Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2010

Lithium pipecolinate as a facile and efficient ligand for copper-catalyzed hydroxylation of aryl halides in water

Linhai Jing,[a,b] Jiangtao Wei,[a] Li Zhou ,[a] Zhiyong Huang,[a] Zhengkai Li,[a] and Xiangge Zhou*[a,c]

[a] Institute of Homogeneous Catalysis, College of Chemistry, Sichuan University, Chengdu 610064, China. [b] Lab of Applied chemistry and pollution control technology, School of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, china [c] State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, China.

Email: zhouxiangge@scu.edu.cn, Fax: +86-28-85412026.

Supplementary Information

Table of Contents

1. General Methods:

Analytical thin layer chromatography (TLC) was performed using Merck silica gel GF254 plates. Column chromatography was performed using silica gel (200-300mesh) eluting with ethyl acetate and petroleum ether or with chloroform and methanol. All products were characterized by their NMR. ^{1}H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra were recorded at 100 MHz (Bruker DPX) with $CDCl_3$ or DMSO-d_6 as solvent. Chemical shifts are reported in ppm using TMS as internal standard. Gas chromatography - mass spectra (GC/MS) were recorded on an Agilent Technologies 6890 N instrument with an Agilent 5973 N mass detector (EI) and a HP5-MS 30 m × 0.25 mm capillary apolar column (Stationary phase: 5% diphenyldimethylpolysiloxane film, 0.25 μm). GC/MS method: Initial temperature: 100 °C; Initial time: 1 min; Ramp: about 6.7 °C/min until 200 °C then 20 min.

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification. 1-Iodo-4-nitrobenzene[1], 1-Iodo-2-nitrobenzene[1] and 1-Chloro-4-iodobenzene[2] were prepared according to the reported procedures. Ligands were prepared according to literature procedure.[3]

2. General procedure for direct hydroxylation of aryl halides:

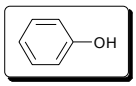
The aryl halide (1.0 mmol), NaOH (3.0 mmol), CuI (0.1 mmol), Lithium

pipecolinate **L4** (0.2 mmol), (n-Bu)$_4$NF (0.2 mmol) and water (3 mL) were put into a Teflon septum screw-capped tube and then sealed in the air. The reaction mixture was stirred at 130 °C for 24 h, then cooled to room temperature and carefully acidified with 1M HCl. After the solvent (H_2O) being removed under reduced pressure, the residue was purified by silica-gel column chromatography to afford the corresponding product. All the products were confirmed by ^{1}H NMR and ^{13}C NMR spectroscopic analysis.

3. Experimental procedures and characterization of products:

Phenol[4] (2a)

Following the general procedure using iodobenzene (112 μL, 1 mmol) provided 80 mg (85% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



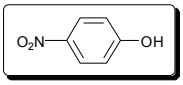
^{1}H NMR (400 MHz, $CDCl_3$): δ 5.52 (s, 1H), 6.83 (d, 2H), 6.90-6.94 (m, 1H), 7.19-7.23 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): 155.16, 129.74, 120.92, 115.39.

MS (EI, M/Z): 94 [M+].

4-Nitrophenol[5] (2b)

Following the general procedure using 1-Iodo-4-nitrobenzene (249 mg, 1 mmol) provided 125 mg (90% yield) of the desired product as a yellow solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



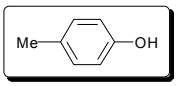
^{1}H NMR (400 MHz, DMSO-d_6): δ 11.08 (br, 1H), 8.14 (d, 2H), 6.96 (d, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): 164.21, 139.93, 126.36, 116.00.

MS (EI, M/Z): 139 [M+].

p-Cresol[4] (2c)

Following the general procedure using 4-iodotoluene (218 mg, 1 mmol) provided 85 mg (79% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



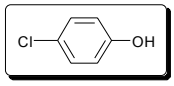
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.98-7.00 (d, 2H), 6.71-6.73 (d, 2H), 5.79 (s, 1H), 2.24 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 152.84, 130.19, 130.18, 115.29, 20.46.

MS (EI, M/Z): 108 [M+].

4-Chlorophenol[4] (2d)

Following the general procedure using 1-Chloro-4-iodobenzene (238 mg, 1 mmol) provided 92 mg (72% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/8).



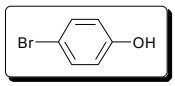
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17-7.20 (d, 2H), 6.75-6.77 (d, 2H), 5.40 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): 153.65, 129.57, 125.83, 116.67.

MS (EI, M/Z): 128 [M+].

4-Bromophenol [4] (2e)

Following the general procedure using 4-iodobromobenzene (282 mg, 1 mmol) provided 138 mg (80% yield) of the desired product as a brown solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



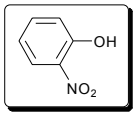
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.34 (d, 2H), 6.71-6.73 (d, 2H), 5.13 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): 154.16, 132.51, 117.19, 113.11.

MS (EI, M/Z): 173 [M+].

o-Nitrophenol[6,7] (2f)

Following the general procedure using 1-Iodo-2-nitrobenzene (249 mg, 1 mmol) provided 118 mg (85% yield) of the desired product as a yellow solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



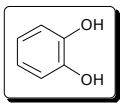
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.59 (s, 1H), 8.10-8.12 (m, 1H), 7.57-7.61 (m, 1H), 7.15-7.18 (m, 1H), 6.98-7.02 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): 154.99, 137.46, 133.55, 124.94, 120.12, 119.84.

MS (EI, M/Z): 139 [M+].

Catechol[8,9] **(2g)**

Following the general procedure using 2-Iodophenol (220 mg, 1 mmol) provided 84 mg (76% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15-1/2).



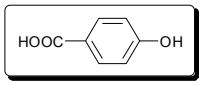
^{1}H NMR (400 MHz, DMSO-d_6): δ 8.80 (s, 2H), 6.72-6.76 (m, 2H), 6.59-6.63 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): 145.19, 119.48, 115.75.

MS (EI, M/Z): 110 [M+].

4-Hydroxybenzoic acid[10] **(2h)**

Following the general procedure using 4-Iodobenzoic acid (248 mg, 1 mmol) provided 99 mg (72% yield) of the desired product as a white solid after purification by flash chromatography (eluent: chloroform/methanol = 20/1-5/1).



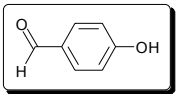
^{1}H NMR (400 MHz, DMSO-d_6): δ 12.44 (br, 1H), 10.23 (s, 1H), 7.81-7.83 (d, 2H), 6.83-6.86 (d, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): 167.21, 161.56, 131.54, 121.35, 115.09.

MS (EI, M/Z): 138 [M+].

4-Hydroxybenzaldehyde[11] **(2i)**

Following the general procedure using 4-Iodobenzaldehyde (232 mg, 1 mmol) provided 85 mg (70% yield) of the desired product as a white yellow solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15-1/4).



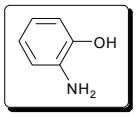
^{1}H NMR (400 MHz, DMSO-d_6): δ 10.61 (s, 1H), 9.80 (s, 1H), 7.76-7.79 (d, 2H), 6.94-6.96 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): 190.77, 163.28, 132.02, 128.40, 115.79.

MS (EI, M/Z): 122 [M+].

2-Aminophenol [12,13] **(2j)**

Following the general procedure using 2-Iodoaniline (219 mg, 1 mmol) provided 81 mg (74% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15-1/2).



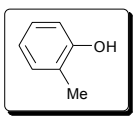
^{1}H NMR (400 MHz, DMSO-d_6): δ 8.92 (s, 1H), 6.62-6.64 (m, 1H), 6.51-6.59 (m, 2H), 6.36-6.40 (m, 1H), 4.45 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): 144.36, 136.84, 119.91, 116.89, 114.87, 114.78.

MS (EI, M/Z): 109 [M+].

o-Cresol[4] (2k)

Following the general procedure using o-bromotoluene (120 µL, 1 mmol) provided 65 mg (60% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



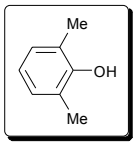
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.06-7.13 (m, 2H), 6.83-6.87 (m, 1H), 6.75-6.77 (m, 1H), 4.73 (s, 1H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 153.62, 131.06, 127.11, 123.89, 120.81, 114.95, 15.73.

MS (EI, M/Z): 108 [M+].

2,6-Dimethylphenol[14,15] (2l)

Following the general procedure using 2-bromo-m-xylene (133 μL, 1 mmol) provided 55 mg (45% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



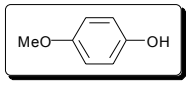
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.97-6.98 (d, 2H), 6.74-6.77 (t, 1H), 4.59 (s, 1H), 2.25 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): 152.13, 128.60, 123.03, 120.23, 15.82.

MS (EI, M/Z): 122 [M+].

4-Methoxyphenol[4] (2m)

Following the general procedure using 4-bromoanisole (125 μL, 1 mmol) provided 77 mg (62% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



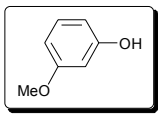
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.76 (d, 4H), 6.00 (s, 1H), 3.74 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 153.41, 149.46, 116.13, 114.97, 55.88.

MS (EI, M/Z): 124 [M+].

m-Methoxyphenol[4] (2n)

Following the general procedure using 3-bromoanisole (127 μL, 1 mmol) provided 74 mg (60% yield) of the desired product as an oil after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



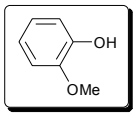
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.08-7.12 (m, 1H), 6.41-6.50 (m, 3H), 6.29 (s, 1H), 3.72 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 160.56, 156.58, 130.35, 108.21, 106.63, 101.67, 55.32.

MS (EI, M/Z): 124 [M+].

2-Methoxyphenol[14,15] (2o)

Following the general procedure using 2-bromoanisole (125 μL, 1 mmol) provided 62 mg (50% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



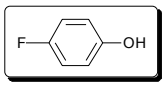
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.92-6.94 (m, 1H), 6.84-6.89 (m, 3H), 5.69 (s, 1H), 3.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 146.64, 145.65, 121.43, 120.17, 114.63, 110.82, 55.79.

MS (EI, M/Z): 124 [M+].

4-Fluorophenol[4] (2p)

Following the general procedure using 1-bromo-4-fluorobenzene (110 μL, 1 mmol) provided 73 mg (65% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



^{1}H NMR (400 MHz, $CDCl_3$): δ 6.90-6.94 (m, 2H), 6.75-6.79 (m, 2H), 5.48 (s, 1H).

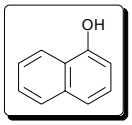
^{13}C NMR (100 MHz, $CDCl_3$): 158.56, 156.19, 150.89, 116.36, 116.28, 116.18, 115.95.

MS (EI, M/Z): 112 [M+].

1-Naphthol[15] (2q)

Following the general procedure using 1-bromonaphthalene (139 μL, 1 mmol) provided 89 mg (62% yield) of the desired product as a white

solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



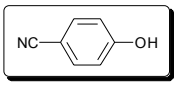
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15-8.18 (m, 1H), 7.79-7.81 (m, 1H), 7.42-7.49 (m, 3H), 7.27-7.30 (m, 1H), 6.77-6.79 (m, 1H), 5.29 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): 151.21, 134.77, 127.75, 126.51, 125.90, 125.39, 124.37, 121.51, 120.83, 108.83.

MS (EI, M/Z): 144 [M+].

4-Hydroxybenzonitrile[5] (2r)

Following the general procedure using 4-bromobenzonitrile (182 mg, 1.0 mmol) provided 95 mg (80% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



^{1}H NMR (400 MHz, DMSO-d_6): δ 10.64 (s, 1H), 7.64-7.66 (d, 2H), 6.91-6.93 (d, 2H).

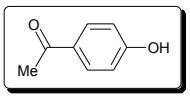
^{13}C NMR (100 MHz, DMSO-d_6): 161.95, 134.50, 119.85, 116.72, 101.38.

MS (EI, M/Z): 119 [M+].

4'-Hydroxyacetophenone[5] (2s)

Following the general procedure using 4'-bromoacetophenone (199 mg, 1

mmol) provided 102 mg (75% yield) of the desired product as a white solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



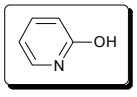
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (s, 1H), 7.91-7.93 (d, 2H), 6.95-6.97 (d, 2H), 2.60 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 199.13, 161.73, 131.26, 129.19, 115.57, 26.19.

MS (EI, M/Z): 136 [M+].

2-Hydroxypyridine[16,17] (2t)

Following the general procedure using 2-bromopyridine (97 μL, 1 mmol) provided 71 mg (75% yield) of the desired product as a white solid after purification by flash chromatography (eluent: chloroform/methanol = 20/1).



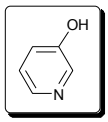
^{1}H NMR (400 MHz, DMSO-d_6): δ 7.37-7.42 (m, 1H), 7.33-7.35 (m, 1H), 6.28-6.31 (m, 1H), 6.12-6.15 (m, 1H).

^{13}C NMR (100 MHz, DMSO-d_6): 162.97, 141.42, 135.83, 120.33, 105.39.

MS (EI, M/Z): 95 [M+].

3-Hydroxypyridine[16,18] (2u)

Following the general procedure using 3-bromopyridine (96 μL, 1 mmol) provided 70 mg (74% yield) of the desired product as a pale yellow after purification by flash chromatography (eluent: chloroform/methanol = 20/1).



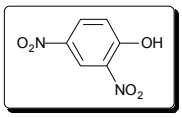
^{1}H NMR (400 MHz, DMSO-d_6): δ 9.89 (s, 1H), 8.14-8.15 (dd, 1H), 8.02-8.04 (dd, 1H), 7.14-7.22 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): 154.08, 140.54, 138.32, 124.46, 122.42.

MS (EI, M/Z): 95 [M+].

2,4-Dinitrophenol[19] (2v)

Following the general procedure using 2,4-dinitrochlorobenzene (203 mg, 1 mmol) provided 129 mg (70% yield) of the desired product as a light yellow solid after purification by flash chromatography (eluent: ethyl acetate/petrol ether = 1/15 – 1/4).



^{1}H NMR (400 MHz, $CDCl_3$): δ 11.04 (s, 1H), 9.08 (d, 1H), 8.46-8.49 (dd, 1H), 7.34-7.37 (d, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): 158.96, 140.17, 132.50, 131.57, 121.81, 121.18.

MS (EI, M/Z): 184 [M+].

References:

1 E. A. Krasnokutskaya, N. I. Semenischeva, V. D. Filimonov and P. Knochel, *Synthesis*, 2007, 81.

2 G. Angelovski, M. D. Keränen, P. Linnepe, S. Grudzielanek and P. Eilbracht, *Adv. Synth. Catal.*, 2006, **348**, 1193.

3 X. H. Liu, B. Qin, X. Zhou, B. He and X. M. Feng, *J. Am. Chem. Soc.*, 2005, **127**, 12224.

4 A. Tlili, N. Xia, F. Monnier and M. Taillefer, *Angew. Chem. Int. Ed.*, 2009, **48**, 8725.

5 L. J. Marshall, K. M. Cable and N. P. Botting, *Tetrahedron*, 2009, **65**, 8165.

6 P. E. Hansen and S. Bolvig, *Magn. Reson. Chem.*, 1997, **35**, 520.

7 M. Shi, S.-C. Cui and W.-P. Yin, *Eur. J. Org. Chem.*, 2005, 2379.

8 H. E. Mabrouk and D. G. Tuck, *J. Chem. Soc., Dalton Trans.*, 1988, 2539.

9 K. S. Webb and S. J. Ruszkay, *Tetrahedron*, 1998, **54**, 401.

10 D. B. Zhao, N. J. Wu, S. Zhang, P. H. Xi, X. Y. Su, J. B. Lan and J. S. You, *Angew. Chem. Int. Ed.*, 2009, **48**, 8729.

11 J. Magano, M. H. Chen, J. D. Clark and T. Nussbaumer, *J. Org. Chem.*, 2006, **71**, 7103.

12 B. Raju, R. Ragul and B. N. Sivasankar, *Indian J. Chem., Sect B*, 2009, **48**, 1315.

13 M. Fujita, M. Nagai and T. Inoue, *Chem. Pharm. Bull.* 1982, **30**, 1151.

14 K. W. Anderson, T. Ikawa, R. E. Tundel and S. L. Buchwald, *J. Am. Chem. Soc.*, 2006, **128**, 10694.

15 T. Schulz, C. Torborg, B. Schäffner, J. Huang, A. Zapf, R. Kadyrov, A. Börner and M. Beller, *Angew. Chem. Int. Ed.*, 2009, **48**, 918.

