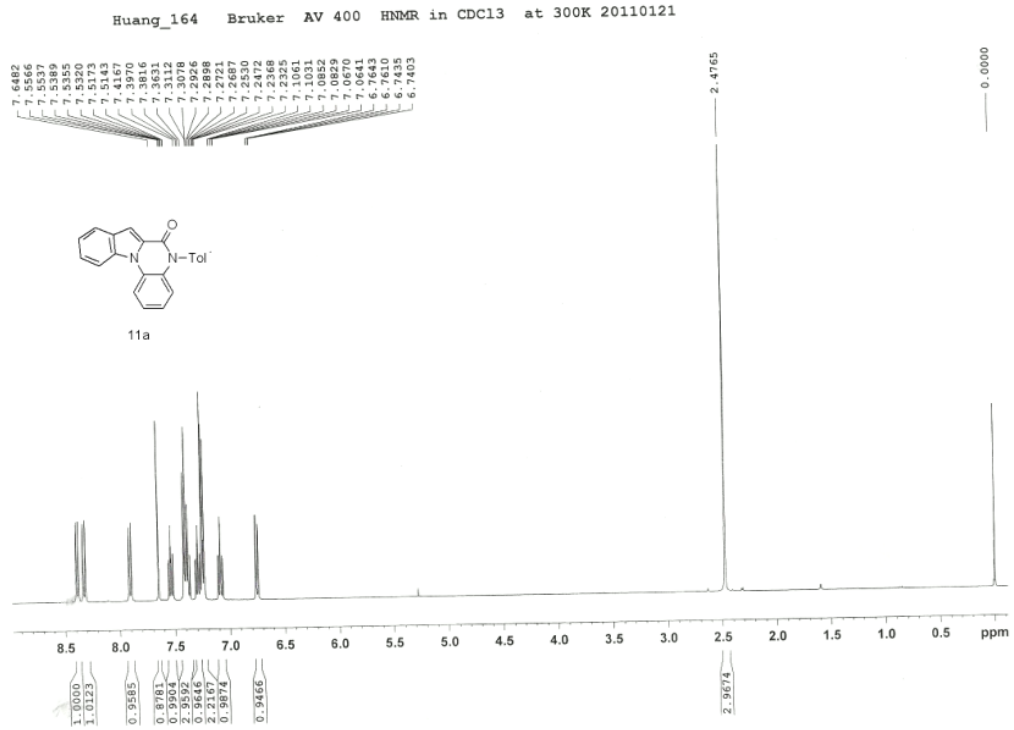

155.29
139.51
135.40
133.66
133.13
131.91
131.12
130.92
129.97
129.49
129.40
129.07
128.84
127.82
127.62
127.49
127.16
126.83
126.24
125.93
124.91
123.94
123.51
122.21
122.02
120.58
120.13
119.88
119.85
119.81
119.77
119.51
116.97
116.47
114.89
114.74
114.69
114.66
114.61
114.32
114.28
113.48
110.05
109.63
77.37
77.05
76.73
29.71
21.35
20.86
1.04
0.00
BRUKER
N-Tol
CF3
5i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

