

## Supporting Information

### **Palladium-catalyzed reductive cleavage of tosylated arene using isopropanol as the mild reducing agent**

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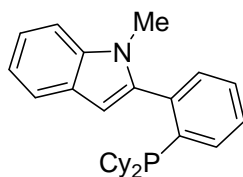
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## 1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All deoxygenative reactions were performed in Rotaflor® (England) resealable screw cap Schlenk flask (approx. 20 mL volume) in the presence of Teflon coated magnetic stirrer bar (4 mm × 10 mm). Methanol, ethanol, *t*-amyl alcohol, *tert*-butanol and *iso*-propanol were distilled from sodium under nitrogen.<sup>1</sup> Thin layer chromatography was performed on Merck precoated silica gel 60 F<sub>254</sub> plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. <sup>1</sup>H NMR spectra were recorded on a Bruker (400 MHz) spectrometer. Spectra were referenced internally to the residual proton resonance in CDCl<sub>3</sub> (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. <sup>13</sup>C NMR spectra were referenced to CDCl<sub>3</sub> (δ 77.0 ppm, the middle peak). Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Bruker APEX 47e FT-ICR mass spectrometer (ESIMS). GC-MS analysis was conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane

calibration standard from HP 6890 GC-FID system. Compounds described in the literatures were characterized by comparison of their  $^1\text{H}$ , and/or  $^{13}\text{C}$  NMR spectra to the previously reported data.

## 2. Preparation of indolyl phosphine ligands

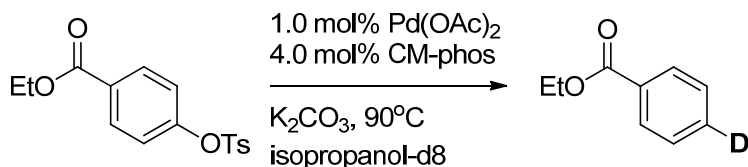


*N*-Methyl-2-(2'-dicyclohexylphosphinophenyl)indole, CM-phos were prepared according to the literature method.<sup>2</sup>

## 3. General procedures for reaction conditions screening and coupling reactions

$\text{Pd}(\text{OAc})_2$  and CM-phos (Pd:L = 1:4) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The tube was evacuated and flushed with nitrogen for several times. Precomplexation was applied by adding freshly distilled dichloromethane (1 mL) and  $\text{Et}_3\text{N}$  (100  $\mu\text{L}$ ) into the tube. The solution was stirred and warmed using a hair drier for about 1 to 2 minutes until the solvent started boiling. The solvent was then evaporated under a high vacuum. Aryl tosylates (1.0 mmol),  $\text{K}_2\text{CO}_3$  (3.0 mmol) were loaded into the tube, and the system was further evacuated and flushed

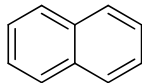
with nitrogen for several times. The solvent *iso*-propanol (3.0 mL) was then added. The tube was stirred at room temperature for several minutes and then placed into a preheated oil bath (90-110 °C) for the time period as indicated in Table. After completion of reaction as judged by GC analysis, the reaction tube was allowed to cool to room temperature and quenched with water and diluted with EtOAc. The organic layer was separated and the aqueous layer was washed with EtOAc. The filtrate was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.



Isopropanol-d<sub>8</sub> was purchased from Cambridge Isotope Laboratories, Inc. and used directly without any purification. Benzoic-4-*d* acid ethyl ester was synthesized by the same procedures using isopropanol-d<sub>8</sub> (instead of isopropanol) as solvent.

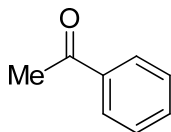
#### 4. Characterization data for deoxygenated products

##### Naphthalene (Table 2, entries 1, 2, 11)<sup>3</sup>



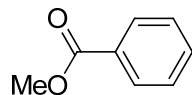
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.58 (dd, *J* = 3.2 Hz, 3.2 Hz 4H), 7.95 (dd, *J* = 3.2 Hz, 3.2 Hz 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 125.7, 127.8, 133.4; MS (EI): *m/z* (relative intensity) 128 (M<sup>+</sup>, 100), 102 (10), 75 (5).

##### Acetophenone (Table 2, entry 3)<sup>4</sup>

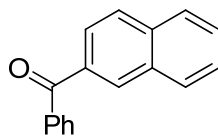


<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.59 (s, 3H), 7.45 (t, *J* = 6.8 Hz, 2H), 7.55 (d, *J* = 6.8 Hz, 1H), 7.95 (d, *J* = 7.2 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 26.5, 128.2, 128.5, 133.1, 137.1, 198.1; MS (EI): *m/z* (relative intensity) 120 (M<sup>+</sup>, 30), 105 (100), 77 (80).

##### Methyl benzoate (Table 2, entry 4)<sup>5</sup>



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 3.91 (s, 3H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 50.3, 128.2, 129.8, 130.2, 133.0, 169.2; MS (EI): *m/z* (relative intensity) 136 (M<sup>+</sup>, 40), 105 (100), 77 (80).

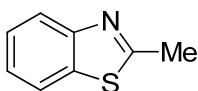
**(Naphthalene-6-yl)(phenyl)methanone (Table 2, entry 5)<sup>6</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.52-7.59 (m, 5H), 6.62-7.65 (m, 6H), 7.89-7.92 (m, 1H);

<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 125.6, 126.6, 127.6, 128.1, 128.2, 129.2, 129.9, 131.7,

132.1, 132.2, 134.6, 135.1, 137.7, 196.5 ; MS (EI): *m/z* (relative intensity) 232 (M<sup>+</sup>, 100),

202 (10), 155 (100).

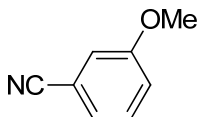
**2-Methylbenzo[d]thiazole (Table 2, entry 6)<sup>7</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.78 (s, 3H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 6.0 Hz,

2H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ

19.8, 121.1, 122.1, 124.4, 125.6, 135.4, 153.1, 166.6, MS (EI): *m/z* (relative intensity)

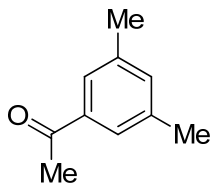
149 (M<sup>+</sup>, 100), 121 (5), 117 (5).

