D-Glucosamine as an Efficient Ligand for Copper-Catalyzed Selective Synthesis of Aniline from Aryl Halides and NaN_3

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Supporting Information

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Experimental Section:

All the reactions were carried out in reaction tube under normal atmospheric air. Commercially available monosaccharide ligands are purchased from Aldrich chemicals. Copper (I) iodide and other copper salts purchased from Alfa Aesar and Aldrich chemicals. Halobenzenes are purchased from Aldrich chemicals, Alfa Aesar, SRL (India) and Awra (India) chemicals. Potassium hydroxide purchased from Ranbaxy (India). *N,N*-dimethylformamide (DMF) 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 on a Bruker 400 MHz instrument. Spectra were reported relative to Me_4Si (δ 0.0 ppm) or residual peak (δ 7.26 ppm). ^{13}C NMR were reported relative to $CDCl_3$ (δ 77.16 ppm). FTIR spectra were recorded on a Nicolet 6700 spectrometer and are reported in frequency of absorption (cm^{-1}). High resolution mass spectra (HRMS) were recorded on Q-Tof Micro mass spectrometer and GCMS.

General Procedure for Aniline Formation from Aryl Halides (0.5 mmol scale) Provided in Table 3.

2 mL of DMF/H_2O (1:1) mixture has taken in 15 mL reaction tube. Argon gas was passed gently for 5 minutes. Aryl halide (0.5 mmol), CuI (9.5 mg, .05 mmol), D-glucosamine (5.4 mg, 0.025 mmol), KI (83 mg, 0.5 mmol) and NaN_3 (97 mg, 1.5 mmol) were then transferred inside the tube along with a magnetic pallet of appropriate size. The reaction tube was then fitted over a preheated oil bath equipped with a magnetic stirrer at 120 ^{o}C. The neck of the reaction tube kept open for 1 minute to remove the pressure generated due to heating. After 1 minute of stirring, the reaction tube was fitted with a stopper and continued stirring for 10 minutes. Then KOH (28 mg, 0.5 mmol) was added either in solid or in water solution (0.5

mL. 1 M) form. The reaction tube was then fitted with a glass stopper properly shielded using Teflon tape and placed in the oil bath. Heating continued for 12 hours with the magnetic stirring (continuation of the reaction for extended time reduce the yield of product for few substrates). The reaction was monitored with TLC checking. After complete disappearance of aryl halide, the reaction mixture was allowed to cool to room temperature. After water/dichloromethane workup the organic phase was evaporated and further purification has done by column chromatography on nutral alumina using ethyl acetate/hexanes as the eluent to afford the aniline.

General Procedure for Aniline synthesis from Aryl Halides (10 mmol scale) Provided in Table 3.

In a 100 ml round bottom flask 10 mL each of DMF and H_2O has taken and argon gas was passed gently for 5 minutes. The reagents CuI (1 mmol, 190 mg) and D-glucosamine (0.5 mmol, 108 mg), KI (10 mmol, 1.67 gm), KOH (10 mmol, 560 mg) and NaN_3 (30 mmol, 2.01 gm) were transferred to the flask. Following this, 4-bromoacetophenone (10 mmol) was added to the reaction mixture. Then the reaction mixture with a condenser was placed in a preheated oil bath at 120 ^oC and stirring continued. The reaction was monitored using TLC. After the completion, the reaction was allowed to cool to room temperature. Then the aniline was extracted from water layer to organic layer by using dichloromethane as solvent. The further purification of aniline was done by column chromatography on silica gel using ethyl acetate/hexanes as the eluent.

Characterization Data:

2-methoxyaniline (Table 3, entries 5 & 6) deep brown liquid; R_f = 0.73 (in 30% EtOAc/Hexane); IR 1038, 1160, 1207, 1297, 1465, 1492, 1601, 2927, 3368, 3463 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.82 (s, 2H), 3.88 (s, 3H), 6.72 - 6.81 (m, 2H), 6.81 - 6.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 110.5, 115.0, 118.5, 121.1, 136.2, 147.3; HRMS [M^++1] Calculated for $C_7H_{10}NO$: 124.0762; found: 124.0758.

3-methoxyaniline (Table 3, entries 7 & 8) dark brown liquid; R_f = 0.54 (in 30% EtOAc/Hexane); IR 1037, 1225, 1270, 1461, 1508, 2926, 3371, 3458 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.72 (s, 2H), 3.78 (s, 3H), 6.26 (t, *J* = 2.0 Hz, 1H), 6.31 (d, *J* = 8 Hz, 1.6 Hz, 1H), 6.29 (d, *J* = 8.4 Hz, 1H), 7.10 (t, *J* = 8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.0, 101.0, 103.8, 107.9, 130.1, 148.0, 160.7; HRMS [M^++1] Calculated for $C_7H_{10}NO$: 124.0762; found: 124.0760.

4-methoxyaniline (Table 3, entries 3 & 4) black solid; MP 56-59 °C. R_f = 0.43 (in 30% EtOAc/Hexane); IR 1031, 1125, 1234, 1458, 1506, 1630, 1858, 2053, 2960, 3345, 3420 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.35 (s, 2H), 3.75 (s, 3H), 6.62 - 6.68 (m, 2H), 6.72 - 6.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 114.9, 116.5, 140.1, 152.8; HRMS [M^++1] Calculated for $C_7H_{10}NO$: 124.0762; found: 124.0768.

4-nitroaniline (Table 3, entries 9,10 & 20) yellow solid; mp 146-149 °C . R_f = 0.31 (in 30% EtOAc/Hexane); IR 1111, 1300, 1473, 1595, 1631, 2362, 3360, 3477 cm^{-1}; ^1H NMR (400 MHz, CD_3OD) δ 4.85 (s, 2H), 6.58 - 6.64 (m, 2H), 7.94 - 8.00 (m, 2H); ^{13}C

NMR (100 MHz, CD_3OD) δ 1 ß.6, 127.3, 138.3, 156.7; HRMS [M^++1] Calculated for $C_6H_7N_2O_2$: 139.0508; found: 139.0506.

3-nitroaniline (Table 3, entry 11) yellow solid; mp 111-114 ^oC; R_f = 0.21 (in 10% EtOAc/Hexane); IR 1084, 1265, 1342, 1482, 1521, 1619, 3327, 3431 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.97 (s, 2H), 6.87 (dd, *J* = 8 Hz, 2 Hz, 1H), 7.18 (t, *J* = 8 Hz, 1H), 7.40 (t, *J* = 2 Hz, 1H), 7.45 - 7.51 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 109.1, 113.2, 120.8, 130.0, 147.6, 149.3; HRMS [M^++1] Calculated for $C_6H_7N_2O_2$: 139.0508; found: 139.0504.

4-aminoacetophenone (Table 3, entry 1 & 2) white solid; mp 103-107 ^oC R_f = 0.30 (in 30% EtOAc/Hexane); IR 1167, 1278, 1358, 1436, 1591, 1649, 3224, 3328 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 4.35 (d, *J* = 56.7 Hz, 2H), 6.57 - 6.69 (m, 2H), 7.73 - 7.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.2, 113.8, 127.6, 130.9, 151.6, 196.7; HRMS [M^++1] Calculated for $C_8H_{10}NO$: 136.0762; found: 136.0759.

3-aminoacetophenone (Table 3, entry 19) white solid; mp 94-98 ^oC; R_f = 0.32 (in 30% EtOAc/Hexane); IR 1015, 1238, 1289, 1323, 1355, 1459, 1491, 1599, 1669, 3369, 3466 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.59 (s, 3H), 3.86 (s, 2H), 6.90 (dd, *J* = 8 Hz, 1.6 Hz, 1H), 7.23 - 7.33 (m, 2H), 7.37 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.8, 114.1, 119.0, 119.8, 129.6, 138.3, 146.8, 198.6; HRMS [M^++1] Calculated for $C_8H_{10}NO$: 136.0762; found: 136.0757.

2-aminoacetophenone (Table 3, entry 18) yellow liquid, R_f = 0.56 (in 20% EtOAc/Hexane); IR 1020, 1162, 1246, 1367, 1447, 1484, 1550, 1632, 2820, 2945, 3340,

3443 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.61 (s, 3H), 6.32 (s, 2H), 6.64 - 6.73 (m, 2H), 7.30 (dt, *J* = 8.4 Hz, 1.2 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.9, 115.8, 117.3, 118.3, 132.1, 134.5, 150.4, 200.9; HRMS [M^++1] Calculated for $C_8H_{10}NO$: 136.0762; found: 136.0761.

4-aminobenzaldehyde (Table 3, entry 12) yellow solid, R_f = 0.15 (in 20% EtOAc/Hexane); IR 1046, 1103, 1163, 1250, 1390, 1440, 1597, 1664, 1706, 2935, 3447 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-D6) δ 4.85 (s, 2H), 6.68 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.4Hz, 2H), 9.55 (s, 1H); ^{13}C NMR (100 MHz, DMSO-D6) δ 114.5, 127.0, 133.7, 156.9, 192.3; HRMS [M^++1] Calculated for C_7H_8NO: 122.0606; found: 122.0601.