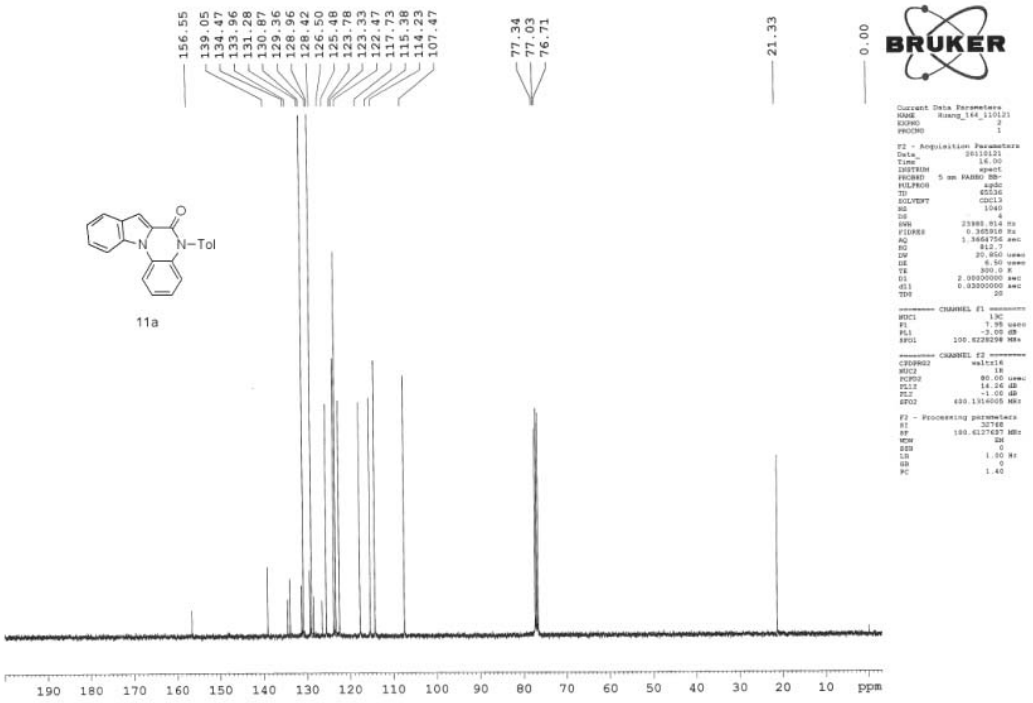

AV 300 H 20101123 hap Huang-118
BRUKER
8.206
8.202
8.131
8.185
8.179
8.175
8.170
7.409
7.382
7.330
7.325
7.317
7.312
7.258
7.210
7.183
7.102
7.086
7.074
7.059
6.997
6.992
6.970
6.965
6.738
6.728
6.726
6.716
2.467
0.000
N-Tol
5j
9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.03
1.01
2.01
1.02
1.02
1.00
3.09

