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Iron-Mediated Direct Arylation with Arylboronic Acids through an Aryl Radical Transfer Pathway

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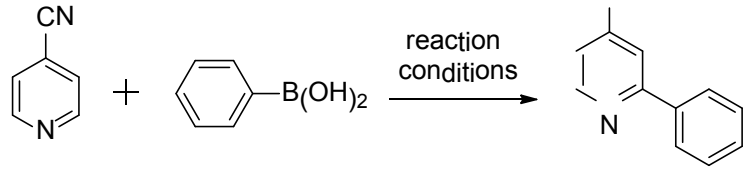
General information:

All reagents were purchased from commercial suppliers and used without further purification. ^{1}H-NMR, ^{13}C-NMR spectra were measured on a Bruker AM400 NMR spectrometer (400 MHz or 100MHz, respectively) with $CDCl_3$ as solvent and recorded in ppm relative to internal tetramethylsilane standard. Mass spectroscopy data of the product was collected on an Agilent 6890-5973N GCMS-EI instrument.

Optimization studies of direct arylation of pyridines

For initial optimization of the reaction conditions, we selected 4-cyanopyridine (**4a**) and benzeneboronic acid (**2a**) as model substrates, and the results are summarized in Table S1.

Table S1: Optimization of direct arylation of pyridines



4a **2a** **5a**

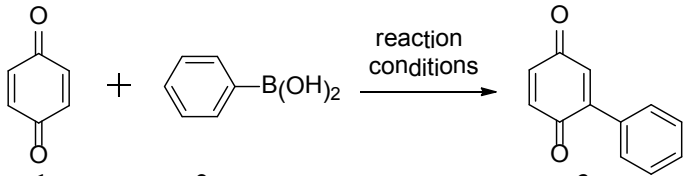
Entry [a]	[Fe] (equiv)	Oxidant (equiv)	Additive (equiv)	Yield(%) [b]
1	FeS(1.0)	$K_2S_2O_8$(3.0)	none	55.9
2	$Fe_2(SO_4)_3$(1.0)	$K_2S_2O_8$(3.0)	none	42.7
3	Fe_2O_3(1.0)	$K_2S_2O_8$(3.0)	none	13.7
4	Fe_3O_4(1.0)	$K_2S_2O_8$(3.0)	none	24.3
5	$FeCl_3 \cdot 6H_2O$(1.0)	$K_2S_2O_8$(3.0)	none	11.9
6	$FeCl_2 \cdot 4H_2O$(1.0)	$K_2S_2O_8$(3.0)	none	trace
7[c]	$Fe(C_2O_4) \cdot 4H_2O$ (1.0)	$K_2S_2O_8$(3.0)	none	68.2
8[c,d]	$Fe(C_2O_4) \cdot 4H_2O$ (1.0)	$K_2S_2O_8$(3.0)	none	56.3
9[c,d]	$Fe(C_2O_4) \cdot 4H_2O$ (1.0)	$K_2S_2O_8$(3.0)	TFA(1.0)	57.0
10	**FeS(1.0)**	**$K_2S_2O_8$(3.0)**	**TFA(1.0)**	**68.6**
11	FeS(1.0)	$K_2S_2O_8$(3.0)	$(COOH)_2$(1.0)	47.6
12	FeS(1.0)	$K_2S_2O_8$(3.0)	H_2SO_4(1.0)	58.6
13	FeS(1.0)	$K_2S_2O_8$(3.0)	HCl(1.0)	26.7
14	FeS (1.0)	$K_2S_2O_8$(3.0)	$(CH_3)_3CCO_2H$(1.0)	30.8
15	FeS (1.0)	$K_2S_2O_8$(3.0)	$Mn(OAc)_3$(1.0)	0
16	FeS (1.0)	Oxone(3.0)	none	0

[a] Reaction conditions: **4a**(0.5 mmol), **2a** (1.5 equiv), 4 mL of solvent (1:1, v/v), 25°C, 40 h. [b] Yield of isolated of 2-arylation product. [c] Ultrapure iron salt (99.999%). [d] 20h.

Optimization studies of direct arylation of quinones

For initial optimization of the reaction conditions, we selected 1,4-benzoquinone (**1a**) and benzeneboronic acid (**2a**) as model substrates, and the results are summarized in Table S2.

Table S2: Optimization of direct arylation of quinones



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

Entry [a]	[Fe] (equiv)	Oxidant (equiv)	Solvent	Yield(%) [b]
1 [c]	$Fe_2(SO_4)_3$(1.0)	$K_2S_2O_8$(3.0)	CH_2Cl_2/H_2O	57.6
2	$Fe_2(SO_4)_3$(1.0)	$K_2S_2O_8$ (3.0)	Acetone/H_2O	5.54
3	$Fe_2(SO_4)_3$(1.0)	$K_2S_2O_8$ (3.0)	EtOAc/H_2O	45.9
4	$Fe_2(SO_4)_3$(1.0)	$K_2S_2O_8$ (3.0)	H_2O	trace
5	$Fe_2(SO_4)_3$(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2	0
6	none	$K_2S_2O_8$(3.0)	CH_2Cl_2/H_2O	trace
7 [d]	$FeCl_3$(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	trace
8 [d]	$FeCl_3 \cdot 6H_2O$(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	trace
9 [d]	$FeSO_4 \cdot 7H_2O$(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	55.5
10 [d]	$Fe(acac)_3$(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	27.5
11	Fe_3O_4(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	17.6
12	FeS(1.0)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	83.9
13	**FeS(0.5)**	**$K_2S_2O_8$ (3.0)**	**CH_2Cl_2/H_2O**	**81.5**
14	FeS (0.25)	$K_2S_2O_8$ (3.0)	CH_2Cl_2/H_2O	63.2
15 [e]	FeS (0.5)	$K_2S_2O_8$ (2.0)	CH_2Cl_2/H_2O	71.6
16 [e]	FeS (0.5)	$K_2S_2O_8$ (1.0)	CH_2Cl_2/H_2O	45.8
17 [e]	FeS (0.5)	Oxone(2.0)	CH_2Cl_2/H_2O	0
18 [e]	FeS (0.5)	H_2O_2(2.0)	CH_2Cl_2/H_2O	0
19 [e]	FeS (0.5)	TBHP(2.0)	CH_2Cl_2/H_2O	0
20 [e]	FeS (0.5)	DTBP(2.0)	CH_2Cl_2/H_2O	0
21	FeS (1.0)	none	CH_2Cl_2/H_2O	0

[a] Reaction conditions (unless otherwise stated): **1a** (0.5 mmol), **2a** (1.5 equiv), 4 mL of solvent (1:1, v/v), 25℃, 24 h. [b] Yield of isolated. [c] 36 h. [d] 60 h. [e] 12 h.

Investigation of radical scavenger effect

Different equivalent amounts of TEMPO were mixed into reaction systems about the direct arylation of 1, 4-benzoquinone or 4-cyanopyridine with benzeneboronic acid, and the results are summarized in Table S3. Radical scavenger reduced the yield obviously.

Table S3: Investigation of radical scavenger effect

Entry	C-H Sources	TEMPO (equiv) [a]	General procedure	Yield(%)	Yield(%)[b]
1	1, 4-benzoquinone or 4-cyanopyridine	1.0	Ⅰ or Ⅱ	22.6 or 27.7	81.5 or 90.3
2	1, 4-benzoquinone or	1.5	Ⅰ or Ⅱ	21.4 or 21.3	81.5 or 90.3

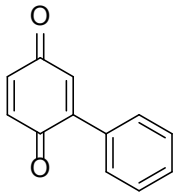
	4-cyanopyridine				
3	1, 4-benzoquinone or 4-cyanopyridine	2.0	Ⅰ or Ⅱ	21.3 or trace	81.5 or 90.3

[a] TEMPO = 2,2,6,6-Tetramethyl-1-piperidinyloxy. [b] No TEMPO was mixed.

General procedure for arylation of quinones with arylboronic acids（Ⅰ）

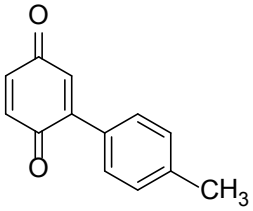
To a test tube equipped with magnetic stir bar was charged with quinone derivative (0.5 mmol, 1.0 equiv), FeS (0.25 mmol, 0.5 equiv), arylboronic acids (0.75 mmol, 1.5 equiv), $K_2S_2O_8$ (1.5 mmol, 3.0 equiv) in solvent (4 mL, 1:1 DCM:H_2O). The test tube was sealed with rubber septum, and stirred for 24 h at room temperature. The resulting solution was directly filtered through a pad of celite and washed with dichloromethane (15 mL). The filtrate was washed with a saturated solution of $NaHCO_3$ (3 x 15 mL) and the aqueous layer was extracted again with dichloromethane (3 x 15 mL). The combined organic layer was concentrated under reduced pressure after had been dried over Na_2SO_4. The crude product was purified by column chromatography using the indicated eluent. The identity and purity of the known product was confirmed by GC-MC, ^{1}H-NMR and ^{13}C-NMR.

2-Phenyl-1, 4-benzoquinone (3a).



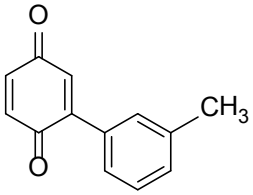
EtOAc/*n*-hexane (1:10); yellow solid (75.1mg, 81.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.47 (br, 5H), 6.89-6.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.5, 186.6, 145.9, 137.1, 136.3, 132.7, 130.1, 129.2, 128.6; MS (EI) *m/z* (%) 184 (M^+,100), 156 (50), 128 (38), 102(32), 82(38).

2-(4-Methylphenyl)-1, 4-benzoquinone (3b).



EtOAc/*n*-hexane (1:10); yellow solid (90.3mg, 91.1%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.39 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 6.87-6.80 (m, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.7, 186.9, 145.9, 140.6, 137.1, 136.2, 132.0, 129.8, 129.3, 129.2, 21.4; MS (EI) *m/z* (%) 198 (M^+,100), 183 (30), 170 (72), 155(20), 141(55), 115(78), 82(64).

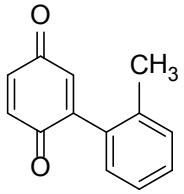
2-(3-Methylphenyl)-1, 4-benzoquinone (3c).



EtOAc/*n*-hexane (1:10); yellow solid (95.7mg, 96.6%); ^{1}H NMR (400 MHz, $CDCl_3$)

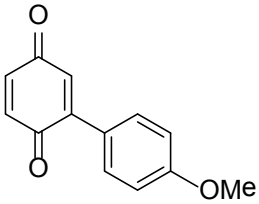
d=7.36-7.26 (m, 4H), 6.88-6.82 (m, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.7, 186.7, 146.2, 138.3, 137.1, 136.2, 132.6, 131.0, 129.8, 128.5, 126.4, 21.4; MS (EI) *m/z* (%) 198 (M^+,100), 183 (30), 170 (72), 155(25), 141(68), 115(72), 82(60).

2-(2-Methylphenyl)-1, 4-benzoquinone (3d).



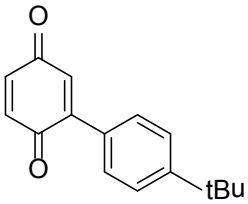
EtOAc/*n*-hexane (1:10); yellow oil (95.8mg, 96.7%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.25 (t, *J* = 7.4 Hz, 1H), 7.18-7.14 (m, 2H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.80-6.74 (m, 2H), 6.63 (d, *J* = 2.2 Hz, 1H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=186.6, 185.2, 147.4, 135.8, 135.3, 135.1, 133.5, 132.0, 129.4, 128.5, 128.2, 124.8, 19.3; MS (EI) *m/z* (%) 198 (M^+,100), 181 (10), 170 (51), 153(12), 141(43), 115(60).

2-(4-Methoxyphenyl)-1, 4-benzoquinone (3e).



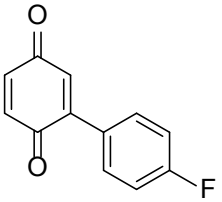
EtOAc/*n*-hexane (1:10); red solid (40.6mg, 37.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.48 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 6.86-6.79 (m, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.7, 187.1, 161.4, 145.2, 137.0, 136.3, 131.1, 130.9, 125.0, 114.2, 55.4; MS (EI) *m/z* (%) 214 (M^+,100), 186 (20), 132 (58), 115(20), 89(20).

2-(4-*tert*-Butylphenyl)-1, 4-benzoquinone (3f).



EtOAc/*n*-hexane (1:10); yellow solid (110.7mg, 92.1%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.47 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 6.88-6.81 (m, 3H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.7, 186.9, 153.7, 145.8, 137.1, 136.3, 132.1, 129.8, 127.4, 125.6, 34.9, 31.2; MS (EI) *m/z* (%) 240 (M^+,5), 225 (95), 197 (27), 184(100).

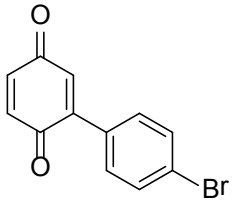
2-(4-Fluorophenyl)-1, 4-benzoquinone (3g).



EtOAc/*n*-hexane (1:10); yellow solid (68.1mg, 67.4%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.51-7.48 (m, 2H), 7.17-7.13 (m, 2H), 6.89-6.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.4, 186.6, 165.2, 144.8, 137.0, 136.4, 132.5, 131.3 (d, *J* = 8.3Hz), 129.5, 115.8 (d, *J* =

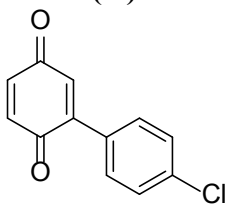
21.8 Hz); MS (EI) *m/z* (%) 202 (M^+,100), 174 (52), 146 (43), 120(42), 82(57).

2-(4-Bromophenyl)-1, 4-benzoquinone (3h).



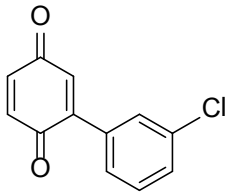
EtOAc/*n*-hexane (1:10); yellow solid (127.7mg, 97.1%); ^{1}H NMR (400 MHz, $CDCl_3$) d= 7.59 (d, *J* = 8.3 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 6.90-6.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.3, 186.3, 144.9, 137.0, 136.4, 132.7, 131.9, 131.5, 130.8, 125.0; MS (EI) *m/z* (%) 263 (M^+,12), 183 (100), 155(30), 127(20), 101(22), 82(27).

2-(4-Chlorophenyl)-1, 4-benzoquinone (3i).



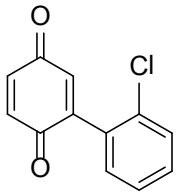
EtOAc/*n*-hexane (1:10); yellow solid (92.8mg, 84.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.44(brs, 4H), 6.90-6.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.4, 186.4, 144.8, 137.0, 136.6, 136.4, 132.7, 131.0, 130.6, 128.9; MS (EI) *m/z* (%) 218 (M^+,41), 183 (100), 155 (57), 136(48), 127(32), 101(29), 82(65).

2-(3-Chlorophenyl)-1, 4-benzoquinone (3j).



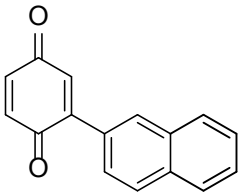
EtOAc/*n*-hexane (1:10); pale yellow solid (97.6mg, 89.3%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.48(s, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 4.4 Hz, 1H), 6.90-6.84 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.3, 186.1, 144.6, 137.0, 136.4, 134.6, 134.3, 133.2, 130.2, 129.8, 129.3, 127.4; MS (EI) *m/z* (%) 218 (M^+,30), 183 (100), 155 (62), 136(39), 127(30), 101(25), 82(54).

2-(2-Chlorophenyl)-1, 4-benzoquinone (3k).



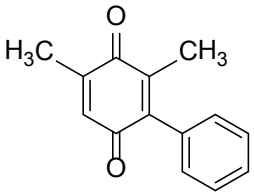
EtOAc/*n*-hexane (1:10); yellow oil (93.6mg, 85.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.46(d, *J* = 7.9 Hz, 1H), 7.41-7.32 (m, 2H), 7.24-7.21 (m, 1H), 6.92-6.85 (m, 2H), 6.80 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.2, 185.1, 146.1, 136.8, 136.5 (d, *J* = 11.8 Hz), 135.0, 133.1, 132.4, 130.8, 130.7, 129.8, 126.8; MS (EI) *m/z* (%) 218 (M^+,27), 183 (100), 155 (78), 136(47), 127(38), 101(35), 82(64).

2- (naphthalen-2-yl) -1,4-benzoquinone (3l).



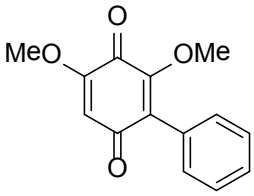
EtOAc/*n*-hexane (1:20); yellow solid (35.7mg, 30.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.05(s, 1H), 7.94-7.86 (m, 3H), 7.58-7.52 (m, 3H), 7.0 (d, *J* = 2.1 Hz, 1H), 6.93-6.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=187.6, 186.9, 145.9, 137.1, 136.3, 133.9, 132.9(2C), 130.1, 129.8, 128.8, 128.3, 127.7, 127.5, 126.7, 125.9; MS (EI) *m/z* (%) 234 (M^+,100), 206 (39), 178 (30), 152(80).

2,6-Dimethyl-3-phenyl-1,4-benzoquinone (3n).



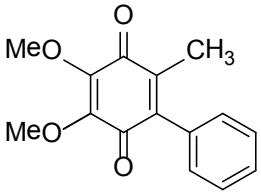
EtOAc/*n*-hexane (1:20); yellow solid (80.2mg, 75.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.45-7.39(m, 3H), 7.16 (d, *J* = 2.0Hz, 1H), 7.14 (d, *J* = 1.2Hz, 1H), 6.66 (d, *J* = 1.0 Hz, 1H), 2.11 (d, *J* = 1.4 Hz, 3H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=188.6, 186.8, 145.6, 143.7, 141.6, 133.2, 132.9, 129.5, 128.5, 128.1, 16.0, 14.1; MS (EI) *m/z* (%) 212 (M^+,100), 197 (37), 183 (16), 169(42), 141(15), 115(32).

2,6-Dimethoxy-3-(4-methylphenyl)-1,4-benzoquinone (3o).



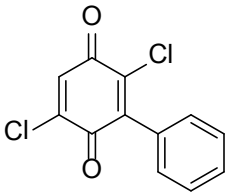
EtOAc/*n*-hexane (1:10); orange solid (105.7mg, 86.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.44-7.39 (m, 3H), 7.32-7.28 (m, 2H), 5.96(s, 1H), 3.85 (s, 3H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=186.7, 178.6, 157.3, 153.9, 130.6, 130.1, 129.2, 128.8, 127.9, 107.2, 61.3, 56.5; MS (EI) *m/z* (%) 244 (M^+,100), 226 (85), 201(94), 145(93), 183 (47).

2,3-Dimethoxy-5-methyl-6-phenyl-1,4-benzoquionone (3q).



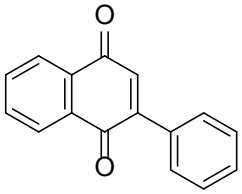
EtOAc/*n*-hexane (1:10); orange oil (42.6mg, 33.0%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.45-7.39 (m, 3H), 7.16-7.13 (m, 2H), 4.06 (s, 3H), 4.02 (s, 3H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=184.8, 183.6, 144.9, 144.1, 141.8, 139.9, 131.3, 129.5, 128.6, 128.1, 61.3, 61.2, 13.8; MS (EI) *m/z* (%) 258 (M^+,100), 213 (66), 187 (30), 159(62), 115(57).

2,5-Dichloro-3-phenyl-1,4-benzoquionone (3r).



EtOAc/*n*-hexane (1:10); orange solid (73.7mg, 58.2%); ^{1}H NMR (400 MHz, $CDCl_3$) d=7.49-7.47 (m, 3H), 7.30-7.27 (m, 2H), 7.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=177.6, 177.2, 144.7, 144.5, 143.7, 133.0, 130.7, 129.9, 129.6, 128.3; MS (EI) *m/z* (%) 252 (M^+,74), 217 (100), 189 (89), 161(25), 136(23), 126(34).

2-phenyl-1,4-naphthoquinone (3s).

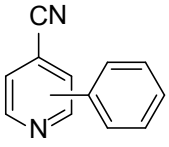


EtOAc/*n*-hexane (1:10); yellow solid (12.9mg, 11.0%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.21-8.18 (m, 1H), 8.14-8.12 (m, 1H), 7.80-7.78 (m, 2H), 7.59-7.57 (m, 2H), 7.49-7.47 (m, 3H), 7.09 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=185.2, 184.4, 148.2, 135.3, 133.9, 133.8, 133.4, 132.5, 132.1, 130.0, 129.4, 128.5, 127.1, 126.0; MS (EI) *m/z* (%) 234 (M^+,100), 206 (65), 178 (24), 104(30), 76(25).

General procedure for arylation of pyridines with arylboronic acids（Ⅱ）

To a test tube equipped with magnetic stir bar was charged with pyridine derivative (0.5 mmol, 1.0 equiv), TFA(1.0 equiv), FeS (0.5 mmol, 1.0 equiv), arylboronic acids (0.75 mmol, 1.5 equiv), $K_2S_2O_8$ (1.5 mmol, 3.0 equiv) in solvent (4 mL, 1:1 DCM:H_2O). The test tube was sealed with rubber septum, and stirred for 40 h at room temperature. The resulting solution was directly filtered through a pad of celite and washed with dichloromethane (15 mL). The filtrate was washed with a saturated solution of $NaHCO_3$ (3 x 15 mL) and the aqueous layer was extracted again with dichloromethane (3 x 15 mL). The combined organic layer was concentrated under reduced pressure after had been dried over Na_2SO_4. The crude product was purified by column chromatography using the indicated eluent. The identity and purity of the known product was confirmed by GC-MC, ^{1}H-NMR and ^{13}C-NMR.

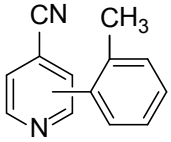
2-phenylisonicotinonitrile (5a-C2), 3-phenylisonicotinonitrile (5a-C3).



EtOAc/*n*-hexane (1:10); C2: pale yellow solid (68.6mg, 76.1%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.86 (dd, *J* = 4.8, 0.6 Hz, 1H), 8.01 (d, *J* = 1.9 Hz, 1H), 7.99 (d, *J* = 1.4 Hz, 1H), 7.95 (s, 1H), 7.51 (d, *J* = 5.6 Hz, 1H), 7.50 (s, 2H), 7.45 (dd, *J* = 5.0, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.8, 150.6, 137.3, 130.2, 129.1, 127.0, 123.2, 122.1, 121.2, 116.7; MS (EI) *m/z* (%) 180 (M^+,100), 153 (16), 126 (10); C3: pale yellow solid (12.8mg, 14.2%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.86(s, 1H), 8.75 (d, *J* = 5.0 Hz, 1H), 7.63 (d, *J* = 5.0 Hz, 1H),

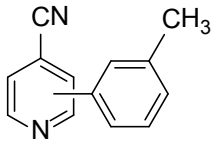
7.60-7.52 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) d=151.0, 148.7, 135.1, 134.4, 129.6, 129.2, 128.8, 126.1, 118.9, 116.3; MS (EI) *m/z* (%) 180 (M^+,100), 153 (28), 126 (10).

2-(*o*-tolyl)isonicotinonitrile (5b-C2), 3-(*o*-tolyl)isonicotinonitrile (5b-C3).



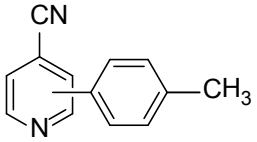
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (72.4mg, 74.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.87 (t, *J* = 4.5 Hz, 1H), 7.64 (d, *J* = 0.9 Hz, 1H), 7.48 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.40-7.30 (m, 4H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=161.5, 150.2, 138.4, 135.9, 131.2, 129.6, 129.3, 126.2, 125.6, 122.9, 120.7, 116.7, 20.3; MS (EI) *m/z* (%) 194 (M^+,100), 167 (40), 139 (12); C3: light yellow oil (16.1mg, 16.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.80(d, *J* = 5.0 Hz, 1H), 8.76 (s, 1H), 7.65 (d, *J* = 5.0 Hz, 1H), 7.45-7.33 (m, 3H), 7.24 (d, *J* = 7.4 Hz, 1H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=151.5, 148.9, 139.3, 136.1, 134.2, 130.8, 129.8, 129.6, 126.2, 125.3, 120.6, 115.8, 19.9; MS (EI) *m/z* (%) 194 (M^+,100), 166 (12).

2-(*m*-tolyl)isonicotinonitrile (5c-C2), 3-(*m*-tolyl)isonicotinonitrile (5c-C3).



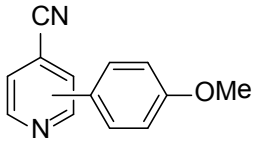
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (67.8mg, 69.8%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.85 (d, *J* = 4.8 Hz, 1H), 7.94 (s, 1H), 7.83 (s, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.45-7.39 (m, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=159.0, 150.6, 138.9, 137.3, 131.0, 129.0, 127.7, 124.1, 123.1, 122.1, 121.1, 116.8, 21.5; MS (EI) *m/z* (%) 194 (M^+,100), 167 (21), 139 (10); C3: pale yellow solid (22.6mg, 23.3%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.85(s, 1H), 8.74 (d, *J* = 5.0 Hz, 1H), 7.61 (d, *J* = 5.0 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 2.1 Hz, 2H), 7.33 (d, *J* = 7.5 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=151.0, 148.6, 139.0, 138.9, 134.4, 130.3, 129.4, 129.0, 126.0, 125.9, 118.8, 116.4, 21.5; MS (EI) *m/z* (%) 194 (M^+,100), 179 (12), 166 (10).

2-(*p*-tolyl)isonicotinonitrile (5d-C2), 3-(*p*-tolyl)isonicotinonitrile (5d-C3).



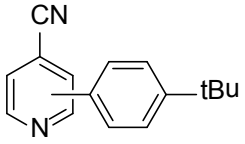
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (61.1mg, 62.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.83 (d, *J* = 5.0 Hz, 1H), 7.91 (d, *J* = 3.4 Hz, 2H), 7.89 (s, 1H), 7.41 (d, *J* = 4.9 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.8, 150.6, 140.5, 134.6, 129.8, 126.9, 122.8, 121.7, 121.1, 116.8, 21.4; MS (EI) *m/z* (%) 194 (M^+,100), 167 (15), 140 (10); C3: pale yellow solid (21.9mg, 22.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.85(s, 1H), 8.72 (d, *J* = 5.0 Hz, 1H), 7.61 (d, *J* = 5.0 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 7.9 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=151.0, 148.4, 139.8, 138.8, 131.5, 129.9, 128.7, 126.0, 118.7, 116.5, 21.3; MS (EI) *m/z* (%) 194 (M^+,100), 179 (10), 166 (10).

2-(4-methoxyphenyl)isonicotinonitrile (5e-C2), 3-(4-methoxyphenyl)isonicotinonitrile (5e-C3).



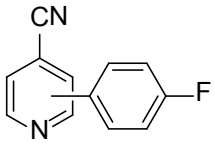
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (54.4mg, 51.8%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.81 (t, *J* = 2.4 Hz, 1H), 7.97 (d, *J* = 8.9 Hz, 2H), 7.88 (s, 1H), 7.37 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=161.4, 158.4, 150.5, 129.9, 128.4, 122.3, 121.3, 121.1, 116.9, 55.4; MS (EI) *m/z* (%) 210 (M^+,100), 195 (17), 167 (26), 140 (21); C3: pale yellow solid (29.3mg, 27.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.84(s, 1H), 8.70 (d, *J* = 5.0 Hz, 1H), 7.60 (d, *J* = 5.0 Hz, 1H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.07 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=160.7, 150.9, 148.1, 138.5, 130.1, 126.7, 126.0, 118.4, 116.6, 114.7, 55.4; MS (EI) *m/z* (%) 210 (M^+,100), 195 (23), 167 (36), 140 (10).

2-(4-*tert*-butylphenyl)isonicotinonitrile (5f-C2), 3-(4-*tert*-butylphenyl)isonicotinonitrile (5f-C3).



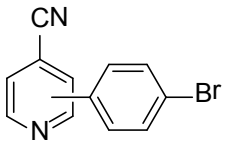
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (85.1mg, 72.0%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.84 (d, *J* = 5.0 Hz, 1H), 7.95 (s, 1H), 7.93 (s, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.41 (dd, *J* = 5.0, 1.3 Hz, 1H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.7, 153.7, 150.6, 134.5, 126.7, 126.1, 122.8, 121.8, 121.1, 116.9, 34.8, 31.2; MS (EI) *m/z* (%) 236 (M^+,24), 221 (100), 193 (19), 181 (15); C3: light yellow oil (29.8mg, 25.2%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.87(s, 1H), 8.72 (d, *J* = 5.0 Hz, 1H), 7.61 (d, *J* = 5.0 Hz, 1H), 7.58-7.53 (m, 4H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) d=152.8, 151.0, 148.4, 138.6, 131.5, 128.5, 126.2, 126.1, 118.6, 116.6, 34.8, 31.2; MS (EI) *m/z* (%) 236 (M^+,29), 221 (100), 205 (13), 193 (26).

2-(4-fluorophenyl)isonicotinonitrile (5g-C2), 3-(4-fluorophenyl)isonicotinonitrile (5g-C3).



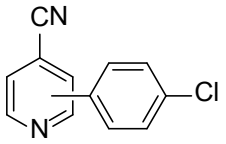
EtOAc/*n*-hexane (1:10); C2: white solid (38.5mg, 38.8%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.84 (dd, *J* = 5.0, 0.7 Hz, 1H), 8.02-7.99 (m, 2H), 7.90 (d, *J* = 0.9 Hz, 1H), 7.45 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.23-7.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=157.7, 150.7, 133.5, 129.0 (d, *J* = 8.6 Hz), 123.1, 121.7, 121.3, 116.6, 116.3, 116.0; MS (EI) *m/z* (%) 198 (M^+,100), 171 (14), 145 (10); C3: pale yellow solid (37.0mg, 37.3%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.84(s, 1H), 8.76 (d, *J* = 5.0 Hz, 1H), 7.63 (d, *J* = 5.0 Hz, 1H), 7.59-7.56 (m, 2H), 7.27-7.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=162.4, 150.8, 148.9, 137.7, 130.8, 130.7, 126.0, 118.9, 116.5, 116.3; MS (EI) *m/z* (%) 198 (M^+,100), 171 (30).

2-(4-bromophenyl)isonicotinonitrile (5h-C2), 3-(4-bromophenyl)isonicotinonitrile (5h-C3).



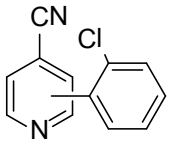
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (19.5mg, 15.1%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.86 (dd, *J* = 5.0, 0.6 Hz, 1H), 7.92 (s, 1H), 7.89 (d, *J* = 8.6 Hz, 2H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.47 (dd, *J* = 5.0, 1.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=157.6, 150.8, 136.2, 132.3, 128.5, 125.0, 123.5, 121.8, 121.4, 116.5; MS (EI) *m/z* (%) 258 (M^+,100), 179 (75), 152 (44), 125 (14); C3: pale yellow solid (33.5mg, 25.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.77 (s, 1H), 8.70 (d, *J* = 5.0 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 5.0 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=150.7, 149.1, 137.6, 133.3, 132.5, 130.3, 126.1, 124.4, 118.8, 116.1; MS (EI) *m/z* (%) 260 (M^+,100), 179 (100), 152 (70), 125 (23).

2-(4-chlorophenyl)isonicotinonitrile (5i-C2), 3-(4-chlorophenyl)isonicotinonitrile (5i-C3).



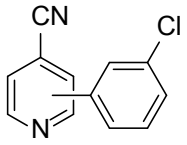
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (30.5mg, 28.4%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.85 (dd, *J* = 4.9, 0.5 Hz, 1H), 7.94 (t, *J* = 9.7 Hz, 3H), 7.50-7.46 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=157.5, 150.7, 136.6, 135.7, 129.3, 128.2, 123.4, 121.8, 121.4, 116.6; MS (EI) *m/z* (%) 214 (M^+,100), 179 (93), 152 (44); C3: pale yellow solid (29.7mg, 27.7%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.84(s, 1H), 8.77 (d, *J* = 5.0 Hz, 1H), 7.63 (d, *J* = 5.0 Hz, 1H), 7.54-7.51 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) d=150.7, 149.1, 137.6, 136.1, 132.8, 130.1, 129.5, 126.1, 118.8, 116.1; MS (EI) *m/z* (%) 214 (M^+,100), 179 (84), 152 (38).

