Supplementary Material (ESI) for Chemical Communications

Supporting Information

Glucosamine as a Green Ligand for Copper-Catalyzed Selective Synthesis of Aniline from Aryl Halides and NH_3

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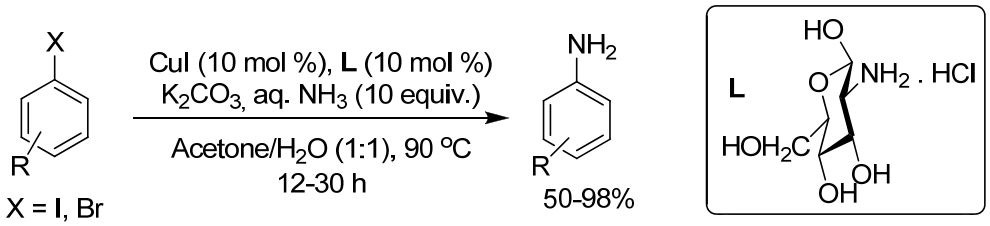
Experimental Section:

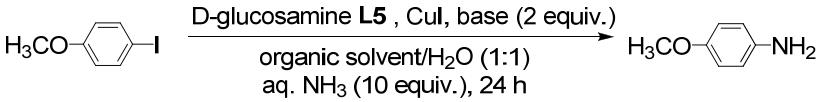
All the reactions were carried out in pressure tube under normal atmospheric air. Commercially available monosaccharide ligands are purchased from Aldrich chemicals. Copper (I) iodide and other copper salts purchased from Alfa Aesar and Aldrich chemicals. Halobenzenes are purchased from Aldrich chemicals, Alfa Aesar, SRL (India) and Awra (India) chemicals. Potassium hydroxide purchased from Ranbaxy (India). Acetone 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 Acetone/H_2O (1:1) mixture has taken in 15 mL reaction tube. Aryl halide (0.5 mmol), CuI (9.5 mg, .05 mmol), D-glucosamine hydrchloride (10.8 mg, 0.05 mmol) and K_2CO_3 (1 mmol, 138 mg) were then transferred to the tube. After 10 minutes of stirring at 90 ^{o}C, 300 μL of aqueous ammonia (28% W/V) was added and the stirring continued at 90 ^{o}C. The reaction was monitored using thin layer chromatographic technique. After complete disappearance of aryl halide, the solvent was evaporated and further purification has done by column chromatography on neutral alumina using ethyl acetate/hexanes as the eluent to afford the aniline.

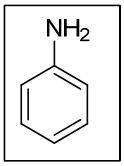
Table 1 Optimization of solvent systems, bases and temperature.



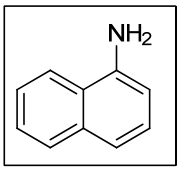
Entry	CuI/**L5** (mol %)	Solvent/H_2O (1:1)	Base	Temp. (^oC)	Yield (%)[a]
1	5:5	Acetone	K_2CO_3	90	57
2	5:10	Acetone	K_2CO_3	90	72
3	**10:10**	**Acetone**	**K_2CO_3**	**90**	**90/20[b]**
4	10:20	Acetone	K_2CO_3	90	75
5	20:20	Acetone	K_2CO_3	90	49
6	10:10	THF	K_2CO_3	90	12
7	10:10	Dioxane	K_2CO_3	90	62
8	10:10	Acetinitrile	K_2CO_3	90	57
9	10:10	DMF	K_2CO_3	90	69
10	10:10	Acetone	Cs_2CO_3	90	73
11	10:10	Acetone	K_3PO_4	90	61
12	10:10	Acetone	NaOAc	90	35
13	10:10	Acetone	Na_2CO_3	90	36
14	10:10	Acetone	KOH	90	36
15	10:10	Acetone	NaOH	90	32
16	10:10	Acetone	NaOMe	90	42
17	10:10	Acetone	K_2CO_3	60	41[c]
18	10:10	Acetone	K_2CO_3	80	62[c]
19	10:10	H_2O	K_2CO_3	90	9
20	10:10	H_2O	K_2CO_3	90	20[d]

[a]Isolated yield. [b]Reaction performed without base. [c]Reaction time was 48 hours. [d]Reaction was performed in water in the presence of 0.5 equiv. of ^{n}-Bu_4NBr.

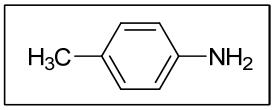
Characterization Data:



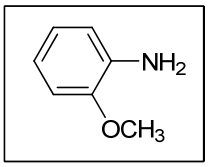
Aniline (Table 2, entry 21) colorless liquid; R_f = 0.55 (in 20% EtOAc/Hexane); IR 1276, 1496, 1610, 3034, 3217, 3356 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.66 (s, 2H), 6.71(d, *J* = 8.0Hz, 2H), 6.80 (t, *J* = 7.6Hz, 1H), 7.19 (t, *J* = 8.0Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.2, 118.6, 129.3, 146.4; GC-MS EI+ : m/z calculated for C_6H_7N: 93.



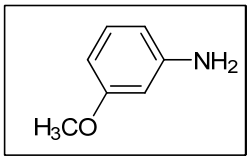
1-Aminonapthalene (Table 2, entry 11) colorless liquid; R_f = 0.34 (in 10% EtOAc/Hexane); IR 1288, 1372, 1403, 1456, 1515, 1585, 1627, 2924 3364 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.13 (s, 2H), 6.77 (d, *J* = 6.8Hz, 1H), 7.30 (t, *J* = 8.8Hz, 2H), 7.45 (d, *J* = 8.0Hz, 2H), 7.80 (dd, *J* = 8.8Hz, 5.6Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 109.8, 119.1, 120.9, 123.8, 125.0, 126.0, 126.4, 128.7, 134.5, 142.2; HRMS [M^++1] Calculated for $C_{10}H_{10}N$: 144.0813; found: 144.0819



4-Aminotoluene (Table 2, entry 16) colorless liquid; R_f = 0.36 (in 10% EtOAc/Hexane); IR 1120, 1267, 1448, 1519, 1627, 2924, 3021, 3217, 3364 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 3H), 6.63 (t, *J* = 6.4Hz, 2H), 7.00 (t, *J* = 8.0Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 115.3, 127.8, 129.8, 143.9; HRMS [M^++1] Calculated for $C_7H_{10}N$: 108.0813; found: 108.0812

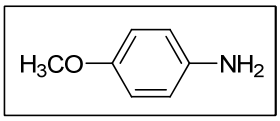


2-methoxyaniline (Table 3, entries 5 & 20) deep brown liquid (eluent: ethyl acetate/hexane = 30:70). R_f = 0.73 (in 30% EtOAc/Hexane); IR 1039, 1160, 1206, 1295, 1465, 1492, 1602, 2927, 3370, 3462 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.79 (s, 2H), 3.86 (s, 3H), 6.68-6.77 (m, 2H), 6.77-6.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.6, 110.6, 115.2, 118.6, 121.2, 136.3, 147.5; HRMS [M^++1] Calculated for $C_7H_{10}NO$: 124.0762; found: 124.0758

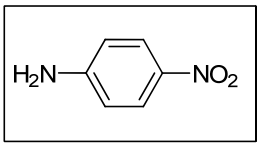


3-methoxyaniline (Table 3, entries 6 & 7) dark brown liquid; R_f = 0.54 (in 30% EtOAc/Hexane); IR 1037, 1224, 1272, 1461, 1507, 2926, 3370, 3458 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.66 (s, 2H), 3.69 (s, 3H), 6.18 (t, *J* = 2.0 Hz, 1H), 6.23 (dd, *J* = 8 Hz, 1.6 Hz, 1H), 6.29 (dd, *J* = 8 Hz, 2.0 Hz, 1H), 7.02 (t, *J* = 8 Hz, 1H); ^{13}C NMR (100 MHz,

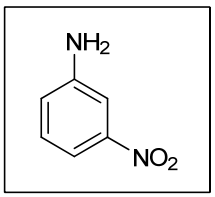
$CDCl_3$) δ 55.0, 101.0, 103.8, 107.9, 130.1, 148.0, 160.7; HRMS [M^++1] Calculated for $C_7H_{10}NO$: 124.0762; found: 124.0760



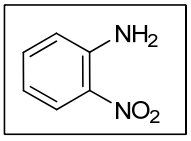
4-methoxyaniline (Table 3, entries 3 & 4) black solid; MP 56-59 ^oC. R_f = 0.43 (in 30% EtOAc/Hexane); IR 1030, 1125, 1233, 1459, 1507, 1629, 1858, 2054, 2960, 3344, 3420 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.43 (s, 2H), 3.75 (s, 3H), 6.62-6.68 (m, 2H), 6.75 (dd, *J* = 6.8 Hz, 2.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 114.9, 116.5, 140.1, 152.9; HRMS [M^++1] Calculated for $C_7H_{10}NO$: 124.0762; found: 124.0768



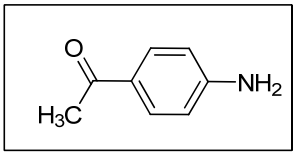
4-nitroaniline (Table 3, entries 8 & 9) yellow solid; MP 146-149 ^oC . R_f = 0.31 (in 30% EtOAc/Hexane); IR 1110, 1300, 1474, 1595, 1630, 2361, 3360, 3479 cm^{-1}; ^1H NMR (400 MHz, CD_3OD) δ 4.40 (s, 2H), 6.59-6.65 (m, 2H), 7.94-8.01 (m, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 113.6, 127.3, 138.3, 156.8; HRMS [M^++1] Calculated for $C_6H_7N_2O_2$: 139.0508; found: 139.0506



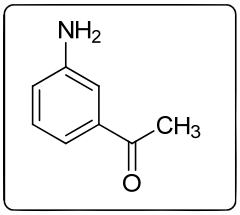
3-nitroaniline (Table 3, entry 10) yellow solid; MP 111-114 ^oC; R_f = 0.21 (in 10% EtOAc/Hexane); IR 1085, 1266, 1342, 1483, 1520, 1619, 3328, 3431 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.04 (s, 2H), 6.78-7.10 (m, 1H), 7.10-7.73 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 109.1, 113.1, 120.7, 130.0, 147.6, 149.3; HRMS [M^++1] Calculated for $C_6H_7N_2O_2$: 139.0508; found: 139.0504



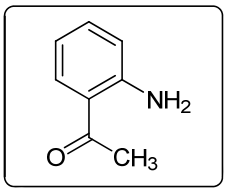
2-Nitroaniline (Table 2, entry 19) yellow solid; MP 70-73 ^oC; R_f = 0.33 (in 10% EtOAc/Hexane); IR 1099, 1250, 1347, 1428, 1501, 1585, 1627, 3354, 3479 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 6.10 (s, 2H), 6.70 (dt, *J* = 8.0Hz, 1.2 Hz, 1H), 6.82 (dd, *J* = 8.4 Hz, 0.8 Hz, 1H), 7.36 (dt, *J* = 8.4 Hz, 1.2 Hz), 8.11 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 117.0, 118.9, 126.2, 132.3, 135.8, 144.8; GC-MS EI+ : m/z calculated for $C_7H_7N_3O$: 138.