4-aminobenzophenone (Table 3, entry 13) yellow solid, mp 121-124 ^{o}C; R_f = 0.20 (in 20% EtOAc/Hexane); IR 1020, 1287, 1321, 1415, 1445, 1593, 1637, 2827, 2945, 3360 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.18 (s, 2H), 6.66 (dd, *J* = 8.4 Hz, 2.0 Hz, 2H), 7.41 - 7.50 (m, 2H), 7.50 - 7.58 (m, 1H), 7.23 (d, *J* = 8.0 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 113.7, 127.5, 128.2, 129.6, 131.5, 133.1, 139.0, 151.1, 195.5; HRMS [M^++1] Calculated for $C_{13}H_{12}NO$: 198.0919; found: 198.0926.

2-aminobenzophenone (Table 3, entry 15) yellow solid, mp 103-107 ^{o}C; R_f = 0.57 (in 20% EtOAc/Hexane); IR 1023, 1114, 1245, 1413, 1450, 1552, 1628, 2524, 2830, 2946, 3367 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.14 (s, 2H), 6.65 (t, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 7.29 - 7.38 (m, 1H), 7.45 - 7.53 (m, 3H), 7.54 - 7.61 (m, 1H), 7.65 - 7.73 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.6, 117.1, 118.3, 128.2, 129.2, 131.2, 134.4, 134.7, 140.2, 151.1, 199.2; HRMS [M^++1] Calculated for $C_{13}H_{12}NO$: 198.0919; found: 198.0910.

3-aminobenzophenone (Table 3, entry 14) yellow solid, mp 81-84 ^{o}C; R_f = 0.29 (in 20% EtOAc/Hexane); IR 1024, 1113, 1321, 1414, 1450, 1649, 2830, 2951, 3390 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 2H), 6.30 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.17 (d, *J* = 7.2 Hz, 2H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.61 (dt, *J* = 7.2 Hz, 1.2 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 116.0, 119.1, 120.8, 128.3, 129.2, 130.2, 132.4, 137.9, 138.8, 146.6, 197.1; HRMS [M^++1] Calculated for $C_{13}H_{12}NO$: 198.0919; found: 198.0916.

(2-amino-5-nitrophenyl)(phenyl)methanone (Table 3, entry 16) yellow solid, mp 166-168 ^{o}C; R_f = 0.31 (in 20% EtOAc/Hexane); IR 1028, 1112, 1262, 1330, 1416, 1452, 1637, 2527, 2834, 2947, 3370 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (d, *J* = 8.4 Hz, 1H), 6.90 (s, 2H), 7.52 (s, 2H), 7.57 - 7.83 (m, 3H), 8.16 (d, *J* = 7.6 Hz, 1H), 8.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 116.1, 116.9, 128.8, 129.2, 129.4, 131.7, 132.3, 136.8, 138.6, 155.4, 198.0; HRMS [M^++1] Calculated for $C_{13}H_{11}N_2O_3$: 243.0770; found: 243.0760.

2-Amino-2',5-dichlorobenzophenone (Table 3, entry 17) yellow solid, mp 87-89 ^{o}C; R_f = 0.29 (in 20% EtOAc/Hexane); IR 1018, 1043, 1232, 1372, 1414, 1452, 1631, 1644, 1708, 2521, 2833, 2941, 2969, 3455 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.46 (s, 2H), 6.68 (d, *J* = 8.8 Hz, 1H), 7.11 (d, *J* = 2.4Hz, 1H), 7.23 (dd, *J* = 8.8Hz, 2.4Hz, 1H), 7.30 (dd, *J* = 7.6Hz, 1.6Hz, 1H), 7.36 (dt, *J* = 7.2Hz, 1.2Hz, 1H), 7.42 (dt, *J* = 8.0Hz, 1.6Hz, 1H), 7.46 (d, *J* = 7.6Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.1, 118.6, 120.2, 126.9, 128.5, 130.2, 130.81, 130.84, 133.3, 135.4, 139.1, 150.0, 196.5; HRMS [M^++1] Calculated for $C_{13}H_{10}Cl_2NO$: 266.0139; found: 266.0134.

1-azido-4-methoxybenzene (Scheme 1, compound 1); Yellow liquid; R_f = 0.4 (in 100% hexane); IR 1029, 1104, 1178, 1245, 1289, 1503, 1636, 2103, 2947, 3428 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.70 (s, 3H), 6.80 (t, J = 4.4 Hz, 2H), 6.84-6.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 115.3, 120.1, 132.5, 157.2; GC-MS EI+ : m/z calculated for $C_7H_7N_3O$: 149.

References

1. (a) Zhao, H.; Fu, H.; Quio, R. *J. Org. Chem.* **2010**, *75*, 3311. (b) Markiewicz, J. T.; Wiest, O.; Helquist, P. *J. Org. Chem.* **2010**, *75*, 4887. (c) Messaoudi, S.; Brion, J-D.; Alami, M. *Adv. Synth. Catal.* **2010**, *352*, 1677.

2. (a) Xia, N.; Taillefer, M. *Angew. Chem. Int. Ed.* **2009**, *48*, 337. (b) Wang, D.; Cai, Q.; Ding, K. *Adv. Synth. Catal.* **2009**, *351*, 1722.

ICP mass analysis for the copper content in the organic phase after aqueous work up.

SOPHISTICATED ANALYTICAL INSTRUMENT FACILITY
IITM, CHENNAI-36
PERKIN ELMER OPTIMA 5300 DV ICP-OES

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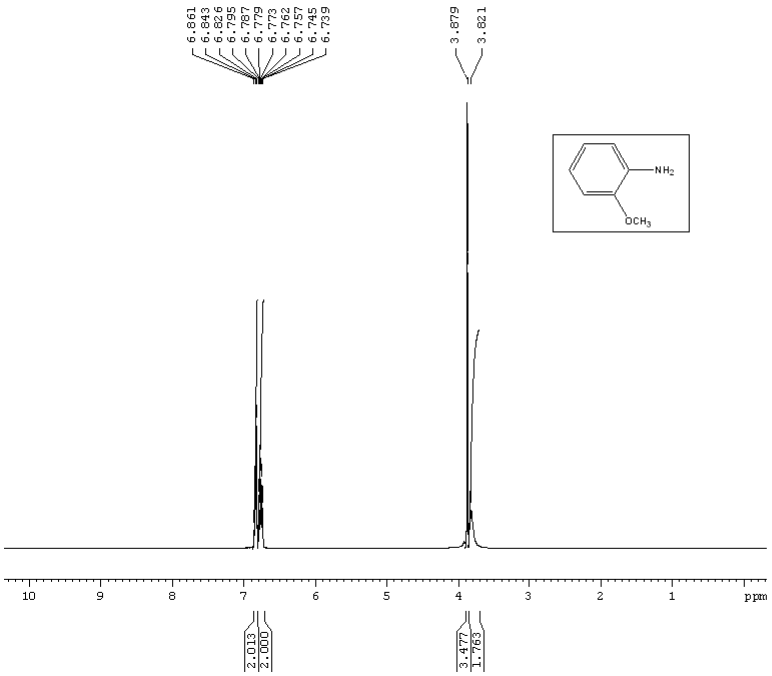
2-Methoxyaniline



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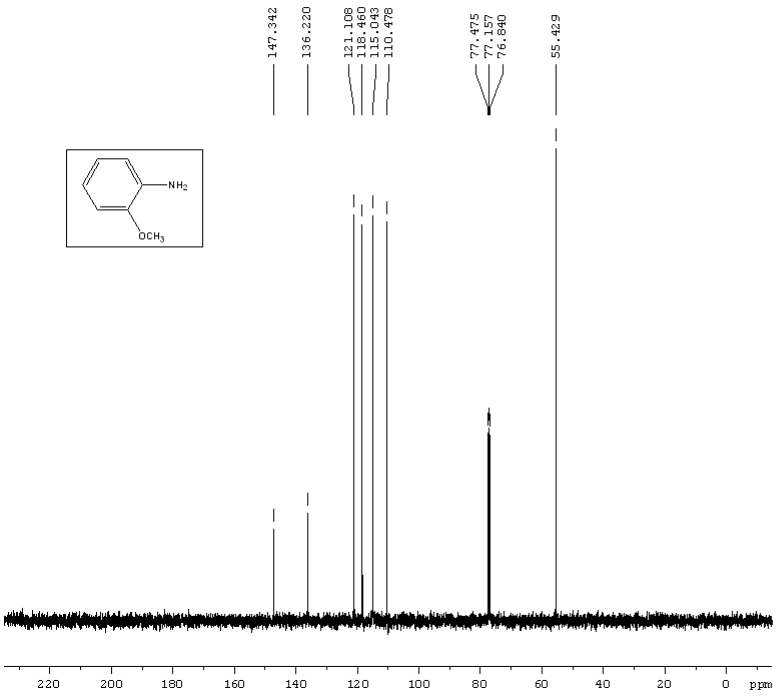

