Supporting Information

D-Glucose as Green Ligand for Selective Copper catalyzed Phenol Formation from Aryl Halides with an Easy Catalyst Removal

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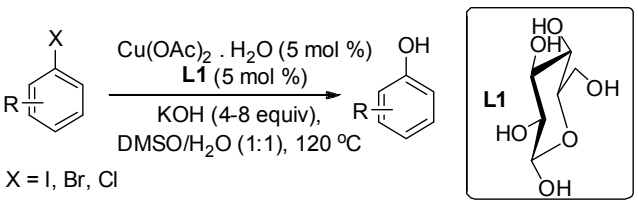
General Experimental Procedures

All the reactions were carried out in 15-20 mL reaction tube under normal atmospheric air. Commercially available D-glucose and other carbohydrates are purchased from Aldrich chemicals. Copper(II) acetate monohydrate along with other copper salts and halobenzenes are purchased from Aldrich chemicals, Alfa Aesar, SRL (India) and Awra chemicals (India). Potassium hydroxide purchased from Ranbaxy (India). Dimethylsulphoxide was purchased from SRL (India) and all these reagents were used without further purification. Reaction temperatures were controlled by Varivolt temperature modulator, melting points were determined using a Guna 230 volts apparatus. Thin-layer chromatography (TLC) was performed using Merck silica gel 60 F254 precoated plates (0.25 mm) and visualized by UV fluorescence lamp. Silica gel (particle size 100-200 mesh) purchased from SRL (India), was used for chromatography. ^{1}H NMR and ^{13}C NMR spectra were recorded at 20°C on a Bruker 400 MHz instrument. Spectra were reported relative to Me_4Si (δ 0.0 ppm) or $CHCl_3$ residual peak (δ 7.26 ppm). ^{13}C 100 MHz NMR were reported relative to $CDCl_3$ (δ 77.16 ppm). All the products were characterized by their NMR, GC/MS and HRMS spectra. The first-order peak patterns are indicated as s (singlet), d (doublet), dd (doublet of doublet), t (triplet), q (quadruplet). Complex non-first-order signals are indicated as m (multiplet). FTIR spectra were recorded on a Nicolet 6700 spectrometer and are reported in frequency of absorption (cm^{-1}). High resolution mass spectrocopy (HRMS) was recorded on Q-Tof Micro mass spectrometer and GCMS recorded on JEOL GCMATE II mass spectrometer.

General Procedure for Hydroxylation of Aryl Halides (0.5 mmol scale) Provided in Table 2.



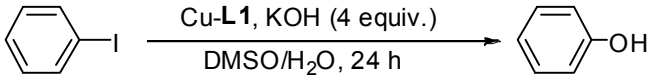
Aryl halide (0.5 mmol), $Cu(OAc)_2.H_2O$ (5 mg, 0.025 mmol) and D-glucose (4.5 mg, 0.025 mmol) were taken in a 15 mL reaction tube. 2 mL of 1:1 mixture of DMSO and

H_2O was added to it followed by KOH pallet (112-228 mg, 2-4 mmol) at room temperature (in case of liquid aryl halides, 0.5 mmol of aryl halide was added after the addition of solvent). Then the reaction tube was fitted with a glass stopper and shielded with Teflon tape. The reaction mixture was heated at 120 ^oC (while heating the reaction muxture, colour of the reaction mixture is changing from blue colour to reddish brown) with occasional mechanical shaking (otherwise KOH sticks to glass wall of the reaction tube). After complete disappearance of aryl halide (the reaction was monitored by TLC), the reaction mixture was allowed to cool to room temperature. Then the reaction mixture was neutralized with few drops of aq. HCl (6 M HCl). In case of water soluble phenols, the solvent was evaporated and the crude residue was purified by column chromatography on silica gel using ethyl acetate/hexanes as eluent to afford the corresponding phenol. In case of water insoluble phenols, the purification was done after water workup.

General Procedure for Hydroxylation of Aryl Halides (10 mmol scale) Provided in Table 2.

In a 100 ml round bottom flask, $Cu(OAc)_2 . H_2O$ (0.5 mmol, 99.5 mg) and D-glucose (0.5 mmol, 90 mg) were taken. 20 mL DMSO and 20 mL H_2O were added to it. Aryl halide (10 mmol) and KOH (60 mmol, 3.36 gm) were added to the reaction mixture. Then the reaction mixture was heated at 120 ^oC and the reaction was monitored using TLC. After the completion, the reaction was allowed to cool to room temperature. The reaction mixture was neutralized with aq. HCl (2 M-6 M HCl), then the phenol was extracted from water layer to organic layer by using dichloromethane as solvent. The further purification of phenol was done by column chromatography on silica gel using ethyl acetate/hexanes as the eluent.

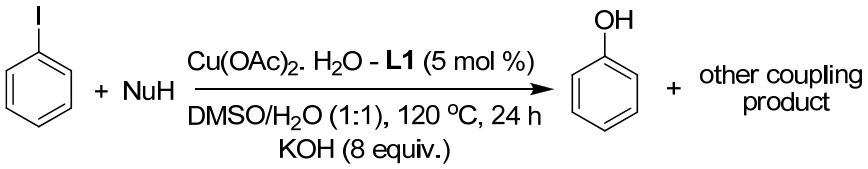
Table 1. Hydroxylation of PhI using various copper sources, solvent ratios, bases and temperature.

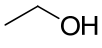
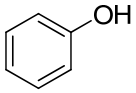
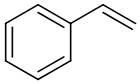
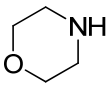


Entry	Cu/**L1**(mol %)	DMSO/H_2O	Temp. (^oC)	Yield(%)[a]
1	CuI/**L1** (20/40)	1:1	120	99
2	$Cu(OAc)_2.H_2O$/**L1** (20/40)	1:1	120	99
3	CuBr/**L1** (20/40)	1:1	120	70
4	CuCl/**L1** (20/40)	1:1	120	55
5	$CuSO_4.H_2O$/**L1** (20/40)	1:1	120	72
6	$CuCl_2$. $2H_2O$/**L1** (20/40)	1:1	120	86
7	$Cu(OAc)_2.H_2O$/**L1** (5/5)	1:1	120	99/0[b]
8	Cu_2O/**L1** (5/5)	1:1	120	20
9	$Cu(OAc)_2.H_2O$/**L1** (5/10)	1:1	120	99
10	$Cu(OAc)_2.H_2O$/**L1** (10/10)	1:1	120	85
11	$Cu(OAc)_2.H_2O$/**L1** (10/20)	1:1	120	75
12	$Cu(OAc)_2.H_2O$/**L1** (20/20)	1:1	120	87
13	$Cu(OAc)_2.H_2O$/**L1** (5/5)	1:9	120	60
14	$Cu(OAc)_2.H_2O$/**L1** (5/5)	2:8	120	70
15	$Cu(OAc)_2.H_2O$/**L1** (5/5)	3:7	120	82
16	$Cu(OAc)_2.H_2O$/**L1** (5/5)	4:6	120	87
17	$Cu(OAc)_2.H_2O$/**L1** (5/5)	H_2O	120	25(48h)
18	$Cu(OAc)_2.H_2O$/**L1** (20/40)	1:1	100	99
19	$Cu(OAc)_2.H_2O$/**L1** (20/40)	1:1	80	50
20	$Cu(OAc)_2.H_2O$/**L1** (5/5)	1:1	100	55
21	$Cu(OAc)_2.H_2O$/**L1** (5/5)	1:1	120	92(34h)[c]
22	$Cu(OAc)_2.H_2O$/**L1** (5/5)	1:1	120	40(34h)[d]

[a] Isolated yield. [b] Reaction without ligand. [c] CsOH is the base. [d] NaOH is the base

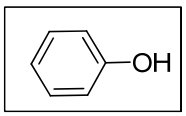
Table 2. Competitive reaction study of hydroxylation of aryl halide in presence of external nucleophiles.[a]



Entry	Nucleophile (1.5 equiv.)[b]	Yield of phenol	Other coupling product
1		90	trace
2		94	0
3		95	0
4		98	0

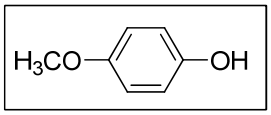
[a] PhI (0.5 mmol), $Cu(OAc)_2$. H_2O (0.025 mmol), D-glucose (0.025 mmol), KOH (4 mmol) in 2 mL DMSO/H_2O at 120 °C. 0.75 mmol of nucleophiles are used unless otherwise mentioned. [b] 10 Equivalents of ethanol (5 mmol) was used.

Characterization data



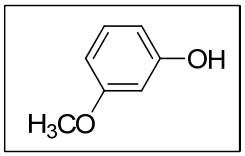
Phenol (Table 3, entry 1):

Following the general method, iodobenzene (56 μL, 0.5 mmol) was reacted with potassium hydroxide (112 mg, 2.0 mmol) to give phenol with 99% yield as colorless liquid with characteristic odor (eluent: ethyl acetate/hexane = 15:85). R_f = 0.28 (in 10% EtOAc in hexane); IR (neat): 1070, 1229, 1369, 1477, 1597, 3339 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 6.38 (s, 1H), 6.82 (td, *J* = 8 Hz, 1.2 Hz, 2H), 6.90 (dt, *J* = 8 Hz, 0.8 Hz, 1H), 7.19 (t, *J* = 8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.5, 121.0, 129.8, 155.3; HRMS [M^++Na] Calculated for C_6H_6ONa: 117.0316; found: 117.0320.



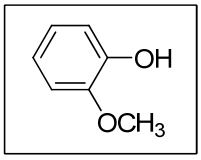
4-Methoxyphenol (Table 3, entry 2)

Following the general method, 4-methoxy-1-iodobenzene (117 mg, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give phenol with 99% yield as white solid (eluent: ethyl acetate/hexane = 20:80). MP 55-57 ^oC. R_f = 0.4 (in 20% EtOAc/Hexane); IR 1031, 1108, 1214, 1337, 1447, 1599, 1718, 2930, 3380 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.81 (s, 3H), 5.71 (s, 1H), 6.70-6.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 115.0, 116.2, 149.6, 153.7; HRMS [M^++K] Calculated for $C_7H_8O_2K$: 163.0161; found: 163.0156.



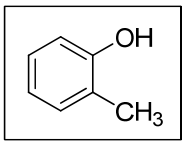
3-Methoxyphenol (Table 3, entry 3)

Following the general method, 3-methoxy-1-iodobenzene (59.5 µL, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give phenol with 99% yield as colorless liquid (eluent: ethyl acetate/hexane = 20:80). R_f = 0.58 (in 20% EtOAc/Hexane); IR 1025, 1099, 1202, 1335, 1440, 1575, 1695, 3000, 3407 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.77 (s, 3H), 6.37 (s, 1H), 6.46 (d, J = 2 Hz, 2H), 6.48 – 6.57 (m, 1H), 7.14 (t, J = 8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 101.7, 106.6, 108.2, 130.4, 156.7, 160.8; HRMS [M^++1] Calculated for $C_7H_9O_2$: 125.0603; found: 125.0603.



2-Methoxyphenol (Table 3, entry 4)

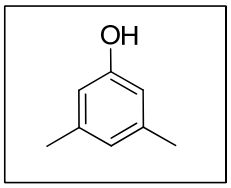
Following the general method, 2-methoxy-1-iodobenzene (66 µL, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give phenol with 52% yield as colorless liquid (eluent: ethyl acetate/hexane = 20:80). R_f = 0.75 (in 20% EtOAc/Hexane); IR 1041, 1154, 1362, 1496, 1603, 1704, 2251, 2954, 3385 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.89 (s, 3H), 5.78 (d, J = 1.2 Hz, 1H), 6.84-6.95 (m, 3H), 6.95-7.06 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.9, 110.8, 114.6, 120.2, 121.5, 145.7, 146.7; GCMS (EI+) : m/z =124.