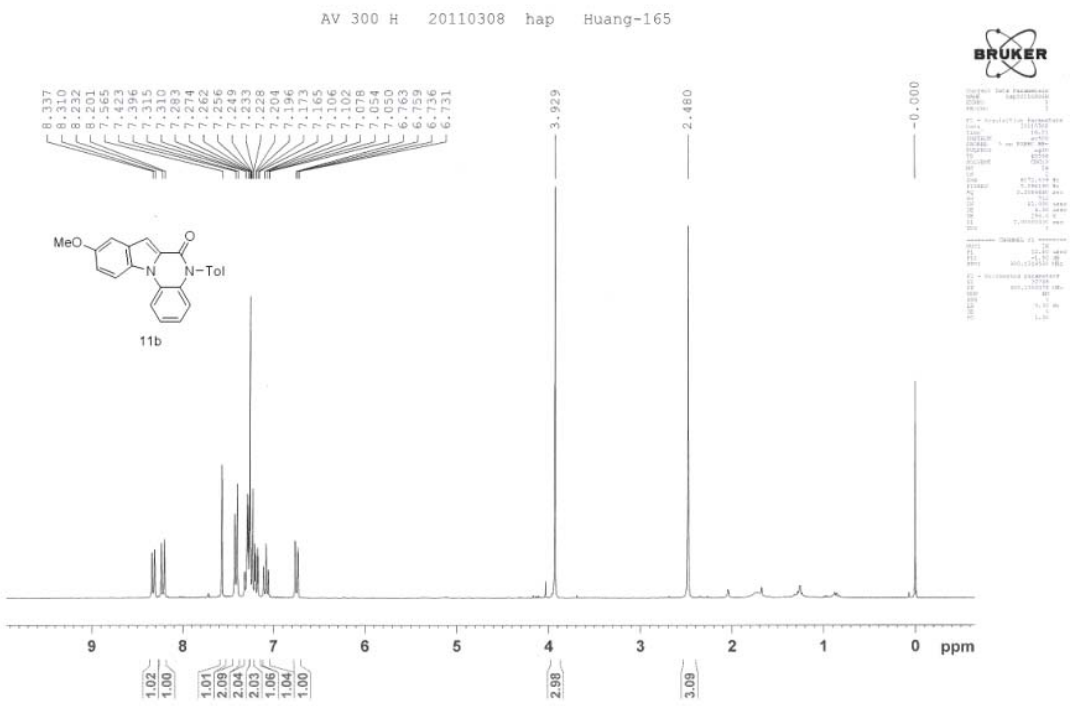

155.04
141.66
139.28
135.75
133.11
130.95
128.93
127.46
124.34
123.41
120.71
117.86
114.71
113.69
77.34
77.03
76.71
21.32
-0.00
BRUKER
N-Tol
5j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Huang_118_101125
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101126
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 912
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1024
DW 20.850 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 11.33 dB
PL2 -4.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

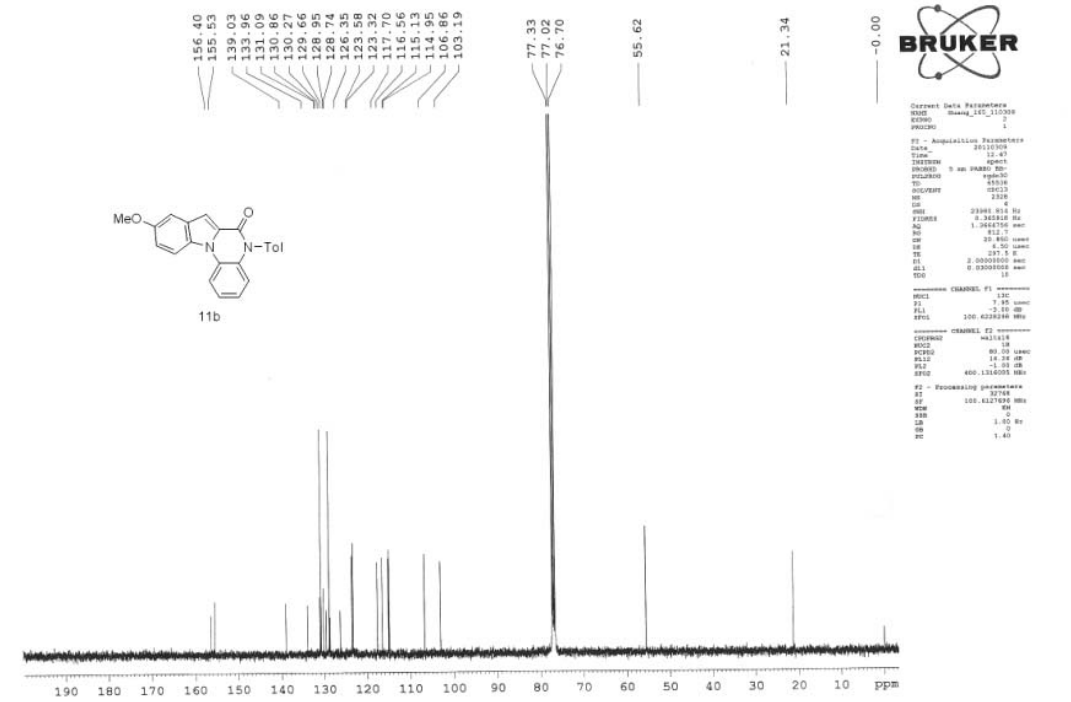

Huang_138 Bruker AV 400 HNMR in CDCl3 at 300K 20110325
8.8167
8.4527
8.4500
7.1991
7.1790
7.1076
7.1046
7.0981
7.0953
7.0058
6.8455
6.8111
6.8035
6.7947
5.5656
3.3199
2.5057
2.4974
2.3649
0.0000
N–Tol
N–Tol
5k
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.9885
1.9674
4.1498
2.0008
4.0000
1.9913
0.9155
6.1450