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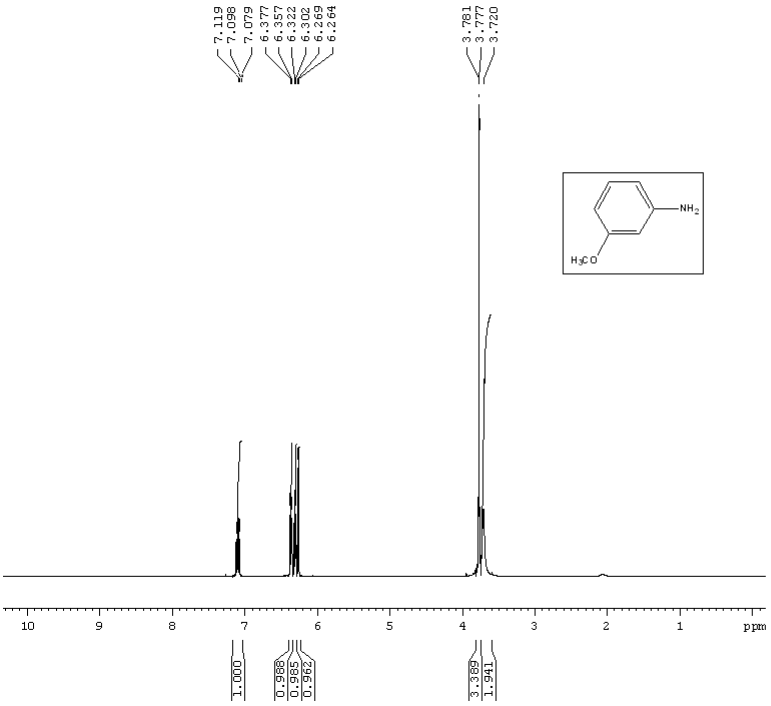
3-Methoxyaniline



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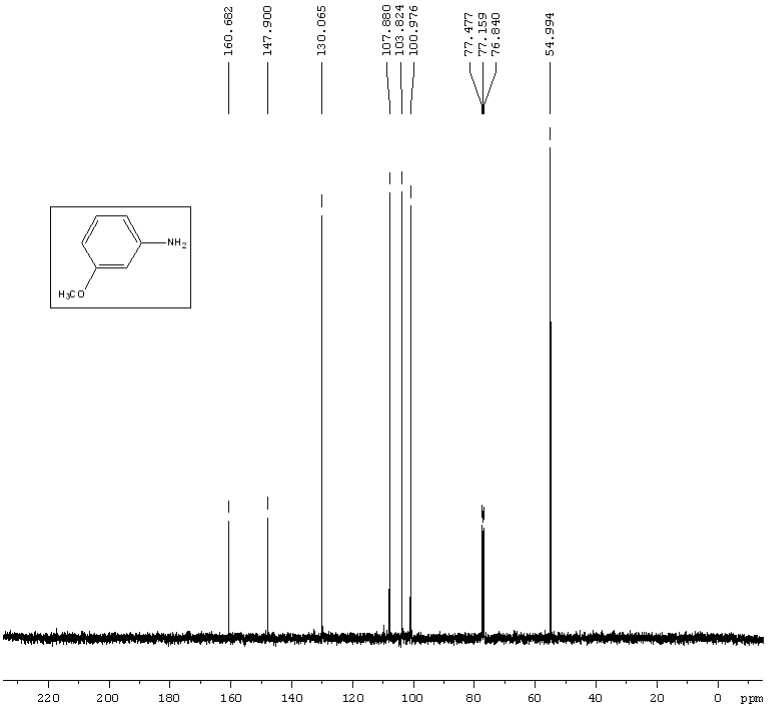

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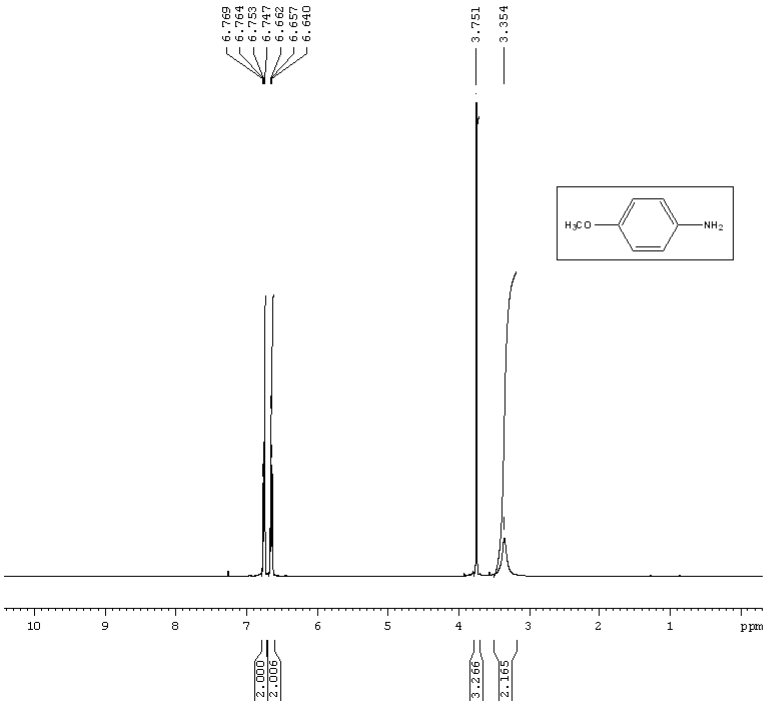
4-Methoxyanisole



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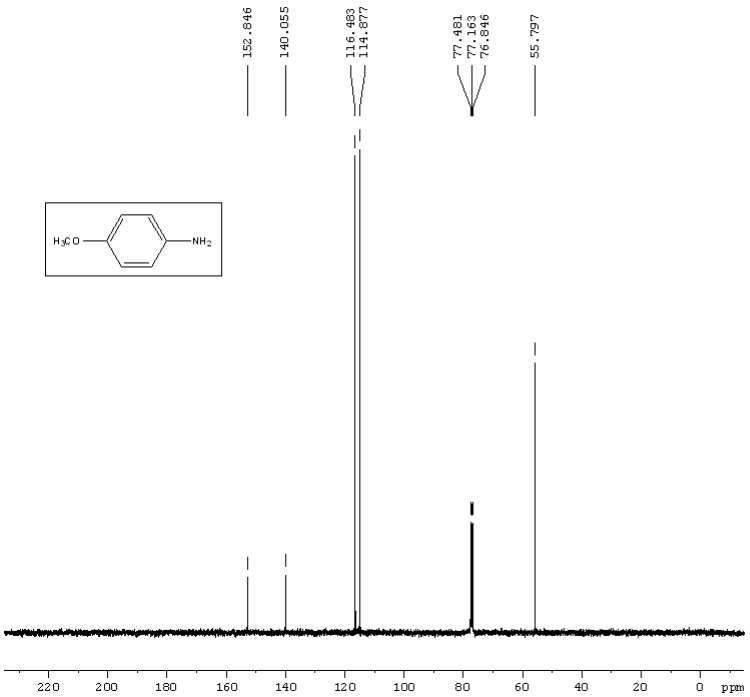

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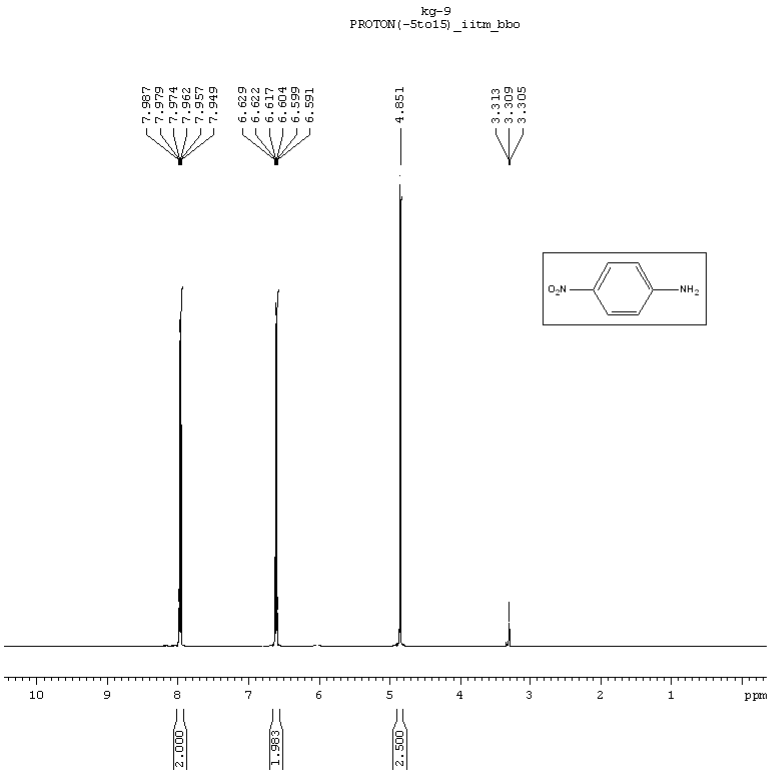
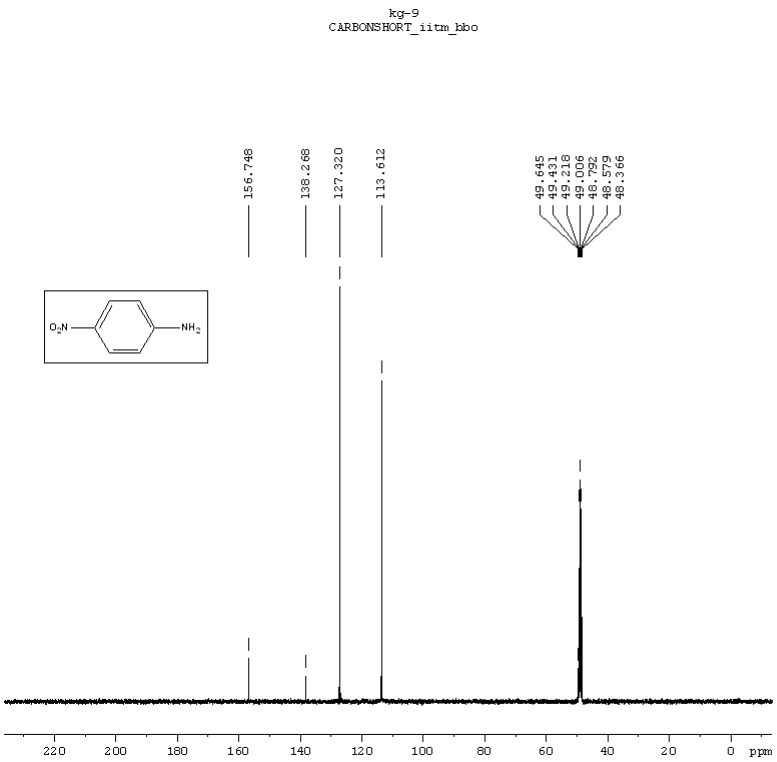
HZCM 1256.28137 Hz/cm