2-Methylphenol (Table 3, entry 5)

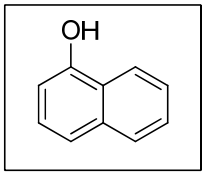
Following the general method, 2-methyl-1-iodobenzene (63.6 µL, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 84% yield as colorless liquid (eluent: ethyl acetate/hexane = 20:80). R_f = 0.78 (in 20% EtOAc/Hexane); IR 1072, 1123, 1273, 1369, 1462, 1639, 1726, 2068, 2959, 3457 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.21 (s, 3H), 6.72 (d, J = 8Hz, 1H), 6.83 (t, J = 7.6 Hz,

1H), 7.04 (t, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.8, 115.1, 120.9, 124.1,127.2, 131.2, 153.6; GCMS (EI+) : *m/z* = 108.



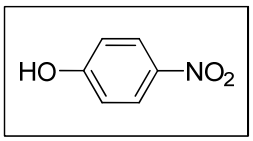
3,5-dimethylphenol (Table 3, entry 6)

Following the general method, 3,5-dimethyl-1-iodobenzene (73µL, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 67% yield as colorless liquid (eluent: ethyl acetate/hexane = 15:85). R_f = 0.58 (in 20% EtOAc/Hexane); IR 1026, 1157, 1252, 1312, 1458, 1630, 2057, 2923, 3457 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 6H), 4.75 (s, 1H), 6.46 (s, 2H), 6.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 113.1, 122.5, 139.6, 155.5; HRMS [M^++1] Calculated for $C_8H_{11}O$: 123.0810; found: 123.0809.



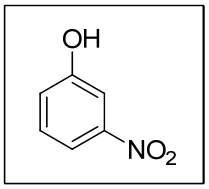
Naphthalene-1-ol (Table 3, entry 7)

Following the general method, 1-iodonapthalene (73µL mg, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 82%, as white solid (eluent: ethyl acetate/hexane = 25:75). MP 94-96 ^{o}C. R_f = 0.62 (in 20% EtOAc/Hexane); IR 1015, 1044, 1082, 1240, 1270, 1386, 3054, 3309 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.41 (s, 1H), 6.79 (s, 1H), 7.25 – 7.39 (m, 1H), 7.39 – 7.59 (m, 3H), 7.81 (s, 1H), 8.18 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.8, 120.8, 121.6, 124.4, 125.4, 126.0, 126.6, 127.8, 134.9, 151.4; HRMS [M^++1] Calculated for $C_{10}H_9O$: 145.0653; found: 145.0658.



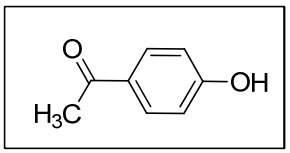
4-Nitrophenol (Table 3, entries 8, 17 & 22)

Following the general method, 4-nitro-1-iodobenzene or 4-nitro-1-bromobenzene or 4-nitro-1-chlorobenzene (124.5 mg or 101 mg or 78.8 mg, 0.5 mmol) was reacted with potassium hydroxide (112 mg, 2.0 mmol) to give corresponding phenol with 99% yield in all cases as yellow solid (eluent: ethyl acetate/hexane = 25:75). MP 110-115 ^{o}C. R_f = 0.32 (in 20% EtOAc/Hexane); IR 1114, 1176, 1204, 1295, 1342, 1498, 1594, 1613, 1638, 3433 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (d, J = 8.8 Hz, 2H), 8.10 (d, J = 9.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.9, 126.5, 141.5, 161.9; HRMS [M^++1] Calculated for $C_6H_6NO_3$: 140.0348; found: 140.0348.



3-Nitrophenol (Table 3, entry 9)

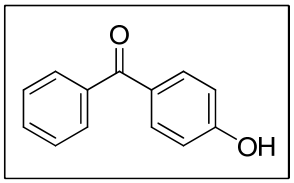
Following the general method, 3-nitro-1-iodobenzene (124.5 mg, 0.5 mmol) was reacted with potassium hydroxide (112 mg, 2.0 mmol) to give corresponding phenol with 83% yield as yellow solid (eluent: ethyl acetate/hexane = 25:75). MP 96-98 ^{o}C. R_f = 0.42 (in 20% EtOAc/Hexane); IR 1213, 1354, 1525, 1620, 3395 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (dd, J = 8 Hz, 3.6Hz, 1H), 7.39 (t, J = 8 Hz, 1H), 7.70 (t, J = 2.4 Hz, 1H), 7.78 (dd, J = 8.4 Hz, 2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 110.6, 115.8, 122.3, 130.4, 149.1, 156.6; HRMS [M^++1] Calculated for $C_6H_6NO_3$: 140.0348; found: 140.0355.



4-Hydroxyacetophenone (Table 3, entries 10 and 15)

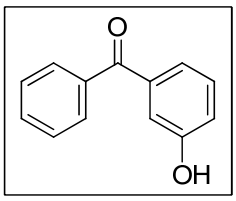
Following the general method, 4-iodoacetophenone or 4-bromoacetophenone (123 mg, or 99.5 mg, 0.5 mmol) was reacted with potassium hydroxide (112 mg, 2.0 mmol) to give

corresponding phenol with 83% or 69% yield, as white solid (eluent: ethyl acetate/hexane = 30:70). MP 109-111 ^{o}C; R_f = 0.29 (in 20% EtOAc/Hexane); IR 1170, 1190, 1343, 1445, 1508, 1593, 1657, 1708, 2956, 3249 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.51 (s, 3H), 6.88 (d, J = 8.8 Hz, 2H), 7.83 (d, J = 8.8 Hz, 2H), 8.22 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.4, 115.7, 129.5, 131.4, 161.8, 199.0; HRMS [M^{+}+1] Calculated for $C_8H_9O_2$: 137.0603; found: 137.0606.



4-Hydroxybenzophenone (Table 3, entries 11 and 21)

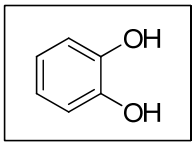
Following the general method, 4-iodobenzophenone or 4-chlorobenzophenone (154 mg or 2.16 gm, 0.5 mmol or 10 mmol) was reacted with potassium hydroxide (168 mg or 3.36 gm, 3.0 mmol or 60 mmol) to give corresponding phenol with 93% or 30% yield as yellow solid (eluent: ethyl acetate/hexane = 25:75). MP 132-135 ^{o}C; IR 1025, 1111, 1282, 1371, 1448, 1597, 1645, 1706, 2834, 2946, 3378 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (dd, J = 8.8, 0.8 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.57 (t, J = 7.6 Hz, 1H), 7.76 (t, J = 8 Hz, 4H) (phenolic proton merged in aromatic zone); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.6, 128.4, 129.4, 130.0, 132.4, 133.3, 138.1, 161.2, 197.3; HRMS [M^{+}+1] Calculated for $C_{13}H_{11}O_2$: 199.0759; found: 199.0768.



3-Hydroxybenzophenone (Table 3, entry 12)

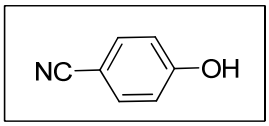
Following the general method, 4-iodobenzophenone (154 mg, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 87% yield as yellow solid (eluent: ethyl acetate/hexane = 25:75). MP 113-115 ^{o}C. IR 1024, 1297, 1418, 1452, 1589, 1653, 2834, 2946, 3348 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 – 7.15 (m, 1H), 7.21 – 7.33 (m, 2H), 7.36 – 7.48 (m, 3H), 7.52 – 7.60 (m, 1H), 7.74

– 7.81 (m, 2H), (phenolic proton merged in aromatic zone); ^{13}C NMR (100 MHz, $CDCl_3$) δ116.8, 120.4, 122.7, 128.4, 129.6, 130.3, 132.9, 137.3, 138.6, 156.4, 197.9; HRMS [M^++1] Calculated for $C_{13}H_{11}O_2$: 199.0759; found: 199.0751.



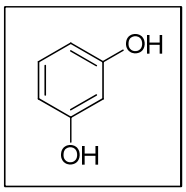
1,2-dihydroxybenzene (Table 3, entries 13, 14, 18 and 20)

Following the general method, 2-bromophenol or 2-iodophenol or 2-iodo-1-bromobenzene or 1,2-diiodobenzene (53.3 µL or 110 mg or 64.2 µL or 65.3 µL, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 70%, 83%, 83%, 54% yield respectively, as colorless liquid (eluent: ethyl acetate/hexane = 30:70). R_f = 0.44 (in 20% EtOAc/Hexane); IR 1095, 1267, 1361, 1467, 1594, 1703, 3340 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.29 (s, 2H), 6.78-6.85 (m, 2H), 6.85-6.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.7, 121.4, 143.6; HRMS $[M+K]^+$ Calculated for $C_6H_6O_2K$: 149.0005; found: 149.0010.



4-hydroxybenzonitrile (Table 3, entry 16)

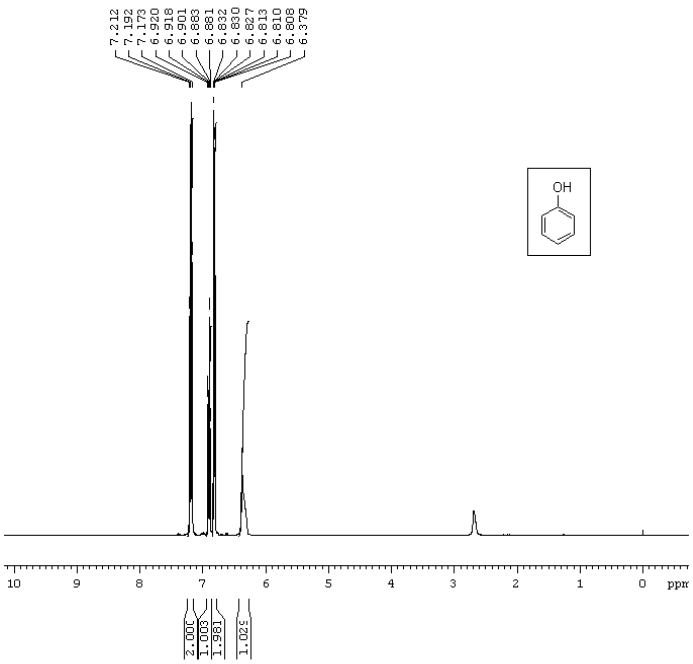
Following the general method, 3-nitro-1-iodobenzene (91 mg, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 99%, as white solid (eluent: ethyl acetate/hexane = 30:70). MP 110-113 ^{o}C. R_f = 0.17 (in 20% EtOAc/Hexane); IR 1114, 1176, 1204, 1295, 1342, 1498, 1594, 1613, 1638, 2162, 3433 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.60 (s, 1H), 7.69 (d, J = 7.6 Hz, 2H), 7.86 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 127.0, 130.1, 131.4, 131.8, 166.8; GCMS (EI+) : m/z =142.