2-(2-chlorophenyl)isonicotinonitrile (5j-C2), 3-(2-chlorophenyl)isonicotinonitrile (5j-C3).



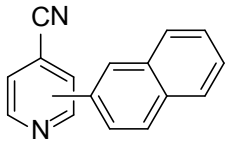
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (46.7mg, 43.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.91 (dd, *J* = 5.0, 0.5 Hz, 1H), 7.94 (s, 1H), 7.62-7.60 (m, 1H), 7.54-7.51 (m, 2H), 7.42-7.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.2, 150.6, 137.2, 132.1, 131.5, 130.7, 130.4, 127.3, 126.6, 123.7，120.4，116.5; MS (EI) *m/z* (%) 214 (M^+,100), 179 (95), 152 (56), 125 (20); C3: pale yellow solid (37.4mg, 17.4%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.82(t, *J* = 2.5 Hz, 2H), 7.67-7.66 (m, 1H), 7.58 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.49-7.41 (m, 2H), 7.37 (dd, *J* = 7.2, 2.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=151.2, 149.0, 137.4, 136.9, 133.2 (d, *J* = 4.4Hz), 132.4, 131.2 (d, *J* = 9.8Hz), 127.3, 125.6, 130.3, 121.3, 115.4; MS (EI) *m/z* (%) 214 (M^+,93), 179 (100), 152 (61), 125 (12).

2-(3-chlorophenyl)isonicotinonitrile (5k-C2), 3-(3-chlorophenyl)isonicotinonitrile (5k-C3).



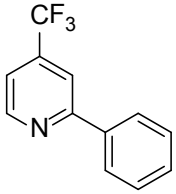
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (52.9mg, 49.3%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.87 (dd, *J* = 5.0, 0.6 Hz, 1H), 8.04 (s, 1H), 7.93 (s, 1H), 7.88-7.7.85 (m, 1H), 7.49 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.46-7.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=157.3, 150.8, 139.0, 135.3, 130.3, 130.2, 127.2, 125.0, 123.8, 122.1, 121.5, 116.5; MS (EI) *m/z* (%) 214 (M^+,100), 179 (72), 145 (10); C3: pale yellow solid (30.8mg, 28.7%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.85(s, 1H), 8.79 (d, *J* = 5.0 Hz, 1H), 7.65 (d, *J* = 5.0 Hz, 1H), 7.56 (d, *J* = 1.4 Hz, 1H), 7.51-7.48 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=150.8, 149.3, 137.3, 136.2, 135.2, 130.4, 129.7, 128.8, 127.1, 126.1, 119.0, 115.9; MS (EI) *m/z* (%) 214 (M^+,100), 179 (72), 152 (24).

2-(naphthalen-2-yl)isonicotinonitrile (5l-C2), 3-(naphthalen-2-yl)isonicotinonitrile (5l-C3),



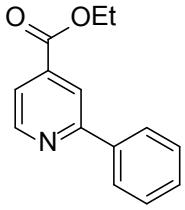
EtOAc/*n*-hexane (1:10); C2: pale yellow solid (28.9mg, 25.1%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.90 (d, *J* = 4.9, 1H), 8.50 (s, 1H), 8.11 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.09 (s, 1H), 7.99-7.96 (m, 2H), 7.89 (t, *J* = 4.3, 1H), 7.56-7.54 (m, 2H), 7.47(dd, *J* = 4.9, 1.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.7, 150.7, 134.5, 134.1, 133.3, 128.9 (2C), 127.8, 127.3, 127.0, 126.7, 123.9, 123.1, 122.3, 121.3, 116.8; MS (EI) *m/z* (%) 230 (M^+,100), 201 (10), 175 (8); C3: pale yellow solid (26.4mg, 22.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.97(s, 1H), 8.78 (d, *J* = 4.6 Hz, 1H), 8.07 (s, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.96-7.91 (m, 2H), 7.69-7.65 (m, 2H), 7.59-7.57 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=151.2, 148.7, 138.8, 133.4, 133.2, 131.8, 129.1, 128.7, 128.5, 127.8, 127.4, 127.0, 126.2, 125.8, 119.1, 116.4; MS (EI) *m/z* (%) 230 (M^+,100), 201 (10), 175 (6).

4-trifluoromethyl -2-phenylpyridine (5m).



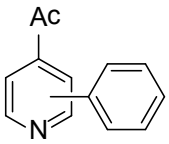
EtOAc/*n*-hexane (1:10); colorless oil (84.6mg, 75.9%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.84 (d, *J* = 5.0 Hz, 1H), 8.02 (dd, *J* = 8.3, 1.6 Hz, 2H)), 7.91 (s, 1H), 7.51-7.45 (m, 3H), 7.42 (d, *J* = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.8, 150.6, 139.0, 138.0, 129.8, 129.0, 127.0, 117.5 (q, J = 3.2 Hz), 116.0 (d, J = 3.6 Hz); MS (EI) *m/z* (%) 223 (M^+,100), 204 (50), 154 (90), 127(45).

ethyl 2-phenylisonicotinate (5n).



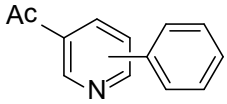
EtOAc/*n*-hexane (1:10); pale yellow oil (68.8mg, 60.6%); The spectroscopic data for these compounds were identical to those reported in the literature: Tetrahedron Letters, 2008, 49, 4349.

4-Acetyl -2-phenylpyridine (5o-C2), 4-Acetyl -3-phenylpyridine (5o-C3).



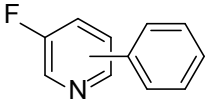
EtOAc/*n*-hexane (1:10); C2: white solid (60.6mg, 61.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.87 (d, *J* = 5.0 Hz, 1H), 8.17 (s, 1H), 8.06-8.04 (m, 2H), 7.65 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.53-7.45 (m, 3H), 2.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=197.5, 158.9, 150.1, 150.8, 143.7, 138.6, 129.5, 128.9, 127.0, 119.7, 118.0, 26.8; MS (EI) *m/z* (%) 197 (M^+,100), 182 (100), 154 (96), 127(80); C3: trace.

3-Acetyl -2-phenylpyridine (5p-C2), 3-Acetyl -4-phenylpyridine(5p-C4), 3-Acetyl -6-phenylpyridine (5p-C6).



EtOAc/*n*-hexane (1:10); C6: white solid (26.4mg, 26.8%); ^{1}H NMR (400 MHz, $CDCl_3$) d=9.24 (d, *J* = 2.0 Hz, 1H), 8.30 (dd, *J* = 8.3, 2.3 Hz, 1H), 8.07 (dd, *J* = 8.2, 1.8 Hz, 2H), 7.85 (dd, *J* = 8.3, 0.6 Hz, 1H), 7.54-7.48 (m, 3H), 2.67(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=196.5, 161.0, 150.1, 138.2, 136.4, 130.6, 130.1, 129.0, 127.4, 120.2, 26.8; MS (EI) *m/z* (%) 197 (M^+,100), 182 (100), 154 (100), 127(90); C2 and C6 (3:1): light yellow oil (37.0mg, 37.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=9.24 (d, *J* = 1.8 Hz, 0.3H), 8.77 (dd, *J* = 4.8, 1.7 Hz, 1H), 8.30 (dd, *J* = 8.4, 2.3 Hz, 0.3H), 8.07 (dd, *J* = 8.2, 1.8 Hz, 0.6H), 7.87 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.74-7.71 (m, 1H), 7.59-7.56 (m, 2H), 7.54-7.52 (m, 1.3H), 7.49-7.47 (m, 2H), 7.37-7.34 (m, 1H), 2.67(s, 1H), 2.07(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=203.7, 199.1, 157.2, 150.9, 150.2, 139.7, 138.2, 136.4, 136.2, 132.3, 130.9, 130.1, 129.4, 129.1, 129.0, 128.8 (2C), 127.4, 121.9, 120.2, 30.3, 26.8; MS (EI) *m/z* (%) 197 (M^+,65), 182 (100), 154 (47), 127(35); C4:trace.

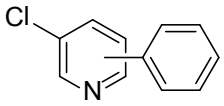
3-fluoro -2-phenylpyridine (5q-C2), 3-fluoro -4-phenylpyridine(5q-C4), 3-fluoro-6-phenylpyridine (5q-C6).



EtOAc/*n*-hexane (1:10); C2: pale yellow solid (18.8mg, 21.7%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.54 (d, *J* = 2.6Hz, 1H), 8.47 (d, *J* = 4.9Hz, 1H), 7.62-7.60 (m, 2H), 7.52-7.46 (m, 3H), 7.42-7.39 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=157.9, 155.4, 146.0 (d, *J* = 5.2Hz), 139.1 (d, *J* = 25.7Hz), 136.1 (d, *J* = 10.7Hz), 132.9, 129.3, 128.8 (d, *J* = 2.4Hz), 124.2; MS (EI) *m/z*

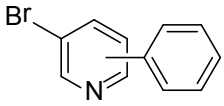
(%) 173 (M^+,100), 146 (26), 125 (13); C4 and C6 : light yellow oil (50.2mg, 58.0%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.53-8.51 (m, 2H), 7.98-7.95 (m, 4H), 7.51-7.42 (m, 8H), 7.28-7.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.8, 156.2, 146.3, 146.2, 145.4 (d, *J* = 5.3Hz), 135.3 (d, *J* = 5.3Hz), 129.2, 128.8 (d, *J* = 5.5Hz), 128.5, 128.4, 127.3, 124.2, 124.0, 123.8, 123.5, 123.4; MS (EI) *m/z* (%) 173 (M^+,100), 154 (16), 140 (24), 125 (14); 173 (M^+,78), 154 (20), 146 (27), 125 (15).

3-chloro -2-phenylpyridine (5r-C2), 3-chloro -4-phenylpyridine(5r-C4), 3-chloro -6-phenylpyridine (5r-C6).



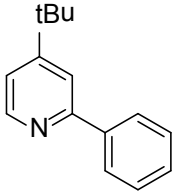
EtOAc/*n*-hexane (1:10); C2: light yellow oil (24.4mg, 25.7%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.60 (dd, *J* = 4.6, 1.4 Hz, 1H), 7.80 (dd, *J* = 4.6, 1.4 Hz, 1H), 7.74-7.72 (m, 2H), 7.50-7.43 (m, 3H), 7.24-7.21 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=156.6, 147.6, 138.2, 138.1, 130.2, 129.3, 128.8, 128.1, 123.1; MS (EI) *m/z* (%) 189 (M^+,95), 154 (100), 127 (70), 77 (38); C6 : pale yellow solid (36.5mg, 38.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.57 (d, *J* = 2.3Hz, 1H), 7.89 (dd, *J* = 8.6, 1.6 Hz, 2H), 7.67-7.60 (m, 2H), 7.43-7.36 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=154.6, 147.5, 137.2, 135.4, 128.3, 129.6, 127.8, 125.8, 120.1; MS (EI) *m/z* (%) 189 (M^+,100), 154 (63), 127 (22), 77 (15). C4: trace.

3-bromo -2-phenylpyridine (5s-C2), 3-bromo -4-phenylpyridine(5s-C4), 3-chloro -6-phenylpyridine (5s-C6).



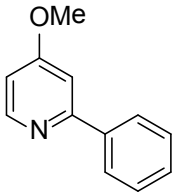
EtOAc/*n*-hexane (1:10); C6: pale yellow solid (12.5mg, 10.7%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.67 (s, 1H), 7.89 (d, *J* = 7.8Hz, 2H), 7.80 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.43-7.36 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) d=155.2, 149.7, 138.3, 137.2, 128.3, 127.9, 125.7, 120.6, 118.3; MS (EI) *m/z* (%) 233 (M^+,100), 154 (57), 127 (43), 77 (28); C2 and C4 : light yellow oil (55.3mg, 47.2%); ^{1}H NMR (400 MHz, $CDCl_3$) d=8.82 (s, 1H), 8.62 (dd, *J* = 4.6, 1.1 Hz, 1H), 8.54 (d, *J* = 4.9Hz, 1H), 7.99 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.68 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.49-7.43 (m, 8H), 7.26 (d, *J* = 2.3 Hz, 1H), 7.16-7.12 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d=158.2, 152.5, 149.7, 148.3, 148.1, 141.3, 139.6, 138.2, 129.3, 128.8, 128.7, 128.4, 128.0, 125.7, 123.3, 120.9, 119.8; MS (EI) *m/z* (%) 233 (M^+,100), 154 (85), 127 (98), 77 (39); 233 (M^+,78), 154 (100), 127 (90), 77 (51).

4-(tert-butyl)-2-phenylpyridine (5t)



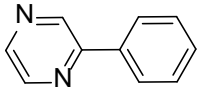
EtOAc/n-hexane (1:10); light yellow oil (72.0mg, 68.2%); The spectroscopic data for these compounds were identical to those reported in the literature: J. Am. Chem. Soc. 2010, 132, 13194

4-methoxy-2-phenylpyridine (5u)



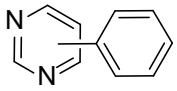
EtOAc/n-hexane (1:10); white solid (32.9mg, 35.6%); The spectroscopic data for these compounds were identical to those reported in the literature: Chem. Commun., 2010, 46, 3384.

2-phenylpyrazine (5v).



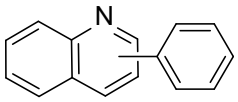
EtOAc/*n*-hexane (1:10); pale yellow solid (41.1mg, 52.6%); ^{1}H NMR (400 MHz, $CDCl_3$) d=9.04(d, *J* = 1.5 Hz, 1H), 8.65-8.64 (m, 1H), 8.52 (d, *J* = 2.5 Hz, 1H), 8.04-8.01 (m, 2H) 7.55-7.47; (m, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) d=152.9, 144.2, 142.9, 142.3, 136.4, 129.9, 129.1, 127.0; MS (EI) *m/z* (%) 156 (M^+,100), 129 (12), 103(54), 76(10).

2-phenylpyrimidine (5w-C2), 4-phenylpyrimidine (5w-C4).



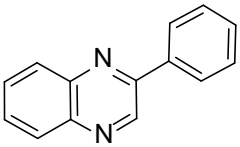
EtOAc/*n*-hexane (1:10); C4: white solid (72.9mg, 93.4%); ^{1}H NMR (400 MHz, $CDCl_3$) d=9.28(d, *J* = 1.1 Hz, 1H), 8.77 (d, *J* = 5.4 Hz, 1H), 8.11-8.08 (m, 2H), 7.73 (dd, *J* = 5.4, 1.4 Hz, 1H); 7.55-7.47 (m, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) d=163.9, 159.1, 157.5, 136.5, 131.1, 129.1, 127.1, 117.0; MS (EI) *m/z* (%) 156 (M^+,100), 129 (12), 103(54), 76(10); C2: trace.

2-phenylquinoline (5x -C2), 4-phenylquinoline (5x -C4).



EtOAc/n-hexane (1:10); C2: pale yellow solid (29.3mg, 28.6%); The spectroscopic data for these compounds were identical to those reported in the literature: Chem. Commun., 2011, 47, 12840. C4: pale yellow oil (21.7mg, 21.1%); The spectroscopic data for these compounds were identical to those reported in the literature: Eur. J. Org. Chem. 2006, 1917.

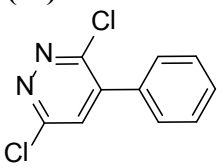
2-phenylquinoxaline (5y).



EtOAc/*n*-hexane (1:10); pale yellow solid (52.1mg, 50.5%); ^{1}H NMR (400 MHz, $CDCl_3$) d=9.34(s, 1H), 8.22-8.12 (m, 4H), 7.82-7.74 (m, 2H), 7.60-7.53 (m, 3H); ^{13}C NMR (100 MHz,

$CDCl_3$) d=151.9, 143.4, 142.3, 141.6, 136.8, 130.3, 130.2, 129.7, 129.6, 129.2, 129.1, 127.6; MS (EI) *m/z* (%) 206 (M^+,100), 179 (100), 152(30), 103(50), 76(66), 50(35).

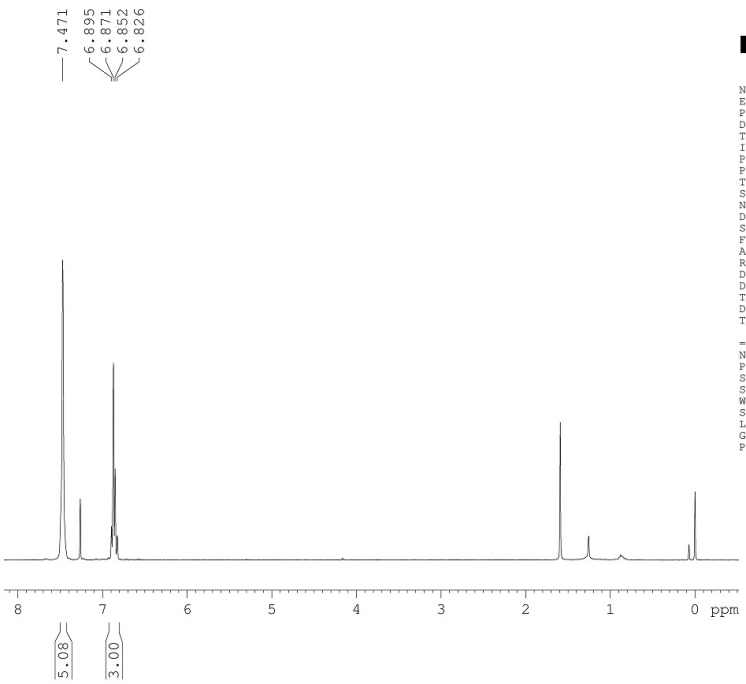
3, 6-dichloro-4-phenylpyridazine (5z).



EtOAc/*n*-hexane (1:10); pale yellow solid (19.5mg, 17.3%); ^1H NMR (400 MHz, $CDCl_3$) d=7.55-7.50 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) d=156.0, 154.9, 142.8, 133.2, 130.4, 129.6, 129.0, 128.9; MS (EI) *m/z* (%) 225(M^+,84), 224 (100), 196(55), 161(53), 136(75), 126(70).

Copies of product ^{1}H NMR and ^{13}C NMR

2-Phenyl-1, 4-benzoquinone (3a)

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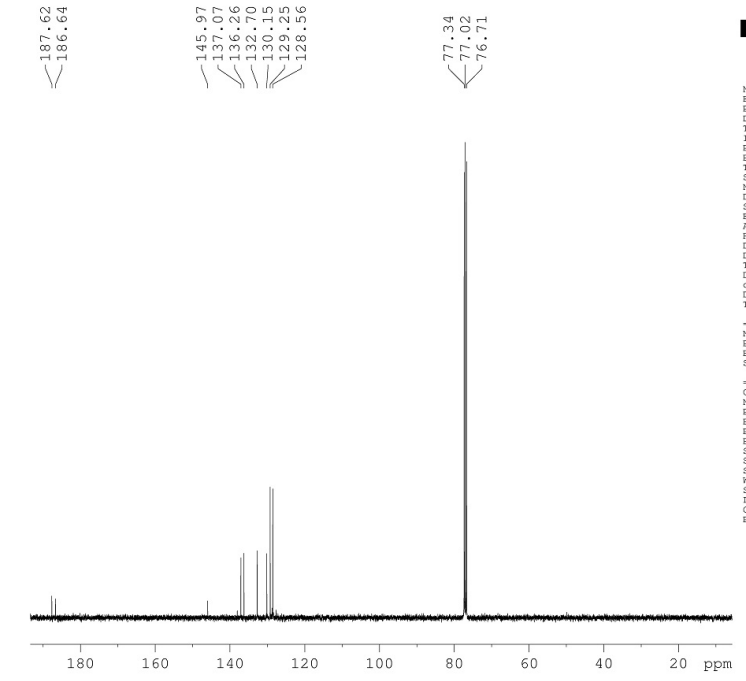


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SF             100.6127690 MHz
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GB                          0
PC                      1.40
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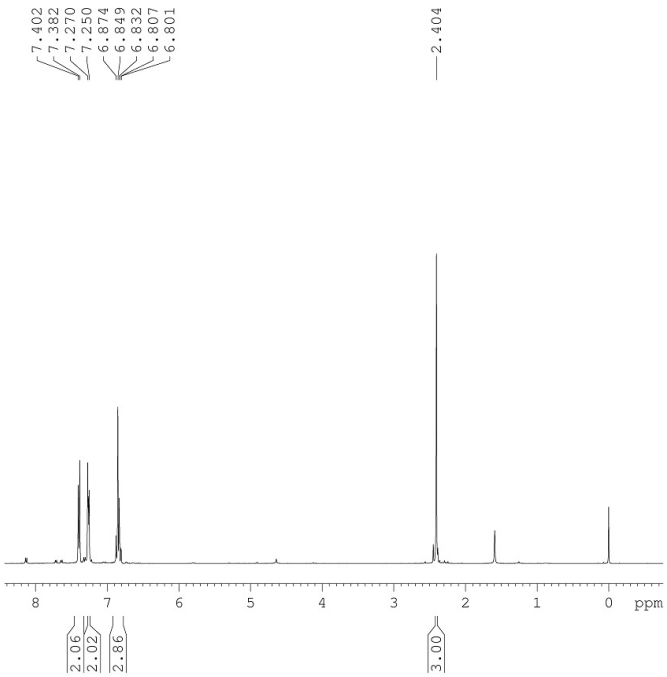
2-(4-Methylphenyl)-1, 4-benzoquinone (3b)

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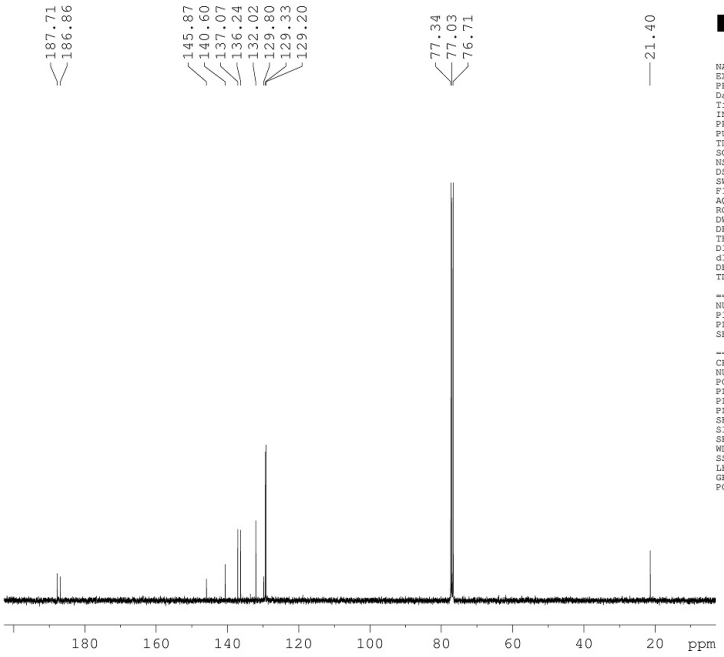
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1             15.84899998 W
SFO1            400.1632013 MHz

F2 - Processing parameters
SI                        65536
SF               400.1600086 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

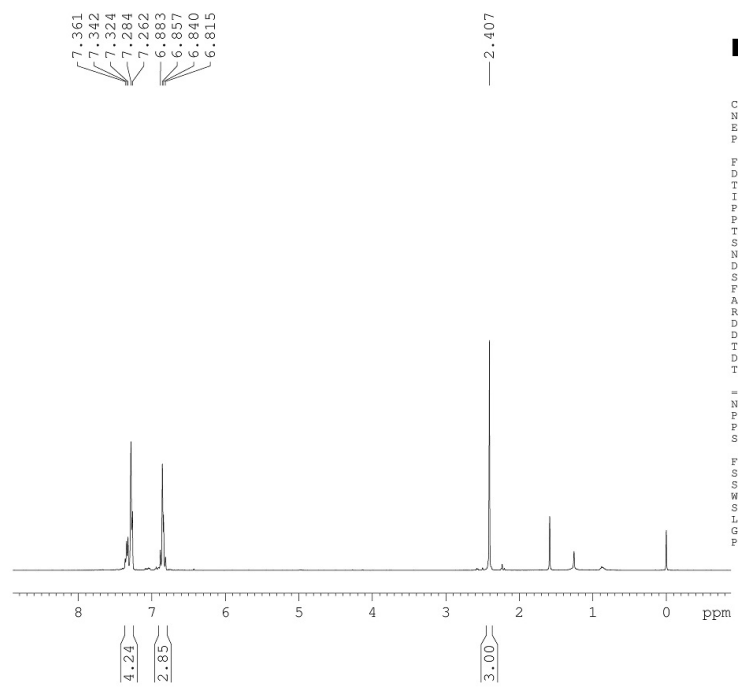



```
NAME          2012-03-21 wangjian-1262
EXPNO                       1
PROCNO                      1
Date_              20120322
Time                  3.14
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      2050
DW                  20.800 usec
DE                   6.50 usec
TE                   297.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                   19.40 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2           400.1316005 MHz
SI                      32768
SF             100.6127690 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

2-(3-Methylphenyl)-1, 4-benzoquinone (3c)

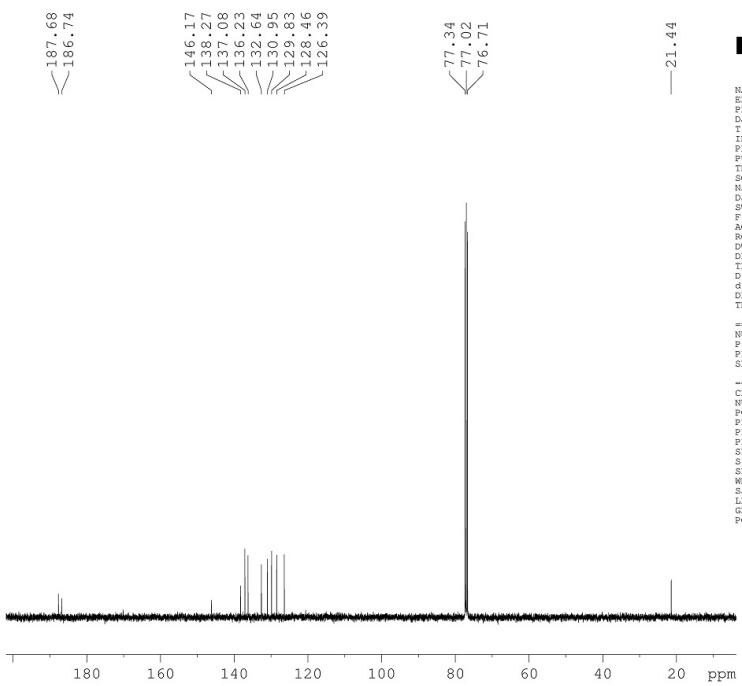



```
Current Data Parameters
NAME                  WJ-1399
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120228
Time                  19.28
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                   177.75
DW                  60.800 usec
DE                   8.00 usec
TE                  294.2 K
D1               1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1            15.84899998 W
SFO1           400.1632013 MHz

F2 - Processing parameters
SI                       65536
SF              400.1600082 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

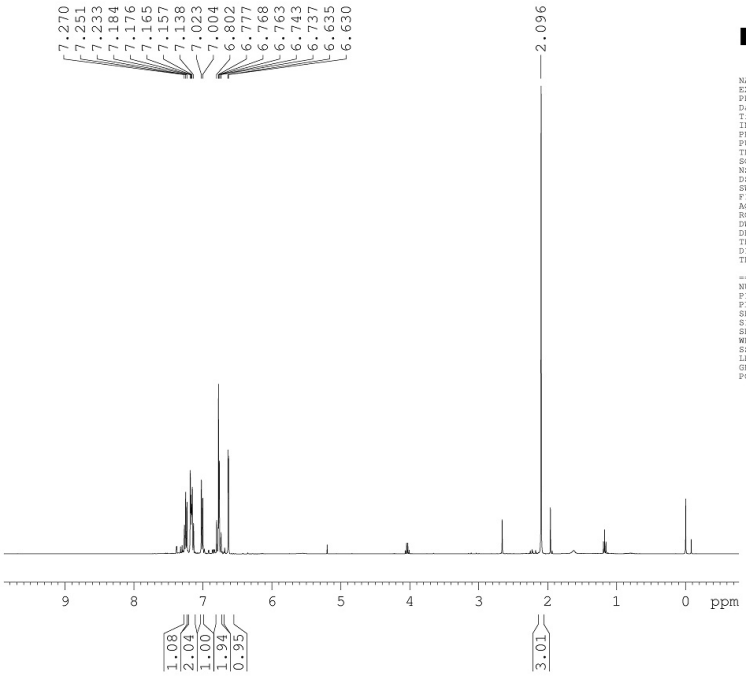


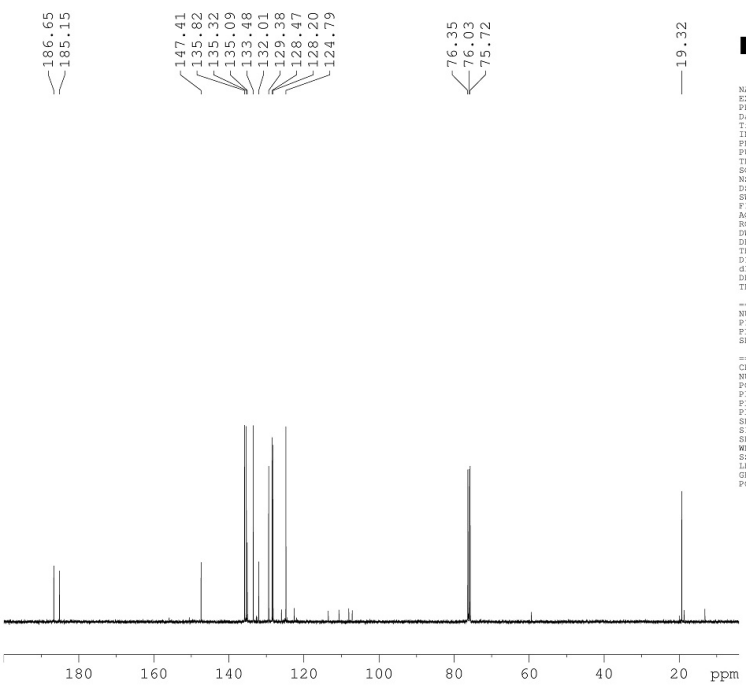

```
NAME        2012-03-21 wangjian-1399
EXPNO                          1
PROCNO                         1
Date_                   20120322
Time                        2.35
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         256
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         2050
DW                       20.800 usec
DE                        6.50 usec
TE                       296.7 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

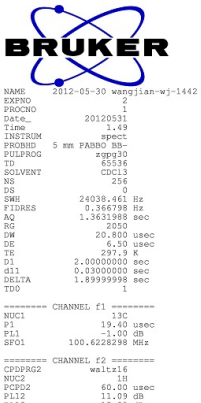
======== CHANNEL f1 ========
NUC1                         13C
P1                        19.40 usec
PL1                       -1.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     60.00 usec
PL12                      11.09 dB
PL13                      13.05 dB
PL2                       -2.00 dB
SFO2              400.1316005 MHz
SI                         32768
SF                100.6127690 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                         1.40
```

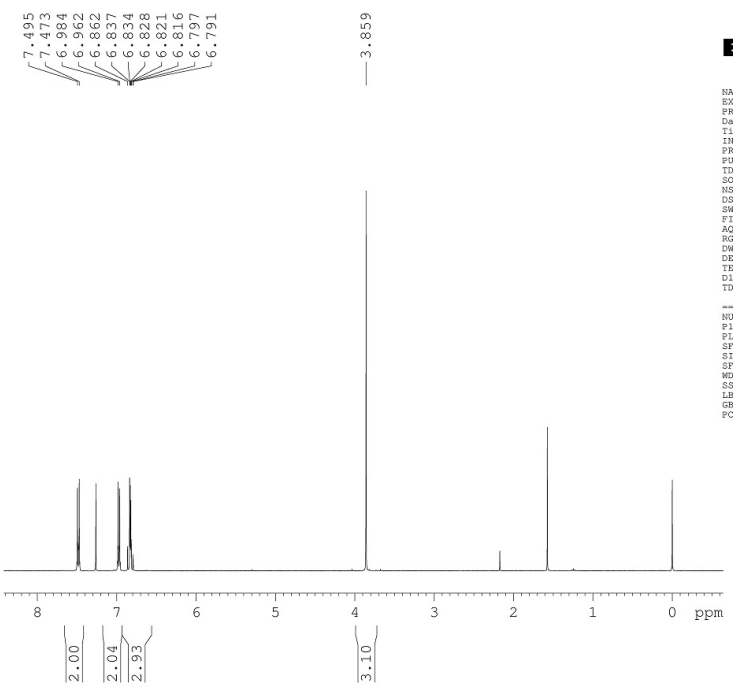
2-(2-Methylphenyl)-1, 4-benzoquinone (3d)