4-Nitroaniline

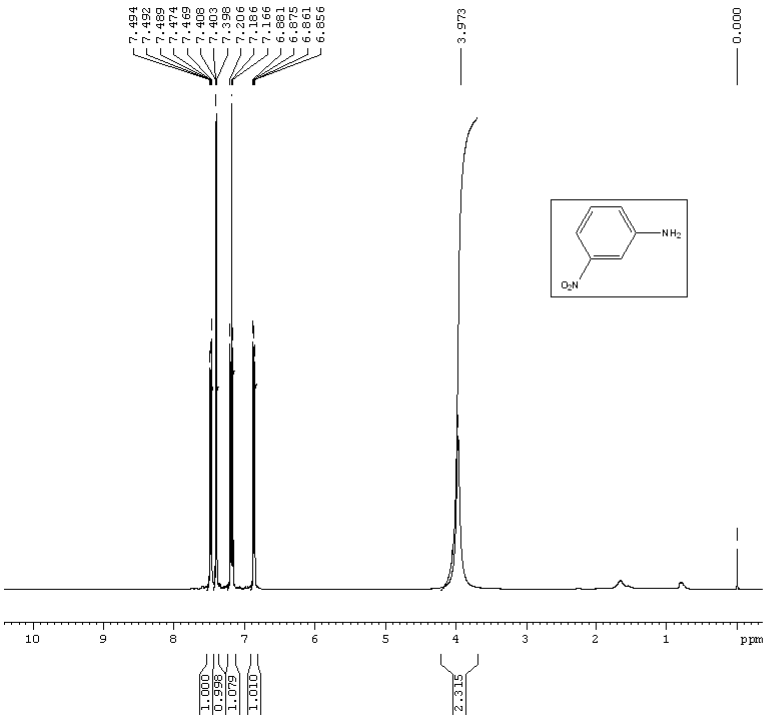



```
Current Data Parameters
NAME                  gsk0611
EXPNO                     138
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                     9.07
INSTRUM                 av400
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                 MeOD
NS                        32
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                       0.0 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                400.1300076 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        3.00
```



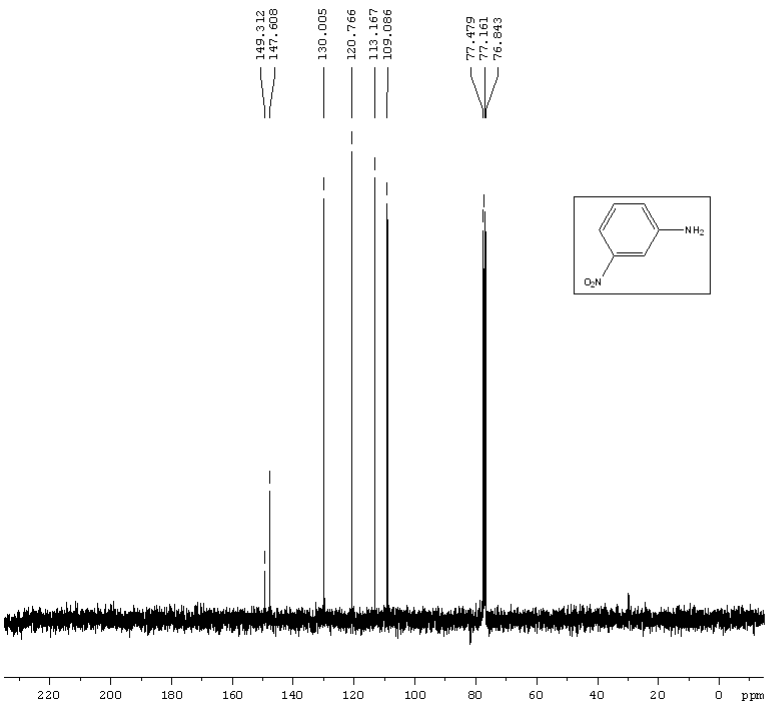

```
Current Data Parameters
NAME                  gsk0611
EXPNO                     139
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                     9.20
INSTRUM                 av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                     16384
SOLVENT                 MeOD
NS                       512
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                       0.0 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                100.6126319 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                    23628.81 Hz
F2P                    -14.877 ppm
F2                     -1496.79 Hz
PPMCM                 12.48630 ppm/cm
HZCM                1256.27966 Hz/cm
```

3-Nitroaniline



BRUKER

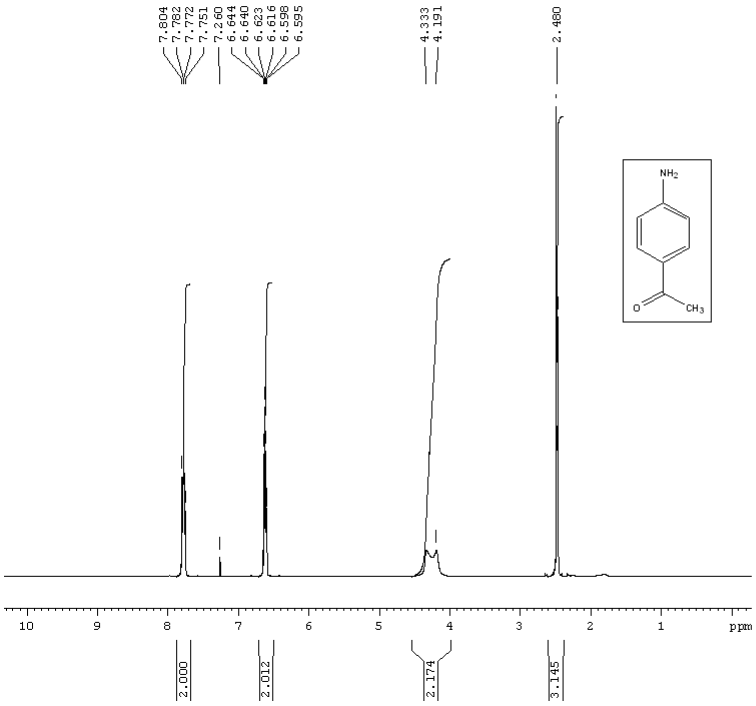
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     150
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                    20.29
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                       80.6
DW                     59.600 usec
DE                      6.00 usec
TE                       0.0 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                400.1300451 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                      3.00
```



BRUKER

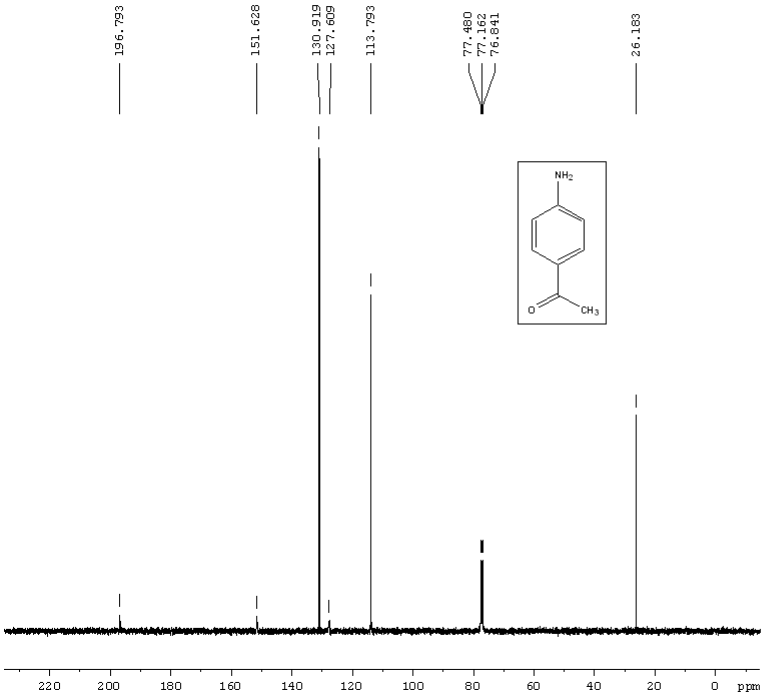
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     151
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                    20.32
INSTRUM                 av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                     16384
SOLVENT                CDCl3
NS                        116
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                       0.0 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                100.6127633 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-Aminoacetophenone



BRUKER

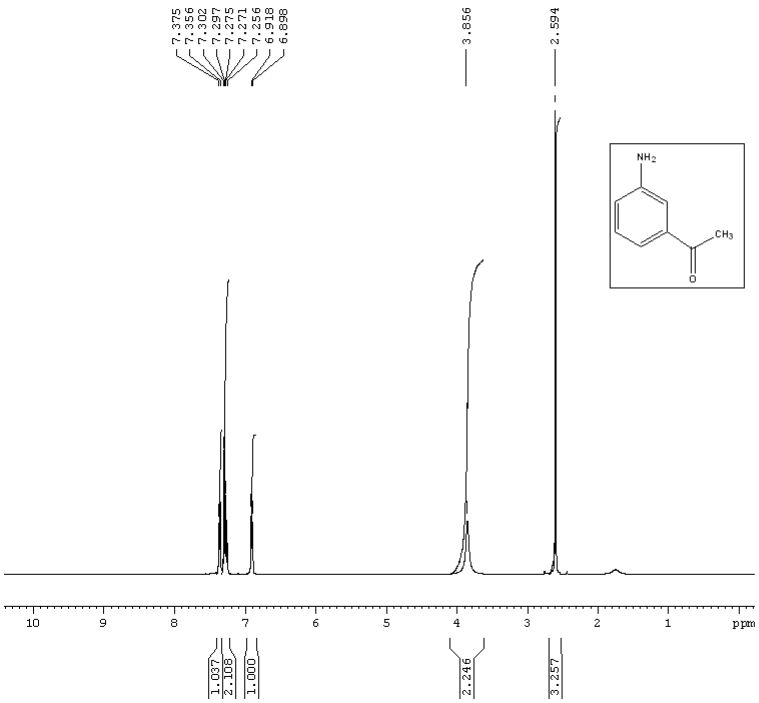
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     108
PROCNO                      1

F2 - Acquisition Parameters
Date_              20110614
Time                  22.01
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                      71.8
DW                 59.600 usec
DE                  6.00 usec
TE                     0.0 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                     10.129 ppm
F1                    4052.73 Hz
F2P                     -1.000 ppm
F2                    -400.13 Hz
PPMCM                  0.55643 ppm/cm
HZCM                 222.64290 Hz/cm
```