**3-Methoxybenzonitrile (Table 2, entry 7)<sup>8</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 3.82 (s, 3H), 7.12-7.14 (m, 2H), 7.20-7.23 (m, 1H),

7.34-7.28 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 55.3, 112.9, 116.7, 118.5, 119.0, 124.2,

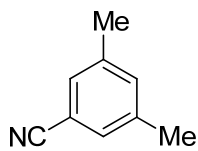
130.1, 159.4, MS (EI): *m/z* (relative intensity) 133 (M<sup>+</sup>, 100), 118 (10), 103 (70).

**1-(3,5-Dimethylphenyl)ethanone (Table 2, entry 8)<sup>9</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.36 (s, 6H), 2.57 (s, 3H), 7.19 (s, 1H), 7.57 (s, 2H), <sup>13</sup>C

NMR (100 MHz, CDCl<sub>3</sub>) δ 21.0, 26.4, 125.9, 134.5, 137.0, 137.9, 198.3, MS (EI): *m/z*

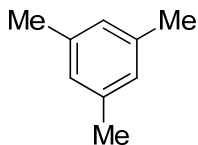
(relative intensity) 148 (M<sup>+</sup>, 50), 133 (100), 105 (70).

**3,5-Dimethyl benzonitrile (Table 2, entry 9)<sup>10</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.35 (s, 3H), 7.22 (s, 1H), 7.25 (s, 2H), <sup>13</sup>C NMR (100

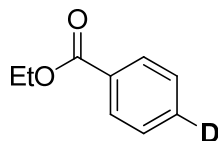
MHz, CDCl<sub>3</sub>) δ 20.8, 111.8, 119.0, 129.4, 134.4, 138.8, MS (EI): *m/z* (relative intensity)

131 (M<sup>+</sup>, 100), 116 (30), 103 (35).

**Mesitylene (Table 2, entry 10)<sup>11</sup>**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.42 (s, 9H), 6.94 (s, 3H), <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ

21.2, 127.0, 137.8, MS (EI): *m/z* (relative intensity) 120 (M<sup>+</sup>, 100), 105 (50), 90 (30).

**Benzoic-4-*d* acid ethyl ester**<sup>12</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.41 (t, *J* = 7.2 Hz, 3H), 4.36-4.42 (q, *J* = 7.2 Hz, 2H),

7.43 (d, *J* = 8.4 Hz, 2H), 8.06-8.08 (dd, *J* = 4.8, 2.0 Hz, 2H), <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

δ 14.2, 60.8, 128.11, 129.4, 130.4, 166.5, MS (EI): *m/z* (relative intensity) 106 (M<sup>+</sup>, 100),

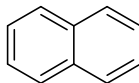
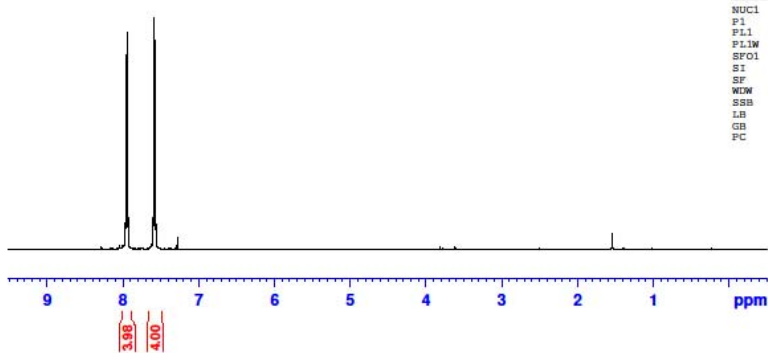
123 (64), 151 (59), HRMS: calcd. for C<sub>9</sub>H<sub>9</sub>DO<sub>2</sub><sup>+</sup>: 151.0744, found 151.0749.



5.  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and HRMS spectra

B806

7.962  
7.953  
7.946  
7.938  
7.595  
7.587  
7.579  
7.571

Table 2  
entries 1, 2 and 11

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EXPNO     1
PROCNO    1
Date_     20110424
Time      18.16
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        4006.410 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         36
DW         124.800 usec
DE         6.50 usec
TE         299.2 K
D1         1.00000000 sec
TD0        1

```

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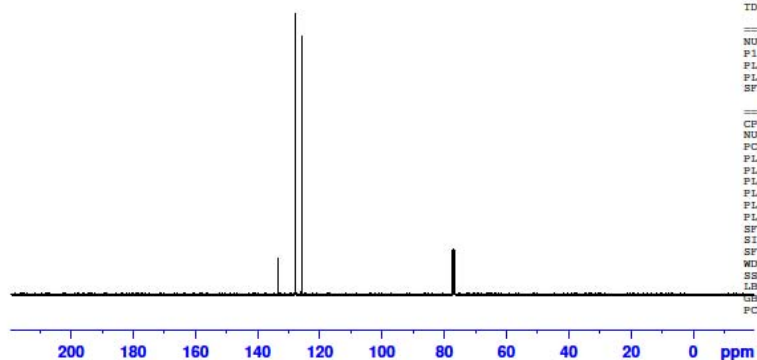
===== CHANNEL f1 =====
NUC1      1H
P1        14.70 usec
PL1       0.00 dB
PL1W      11.88122272 W
SFO1      400.1318007 MHz
SI        32768
SF        400.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```

B806C

133.45  
127.86  
125.79

77.32  
77.00  
76.68



```

NAME      B806
EXPNO     2
PROCNO    1
Date_     20110424
Time      18.19
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         32
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         300.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -2.00 dB
PL1W      58.52175522 W
SFO1      100.6228298 MHz

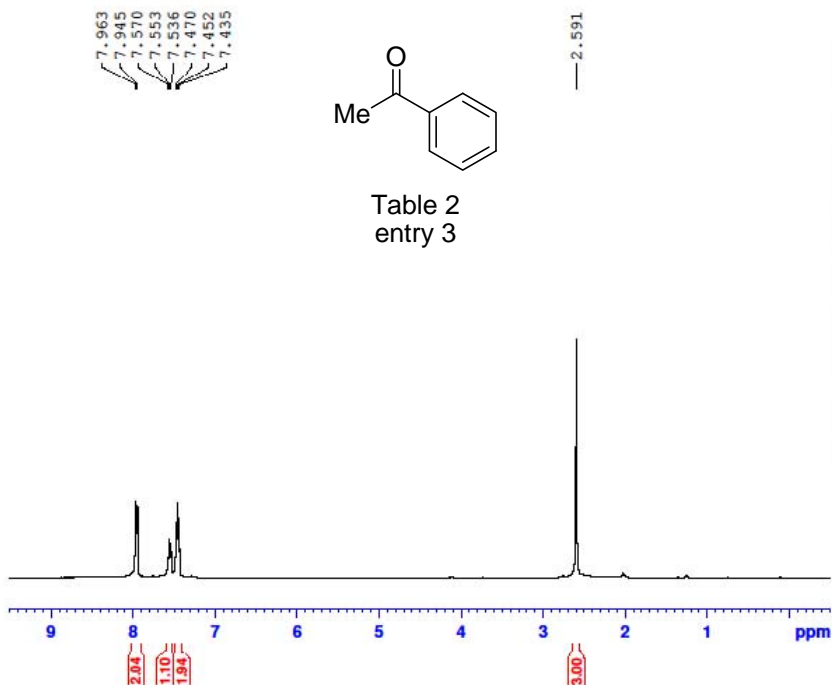
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===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       0.00 dB
PL12      15.00 dB
PL13      15.00 dB
PL2W      11.88122272 W
PL12W     0.37571725 W
PL13W     0.37571725 W
SFO2      400.1316005 MHz
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SF        100.6127817 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