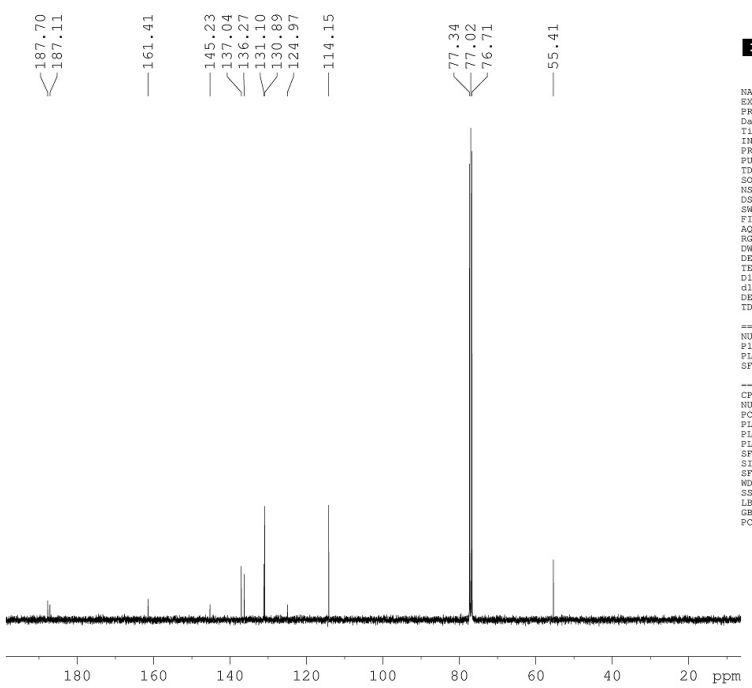


2-(4-Methoxyphenyl)-1, 4-benzoquinone (3e)




```
NAME          2012-04-20 wangjian-1415
EXPNO                    1
PROCNO                   1
Date_             20120420
Time                 1.14
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    406
DW                60.800 usec
DE                 6.50 usec
TE                294.9 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.30 usec
PL1                 -2.00 dB
SFO1          400.1324710 MHz
SI                  32768
SF            400.1300088 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

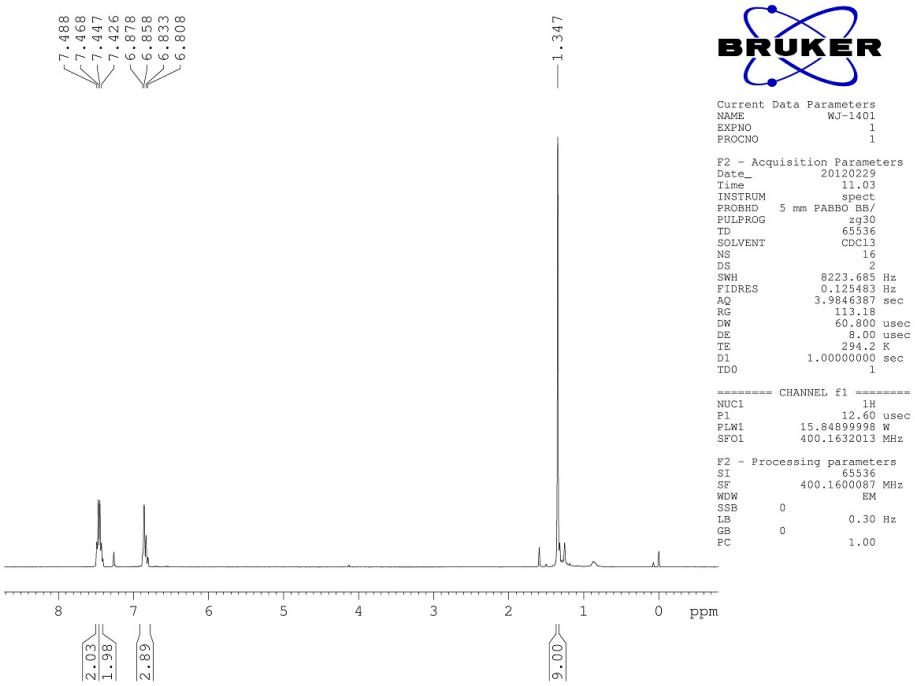



```
NAME          2012-04-20 wangjian-1415
EXPNO                    2
PROCNO                   1
Date_             20120420
Time                 1.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   2050
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  19.40 usec
PL1                 -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               60.00 usec
PL12                11.09 dB
PL13                13.05 dB
PL2                 -2.00 dB
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

2-(4-*tert*-Butylphenyl)-1, 4-benzoquinone (3f)

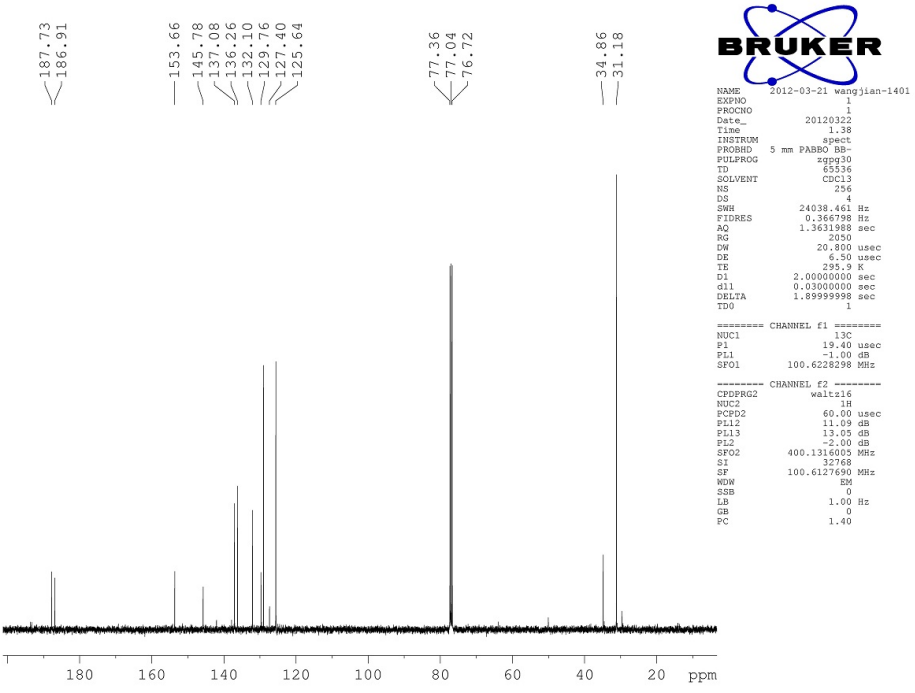



```
Current Data Parameters
NAME                  WJ-1401
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120229
Time                  11.03
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    113.18
DW                   60.800 usec
DE                    8.00 usec
TE                   294.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1             15.84899998 W
SFO1            400.1632013 MHz

F2 - Processing parameters
SI                       65536
SF                400.1600087 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

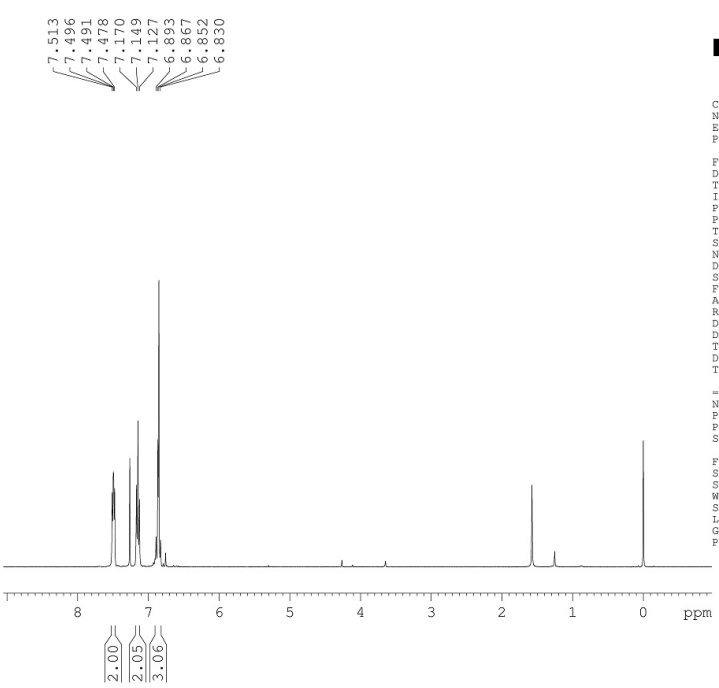



```
NAME          2012-03-21 wangjian-1401
EXPNO                       1
PROCNO                      1
Date_              20120322
Time                  1.38
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                   20.800 usec
DE                    6.50 usec
TE                   295.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      19.40 usec
PL1                     -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   60.00 usec
PL12                    11.09 dB
PL13                    13.05 dB
PL2                     -2.00 dB
SFO2           400.1316005 MHz
SI                      32768
SF             100.6127690 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

2-(4-Fluorophenyl)-1, 4-benzoquinone (3g)

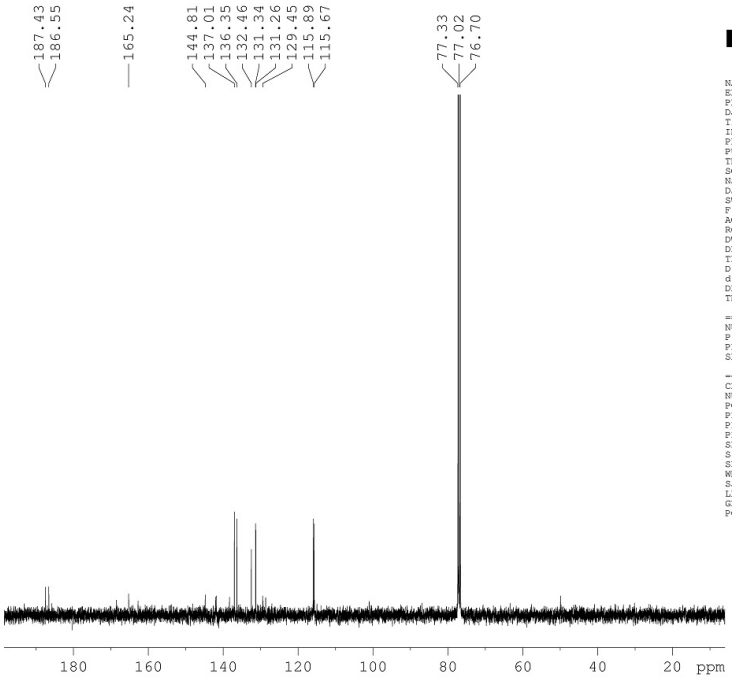



```
Current Data Parameters
NAME                  WJ-1264
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120228
Time                  18.32
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    197.41
DW                   60.800 usec
DE                    8.00 usec
TE                   294.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1             15.84899998 W
SFO1            400.1632013 MHz

F2 - Processing parameters
SI                        65536
SF               400.1600074 MHz
WDW                         EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

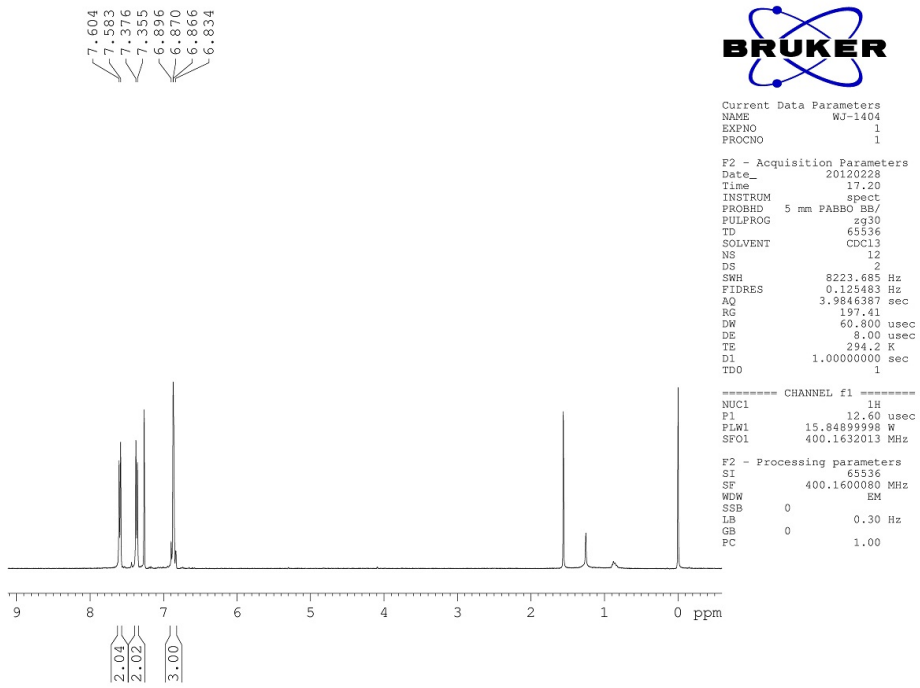



```
NAME        2012-03-21 wangjian-1264
EXPNO                       1
PROCNO                      1
Date_              20120322
Time                  4.11
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      2050
DW                   20.800 usec
DE                    6.50 usec
TE                   298.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      19.40 usec
PL1                     -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                       1H
PCPD2                 60.00 usec
PL12                  11.09 dB
PL13                  13.05 dB
PL2                   -2.00 dB
SFO2           400.1316005 MHz
SI                     32768
SF             100.6127690 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

2-(4-Bromophenyl)-1, 4-benzoquinone (3h)

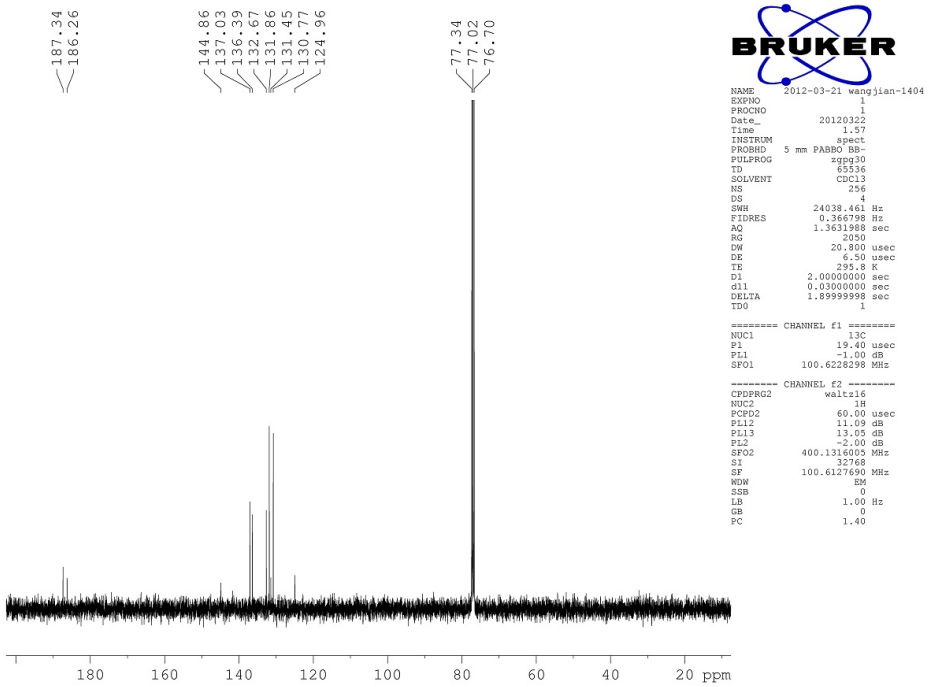



```
Current Data Parameters
NAME                  WJ-1404
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120228
Time                  17.20
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                    197.41
DW                   60.800 usec
DE                    8.00 usec
TE                   294.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                        1H
P1                       12.60 usec
PLW1             15.84899998 W
SFO1             400.1632013 MHz

F2 - Processing parameters
SI                        65536
SF               400.1600080 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

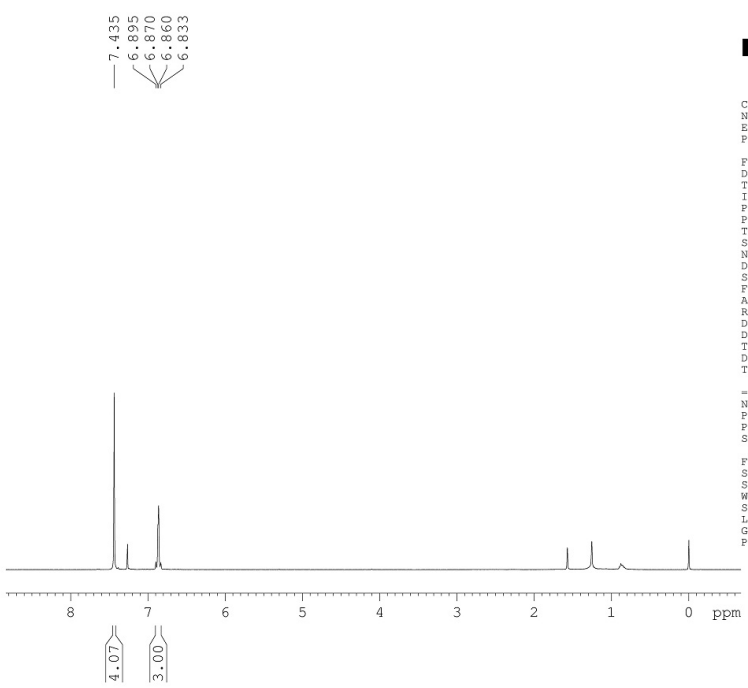



```
NAME        2012-03-21 wangjian-1404
EXPNO                       1
PROCNO                      1
Date_              20120322
Time                  1.57
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                     2050
DW                   20.800 usec
DE                    6.50 usec
TE                   295.8 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                       19.40 usec
PL1                      -1.00 dB
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    60.00 usec
PL12                     11.09 dB
PL13                     13.05 dB
PL2                      -2.00 dB
SFO2            400.1316005 MHz
SI                       32768
SF              100.6127690 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

2-(4-Chlorophenyl)-1, 4-benzoquinone (3i)

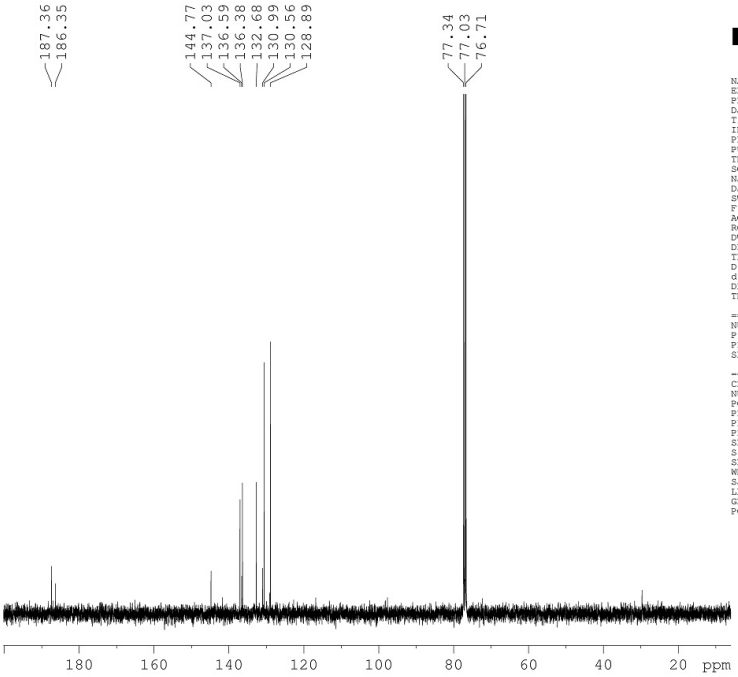



```
Current Data Parameters
NAME                  WJ-1402
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120228
Time                  16.17
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    197.41
DW                  60.800 usec
DE                   8.00 usec
TE                  294.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1            15.84899998 W
SFO1           400.1632013 MHz

F2 - Processing parameters
SI                        65536
SF               400.1600075 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

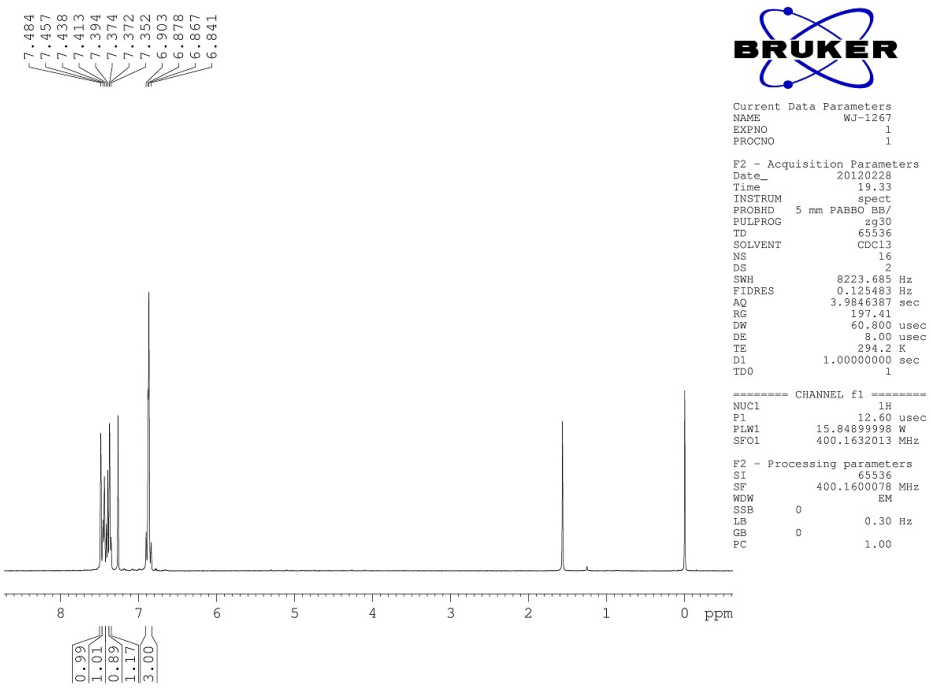



```
NAME        2012-03-21 wangjian-1402
EXPNO                       1
PROCNO                      1
Date_              20120322
Time                  1.19
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     2050
DW                  20.800 usec
DE                   6.50 usec
TE                  295.3 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      19.40 usec
PL1                     -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                       1H
PCPD2                   60.00 usec
PL12                    11.09 dB
PL13                    13.05 dB
PL2                     -2.00 dB
SFO2           400.1316005 MHz
SI                      32768
SF             100.6127690 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

2-(3-Chlorophenyl)-1, 4-benzoquinone (3j)

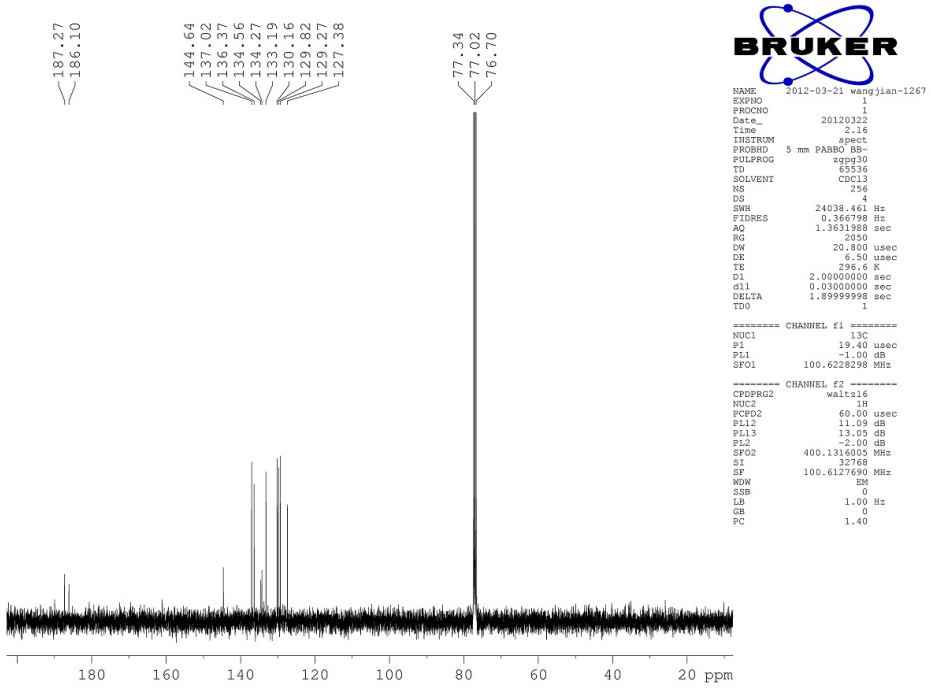



```
Current Data Parameters
NAME                  WJ-1267
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120228
Time                  19.33
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    197.41
DW                  60.800 usec
DE                   8.00 usec
TE                  294.2 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1           15.84899998 W
SFO1           400.1632013 MHz

F2 - Processing parameters
SI                       65536
SF              400.1600078 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

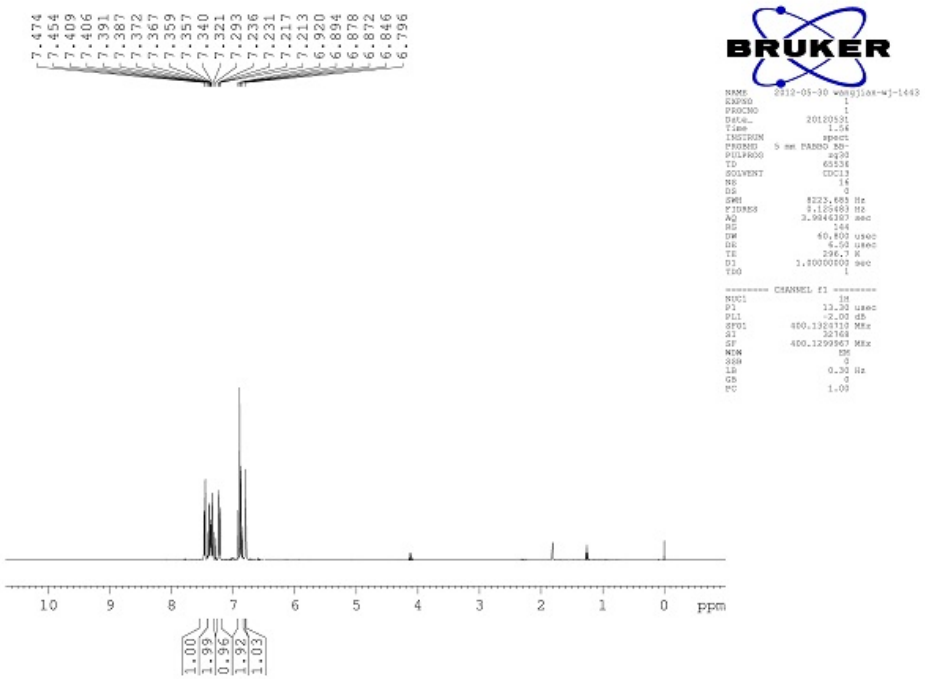


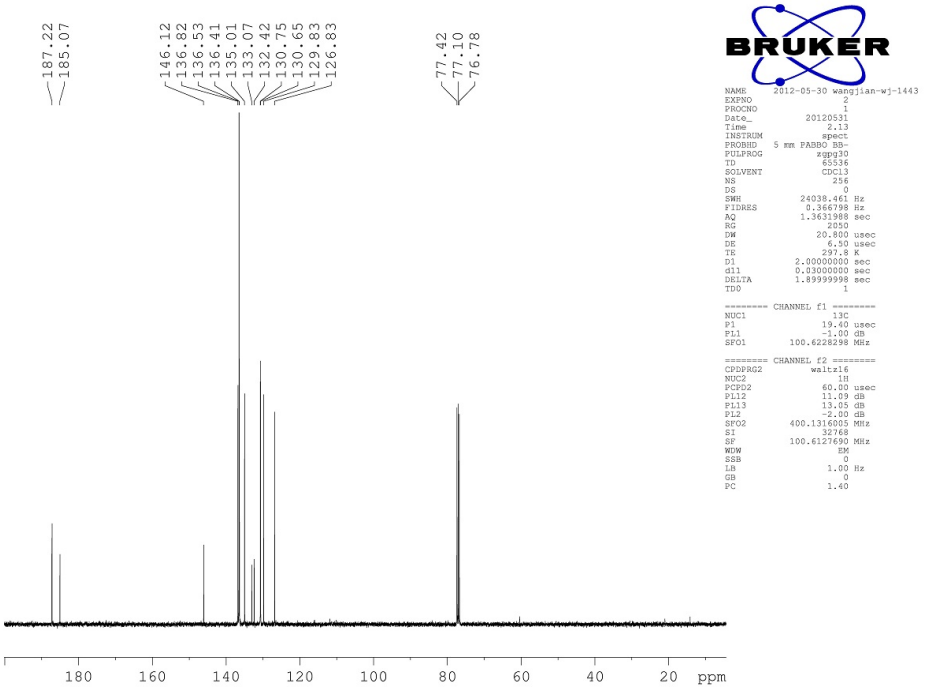

```
NAME      2012-03-21 wangjian-1267
EXPNO                       1
PROCNO                      1
Date_              20120322
Time                  2.16
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  296.6 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      19.40 usec
PL1                     -1.00 dB
SFO1           100.6228298 MHz

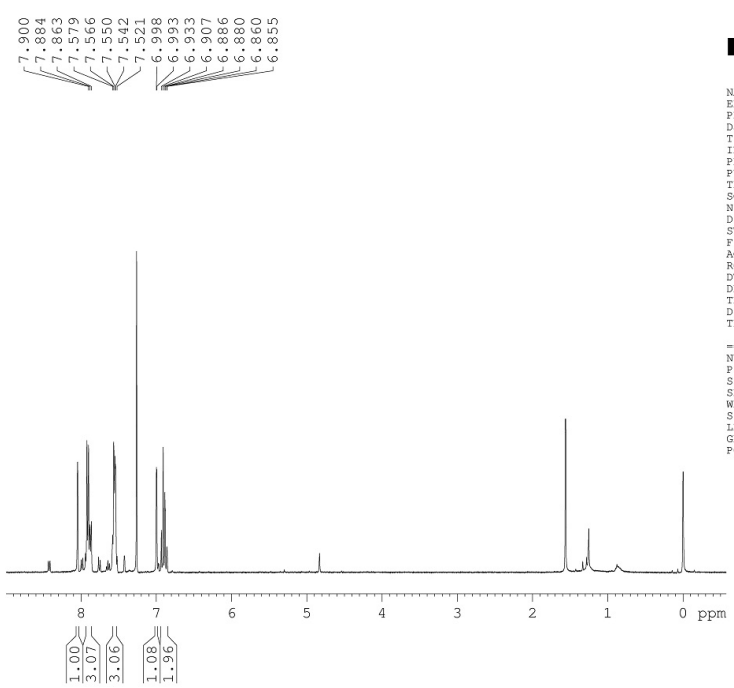
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   60.00 usec
PL12                    11.09 dB
PL13                    13.05 dB
PL2                     -2.00 dB
SFO2           400.1316005 MHz
SI                      32768
SF             100.6127690 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

2-(2-Chlorophenyl)-1, 4-benzoquinone (3k)



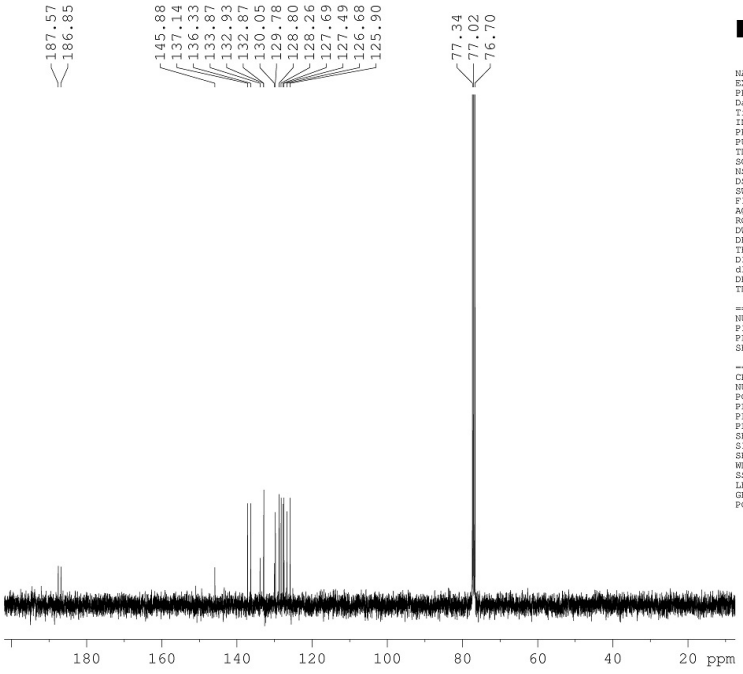


2- (naphthalen-2-yl) -1,4-benzoquinone (3l)




```
NAME                 WJ-1270
EXPNO                      1
PROCNO                     1
Date_             20120229
Time                  14.11
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                         8
DS                         2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                   197.41
DW                 60.800 usec
DE                  8.00 usec
TE                  294.2 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    12.60 usec
SI                        65536
SF             400.1600083 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                    1.00
```