1,3-dihydroxybenzene (Table 3, entry 19)

Following the general method, 1,3-diiodobenzene (165 mg, 0.5 mmol) was reacted with potassium hydroxide (224 mg, 4.0 mmol) to give corresponding phenol with 80% yield as colorless liquid (eluent: ethyl acetate/hexane = 25:75). R_f = 0.52 (in 20% EtOAc/Hexane); IR 1235, 1462, 1582, 1639, 3467 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 5.18 (s, 2H), 6.78-6.83(m, 1H), 6.96 (t, J = 8 Hz, 1H), 7.20-7.29 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.1, 124.7, 130.1, 131.1; HRMS $[M+K]^+$ Calculated for $C_6H_6O_2K$: 149.0005; found: 149.0002

Phenol (^{1}H & ^{13}C)

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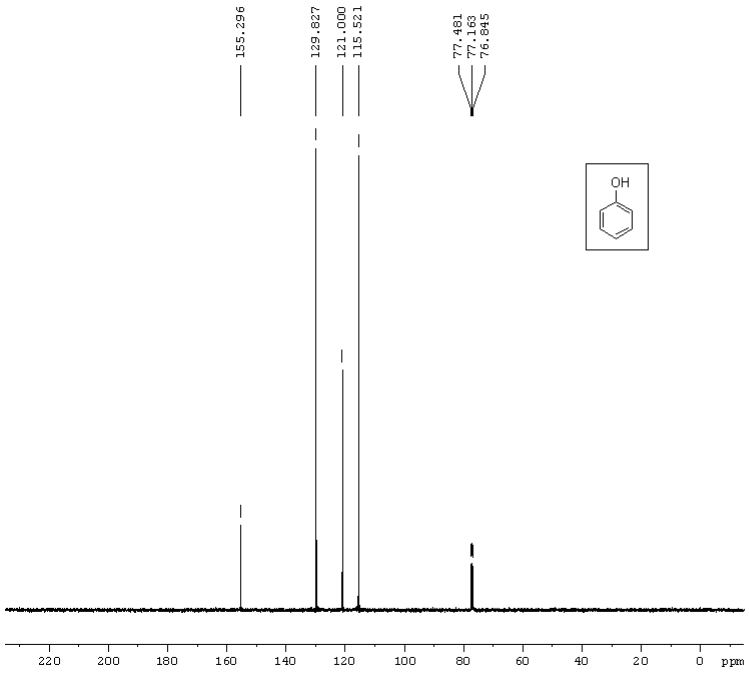
Current Data Parameters
NAME                  gsk0610
EXPNO                     186
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100626
Time                  22.42
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        9
DS                        4
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                     25.4
DW                   59.600 usec
DE                    6.00 usec
TE                   300.2 K
D1                0.50000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SFO1             400.1319460 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300571 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         3.00

1D NMR plot parameters
CX                        20.00 cm
CY                        10.00 cm
F1P                       10.000 ppm
F1                      4001.30 Hz
F2P                       -1.000 ppm
F2                      -400.13 Hz
PPMCM                     0.55000 ppm/cm
HZCM                  220.07153 Hz/cm
```

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Current Data Parameters
NAME                  gsk0610
EXPNO                     187
PROCNO                      1

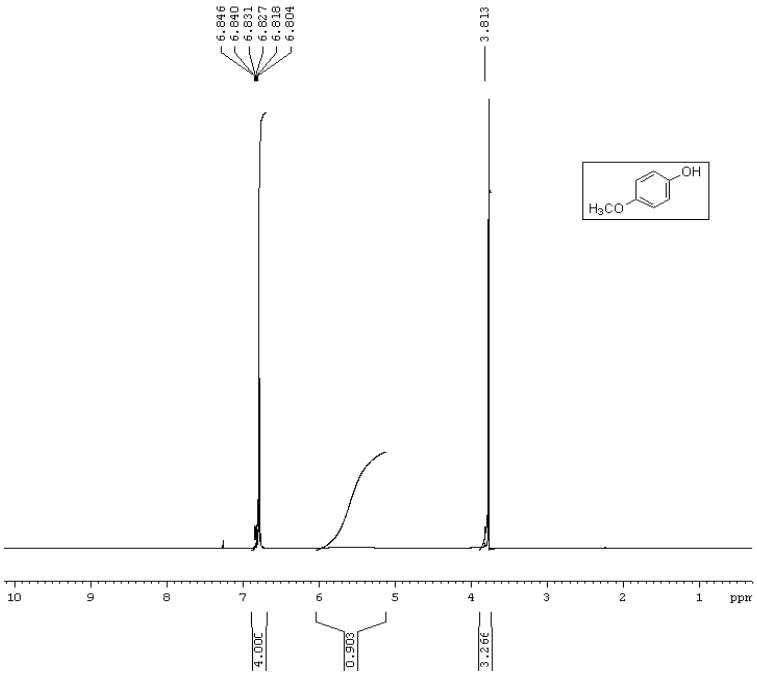
F2 - Acquisition Parameters
Date_              20100626
Time                  22.45
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                       88
DS                        4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                   14596.5
DW                   19.900 usec
DE                    6.00 usec
TE                   300.2 K
D1                1.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     12.50 usec
PL1                     0.00 dB
SFO1             100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SFO2             400.1320007 MHz

F2 - Processing parameters
SI                        65536
SF               100.6127737 MHz
WDW                          EM
SSB                           0
LB                         2.00 Hz
GB                            0
PC                         1.40
```

4-Methoxyphenol (^{1}H & ^{13}C)




```
Current Data Parameters
NAME                  gsk0610
EXPNO                      65
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100608
Time                    5.27
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        4
SWH                8389.262 Hz
FIDRES            0.256020 Hz
AQ                1.9530228 sec
RG                       57
DW                   59.600 usec
DE                    6.00 usec
TE                   295.5 K
D1                0.50000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    11.55 usec
PL1                    3.00 dB
SFO1           400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF                400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        3.00

1D NMR plot parameters
CX                       20.00 cm
CY                       10.00 cm
F1P                    10.000 ppm
F1                   4001.30 Hz
F2P                   -1.000 ppm
F2                   -400.13 Hz
PPMCM                 0.55000 ppm/cm
HZCM                220.07150 Hz/cm
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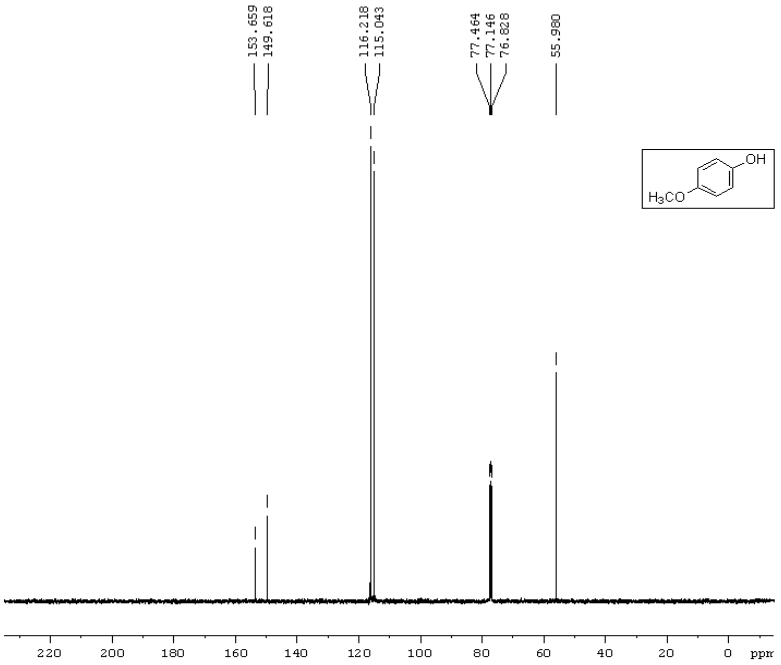



```
Current Data Parameters
NAME                  gsk0610
EXPNO                      66
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100608
Time                    5.35
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      464
DS                        4
SWH               25125.629 Hz
FIDRES            1.533547 Hz
AQ                0.3260916 sec
RG                     6502
DW                   19.900 usec
DE                    6.00 usec
TE                   296.3 K
D1                1.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

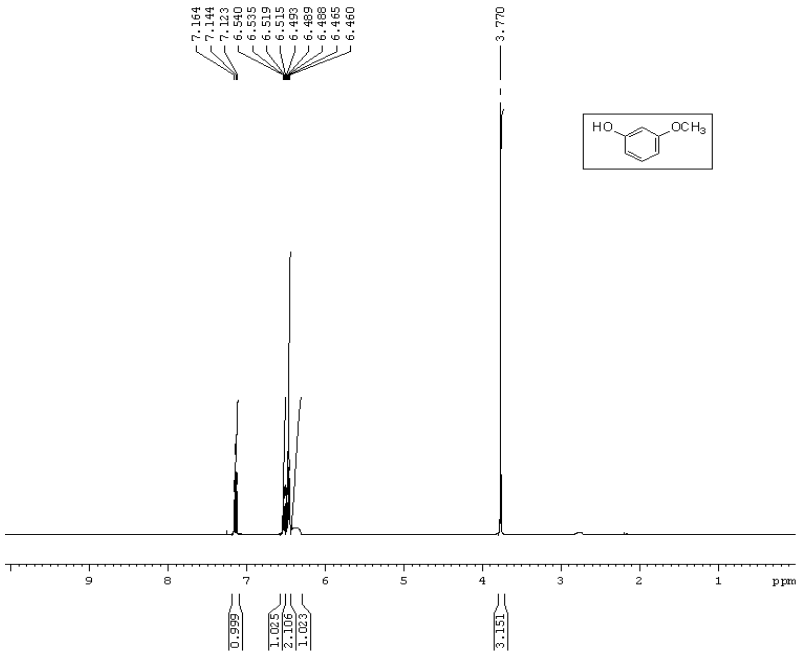
======== CHANNEL f1 ========
NUC1                    13C
P1                    12.50 usec
PL1                    0.00 dB
SFO1           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    3.00 dB
PL12                  19.81 dB
PL13                  20.23 dB
SFO2           400.1320007 MHz

F2 - Processing parameters
SI                       65536
SF                100.6127651 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       20.00 cm
CY                        9.94 cm
F1P                    234.849 ppm
F1                   23628.84 Hz
F2P                   -14.877 ppm
F2                   -1496.79 Hz
PPMCM                12.48630 ppm/cm
HZCM              1256.28125 Hz/cm
```

3-Methoxyphenol (^{1}H & ^{13}C)

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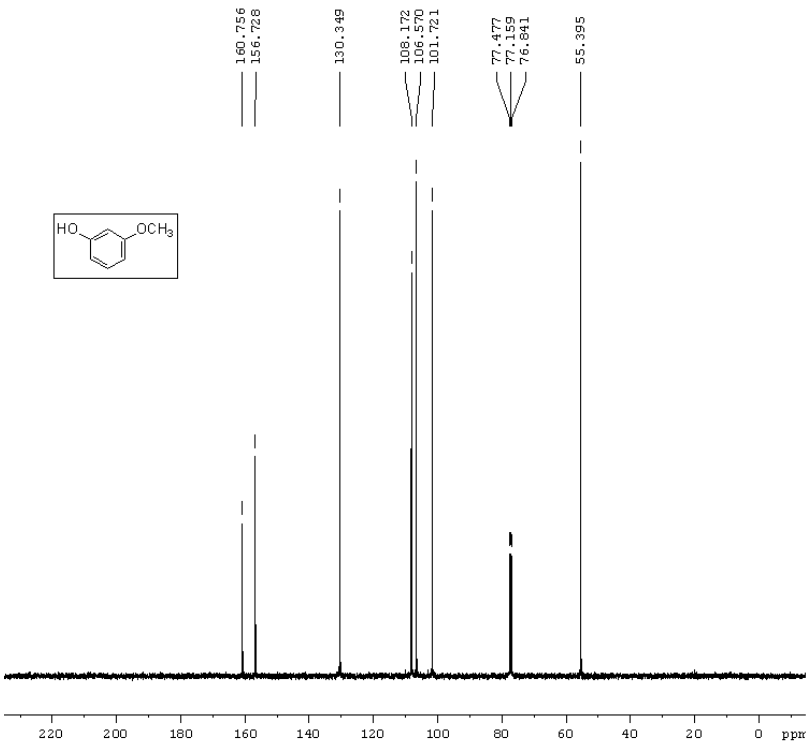
Current Data Parameters
NAME                  KG
EXPNO                 71
PROCNO                1

F2 - Acquisition Parameters
Date_              20100608
Time                  6.22
INSTRUM               av400
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      20
DS                       4
SWH               8389.262 Hz
FIDRES            0.256020 Hz
AQ                1.9530228 sec
RG                     25.4
DW                59.600 usec
DE                 6.00 usec
TE                 295.4 K
D1              0.50000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.55 usec
PL1                 3.00 dB
SFO1          400.1319460 MHz

F2 - Processing parameters
SI                   16384
SF            400.1300170 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   3.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.00 cm
F1P                 10.000 ppm
F1                4001.30 Hz
F2P                -1.000 ppm
F2                -400.13 Hz
PPMCM              0.55000 ppm/cm
HZCM             220.07150 Hz/cm
```




```
Current Data Parameters
NAME              gsk0610
EXPNO                  72
PROCNO                  1

F2 - Acquisition Parameters
Date_              20100608
Time                  6.27
INSTRUM               av400
PROBHD    5 mm BBO BB-1H
PULPROG           zgpg30
TD                   16384
SOLVENT              CDCl3
NS                     260
DS                       4
SWH              25125.629 Hz
FIDRES            1.533547 Hz
AQ                0.3260916 sec
RG                   9195.2
DW                19.900 usec
DE                 6.00 usec
TE                 296.1 K
D1              1.00000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

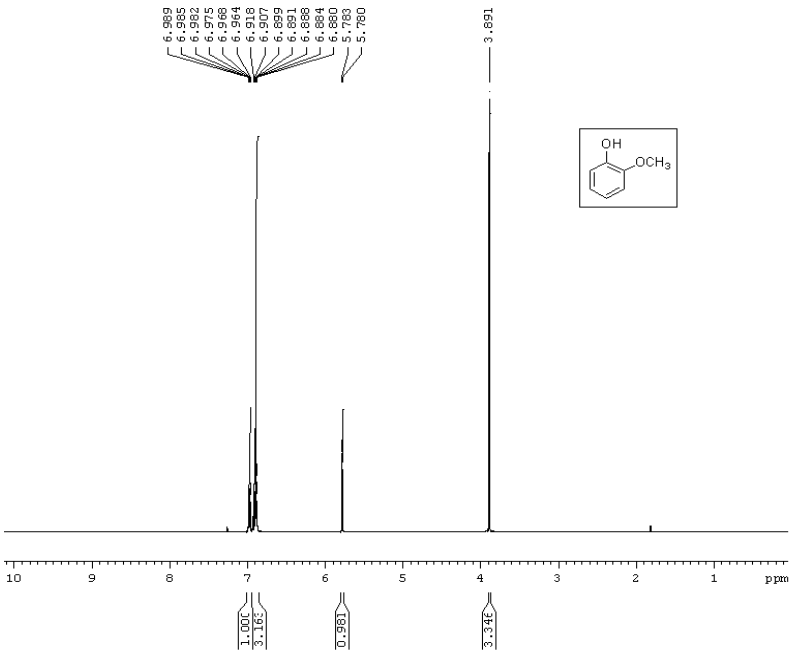
======== CHANNEL f1 ========
NUC1                  13C
P1                 12.50 usec
PL1                 0.00 dB
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 3.00 dB
PL12               19.81 dB
PL13               20.23 dB
SFO2          400.1320007 MHz

F2 - Processing parameters
SI                   65536
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
CY                   9.94 cm
F1P                234.849 ppm
F1               23628.84 Hz
F2P                -14.877 ppm
F2               -1496.79 Hz
PPMCM             12.48630 ppm/cm
HZCM           1256.28137 Hz/cm
```