B788



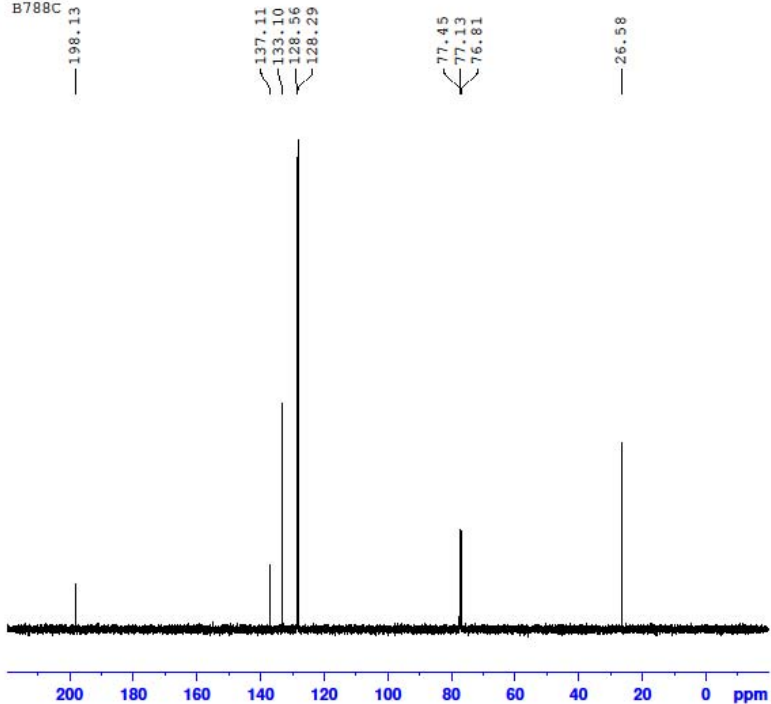
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PROCNO        1
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Time         17.23
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PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            1
RW           124.800 usec
DE            6.50 usec
TE            300.5 K
D1            1.0000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
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WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

B788C



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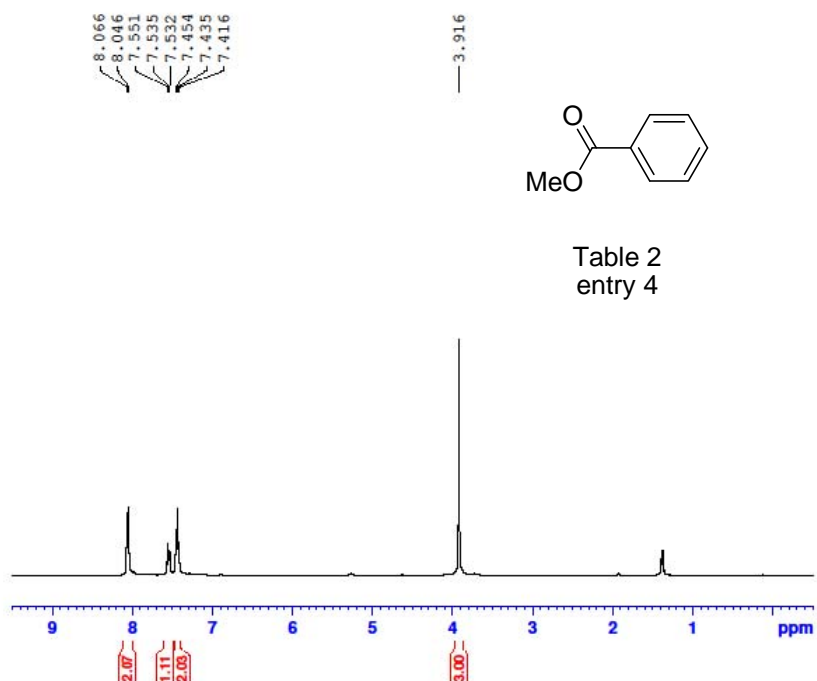
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PROCNO        1
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Time         17.30
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TD            65536
SOLVENT       CDCl3
NS            15
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            228
RW           20.800 usec
DE            6.50 usec
TE            298.5 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127690 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

B789



```

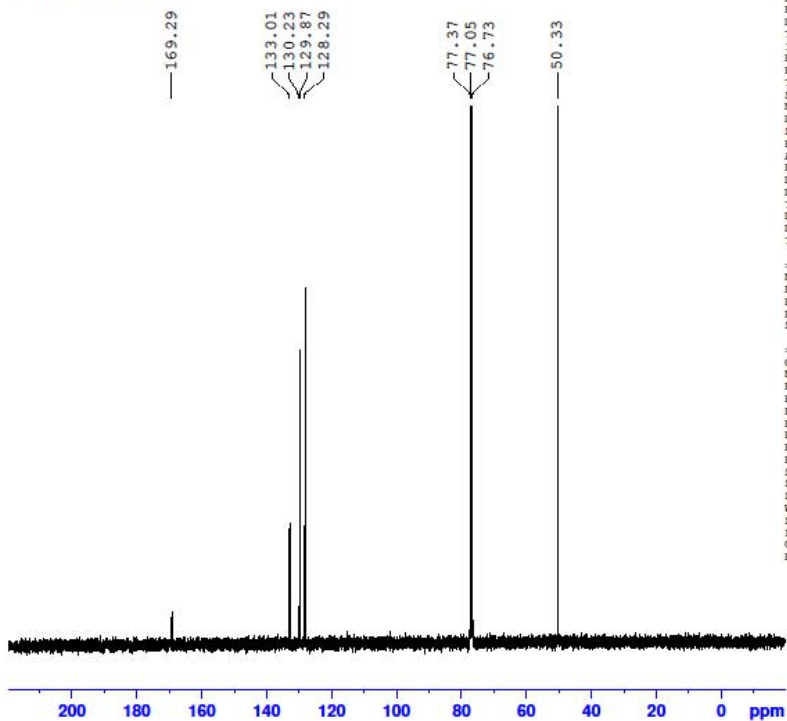
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EXPNO         1
PROCNO        1
Date_         20110329
Time          16.53
INSTRUM       spect
PROBHD        5 mm PAHBO BB-
PULPROG       zg30
ID            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            1
LW           124.800 usec
DE            6.50 usec
TE            300.4 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

Table 2  
entry 4

PCKinEntry3 (B789) C