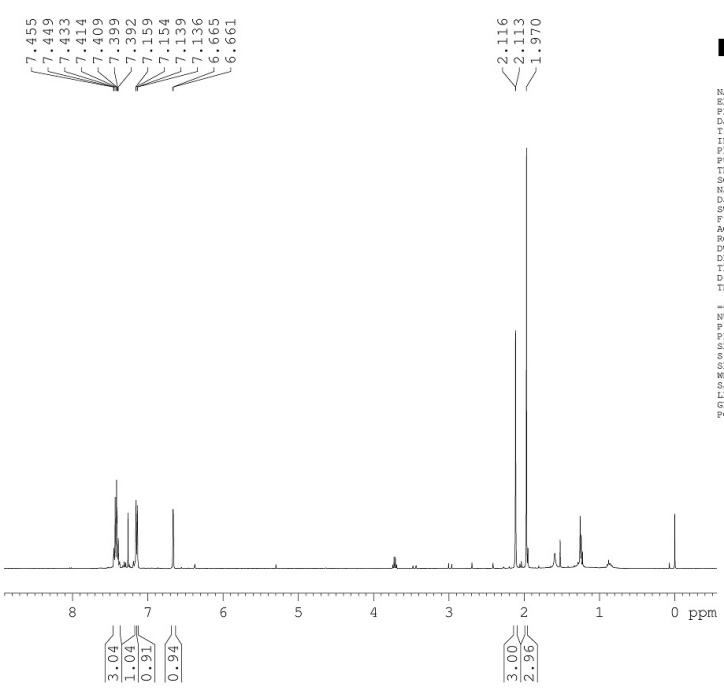



```
NAME      2012-05-25 wangjian-1270
EXPNO                      1
PROCNO                     1
Date_             20120524
Time                  23.12
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      181
DW                 20.800 usec
DE                  6.50 usec
TE                  297.7 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                    19.40 usec
PL1                   -1.00 dB
SFO1           100.6228298 MHz

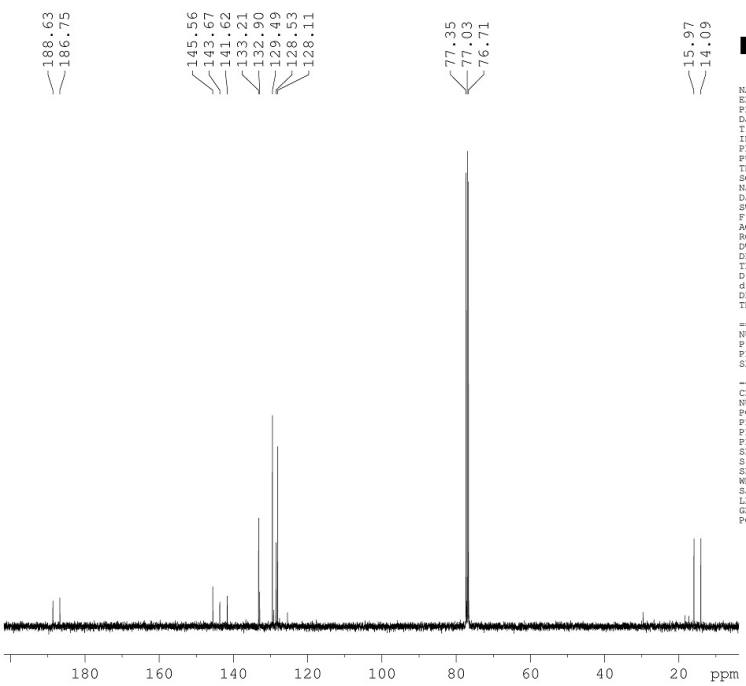
======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 60.00 usec
PL12                  11.09 dB
PL13                  13.05 dB
PL2                   -2.00 dB
SFO2           400.1316005 MHz
SI                        32768
SF             100.6127690 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

2,6-Dimethyl-3-phenyl-1,4-benzoquinone (3n)




```
NAME          2012-04-20 wangjian-1421
EXPNO                    1
PROCNO                   1
Date_             20120420
Time                 1.57
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    256
DW                60.800 usec
DE                 6.50 usec
TE                294.9 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.30 usec
PL1                 -2.00 dB
SFO1          400.1324710 MHz
SI                  32768
SF            400.1300093 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

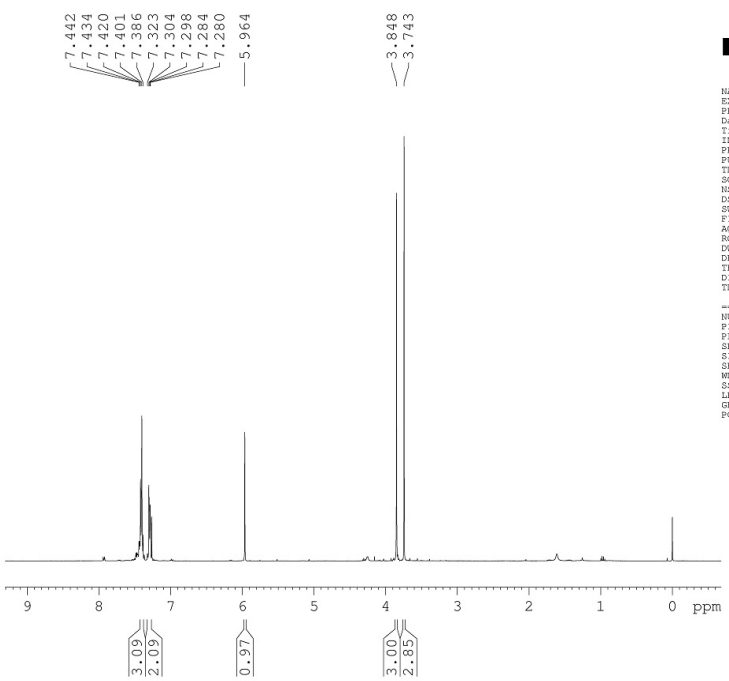



```
NAME          2012-04-20 wangjian-1421
EXPNO                    2
PROCNO                   1
Date_             20120420
Time                 2.13
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   1820
DW                20.800 usec
DE                 6.50 usec
TE                296.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  19.40 usec
PL1                 -1.00 dB
SFO1          100.6228298 MHz

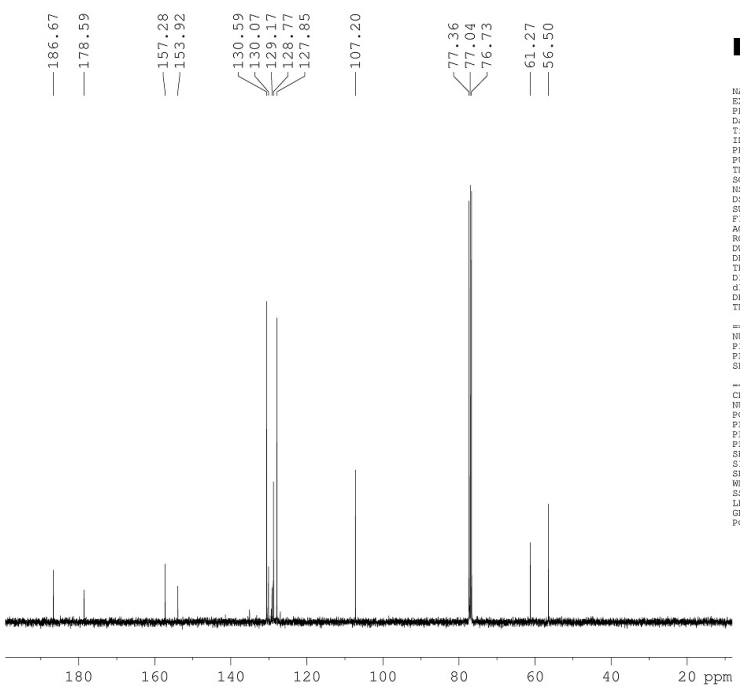
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               60.00 usec
PL12                11.09 dB
PL13                13.05 dB
PL2                 -2.00 dB
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

2,6-Dimethoxy-3-(4-methylphenyl)-1,4-benzoquinone (3o)




```
NAME            2012-05-25 wangjian-1437
EXPNO                    1
PROCNO                   1
Date_             20120525
Time                 19.03
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      228
DW                   60.800 usec
DE                    6.50 usec
TE                  296.5 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.30 usec
PL1                  -2.00 dB
SFO1            400.1324710 MHz
SI                    32768
SF              400.1300088 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

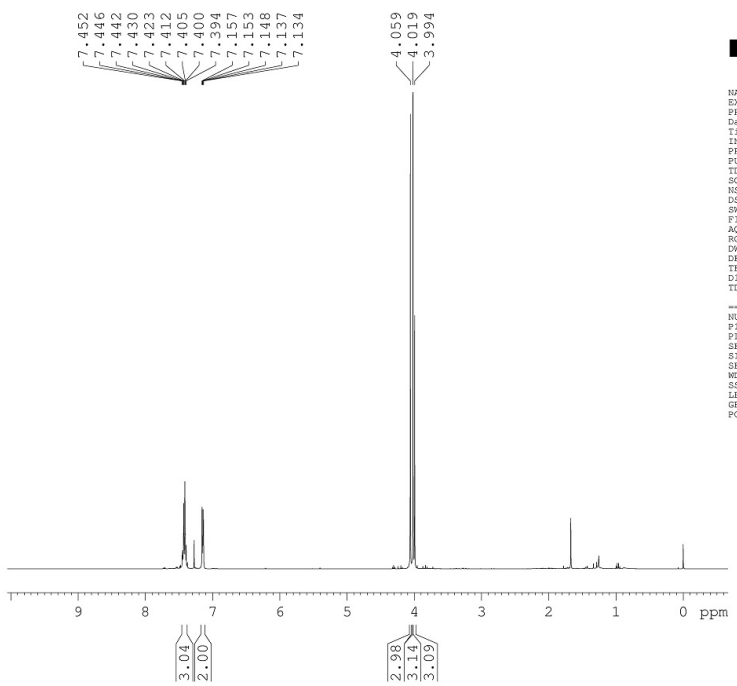



```
NAME            2012-05-25 wangjian-1437
EXPNO                    2
PROCNO                   1
Date_             20120525
Time                 19.20
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     2050
DW                   20.800 usec
DE                    6.50 usec
TE                  297.6 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   19.40 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

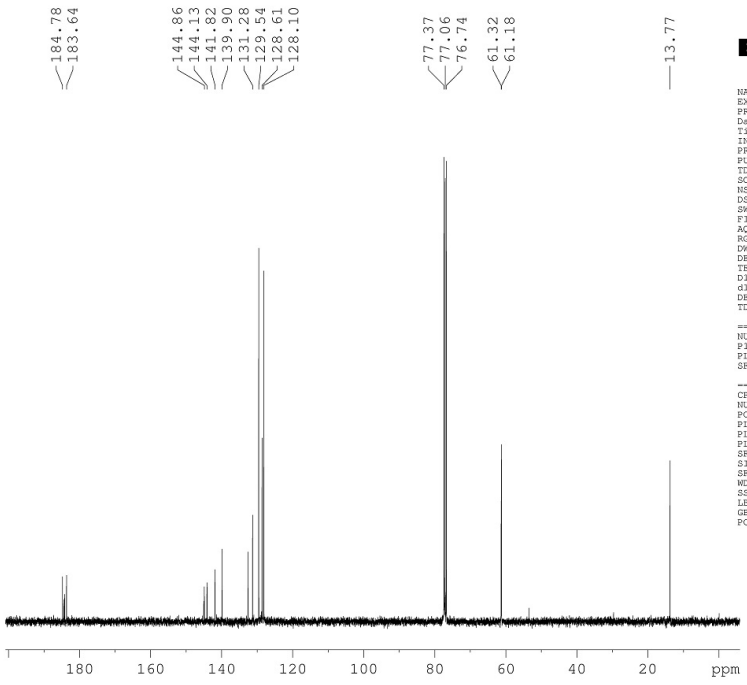
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2            400.1316005 MHz
SI                    32768
SF              100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2,3-Dimethoxy-5-methyl-6-phenyl-1,4-benzoquionone (3q)




```
NAME          2012-05-25 wangjian-1440
EXPNO                  1
PROCNO                 1
Date_           20120525
Time              19.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   161
DW                60.800 usec
DE                 6.50 usec
TE                296.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1          400.1324710 MHz
SI                 32768
SF            400.1300045 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

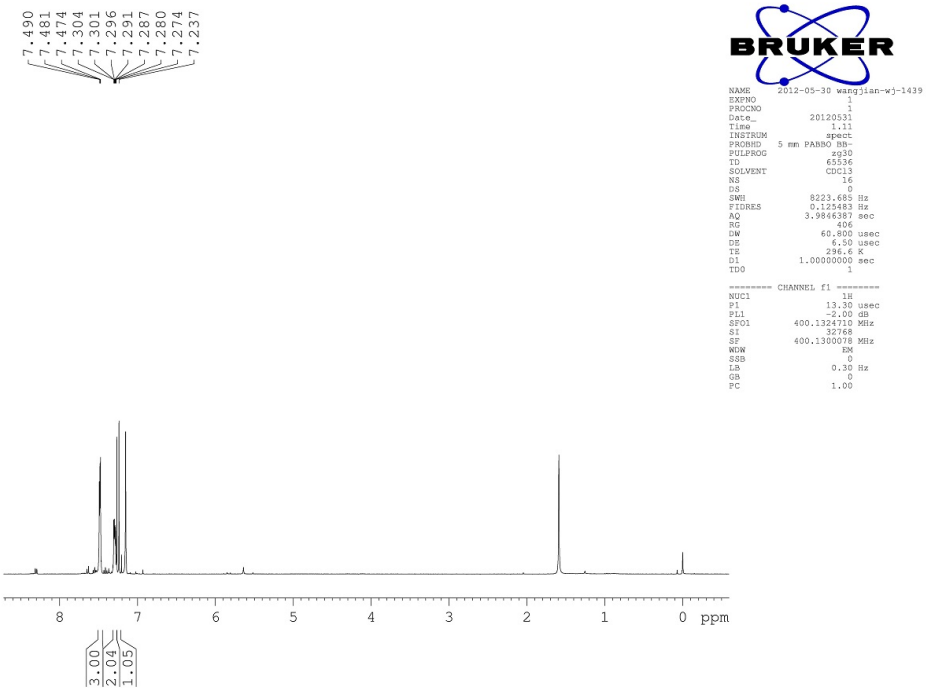


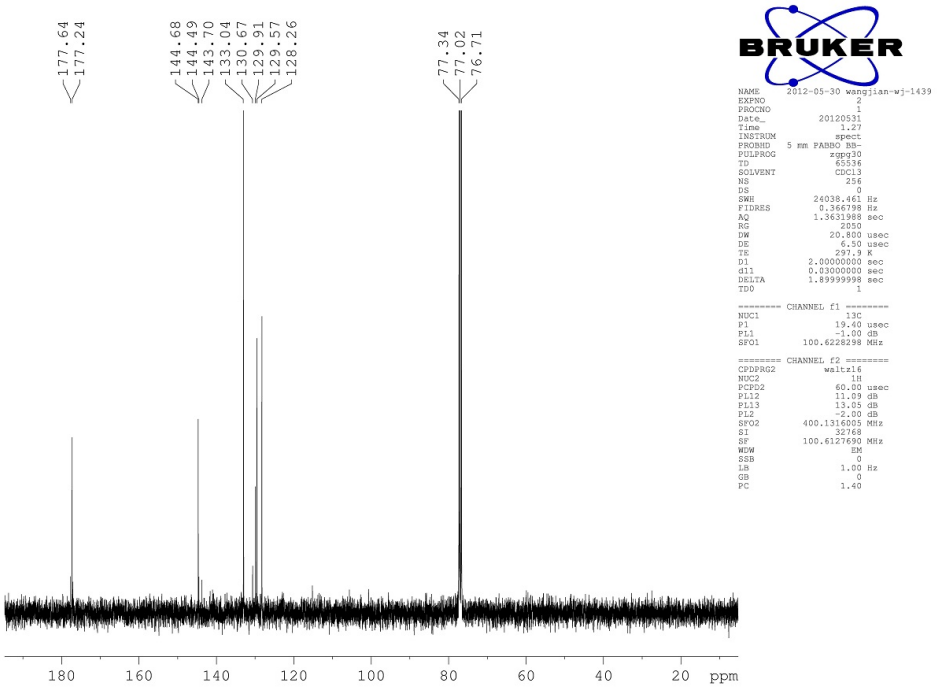

```
NAME          2012-05-25 wangjian-1440
EXPNO                  2
PROCNO                 1
Date_           20120525
Time              19.42
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1          100.6228298 MHz

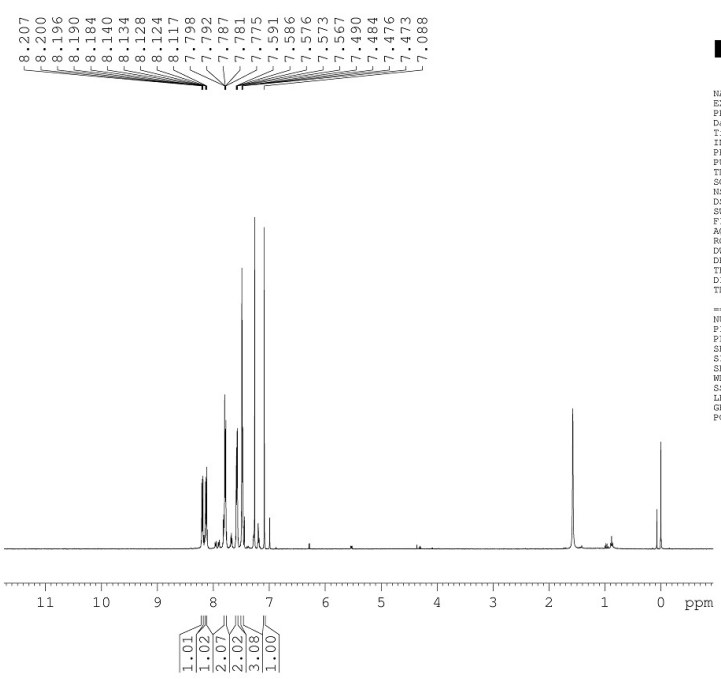
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

2,5-Dichloro-3-phenyl-1,4-benzoquionone (3r)



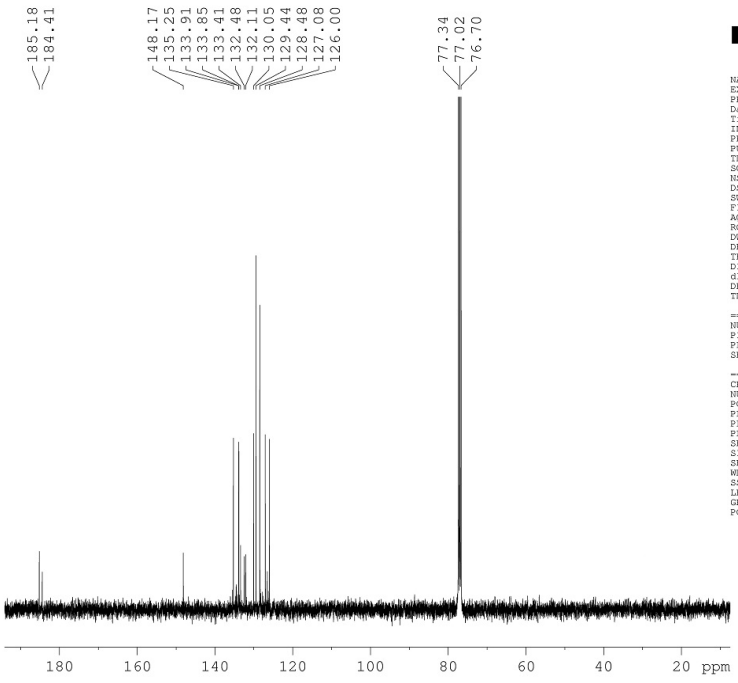


2-phenyl-1,4-naphthoquinone (3s)




```
NAME          2012-05-25 wangjian-1419
EXPNO                    1
PROCNO                   1
Date_             20120525
Time                 17.58
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     406
DW                  60.800 usec
DE                   6.50 usec
TE                  296.3 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.30 usec
PL1                  -2.00 dB
SFO1           400.1324710 MHz
SI                   32768
SF             400.1300094 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

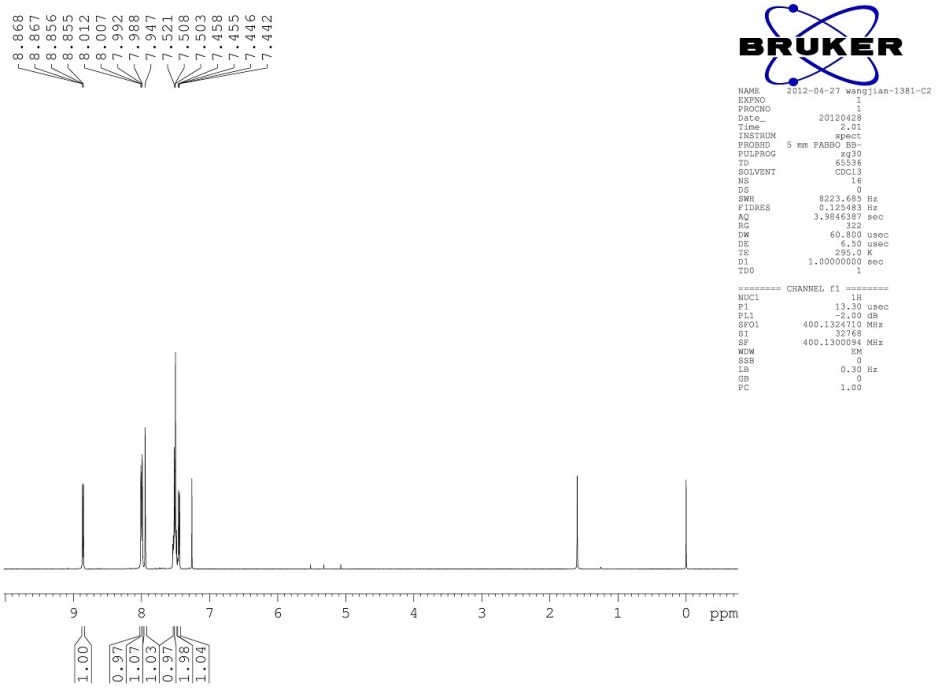


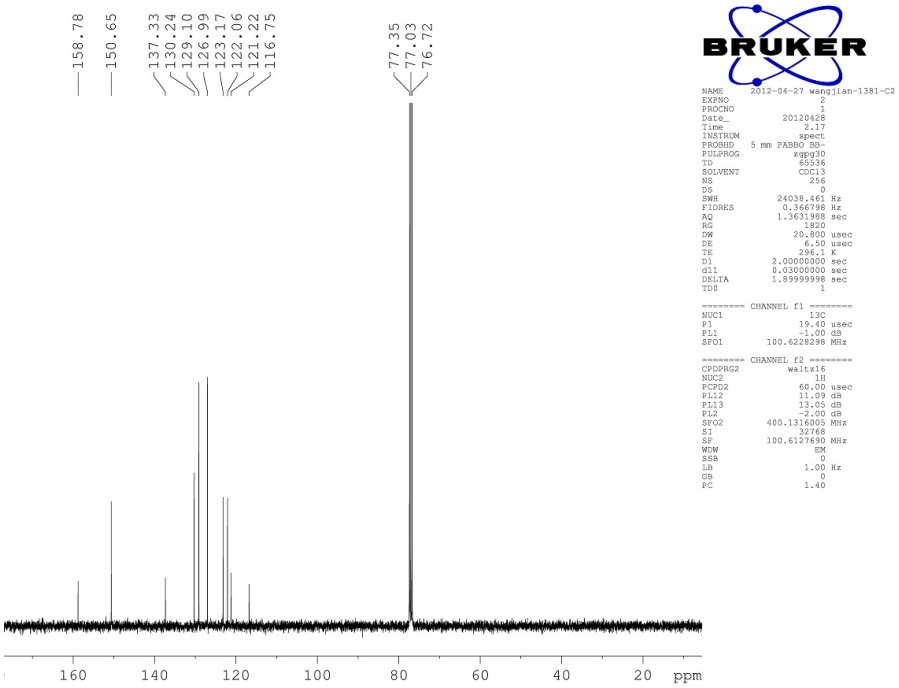

```
NAME          2012-05-25 wangjian-1419
EXPNO                    2
PROCNO                   1
Date_             20120525
Time                 18.58
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  297.6 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   19.40 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

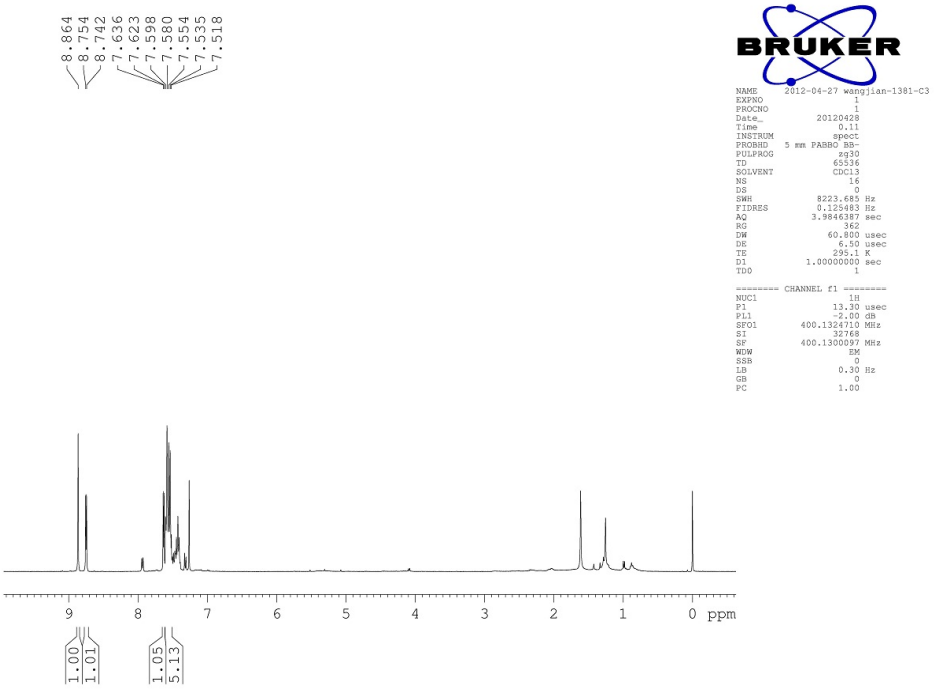
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2           400.1316005 MHz
SI                   32768
SF             100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2-phenylisonicotinonitrile (5a-C2)



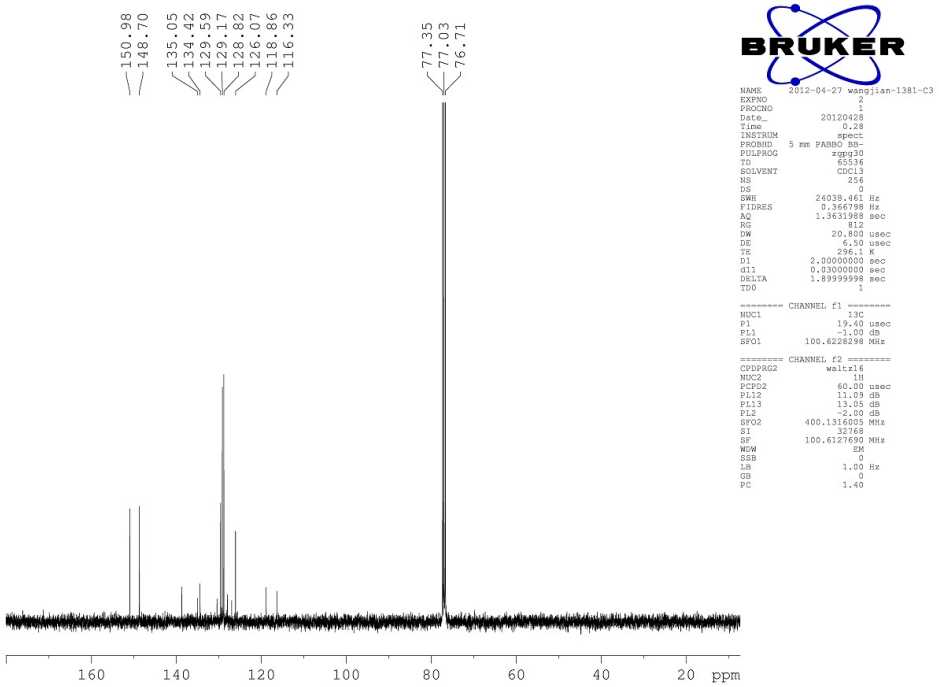


3-phenylisonicotinonitrile (5a-C3)




```
NAME        2012-04-27 wangjian-1381-C3
EXPNO                  1
PROCNO                 1
Date_           20120428
Time                0.11
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                   362
DW               60.800 usec
DE                6.50 usec
TE                295.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.30 usec
PL1               -2.00 dB
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300097 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