BRUKER

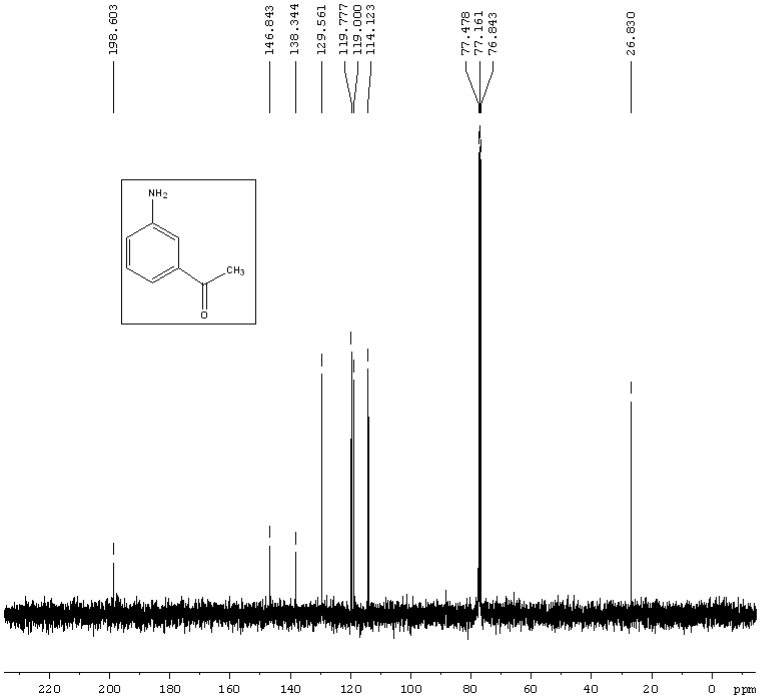
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     111
PROCNO                      1

F2 - Acquisition Parameters
Date_              20110614
Time                  22.17
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      512
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                     0.0 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                 100.6127614 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
```

3-Aminoacetophenone



BRUKER

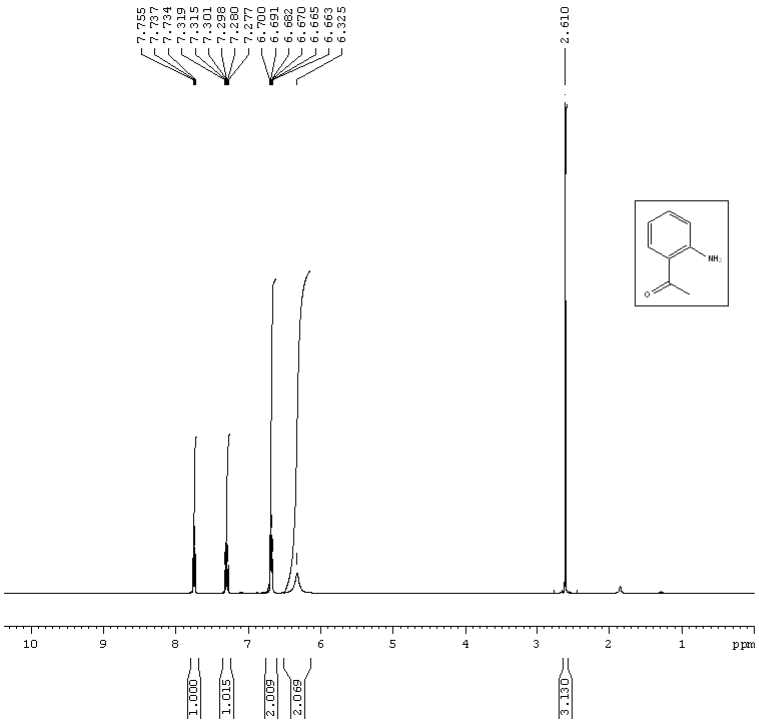
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     117
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                     6.36
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        19
DS                         4
SWH                 8389.262 Hz
FIDRES              0.256020 Hz
AQ                  1.9530228 sec
RG                      143.7
DW                     59.600 usec
DE                      6.00 usec
TE                       0.0 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
```



BRUKER

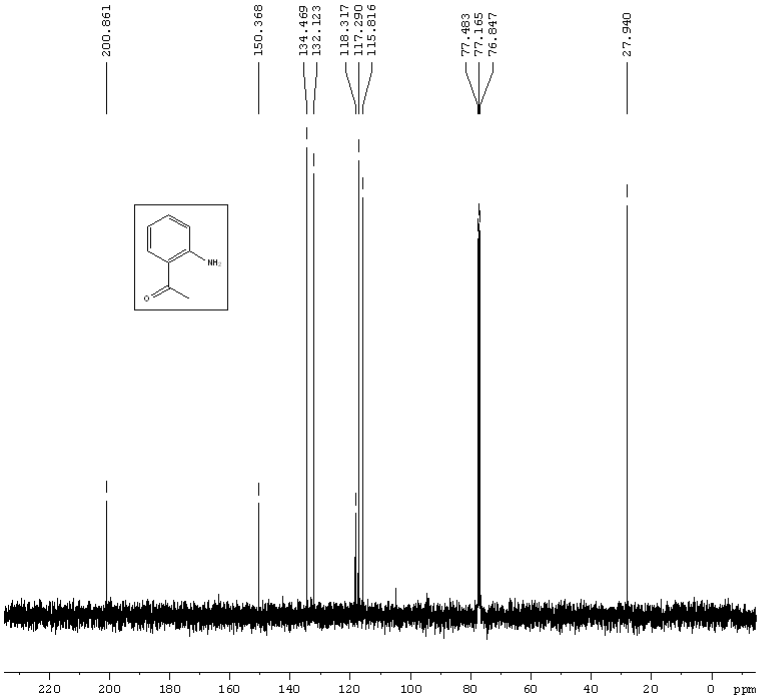
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     118
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                     6.41
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                     16384
SOLVENT                CDCl3
NS                       185
DS                         4
SWH                25125.629 Hz
FIDRES              1.533547 Hz
AQ                  0.3260916 sec
RG                      16384
DW                     19.900 usec
DE                      6.00 usec
TE                       0.0 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                100.6127599 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
```

2-Aminoacetophenone



BRUKER

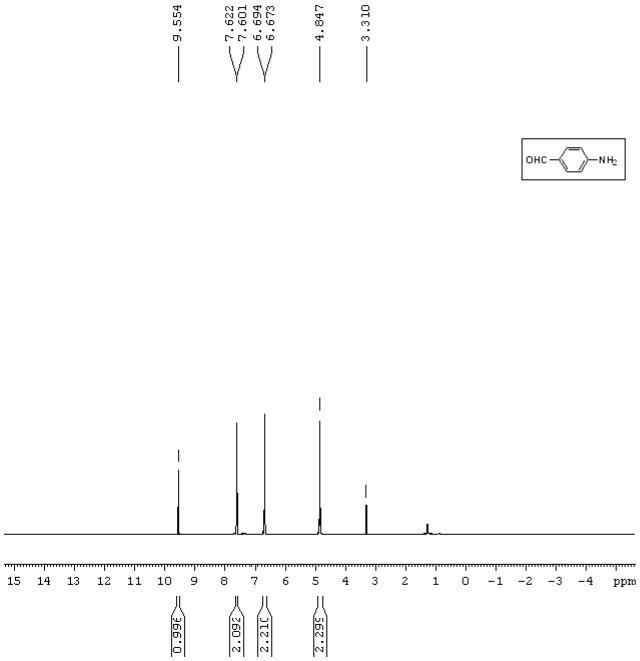
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     125
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                     7.21
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                         64
DW                     59.600 usec
DE                      6.00 usec
TE                       0.0 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
```