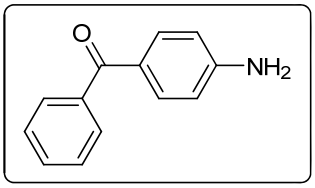
4-aminoacetophenone (Table 3, entry 1 & 2) white solid; MP 103-107 ^{o}C R_f = 0.30 (in 30% EtOAc/Hexane); IR 1169, 1276, 1360, 1435, 1589, 1647, 3223, 3329 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.49 (s, 3H), 4.35 (s, 2H), 6.60-6.67 (m, 2H), 7.76-7.82 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.1, 113.7, 127.5, 130.8, 151.5, 196.7; HRMS [M^{+}+1] Calculated for $C_8H_{10}NO$: 136.0762; found: 136.0759



3-aminoacetophenone (Table 3, entry 18) white solid; MP 94-98 ^{o}C; R_f = 0.32 (in 30% EtOAc/Hexane); IR 1017, 1239, 1288, 1323, 1356, 1459, 1490, 1599, 1669, 3370, 3467 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (s, 3H), 3.81 (s, 2H), 6.87 (dd, *J* = 8 Hz, 1.6 Hz, 1H), 7.17-7.29 (m, 2H), 7.33 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.8, 114.1, 119.0, 119.8, 129.6, 138.4, 146.9, 198.6; HRMS [M^{+}+1] Calculated for $C_8H_{10}NO$: 136.0762; found: 136.0757

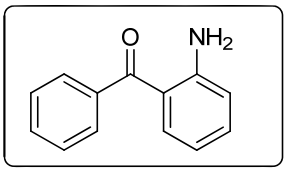


2-aminoacetophenone (Table 3, entry 17) yellow liquid, R_f = 0.56 (in 20% EtOAc/Hexane); IR 1024, 1163, 1245, 1365, 1449, 1484, 1552, 1630, 2835, 2947, 3341, 3440 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (s, 3H), 6.58-6.73 (m, 2H), 7.21-7.32 (m, 1H), 7.70 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.9, 115.8, 117.3, 118.3, 132.1, 134.5, 150.3, 200.8; HRMS [M^{+}+1] Calculated for $C_8H_{10}NO$: 136.0762; found: 136.0761

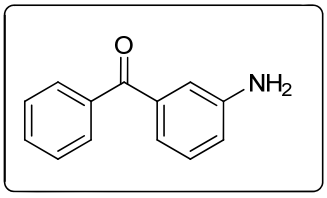


4-aminobenzophenone (Table 3, entry 12) yellow solid, MP 121-124 ^{o}C; R_f = 0.20 (in 20% EtOAc/Hexane); IR 1024, 1289, 1321, 1415, 1448, 1594, 1636,

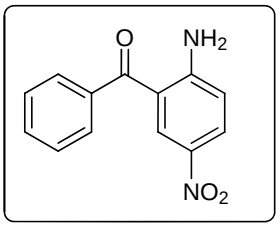
2835, 2947, 3367 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.19 (s, 2H), 6.66 (d, *J* = 8.8 Hz, 2H), 7.41-7.49 (m, 2H), 7.49-7.58 (m, 1H), 7.68-7.79 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 113.7, 127.4, 128.2, 129.6, 131.5, 133.0, 139.0, 151.1, 195.4; HRMS [M^++1] Calculated for $C_{13}H_{12}NO$: 198.0919; found: 198.0926



2-aminobenzophenone (Table 3, entry 14) yellow solid, MP 103-107 ^oC; R_f = 0.57 (in 20% EtOAc/Hexane); IR 1024, 1113, 1247, 1415, 1451, 1551, 1628, 2524, 2834, 2947, 3367 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 6.10 (s, 2H), 6.60 (t, *J* = 7.6 Hz, 1H), 7.25-7.34 (m, 1H), 7.41-7.49 (m, 3H), 7.49-7.56 (m, 1H), 7.61-7.69 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.6, 117.1, 118.3, 128.2, 129.2, 131.1, 134.3, 134.7, 140.2, 151.0, 199.2; HRMS [M^++1] Calculated for $C_{13}H_{12}NO$: 198.0919; found: 198.0910



3-aminobenzophenone (Table 3, entry 13) yellow solid, MP 81-84 ^oC; R_f = 0.29 (in 20% EtOAc/Hexane); IR 1023, 1112, 1321, 1413, 1452, 1648, 2834, 2950, 3390 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.82 (s, 2H), 6.86-6.93 (m, 1H), 7.10-7.16 (m, 2H), 7.21-7.285 (m, 1H), 7.43-7.51 (m, 2H), 7.54-7.61 (m, 1H), 7.77-7.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 116.0, 119.1, 120.7, 128.3, 129.2, 130.1, 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

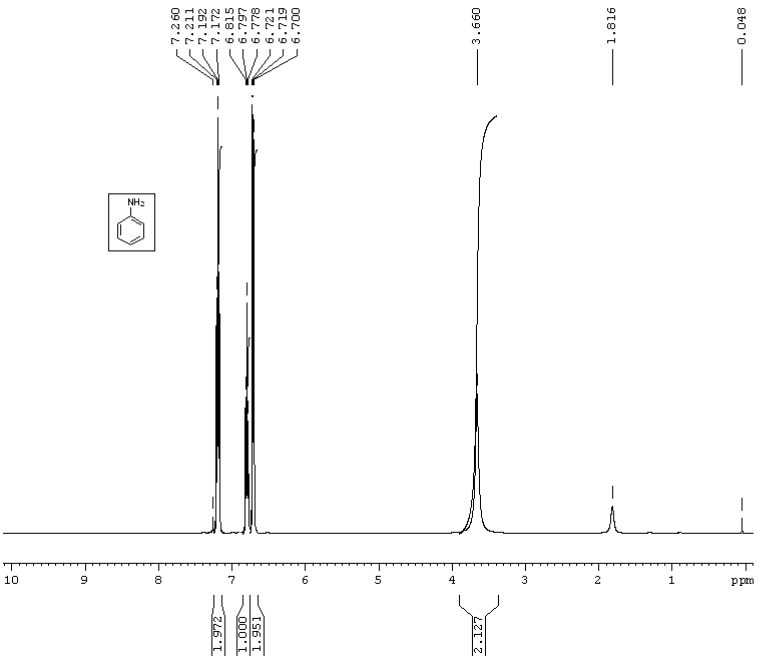


(2-amino-5-nitrophenyl)(phenyl)methanone (Table 3, entry 15) yellow solid, MP 166-168 ^oC; R_f = 0.31 (in 20% EtOAc/Hexane); IR 1027, 1112, 1259, 1332, 1416, 1452, 1635, 2524, 2834, 2947, 3372 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 6.76 (d, *J* = 9.2 Hz, 1H), 6.91 (s, 2H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 2H), 8.16 (dd, *J* = 9.2 Hz, 1H), 8.48 (d, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 116.1, 116.9, 128.7, 129.2, 129.4, 131.7, 132.3, 136.7, 138.5, 155.4, 198.0; HRMS [M^++1] Calculated for $C_{13}H_{11}N_2O_3$: 243.0770; found: 243.0760

References

1. Z. Wu, Z. Jiang, D. Wu, H. Xiang, X. Zhao, *Eur. J. Org. Chem*., 2010, 1854
2. F. Meng, X. Zhu, Y. Li, J. Xie, B. Wang, J. Yao, Y. Wan, *Eur. J. Org. Chem*., 2010, 6149.
3. N. Xia, M. Taillefer, *Angew. Chem. Int. Ed.*, 2009, **48**, 337.