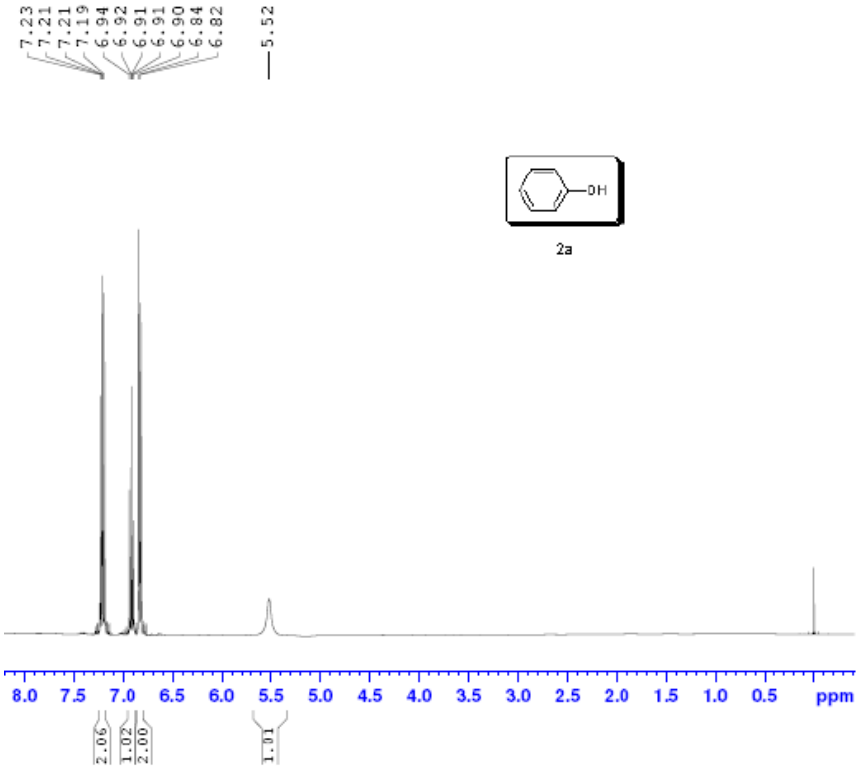
16 D. G. De Kowalewski, R. H. Contreras and C. De Los Santos, *J. Mol. Struct.*, 1989, **213**, 201.

17 D. W. Aksnes and H. Kryvi, *Acta. Chem. Scand.*, 1972, **26**, 2255.

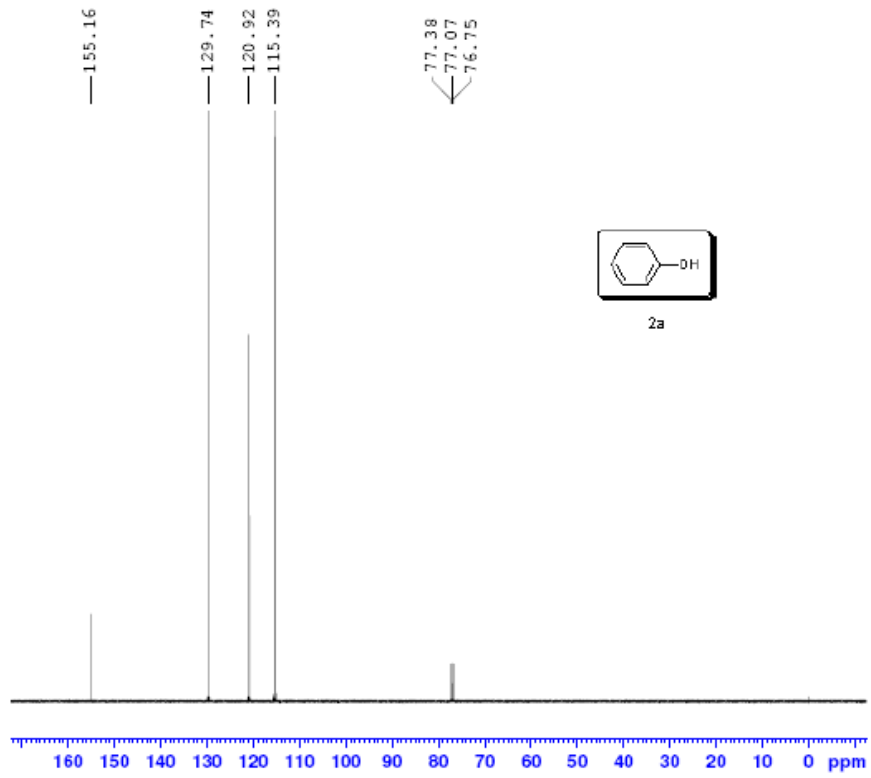
18 U. Vögeli and W. v. Philipsborn, *Org. Magn. Reson.*, 1973, **5**, 551.

19 M. Terrazas, X. Ariza, J. Farras and J. Vilarrasa, *Chem. Commun.*, 2005, 3968.

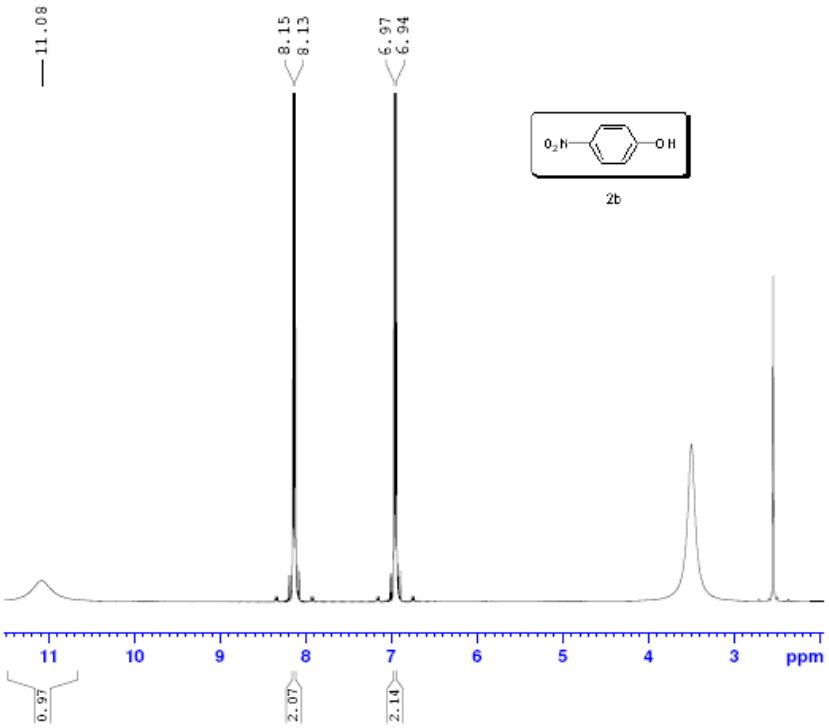
4. NMR spectra of compounds:



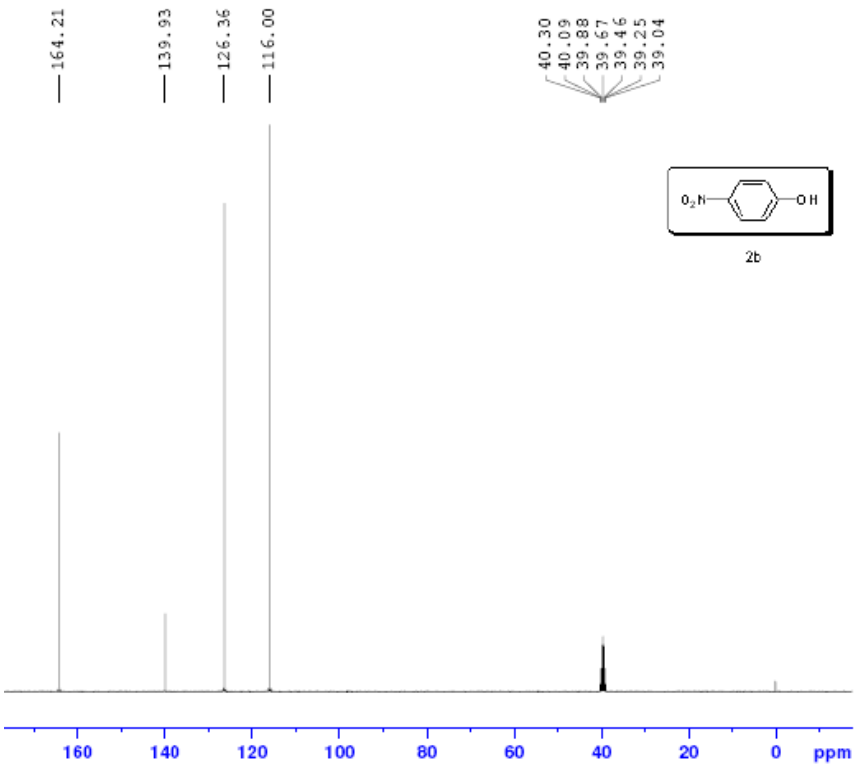

```
NAME            2010-02-20 PhOH-H
EXPNO                        1
PROCNO                       1
Date_                 20100220
Time                     16.33
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg
TD                        32768
SOLVENT                 CDCl3
NS                           32
DS                            0
SWH                  6009.615 Hz
FIDRES               0.183399 Hz
AQ                   2.7263477 sec
RG                        90.5
DW                      83.200 usec
DE                        6.50 usec
TE                      290.6 K
D1                   5.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       12.50 usec
PL1                      -2.60 dB
PL1W                17.82643890 W
SFO1               400.1516006 MHz
SI                        32768
SF                 400.1500387 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```



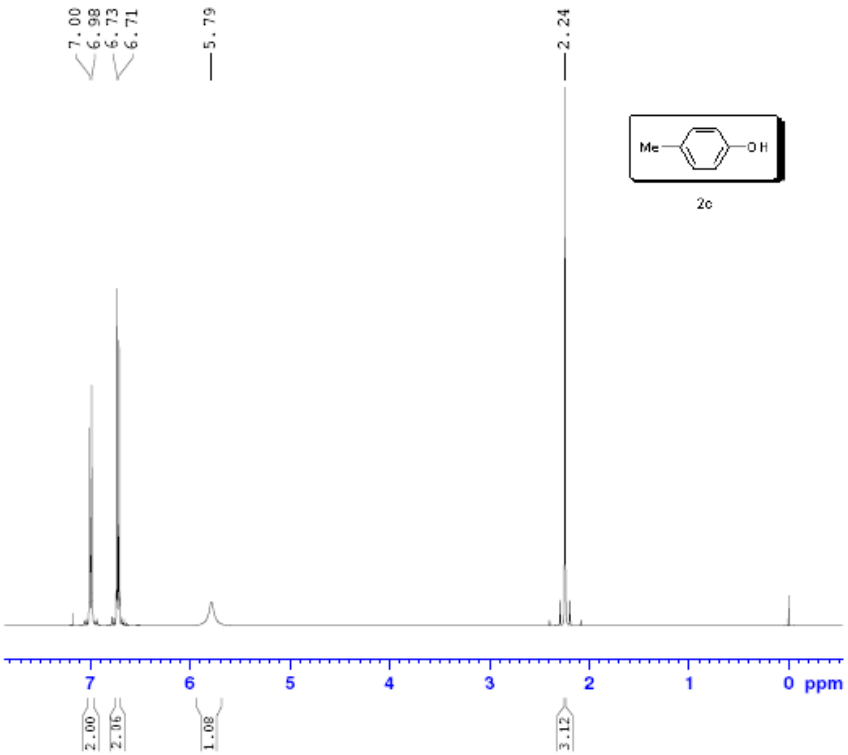

```
EXPNO                        1
PROCNO                       1
Date_                 20100220
Time                     17.18
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg
TD                       262144
SOLVENT                 CDCl3
NS                          128
DS                            0
SWH                 20161.291 Hz
FIDRES               0.076909 Hz
AQ                   6.5012212 sec
RG                        90.5
DW                      24.800 usec
DE                        6.50 usec
TE                      293.4 K
D1                  10.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.30 usec
PL1                      -2.00 dB
PL1W                54.14257431 W
SFO1               100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                      -2.60 dB
PL12                     14.50 dB
PL13                     14.50 dB
PL2W                17.82643890 W
PL12W                0.34758785 W
PL13W                0.34758785 W
SFO2               400.1520008 MHz
SI                       131072
SF                 100.6178087 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
```



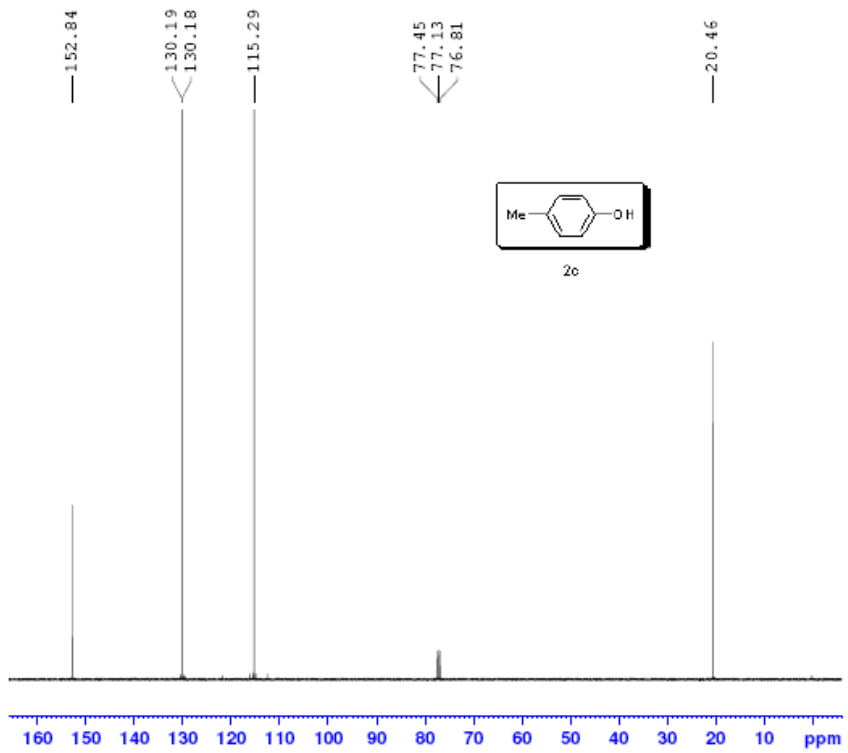

```
NAME            2010-02-22 p-NO2-Ph-H
EXPNO                    1
PROCNO                   1
Date_             20100222
Time                 22.31
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT                DMSO
NS                       32
DS                        0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                     28.5
DW                83.200 usec
DE                 6.50 usec
TE                 297.3 K
D1              5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  12.50 usec
PL1                 -2.60 dB
PL1W          17.82643890 W
SFO1          400.1516006 MHz
SI                   32768
SF            400.1499855 MHz
WDW                     no
SSB                      0
LB                  0.00 Hz
GB                       0
PC                    1.00
```



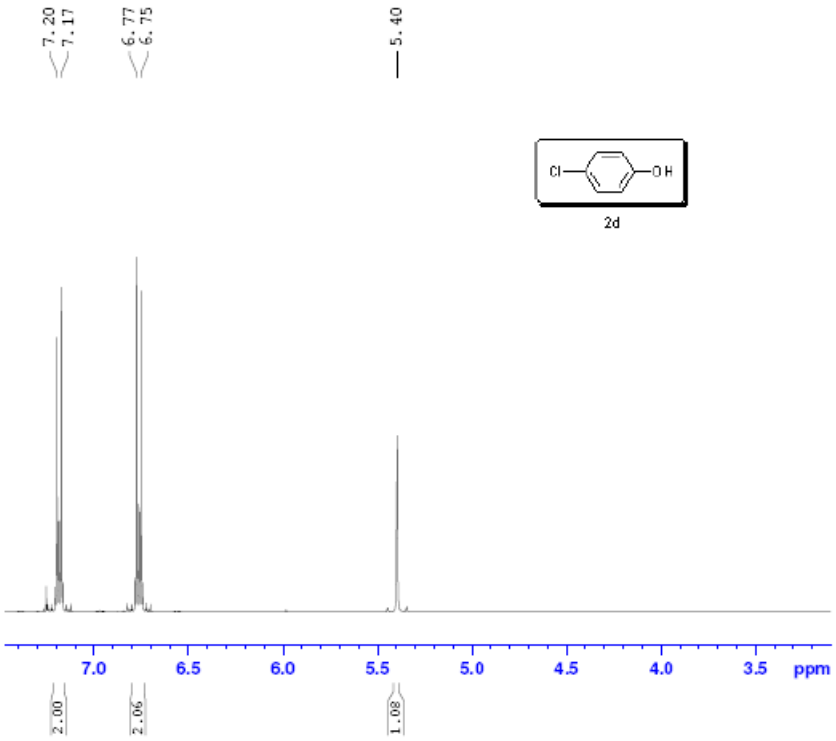