```

NAME          PCKinEntry3
EXPNO         1
PROCNO        1
Date_         20140415
Time          12.03
INSTRUM       spect
PROBHD        5 mm PAHBO BB-
PULPROG       zgpg30
ID            65536
SOLVENT       CDCl3
NS            290
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
LW           20.800 usec
DE            6.50 usec
TE            298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
  
```

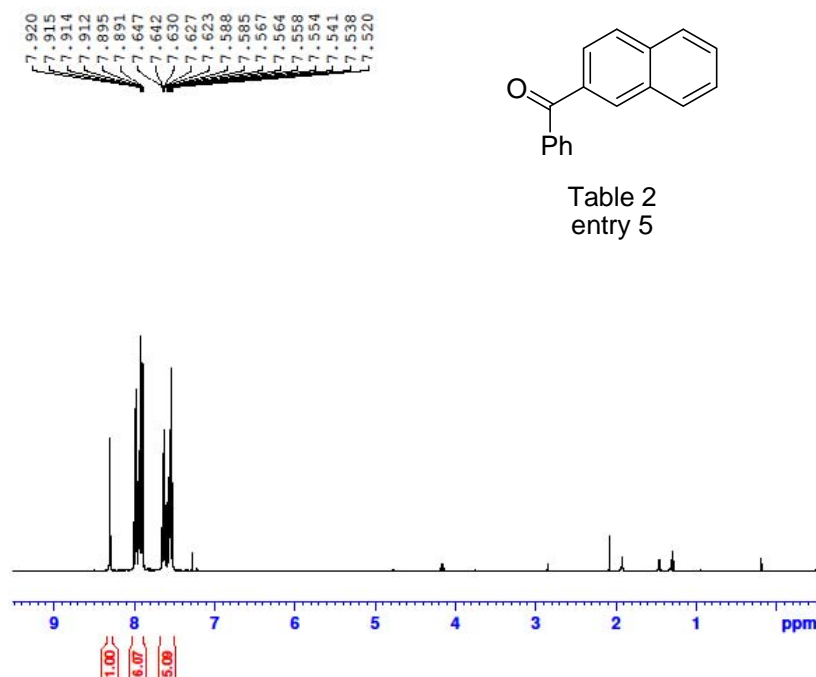
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===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL12W         11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127754 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

B799

Table 2  
entry 5

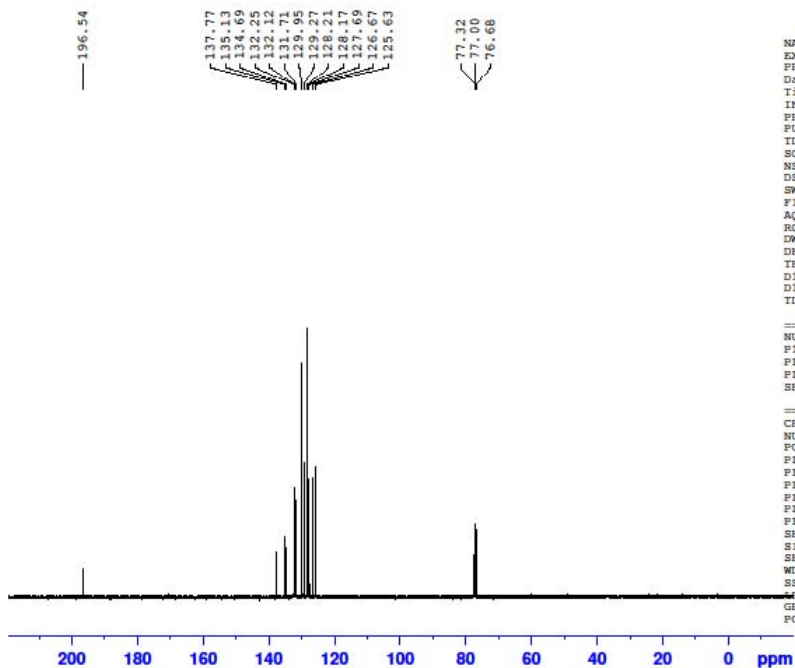
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PROCNO        1
Date_         20110408
Time         16.13
INSTRUM       spect
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PULPROG       zg30
TD            32768
SOLVENT       cdcl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            22.6
DW            124.800 usec
DE            6.50 usec
TE            298.6 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W         11.88122272 W
SFO1         400.1318007 MHz
SI            32768
SF           400.1300000 MHz
WDM           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

B799C



```

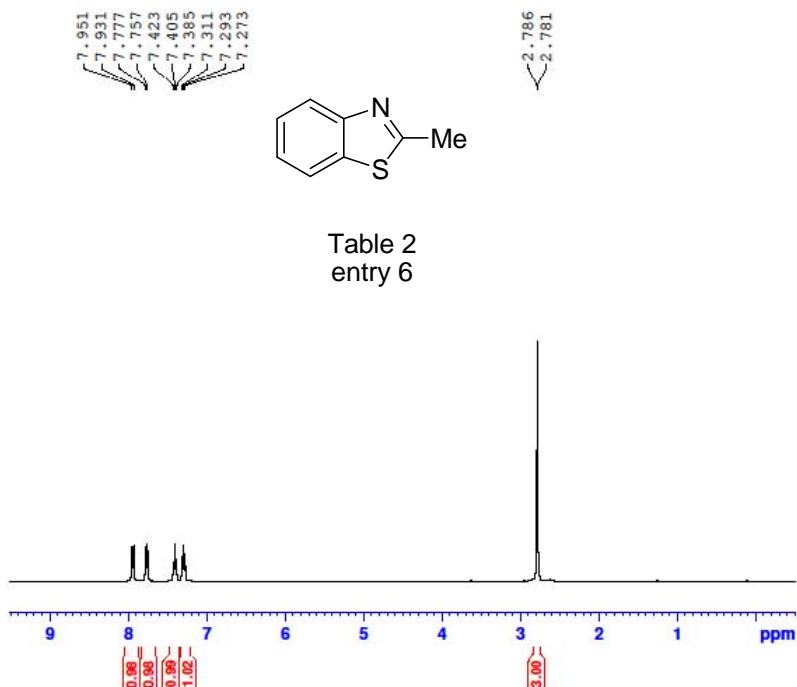
NAME          B799
EXPNO         2
PROCNO        1
Date_         20110408
Time         16.15
INSTRUM       spect
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PULPROG       zgpg30
TD            65536
SOLVENT       cdcl3
NS            32
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            299.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W         58.52175522 W
SFO1         100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12         15.00 dB
PL13         15.00 dB
PL2W         11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2         400.1316005 MHz
SI            32768
SF           100.6127868 MHz
WDM           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