Aniline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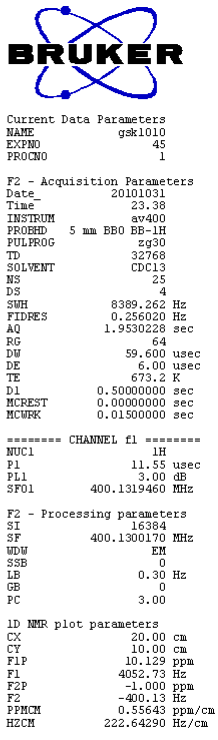
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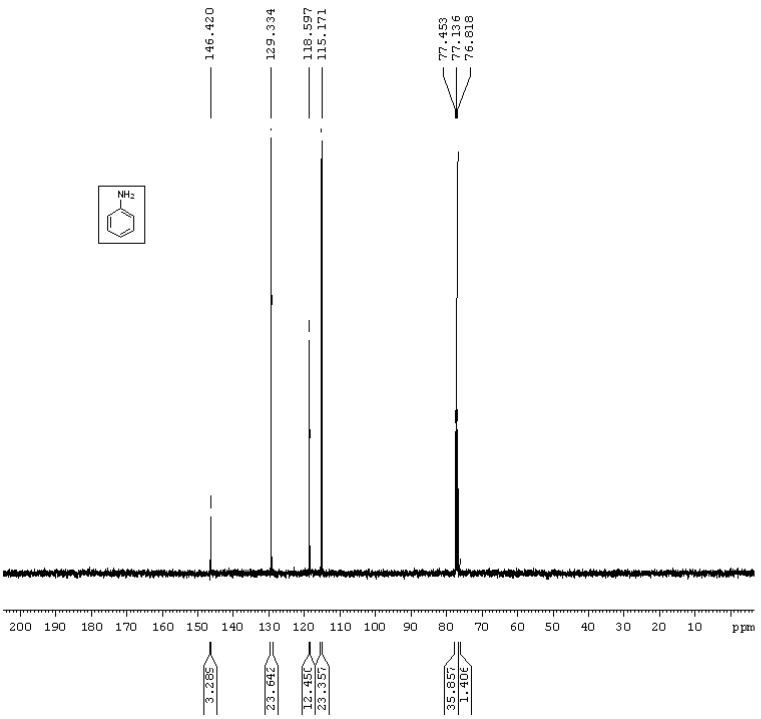
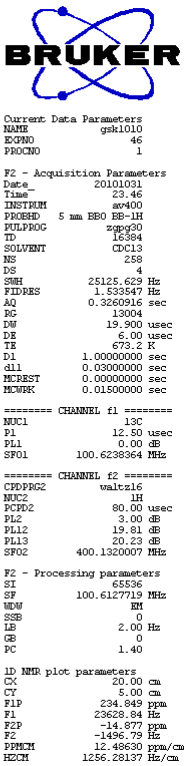
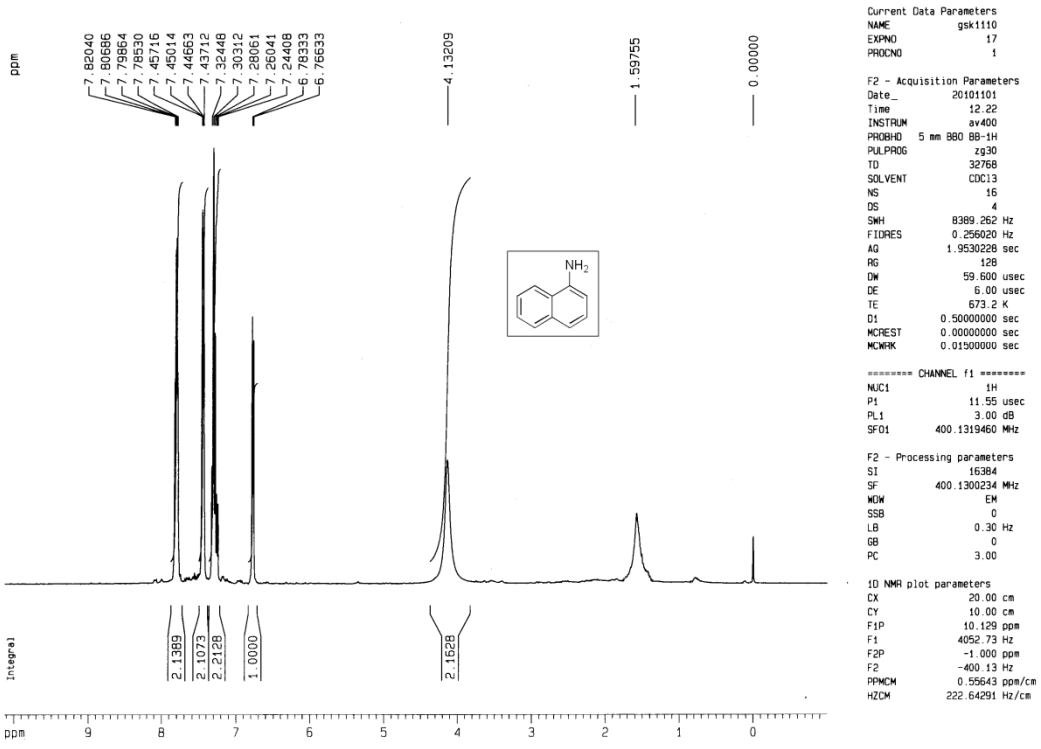
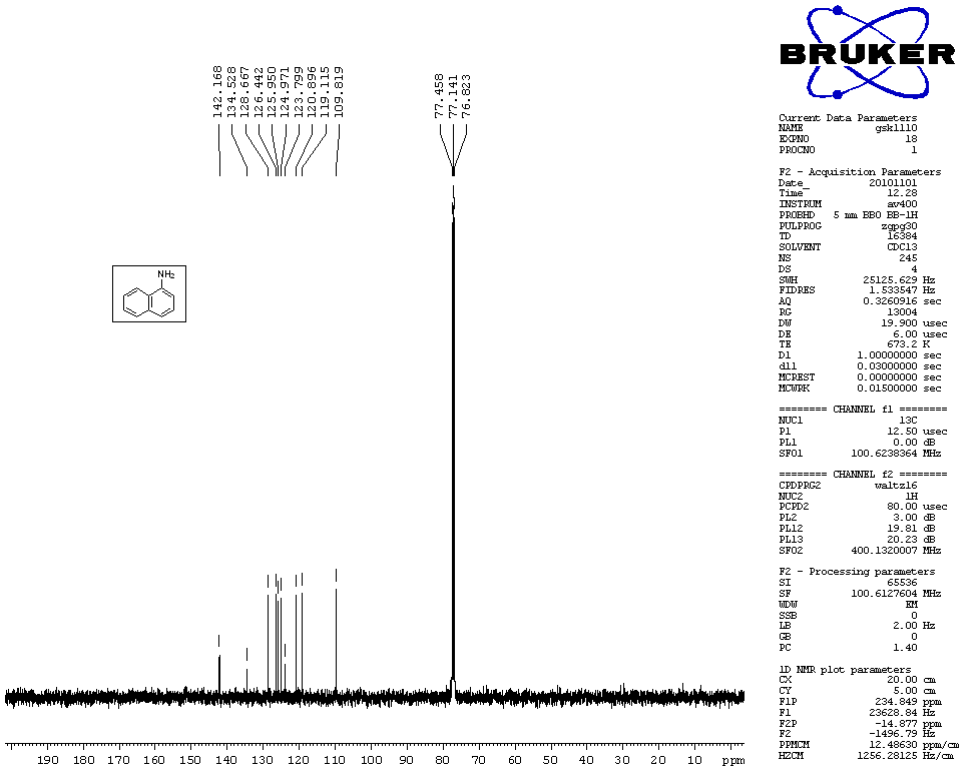
PPMCM 0.55643 ppm/cm
HZCM 222.64290 Hz/cm


146.420
129.334
118.597
115.171
77.453
77.136
76.818
NH2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
3.285
23.642
12.450
23.357
35.857
1.406

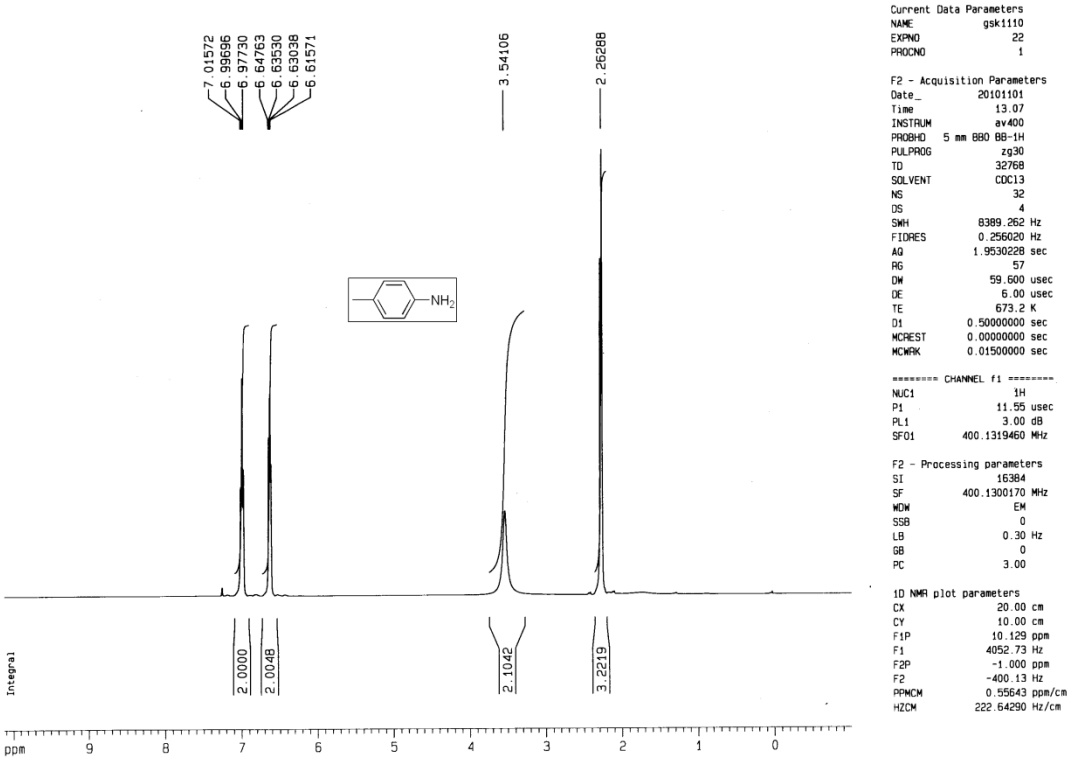

BRUKER
Current Data Parameters
NAME gsk1010
EXPNO 46
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101031
Time 23.46
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 258
DS 4
SWH 25125.629 Hz
FIDRES 1.533547 Hz
AQ 0.3260916 sec
RG 13004
DW 19.900 usec
DE 6.00 usec
TE 673.2 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 100.6127719 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-Aminonapthaline