```
NAME            2010-02-22 p-NO2-Ph-C
EXPNO                    1
PROCNO                   1
Date_             20100222
Time                 23.35
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg
TD                  262144
SOLVENT                DMSO
NS                      128
DS                        0
SWH              27173.912 Hz
FIDRES            0.103660 Hz
AQ                4.8234997 sec
RG                     90.5
DW                18.400 usec
DE                 6.50 usec
TE                 298.7 K
D1             10.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.30 usec
PL1                -2.00 dB
PL1W          54.14257431 W
SFO1          100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2              90.00 usec
PL2                -2.60 dB
PL12               14.50 dB
PL13               14.50 dB
PL2W          17.82643890 W
PL12W          0.34758785 W
PL13W          0.34758785 W
SFO2          400.1520008 MHz
SI                  131072
SF            100.6178087 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.40
```



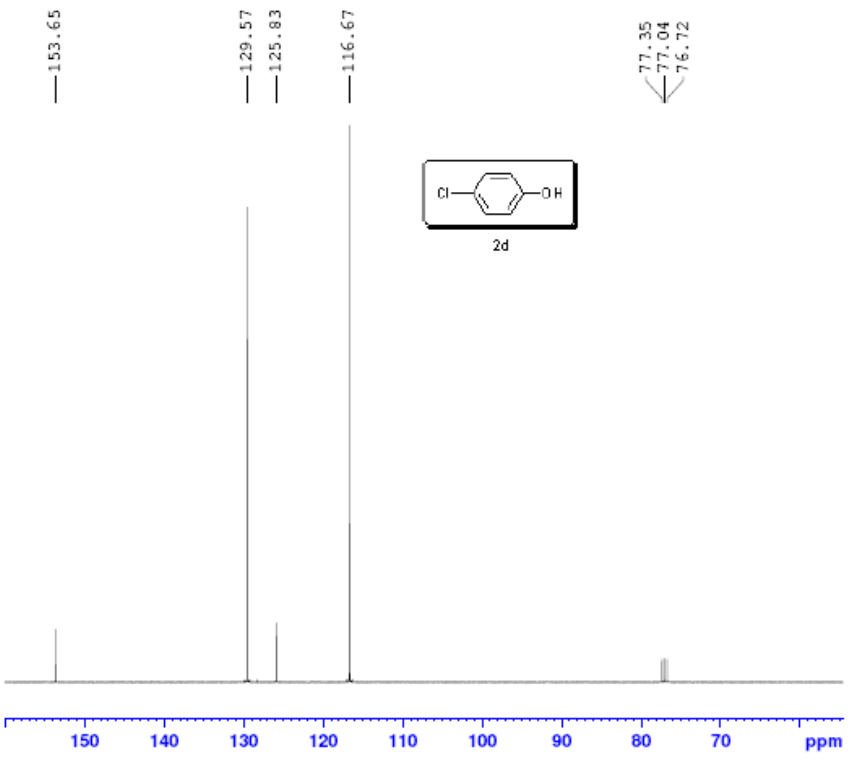

```
NAME            2010-02-21 p-Me-Ph-H
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                 16.37
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                    14.2
DW                  83.200 usec
DE                   6.50 usec
TE                  292.4 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PLW1             17.82643890 W
SFO1            400.1516006 MHz
SI                   32768
SF               400.1500444 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



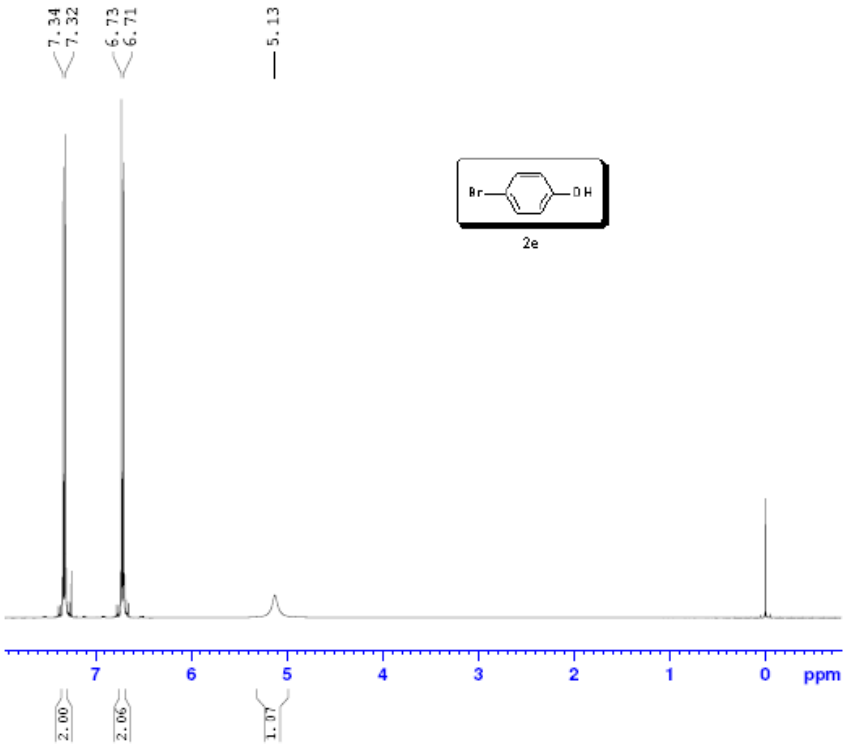

```
NAME            2010-02-21 p-Me-Ph-C
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                 18.10
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zgpg
TD                  262144
SOLVENT              CDCl3
NS                     128
DS                       0
SWH              20161.291 Hz
FIDRES            0.076909 Hz
AQ                6.5012212 sec
RG                    90.5
DW                  24.800 usec
DE                   6.50 usec
TE                  294.7 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                  -2.00 dB
PLW1             54.14257431 W
SFO1            100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W             17.82643890 W
PL12W             0.34758785 W
PL13W             0.34758785 W
SFO2            400.1520009 MHz
SI                  131072
SF               100.6178087 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
```



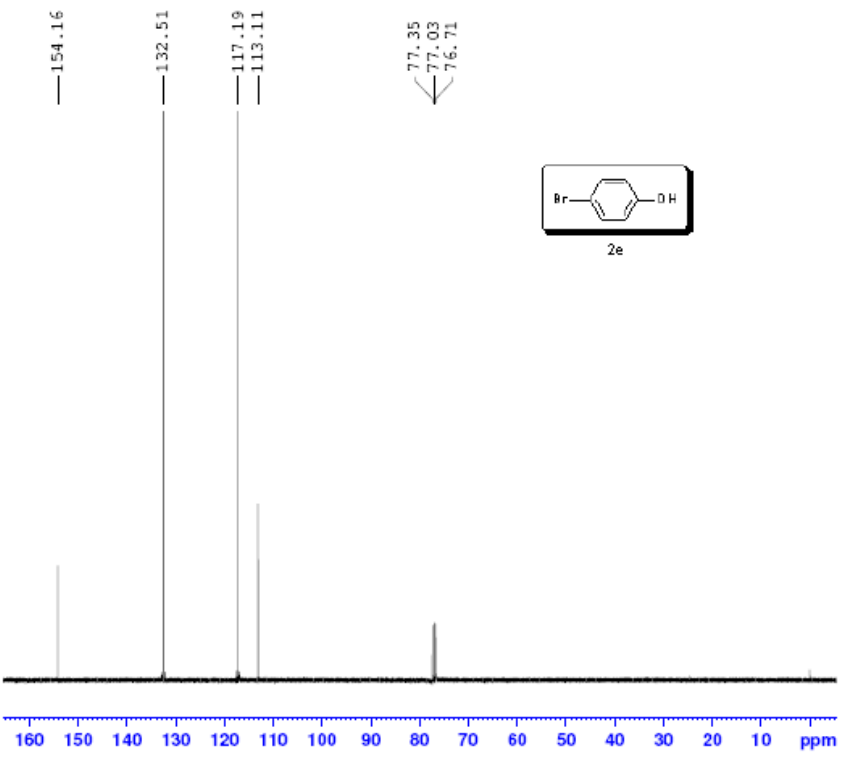

```
NAME          2010-02-22 p-Cl-Ph-H
EXPNO                  1
PROCNO                 1
Date_           20100222
Time               16.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG                zg
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH            6009.615 Hz
FIDRES         0.183399 Hz
AQ             2.7263477 sec
RG                  90.5
DW                 83.200 usec
DE                  6.50 usec
TE                292.5 K
D1             5.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.50 usec
PL1                -2.60 dB
PL1W        17.82643890 W
SFO1        400.1516006 MHz
SI                 32768
SF          400.1500115 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```



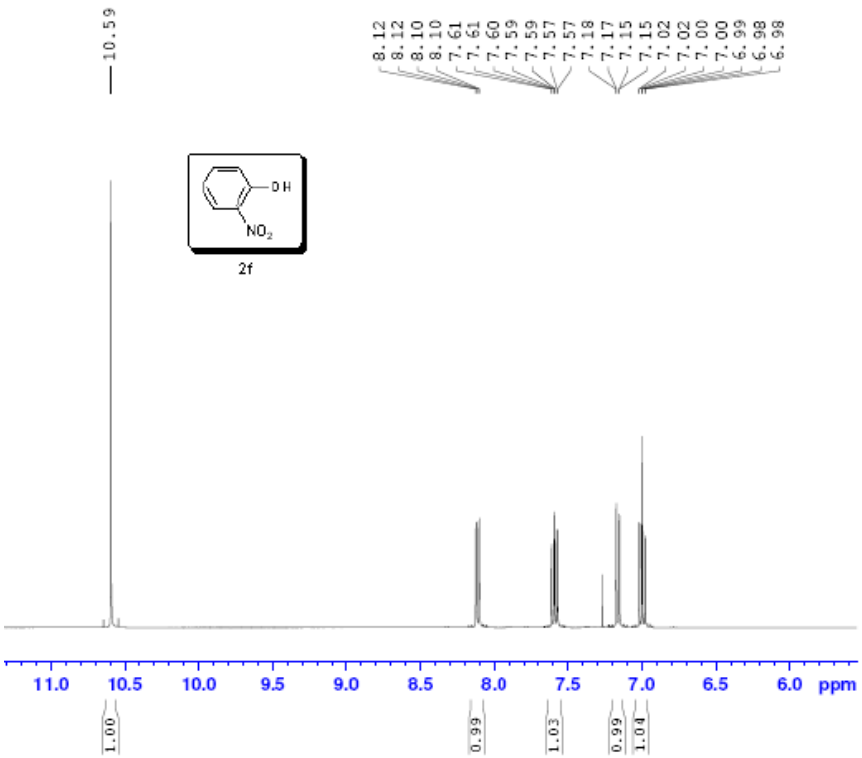

```
NAME          2010-02-22 p-Cl-Ph-C
EXPNO                  1
PROCNO                 1
Date_           20100222
Time               17.23
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                262144
SOLVENT            CDCl3
NS                   128
DS                     0
SWH           20161.291 Hz
FIDRES         0.076909 Hz
AQ             6.5012212 sec
RG                  90.5
DW                 24.800 usec
DE                  6.50 usec
TE                294.5 K
D1            10.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.30 usec
PL1                -2.00 dB
PL1W        54.14257431 W
SFO1        100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -2.60 dB
PL12               14.50 dB
PL13               14.50 dB
PL2W        17.82643890 W
PL12W        0.34758785 W
PL13W        0.34758785 W
SFO2        400.1520009 MHz
SI                131072
SF          100.6178087 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```



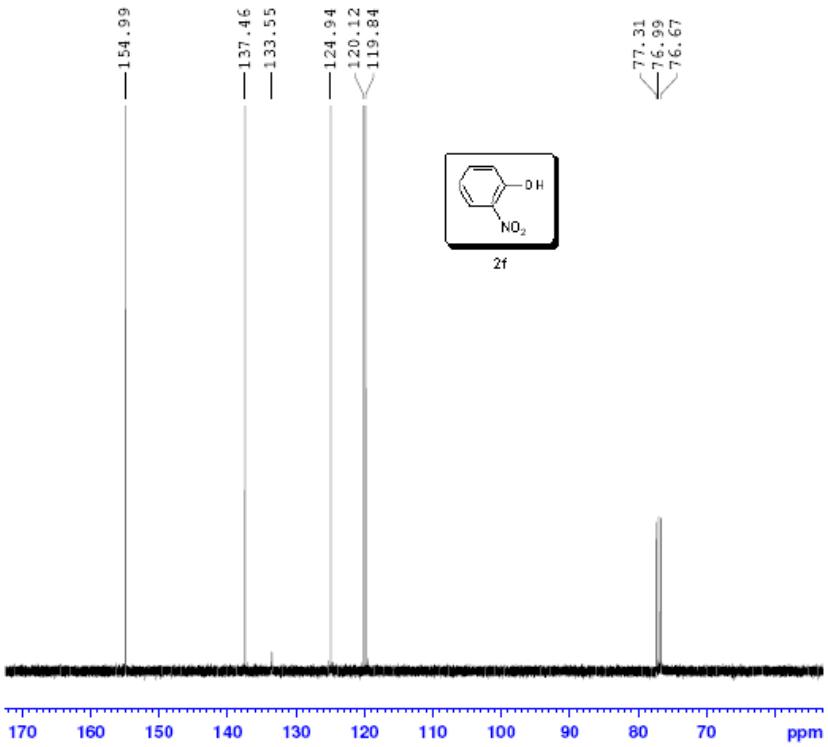

```
NAME            2010-02-21 p-Br-Ph-H
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                16.24
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7263477 sec
RG                    90.5
DW                83.200 usec
DE                 6.50 usec
TE                292.3 K
D1               5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                 12.50 usec
PL1                -2.60 dB
PL1W         17.82643890 W
SFO1         400.1516006 MHz
SI                   32768
SF           400.1500119 MHz
WDW                     no
SSB                      0
LB                 0.00 Hz
GB                       0
PC                 1.00
```