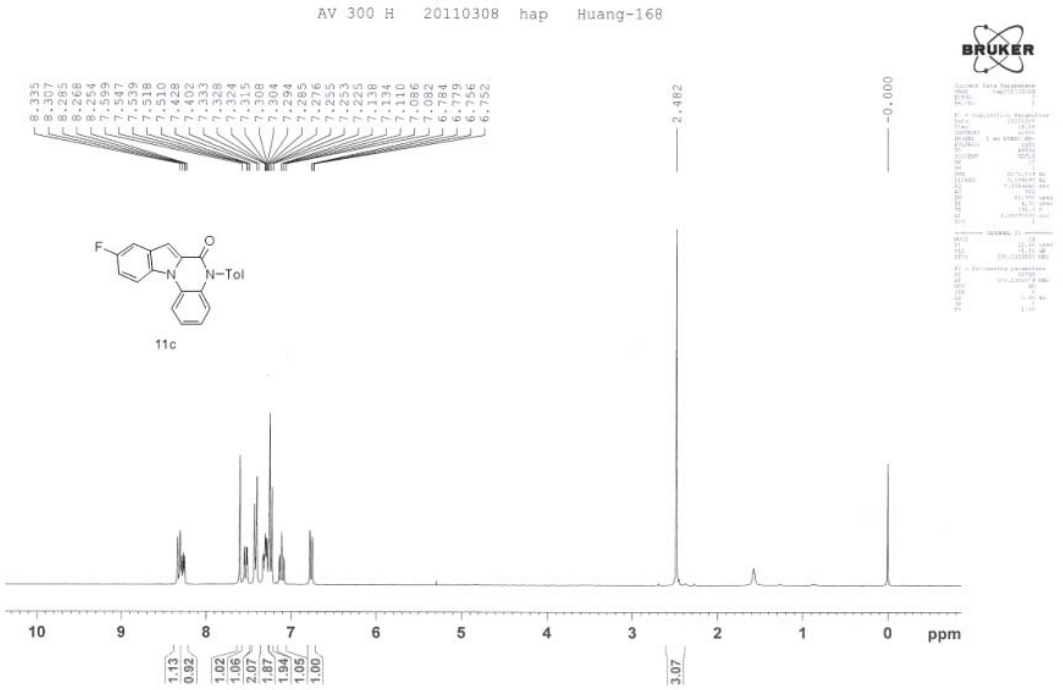

154.53
138.51
133.96
130.42
129.36
129.24
123.12
119.43
119.29
113.73
113.23
105.88
102.20
40.43
40.22
40.01
39.80
39.59
21.15
N–Tol
N–Tol
5k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