2-Methoxyphenol (^{1}H & ^{13}C)




```
Current Data Parameters
NAME                  gsk0610
EXPNO                      69
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100608
Time                    6.05
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        4
SWH                8389.262 Hz
FIDRES                0.256020 Hz
AQ                 1.9530228 sec
RG                       40.3
DW                     59.600 usec
DE                      6.00 usec
TE                     295.5 K
D1                 0.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      11.55 usec
PL1                      3.00 dB
SF01             400.1319460 MHz

F2 - Processing parameters
SI                        16384
SF                 400.1300175 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         3.00

1D NMR plot parameters
CX                        20.00 cm
CY                        10.00 cm
F1P                      10.000 ppm
F1                     4001.30 Hz
F2P                      -1.000 ppm
F2                     -400.13 Hz
PPMCM                  0.55000 ppm/cm
HZCM                 220.07150 Hz/cm
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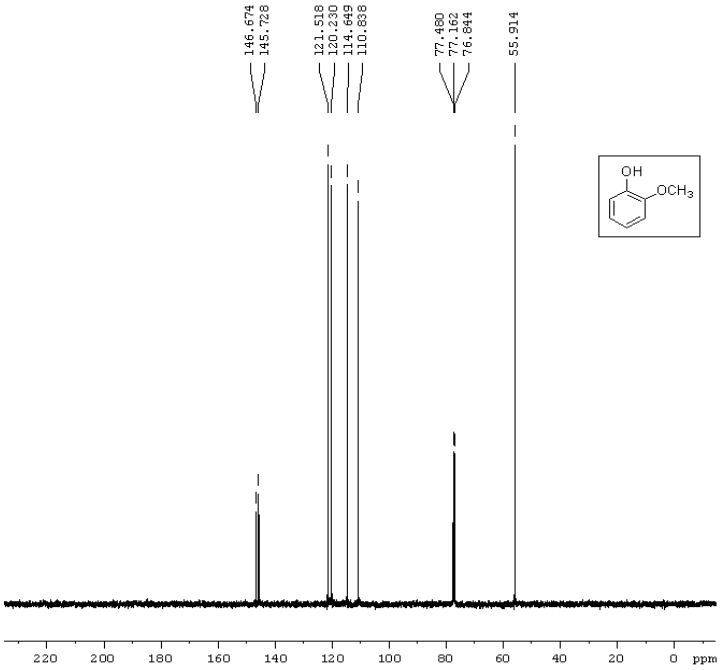


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Current Data Parameters
NAME                  gsk0610
EXPNO                      70
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100608
Time                    6.12
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      253
DS                        4
SWH               25125.629 Hz
FIDRES                1.533547 Hz
AQ                 0.3260916 sec
RG                     9195.2
DW                     19.900 usec
DE                      6.00 usec
TE                     296.3 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

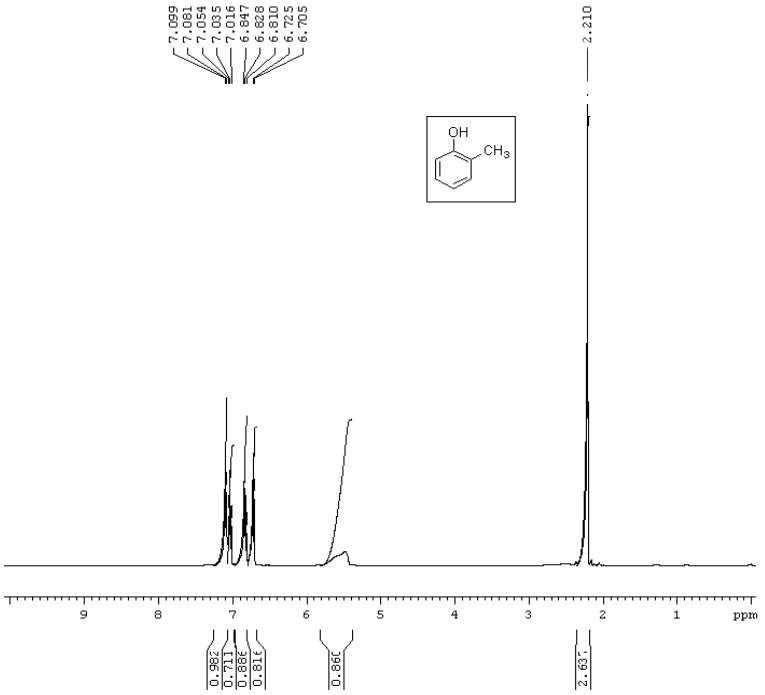
======== CHANNEL f1 ========
NUC1                      13C
P1                      12.50 usec
PL1                      0.00 dB
SF01             100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      3.00 dB
PL12                    19.81 dB
PL13                    20.23 dB
SF02             400.1320007 MHz

F2 - Processing parameters
SI                        65536
SF                 100.6127690 MHz
WDW                          EM
SSB                           0
LB                         2.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                        20.00 cm
CY                         9.94 cm
F1P                      234.849 ppm
F1                     23628.84 Hz
F2P                      -14.877 ppm
F2                     -1496.79 Hz
PPMCM                  12.48630 ppm/cm
HZCM                 1256.28137 Hz/cm
```

2-Methylphenol (^{1}H & ^{13}C)

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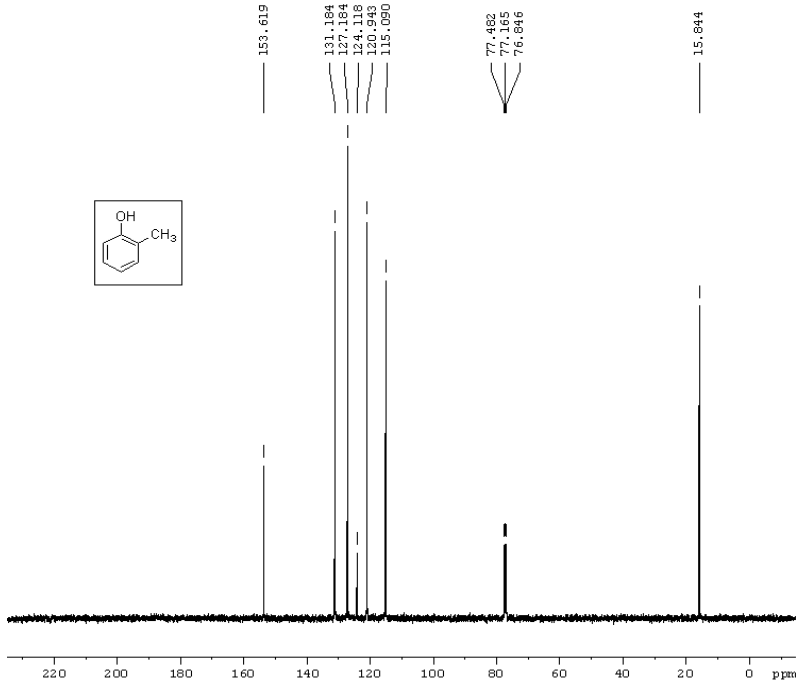
Current Data Parameters
NAME                  gsk0610
EXPNO                      108
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20100612
Time                     15.29
INSTRUM                  av400
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      32768
SOLVENT                  CDCl3
NS                          32
DS                           4
SWH                 8389.262 Hz
FIDRES              0.256020 Hz
AQ                  1.9530228 sec
RG                          18
DW                     59.600 usec
DE                      6.00 usec
TE                     293.1 K
D1                  0.50000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                      11.55 usec
PL1                      3.00 dB
SFO1             400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF                400.1300738 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        3.00

1D NMR plot parameters
CX                       20.00 cm
CY                       10.00 cm
F1P                     10.000 ppm
F1                    4001.30 Hz
F2P                     -1.000 ppm
F2                    -400.13 Hz
PPMCM                  0.55000 ppm/cm
HZCM                 220.07153 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0610
EXPNO                      109
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20100612
Time                     15.32
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PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      16384
SOLVENT                  CDCl3
NS                         124
DS                           4
SWH                25125.629 Hz
FIDRES              1.533547 Hz
AQ                  0.3260916 sec
RG                        6502
DW                     19.900 usec
DE                      6.00 usec
TE                     293.7 K
D1                  1.00000000 sec
d11                 0.03000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

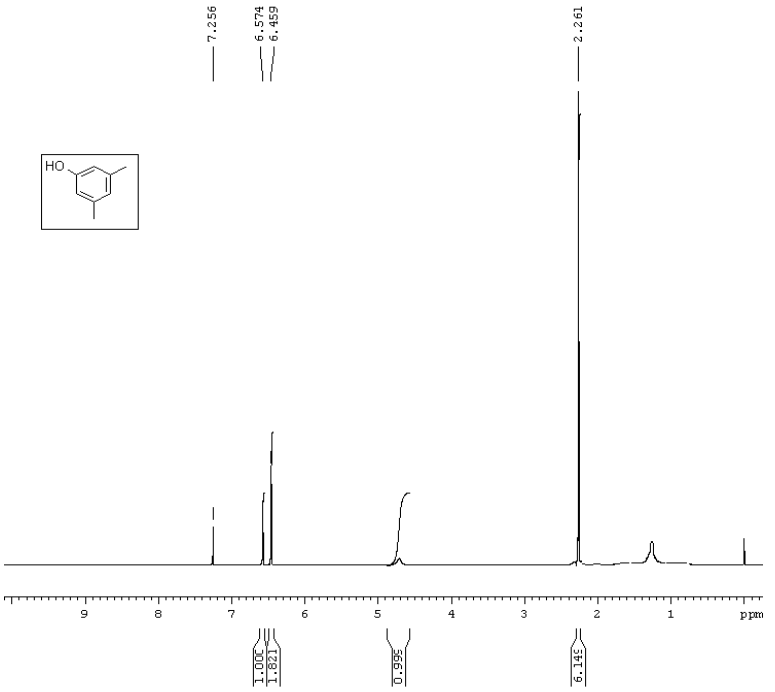
======== CHANNEL f1 ========
NUC1                       13C
P1                      12.50 usec
PL1                      0.00 dB
SFO1             100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      3.00 dB
PL12                    19.81 dB
PL13                    20.23 dB
SFO2             400.1320007 MHz