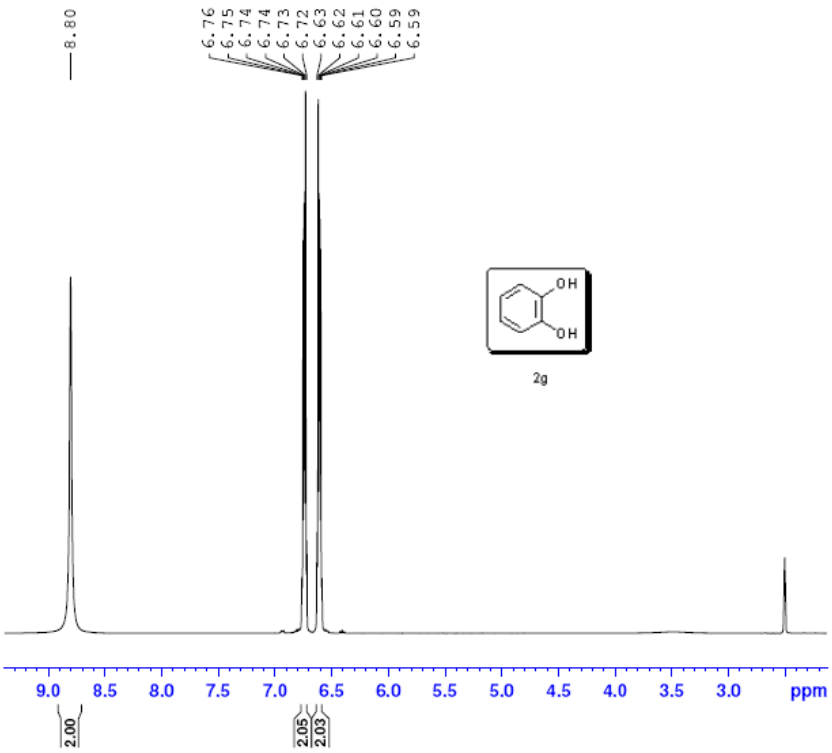

```
NAME            2010-02-21 Br-Ph-C
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                17.25
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zgpg
TD                  262144
SOLVENT              CDCl3
NS                     128
DS                       0
SWH              20161.291 Hz
FIDRES           0.076909 Hz
AQ               6.5012212 sec
RG                    90.5
DW                24.800 usec
DE                 6.50 usec
TE                294.9 K
D1              10.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.30 usec
PL1                -2.00 dB
PL1W         54.14257431 W
SFO1         100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2              90.00 usec
PL2                -2.60 dB
PL12               14.50 dB
PL13               14.50 dB
PL2W         17.82643890 W
PL12W         0.34758785 W
PL13W         0.34758785 W
SFO2         400.1520009 MHz
SI                  131072
SF           100.6178087 MHz
WDW                     no
SSB                      0
LB                 0.00 Hz
GB                       0
PC                 1.40
```



```
NAME            2010-02-20 o-NO2-Ph-H
EXPNO                    1
PROCNO                   1
Date_             20100220
Time                 23.57
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                zg
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7263477 sec
RG                    90.5
DW                83.200 usec
DE                 6.50 usec
TE                294.5 K
D1               5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.50 usec
PL1                 -2.60 dB
PL1W          17.82643890 W
SFO1          400.1516006 MHz
SI                   32768
SF            400.1500055 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

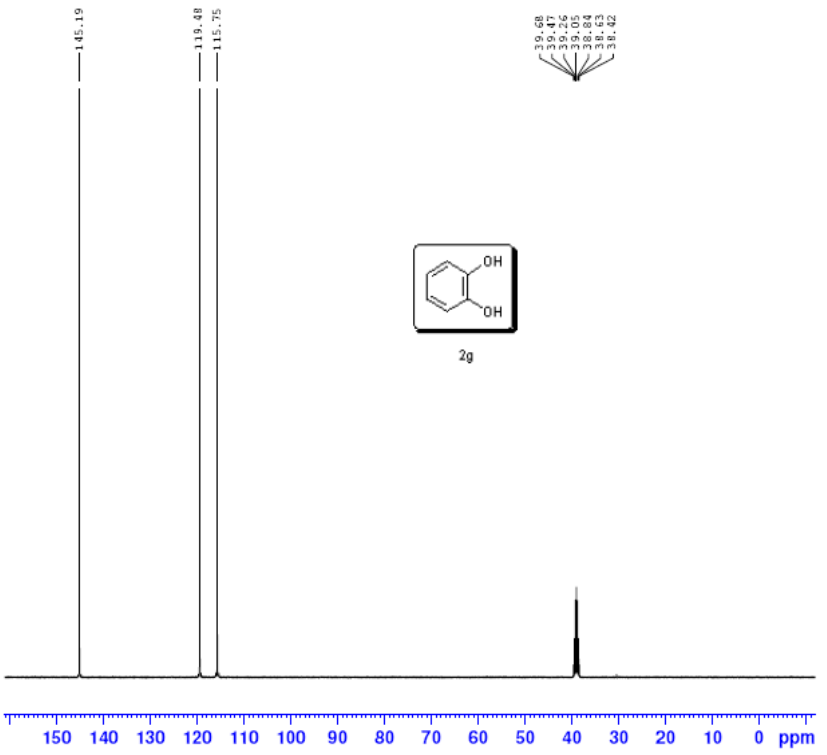


```
NAME            2010-02-20 o-NO2-PhOH-C
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                 0.54
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg
TD                  262144
SOLVENT              CDCl3
NS                     128
DS                       0
SWH             20161.291 Hz
FIDRES           0.076909 Hz
AQ               6.5012212 sec
RG                    90.5
DW                24.800 usec
DE                 6.50 usec
TE                295.6 K
D1              10.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.30 usec
PL1                 -2.00 dB
PL1W          54.14257431 W
SFO1          100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2               90.00 usec
PL2                 -2.60 dB
PL12                14.50 dB
PL13                14.50 dB
PL2W          17.82643890 W
PL12W          0.34758785 W
PL13W          0.34758785 W
SFO2          400.1520008 MHz
SI                  131072
SF            100.6178087 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
```



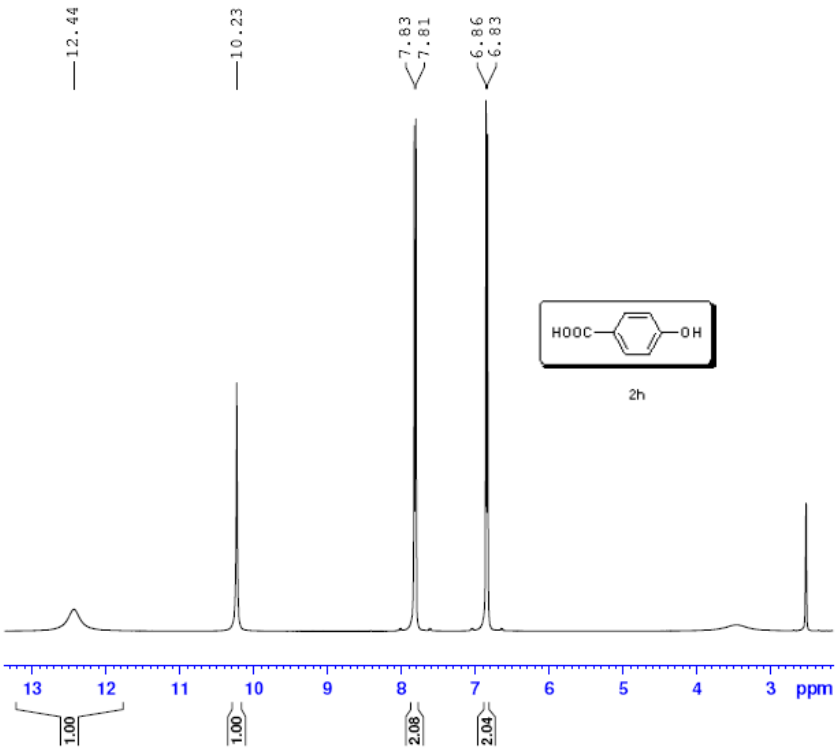
BRUKER

```
Current Data Parameters
NAME                  04212010
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20100421
Time                    13.21
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         0
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                       80.6
DW                     60.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     12.00 usec
PL1                    -2.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                     32768
SF                400.1300023 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



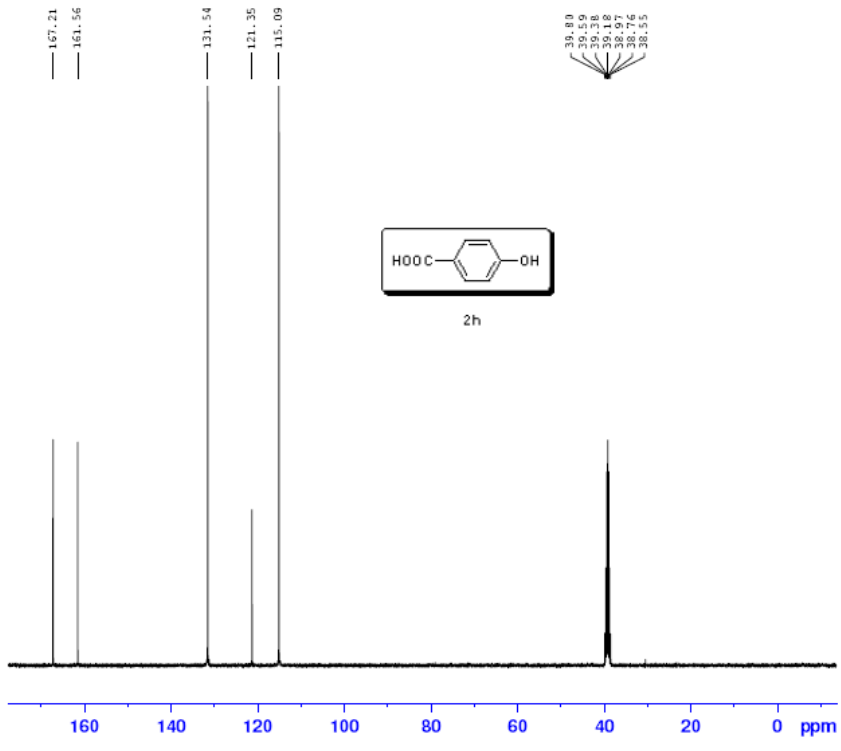
BRUKER

```
Current Data Parameters
NAME                  04212010
EXPNO                       12
PROCNO                       1

F2 - Acquisition Parameters
Date_              20100421
Time                    14.32
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                     65536
SOLVENT                 DMSO
NS                       128
DS                         0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631888 sec
RG                      2050
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                     15.50 usec
PL1                    -1.00 dB
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  60.00 usec
PL12                   11.35 dB
PL13                   13.05 dB
PL2                    -2.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF                100.6128193 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```



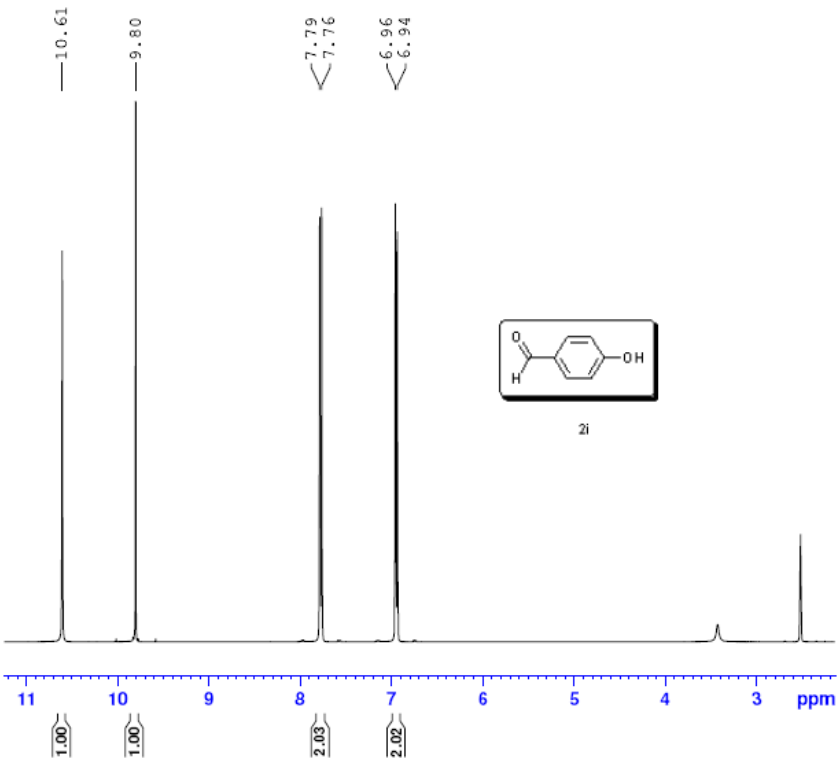
BRUKER

```
Current Data Parameters
NAME                  04212010
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20100421
Time                   13.11
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        0
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                       128
DW                  60.800 usec
DE                   6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       12.00 usec
PL1                      -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       32768
SF                400.1299943 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```



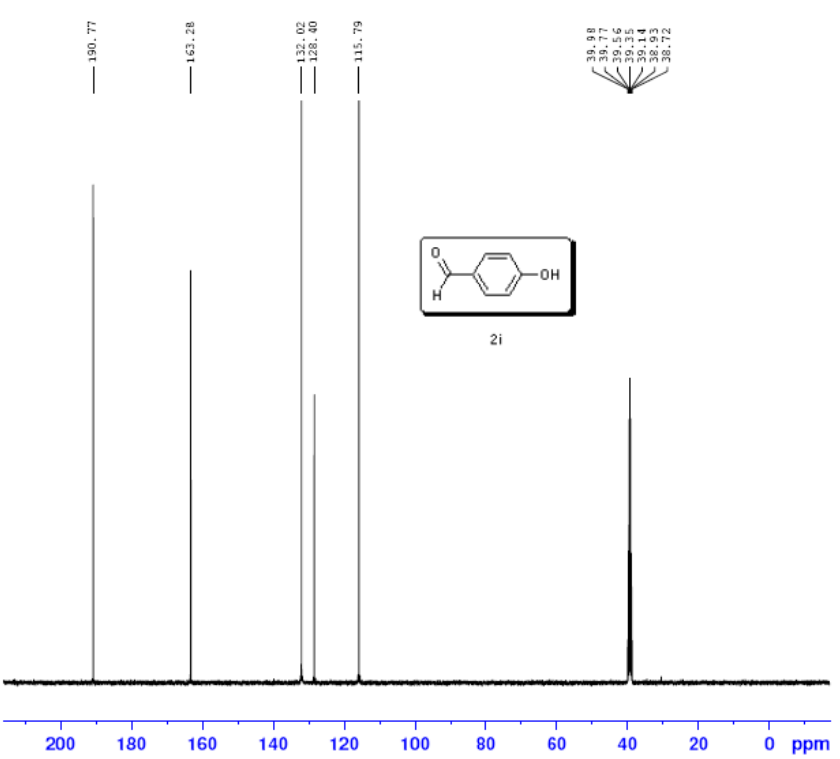
BRUKER

```
Current Data Parameters
NAME                  04212010
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_              20100421
Time                   14.11
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      128
DS                        0
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                     2050
DW                  20.800 usec
DE                   6.50 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       15.50 usec
PL1                      -1.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    60.00 usec
PL12                     11.35 dB
PL13                     13.05 dB
PL2                      -2.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                100.6128193 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```



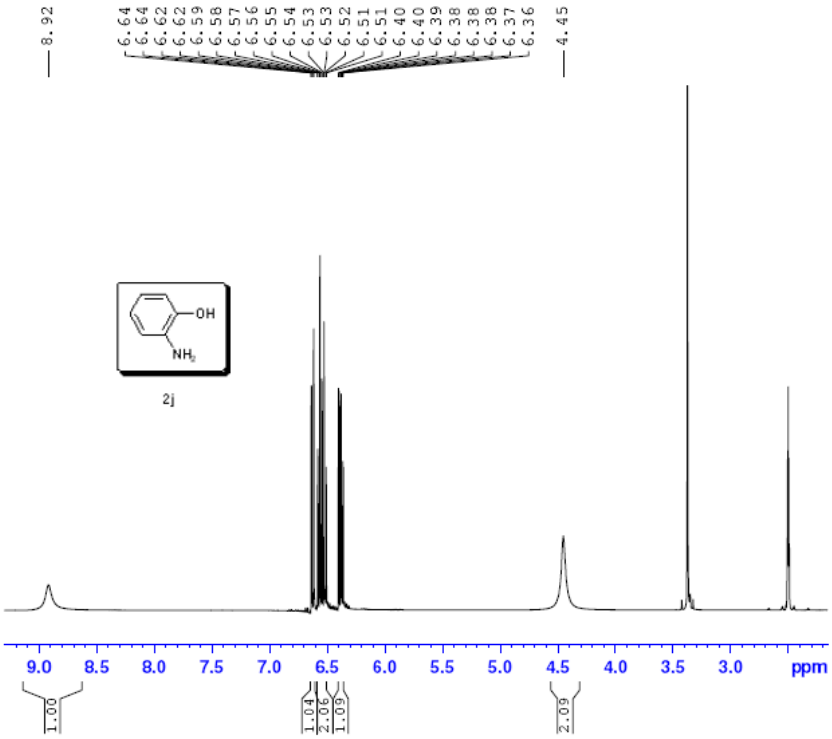
BRUKER

```
Current Data Parameters
NAME                 04212010
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100421
Time                   13.16
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        0
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      128
DW                   60.800 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.00 usec
PL1                     -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                400.1299962 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