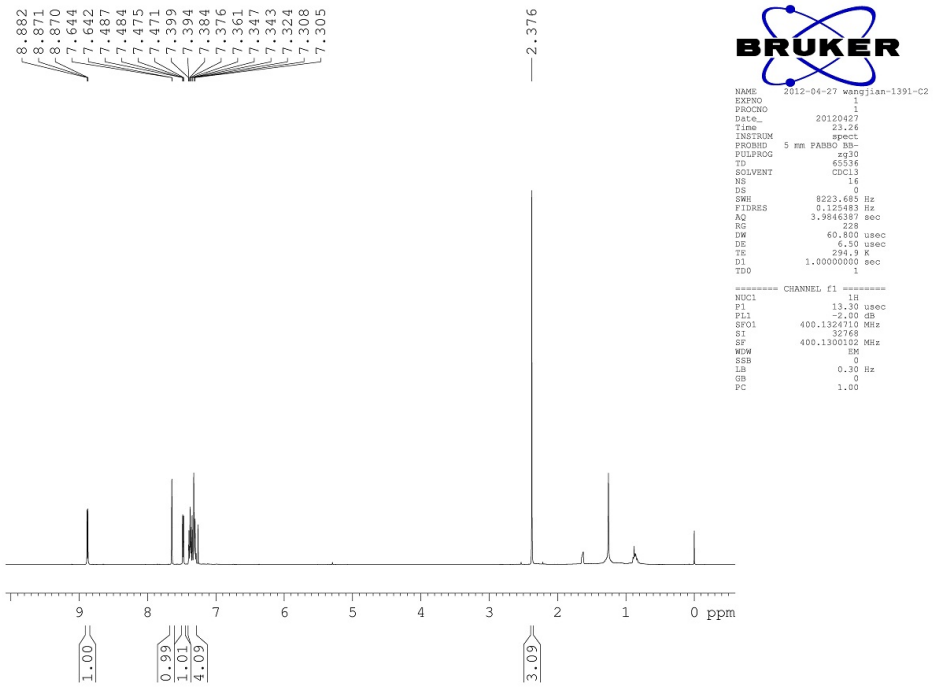


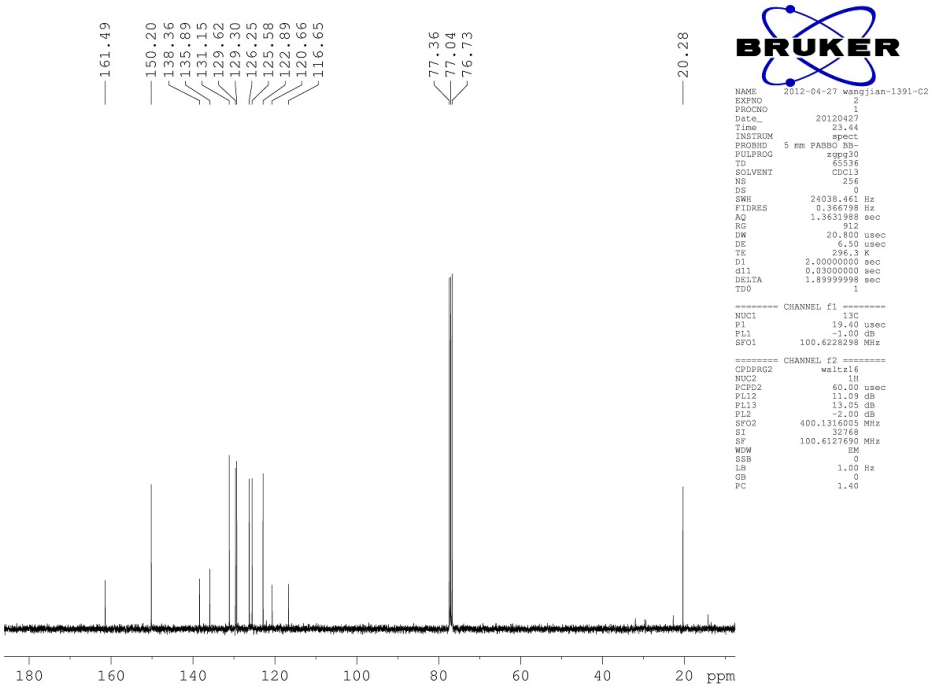

```
NAME        2012-04-27 wangjian-1381-C3
EXPNO                  2
PROCNO                 1
Date_           20120428
Time                0.28
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                   812
DW               20.800 usec
DE                6.50 usec
TE                296.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                19.40 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

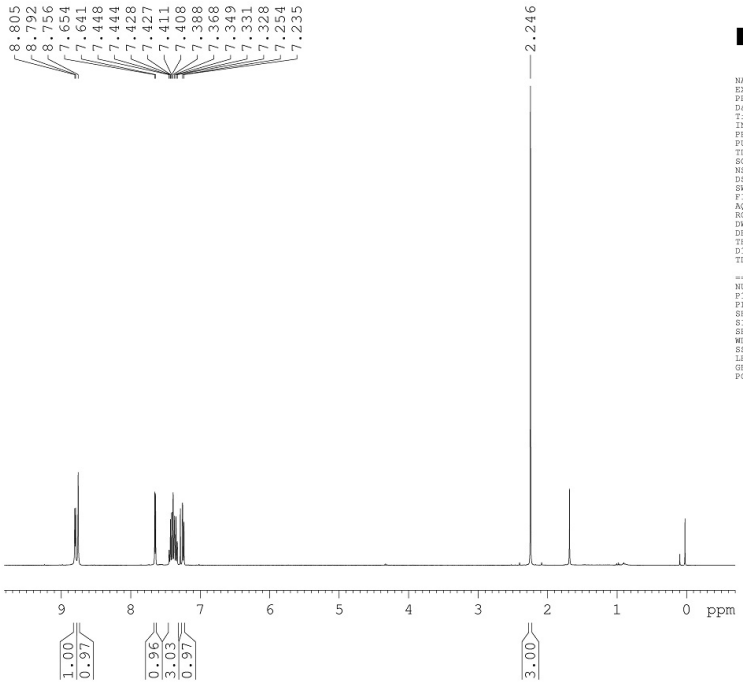
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

2-(*o*-tolyl)isonicotinonitrile (5b-C2)



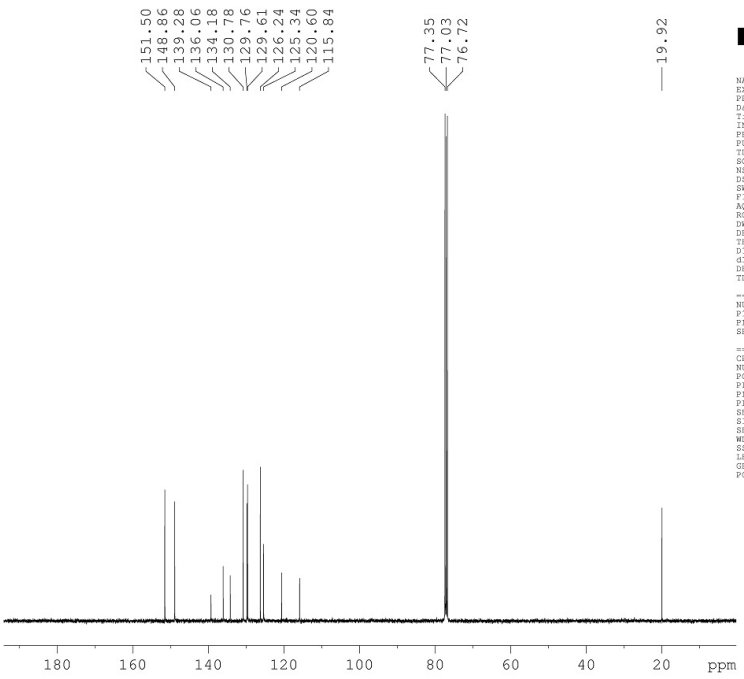


3-(*o*-tolyl)isonicotinonitrile (5b-C3)




```
NAME          2012-05-25 wangjian-1391-C3
EXPNO                  1
PROCNO                 1
Date_           20120524
Time               23.23
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                  90.5
DW                60.800 usec
DE                 6.50 usec
TE                296.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

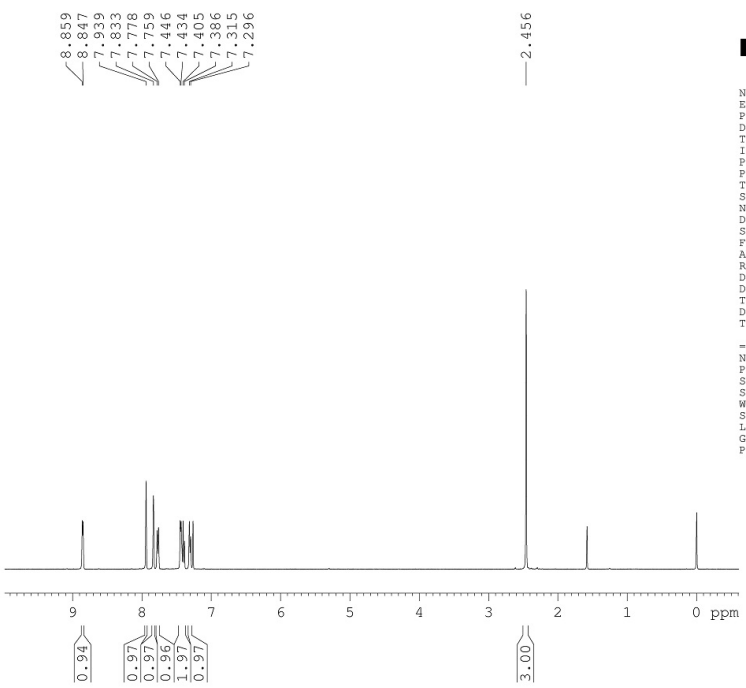



```
NAME          2012-05-25 wangjian-1391-C3
EXPNO                  2
PROCNO                 1
Date_           20120525
Time               0.21
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   181
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1             2.00000000 sec
D11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

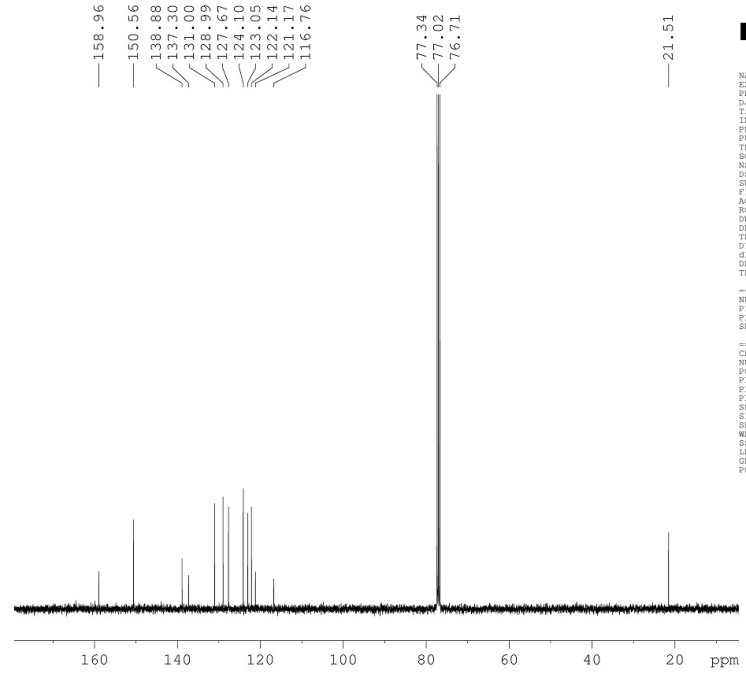
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

2-(*m*-tolyl)isonicotinonitrile (5c-C2)




```
NAME                WJ-1392-C2
EXPNO                        1
PROCNO                       1
Date_                 20120228
Time                     17.14
INSTRUM                  spect
PROBHD   5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           4
DS                           2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                      197.41
DW                      60.800 usec
DE                       8.00 usec
TE                      294.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       12.60 usec
SI                       65536
SF                 400.1600084 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

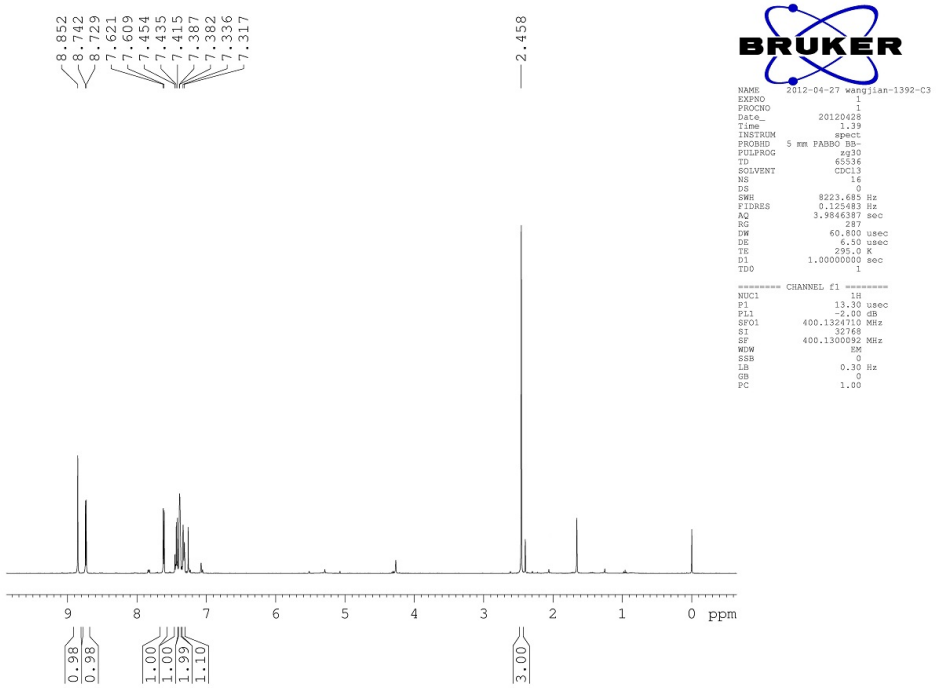



```
NAME      2012-03-21 wangjian-1392-C2
EXPNO                        1
PROCNO                       1
Date_                 20120322
Time                     3.52
INSTRUM                  spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         256
DS                           4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                        2050
DW                      20.800 usec
DE                       6.50 usec
TE                      297.7 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                       19.40 usec
PL1                      -1.00 dB
SFO1               100.6228298 MHz

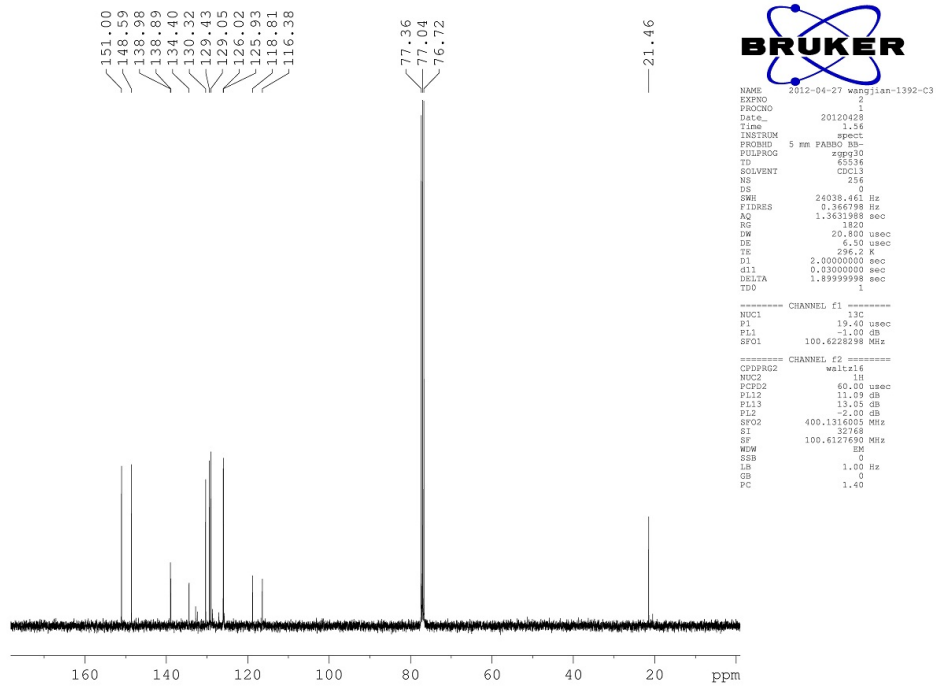
======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    60.00 usec
PL12                     11.09 dB
PL13                     13.05 dB
PL2                      -2.00 dB
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6127694 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

3-(*m*-tolyl)isonicotinonitrile (5c-C3)




```
NAME          2012-04-27 wangjian-1392-C3
EXPNO                    1
PROCNO                   1
Date_             20120428
Time                 1.39
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    287
DW                 60.800 usec
DE                  6.50 usec
TE                 295.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1          400.1324710 MHz
SI                  32768
SF            400.1300092 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

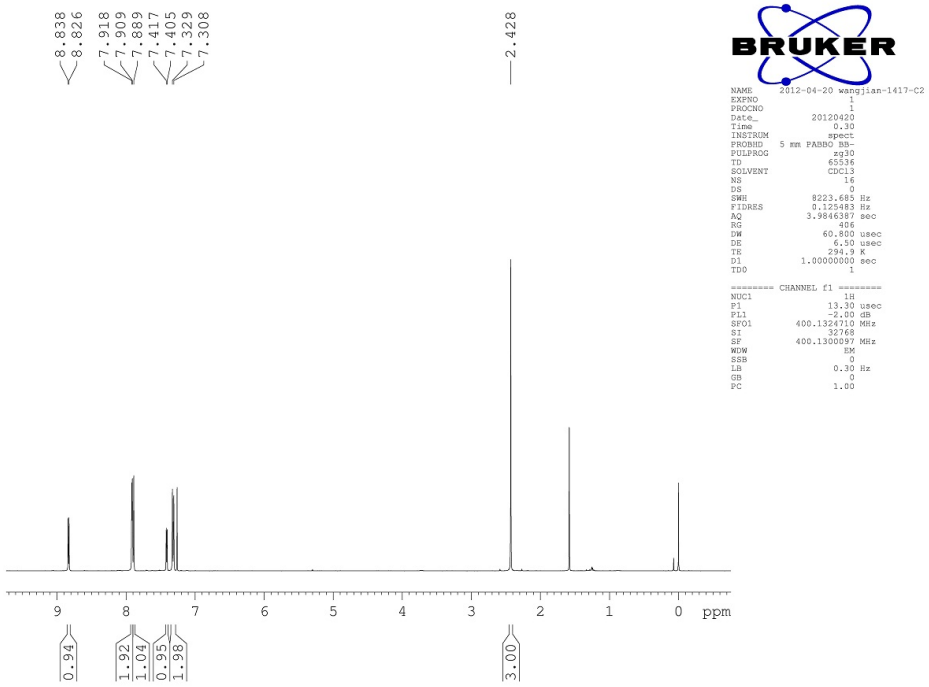



```
NAME          2012-04-27 wangjian-1392-C3
EXPNO                    2
PROCNO                   1
Date_             20120428
Time                 1.56
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   1820
DW                 20.800 usec
DE                  6.50 usec
TE                 296.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1          100.6228298 MHz

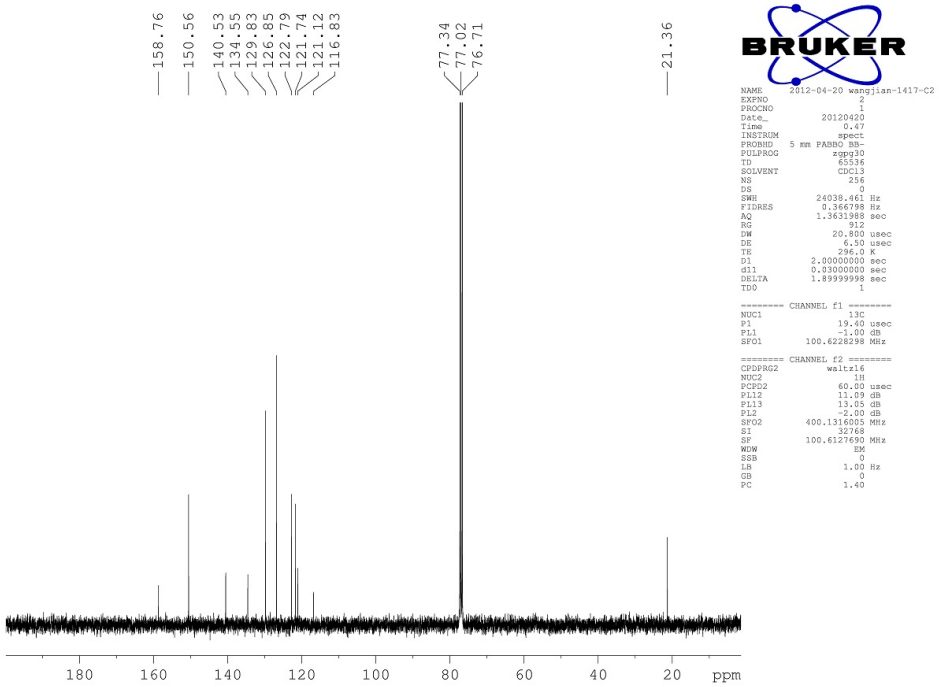
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

2-(*p*-tolyl)isonicotinonitrile (5d-C2)




```
NAME        2012-04-20 wangjian-1417-C2
EXPNO                1
PROCNO               1
Date_         20120420
Time              0.30
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                 406
DW              60.800 usec
DE               6.50 usec
TE              294.9 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               13.30 usec
PL1              -2.00 dB
SFO1        400.1324710 MHz
SI                32768
SF          400.1300097 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

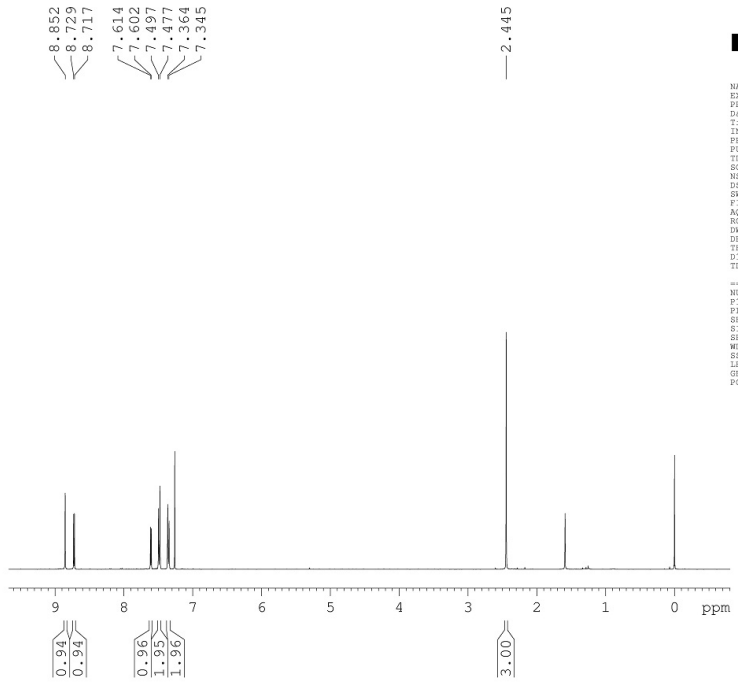


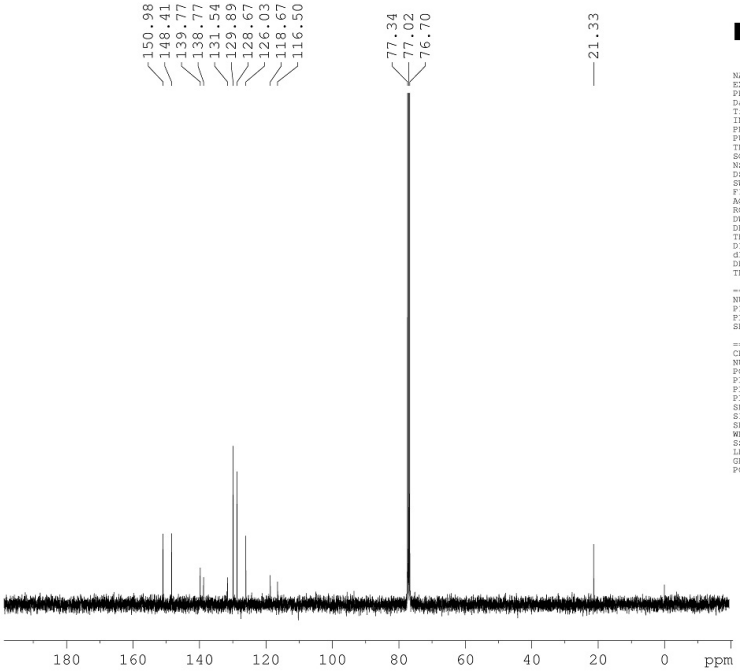

```
NAME        2012-04-20 wangjian-1417-C2
EXPNO                2
PROCNO               1
Date_         20120420
Time              0.47
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG        zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                 912
DW              20.800 usec
DE               6.50 usec
TE              296.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  1

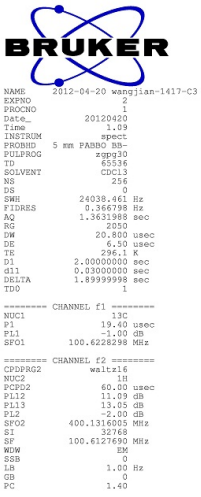
======== CHANNEL f1 ========
NUC1                13C
P1               19.40 usec
PL1              -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            60.00 usec
PL12             11.09 dB
PL13             13.05 dB
PL2              -2.00 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6127690 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

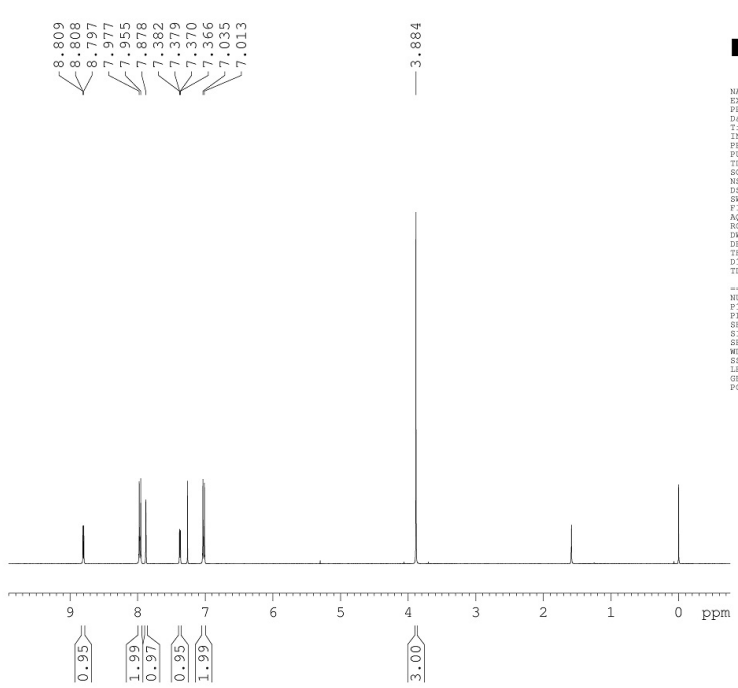
3-(*p*-tolyl)isonicotinonitrile (5d-C3)





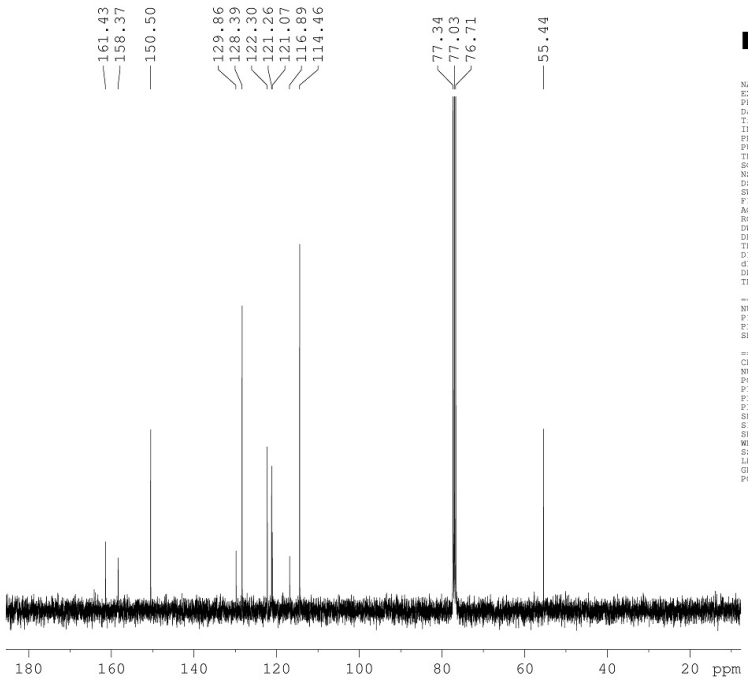


2-(4-methoxyphenyl)isonicotinonitrile (5e-C2)




```
NAME        2012-04-20 wangjian-1416-C2
EXPNO                  1
PROCNO                 1
Date_           20120419
Time               23.47
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   406
DW                60.800 usec
DE                 6.50 usec
TE                294.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300090 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

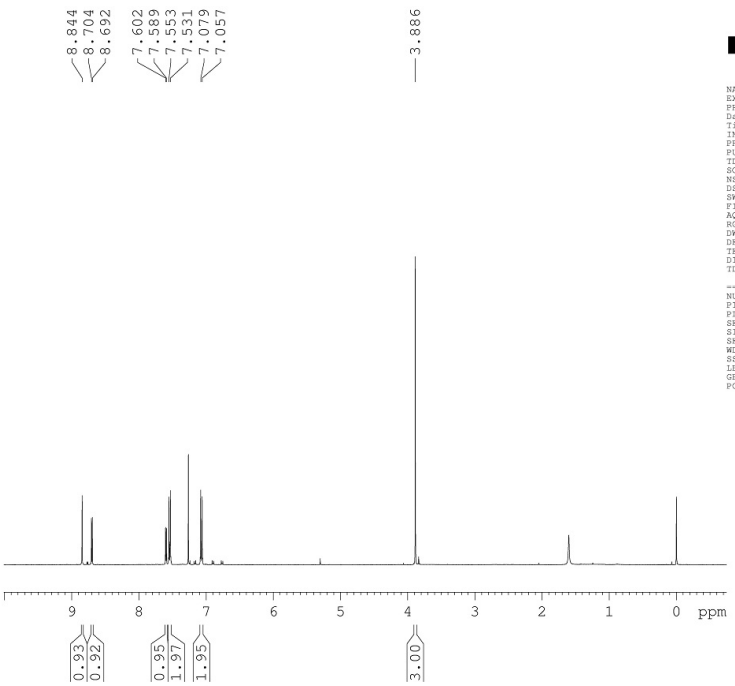



```
NAME        2012-04-20 wangjian-1416-C2
EXPNO                  2
PROCNO                 1
Date_           20120420
Time               0.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

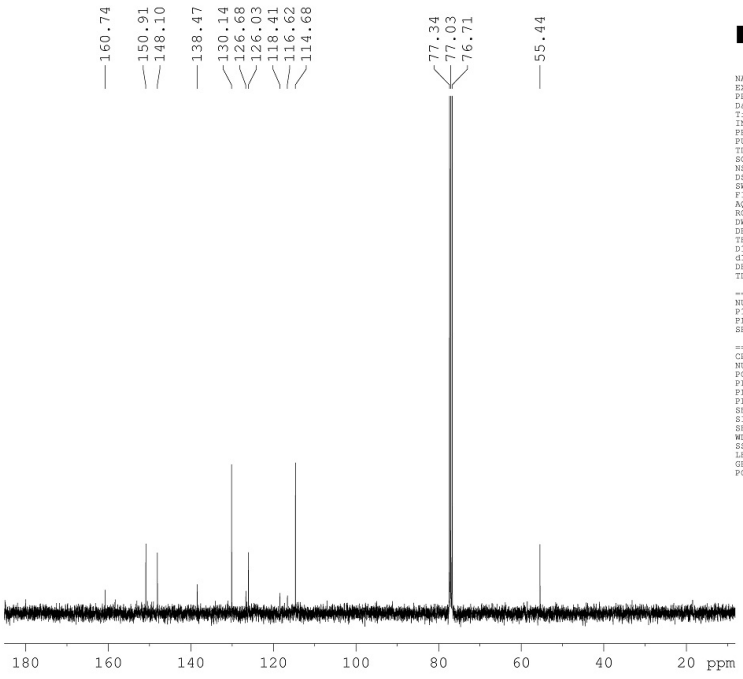
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

3-(4-methoxyphenyl)isonicotinonitrile (5e-C3)




```
NAME          2012-04-20 wangjian-1416-C3
EXPNO                    1
PROCNO                   1
Date_             20120420
Time                  0.08
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     406
DW                  60.800 usec
DE                   6.50 usec
TE                  294.9 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.30 usec
PL1                 -2.00 dB
SFO1          400.1324710 MHz
SI                   32768
SF            400.1300088 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

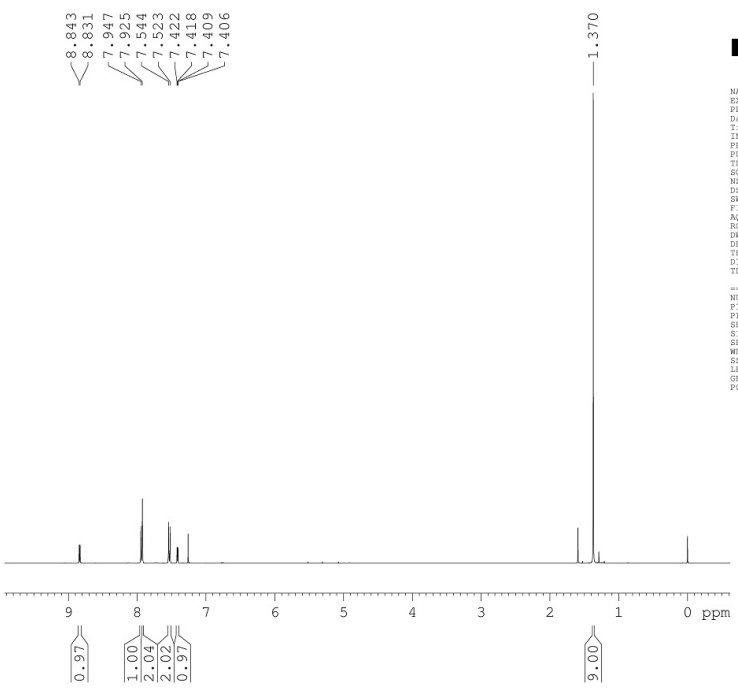



```
NAME          2012-04-20 wangjian-1416-C3
EXPNO                    2
PROCNO                   1
Date_             20120420
Time                  0.25
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  295.8 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  19.40 usec
PL1                 -1.00 dB
SFO1          100.6228298 MHz

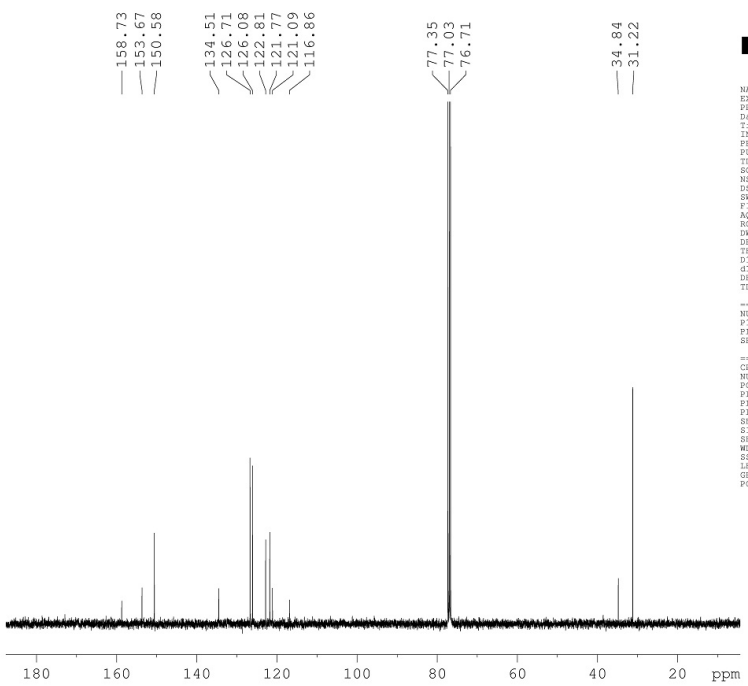
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2               60.00 usec
PL12                11.09 dB
PL13                13.05 dB
PL2                 -2.00 dB
SFO2          400.1316005 MHz
SI                   32768
SF            100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

2-(4-*tert*-butylphenyl)isonicotinonitrile (5f-C2)