F2 - Processing parameters
SI                       65536
SF                100.6127802 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       20.00 cm
CY                        9.94 cm
F1P                     234.849 ppm
F1                    23628.84 Hz
F2P                     -14.877 ppm
F2                    -1496.79 Hz
PPMCM                  12.48630 ppm/cm
HZCM                 1256.28149 Hz/cm
```

3,5-dimethylphenol (^{1}H & ^{13}C)

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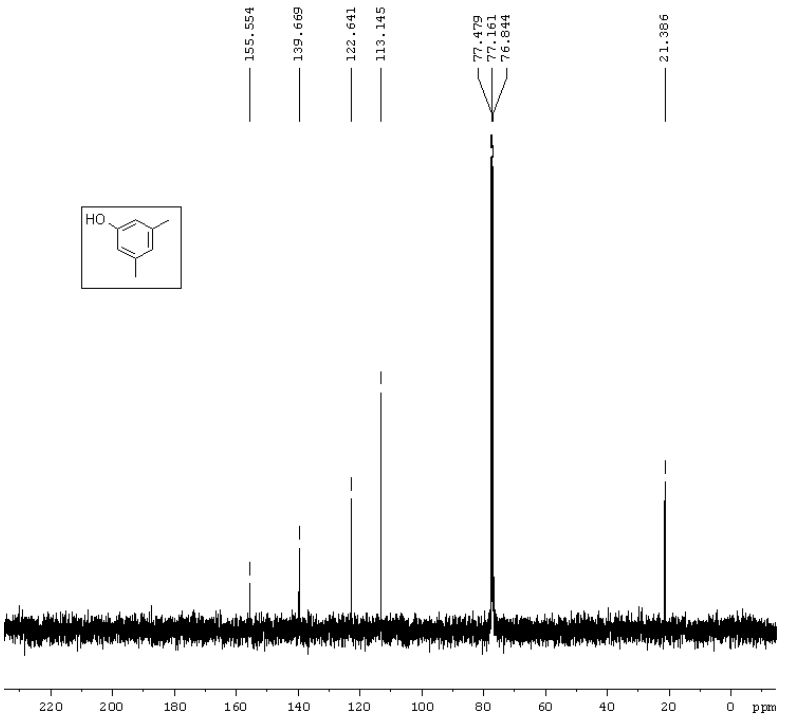
Current Data Parameters
NAME                  gsk0610
EXPNO                     180
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100626
Time                  21.51
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        4
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                     203.2
DW                    59.600 usec
DE                     6.00 usec
TE                    300.2 K
D1                 0.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SFO1           400.1319460 MHz

F2 - Processing parameters
SI                     16384
SF                400.1300190 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      3.00

1D NMR plot parameters
CX                     20.00 cm
CY                      6.00 cm
F1P                   10.000 ppm
F1                  4001.30 Hz
F2P                   -1.000 ppm
F2                  -400.13 Hz
PPMCM                 0.55000 ppm/cm
HZCM                220.07150 Hz/cm
```

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Current Data Parameters
NAME                  gsk0310
EXPNO                      34
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100303
Time                  15.27
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      223
DS                        4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                   18390.4
DW                    19.900 usec
DE                     6.00 usec
TE                    294.7 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

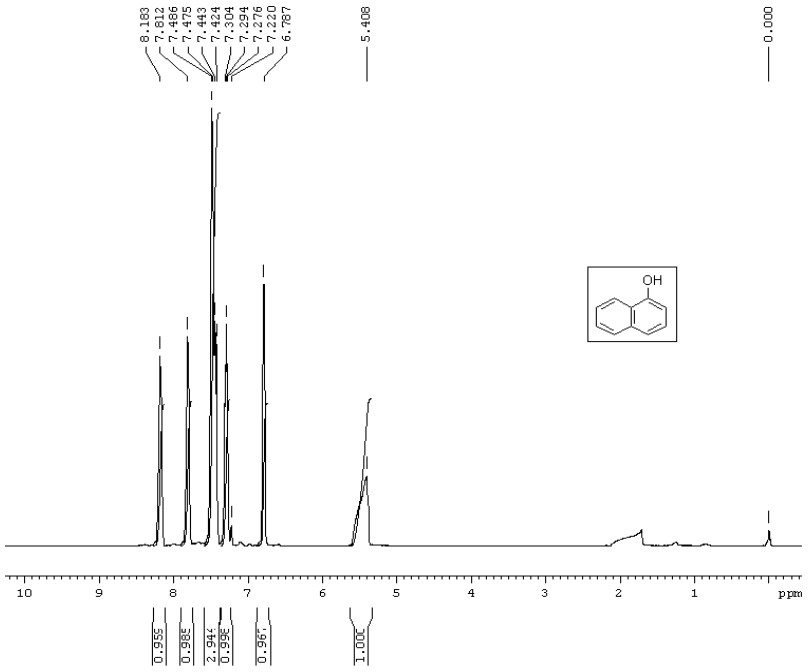
======== CHANNEL f1 ========
NUC1                      13C
P1                     12.50 usec
PL1                     0.00 dB
SFO1           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SFO2           400.1320007 MHz

F2 - Processing parameters
SI                     65536
SF                100.6127595 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     20.00 cm
CY                      9.94 cm
F1P                   234.849 ppm
F1                  23628.84 Hz
F2P                  -14.877 ppm
F2                  -1496.79 Hz
PPMCM                 12.48630 ppm/cm
HZCM               1256.28125 Hz/cm
```

Naphthalene-1-ol (^{1}H & ^{13}C)



BRUKER

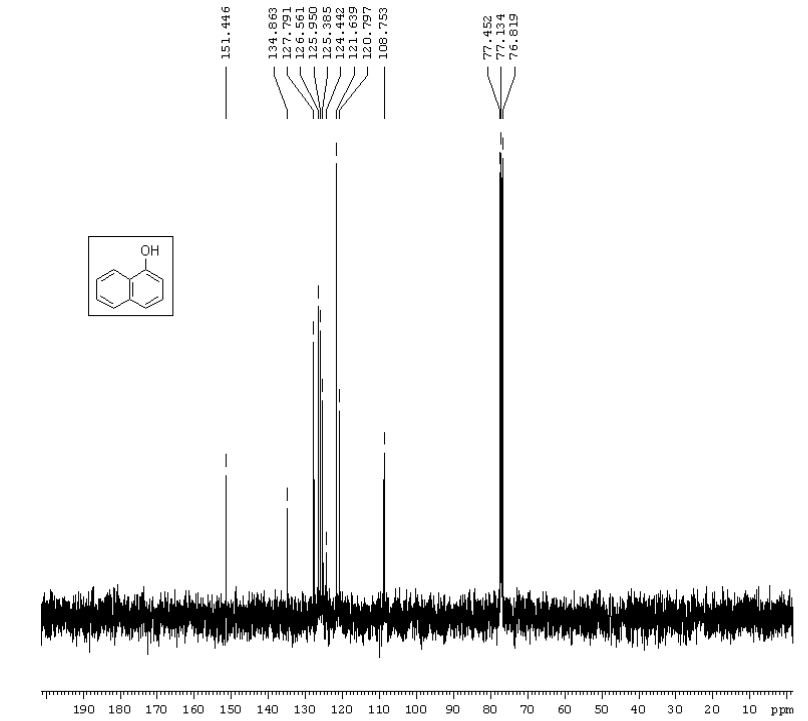
```
Current Data Parameters
NAME                  gsk1010
EXPNO                      41
PROCNO                      1

F2 - Acquisition Parameters
Date_               20101031
Time                   23.08
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        4
SWH                8389.262 Hz
FIDRES                0.256020 Hz
AQ                 1.9530228 sec
RG                      114
DW                    59.600 usec
DE                     6.00 usec
TE                    673.2 K
D1                 0.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SFO1           400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF                 400.1300293 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        3.00

1D NMR plot parameters
CX                       20.00 cm
CY                       10.00 cm
F1P                     10.129 ppm
F1                    4052.73 Hz
F2P                     -1.000 ppm
F2                    -400.13 Hz
PPMCM                  0.55643 ppm/cm
HZCM                 222.64291 Hz/cm
```



BRUKER

```
Current Data Parameters
NAME                  gsk1010
EXPNO                      42
PROCNO                      1

F2 - Acquisition Parameters
Date_               20101031
Time                   23.11
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      156
DS                        4
SWH               25125.629 Hz
FIDRES                1.533547 Hz
AQ                 0.3260916 sec
RG                      13004
DW                    19.900 usec
DE                     6.00 usec
TE                    673.2 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

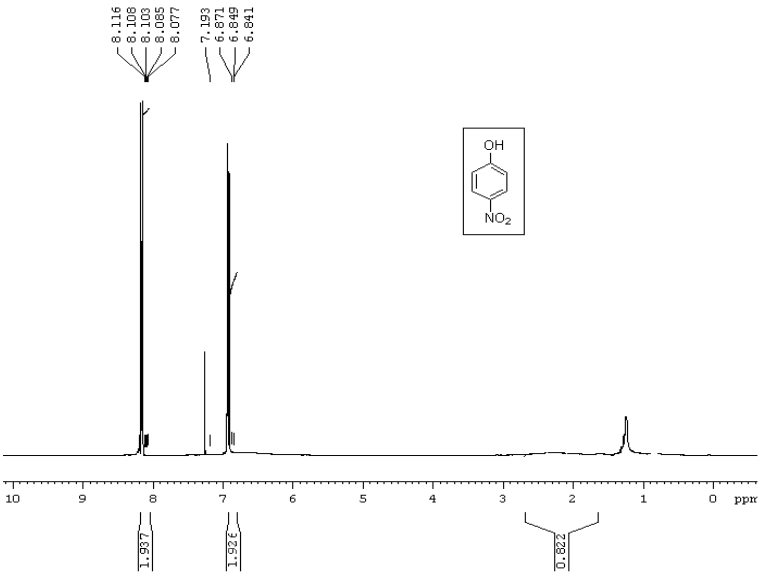
======== CHANNEL f1 ========
NUC1                      13C
P1                     12.50 usec
PL1                     0.00 dB
SFO1           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SFO2           400.1320007 MHz

F2 - Processing parameters
SI                       65536
SF                 100.6127642 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       20.00 cm
CY                        5.00 cm
F1P                    234.849 ppm
F1                   23628.84 Hz
F2P                    -14.877 ppm
F2                    -1496.79 Hz
PPMCM                 12.48630 ppm/cm
HZCM                1256.28125 Hz/cm
```

4-Nitrophenol (^{1}H & ^{13}C)



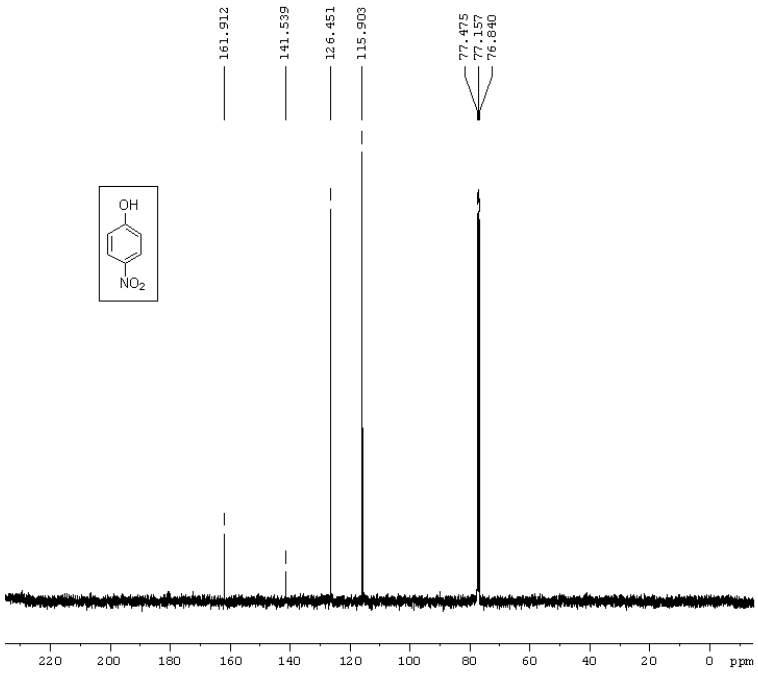