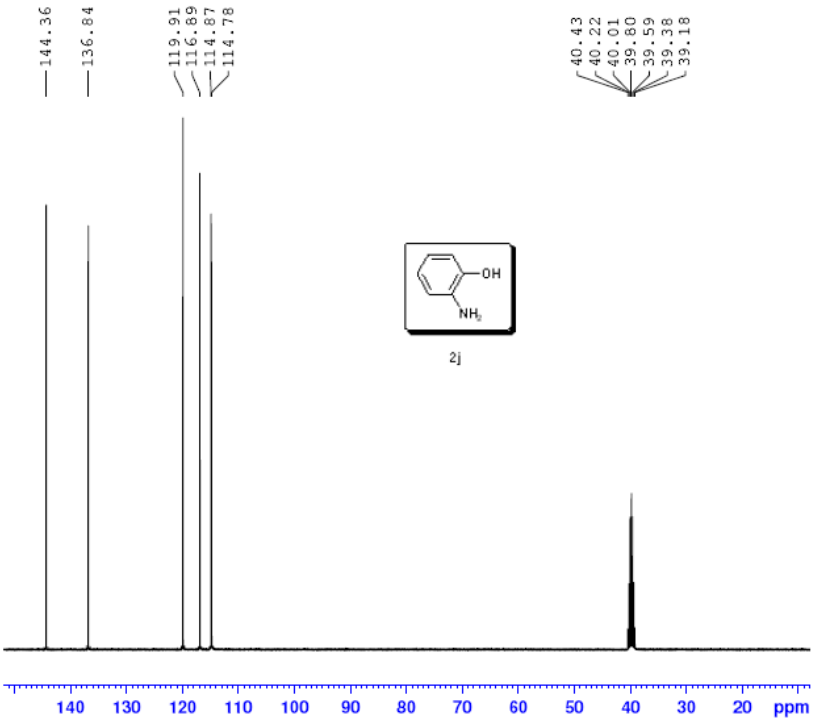


BRUKER

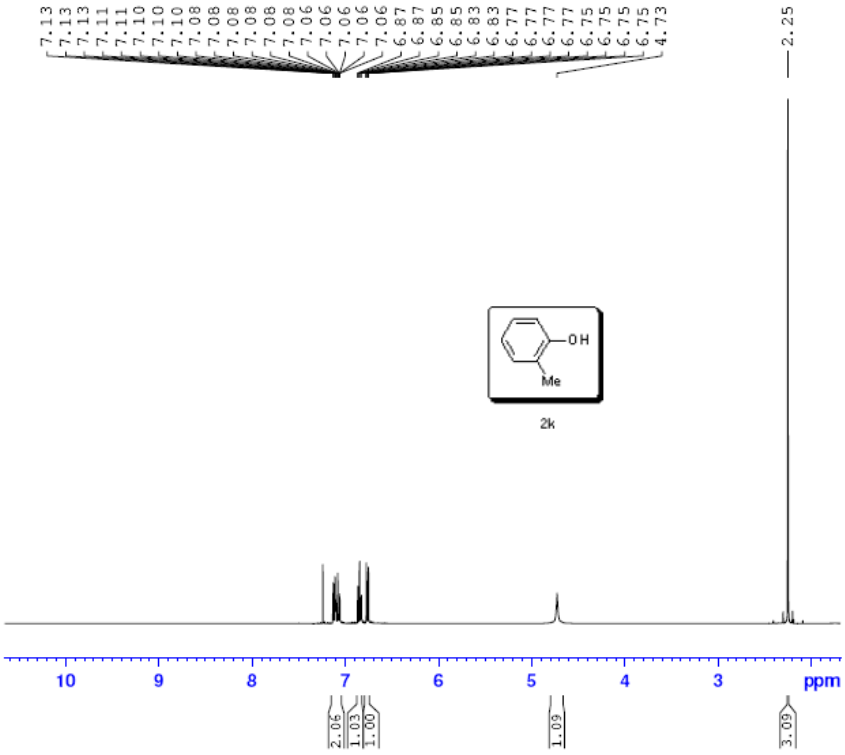
```
Current Data Parameters
NAME                 04212010
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_               20100421
Time                   14.21
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                      128
DS                        0
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                     2050
DW                   20.800 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      15.50 usec
PL1                     -1.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   60.00 usec
PL12                    11.35 dB
PL13                    13.05 dB
PL2                     -2.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6128193 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```



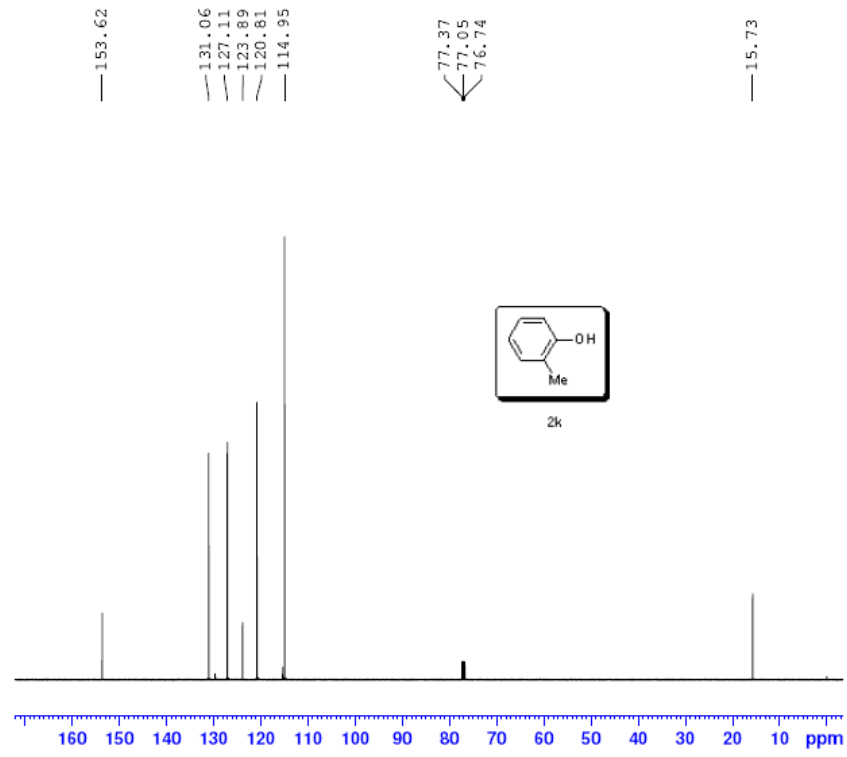

```
NAME            2010-02-22 o-NH2-Ph-H
EXPNO                    1
PROCNO                   1
Date_             20100222
Time                 20.51
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT               DMSO
NS                      32
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                     90.5
DW                 83.200 usec
DE                  6.50 usec
TE                 296.1 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.82643890 W
SFO1            400.1516006 MHz
SI                   32768
SF              400.1500016 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



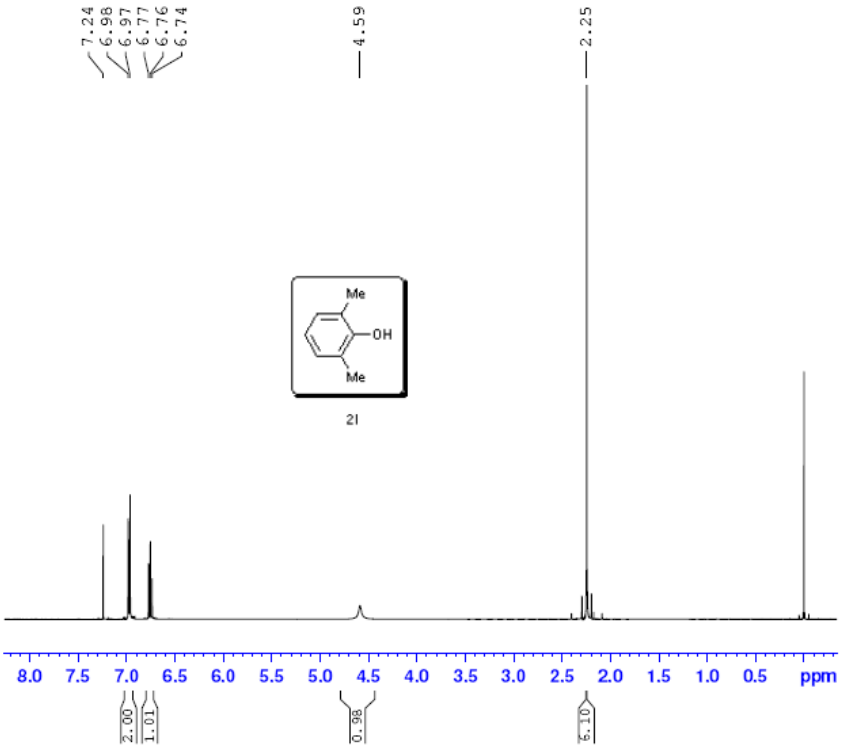

```
NAME            2010-02-22 o-NH2-Ph-C
EXPNO                    1
PROCNO                   1
Date_             20100222
Time                 22.20
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg
TD                  262144
SOLVENT               DMSO
NS                     128
DS                       0
SWH              20161.291 Hz
FIDRES            0.076909 Hz
AQ                6.5012212 sec
RG                     90.5
DW                 24.800 usec
DE                  6.50 usec
TE                 298.8 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W            54.14257431 W
SFO1            100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W            17.82643990 W
PL12W            0.34758785 W
PL13W            0.34758785 W
SFO2            400.1520008 MHz
SI                  131072
SF              100.6178087 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.40
```



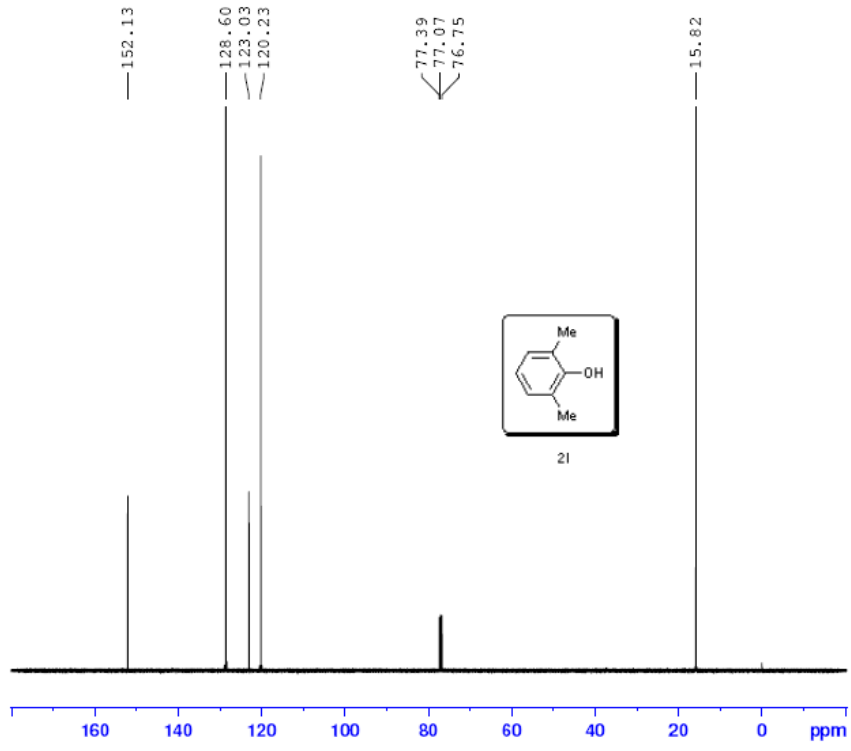
```
NAME            2010-02-21 o-Me-Ph-H
EXPNO                     1
PROCNO                    1
Date_              20100221
Time                  19.26
INSTRUM               spect
PROBHD     5 mm PABBO BB-
PULPROG                zg
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                     90.5
DW                   83.200 usec
DE                    6.50 usec
TE                   293.6 K
D1                5.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.82643890 W
SFO1            400.1516006 MHz
SI                    32768
SF              400.1500163 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.00
```



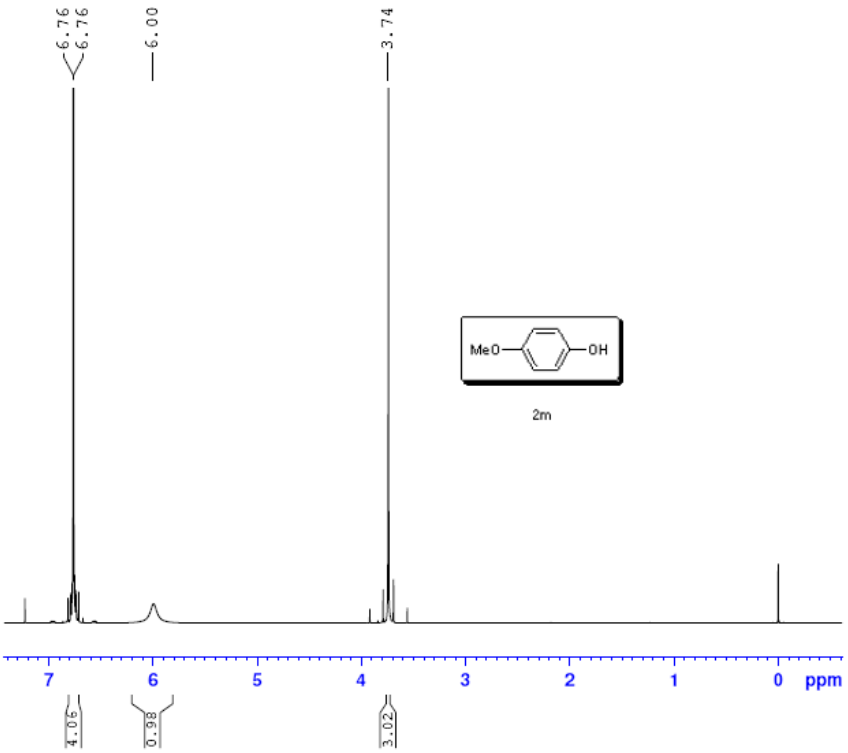
```
NAME            2010-02-21 o-Me-Ph-C
EXPNO                     1
PROCNO                    1
Date_              20100221
Time                  20.05
INSTRUM               spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg
TD                   262144
SOLVENT               CDCl3
NS                      256
DS                        0
SWH              20161.291 Hz
FIDRES            0.076909 Hz
AQ                6.5012212 sec
RG                     90.5
DW                   24.800 usec
DE                    6.50 usec
TE                   295.8 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W            54.14257431 W
SFO1            100.6259474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W            17.82643890 W
PL12W            0.34758785 W
PL13W            0.34758785 W
SFO2            400.1520008 MHz
SI                   131072
SF              100.6179087 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.40
```



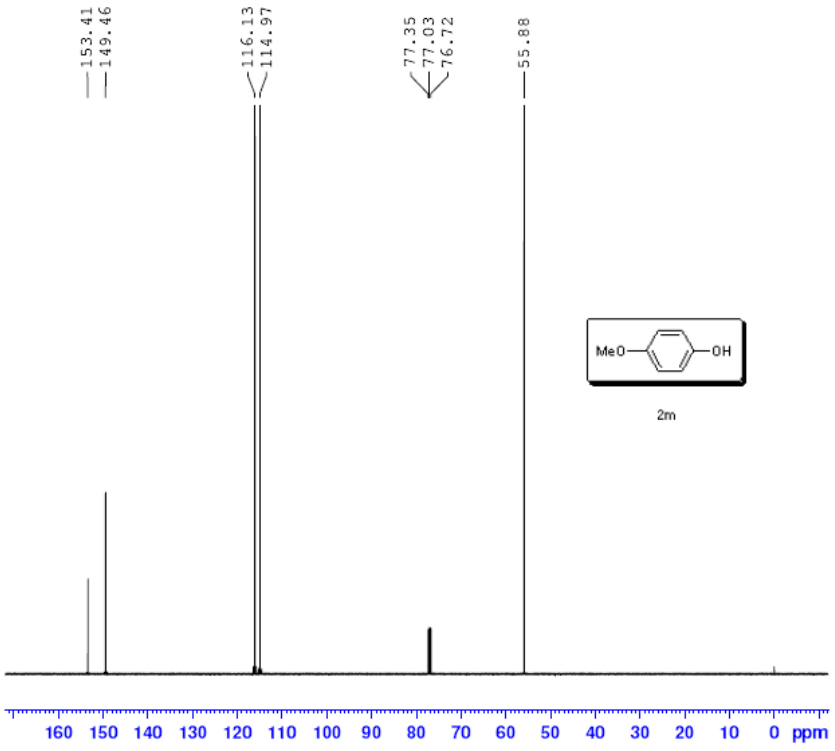

```
NAME          2010-02-21 2,6-dimethyl-Ph-H
EXPNO                  1
PROCNO                 1
Date_           20100221
Time               18.38
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7263477 sec
RG                  90.5
DW                 83.200 usec
DE                  6.50 usec
TE                294.2 K
D1              5.00000000 sec
TD0                    1

====== CHANNEL f1 ======
NUC1                  1H
P1                 12.50 usec
PL1                -2.60 dB
PL1W           17.82643890 W
SFO1          400.1516006 MHz
SI                 32768
SF            400.1500150 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```



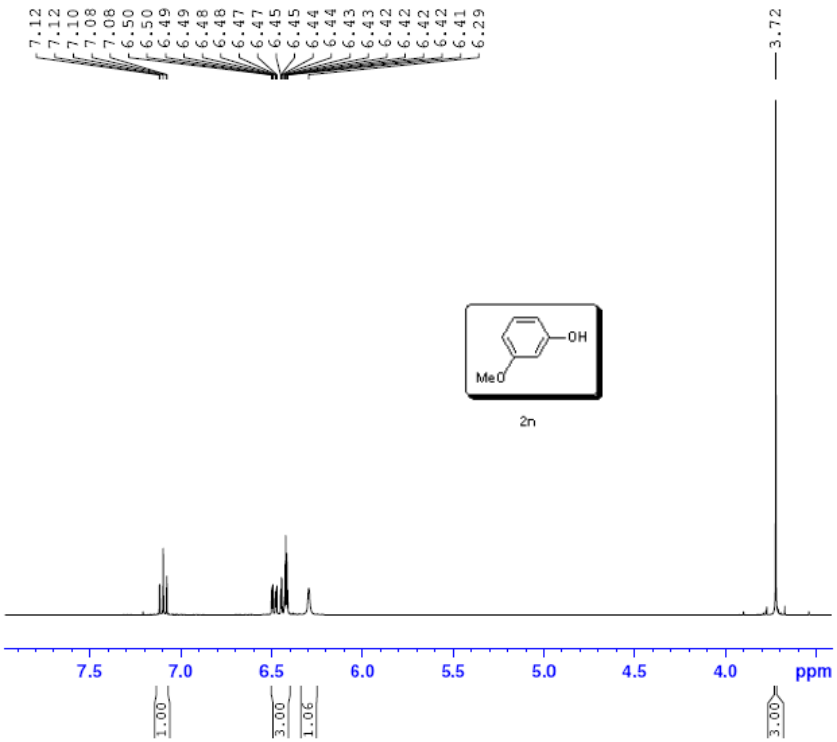