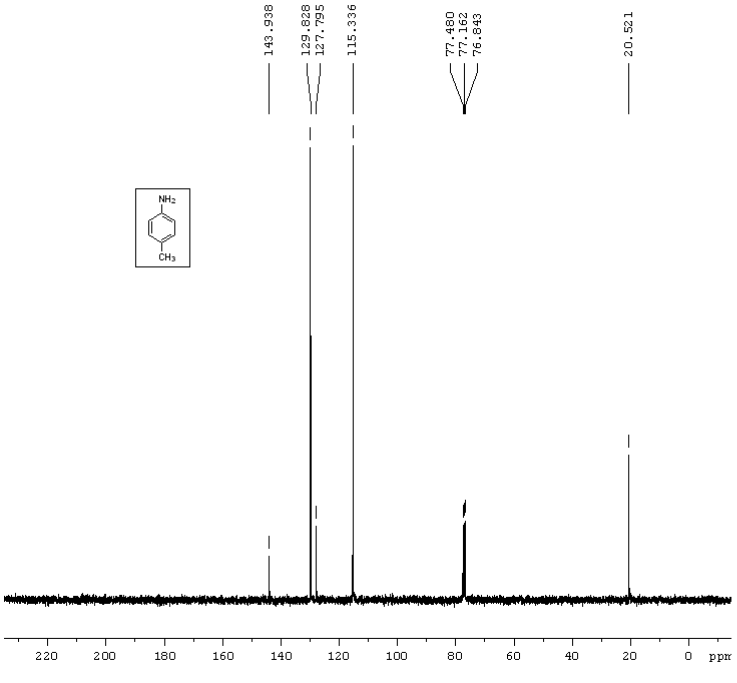




4-Aminotoluene

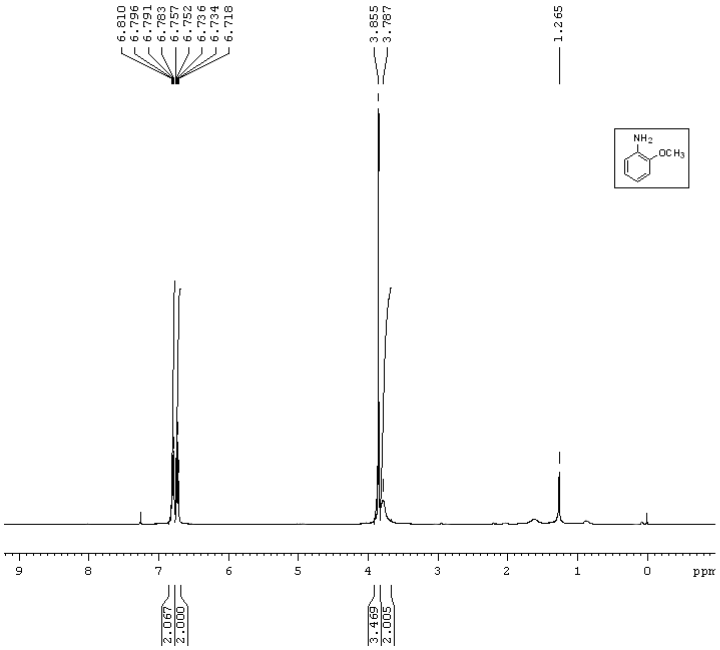



```
Current Data Parameters
NAME                  gsk1110
EXPNO                      22
PROCNO                      1

F2 - Acquisition Parameters
Date_               20101101
Time                   13.07
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                   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                400.1300170 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
```



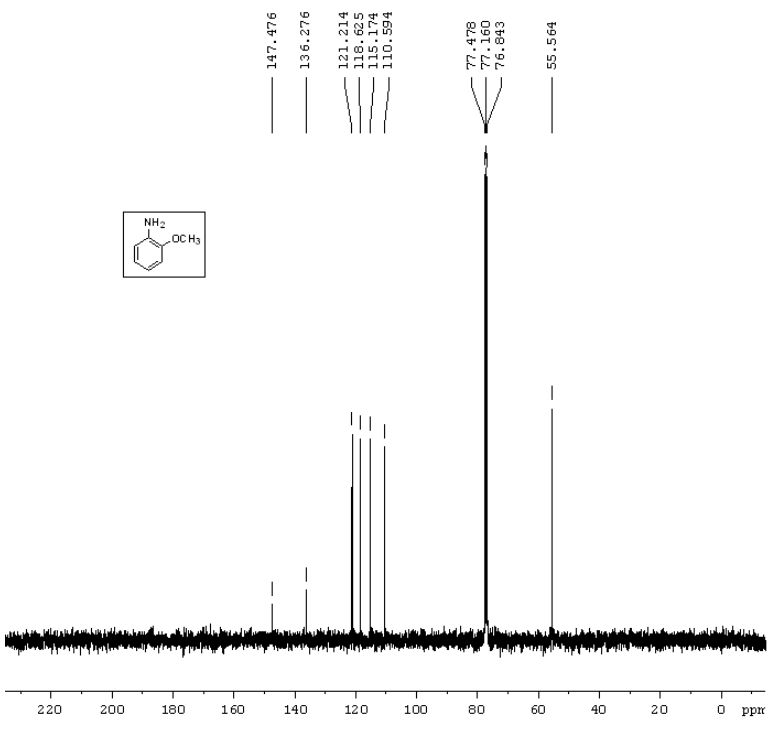

```
Current Data Parameters
NAME                  gsk0810
EXPNO                       6
PROCNO                      1

F2 - Acquisition Parameters
Date_               20101001
Time                   18.06
INSTRUM                av400
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                     16384
SOLVENT               CDCl3
NS                       144
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                   300.0 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-methoxyaniline



BRUKER

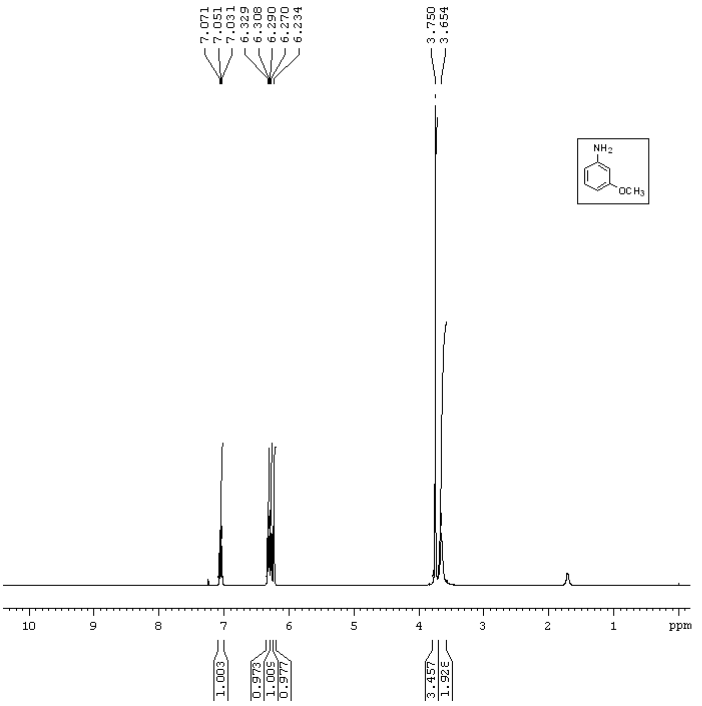
```
Current Data Parameters
NAME                  gsk0810
EXPNO                     112
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100811
Time                  14.41
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                    161.3
DW                   59.600 usec
DE                    6.00 usec
TE                   299.2 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               400.1300175 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                 222.64290 Hz/cm
```



BRUKER

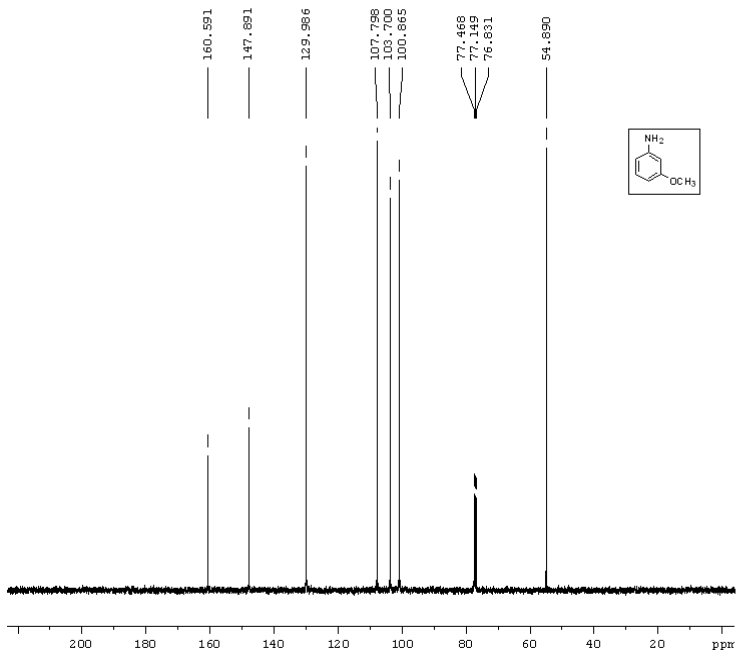
```
Current Data Parameters
NAME                  gsk0810
EXPNO                     113
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100811
Time                  14.43
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                   299.6 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                         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-methoxyaniline