B794



```

NAME          h794
EXPNO         1
PROCNO        1
Date_         20110331
Time         11.59
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
ID            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            1
DW            124.800 usec
DE            6.50 usec
TE            298.9 K
D1            1.00000000 sec
TD0           1

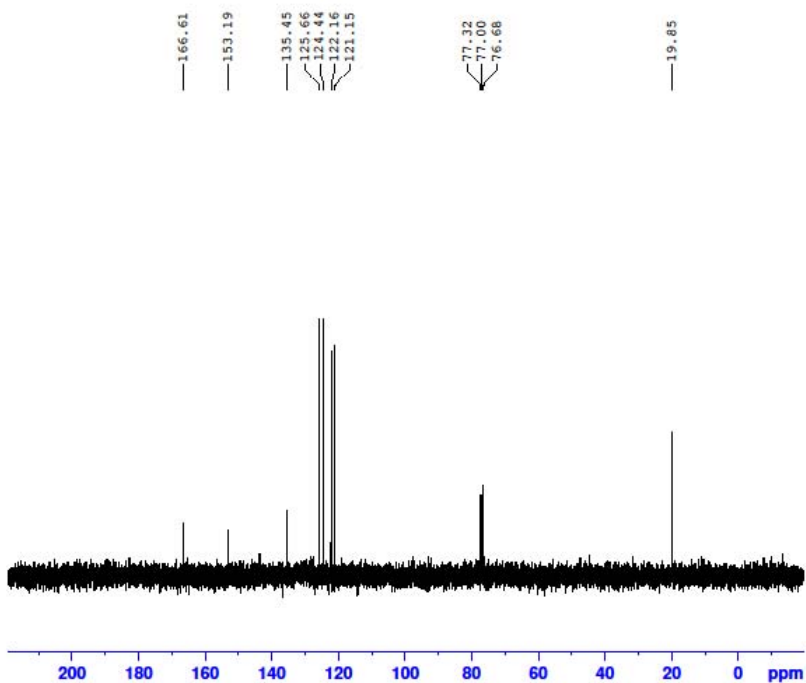
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

B794C



```

NAME          B794
EXPNO         2
PROCNO        1
Date_         20110331
Time         12.07
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
ID            65536
SOLVENT       CDCl3
NS            32
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            1
DW            20.800 usec
DE            6.50 usec
TE            299.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

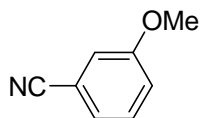
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2            0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL1W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127898 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

B807

Table 2  
entry 7

```

NAME          B807
EXPNO         1
PROCNO        1
Date_         20110424
Time          18.05
INSTRUM       spect
PROBHD        5 mm FAHBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            22.6
DW            124.800 usec
DE            6.50 usec
TE            299.1 K
D1            1.0000000 sec
TD0           1

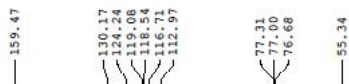
```

```

===== CHANNEL F1 =====
NUC1           1H
P1             14.70 usec
PL1            0.00 dB
PL1W           11.88122272 W
SFO1           400.1318007 MHz
SI             32768
SF            400.1300000 MHz
WDW            EM
SBB            0
LB             0.30 Hz
GB             0
PC             1.00

```

B807C



```

NAME          B807
EXPNO         2
PROCNO        1
Date_         20110424
Time          18.09
INSTRUM       spect
PROBHD        5 mm FAHBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

```

```

===== CHANNEL F1 =====
NUC1           13C
P1             9.50 usec
PL1            -2.00 dB
PL1W           58.52175522 W
SFO1           100.6228298 MHz

```

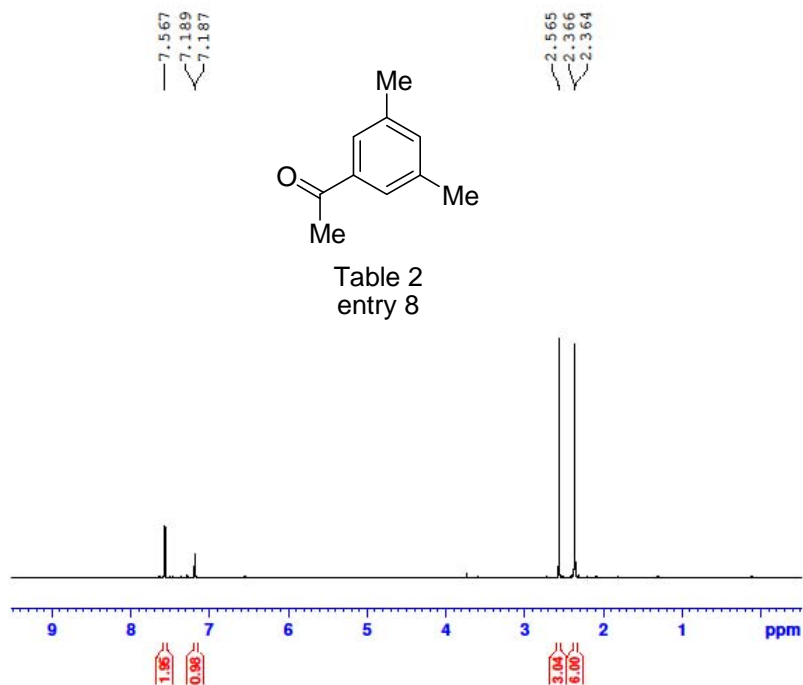
```

===== CHANNEL F2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2            0.00 dB
PL12           15.00 dB
PL13           15.00 dB
PL2W           11.88122272 W
PL12W          0.37571725 W
PL13W          0.37571725 W
SFO2           400.1316005 MHz
SI             32768
SF            100.6127868 MHz
WDW            EM
SBB            0
LB             1.00 Hz
GB             0
PC             1.40