```
Current Data Parameters
NAME                  gsk0310
EXPNO                     193
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100317
Time                    16.08
INSTRUM                 av400
PROBHD   5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                 8389.262 Hz
FIDRES                 0.256020 Hz
AQ                  1.9530228 sec
RG                       256
DW                    59.600 usec
DE                     6.00 usec
TE                     294.9 K
D1                  0.50000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.55 usec
PL1                     3.00 dB
SF01           400.1319460 MHz

F2 - Processing parameters
SI                         16384
SF                 400.1300443 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          3.00

1D NMR plot parameters
CX                         20.00 cm
CY                          6.00 cm
F1P                        10.129 ppm
F1                       4052.73 Hz
F2P                       -1.000 ppm
F2                      -400.13 Hz
PPMCM                    0.55643 ppm/cm
HZCM                   222.64291 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0310
EXPNO                     204
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100317
Time                    20.40
INSTRUM                 av400
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                     16384
SOLVENT                CDCl3
NS                        468
DS                         4
SWH                25125.629 Hz
FIDRES                 1.533547 Hz
AQ                  0.3260916 sec
RG                     18390.4
DW                    19.900 usec
DE                     6.00 usec
TE                     296.4 K
D1                  1.00000000 sec
d11                 0.03000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

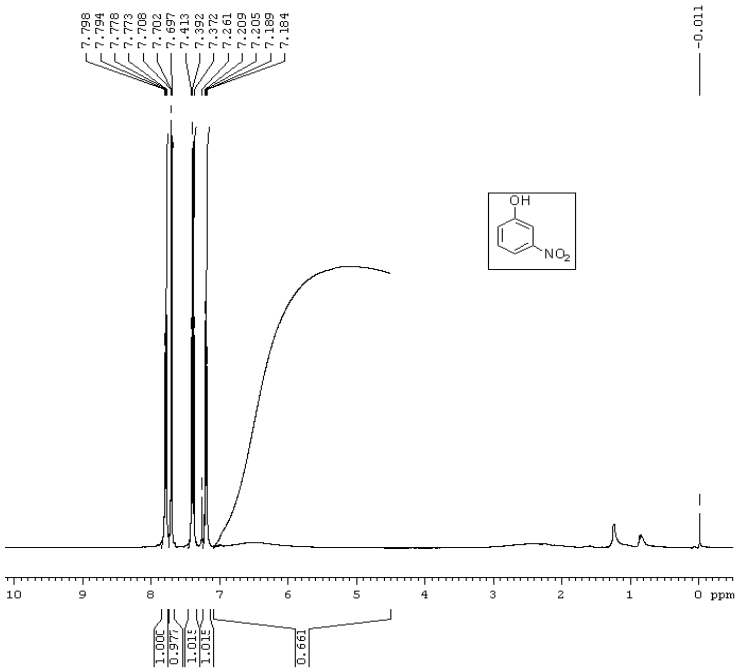
======== CHANNEL f1 ========
NUC1                      13C
P1                     12.50 usec
PL1                     0.00 dB
SF01           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SF02           400.1320007 MHz

F2 - Processing parameters
SI                         65536
SF                 100.6127591 MHz
WDW                           EM
SSB                            0
LB                          2.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                         20.00 cm
CY                          9.94 cm
F1P                      234.849 ppm
F1                     23628.94 Hz
F2P                      -14.877 ppm
F2                     -1496.79 Hz
PPMCM                   12.48630 ppm/cm
HZCM                 1256.28125 Hz/cm
```

3-Nitrophenol (^{1}H & ^{13}C)



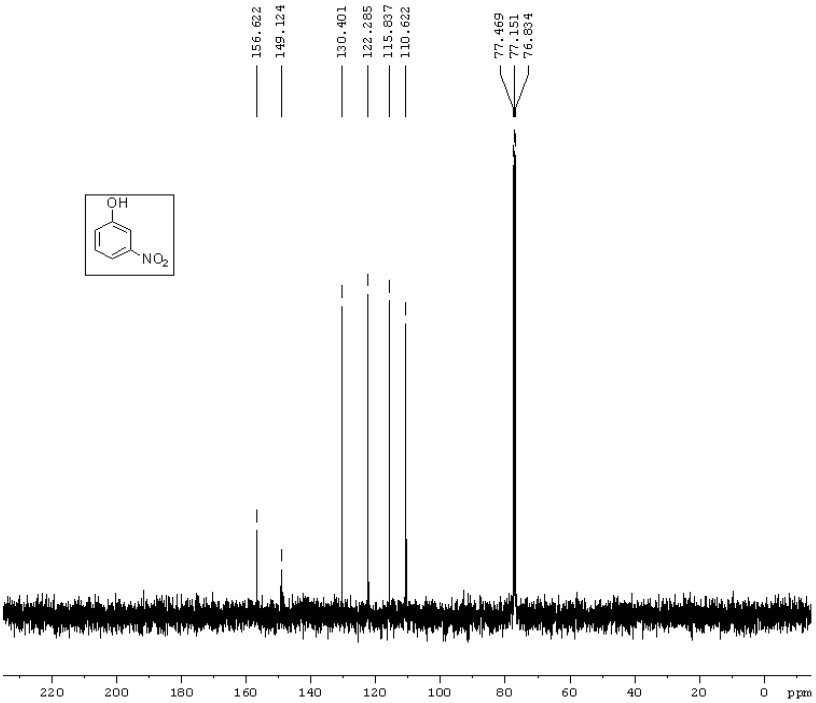

```
Current Data Parameters
NAME                  gsk0610
EXPNO                      92
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100612
Time                   8.52
INSTRUM               av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       22
DS                        4
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                       128
DW                    59.600 usec
DE                     6.00 usec
TE                    293.1 K
D1                 0.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SF01             400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF               400.1300165 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        3.00

1D NMR plot parameters
CX                       20.00 cm
CY                        5.00 cm
F1P                      10.000 ppm
F1                     4001.30 Hz
F2P                      -1.000 ppm
F2                     -400.13 Hz
PPMCM                  0.55000 ppm/cm
HZCM                 220.07150 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0610
EXPNO                      93
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100612
Time                   8.54
INSTRUM               av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                       56
DS                        4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                     6502
DW                    19.900 usec
DE                     6.00 usec
TE                    293.4 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

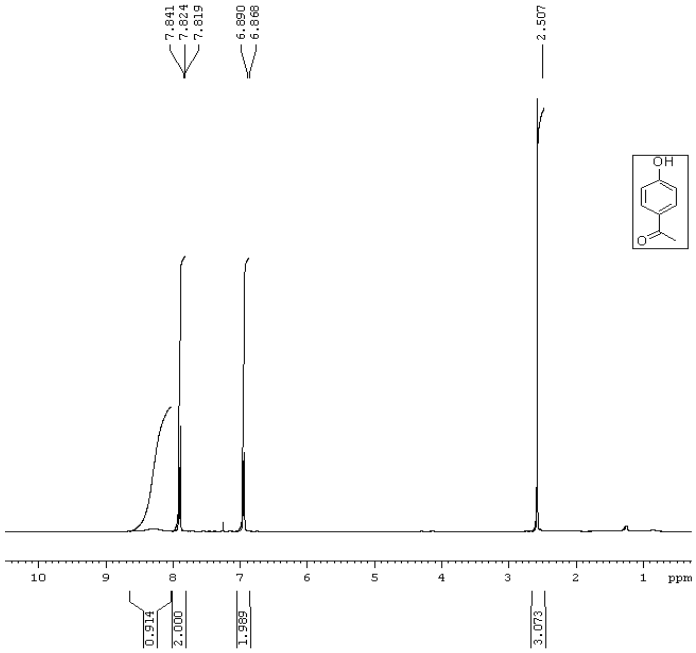
======== CHANNEL f1 ========
NUC1                     13C
P1                     12.50 usec
PL1                     0.00 dB
SF01             100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SF02             400.1320007 MHz

F2 - Processing parameters
SI                       65536
SF               100.6127624 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       20.00 cm
CY                        9.94 cm
F1P                    234.849 ppm
F1                   23628.84 Hz
F2P                    -14.877 ppm
F2                   -1496.79 Hz
PPMCM                 12.48630 ppm/cm
HZCM                1256.28125 Hz/cm
```

4-Hydroxyacetophenone (^{1}H & ^{13}C)



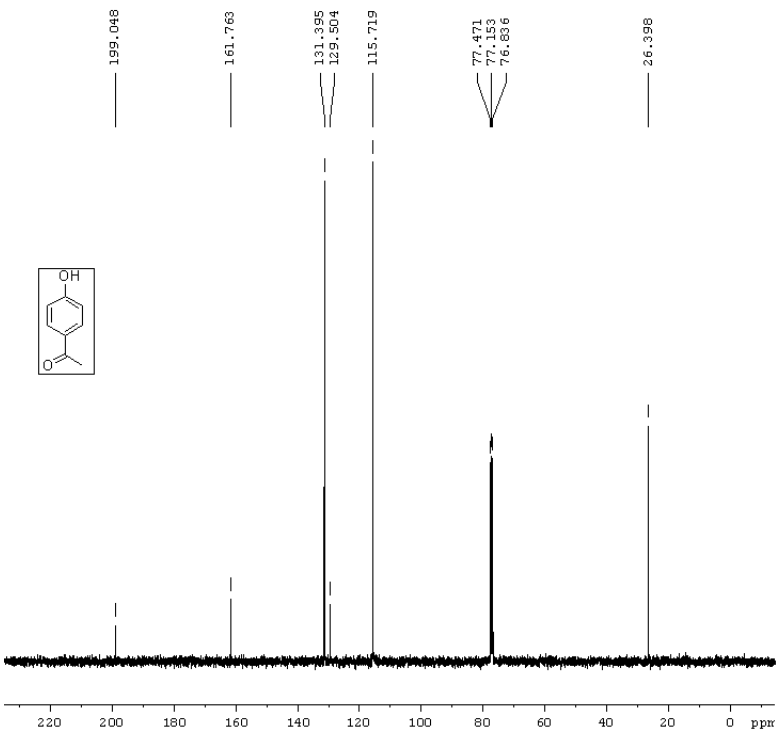

```
Current Data Parameters
NAME                  gsk0510
EXPNO                      54
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100511
Time                  12.31
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       21
DS                        4
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                      80.6
DW                   59.600 usec
DE                    6.00 usec
TE                   297.8 K
D1                0.50000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SF01           400.1319460 MHz

F2 - Processing parameters
SI                    16384
SF               400.1300180 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     3.00

1D NMR plot parameters
CX                    20.00 cm
CY                     5.05 cm
F1P                  10.129 ppm
F1                 4052.73 Hz
F2P                  -1.000 ppm
F2                 -400.13 Hz
PPMCM                0.55643 ppm/cm
HZCM               222.64290 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0510
EXPNO                      55
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100511
Time                  12.36
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      209
DS                        4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                   18390.4
DW                   19.900 usec
DE                    6.00 usec
TE                   298.5 K
D1                1.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