BRUKER

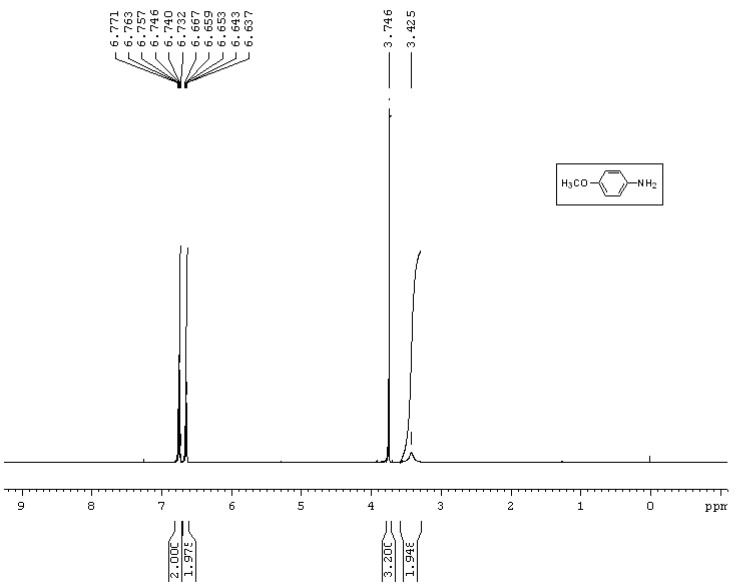
```
Current Data Parameters
NAME                  gsk1110
EXPNO                      19
PROCNO                      1

F2 - Acquisition Parameters
Date_               20101101
Time                   12.37
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                    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                400.1300238 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

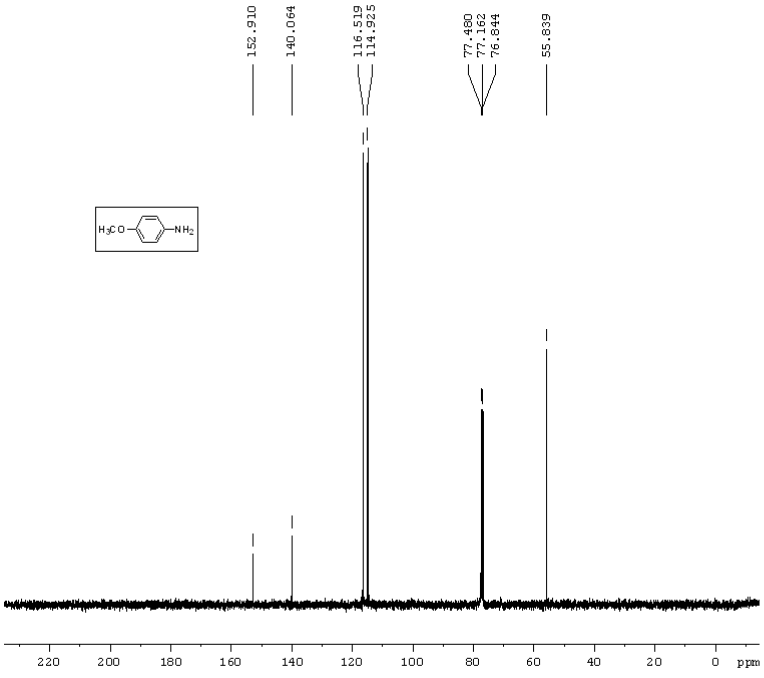
```
Current Data Parameters
NAME                  gsk0810
EXPNO                     214
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100830
Time                   14.54
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    16384
SOLVENT                CDCl3
NS                       245
DS                         4
SWH                25125.629 Hz
FIDRES              1.533547 Hz
AQ                  0.3260916 sec
RG                    20642.5
DW                    19.900 usec
DE                     6.00 usec
TE                    296.8 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                100.6127932 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               1256.28162 Hz/cm
```

4-methoxyanisole



BRUKER

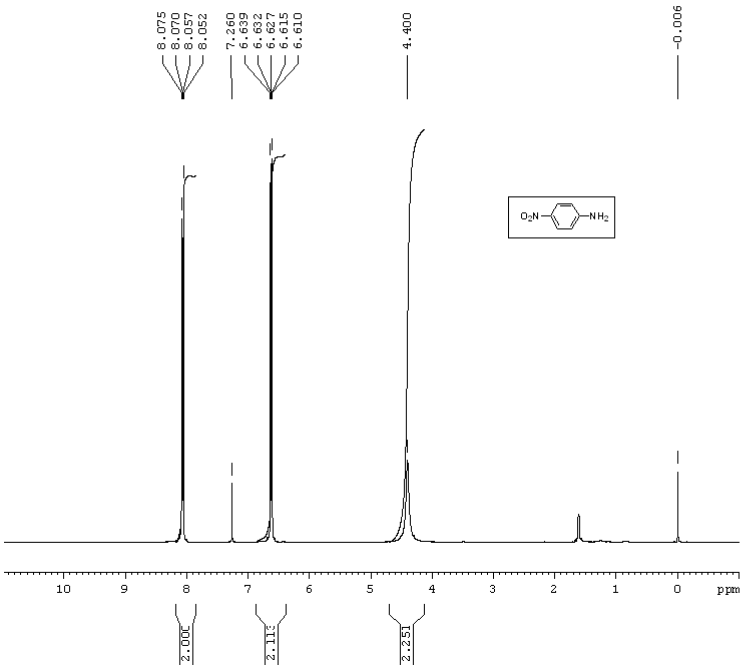
```
Current Data Parameters
NAME                 gsk0810
EXPNO                    114
PROCNO                     1

F2 - Acquisition Parameters
Date_               20100811
Time                   16.57
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                    299.2 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               400.1300170 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      3.00

1D NMR plot parameters
CX                     20.00 cm
CY                      8.24 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

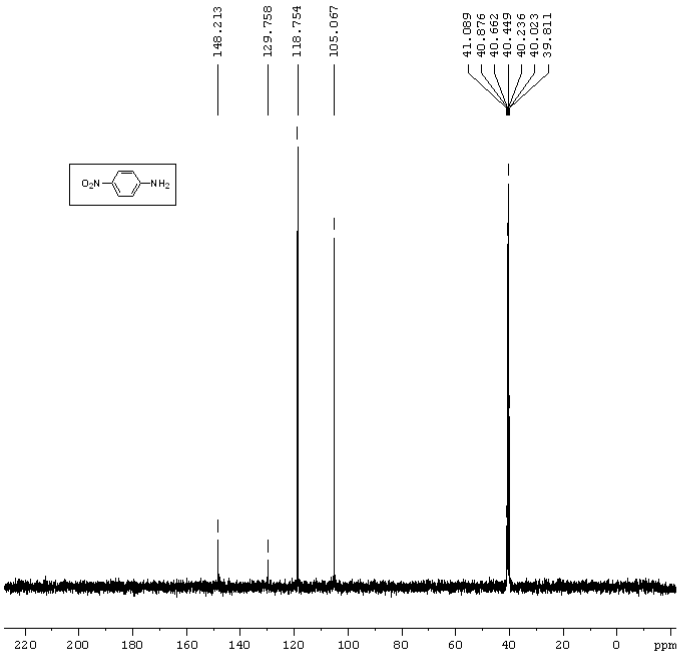
```
Current Data Parameters
NAME                 gsk0810
EXPNO                    115
PROCNO                     1

F2 - Acquisition Parameters
Date_               20100811
Time                   17.00
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT                CDCl3
NS                       300
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                    299.8 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               100.6127630 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-nitroaniline



BRUKER

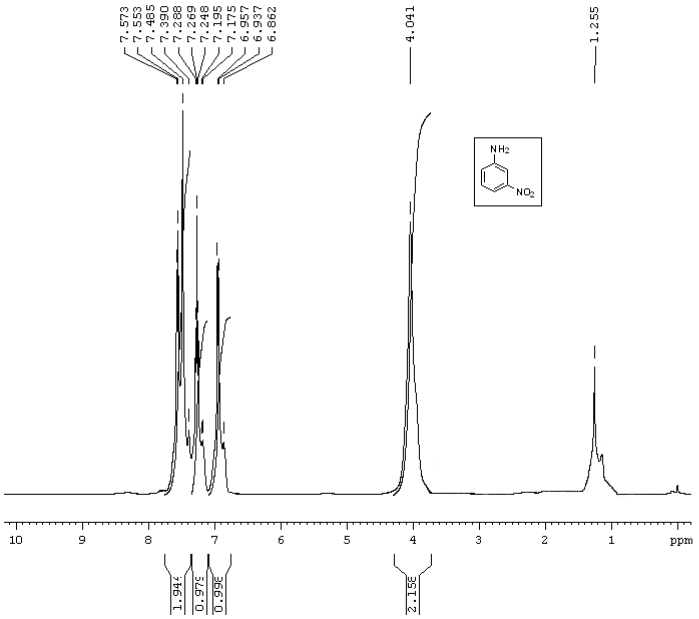
```
Current Data Parameters
NAME                  gsk0810
EXPNO                     135
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100816
Time                    20.40
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                    298.8 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                400.1300175 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                 222.64290 Hz/cm
```



BRUKER

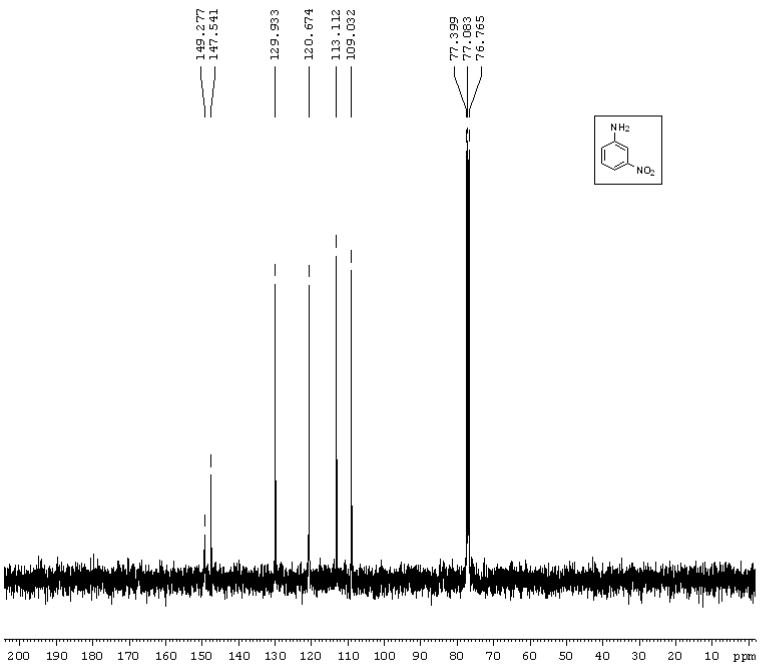
```
Current Data Parameters
NAME                  gsk0810
EXPNO                     169
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100730
Time                     9.42
INSTRUM                 av400
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                     16384
SOLVENT                MeOD
NS                       213
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                    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
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                100.6134909 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                    23629.01 Hz
F2P                     -14.877 ppm
F2                    -1496.80 Hz
PPMCM                 12.48630 ppm/cm
HZCM                1256.29028 Hz/cm
```

3-nitroaniline



BRUKER

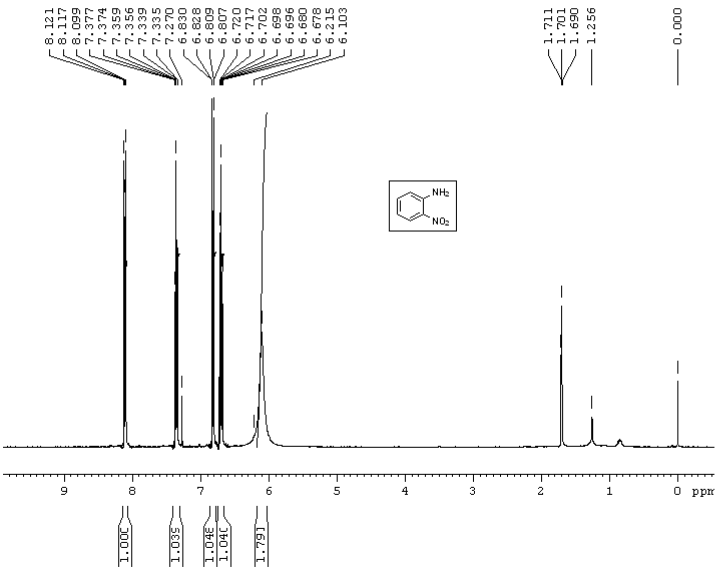
```
Current Data Parameters
NAME                  gskl110
EXPNO                      13
PROCNO                      1