```
NAME          2010-02-21 2,6-dimethyl-Ph-C
EXPNO                  1
PROCNO                 1
Date_           20100221
Time               21.32
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                262144
SOLVENT            CDCl3
NS                   256
DS                     0
SWH            20161.291 Hz
FIDRES          0.076909 Hz
AQ              6.5012212 sec
RG                  90.5
DW                 24.800 usec
DE                  6.50 usec
TE                295.7 K
D1             10.00000000 sec
D11             0.03000000 sec
TD0                    1

====== CHANNEL f1 ======
NUC1                  13C
P1                  9.30 usec
PL1                -2.00 dB
PL1W           54.14257431 W
SFO1          100.6258474 MHz

====== CHANNEL f2 ======
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -2.60 dB
PL2L2              14.50 dB
PL2L3              14.50 dB
PL2W           17.82643890 W
PL12W           0.34758785 W
PL13W           0.34758785 W
SFO2          400.1520098 MHz
SI                131072
SF            100.6178087 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.40
```



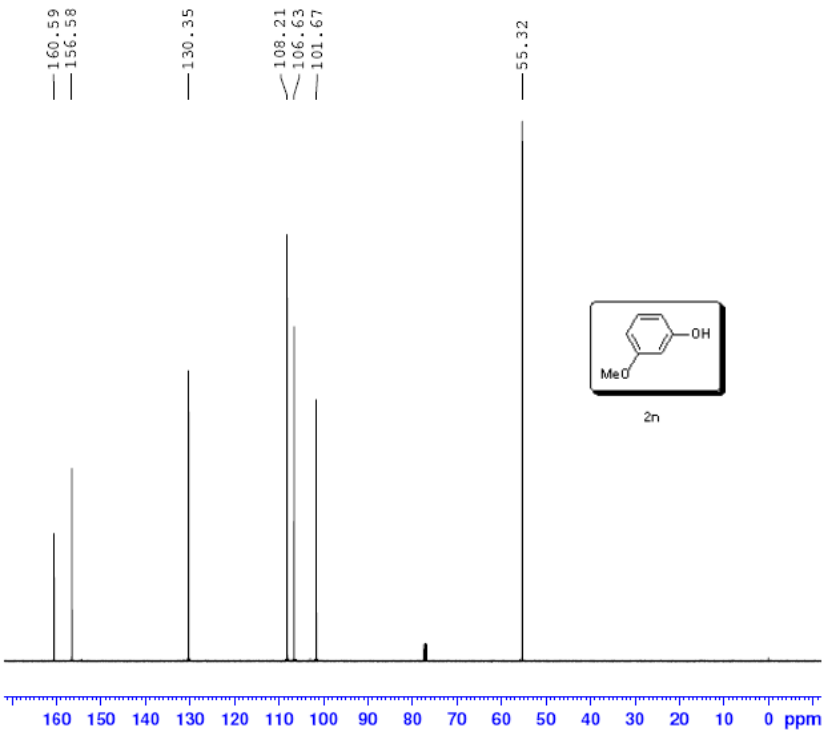

```
NAME            2010-02-20 p-OMePh-H
EXPNO                    1
PROCNO                   1
Date_                20100220
Time                    22.50
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg
TD                      32768
SOLVENT                 CDCl3
NS                         32
DS                          0
SWH                  6009.615 Hz
FIDRES               0.183399 Hz
AQ                   2.7263477 sec
RG                         16
DW                     83.200 usec
DE                      6.50 usec
TE                     294.4 K
D1                   5.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.50 usec
PL1                     -2.60 dB
PL1W                17.92643890 W
SFO1                400.1516006 MHz
SI                      32768
SF                  400.1500206 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.00
```



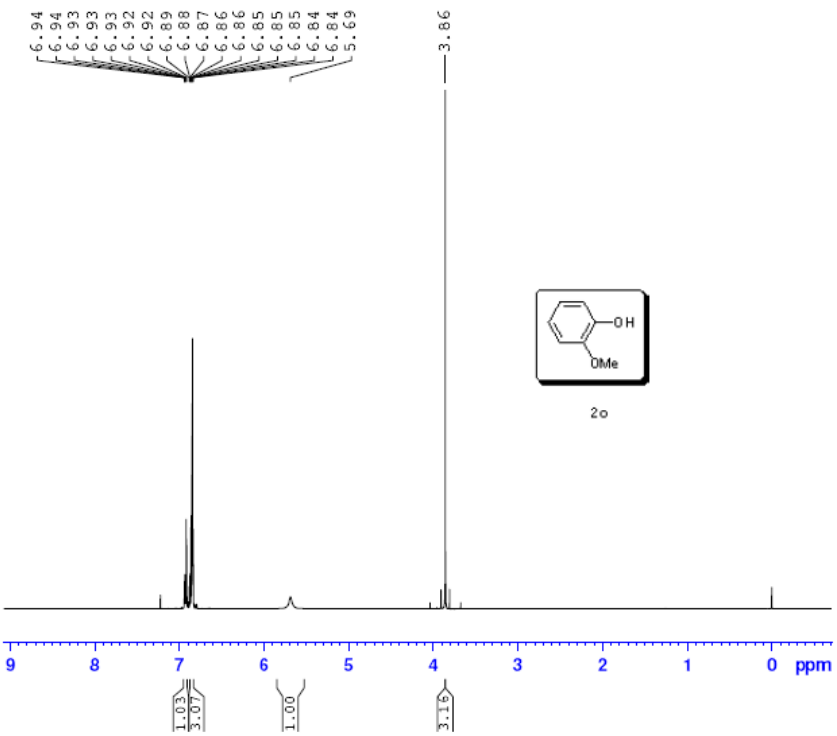

```
NAME            2010-02-20 p-OMePh-C
EXPNO                    1
PROCNO                   1
Date_                20100220
Time                    22.00
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg
TD                     262144
SOLVENT                 CDCl3
NS                        512
DS                          0
SWH                 20161.291 Hz
FIDRES               0.076909 Hz
AQ                   6.5012212 sec
RG                       90.5
DW                     24.800 usec
DE                      6.50 usec
TE                     296.1 K
D1                  10.00000000 sec
D11                  0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.30 usec
PL1                     -2.00 dB
PL1W                54.14257431 W
SFO1                100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL2                     -2.60 dB
PL12                    14.50 dB
PL13                    14.50 dB
PL2W                17.92643890 W
PL12W                0.34759795 W
PL13W                0.34759795 W
SFO2                400.1520008 MHz
SI                      131072
SF                  100.6179097 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.40
```



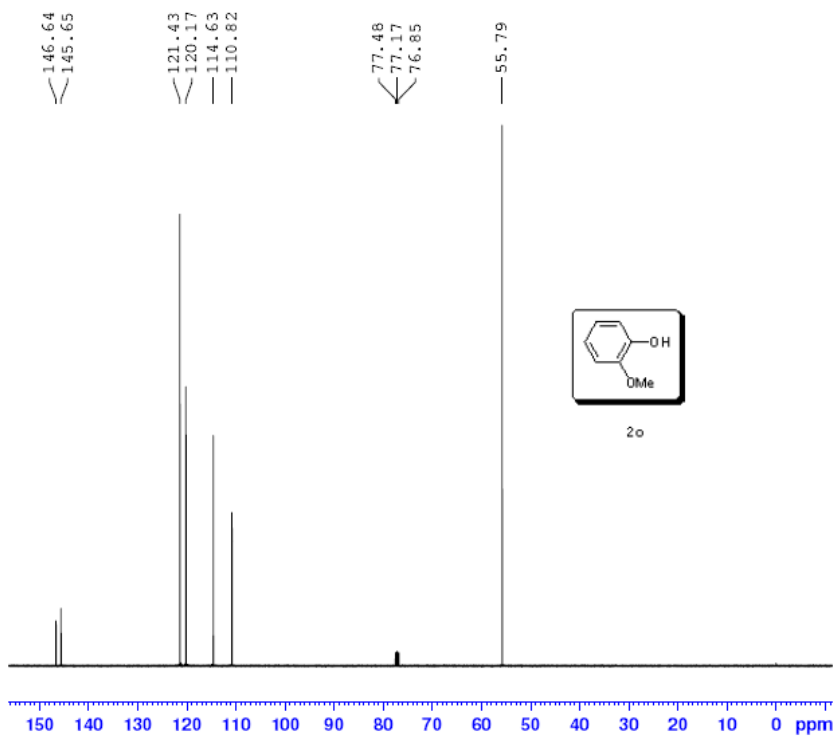

```
NAME            2010-02-22 m-OMe-Ph-H-2
EXPNO                    1
PROCNO                   1
Date_             20100223
Time                 3.07
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG                zg
TD                  32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                     14.2
DW                 83.200 usec
DE                  6.50 usec
TE                 298.2 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.82643890 W
SFO1           400.1516006 MHz
SI                   32768
SF             400.1500288 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



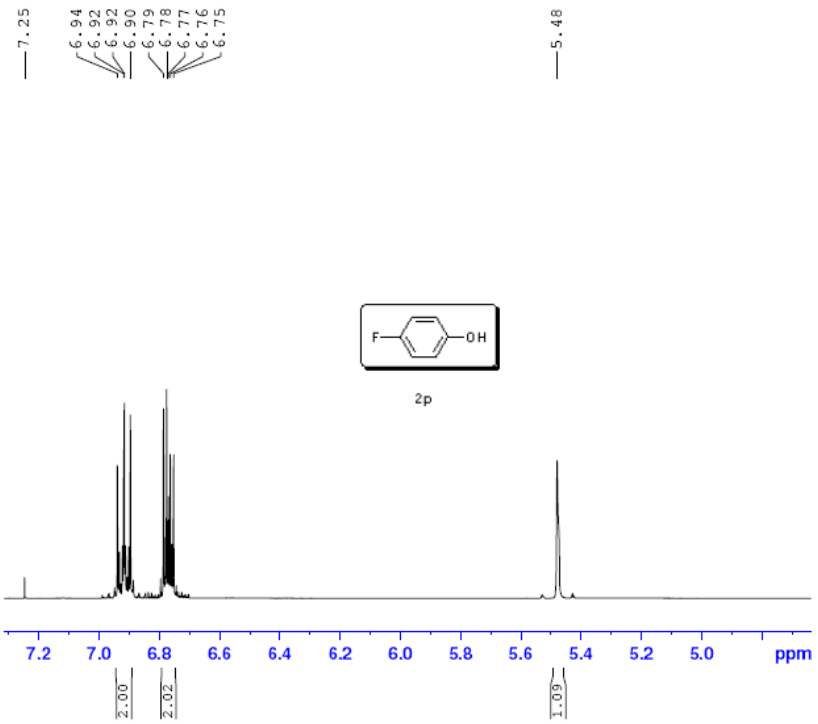

```
NAME          2010-02-20 m-OMePh-C
EXPNO                    1
PROCNO                   1
Date_             20100220
Time                23.46
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                  262144
SOLVENT              CDCl3
NS                      128
DS                       0
SWH              20161.291 Hz
FIDRES            0.076909 Hz
AQ                6.5012212 sec
RG                     90.5
DW                 24.800 usec
DE                  6.50 usec
TE                 295.8 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.30 usec
PL1                 -2.00 dB
PL1W            54.14257431 W
SFO1           100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                 -2.60 dB
PL12                14.50 dB
PL13                14.50 dB
PL2W            17.82643890 W
PL12W            0.34759795 W
PL13W            0.34759795 W
SFO2           400.1520008 MHz
SI                  131072
SF             100.6179087 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
```




```
NAME            2010-02-20 0-OMePh-H
EXPNO                    1
PROCNO                   1
Date_             20100220
Time                 22.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                  zg
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                     25.4
DW                  83.200 usec
DE                   6.50 usec
TE                  294.8 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.82643890 W
SFO1            400.1516006 MHz
SI                    32768
SF              400.1500224 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

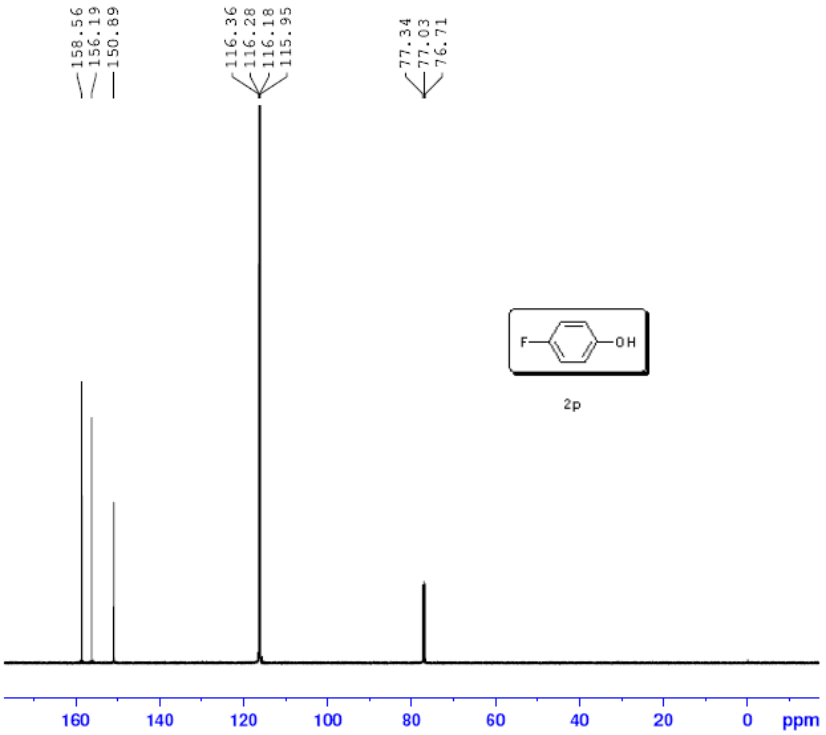