BRUKER

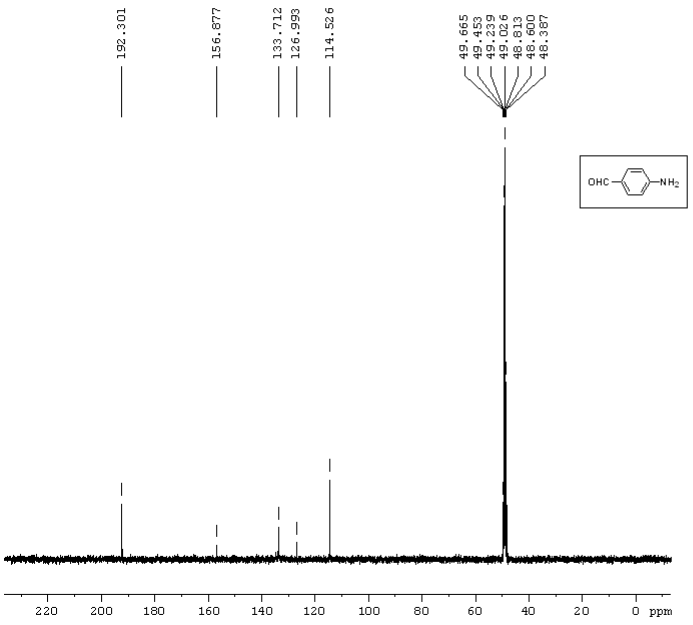
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     126
PROCNO                      1

F2 - Acquisition Parameters
Date_                20110615
Time                     7.24
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                      16384
SOLVENT                 CDCl3
NS                         86
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                       0.0 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                100.6127690 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
```

4-Aminobenzaldehyde



BRUKER

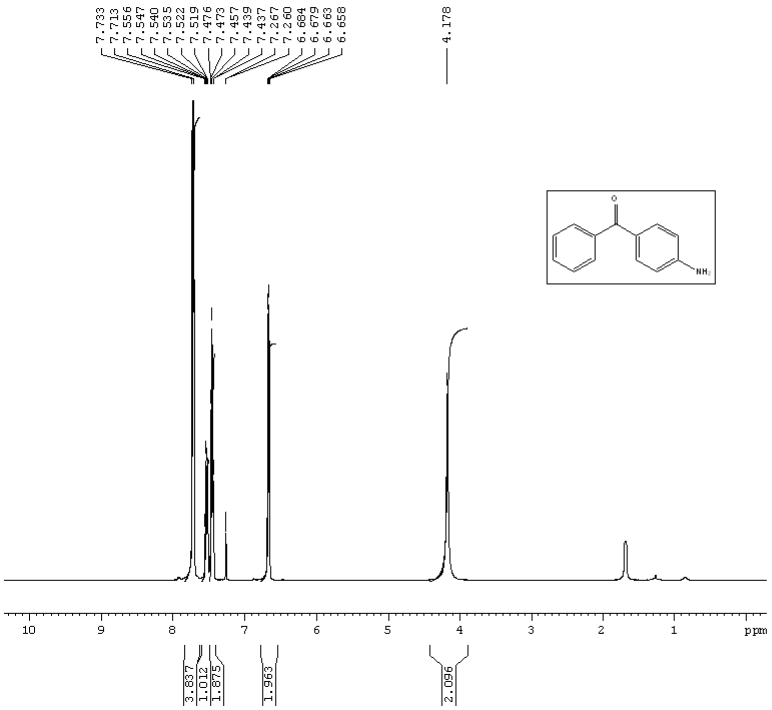
```
Current Data Parameters
NAME                 gskl110
EXPNO                     15
PROCNO                     1

F2 - Acquisition Parameters
Date_              20101101
Time                   12.05
INSTRUM                av400
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                MeOD
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
SF01             400.1319460 MHz

F2 - Processing parameters
SI                       16384
SF               400.1300071 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
```



BRUKER

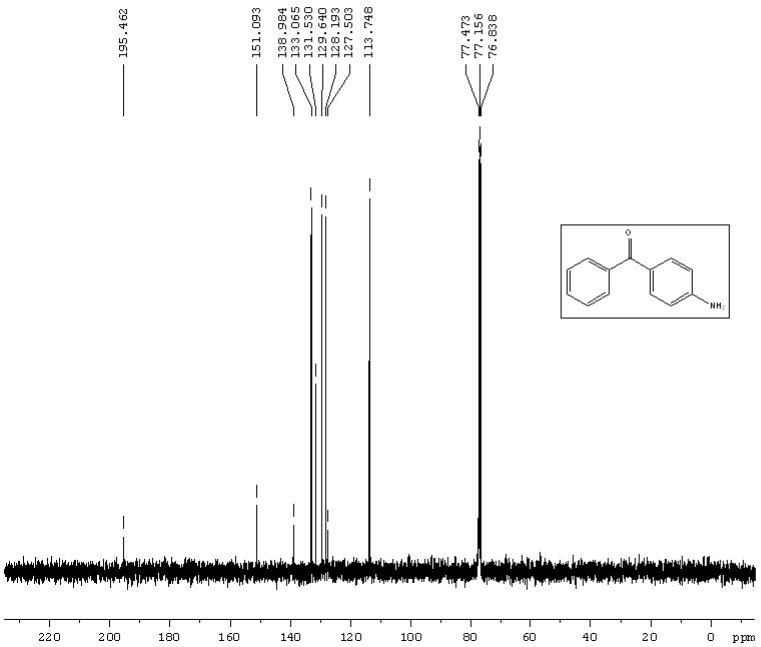
```
Current Data Parameters
NAME                 gskl110
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20101101
Time                   12.15
INSTRUM                av400
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    16384
SOLVENT                MeOD
NS                       364
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
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               100.6126261 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                    23628.80 Hz
F2P                    -14.877 ppm
F2                    -1496.79 Hz
PPMCM                 12.48630 ppm/cm
HZCM                1256.27954 Hz/cm
```

4-Aminobezophenone



BRUKER

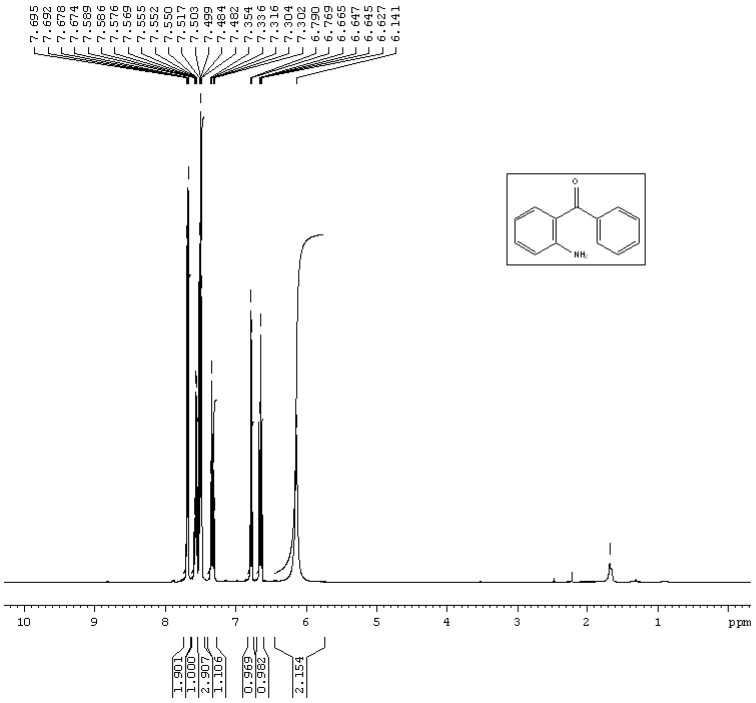
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     119
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110615
Time_                   6.46
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                     161.3
DW                  59.600 usec
DE                   6.00 usec
TE                     0.0 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            400.1300155 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                    3.00
```