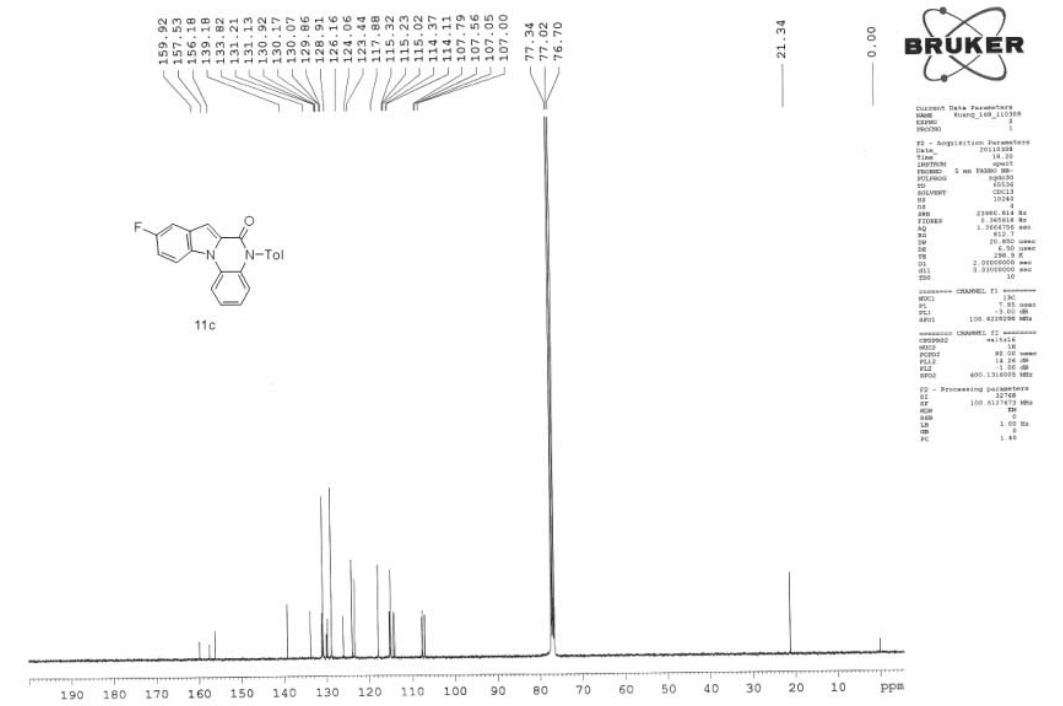

Huang_164 Bruker AV 400 HNMR in CDCl3 at 300K 20110121
7.6482
7.5566
7.5537
7.5389
7.5355
7.5320
7.5173
7.5143
7.4167
7.3970
7.3816
7.3631
7.3112
7.3078
7.2926
7.2898
7.2721
7.2687
7.2530
7.2472
7.2368
7.2235
7.1061
7.1031
7.0852
7.0829
7.0670
7.0641
6.7643
6.7610
6.7435
6.7403
2.4765
0.0000
N
N–Tol
11a
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
1.0000
1.0123
0.9585
0.8781
0.9904
0.9902
2.9646
2.2167
0.9874
0.9466
2.9674