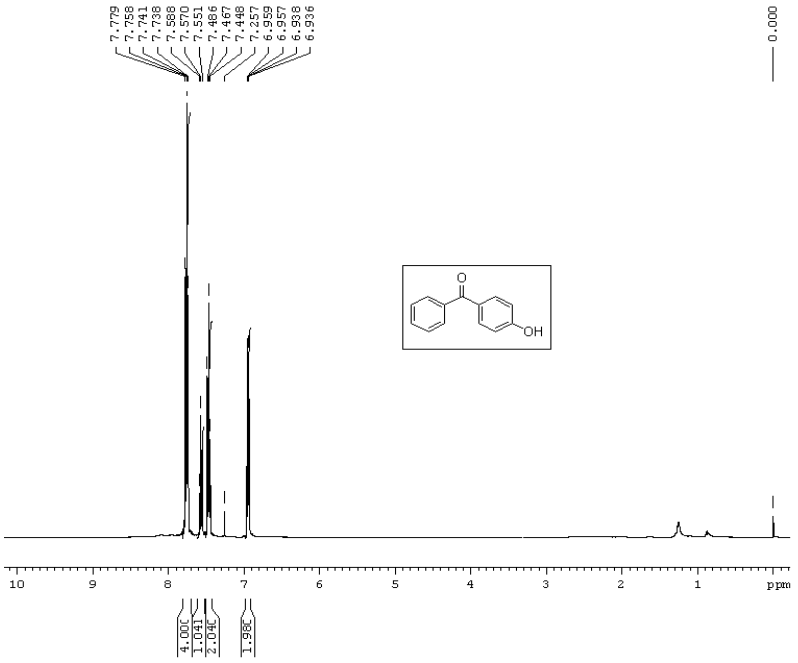
======== CHANNEL f1 ========
NUC1                     13C
P1                     12.50 usec
PL1                     0.00 dB
SF01           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SF02           400.1320007 MHz

F2 - Processing parameters
SI                    65536
SF               100.6127614 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                    20.00 cm
CY                     9.94 cm
F1P                  234.849 ppm
F1                 23628.84 Hz
F2P                  -14.877 ppm
F2                 -1496.79 Hz
PPMCM                12.48630 ppm/cm
HZCM               1256.28125 Hz/cm
```

4-Hydroxybenzophenone (^{1}H & ^{13}C)



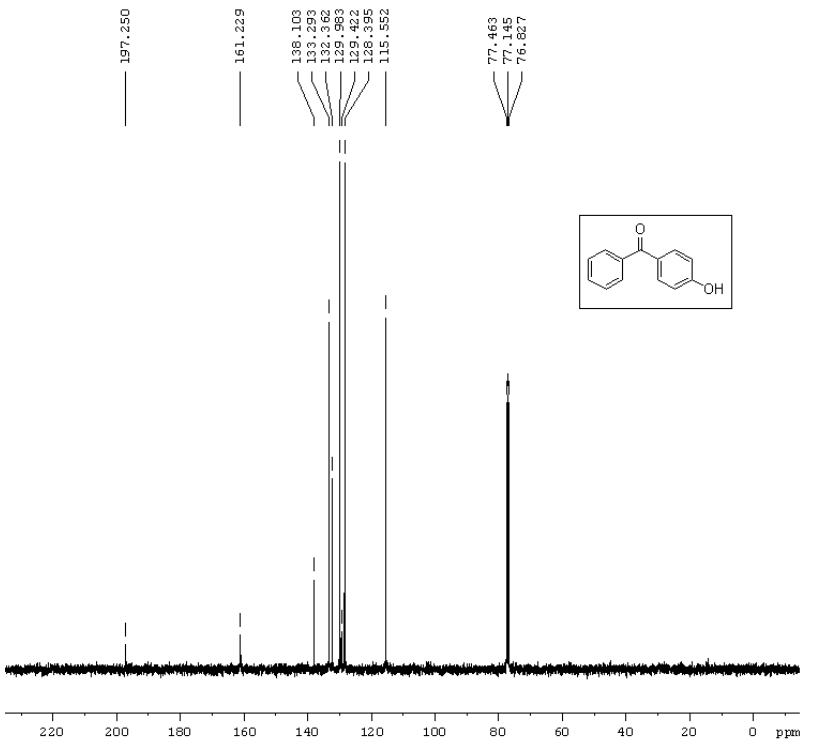

```
Current Data Parameters
NAME                  gsk0910
EXPNO                      49
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100911
Time               11.18
INSTRUM            av400
PROBHD    5 mm BBO BB-1H
PULPROG            zg30
TD                 32768
SOLVENT            CDCl3
NS                 32
DS                 4
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                 90.5
DW                 59.600 usec
DE                 6.00 usec
TE                 297.3 K
D1                 0.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1               1H
P1                 11.55 usec
PL1                3.00 dB
SFO1               400.1319460 MHz

F2 - Processing parameters
SI                 16384
SF                 400.1300184 MHz
WDW                EM
SSB                0
LB                 0.30 Hz
GB                 0
PC                 3.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P                10.129 ppm
F1                 4052.73 Hz
F2P                -1.000 ppm
F2                 -400.13 Hz
PPMCM              0.55643 ppm/cm
HZCM               222.64290 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0910
EXPNO                      50
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100911
Time               11.22
INSTRUM            av400
PROBHD    5 mm BBO BB-1H
PULPROG            zgpg30
TD                 16384
SOLVENT            CDCl3
NS                 361
DS                 4
SWH                25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                 13004
DW                 19.900 usec
DE                 6.00 usec
TE                 297.9 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

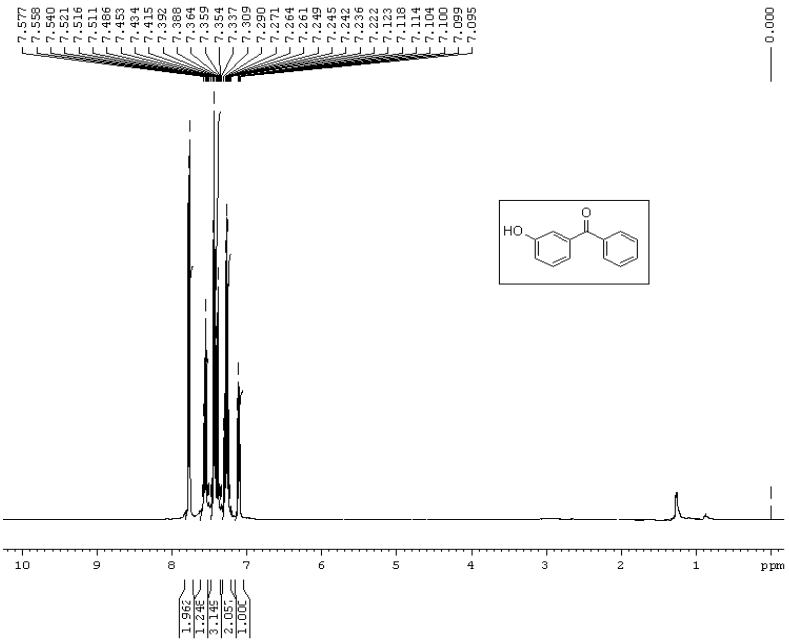
======== CHANNEL f1 ========
NUC1               13C
P1                 12.50 usec
PL1                0.00 dB
SFO1               100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2               1H
PCPD2              80.00 usec
PL2                3.00 dB
PL12               19.81 dB
PL13               20.23 dB
SFO2               400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF                 100.6127627 MHz
WDW                EM
SSB                0
LB                 2.00 Hz
GB                 0
PC                 1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 5.00 cm
F1P                234.849 ppm
F1                 23628.84 Hz
F2P                -14.877 ppm
F2                 -1496.79 Hz
PPMCM              12.48830 ppm/cm
HZCM               1256.28125 Hz/cm
```

3-Hydroxybenzophenone (^{1}H & ^{13}C)



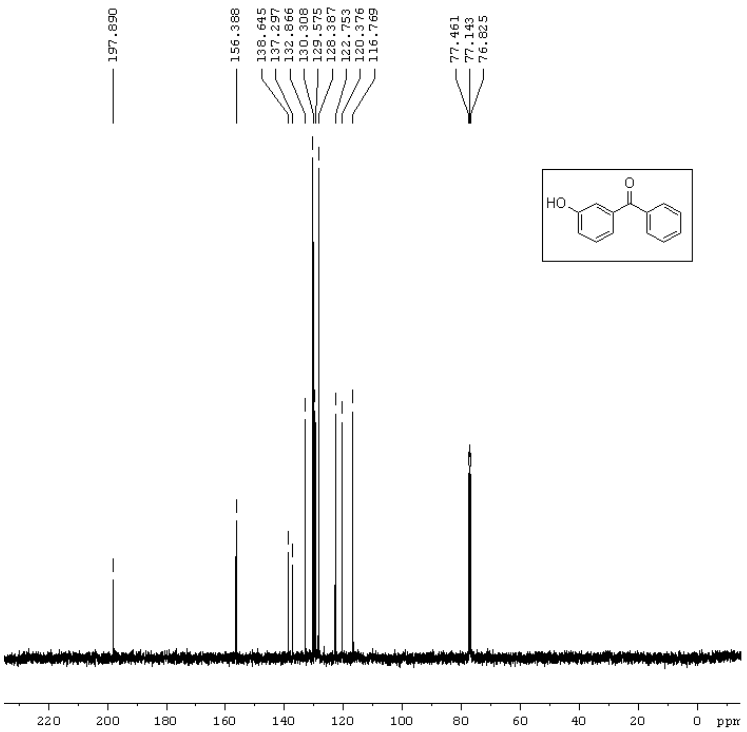
Current Data Parameters
NAME gsk0910
EXPNO 47
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100911
Time 11.05
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 57
DW 59.600 usec
DE 6.00 usec
TE 297.3 K
D1 0.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.55 usec
PL1 3.00 dB
SFO1 400.1319460 MHz

F2 - Processing parameters
SI 16384
SF 400.1300208 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 3.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.129 ppm
F1 4052.73 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.55643 ppm/cm
HZCM 222.64291 Hz/cm



Current Data Parameters
NAME gsk0910
EXPNO 48
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100911
Time 11.07
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 66
DS 4
SWH 25125.629 Hz
FIDRES 1.533547 Hz
AQ 0.3260916 sec
RG 13004
DW 19.900 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

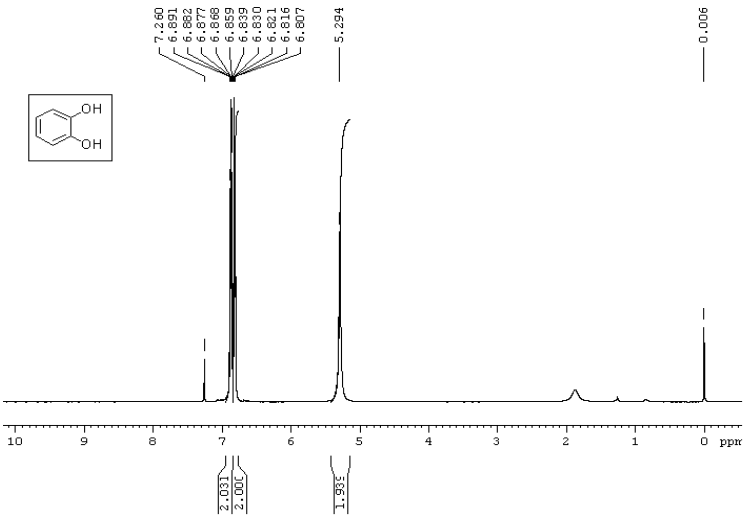
======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SFO1 100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 19.81 dB
PL13 20.23 dB
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 65536
SF 100.6127669 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 234.849 ppm
F1 23628.84 Hz
F2P -14.877 ppm
F2 -1496.79 Hz
PPMCM 12.48630 ppm/cm
HZCM 1256.28137 Hz/cm

1,2-dihydroxybenzene (^{1}H & ^{13}C)



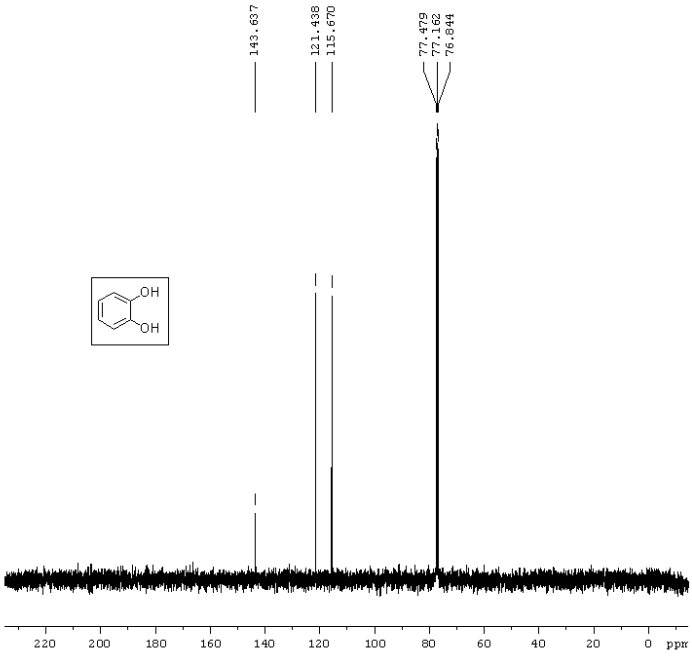