BRUKER

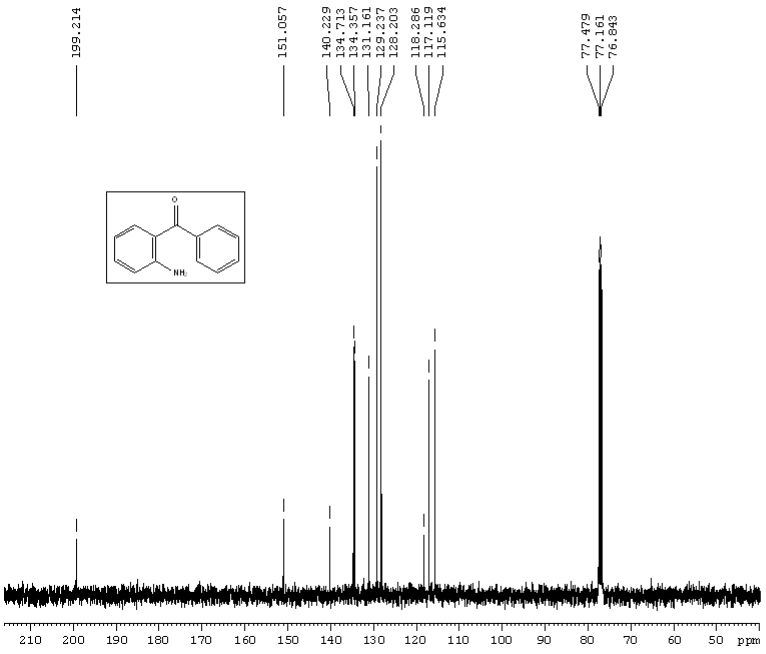
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     120
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110615
Time_                   6.48
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      241
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                     0.0 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            100.6127603 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
```

2-Aminobenzophenone



BRUKER

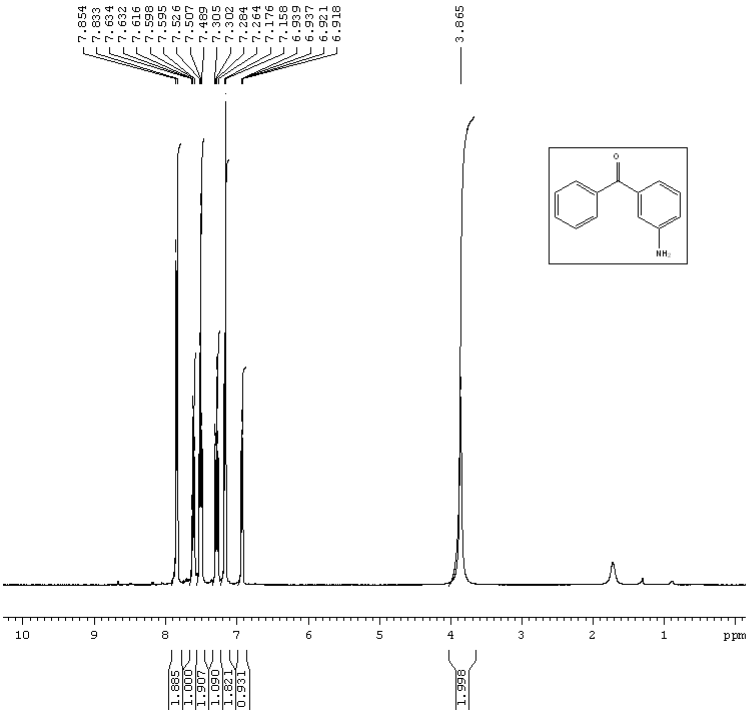
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     109
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110614
Time                   22.08
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                       128
DW                    59.600 usec
DE                     6.00 usec
TE                      0.0 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
```

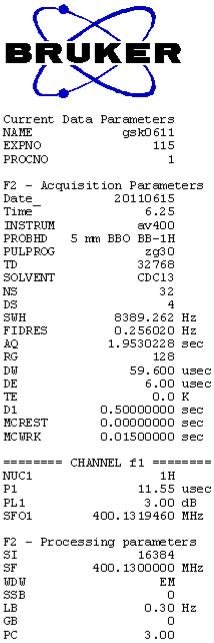


BRUKER

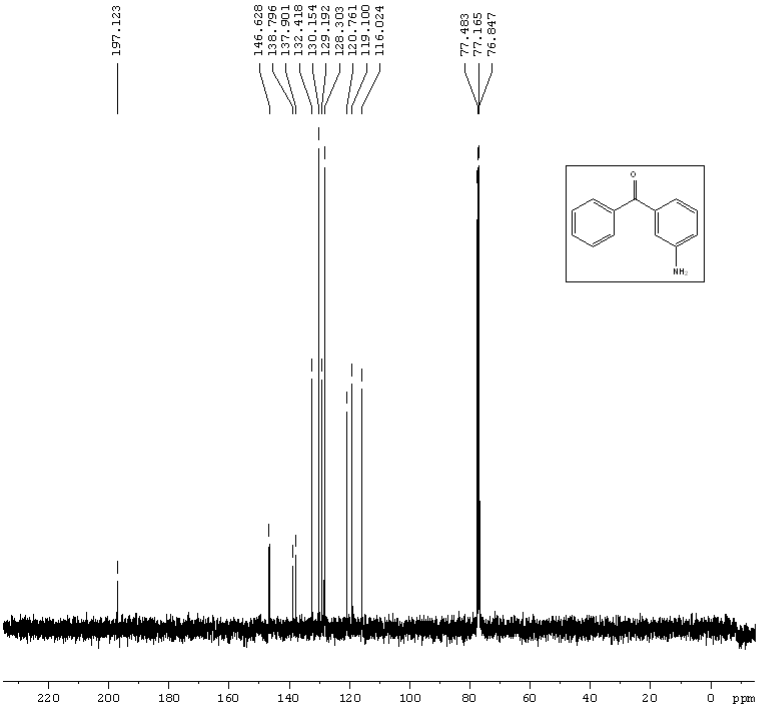
```
Current Data Parameters
NAME                  gsk0611
EXPNO                     110
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110614
Time                   22.12
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT                CDCl3
NS                       184
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                      0.0 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                100.6127603 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
```

3-Aminobenzophenone



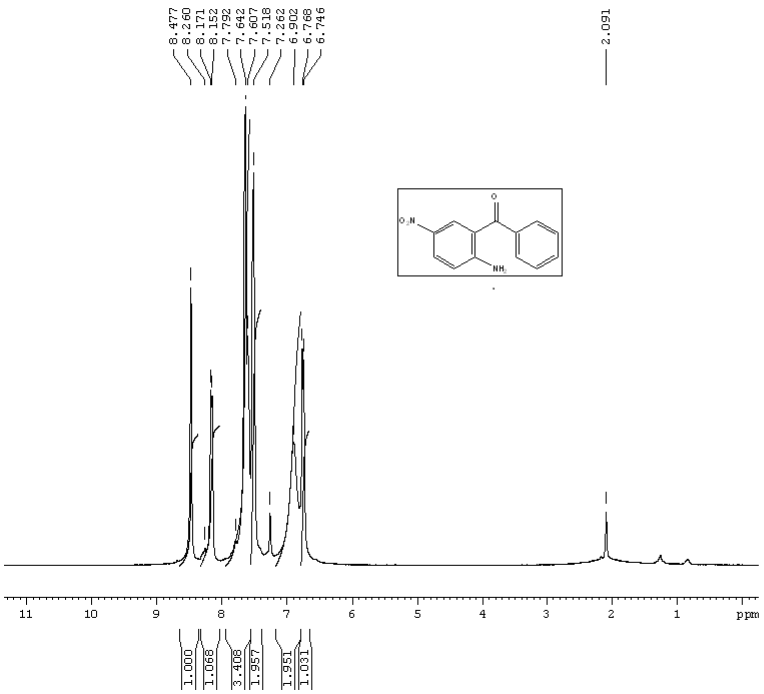


```
Current Data Parameters
NAME                  gsk0611
EXPNO                     115
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110615
Time                    6.25
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                       128
DW                    59.600 usec
DE                     6.00 usec
TE                      0.0 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
```