```
NAME        2012-04-27 wangjian-1395-C2
EXPNO                1
PROCNO               1
Date_         20120428
Time              0.55
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                 287
DW               60.800 usec
DE                6.50 usec
TE               295.1 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               13.30 usec
PL1              -2.00 dB
SFO1        400.1324710 MHz
SI                32768
SF          400.1300096 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

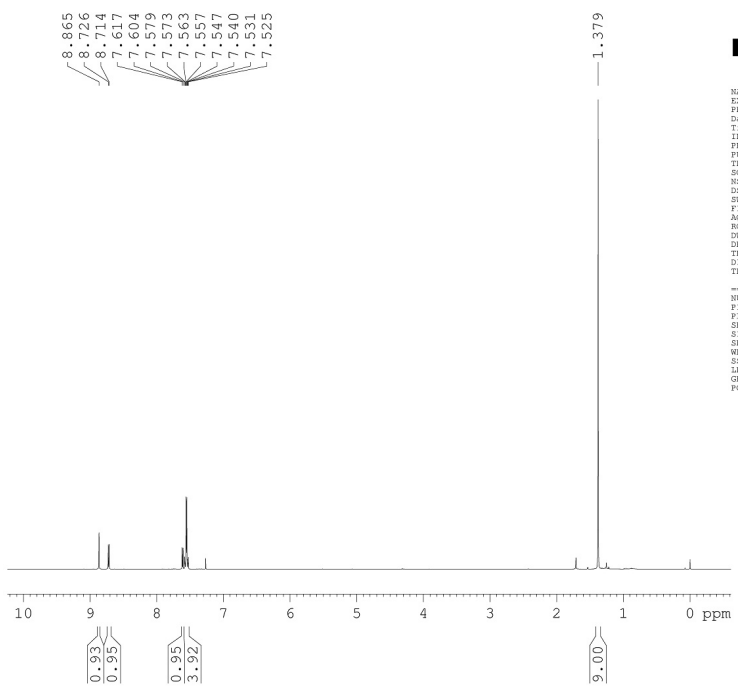


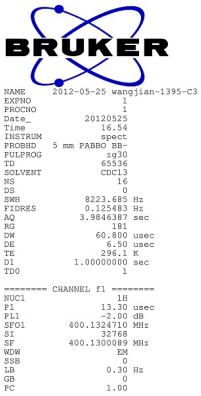

```
NAME        2012-04-27 wangjian-1395-C2
EXPNO                2
PROCNO               1
Date_         20120428
Time              1.11
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG        zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                1030
DW               20.800 usec
DE                6.50 usec
TE               296.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  1

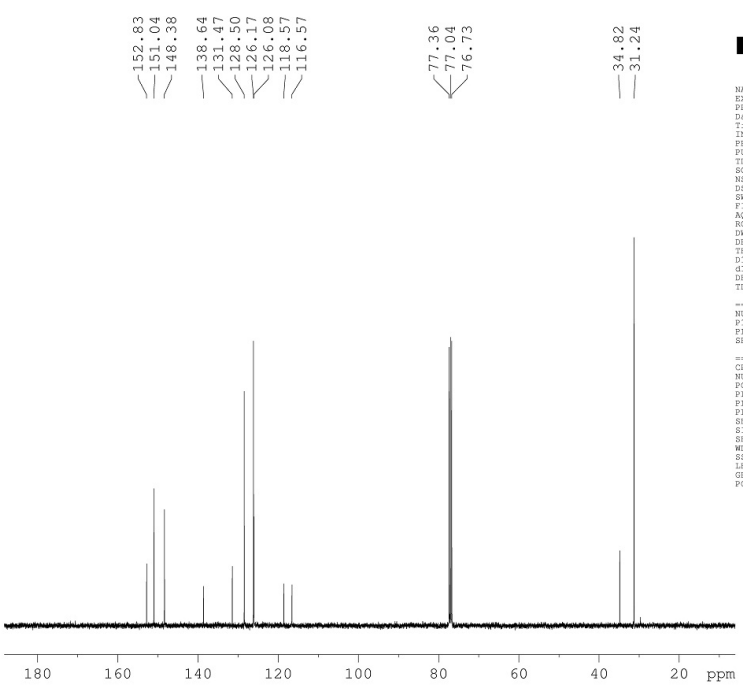
======== CHANNEL f1 ========
NUC1                13C
P1               19.40 usec
PL1              -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            60.00 usec
PL12             11.09 dB
PL13             13.05 dB
PL2              -2.00 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

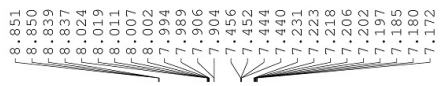
3-(4-*tert*-butylphenyl)isonicotinonitrile (5f-C3)





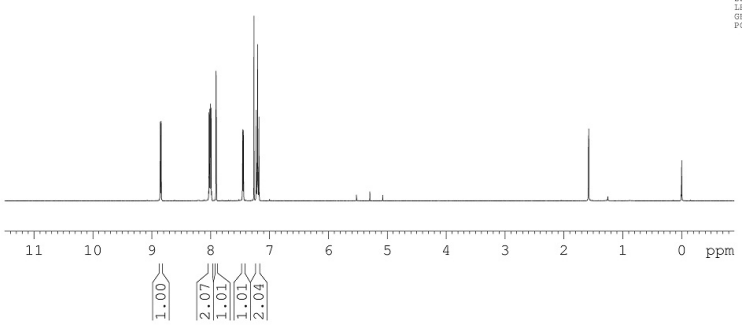


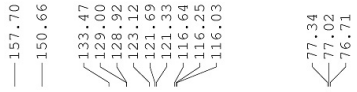
2-(4-fluorophenyl)isonicotinonitrile (5g-C2)



```
NAME          2012-04-27 wangjian-1379-C2
EXPNO                    1
PROCNO                   1
Date_             20120428
Time                 1.16
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    406
DW                60.800 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1         400.1324710 MHz
SI                  32768
SF           400.1300087 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

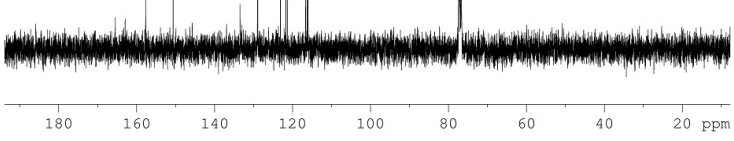




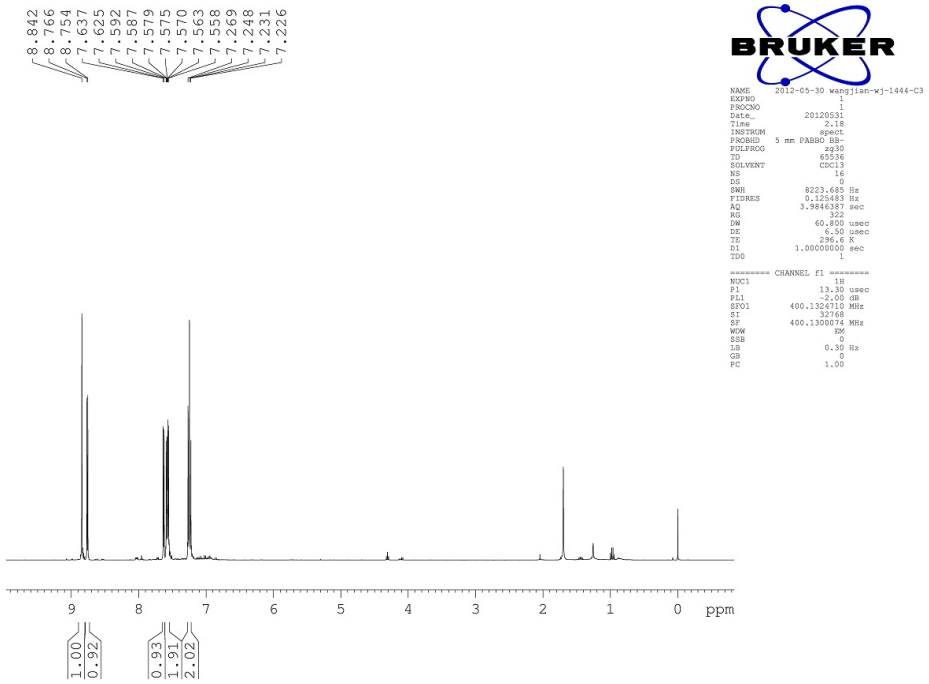
```
NAME          2012-04-27 wangjian-1379-C2
EXPNO                    2
PROCNO                   1
Date_             20120428
Time                 1.34
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    812
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

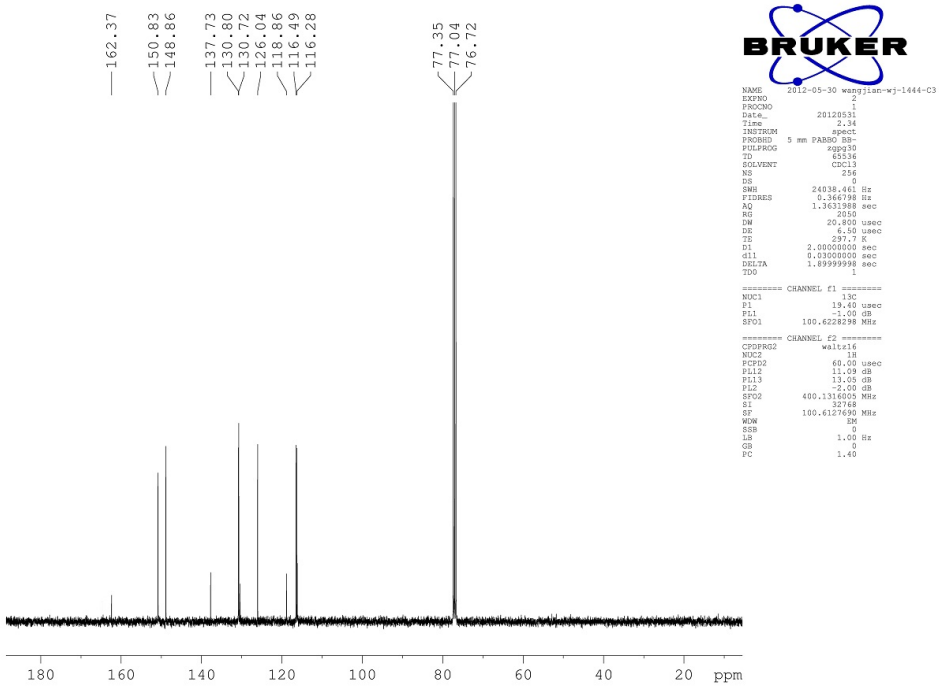
======== CHANNEL f1 ========
NUC1                   13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2         400.1316005 MHz
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 1.40
```

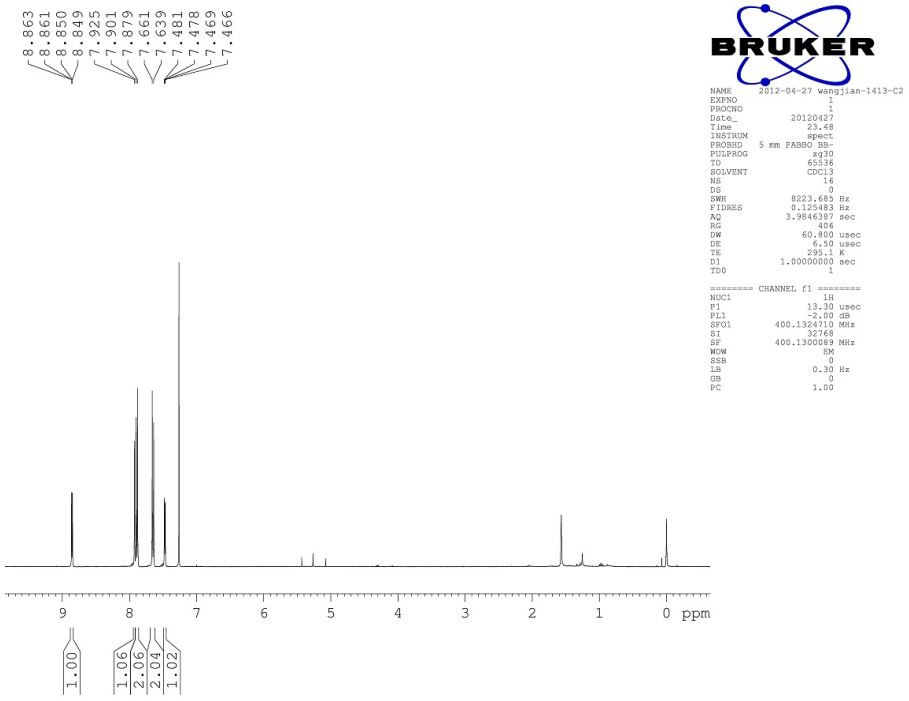


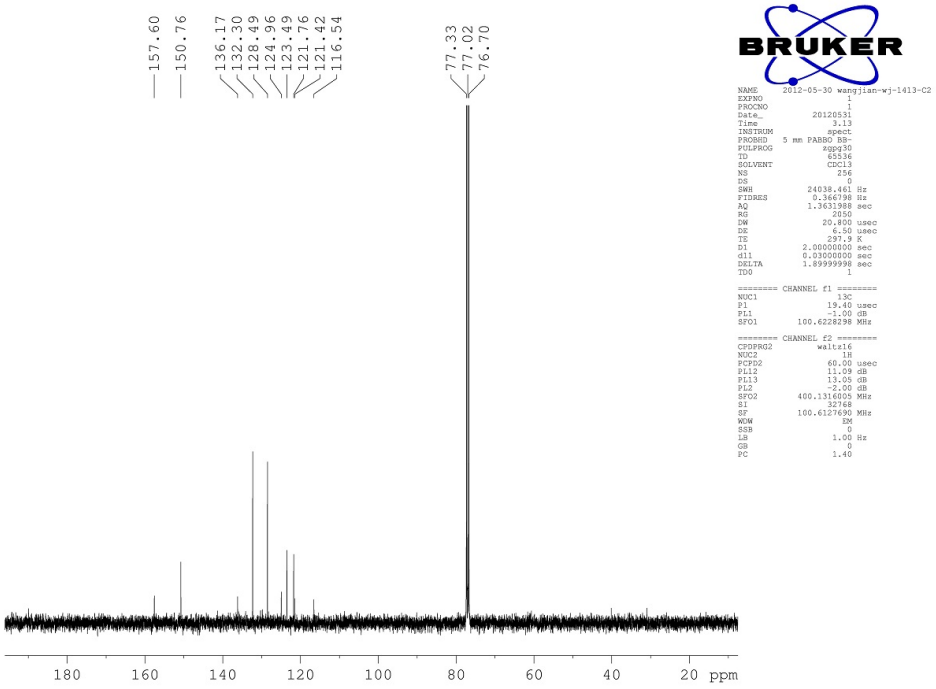
3-(4-fluorophenyl)isonicotinonitrile (5g-C3)



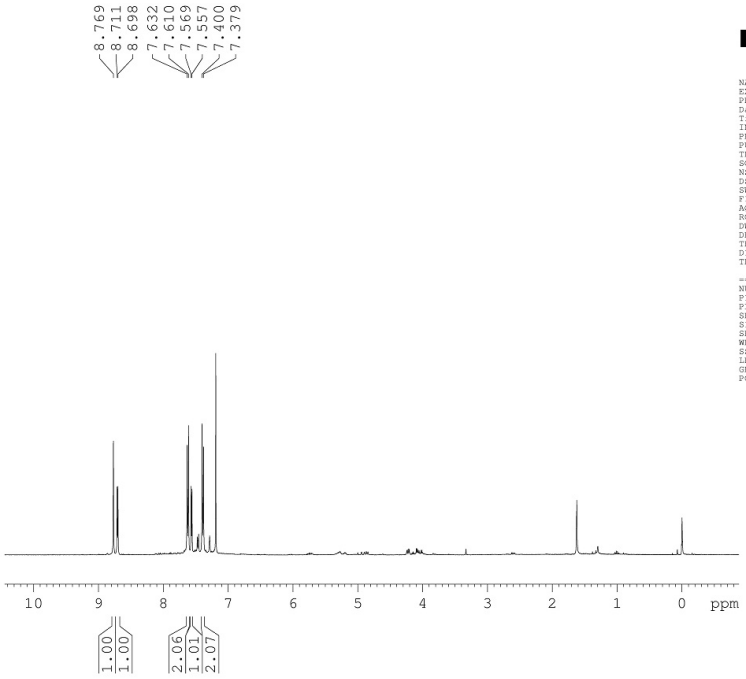


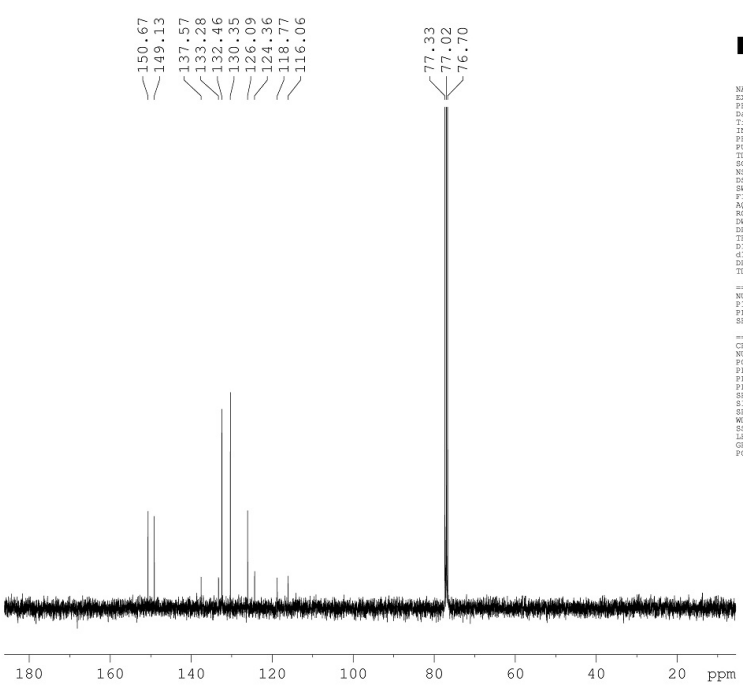
2-(4-bromophenyl)isonicotinonitrile (5h-C2)



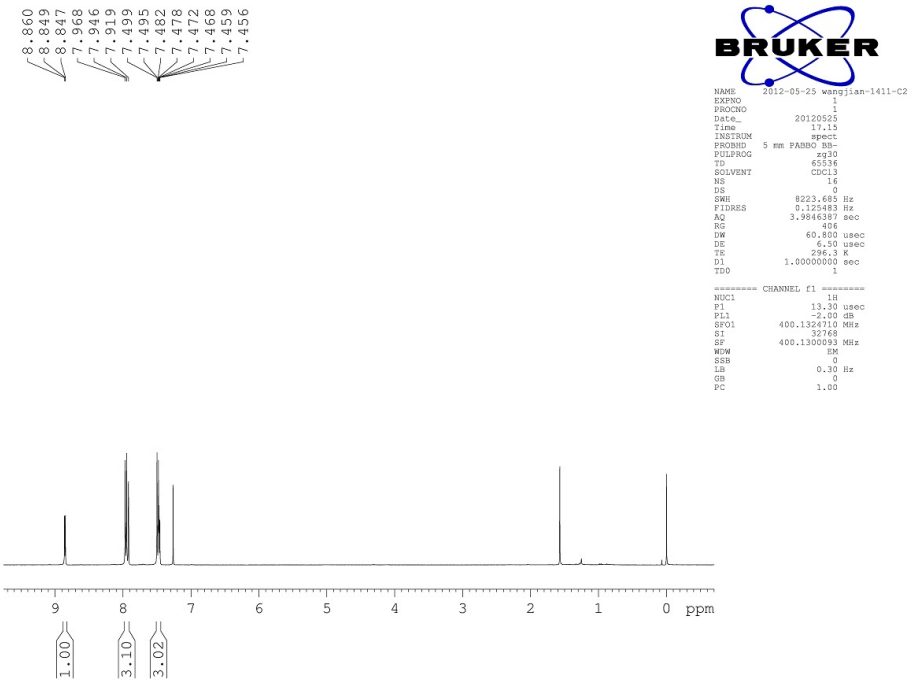


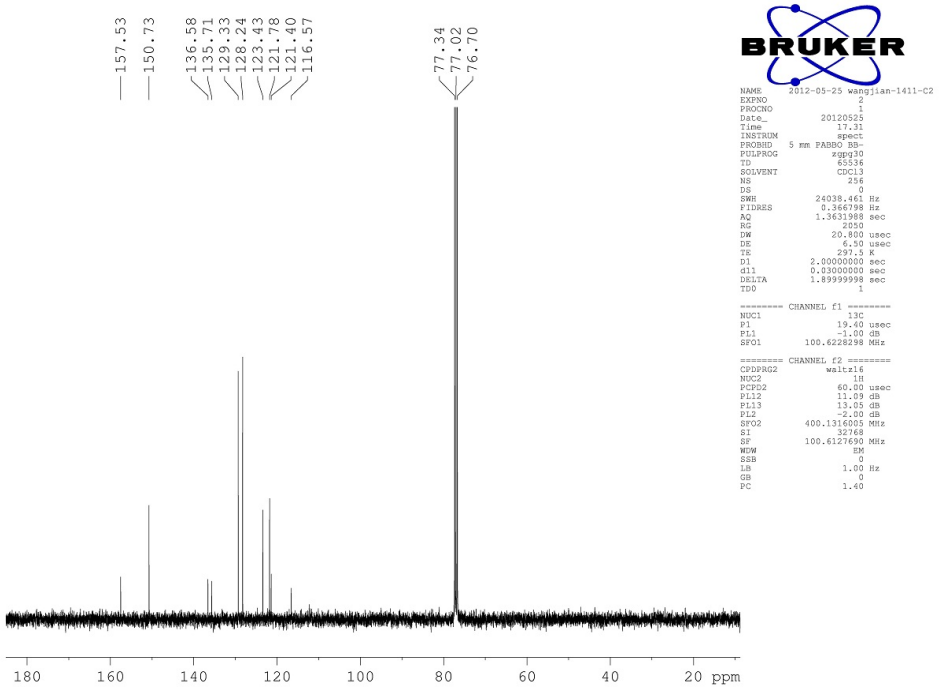
3-(4-bromophenyl)isonicotinonitrile (5h-C3)



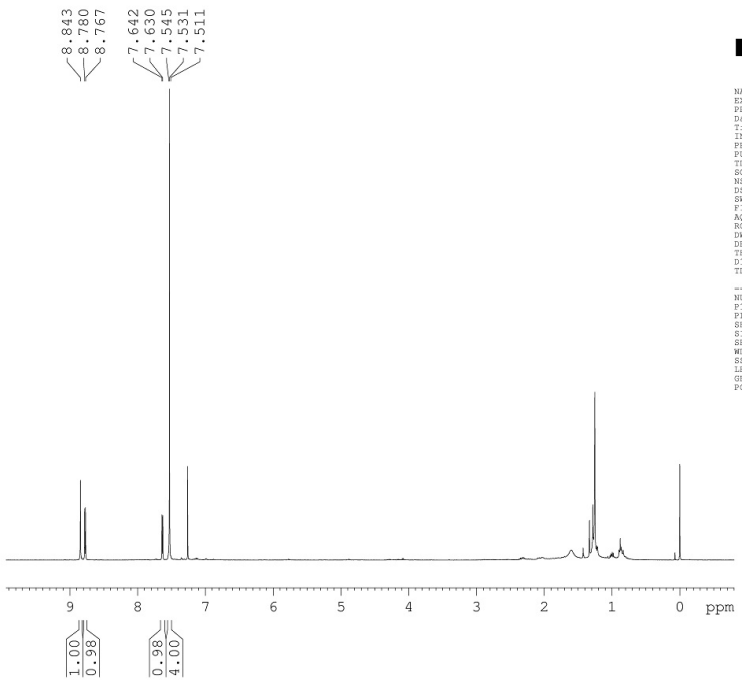


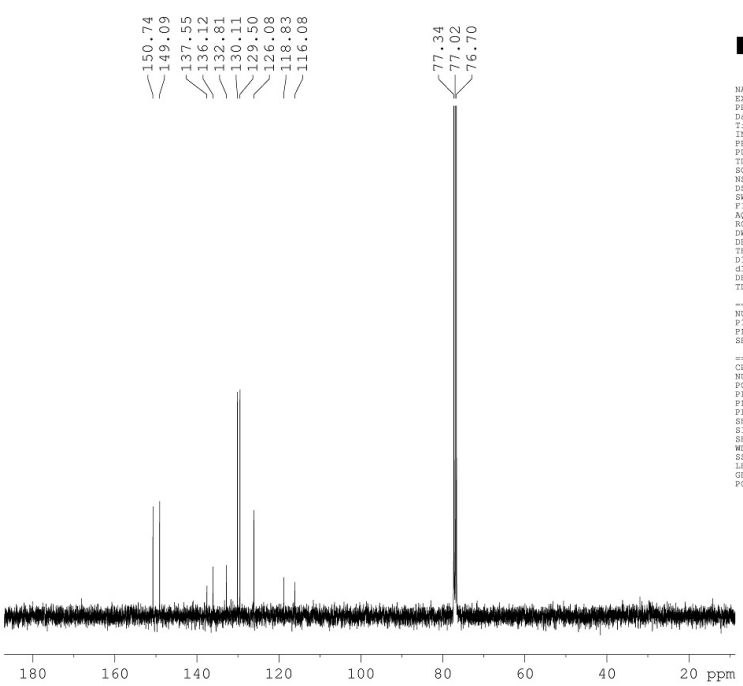
2-(4-chlorophenyl)isonicotinonitrile (5i-C2)

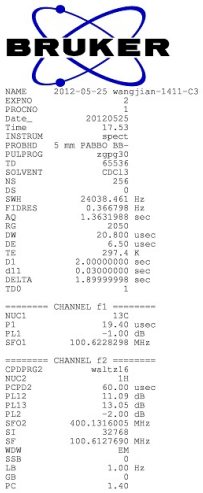




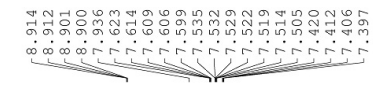
3-(4-chlorophenyl)isonicotinonitrile (5i-C3)

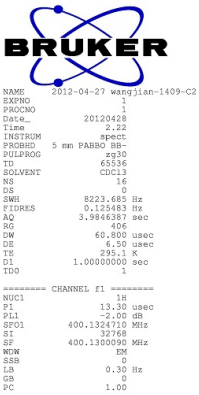


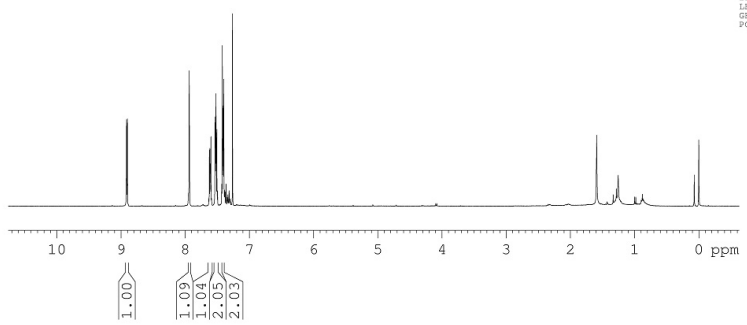


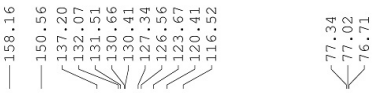


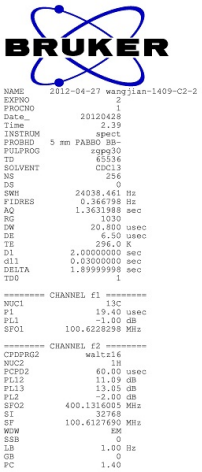
2-(2-chlorophenyl)isonicotinonitrile (5j-C2)

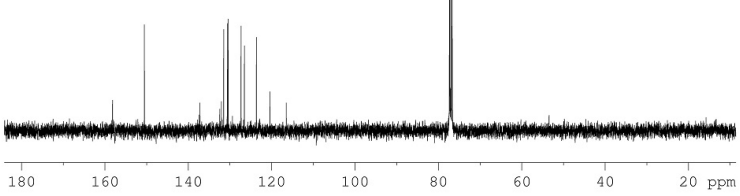




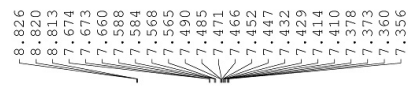


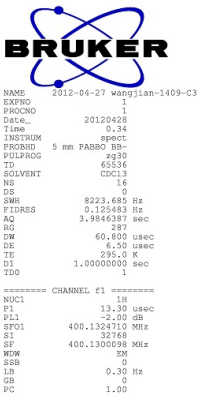


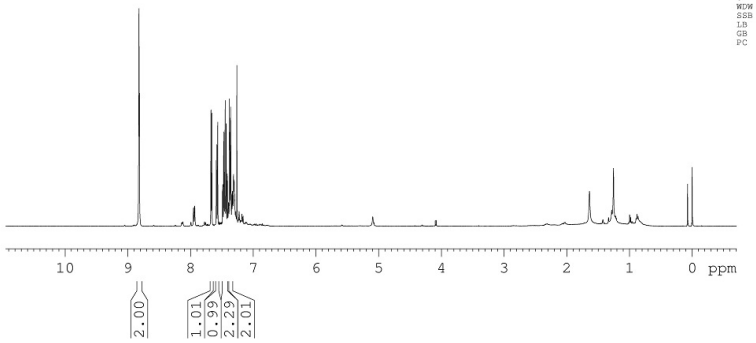


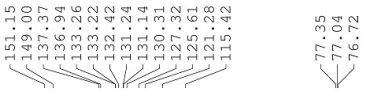


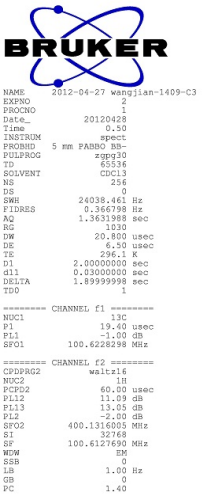
3-(2-chlorophenyl)isonicotinonitrile (5j-C3)