```
NAME            2010-02-20 o-omeph-c
EXPNO                    1
PROCNO                   1
Date_             20100220
Time                 18.44
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg
TD                   262144
SOLVENT               CDCl3
NS                      128
DS                        0
SWH              20161.291 Hz
FIDRES            0.076909 Hz
AQ                6.5012212 sec
RG                     90.5
DW                  24.800 usec
DE                   6.50 usec
TE                  295.1 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W            54.14257431 W
SFO1            100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W            17.82643890 W
PL12W            0.34758785 W
PL13W            0.34758785 W
SFO2            400.1520009 MHz
SI                   131072
SF              100.6178087 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
```



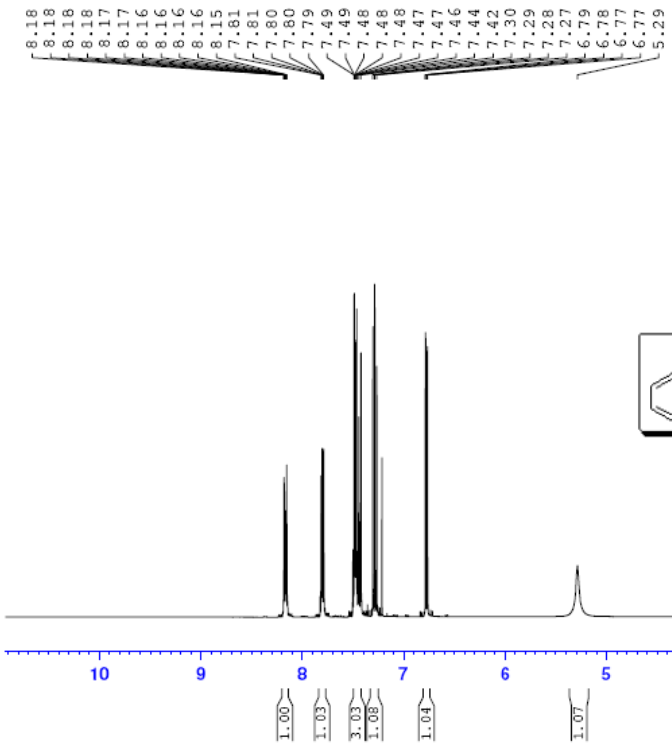
BRUKER

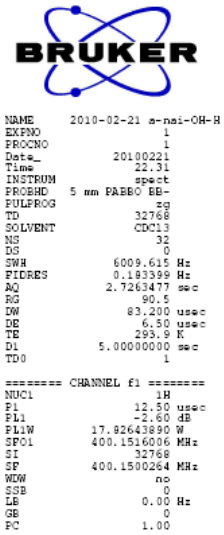
```
NAME          2010-02-22 p-F-Ph-H
EXPNO                   1
PROCNO                  1
Date_            20100222
Time                16.35
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7263477 sec
RG                    28.5
DW                  83.200 usec
DE                   6.50 usec
TE                  292.7 K
D1               5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W          17.82643890 W
SFO1          400.1516006 MHz
SI                   32768
SF            400.1500136 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



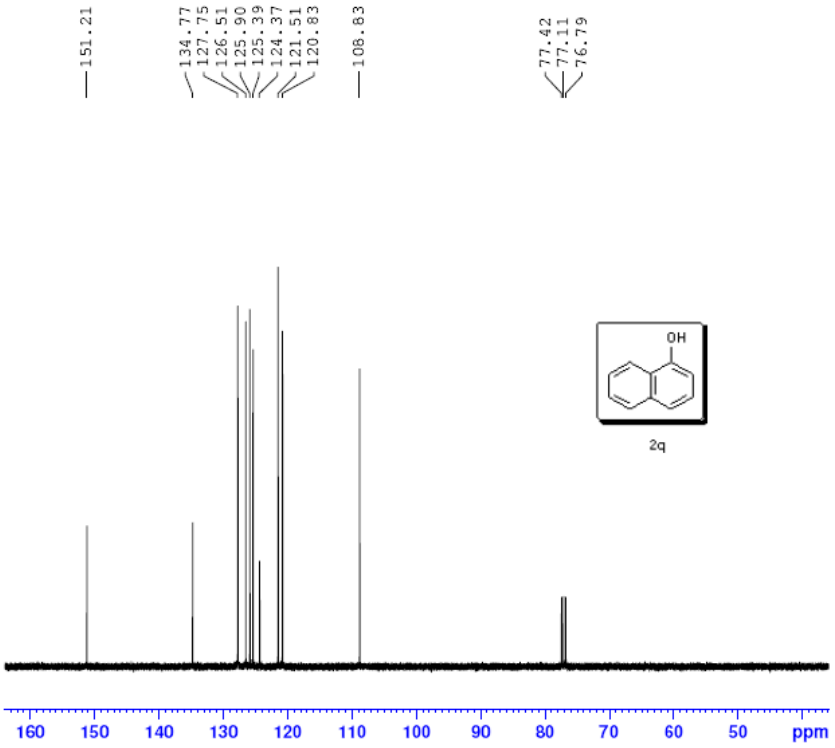
BRUKER

```
NAME          2010-02-22 p-F-Ph-C
EXPNO                   1
PROCNO                  1
Date_            20100222
Time                18.06
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg
TD                  262144
SOLVENT              CDCl3
NS                     128
DS                       0
SWH             20161.291 Hz
FIDRES           0.076909 Hz
AQ               6.5012212 sec
RG                    90.5
DW                  24.800 usec
DE                   6.50 usec
TE                  294.9 K
D1              10.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W          54.14257431 W
SFO1          100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W          17.82643890 W
PL12W          0.34758785 W
PL13W          0.34758785 W
SFO2          400.1520008 MHz
SI                  131072
SF            100.6178087 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.40
```

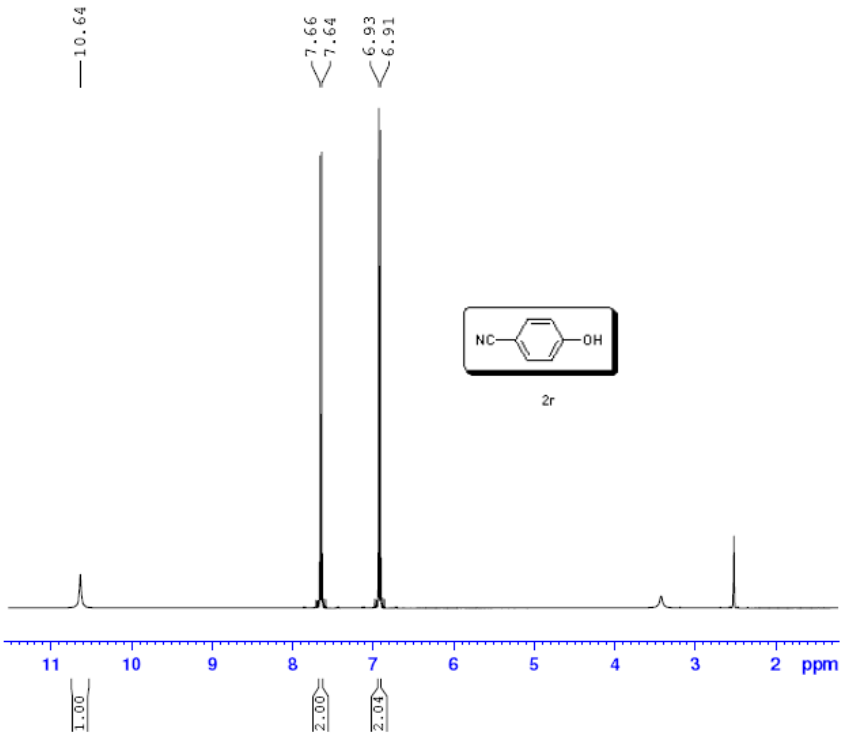




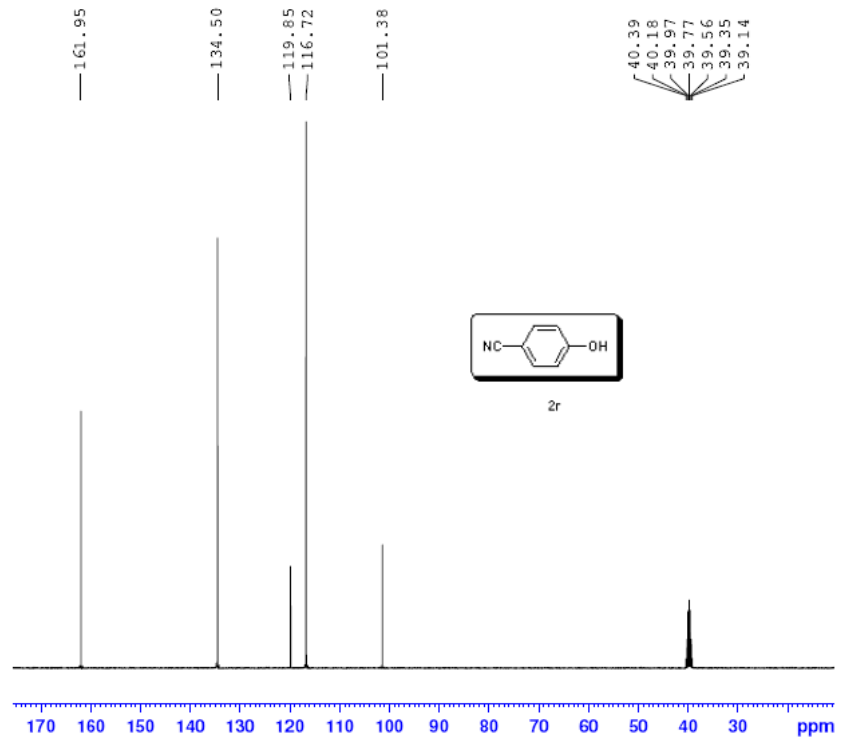

```
NAME            2010-02-21 a-nai-OH-H
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                 22.31
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7263477 sec
RG                    90.5
DW                83.200 usec
DE                 6.50 usec
TE                 293.9 K
D1              5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W          17.82643890 W
SFO1          400.1516006 MHz
SI                   32768
SF            400.1500264 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



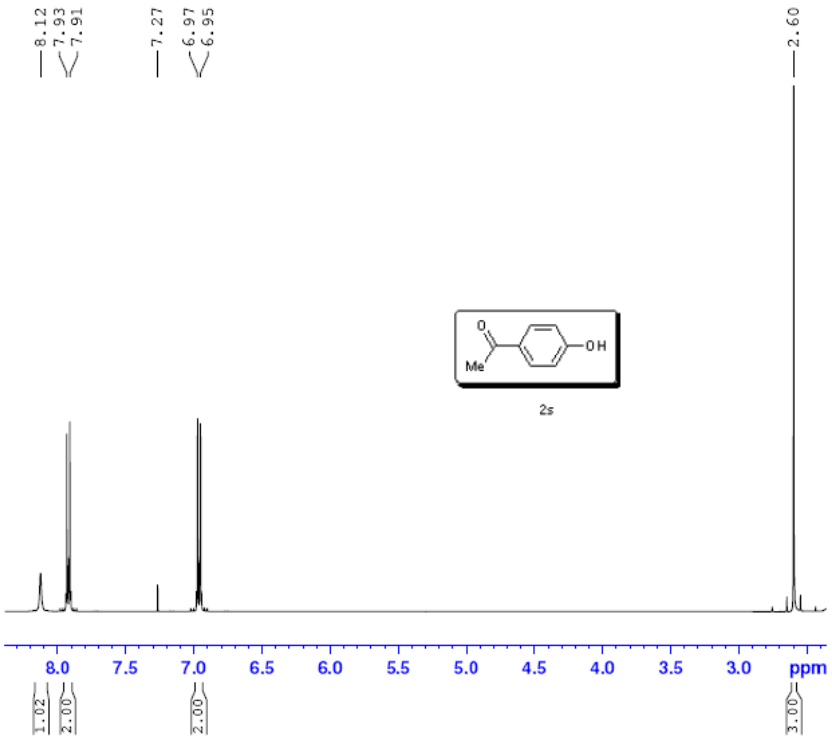

```
NAME            2010-02-21 a-nai-OH-C
EXPNO                    1
PROCNO                   1
Date_             20100221
Time                 23.22
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg
TD                 262144
SOLVENT              CDCl3
NS                     128
DS                       0
SWH             20161.291 Hz
FIDRES           0.076909 Hz
AQ               6.5012212 sec
RG                    90.5
DW                24.800 usec
DE                 6.50 usec
TE                 295.4 K
D1              10.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W          54.14257431 W
SFO1          100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W          17.82643890 W
PL12W          0.34758785 W
PL13W          0.34758785 W
SFO2          400.1520009 MHz
SI                  131072
SF            100.6178097 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
```



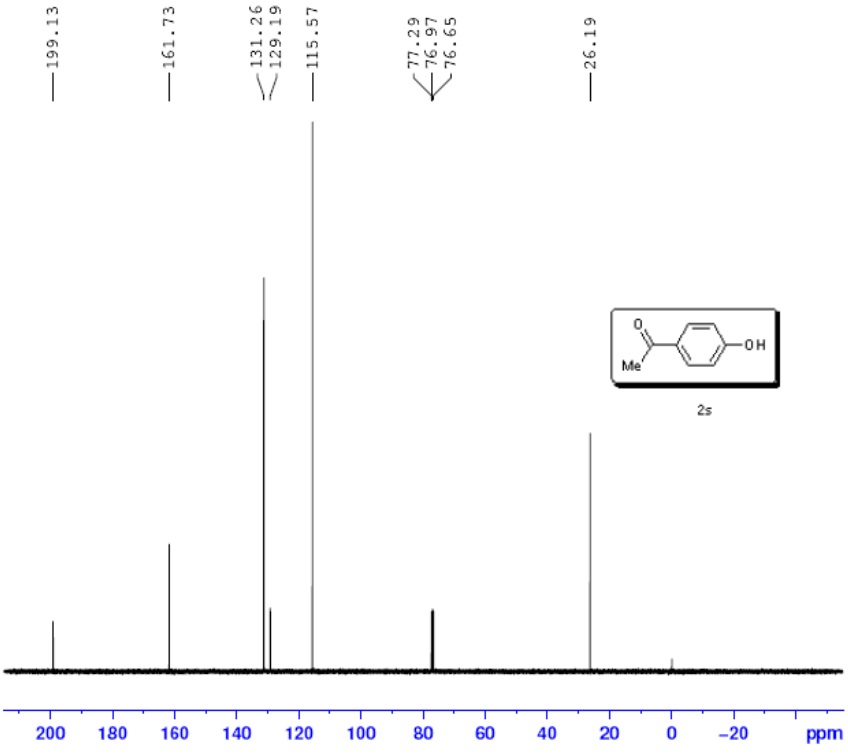

```
NAME            2010-02-22 p-CN-Ph-H
EXPNO                    1
PROCNO                   1
Date_             20100222
Time                 20.40
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT               DMSO
NS                      32
DS                       0
SWH               6009.615 Hz
FIDRES           0.183399 Hz
AQ                2.7263477 sec
RG                    90.5
DW                  83.200 usec
DE                   6.50 usec
TE                  295.2 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.92643890 W
SFO1           400.1516006 MHz
SI                   32768
SF             400.1499926 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```