```

200 180 160 140 120 100 80 60 40 20 0 ppm

B797



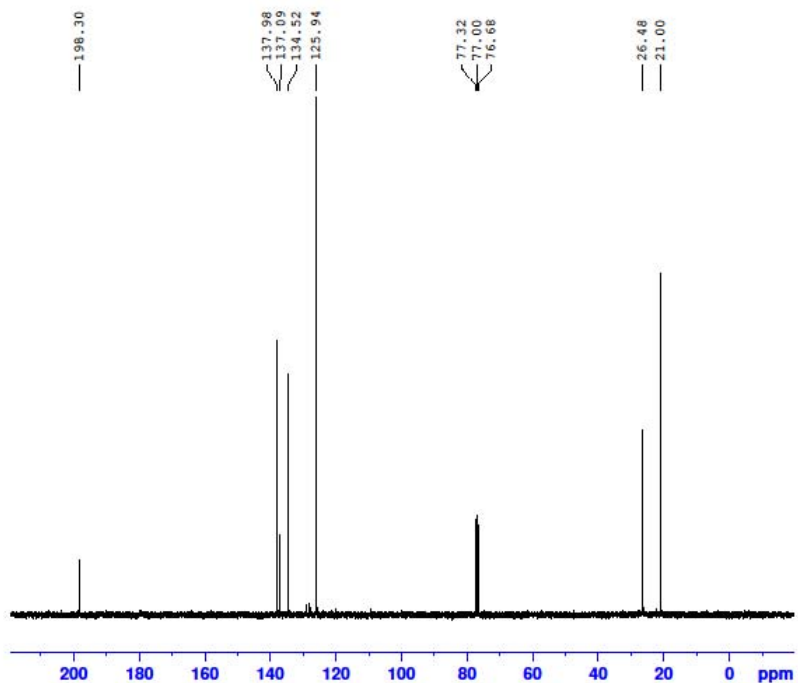
```

NAME          B797
EXPNO         1
PROCNO        1
Date_         20110401
Time          18.30
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            1
DM            124.800 usec
DE            6.50 usec
TE            299.2 K
D1            1.0000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W         11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

B797C



```

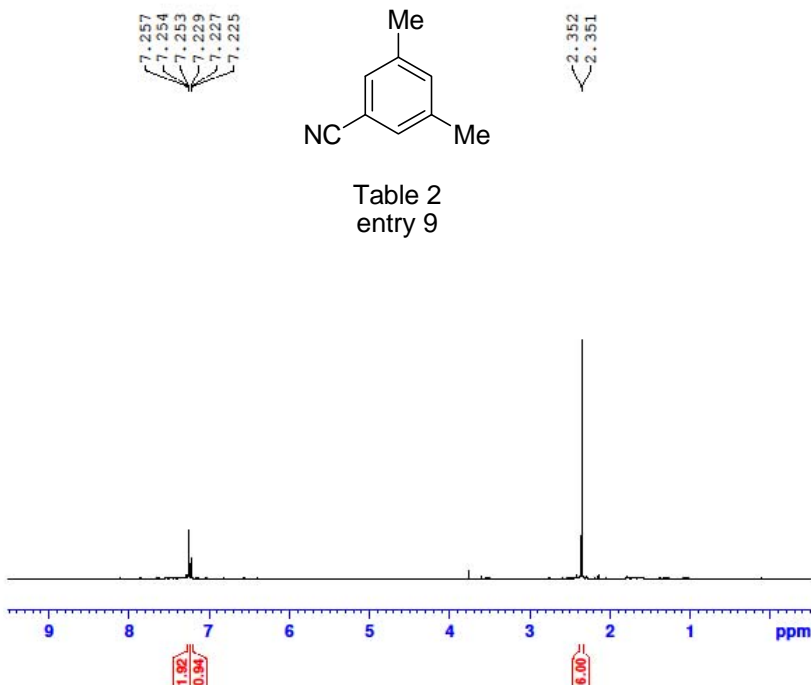
NAME          B797
EXPNO         2
PROCNO        1
Date_         20110401
Time          18.33
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            12.7
DM            20.800 usec
DE            6.50 usec
TE            300.1 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W         58.52175522 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CFDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12         15.00 dB
PL13         15.00 dB
PL12W        11.88122272 W
PL13W        0.37571725 W
PL13W        0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127854 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

B805



```

NAME          B805
EXPNO         3
PROCNO        1
Date_         20110408
Time          16.06
INSTRUM       spect
PROBHD        5 mm FAMB0 BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            22.6
DW            124.800 usec
DE            6.50 usec
TE            298.4 K
D1            1.0000000 sec
TD0           1

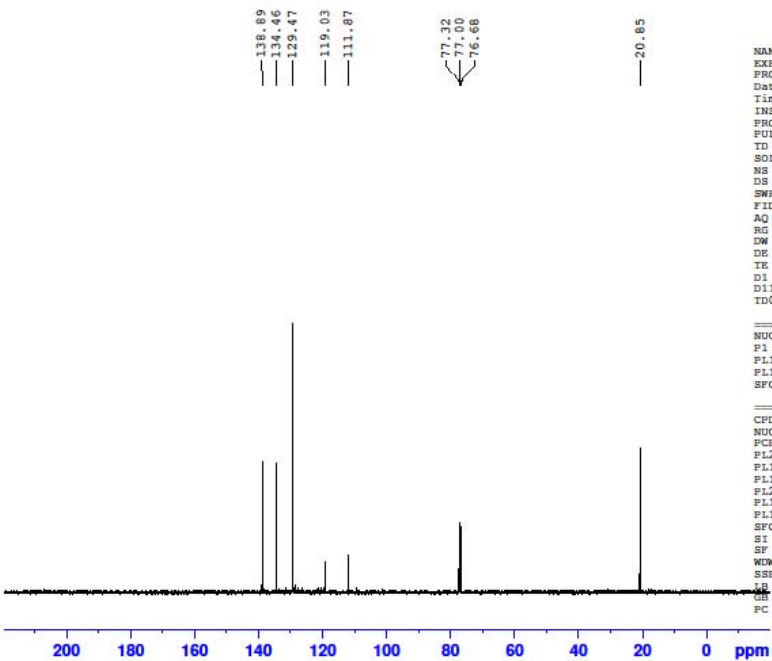
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W          11.88122272 W
SFO1          400.1318007 MHz
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```

B805C