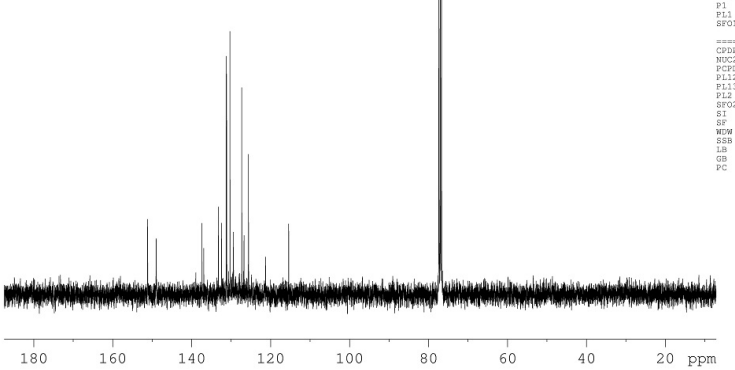




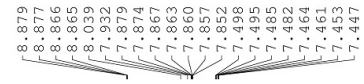






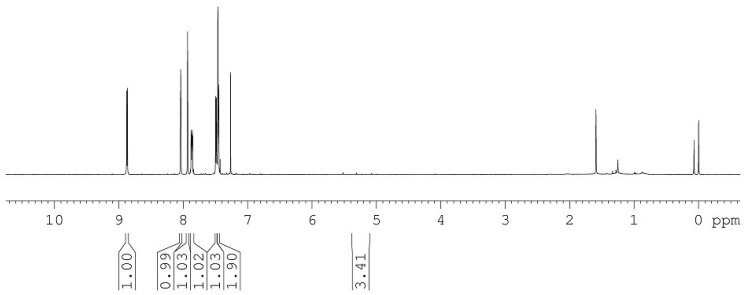


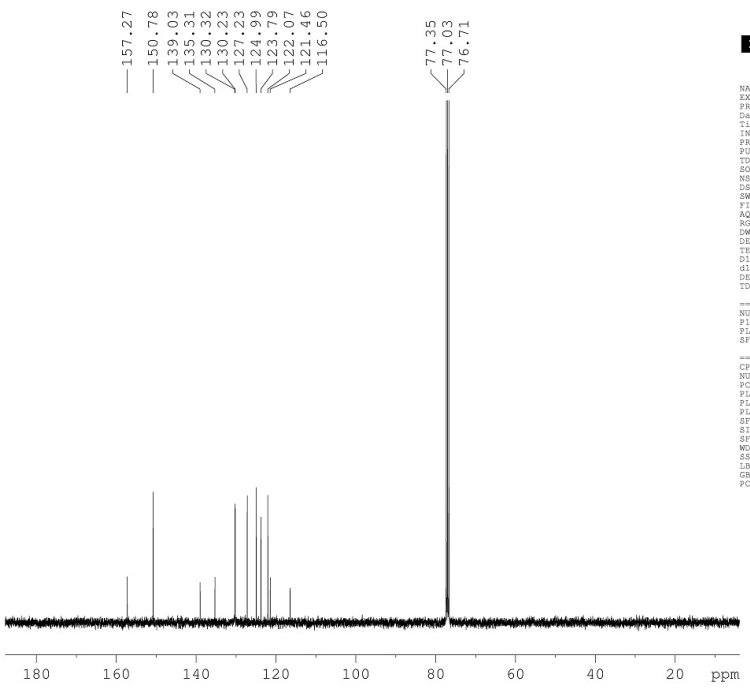
2-(3-chlorophenyl)isonicotinonitrile (5k-C2)




```
NAME            2012-04-27 wangjian-1410-C2
EXPNO                    1
PROCNO                   1
Date_             20120427
Time                 22.42
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    322
DW                 60.800 usec
DE                  6.50 usec
TE                 294.6 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.30 usec
PL1                 -2.00 dB
SFO1          400.1324710 MHz
SI                  32768
SF            400.1300086 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



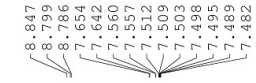


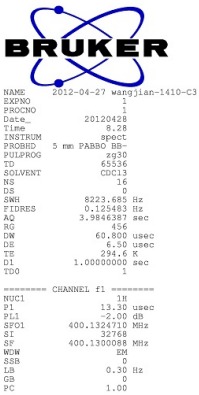

```
NAME            2012-04-27 wangjian-1410-C2
EXPNO                    2
PROCNO                   1
Date_             20120427
Time                 22.59
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                   1030
DW                 20.800 usec
DE                  6.50 usec
TE                 296.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

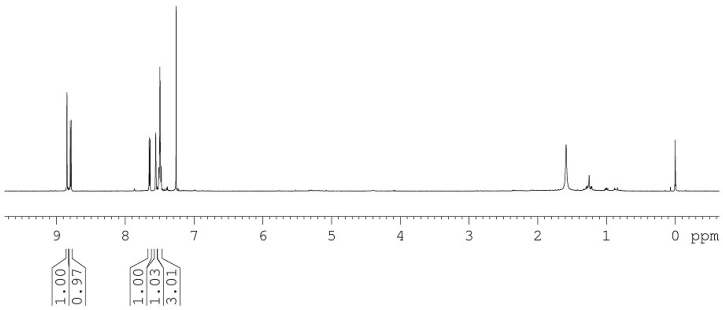
======== CHANNEL f1 ========
NUC1                   13C
P1                  19.40 usec
PL1                 -1.00 dB
SFO1          100.6228298 MHz

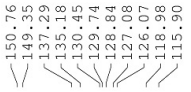
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2               60.00 usec
PL12                11.09 dB
PL13                13.05 dB
PL2                 -2.00 dB
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

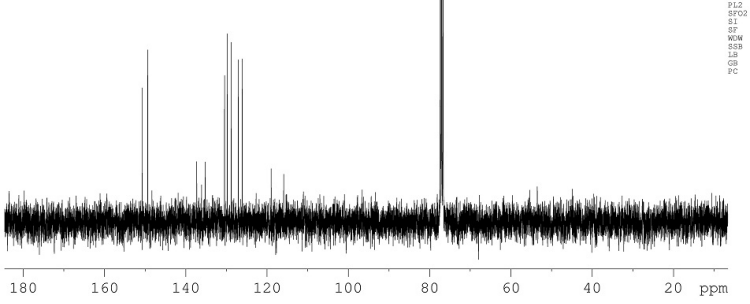
3-(3-chlorophenyl)isonicotinonitrile (5k-C3)



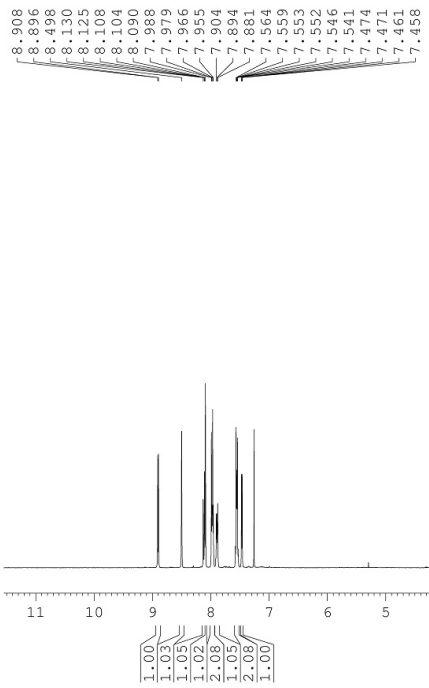


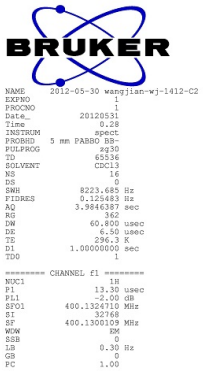


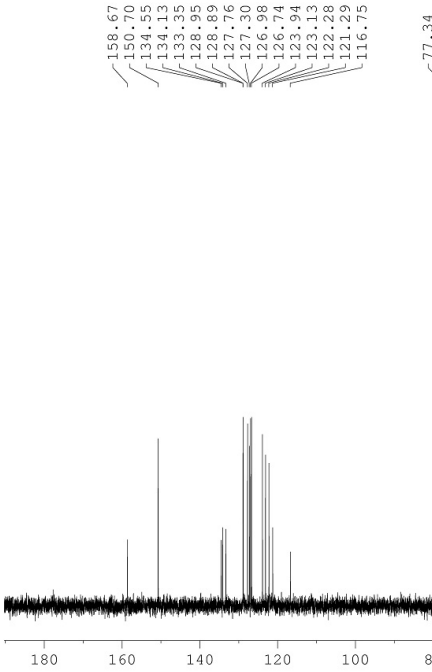




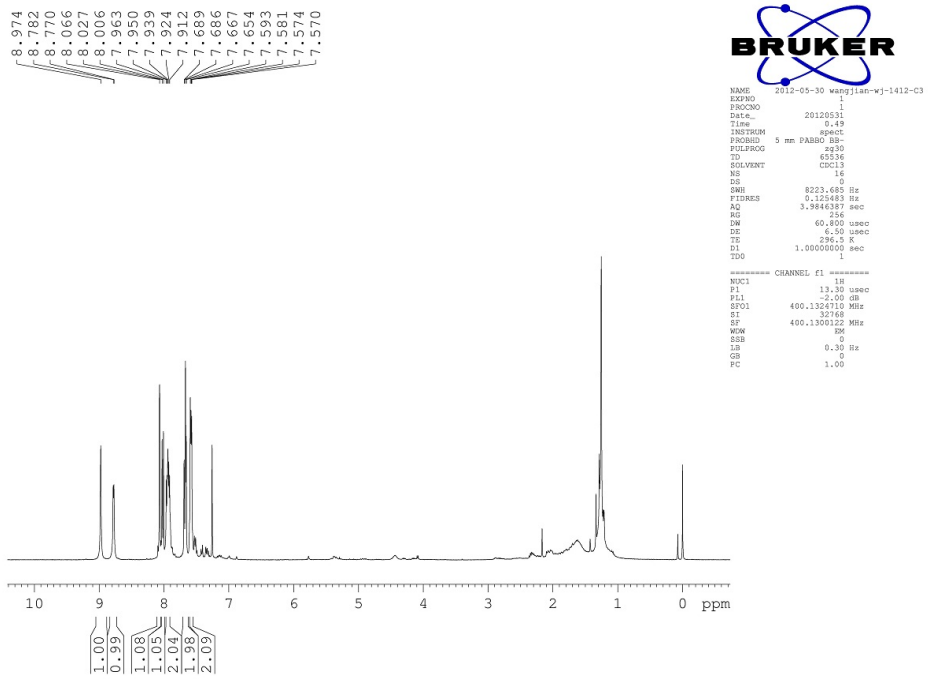
2-(naphthalen-2-yl)isonicotinonitrile (5l-C2)

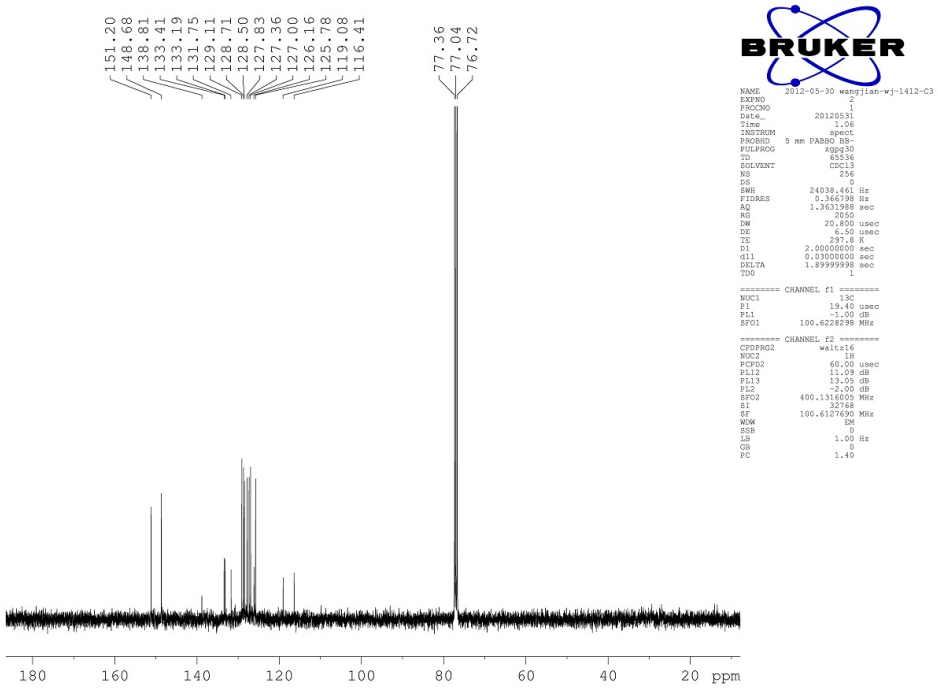




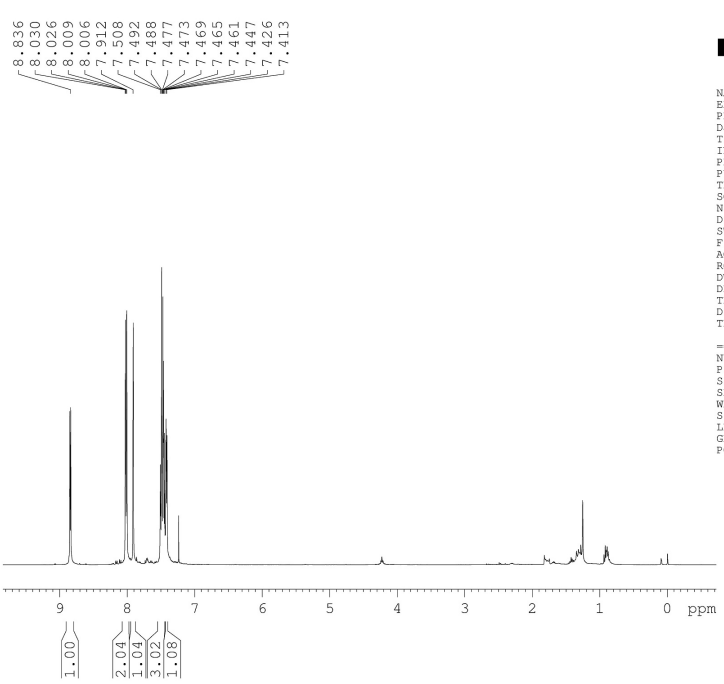


3-(naphthalen-2-yl)isonicotinonitrile (5l-C3)



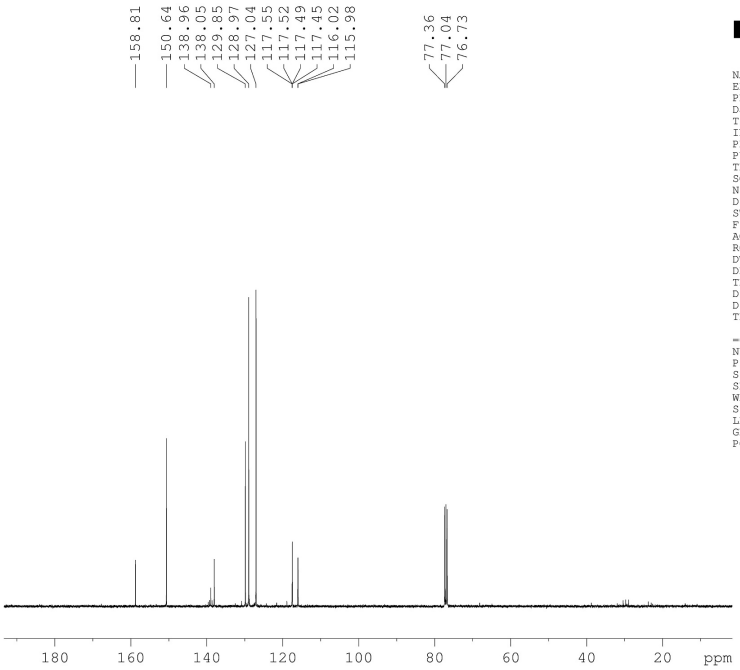


4-trifluoromethyl -2-phenylpyridine (5m)




```
NAME          yxq-20120905-1663
EXPNO                        7
PROCNO                       1
Date_                 20120905
Time                     23.58
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                       32.31
DW                      60.800 usec
DE                       6.50 usec
TE                      300.1 K
D1                 1.00000000 sec
TD0                          1

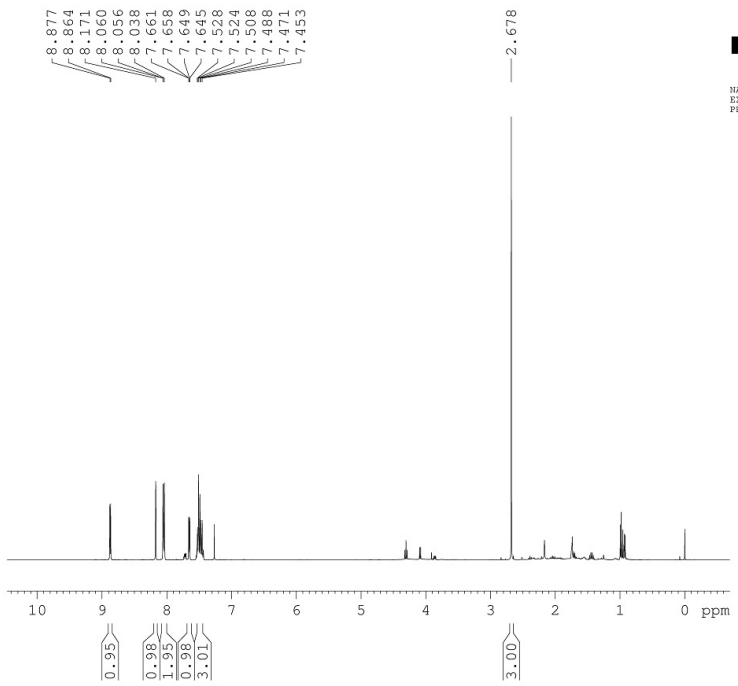
======== CHANNEL f1 ========
NUC1                        1H
P1                        9.93 usec
SI                       65536
SF                 400.1300181 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

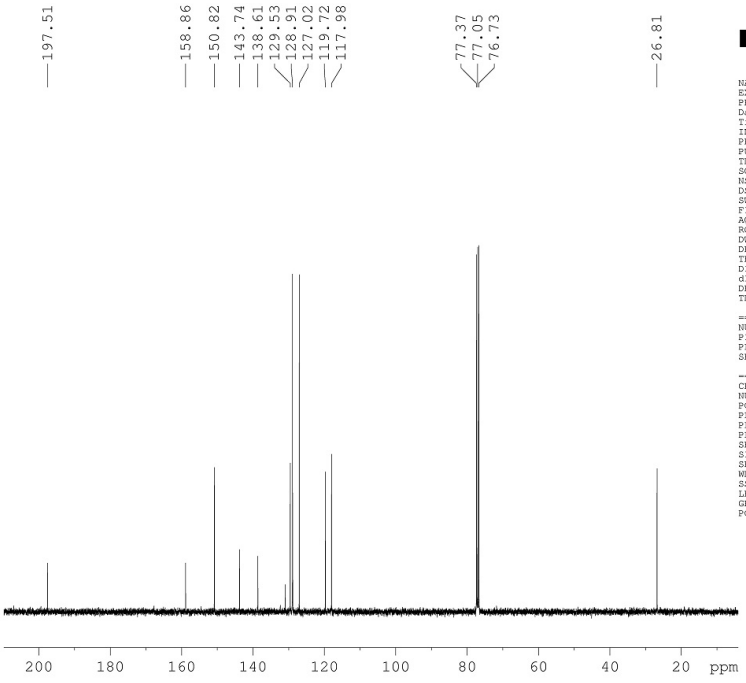



```
NAME          yxq-20120905-1663
EXPNO                        8
PROCNO                       1
Date_                 20120906
Time                      0.13
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        256
DS                          0
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                      181.24
DW                      20.800 usec
DE                       6.50 usec
TE                      300.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.63 usec
SI                       32768
SF                 100.6127690 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

4-Acetyl -2-phenylpyridine (5o-C2)



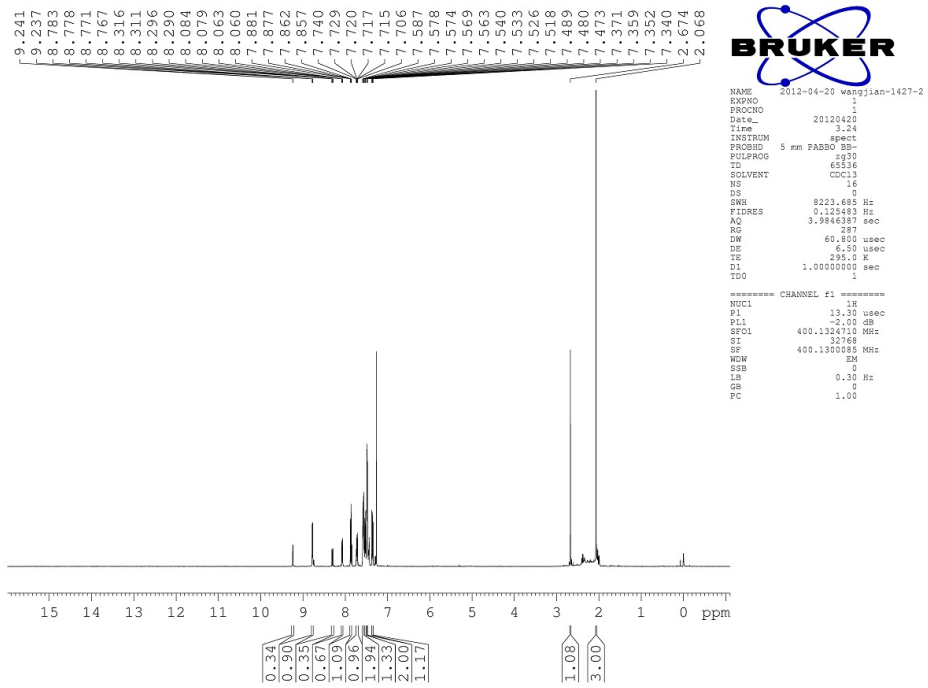


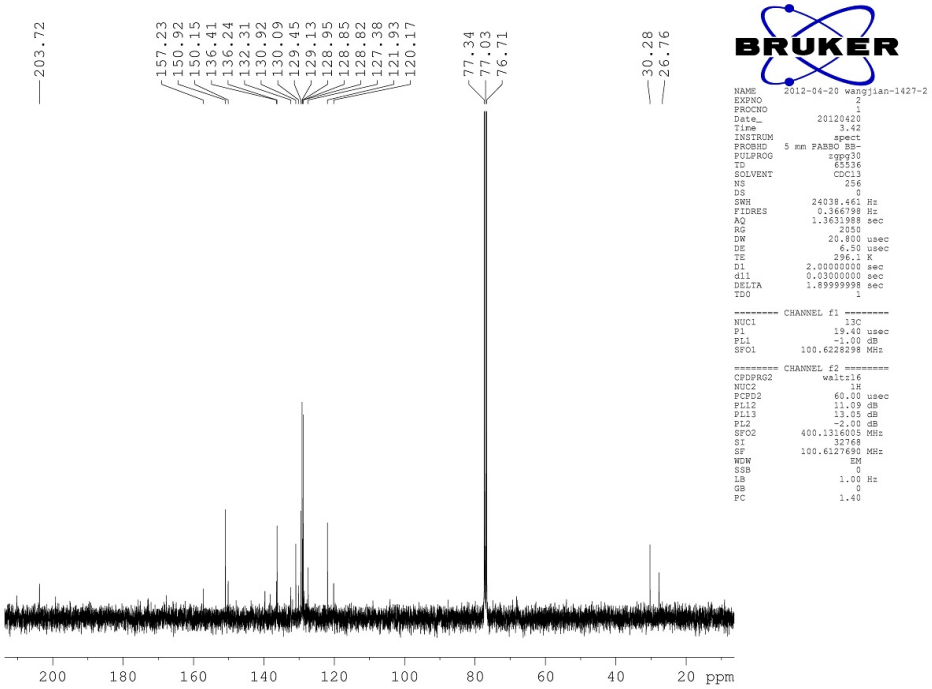

```
EXPNO                  2
PROCNO                 1
Date_           20120412
Time               11.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    0
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               296.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

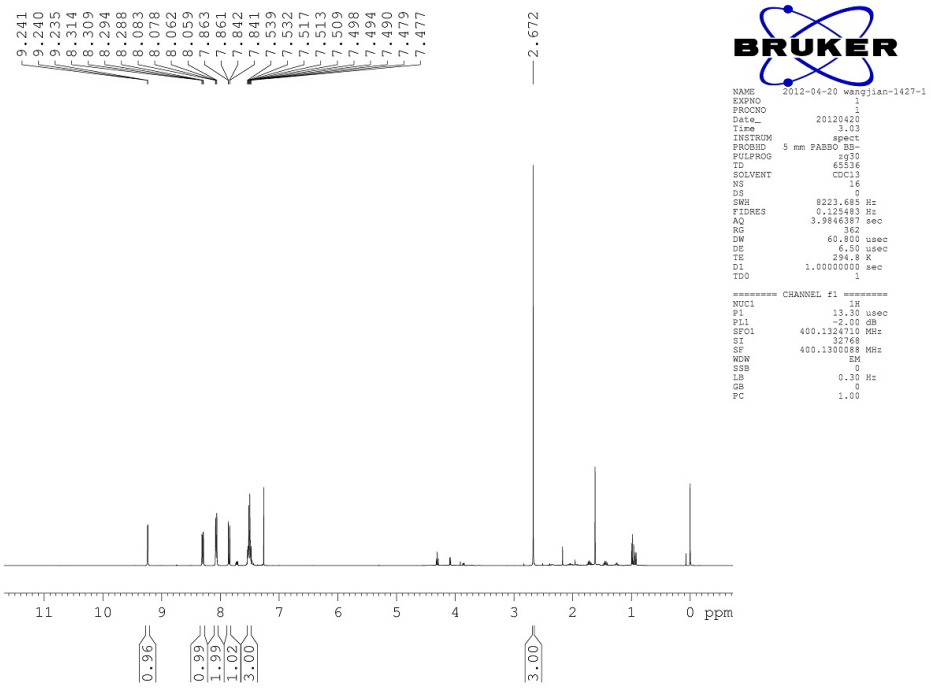
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

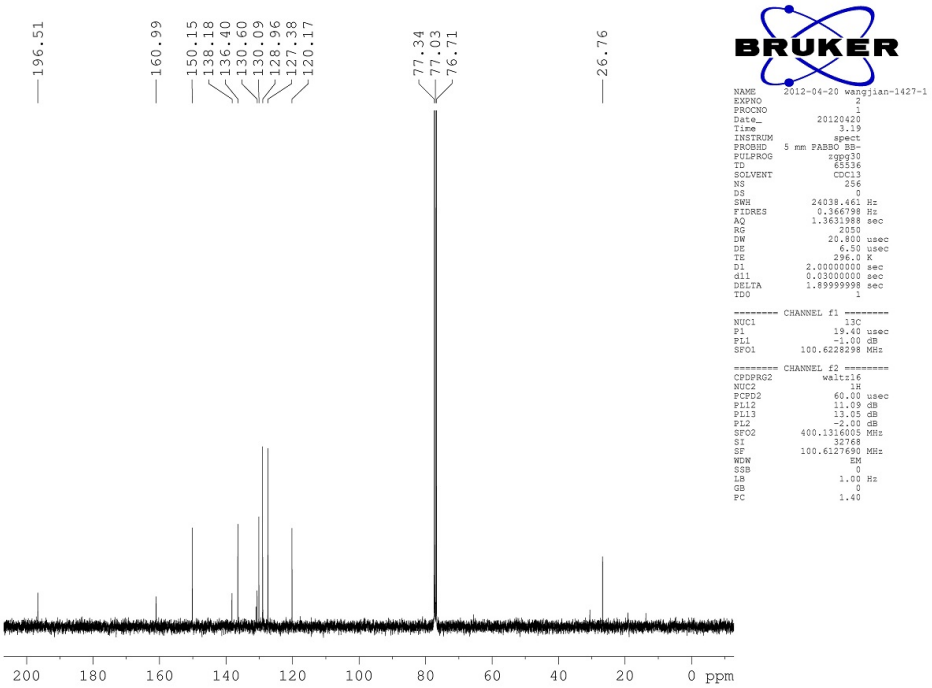
3-Acetyl -2-phenylpyridine (5p-C2) and 3-Acetyl-6-phenylpyridine (5p-C6)



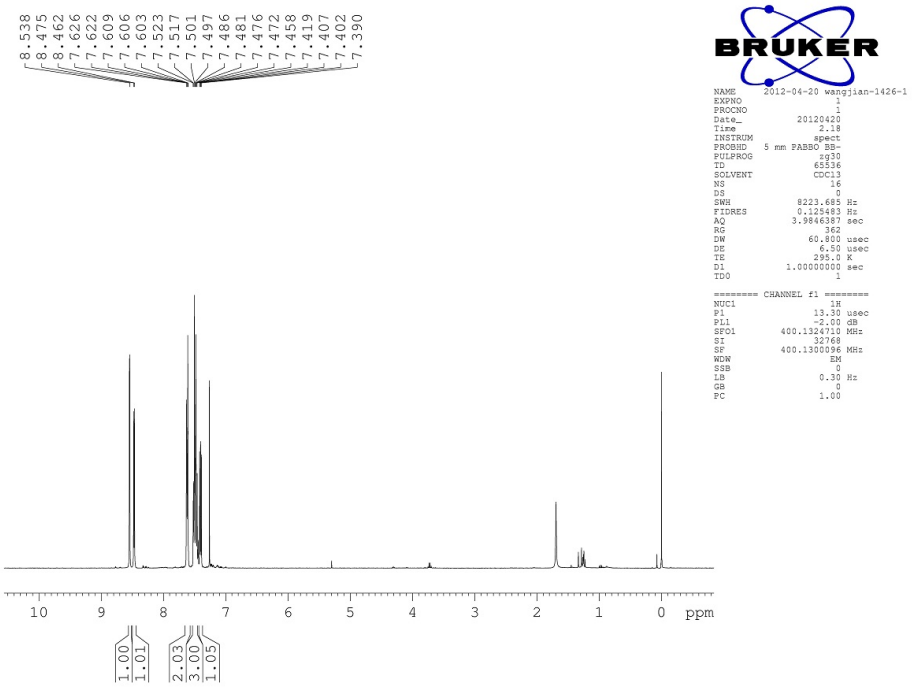


3-Acetyl-6-phenylpyridine (5p-C6)



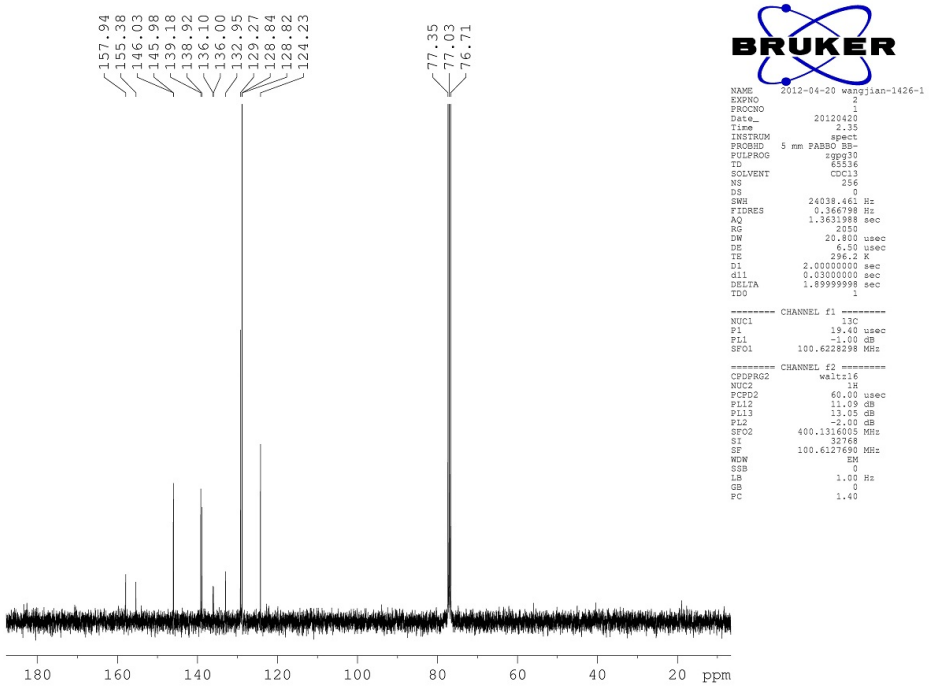


3-fluoro -2-phenylpyridine (5q-C2)




```
NAME        2012-04-20 wangjian-1426-1
EXPNO                1
PROCNO               1
Date_         20120420
Time              2.18
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                 362
DW              60.800 usec
DE               6.50 usec
TE              295.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               13.30 usec
PL1              -2.00 dB
SFO1        400.1324710 MHz
SI                32768
SF          400.1300096 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