F2 - Acquisition Parameters
Date_              20101101
Time                   11.48
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                    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                400.1300129 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

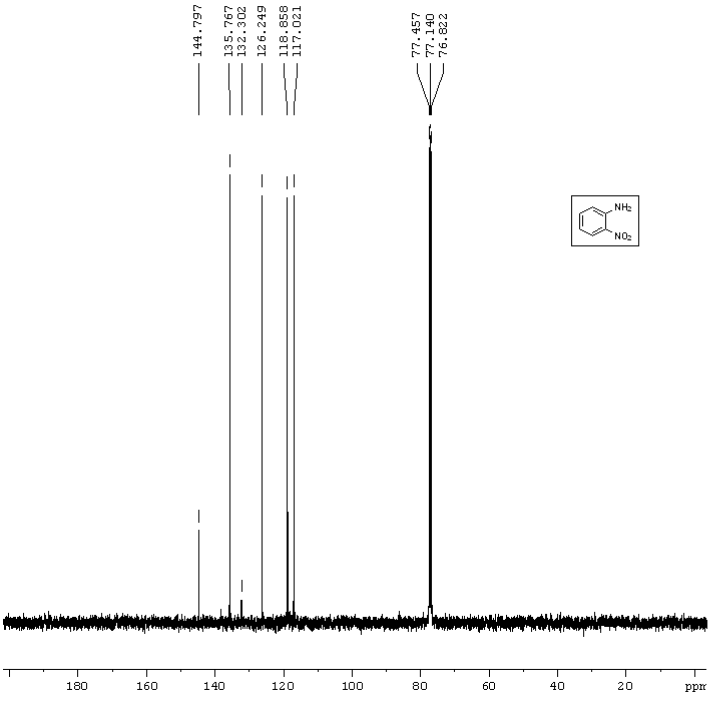
```
Current Data Parameters
NAME                  gskl110
EXPNO                      14
PROCNO                      1

F2 - Acquisition Parameters
Date_              20101101
Time                   11.54
INSTRUM                av400
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                      300
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                    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                100.6127690 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-Nitroaniline



BRUKER

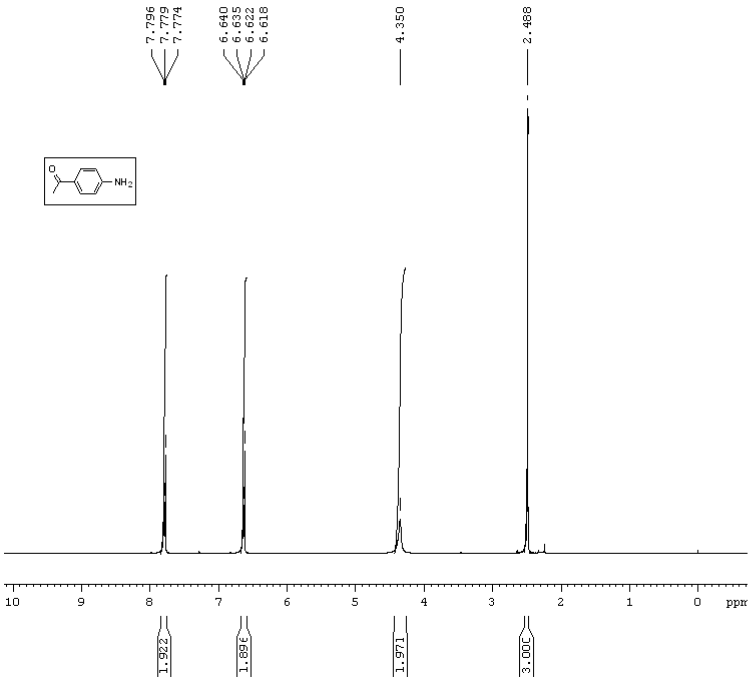
```
Current Data Parameters
NAME                 gsk1010
EXPNO                     43
PROCNO                     1

F2 - Acquisition Parameters
Date_               20101031
Time                   23.18
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                     101.6
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                400.1300131 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
```



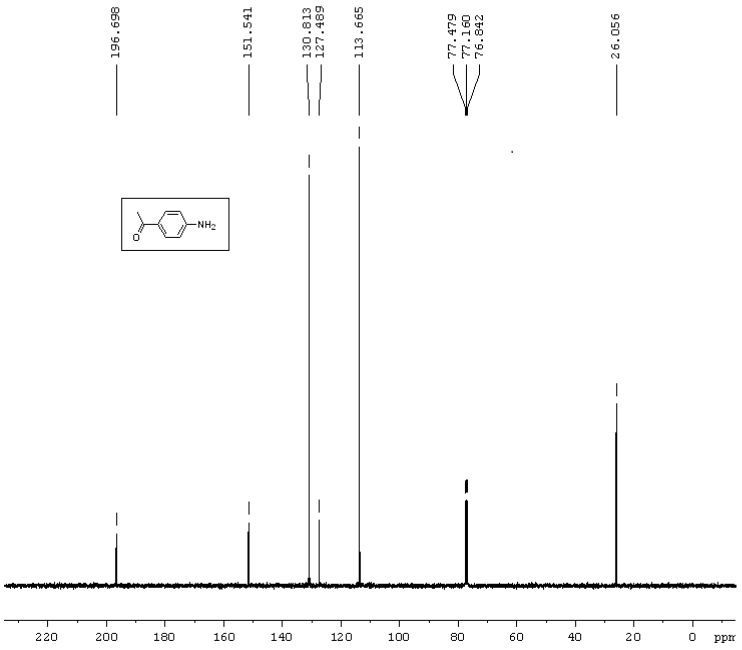
BRUKER

```
Current Data Parameters
NAME                 gsk1010
EXPNO                     44
PROCNO                     1

F2 - Acquisition Parameters
Date_               20101031
Time                   23.25
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                    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                100.6127646 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

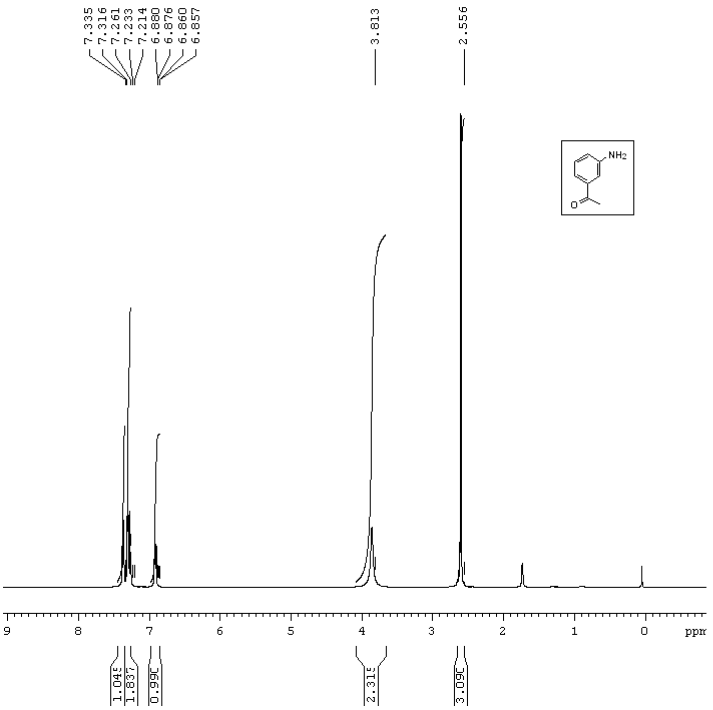



```
Current Data Parameters
NAME                  gsk0810
EXPNO                     148
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100817
Time                    22.31
INSTRUM                  av400
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                         11
DS                          4
SWH                  8389.262 Hz
FIDRES               0.256020 Hz
AQ                   1.9530228 sec
RG                        45.3
DW                      59.600 usec
DE                        6.00 usec
TE                       298.6 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                400.1300085 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                 222.64290 Hz/cm
```

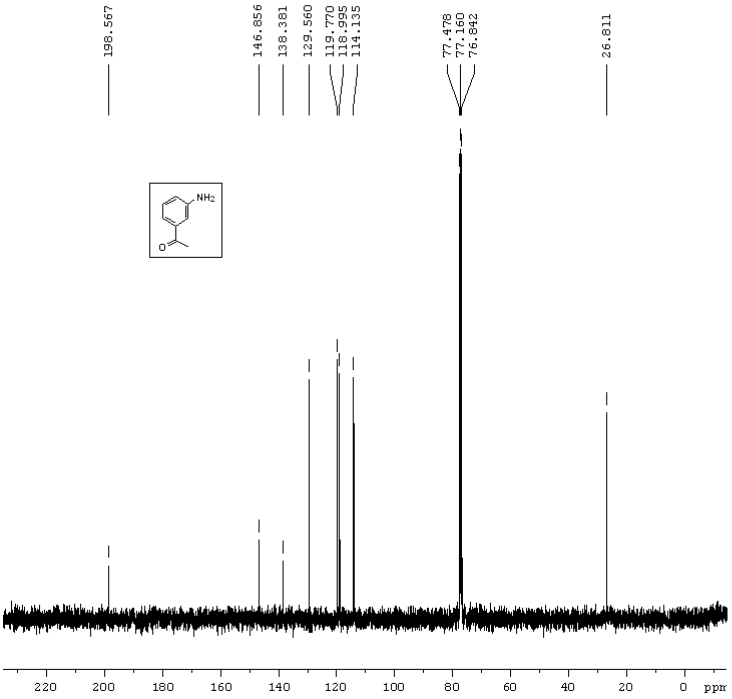



```
Current Data Parameters
NAME                  gsk0810
EXPNO                     149
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100817
Time                    22.40
INSTRUM                  av400
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      16384
SOLVENT                 CDCl3
NS                        424
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                       299.4 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
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                100.6127729 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
```