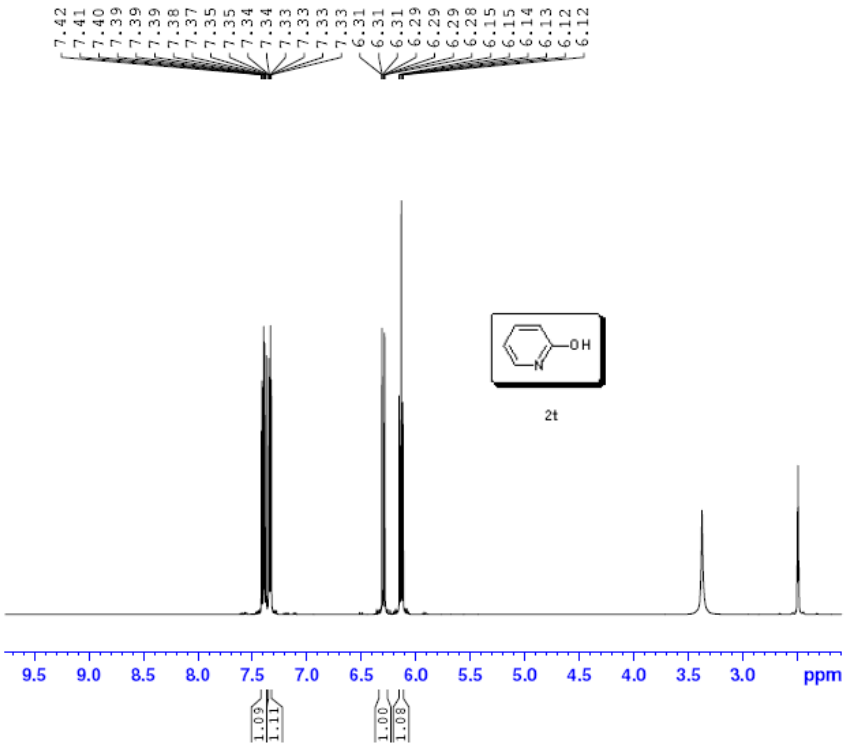

```
NAME            2010-02-22 p-CN-Ph-C
EXPNO                    1
PROCNO                   1
Date_             20100222
Time                 21.40
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG              zgpg
TD                  262144
SOLVENT               DMSO
NS                     128
DS                       0
SWH              20161.291 Hz
FIDRES           0.076909 Hz
AQ                6.5012212 sec
RG                    90.5
DW                  24.800 usec
DE                   6.50 usec
TE                  298.2 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W            54.14257431 W
SFO1           100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W            17.92643890 W
PL12W            0.34759795 W
PL13W            0.34759795 W
SFO2           400.1520008 MHz
SI                  131072
SF             100.6179097 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.40
```



```
NAME            2010-03-02 p-OH-benyitong-H
EXPNO                    1
PROCNO                   1
Date_             20100302
Time                 20.54
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                    90.5
DW                  83.200 usec
DE                   6.50 usec
TE                  293.9 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.92643890 W
SFO1            400.1516006 MHz
SI                   32768
SF              400.1500062 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

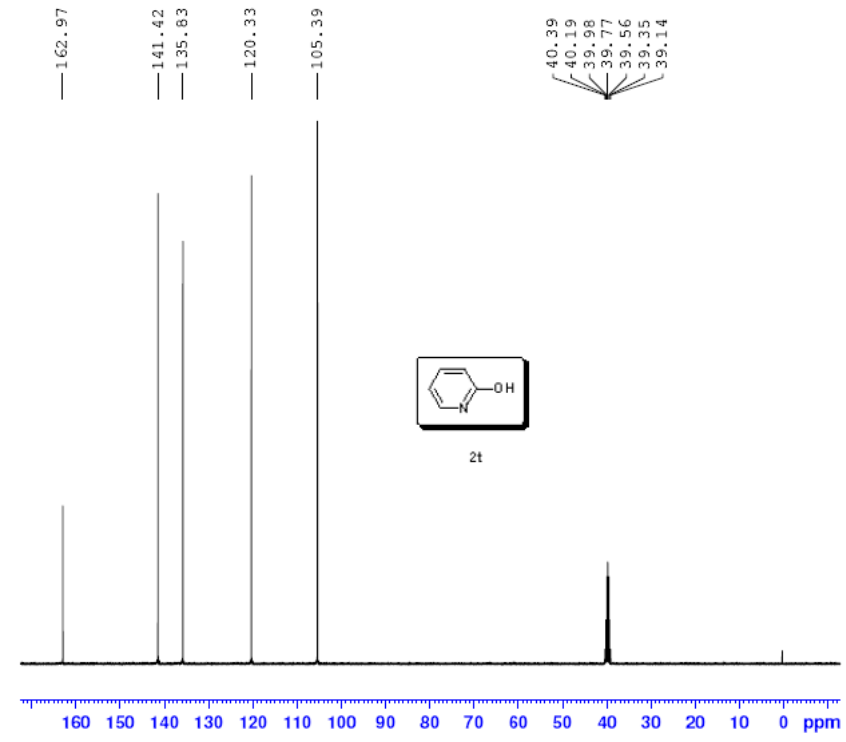


```
NAME            2010-02-22 p-OH-benyitong-C-2
EXPNO                    1
PROCNO                   1
Date_             20100223
Time                 1.05
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg
TD                  262144
SOLVENT              CDCl3
NS                     128
DS                       0
SWH              27173.912 Hz
FIDRES            0.103660 Hz
AQ                4.8234997 sec
RG                    90.5
DW                  18.400 usec
DE                   6.50 usec
TE                  299.2 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13c
P1                    9.30 usec
PL1                  -2.00 dB
PL1W            54.14257431 W
SFO1            100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W            17.82643890 W
PL12W            0.34758785 W
PL13W            0.34758785 W
SFO2            400.1520008 MHz
SI                  131072
SF              100.6178087 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
```



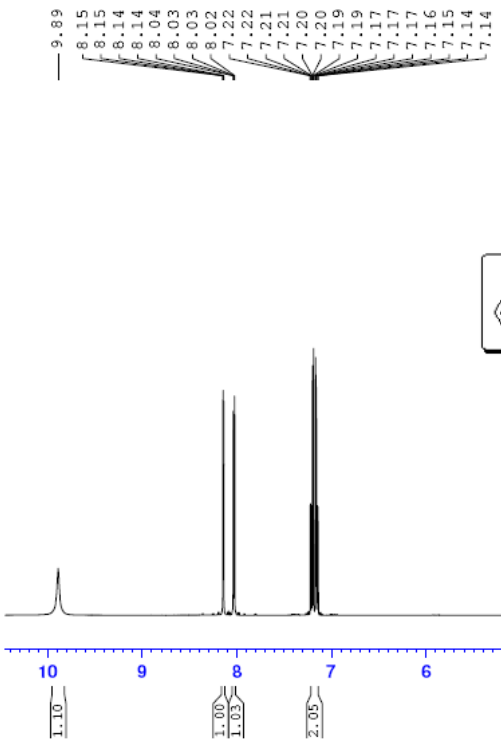
BRUKER

```
NAME            2010-02-22 2-OH-Py-H
EXPNO                    1
PROCNO                   1
Date_             20100223
Time                 3.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG                zg
TD                   32768
SOLVENT               DMSO
NS                      32
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7263477 sec
RG                     90.5
DW                  83.200 usec
DE                   6.50 usec
TE                  298.2 K
D1                5.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.50 usec
PL1                  -2.60 dB
PL1W            17.82643890 W
SFO1           400.1516006 MHz
SI                   32768
SF             400.1500056 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

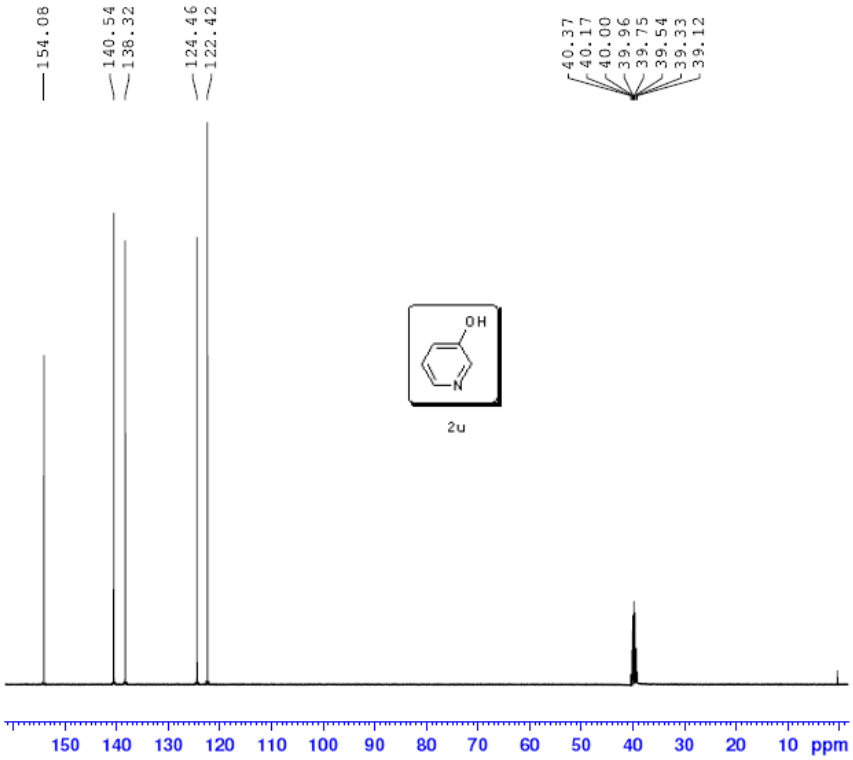


BRUKER

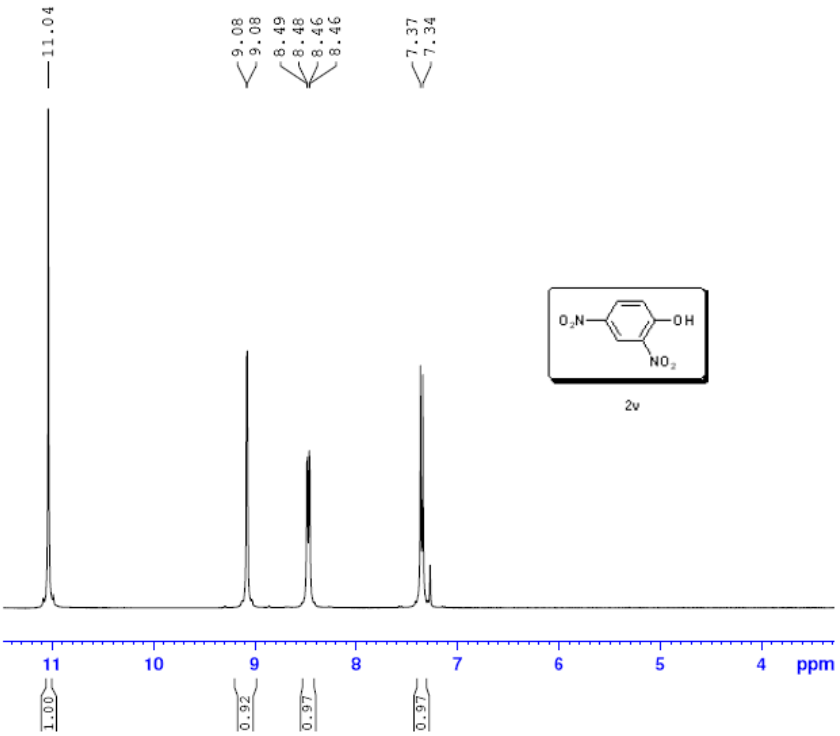
```
NAME            2010-02-22 2-OH-Py-C
EXPNO                    1
PROCNO                   1
Date_             20100223
Time                 4.44
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                  262144
SOLVENT               DMSO
NS                      64
DS                       0
SWH              27173.912 Hz
FIDRES            0.103660 Hz
AQ                4.8234997 sec
RG                     90.5
DW                  18.400 usec
DE                   6.50 usec
TE                  299.4 K
D1               10.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                  -2.00 dB
PL1W            54.14257431 W
SFO1           100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.60 dB
PL12                 14.50 dB
PL13                 14.50 dB
PL2W            17.82643890 W
PL12W            0.34758785 W
PL13W            0.34758785 W
SFO2           400.1520008 MHz
SI                  131072
SF             100.6178087 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.40
```



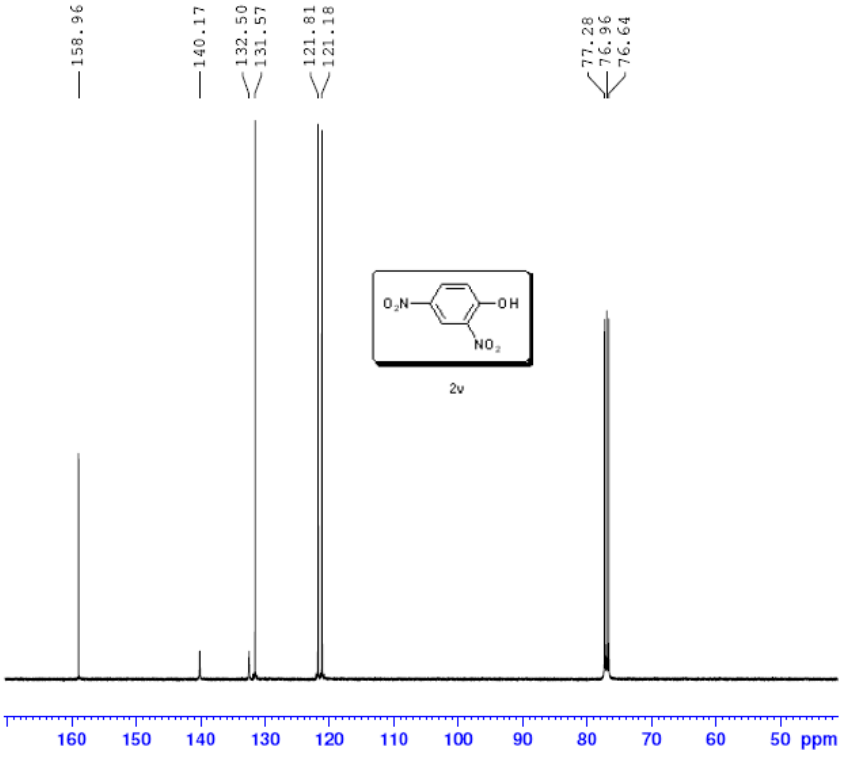

```
NAME        2010-02-22 3-OH-Py-H
EXPNO                          1
PROCNO                         1
Date_                   20100223
Time_                       3.18
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                       zg
TD                         32768
SOLVENT                     DMSO
NS                            32
DS                             0
SWH                     6009.615 Hz
FIDRES                  0.183399 Hz
AQ                      2.7263477 sec
RG                           90.5
DW                         83.200 usec
DE                          6.50 usec
TE                        297.8 K
D1                     5.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         12.50 usec
PL1                        -2.60 dB
PL1W                17.92643890 W
SFO1                400.1516006 MHz
SI                         32768
SF                  400.1499960 MHz
WDW                           no
SSB                            0
LB                          0.00 Hz
GB                             0
PC                          1.00
```

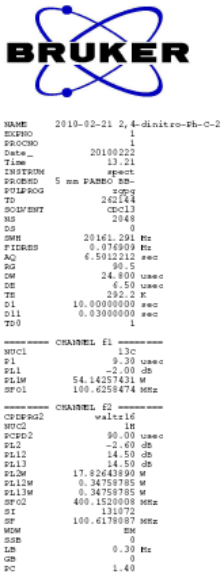



```
NAME        2010-02-22 3-OH-Py-C
EXPNO                          1
PROCNO                         1
Date_                   20100223
Time_                       4.23
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                    zgpg
TD                        262144
SOLVENT                     DMSO
NS                           128
DS                             0
SWH                    26041.666 Hz
FIDRES                  0.099341 Hz
AQ                      5.0332146 sec
RG                           90.5
DW                         19.200 usec
DE                          6.50 usec
TE                        299.4 K
D1                    10.00000000 sec
D11                    0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          13C
P1                          9.30 usec
PL1                        -2.00 dB
PL1W                54.14257431 W
SFO1                100.6258474 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                          1H
PCPD2                      90.00 usec
PL2                        -2.60 dB
PL12                       14.50 dB
PL13                       14.50 dB
PL2W                17.92643890 W
PL12W                0.34758785 W
PL13W                0.34758785 W
SFO2                400.1520008 MHz
SI                        131072
SF                  100.6179087 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.40
```


11.04
9.08
9.08
8.49
8.48
8.46
8.46
7.37
7.34
O2N
OH
NO2
2v
11
10
9
8
7
6
5
4
ppm
1.00
0.92
0.97
0.97


BRUKER
NAME 2010-02-20 2,4-dinitro-PhOH-H
EXPNO 1
PROCNO 1
Date_ 20100221
Time 0.10
INSTRM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 90.5
DW 83.200 usec
DE 6.50 usec
TE 294.6 K
D1 5.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -2.60 dB
PLW1 17.82643890 W
SFO1 400.1516006 MHz
SI 32768
SF 400.1500033 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00


158.96
140.17
132.50
131.57
121.81
121.18
77.28
76.96
76.64
O2N
OH
NO2
2v
160
150
140
130
120
110
100
90
80
70
60
50
ppm


BRUKER
NAME 2010-02-21 2,4-dinitro-Ph-C-2
EXPNO 1
PROCNO 1
Date_ 20100222
Time 13.21
INSTRM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 2048
DS 0
SWH 20161.291 Hz
FIDRES 0.076909 Hz
AQ 6.50122112 sec
RG 90.5
DW 24.800 usec
DE 6.50 usec
TE 292.2 K
D1 10.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 -2.00 dB
PLW1 54.14257431 W
SFO1 100.6258474 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.09 usec
PL2 -2.60 dB
PL12 14.50 dB
PL13 14.50 dB
PL2W 17.82643890 W
PL12W 0.34758785 W
PL13W 0.34758785 W
SFO2 400.1520008 MHz
SI 131072
SF 100.6178987 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40