```

NAME          B805
EXPNO         2
PROCNO        1
Date_         20110408
Time          16.08
INSTRUM       spect
PROBHD        5 mm FAMB0 BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            299.3 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0           1

```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W          58.52175522 W
SFO1          100.6228298 MHz

```

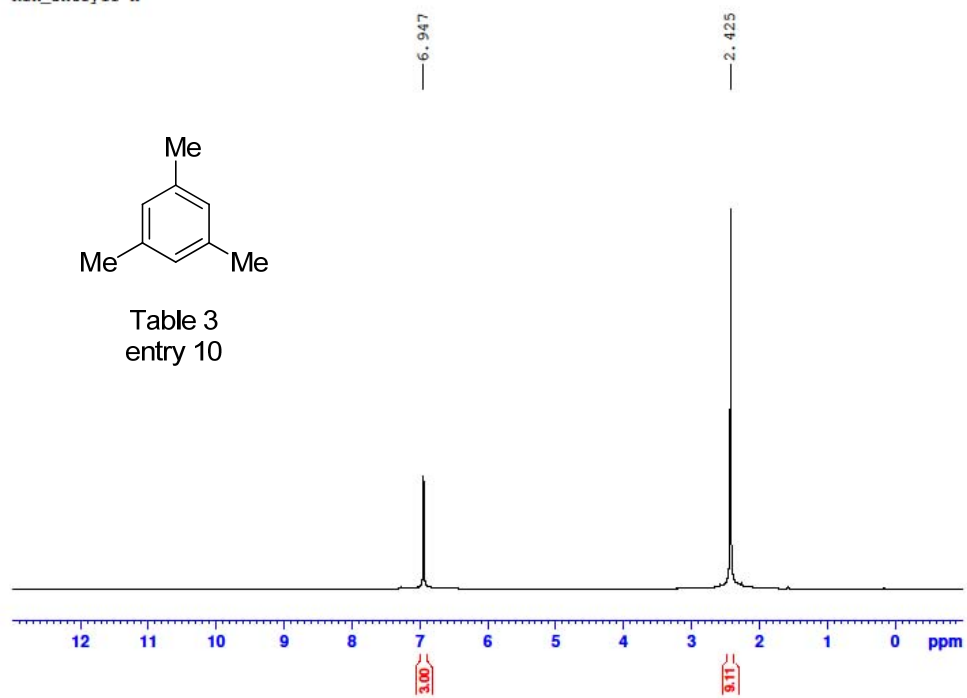
```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL13          15.00 dB
PL2W          11.88122272 W
PL12W         0.37571725 W
PL13W         0.37571725 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127846 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

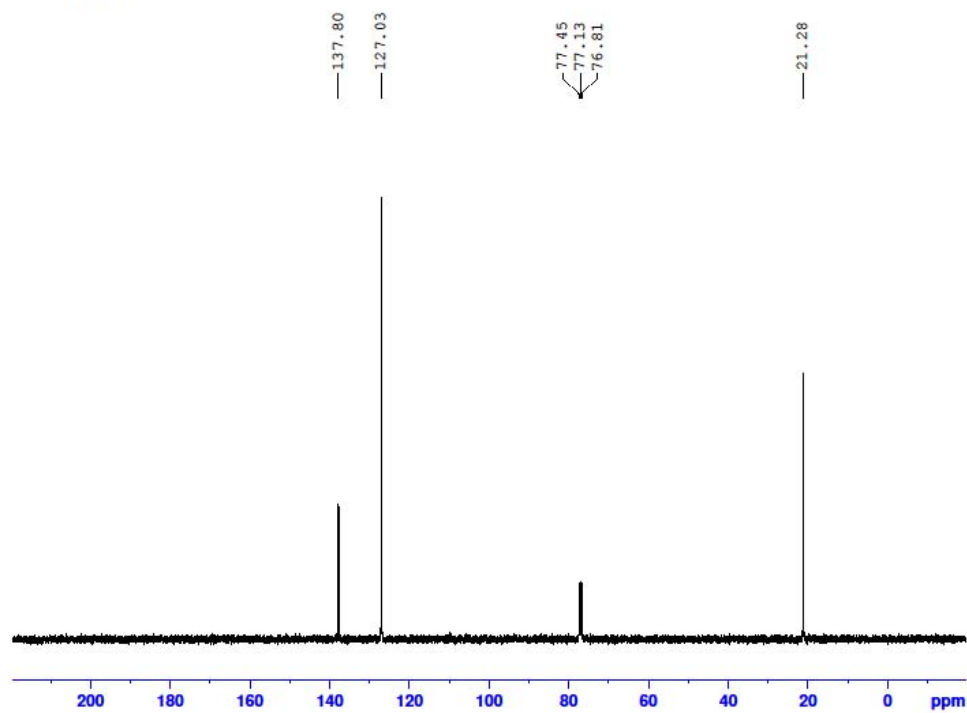
```