```
Current Data Parameters
NAME                  gsk0710
EXPNO                     110
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100721
Time                   10.44
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    16384
SOLVENT               CDCl3
NS                       32
DS                        0
SWH                8389.262 Hz
FIDRES             0.512040 Hz
AQ                 0.9765364 sec
RG                     287.4
DW                    59.600 usec
DE                     6.00 usec
TE                    298.5 K
D1                 0.50000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SFO1          400.1319460 MHz

F2 - Processing parameters
SI                      131072
SF            400.1300173 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      3.00

1D NMR plot parameters
CX                     20.00 cm
CY                     10.00 cm
F1P                   10.129 ppm
F1                   4052.73 Hz
F2P                   -1.000 ppm
F2                   -400.13 Hz
PPMCM                 0.55643 ppm/cm
HZCM                222.64290 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0710
EXPNO                     111
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100721
Time                   10.49
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG               zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      161
DS                        4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                     13004
DW                    19.900 usec
DE                     6.00 usec
TE                    299.2 K
D1                 1.00000000 sec
d11                0.03000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

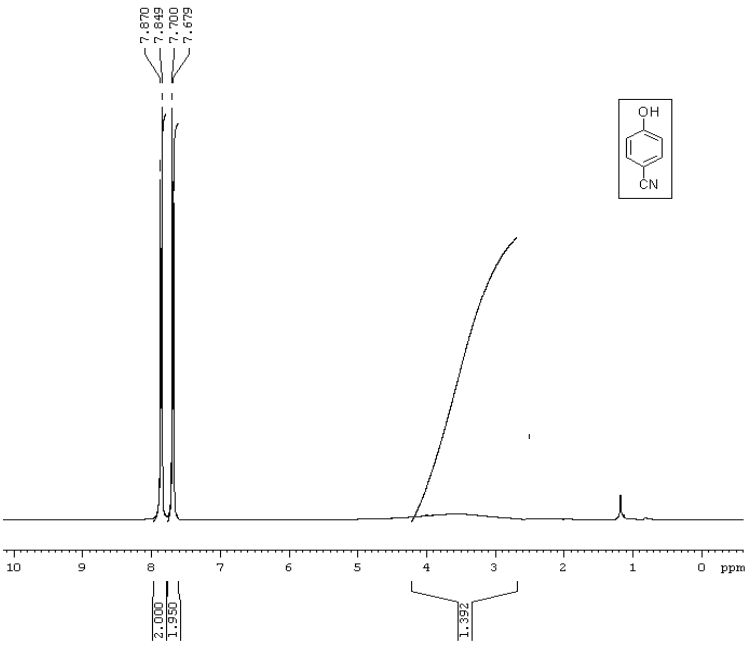
======== CHANNEL f1 ========
NUC1                      13C
P1                     12.50 usec
PL1                     0.00 dB
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SFO2          400.1320007 MHz

F2 - Processing parameters
SI                      65536
SF            100.6127576 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     20.00 cm
CY                      5.00 cm
F1P                   234.849 ppm
F1                  23628.84 Hz
F2P                  -14.877 ppm
F2                  -1496.79 Hz
PPMCM                12.48630 ppm/cm
HZCM              1256.28125 Hz/cm
```

4-hydroxybenzonitrile (^{1}H & ^{13}C)



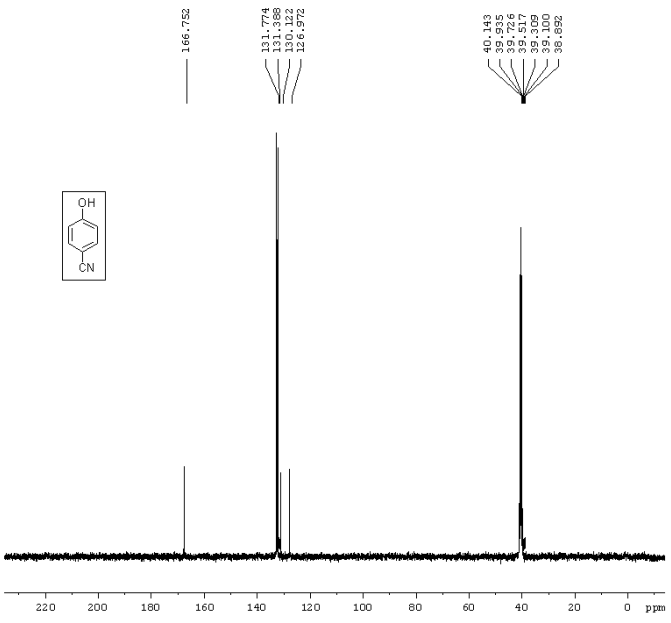

```
Current Data Parameters
NAME                  gsk0610
EXPNO                     134
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100616
Time                   18.00
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       32
DS                        4
SWH                8389.262 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                       57
DW                  59.600 usec
DE                   6.00 usec
TE                   293.4 K
D1                0.50000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.55 usec
PL1                     3.00 dB
SFO1             400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF                400.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        3.00

1D NMR plot parameters
CX                       20.00 cm
CY                       10.00 cm
F1P                     10.000 ppm
F1                    4001.30 Hz
F2P                     -1.000 ppm
F2                    -400.13 Hz
PPMCM                 0.55000 ppm/cm
HZCM                220.07150 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0610
EXPNO                     135
PROCNO                      1

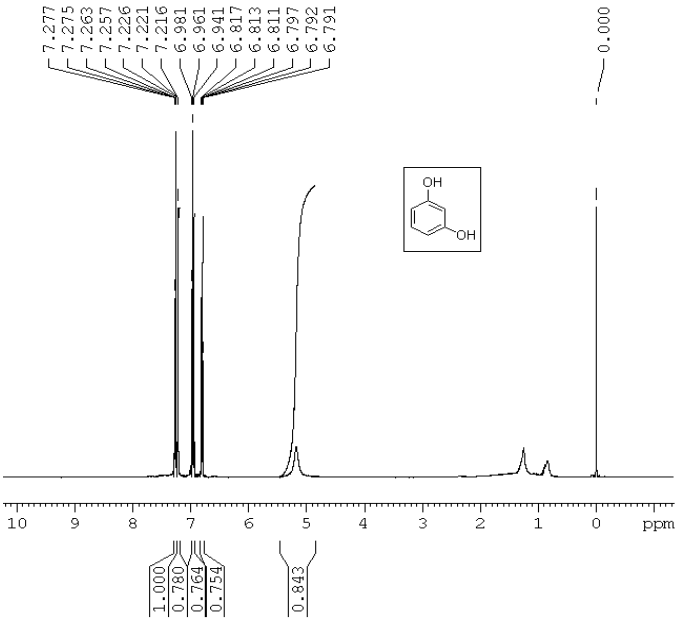
F2 - Acquisition Parameters
Date_               20100616
Time                   18.05
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    16384
SOLVENT                DMSO
NS                       229
DS                        4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                   10321.3
DW                  19.900 usec
DE                   6.00 usec
TE                   294.0 K
D1                1.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     12.50 usec
PL1                     0.00 dB
SFO1            100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                     3.00 dB
PL12                   19.81 dB
PL13                   20.23 dB
SFO2             400.1320007 MHz

F2 - Processing parameters
SI                       65536
SF                100.6128051 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40
```

1,3-dihydroxybenzene (^{1}H & ^{13}C)



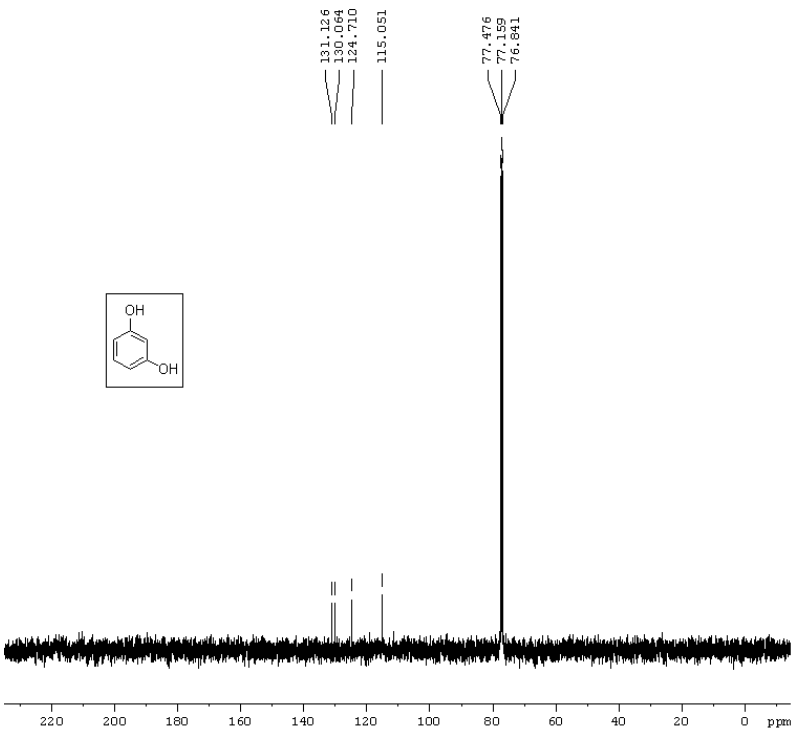

```
Current Data Parameters
NAME                  gsk0610
EXPNO                      94
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100612
Time                    9.03
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                 8389.262 Hz
FIDRES                 0.256020 Hz
AQ                  1.9530228 sec
RG                       322.5
DW                    59.600 usec
DE                     6.00 usec
TE                     293.1 K
D1                  0.50000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      11.55 usec
PL1                      3.00 dB
SF01             400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF                400.1300160 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                        3.00

1D NMR plot parameters
CX                      20.00 cm
CY                      10.00 cm
F1P                    10.000 ppm
F1                   4001.30 Hz
F2P                    -1.000 ppm
F2                   -400.13 Hz
PPMCM                 0.55000 ppm/cm
HZCM                220.07150 Hz/cm
```




```
Current Data Parameters
NAME                  gsk0610
EXPNO                      95
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100612
Time                    9.07
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                     16384
SOLVENT                CDCl3
NS                       172
DS                         4
SWH                25125.629 Hz
FIDRES                 1.533547 Hz
AQ                  0.3260916 sec
RG                      14596.5
DW                    19.900 usec
DE                     6.00 usec
TE                     293.5 K
D1                  1.00000000 sec
d11                 0.03000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      12.50 usec
PL1                      0.00 dB
SF01             100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                      3.00 dB
PL12                    19.81 dB
PL13                    20.23 dB
SF02             400.1320007 MHz

F2 - Processing parameters
SI                       65536
SF                100.6127587 MHz
WDW                         EM
SSB                          0
LB                      2.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                      20.00 cm
CY                       9.94 cm
F1P                    234.849 ppm
F1                   23628.84 Hz
F2P                    -14.877 ppm
F2                   -1496.79 Hz
PPMCM                 12.48630 ppm/cm
HZCM                1256.28125 Hz/cm
```