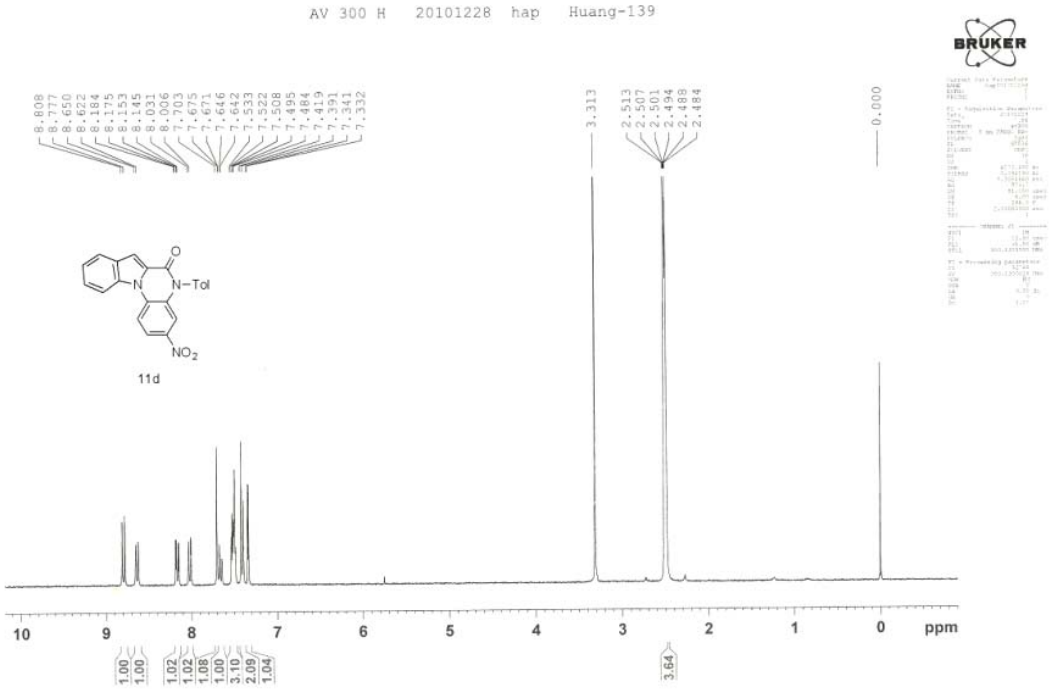

156.55
139.05
134.47
133.96
131.28
130.87
129.36
128.96
128.42
126.50
125.48
123.78
123.33
122.47
117.73
115.38
114.23
107.47
77.34
77.03
76.71
21.33
0.00
BRUKER
N
N–Tol
11a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

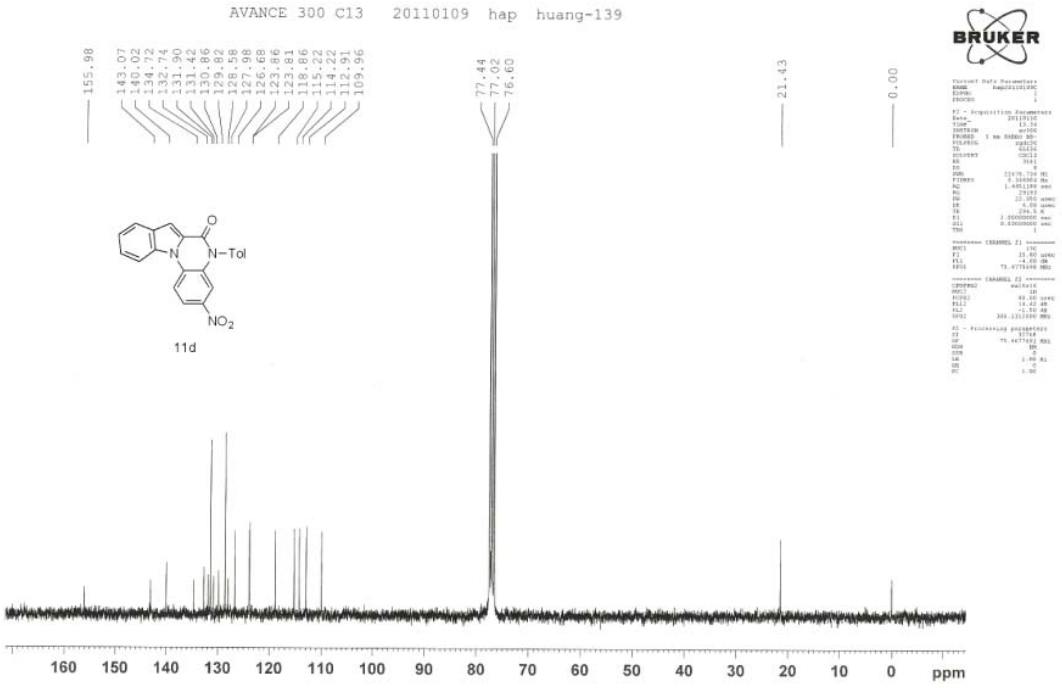

AV 300 H 20110308 hap Huang-165
BRUKER
8.337
8.310
8.232
8.201
7.565
7.423
7.396
7.315
7.310
7.283
7.274
7.262
7.256
7.249
7.233
7.228
7.204
7.196
7.173
7.165
7.106
7.102
7.078
7.054
7.050
6.763
6.759
6.736
6.731
3.929
2.480
0.000
MeO
N
N-Tol
O
11b
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.00
1.01
2.09
2.04
2.03
1.06
1.04
1.00
2.98
3.09