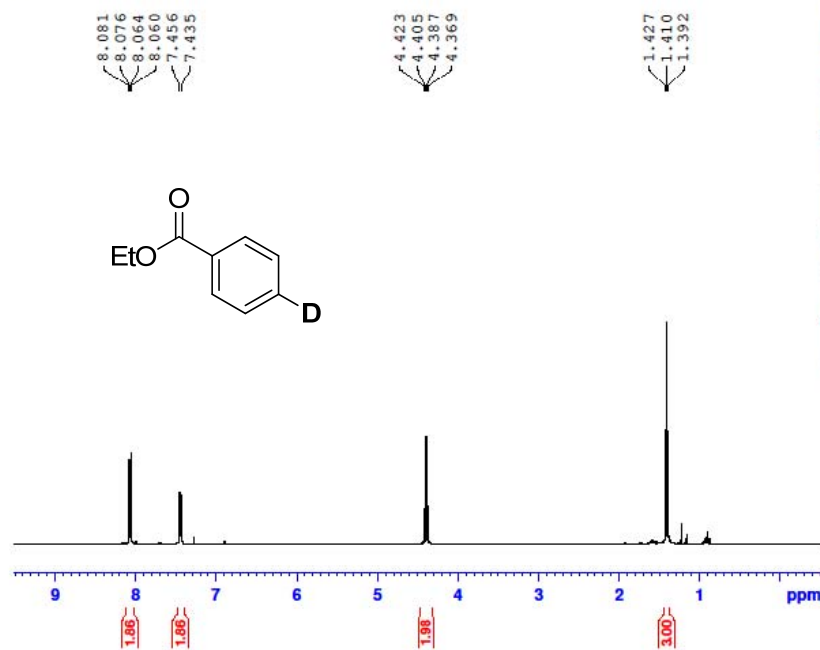
Kin\_entry11 H



Kin\_entry11 C



B1030



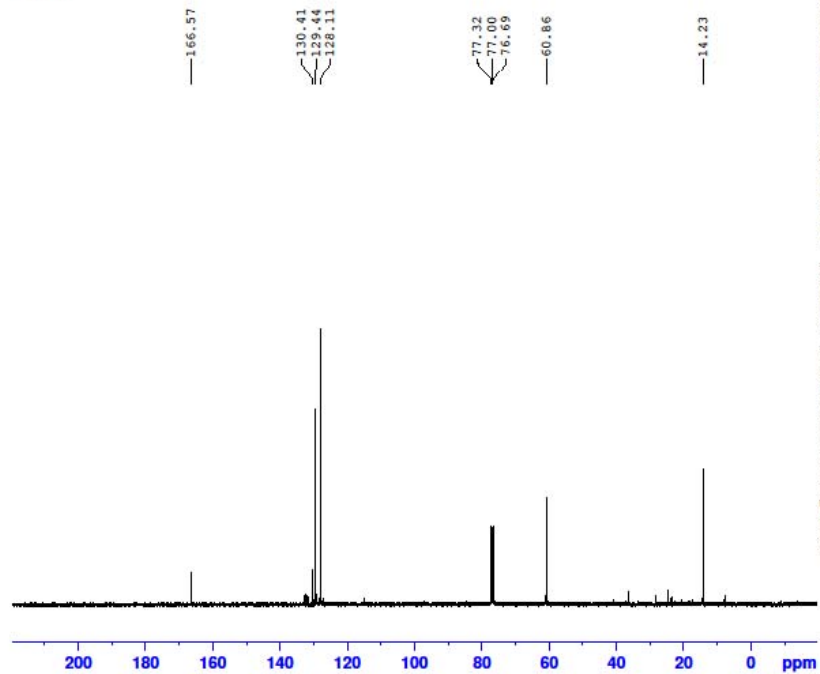
```

NAME          B1030
EXPNO         1
PROCNO        1
Date_         20130902
Time         15.35
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           4006.410 Hz
FIDRES       0.122266 Hz
AQ           4.0894966 sec
RG           25.4
DW           124.800 usec
DE           6.50 usec
TE           295.7 K
D1           1.0000000 sec
D11          1
D10          1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.70 usec
PL1           0.00 dB
PL1W         11.88122272 W
SFO1         400.1318007 MHz
SI           32768
SF           400.1300000 MHz
WDW           EM
SSB           0
LB           0.30 Hz
GB           0
PC           1.00
  
```

B1030C



```

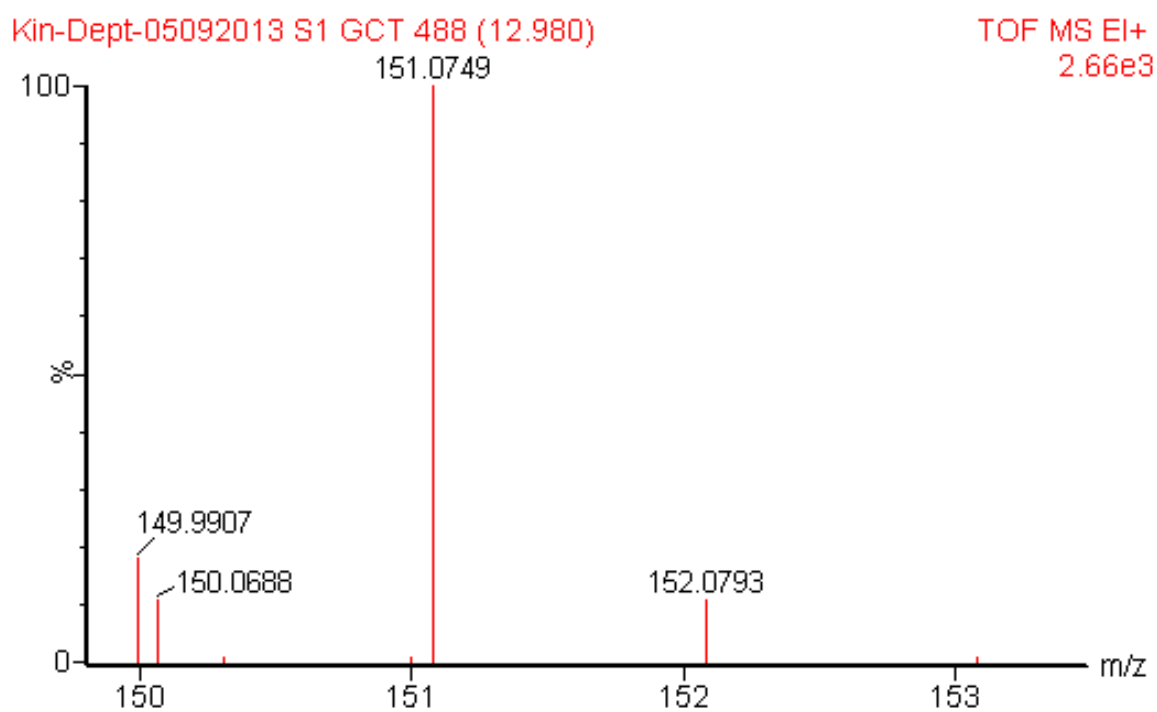
NAME          B1030
EXPNO         2
PROCNO        1
Date_         20130902
Time         15.43
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            64
DS            2
SWH           24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3631988 sec
RG           203
DW           20.800 usec
DE           6.50 usec
TE           297.0 K
D1           2.0000000 sec
D11          0.0300000 sec
D10          1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -2.00 dB
PL1W         58.52175522 W
SFO1         100.6228298 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           0.00 dB
PL12         15.00 dB
PL13         15.00 dB
PL2W         11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127773 MHz
WDW           EM
SSB           0
LB           1.00 Hz
GB           0
PC           1.40
  
```



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
151.0749	151.0744	0.5	3.3	5.0	13.2	C <sub>9</sub> H <sub>9</sub> DO <sub>2</sub>

## 6. References

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