3-Aminoacetophenone

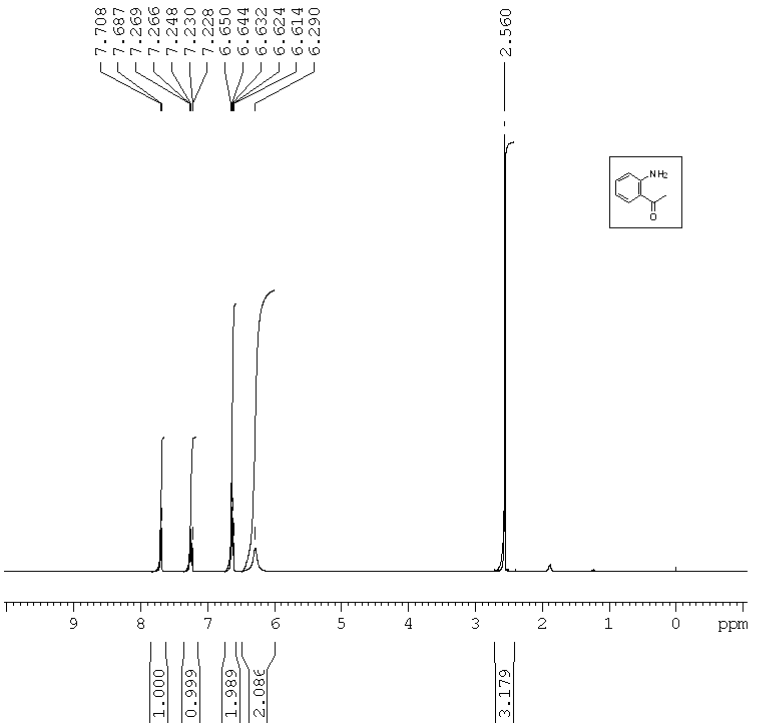



```
Current Data Parameters
NAME                  gsk0810
EXPNO                     205
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100827
Time                  15.56
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                C6D6
NS                       32
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                    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
SF01             400.1319460 MHz

F2 - Processing parameters
SI                        16384
SF               400.1300052 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
```




```
Current Data Parameters
NAME                  gsk0810
EXPNO                     206
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100827
Time                  16.02
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT                C6D6
NS                      279
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                    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
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               100.6127610 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



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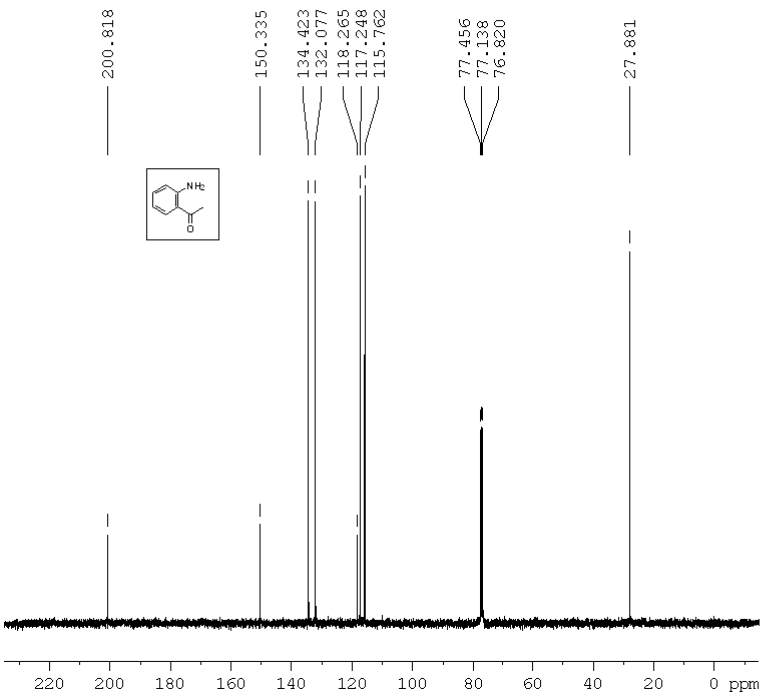
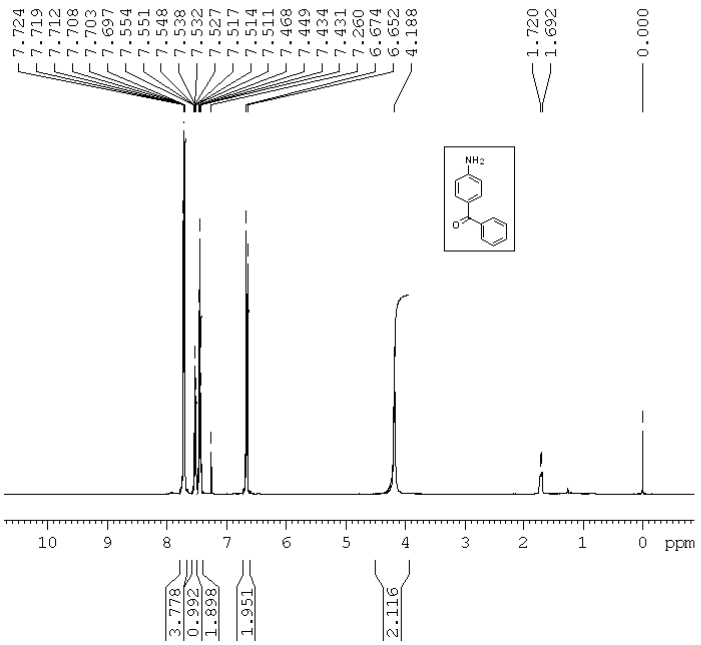
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      42
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100911
Time                    10.26
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                       50.8
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                400.1300179 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

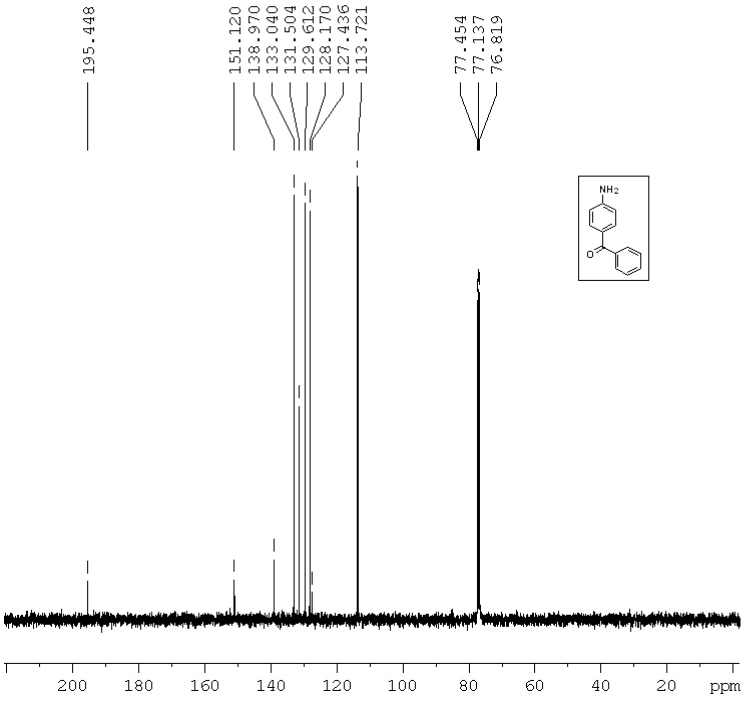
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      43
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100911
Time                    10.36
INSTRUM                 av400
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                     16384
SOLVENT                 CDCl3
NS                        375
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                     298.1 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
```

4-Aminobezophenone



BRUKER

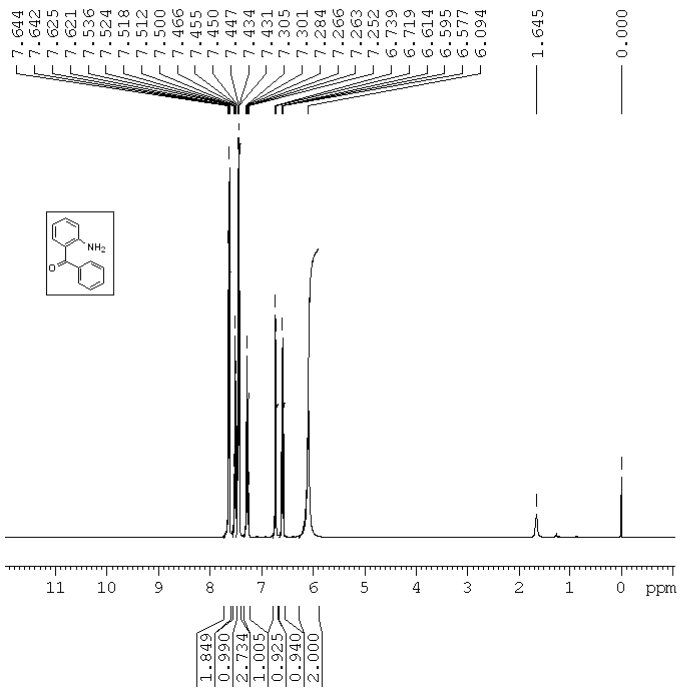
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      55
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100911
Time                   12.53
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                     297.2 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                400.1300172 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         3.00
```



BRUKER

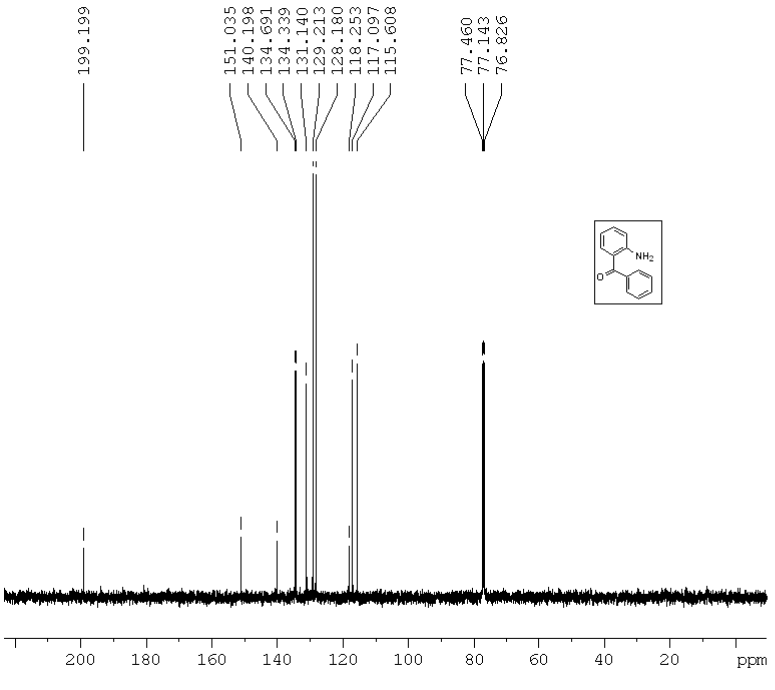
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      56
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100911
Time                   13.00
INSTRUM                av400
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                    16384
SOLVENT               CDCl3
NS                       329
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                100.6127631 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
```