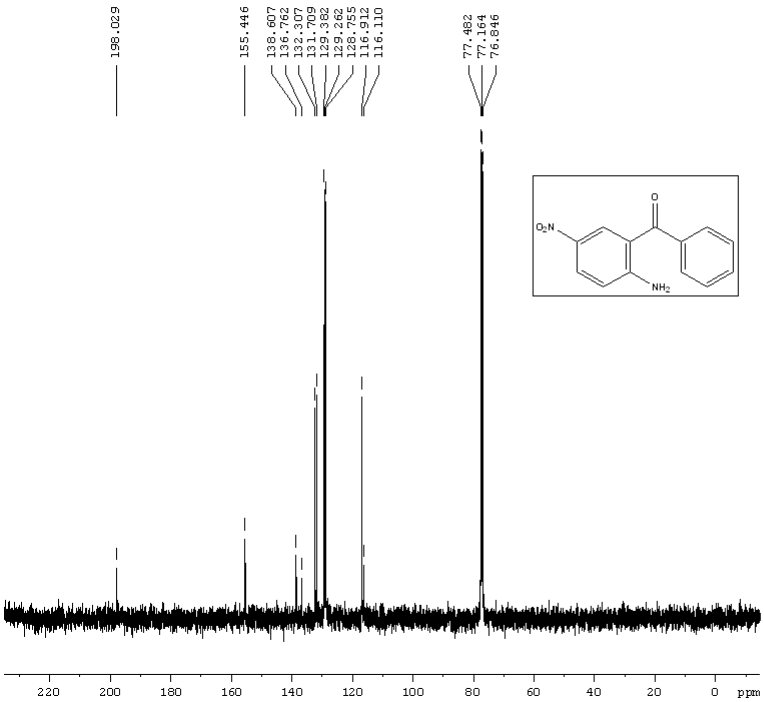


```
Current Data Parameters
NAME                  gsk0611
EXPNO                     116
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110615
Time                    6.28
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT                CDCl3
NS                       225
DS                         4
SWH               25125.629 Hz
FIDRES             1.533547 Hz
AQ                 0.3260916 sec
RG                   11585.2
DW                   19.900 usec
DE                     6.00 usec
TE                      0.0 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             100.6127690 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
```

(2-Amino-5-nitrophenyl)(phenyl)methanone

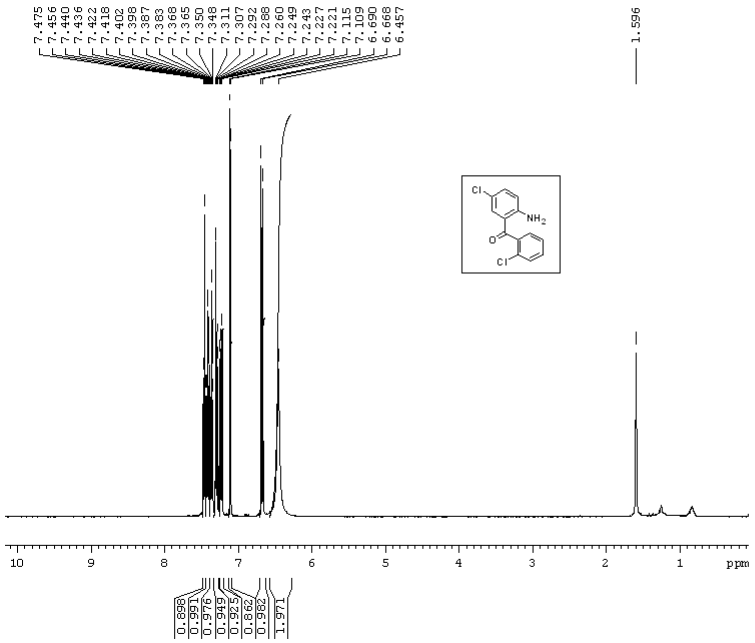



```
Current Data Parameters
NAME                  gsk0611
EXPNO                     127
PROCNO                      1

F2 - Acquisition Parameters
Date_              20110615
Time                   7.31
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                     143.7
DW                    59.600 usec
DE                     6.00 usec
TE                      0.0 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                400.1300165 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      3.00
```




```
Current Data Parameters
NAME                  gsk0611
EXPNO                     128
PROCNO                      1

F2 - Acquisition Parameters
Date_              20110615
Time                   7.38
INSTRUM               av400
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      512
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                      0.0 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            100.6127599 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
```

(2-Amino-5-chlorophenyl)(2-chlorophenyl)methanone



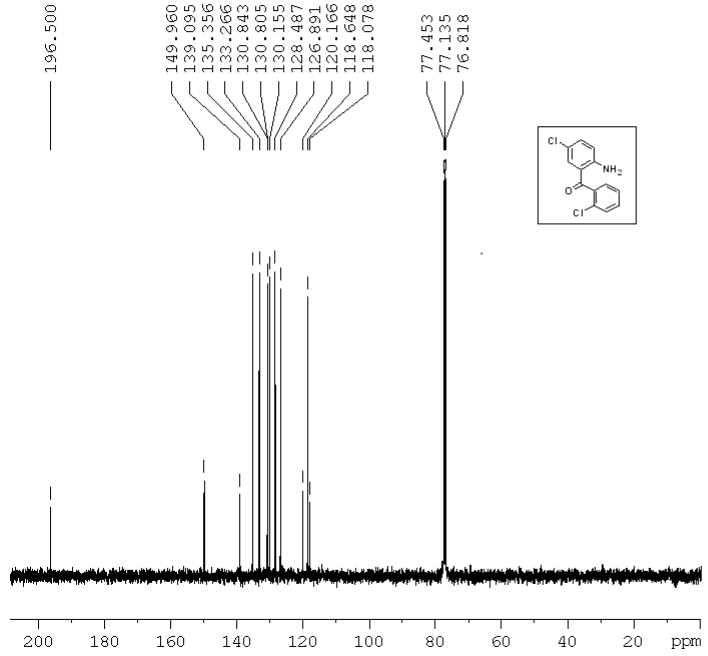
Current Data Parameters
NAME gsk0111
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110119
Time 7.17
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 228.1
DW 59.600 usec
DE 6.00 usec
TE 295.0 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 10.129 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 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100911
Time 12.07
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 512
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 298.0 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

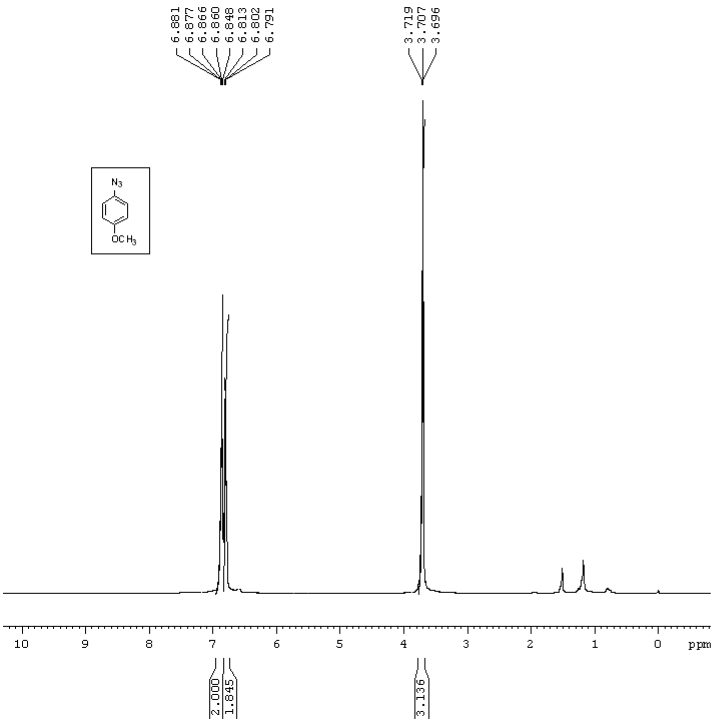
======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SF01 100.6238364 MHz

======== 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 100.6127623 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

1-Azido-4-methoxybenzene



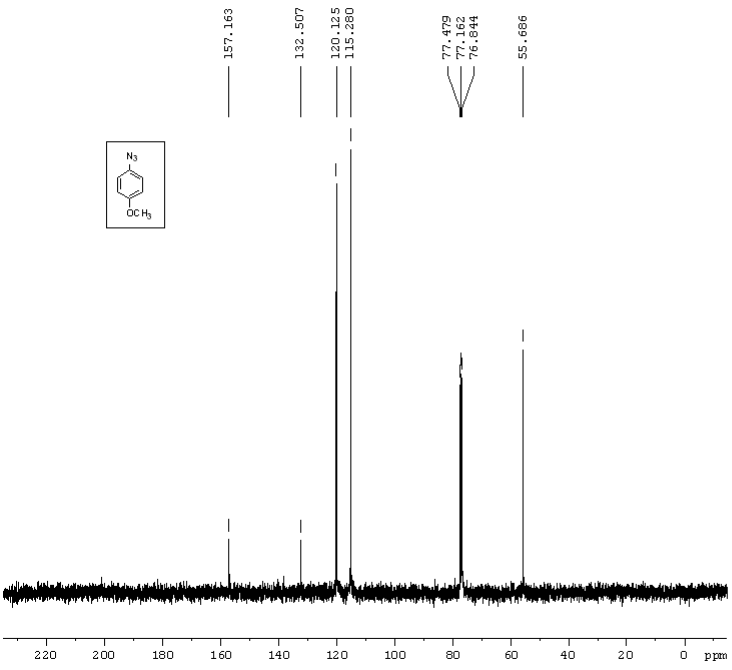
Current Data Parameters
NAME gsk0111
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110107
Time 17.04
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 301.6 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 400.1300526 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 222.64293 Hz/cm



Current Data Parameters
NAME gsk0111
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110107
Time 17.20
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 242
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 304.1 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 100.6127587 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