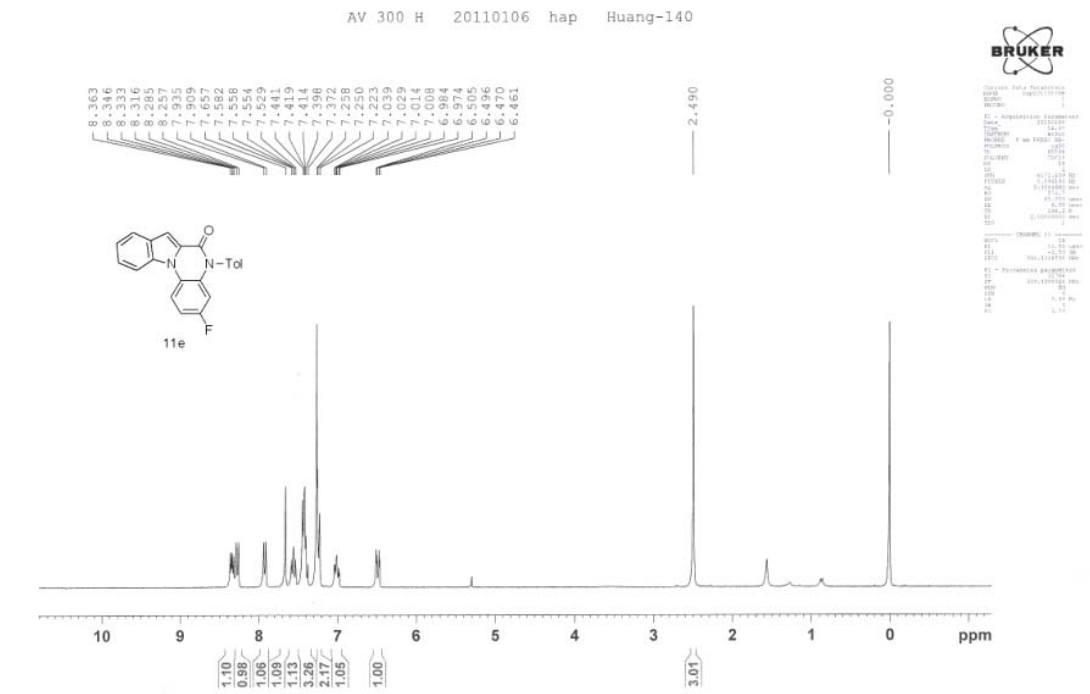

156.40
155.53
139.03
133.96
131.09
130.86
130.27
129.66
128.95
128.74
126.35
123.58
123.32
117.70
116.56
115.13
114.95
106.86
103.19
77.33
77.02
76.70
55.62
21.34
0.00
BRUKER
MeO
N
N-Tol
O
11b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