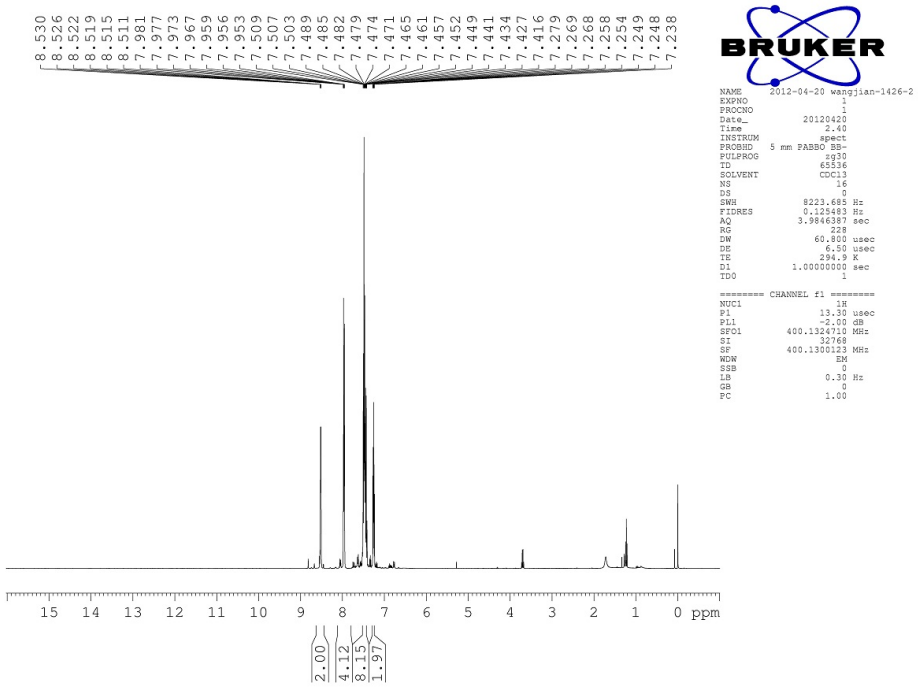


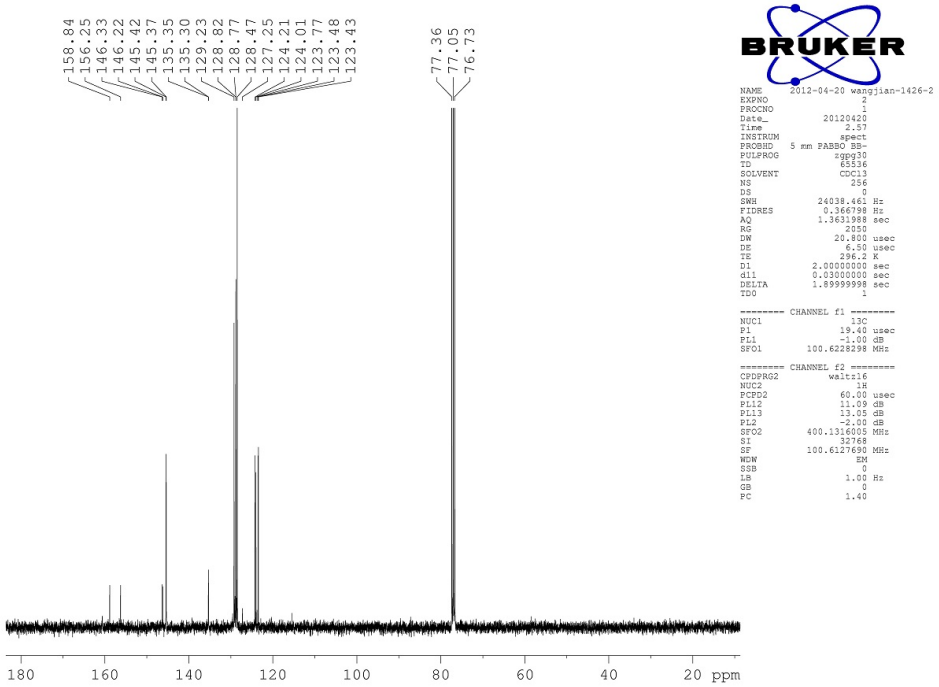

```
NAME        2012-04-20 wangjian-1426-1
EXPNO                2
PROCNO               1
Date_         20120420
Time              2.35
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG        zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                2050
DW              20.800 usec
DE               6.50 usec
TE              296.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               19.40 usec
PL1              -1.00 dB
SFO1        100.6228298 MHz

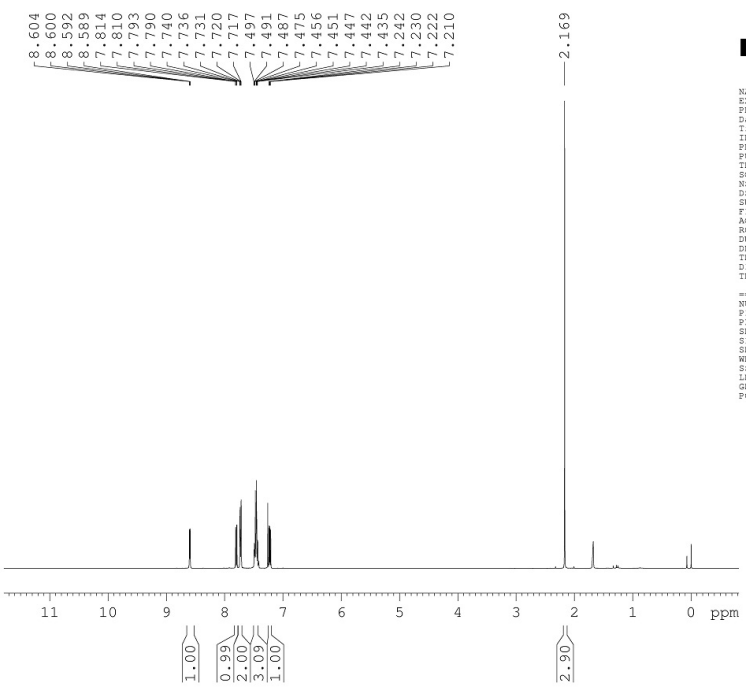
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            60.00 usec
PL12             11.09 dB
PL13             13.05 dB
PL2              -2.00 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

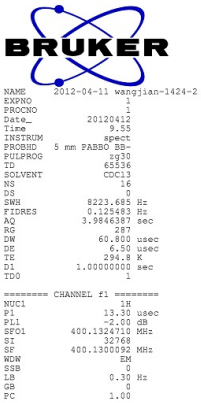
3-fluoro -4-phenylpyridine(5q-C4) and 3-fluoro-6-phenylpyridine (5q-C6)

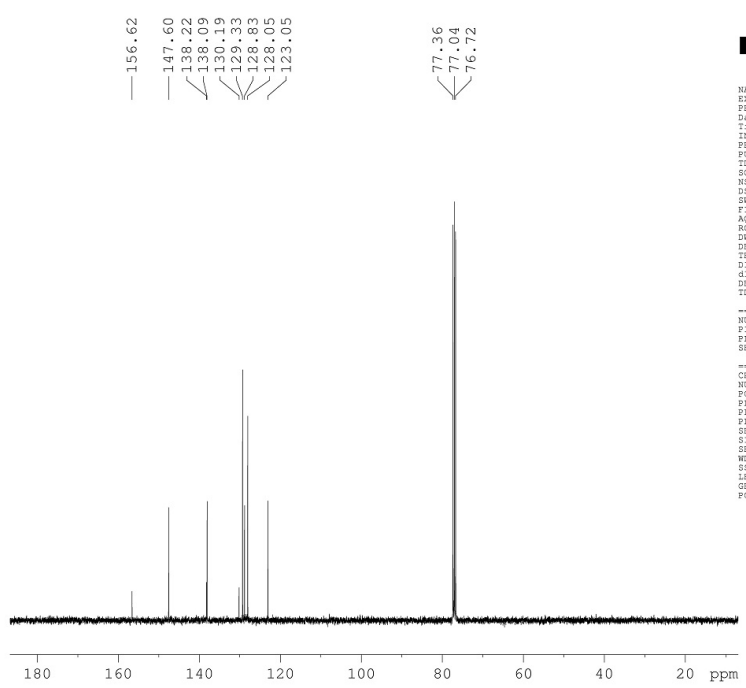


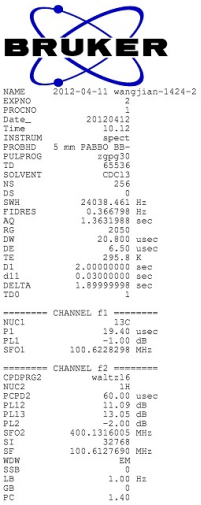


3-chloro -2-phenylpyridine (5r-C2)

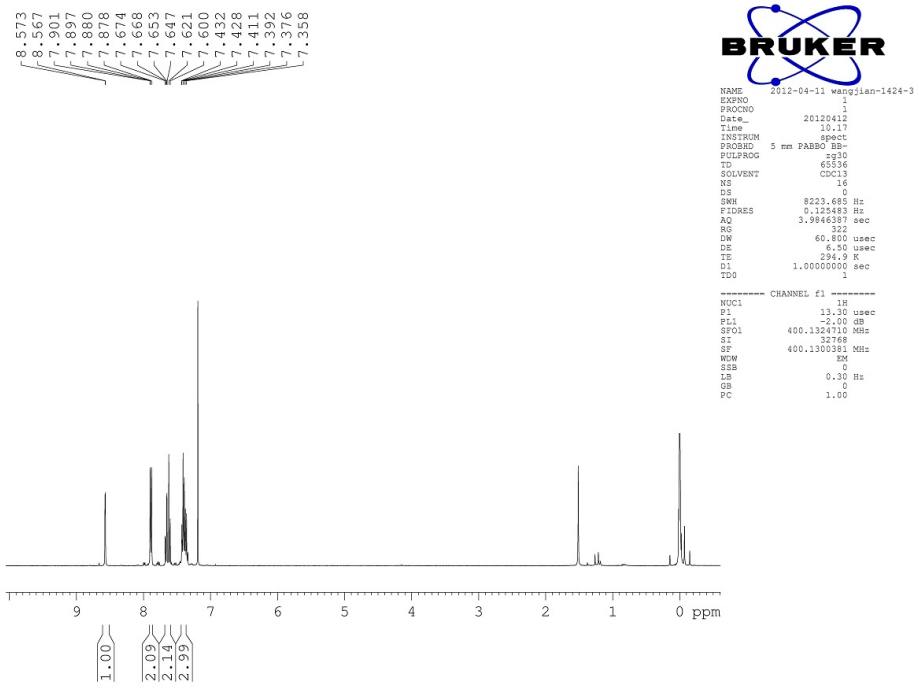






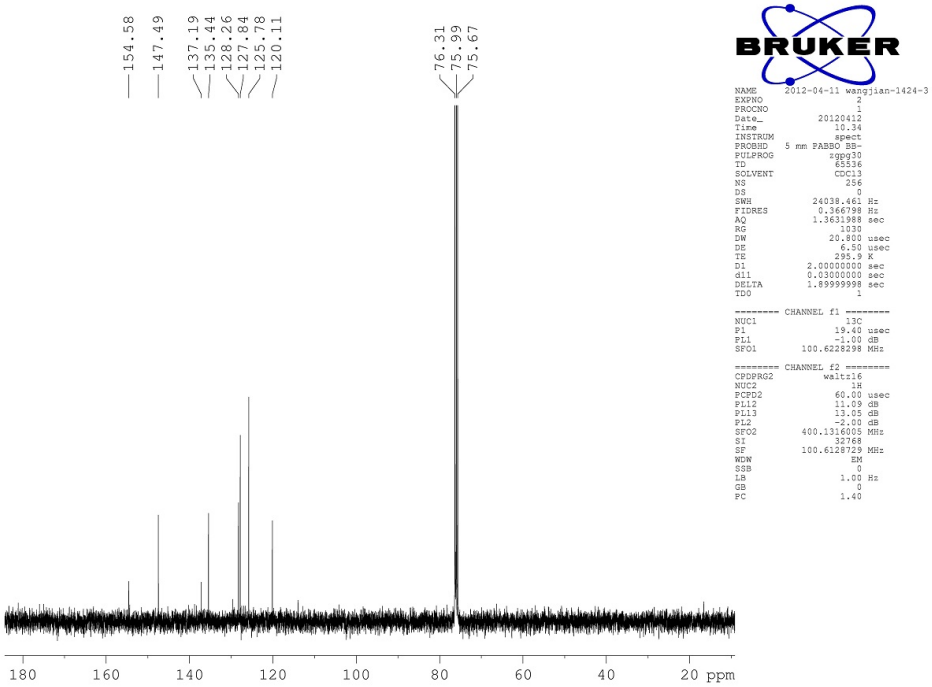


3-chloro-6-phenylpyridine (5r-C6)




```
NAME        2012-04-11 wangjian-1424-3
EXPNO                 1
PROCNO                1
Date_          20120412
Time              10.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  322
DW             60.800 usec
DE              6.50 usec
TE             294.9 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.30 usec
PL1               -2.00 dB
SFO1        400.1324710 MHz
SI                32768
SF          400.1300381 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

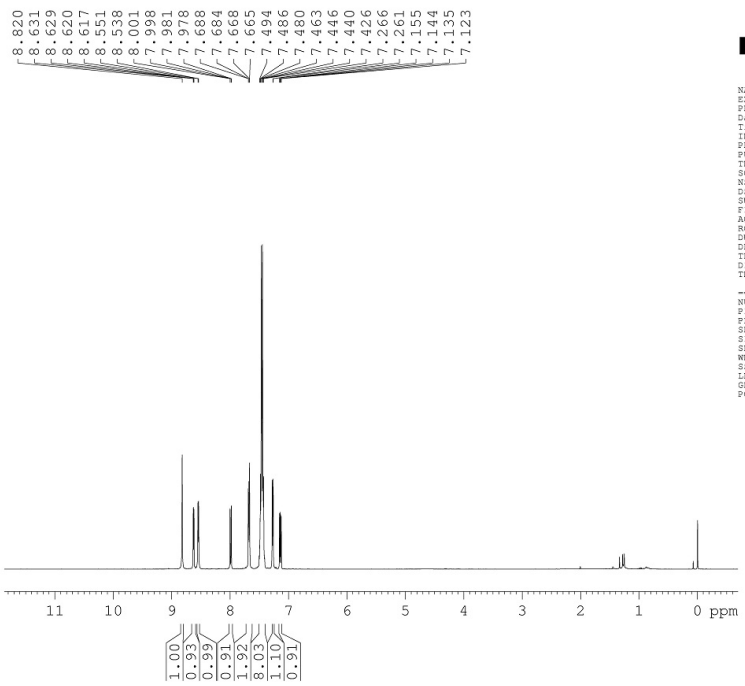



```
NAME        2012-04-11 wangjian-1424-3
EXPNO                 2
PROCNO                1
Date_          20120412
Time              10.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                  256
DS                    0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                 1030
DW             20.800 usec
DE              6.50 usec
TE             295.9 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                19.40 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6128729 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

3-bromo -2-phenylpyridine (5s-C2) and 3-bromo -4-phenylpyridine(5s-C4)



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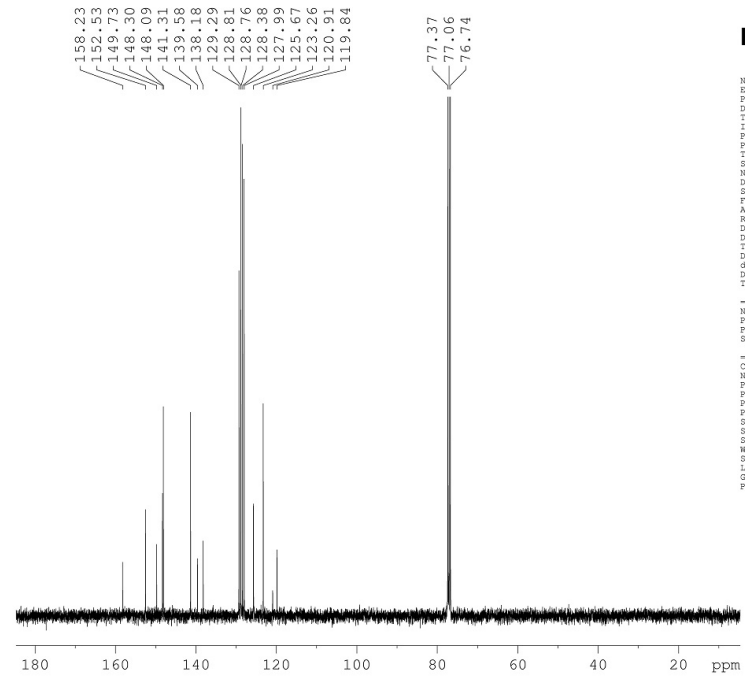
```
NAME          2012-04-11 wangjian-1425-1
EXPNO                  1
PROCNO                 1
Date_           20120412
Time               10.40
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                   228
DW               60.800 usec
DE                6.50 usec
TE                295.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.30 usec
PL1               -2.00 dB
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300098 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



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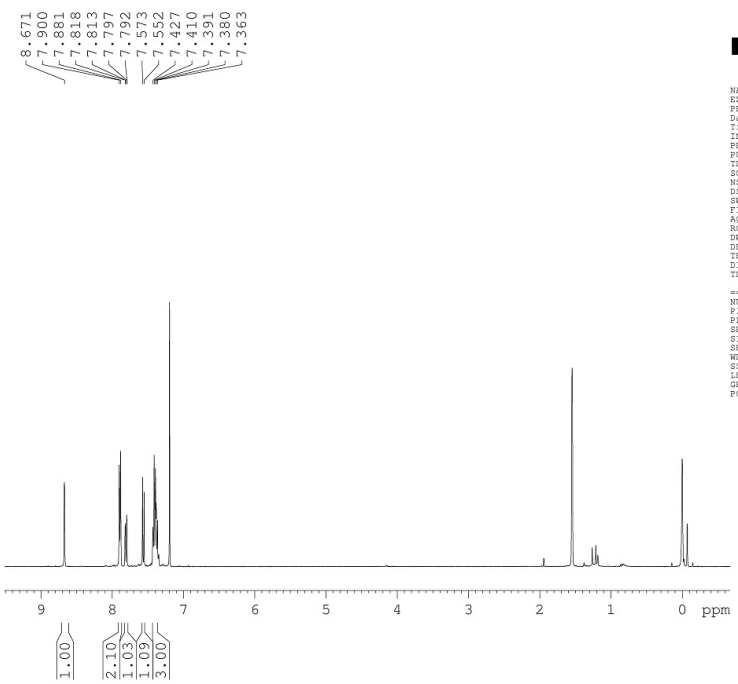
```
NAME          2012-04-11 wangjian-1425-1
EXPNO                  2
PROCNO                 1
Date_           20120412
Time               10.56
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  2050
DW               20.800 usec
DE                6.50 usec
TE                296.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                19.40 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

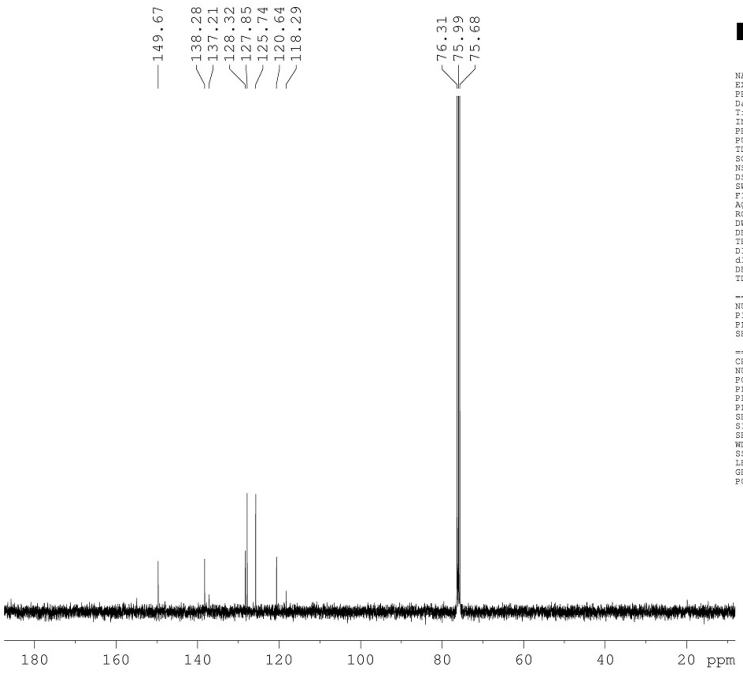
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

3-bromo-6-phenylpyridine (5s-C6)




```
NAME        2012-04-11 wangjian-1425-2
EXPNO                 1
PROCNO                1
Date_          20120412
Time              11.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ             3.9846387 sec
RG                  362
DW                60.800 usec
DE                 6.50 usec
TE                294.8 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300365 MHz
WDW                   EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

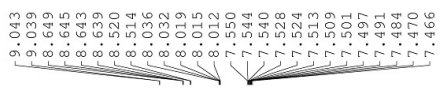



```
NAME        2012-04-11 wangjian-1425-2
EXPNO                 2
PROCNO                1
Date_          20120412
Time              11.18
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                  256
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 2050
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

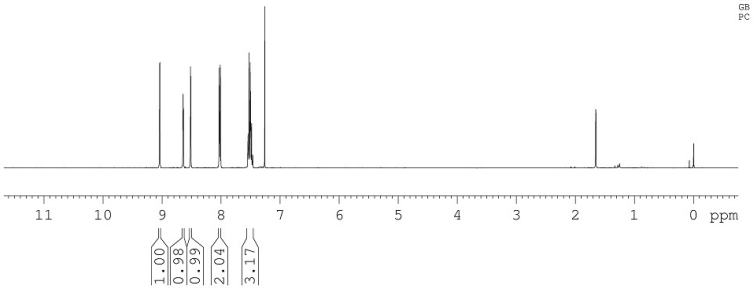
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6128726 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

2-phenylpyrazine (5v)



```
NAME          2012-04-11 wangjian-1430
EXPNO                  1
PROCNO                 1
Date_           20120412
Time               11.44
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   362
DW                60.800 usec
DE                 6.50 usec
TE                294.8 K
D1             1.00000000 sec
TD0                    1

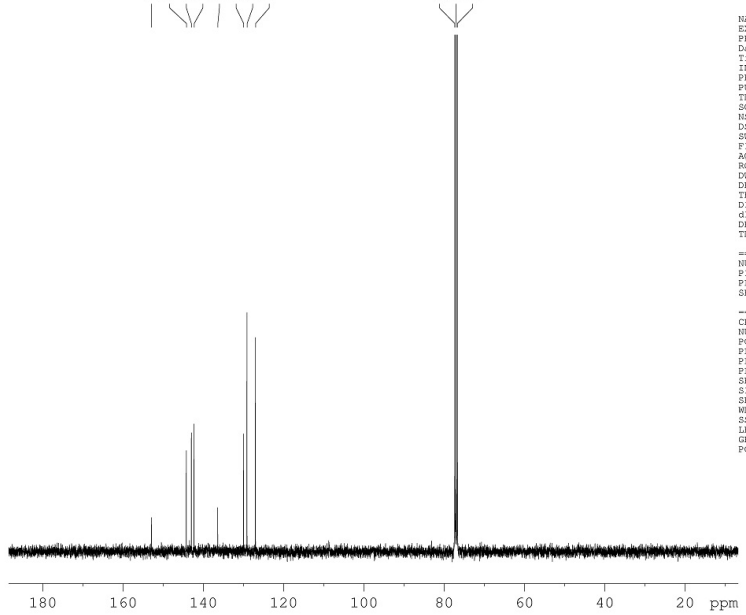
======== CHANNEL f1 ========
NUC1                  1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1          400.1324710 MHz
SI                 32768
SF            400.1300085 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



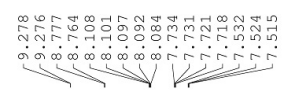
```
NAME          2012-04-11 wangjian-1430
EXPNO                  2
PROCNO                 1
Date_           20120412
Time               12.01
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

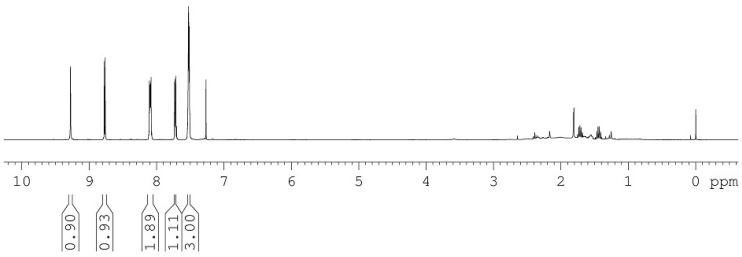


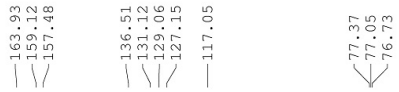
4-phenylpyrimidine (5w-C4)



```
NAME            2012-04-11 wangjian-1431
EXPNO                    1
PROCNO                   1
Date_             20120412
Time                 12.06
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     181
DW                  60.800 usec
DE                   6.50 usec
TE                  295.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.30 usec
PL1                 -2.00 dB
SFO1          400.1324710 MHz
SI                   32768
SF            400.1300067 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

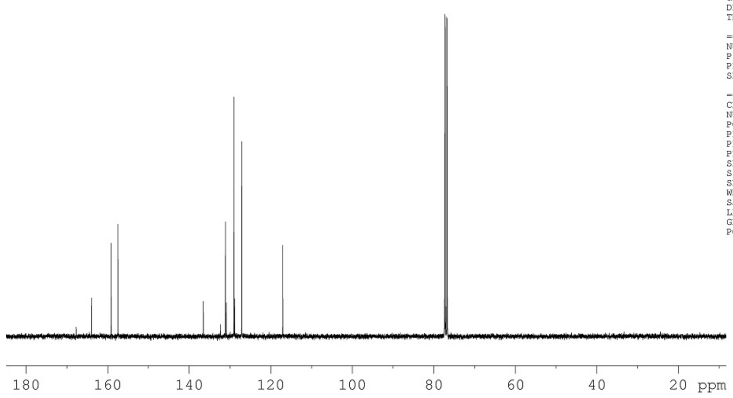




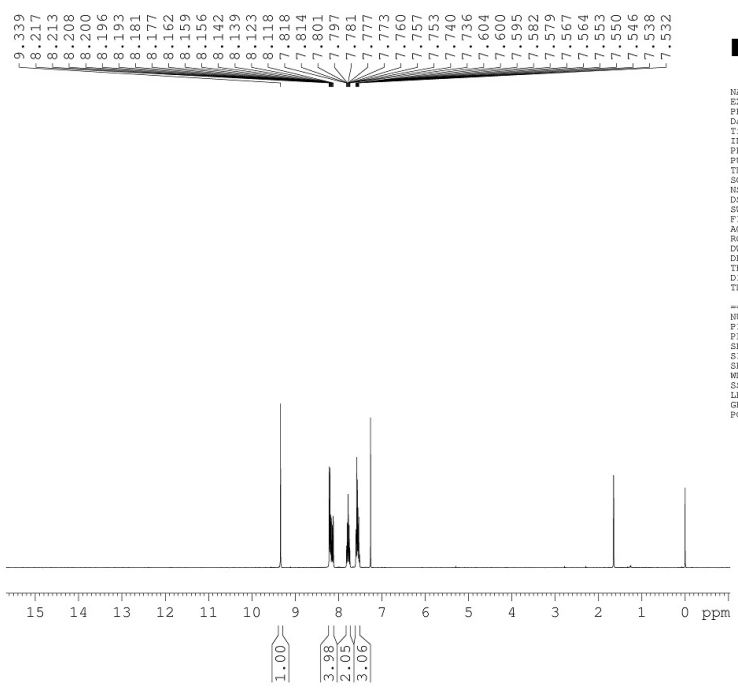
```
NAME            2012-04-11 wangjian-1431
EXPNO                    2
PROCNO                   1
Date_             20120412
Time                 12.23
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  296.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                  19.40 usec
PL1                 -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               60.00 usec
PL12                11.09 dB
PL13                13.05 dB
PL2                 -2.00 dB
SFO2          400.1316005 MHz
SI                   32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



2-phenylquinoxaline (5y)



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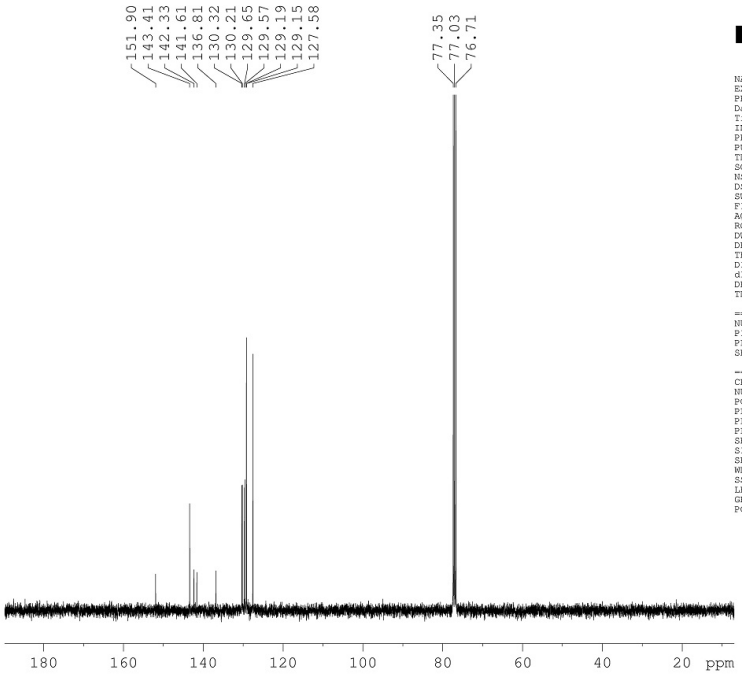
```
NAME          2012-04-11 wangjian-1432
EXPNO                    1
PROCNO                   1
Date_             20120412
Time                 12.28
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      362
DW                   60.800 usec
DE                    6.50 usec
TE                  294.8 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.30 usec
PL1                  -2.00 dB
SFO1           400.1324710 MHz
SI                    32768
SF             400.1300094 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



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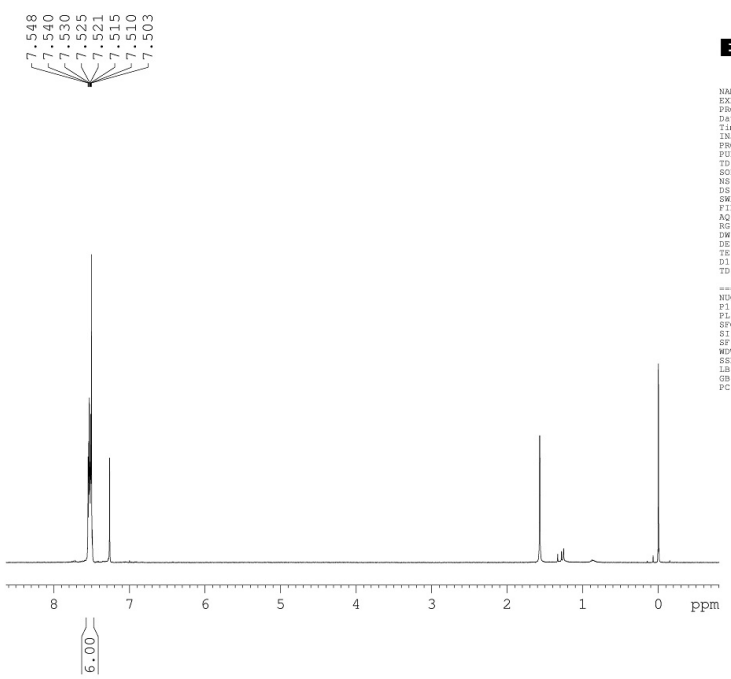
```
NAME          2012-04-11 wangjian-1432
EXPNO                    2
PROCNO                   1
Date_             20120412
Time                 12.45
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     2050
DW                   20.800 usec
DE                    6.50 usec
TE                  295.9 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   19.40 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

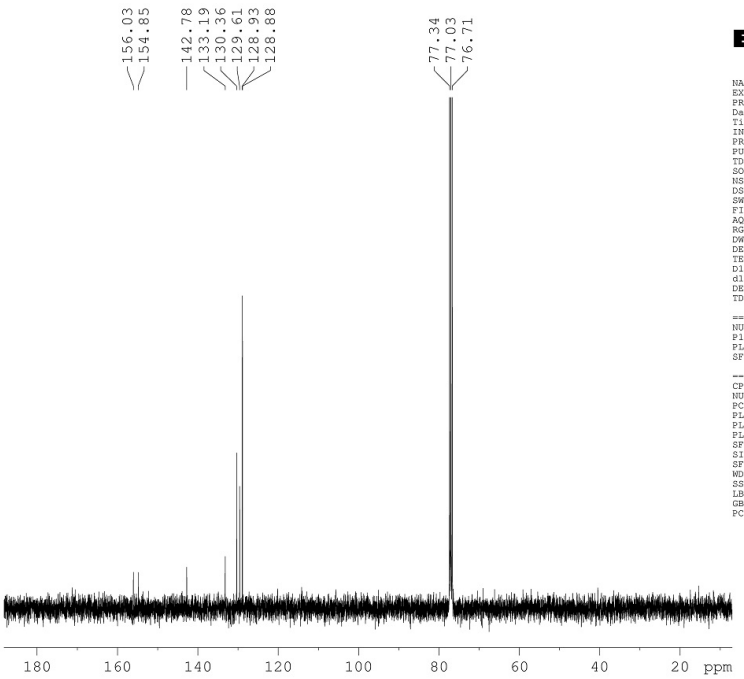
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

3, 6-dichloro-4-phenylpyridazine (5z)




```
NAME          2012-05-30 wangjian-wj-1436
EXPNO                  1
PROCNO                 1
Date_           20120531
Time                0.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES             0.125483 Hz
AQ              3.9846387 sec
RG                   512
DW                60.800 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.30 usec
PL1                -2.00 dB
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300092 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME          2012-04-11 wangjian-1436
EXPNO                  2
PROCNO                 1
Date_           20120412
Time                13.28
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631988 sec
RG                  1620
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 19.40 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              60.00 usec
PL12               11.09 dB
PL13               13.05 dB
PL2                -2.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```