2-Aminobenzophenone



BRUKER

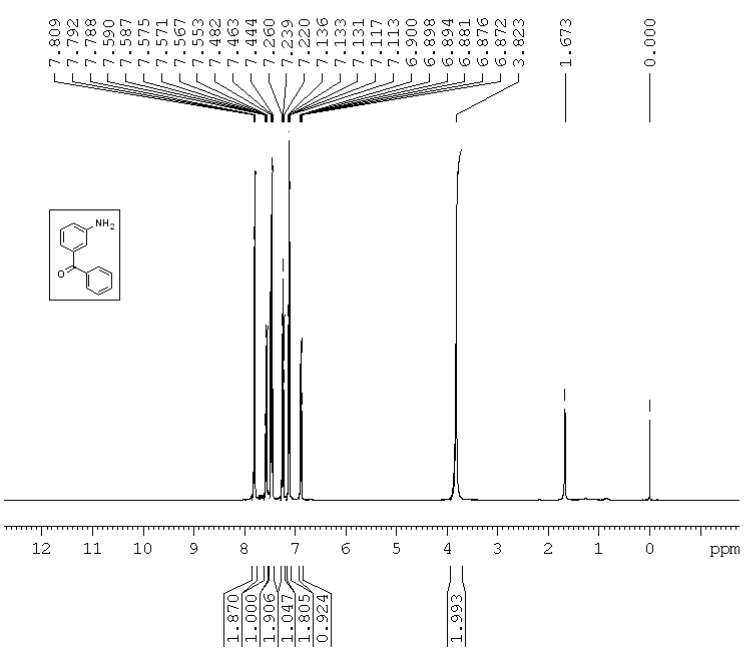
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      53
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100911
Time                    12.36
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                      101.6
DW                     59.600 usec
DE                      6.00 usec
TE                     297.2 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                 400.1300203 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         3.00
```



BRUKER

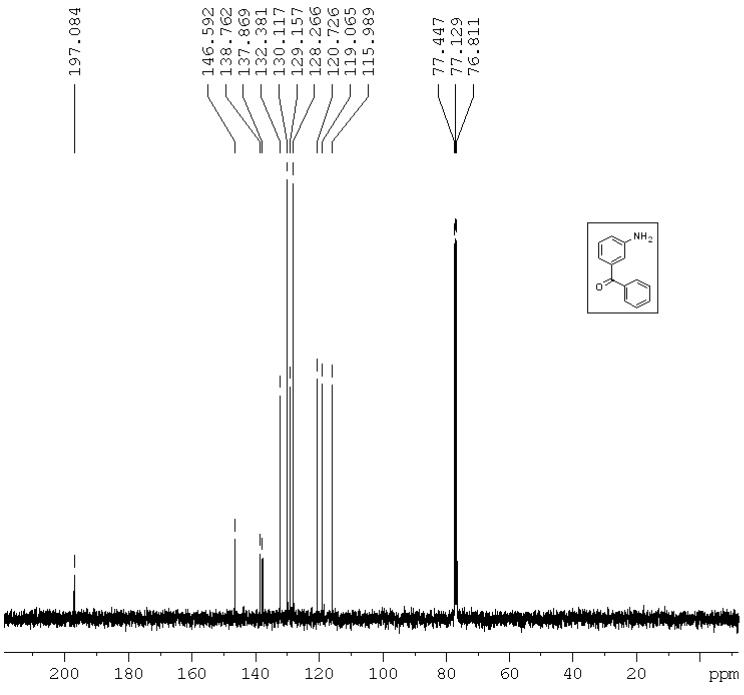
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      54
PROCNO                      1

F2 - Acquisition Parameters
Date_                20100911
Time                    12.41
INSTRUM                 av400
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                     16384
SOLVENT                CDCl3
NS                       211
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                 100.6127631 MHz
WDW                          EM
SSB                           0
LB                         2.00 Hz
GB                            0
PC                         1.40
```

3-Aminobenzophenone



BRUKER

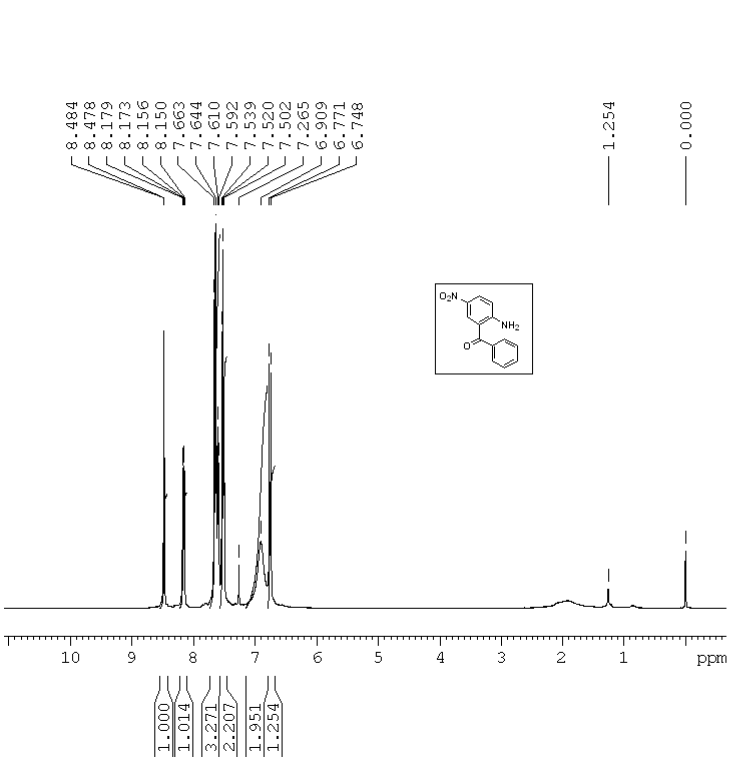
```
Current Data Parameters
NAME                  gsk0910
EXPNO                      45
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100911
Time                   10.46
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                    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                400.1300172 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
```

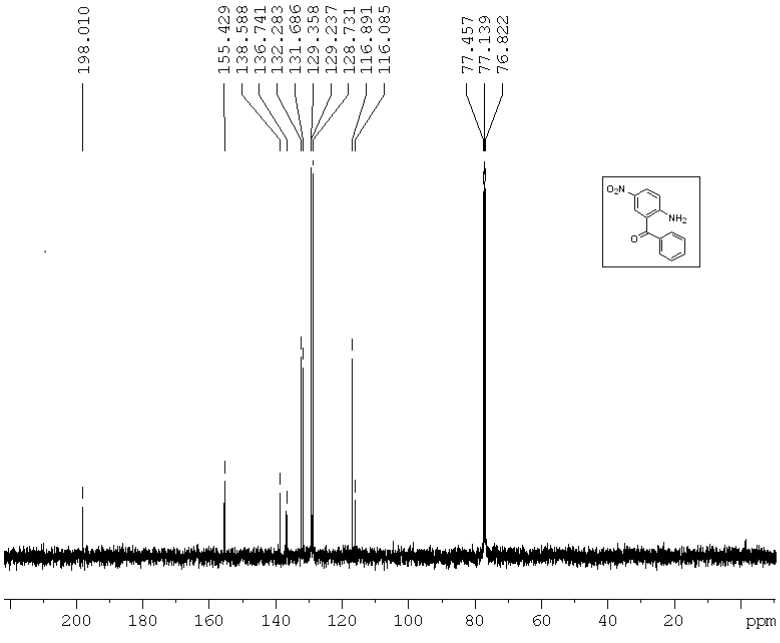


BRUKER

```
Current Data Parameters
NAME                  gsk0910
EXPNO                      46
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100911
Time                   10.54
INSTRUM                av400
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                     16384
SOLVENT                CDCl3
NS                       311
DS                         4
SWH               25125.629 Hz
FIDRES                1.533547 Hz
AQ                 0.3260916 sec
RG                   20642.5
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
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                100.6127634 MHz
WDW                       EM
SSB                        0
LB                     2.00 Hz
GB                         0
PC                      1.40
```

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





Current Data Parameters
NAME gsk0910
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100911
Time 13.34
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 297.2 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 400.1300152 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 3.00

Current Data Parameters
NAME gsk0910
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100911
Time 13.41
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 16384
SOLVENT CDCl3
NS 283
DS 4
SWH 25125.629 Hz
FIDRES 1.533547 Hz
AQ 0.3260916 sec
RG 20642.5
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 100.6127623 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