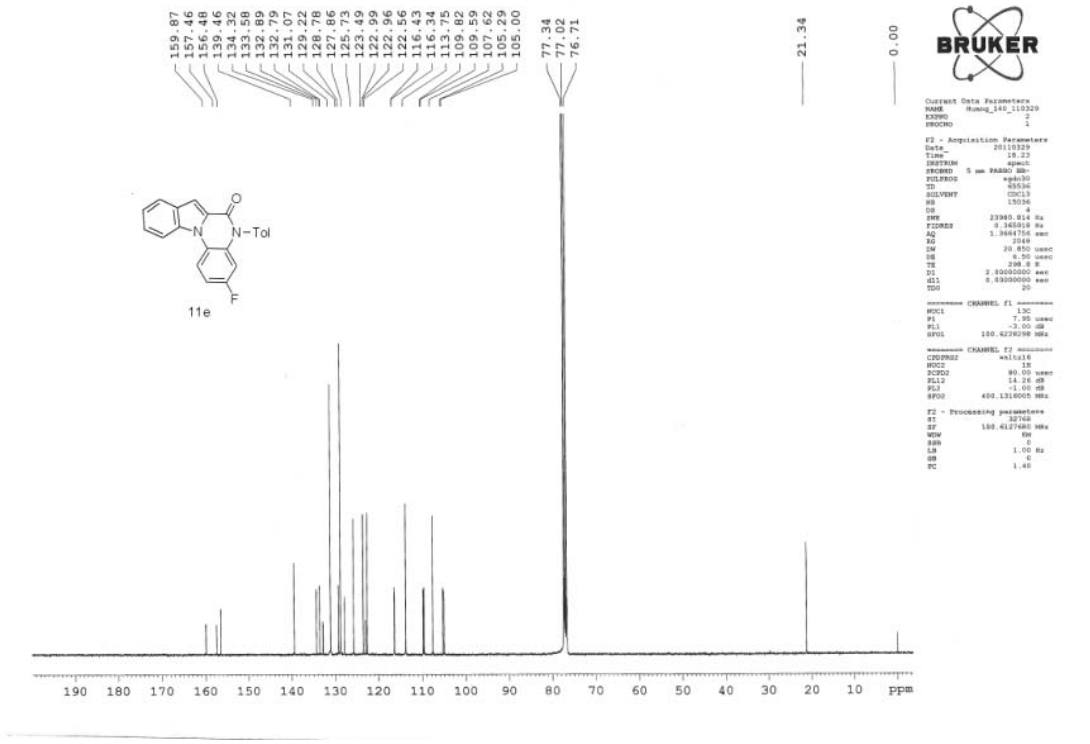

AV 300 H 20110308 hap Huang-168
BRUKER
8.335
8.307
8.285
8.268
8.254
7.599
7.547
7.539
7.518
7.510
7.428
7.402
7.333
7.328
7.324
7.315
7.308
7.304
7.294
7.285
7.276
7.255
7.253
7.225
7.138
7.134
7.110
7.086
7.082
6.784
6.779
6.756
6.752
2.482
0.000
F
O
N
N–Tol
11c
10
9
8
7
6
5
4
3
2
1
0
ppm
1.13
0.92
1.02
1.06
2.07
1.87
1.94
1.05
1.00
3.07


159.92
157.53
156.18
139.18
133.82
131.21
131.13
130.92
130.17
130.07
129.86
128.91
126.16
124.06
123.44
117.88
115.32
115.23
115.02
114.37
114.11
107.79
107.56
107.05
107.00
77.34
77.02
76.70
21.34
0.00
BRUKER
F
O
N
N–Tol
11c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


AV 300 H 20101228 hap Huang-139
BRUKER
8.808
8.777
8.650
8.622
8.184
8.175
8.153
8.145
8.031
8.006
7.703
7.675
7.671
7.646
7.642
7.533
7.522
7.508
7.495
7.484
7.419
7.391
7.341
7.332
3.313
2.513
2.507
2.501
2.494
2.488
2.484
0.000
N–Tol
NO2
11d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.02
1.02
1.08
1.00
3.10
2.09
1.04
3.64


AVANCE 300 C13 20110109 hap huang-139
BRUKER
155.98
143.07
140.02
134.72
132.74
131.90
131.42
130.86
129.82
128.58
127.98
126.68
123.86
123.81
118.86
115.22
114.22
112.91
109.96
77.44
77.02
76.60
21.43
0.00
N–Tol
NO2
11d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


AV 300 H 20110106 hap Huang-140
BRUKER
8.363
8.346
8.333
8.316
8.285
8.257
7.935
7.909
7.657
7.582
7.558
7.554
7.529
7.441
7.419
7.414
7.398
7.372
7.258
7.250
7.223
7.039
7.029
7.014
7.008
6.984
6.974
6.505
6.496
6.470
6.461
2.490
0.000
N-Tol
F
11e
10 9 8 7 6 5 4 3 2 1 0 ppm
1.10 0.98 1.06 1.09 1.13 3.26 2.17 1.05 1.00 3.01


159.87
157.46
156.48
139.46
134.32
133.58
132.89
132.79
131.07
129.22
128.78
127.86
125.73
123.49
122.99
122.96
122.56
116.43
116.34
113.75
109.82
109.59
107.62
105.29
105.00
77.34
77.02
76.71
21.34
0.00
BRUKER
N-Tol
F
11e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm