Supporting information for

# O-Allylation of phenols with allylic acetates in aqueous medium using a magnetically separable catalytic system

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## General Consideration

All the reactions were carried out in refluxing water under open aerial atmosphere. All the reagents were purchased from Sigma-Aldrich Chemical Co. and were used directly without further any purification. NMR spectra were obtained using the Brucker AVANCE 300MHz spectrometer using $CDCl_3$ as solvent. Chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. IR spectra were taken on Perkin Elmer Spectrum 2000 FT-IR spectrometer. Reactions were monitored by thin layer chromatography. Elemental analyses of the products were performed on a Costech Analytical - ECS 4010 Elemental analyzer. Elemental analyses of the catalyst before as well as after the reactions were performed on a Perkin Elmer Optima 3300 DV ICP-AES. Five mg of each sample was dissolved in 2.5 mL of concentrated aqua regia and the volume was adjusted to 50 mL in a volumetric flask. This solution was then used for the elemental analysis. TEM micrographs were recorded on TEM; Philips, CM20 microscope at an operating voltage of 200 kV. The particles were dispersed in ethanol by ultrasonication, loaded on a carbon coated copper grid, and then allowed to dry at room temperature before recording the micrographs.

## Synthesis of magnetic nano-ferrites

$FeSO_4.7H_2O$ (13.9 g) and $Fe_2(SO_4)_3$ (20 g) were dissolved in 500 mL water in a 1000 mL beaker. Ammonium hydroxide (25%) was added slowly to adjust the pH of the solution to 10. The reaction mixture was then continually stirred for 1 h at 60 $^{o}$C. The precipitated nanoparticles were separated magnetically, washed with water until the pH reached 7, and then dried under a vacuum at 60 $^{o}$C for 2 h. This magnetic nano-ferrite ($Fe_3O_4$) was then used for further chemical modification.

## Surface functionalization of nano-ferrites

Nano-$Fe_3O_4$ (2 g) was dispersed in 25 mL water by sonication for 30 min. Dopamine hydrochloride (2 g) dissolved in 5 mL of water was added to this solution and again sonicated for 2 h. The amine-functionalized nanomaterial was then precipitated using acetone, isolated by centrifugation, and dried under vacuum at 60 $^{o}$C for 2 h.

## Synthesis of [$Fe_3O_4$-Dopamine-Pd] catalyst

Dopamine functionalized nano-ferrite (1 g) was dispersed in MeOH (25 mL) by stirring. $PdCl_2$ (200 mg) was added slowly to the suspension and the solution was stirred for 10 min. Ammonium hydroxide (25%) was added drop wise to bring the pH of the medium 9. The mixture was stirred at room temperature for 24 h. The nano catalyst was separated out using an external magnet. It was washed with acetone for three times and was dried under vacuum at 60 $^{o}$C for 2 h.

## *O*-Allylation of phenols by allylic acetates using [$Fe_3O_4$-Dopamine-Pd] catalyst

A mixture of phenol (1 mmol), allylic acetate (1 mmol), $NaHCO_3$ (2 mmol) and Pd-catalyst (50 mg, 4.8 mol%) was taken in 2.5 mL of water. The aqueous reaction mixture was heated to reflux for required time period as indicated in Table 2. The progress of the reaction was monitored by TLC. Standard work-up with ethyl acetate followed by simple column chromatography provided the pure product. All products listed in Table 3 were known in the literature (except entry 6 and 11) and were identified by comparison of their FT-IR, $^1$H and $^{13}$C NMR with literature data. The products of entries 6 and 11, Table 3, were characterized by FT-IR, $^1$H and $^{13}$C NMR spectroscopy and elemental analysis.

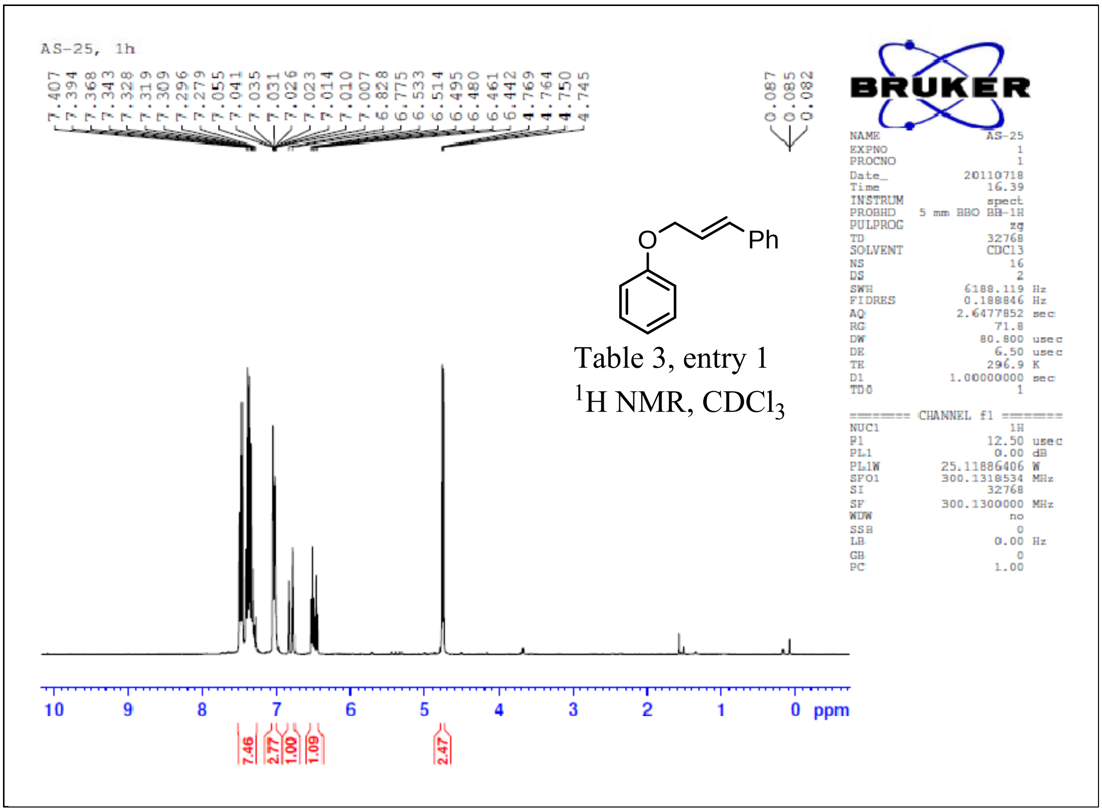

Table 3, entry 1
$^1$H NMR, $CDCl_3$

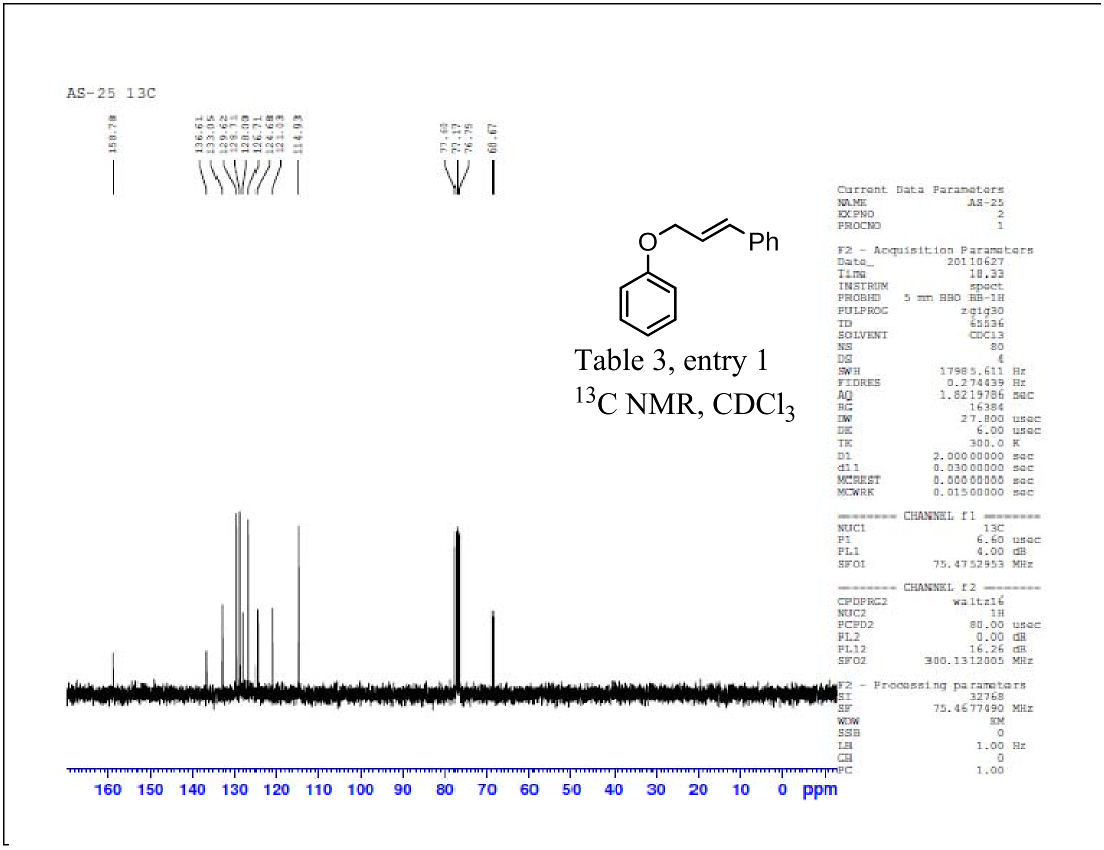

Table 3, entry 1
$^{13}$C NMR, $CDCl_3$

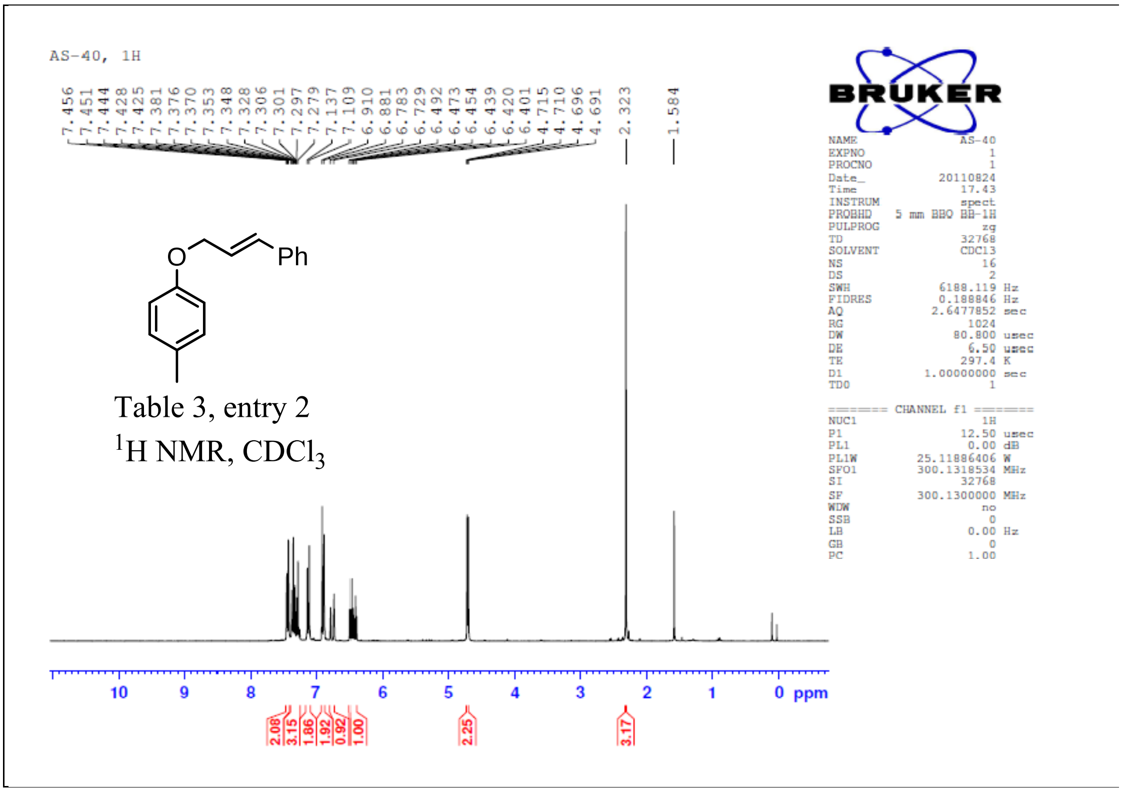

Table 3, entry 2
$^{1}$H NMR, $CDCl_3$

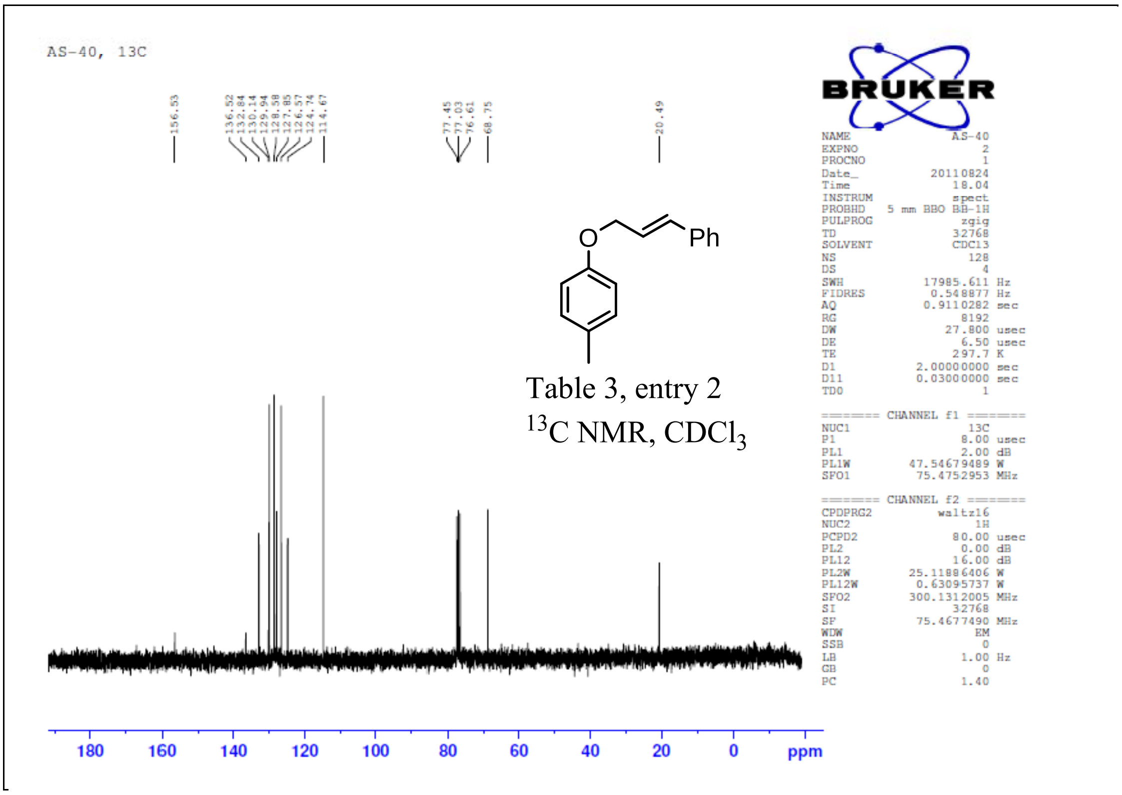

Table 3, entry 2
$^{13}C$ NMR, $CDCl_3$

```
NAME                AS-40
EXPNO                   2
PROCNO                  1
Date_            20110824
Time                18.04
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgig
TD                  32768
SOLVENT             CDCl3
NS                    128
DS                      4
SWH             17985.611 Hz
FIDRES           0.548877 Hz
AQ              0.9110282 sec
RG                   8192
DW                 27.800 usec
DE                   6.50 usec
TE                  297.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.00 usec
PL1                  2.00 dB
PL1W          47.54679489 W
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                16.00 dB
PL2W          25.11886406 W
PL12W          0.63095737 W
SFO2          300.1312005 MHz
SI                  32768
SF             75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

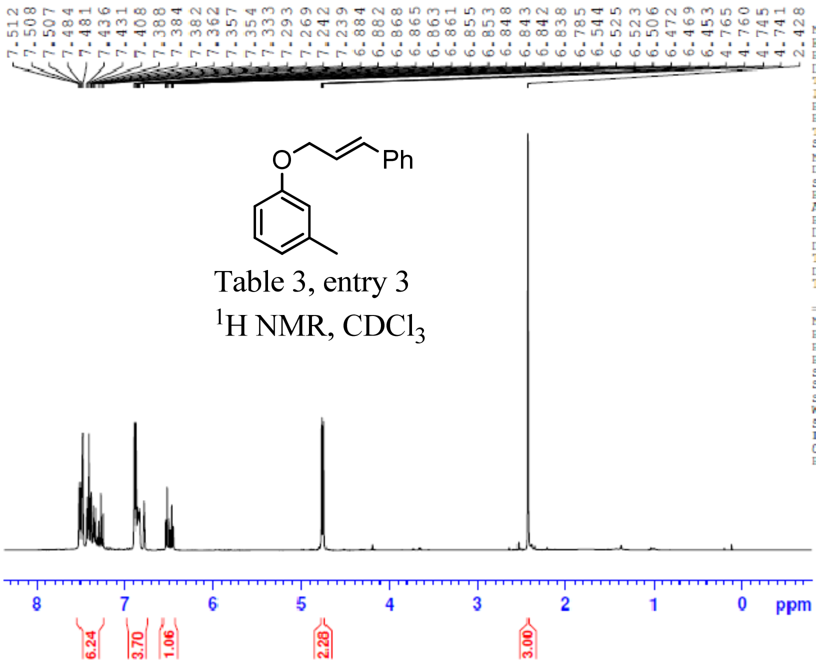

Table 3, entry 3
$^1$H NMR, $CDCl_3$

```
NAME                AS-32
EXPNO                   1
PROCNO                  1
Date_            20110719
Time                14.59
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.188846 Hz
AQ              2.6477852 sec
RG                   35.9
DW                 80.800 usec
DE                   6.50 usec
TE                  297.3 K
D1             1.00000000 sec
TD0                     1

======= CHANNEL f1 =======
NUC1                   1H
P1                  12.50 usec
PL1                  0.00 dB
PL1W          25.11886406 W
SFO1          300.1318534 MHz
SI                  32768
SF            300.1300000 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

AS-32, 13C

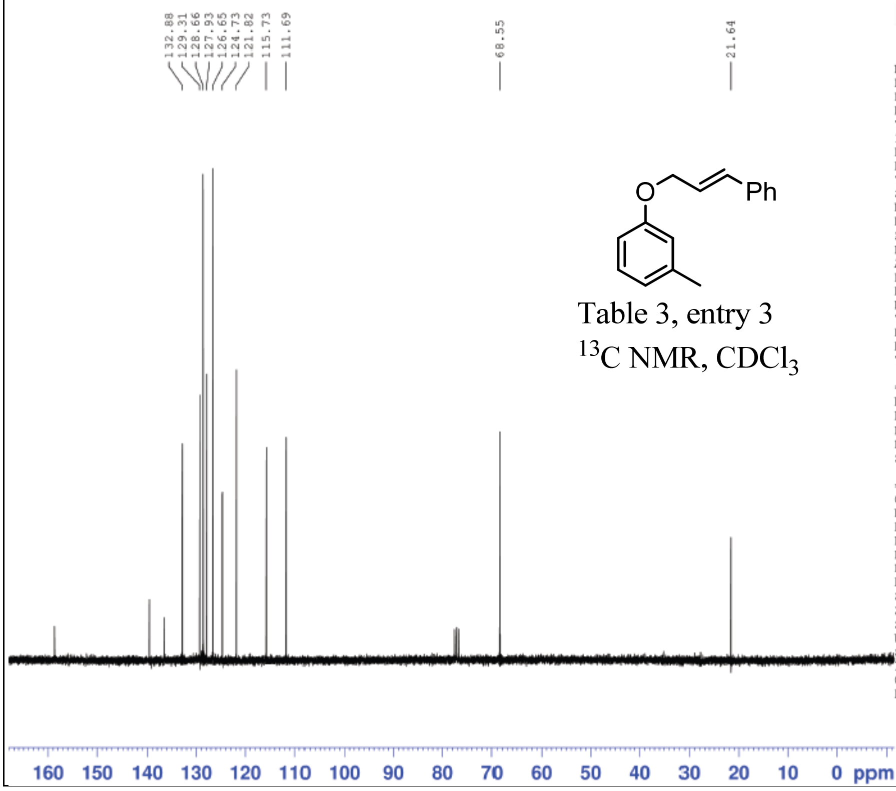

Table 3, entry 3
$^{13}$C NMR, $CDCl_3$

```
NAME                AS-32
EXPNO                   2
PROCNO                  1
Date_            20110719
Time                15.25
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgig
TD                  32768
SOLVENT             CDCl3
NS                    128
DS                      4
SWH             17985.611 Hz
FIDRES           0.548877 Hz
AQ              0.9110282 sec
RG                   28.5
DW                 27.800 usec
DE                   6.50 usec
TE                  297.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.00 usec
PL1                  2.00 dB
PL1W          47.54679489 W
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                16.00 dB
PL2W          25.11886406 W
PL12W          0.63095737 W
SFO2          300.1312005 MHz
SI                  32768
SF             75.4677490 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
```

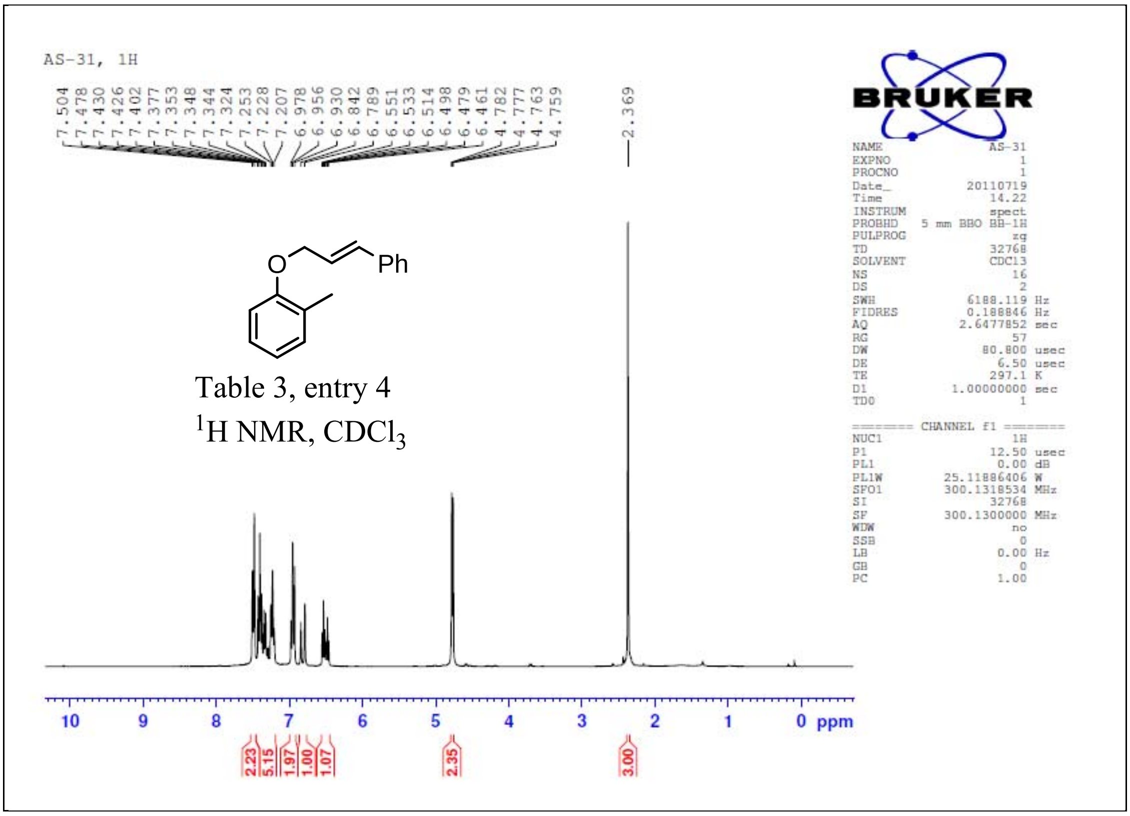

Table 3, entry 4
$^{1}H$ NMR, $CDCl_3$

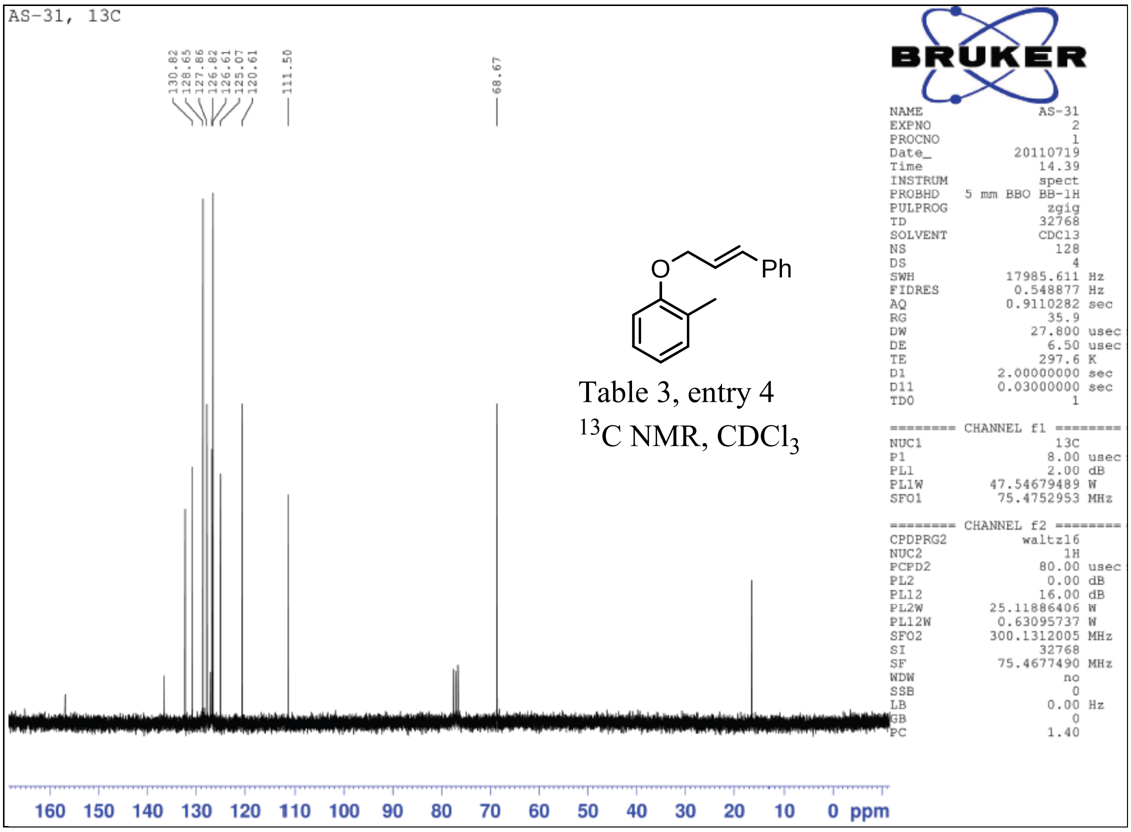

Table 3, entry 4
$^{13}C$ NMR, $CDCl_3$

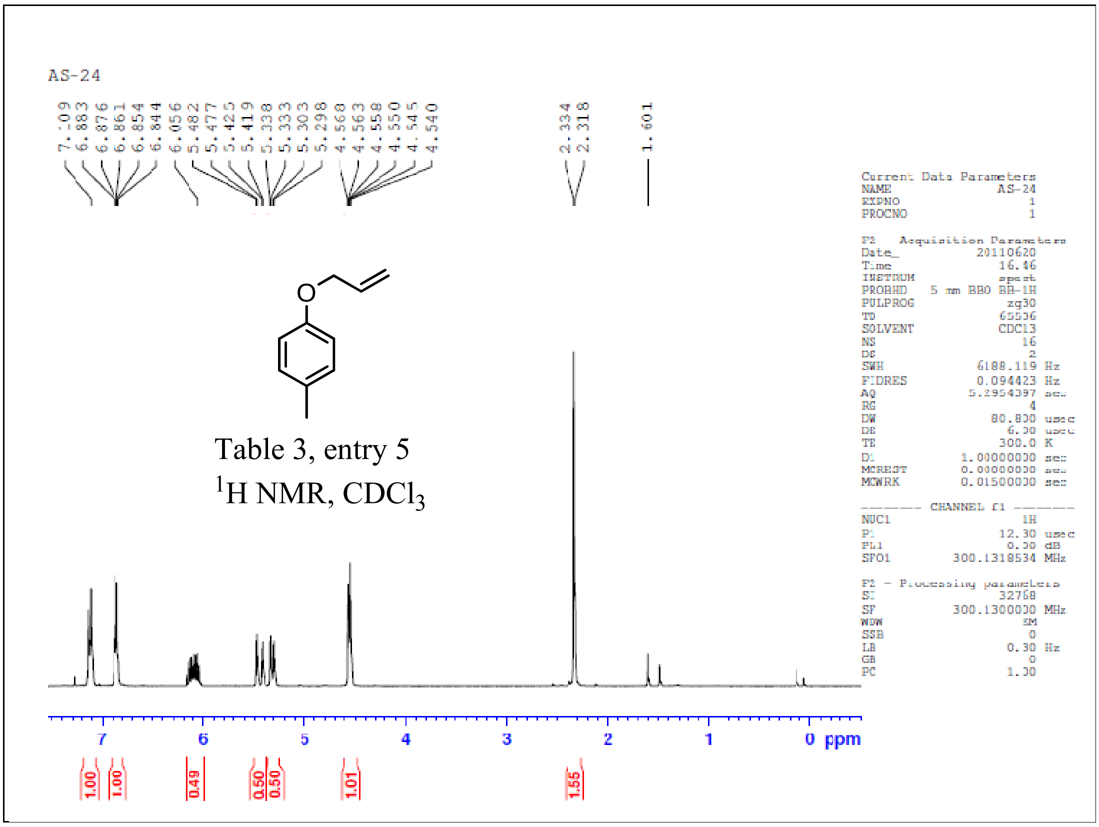

Table 3, entry 5
$^1$H NMR, $CDCl_3$

```
Current Data Parameters
NAME               AS-24
EXPNO                  1
PROCNO                 1

F2   Acquisition Parameters
Date_           20110620
Time               16.46
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6188.119 Hz
FIDRES          0.094423 Hz
AQ             5.2954397 sec
RG                     4
DW                80.800 usec
DE                  6.00 usec
TE                 300.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.30 usec
PL1                 0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

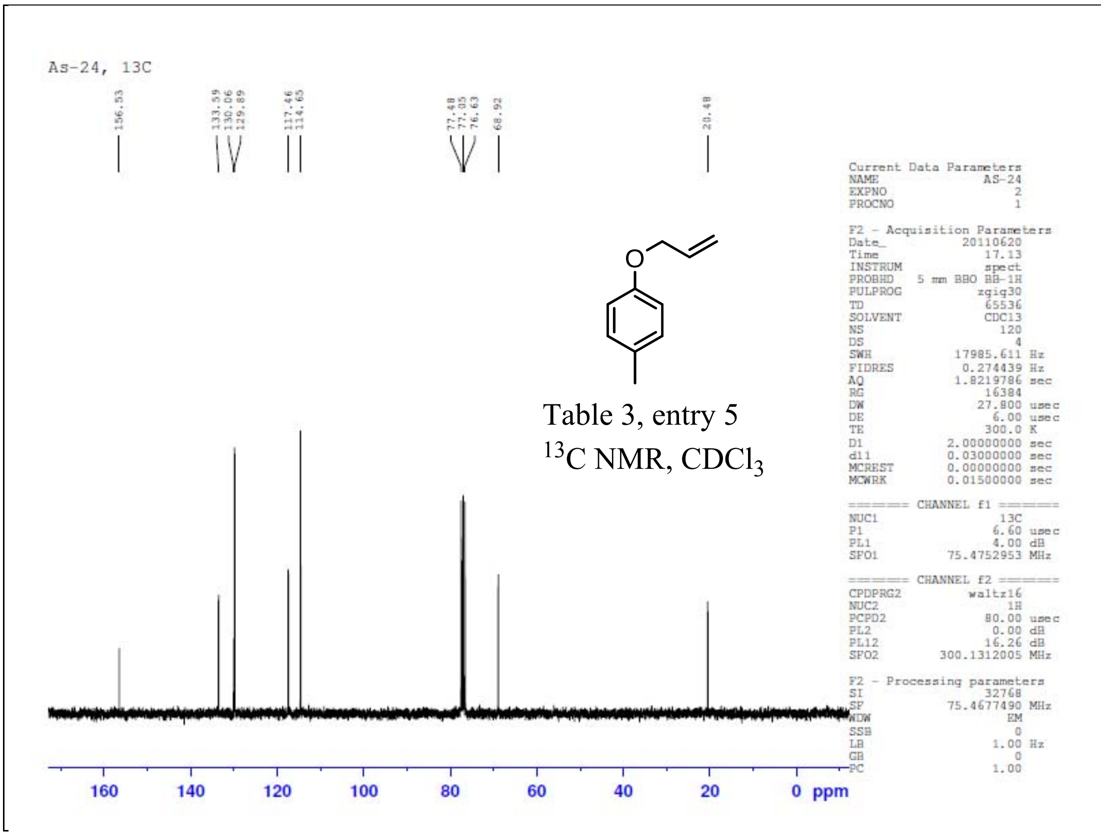

Table 3, entry 5
$^{13}$C NMR, $CDCl_3$

```
Current Data Parameters
NAME               AS-24
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110620
Time               17.13
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgig30
TD                 65536
SOLVENT            CDCl3
NS                   120
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ             1.8219786 sec
RG                 16384
DW                27.800 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.60 usec
PL1                 4.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               16.26 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

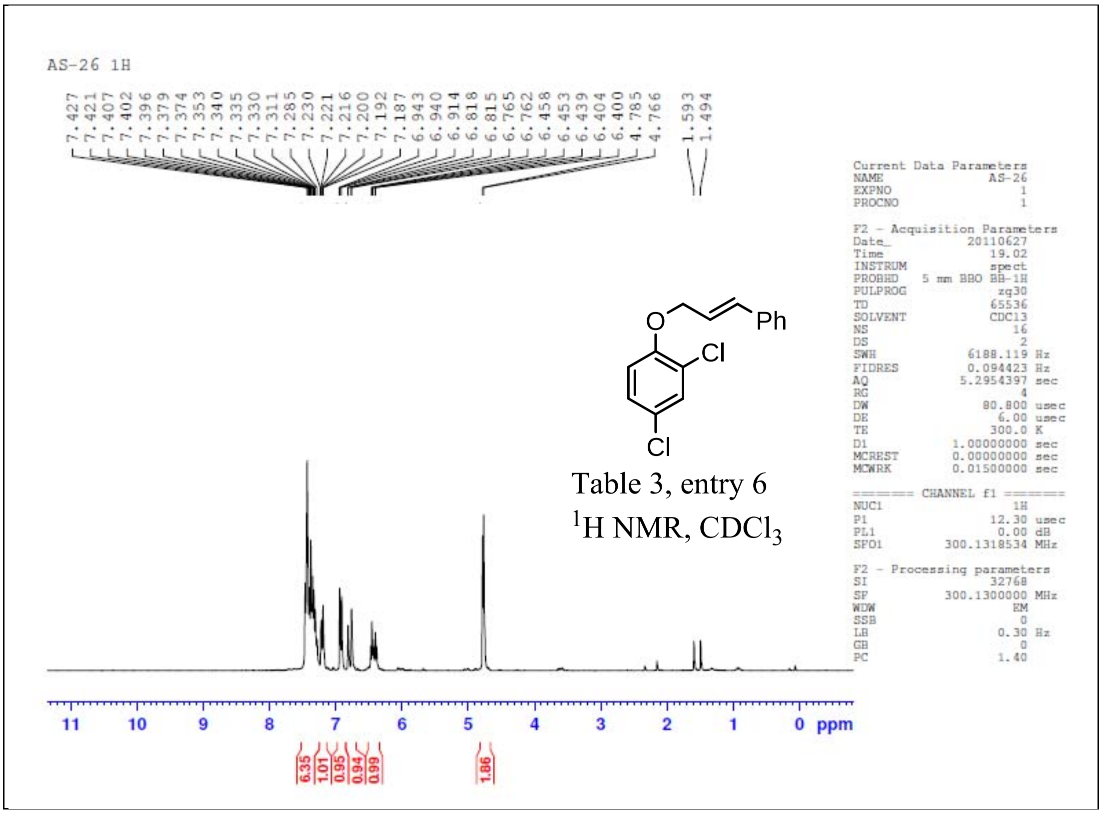

Table 3, entry 6
$^{1}$H NMR, $CDCl_3$

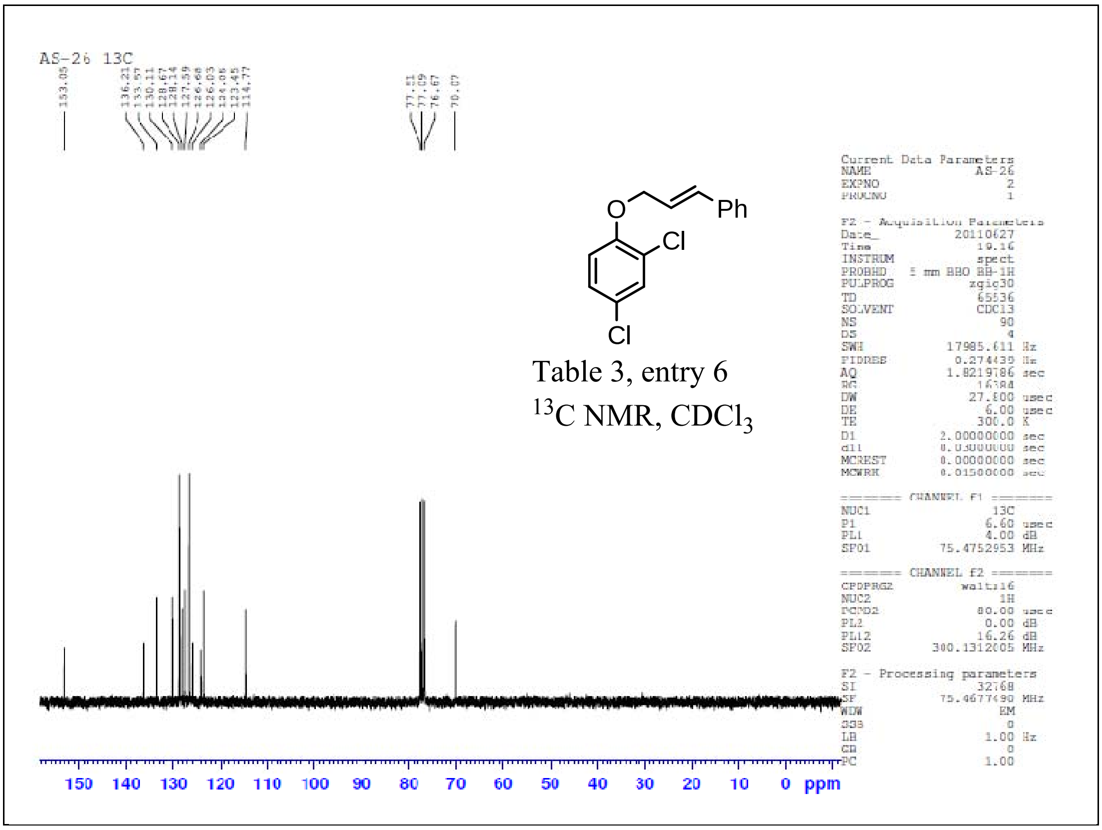

Table 3, entry 6
$^{13}$C NMR, $CDCl_3$

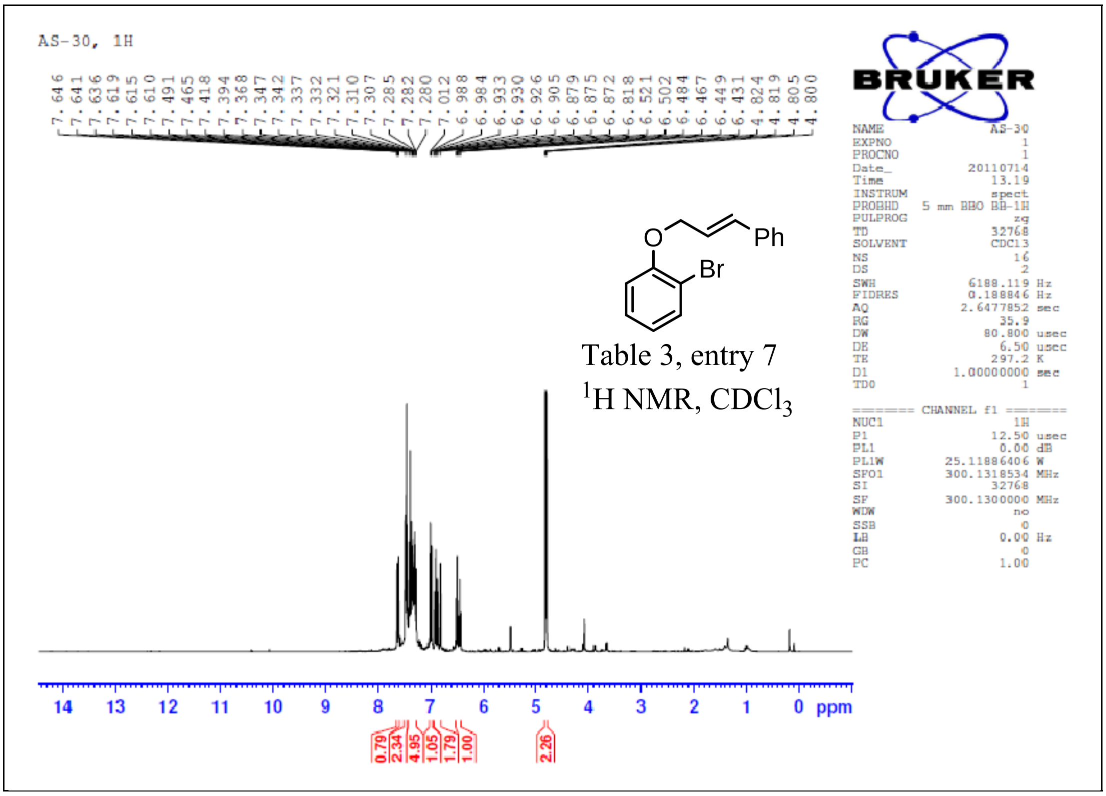

Table 3, entry 7
$^1$H NMR, $CDCl_3$

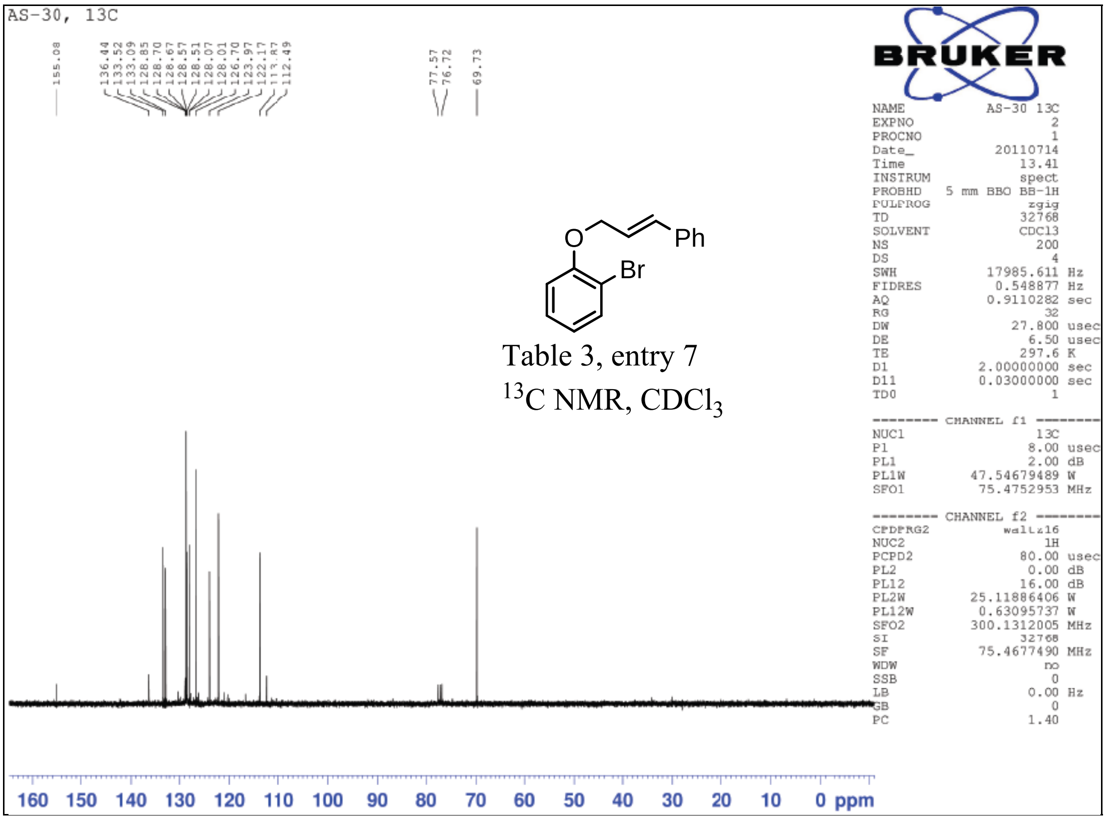

Table 3, entry 7
$^{13}$C NMR, $CDCl_3$

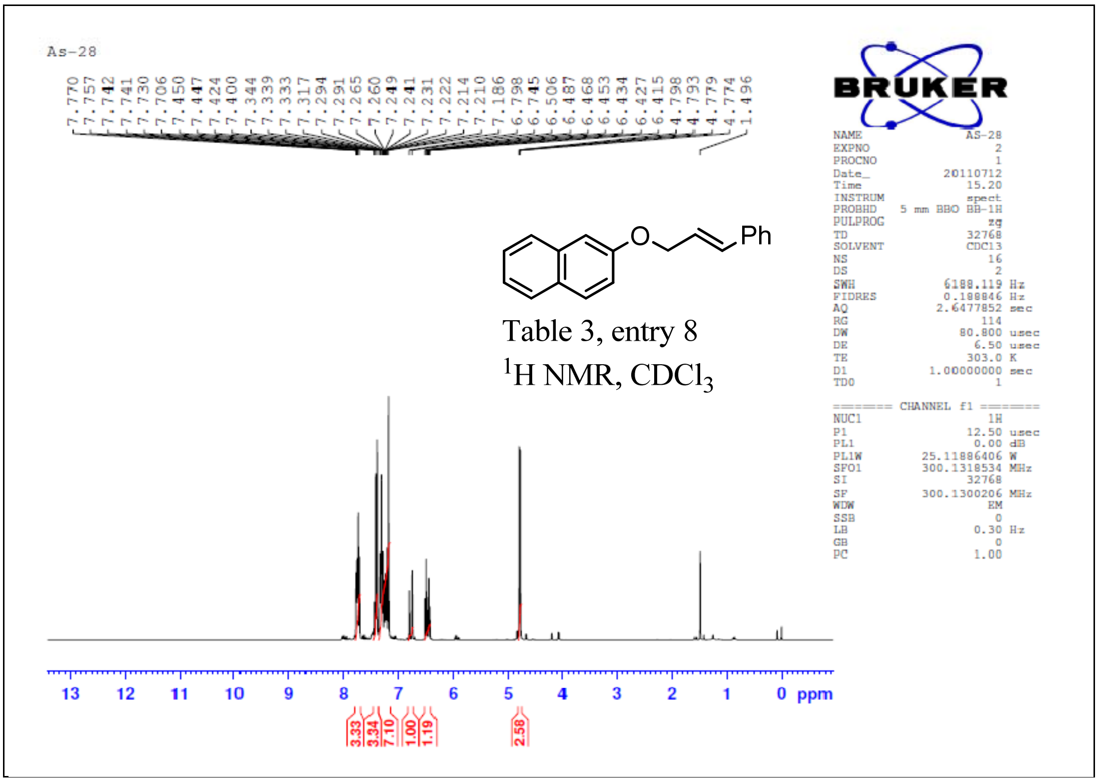

Table 3, entry 8
$^{1}H$ NMR, $CDCl_3$

```
NAME                AS-28
EXPNO                   2
PROCNO                  1
Date_            20110712
Time                15.20
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                  32768
SOLVENT             CDC13
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.188846 Hz
AQ              2.6477852 sec
RG                    114
DW                 80.800 usec
DE                   6.50 usec
TE                  303.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.50 usec
PL1                  0.00 dB
PL1W          25.11886406 W
SFO1          300.1318534 MHz
SI                  32768
SF            300.1300206 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

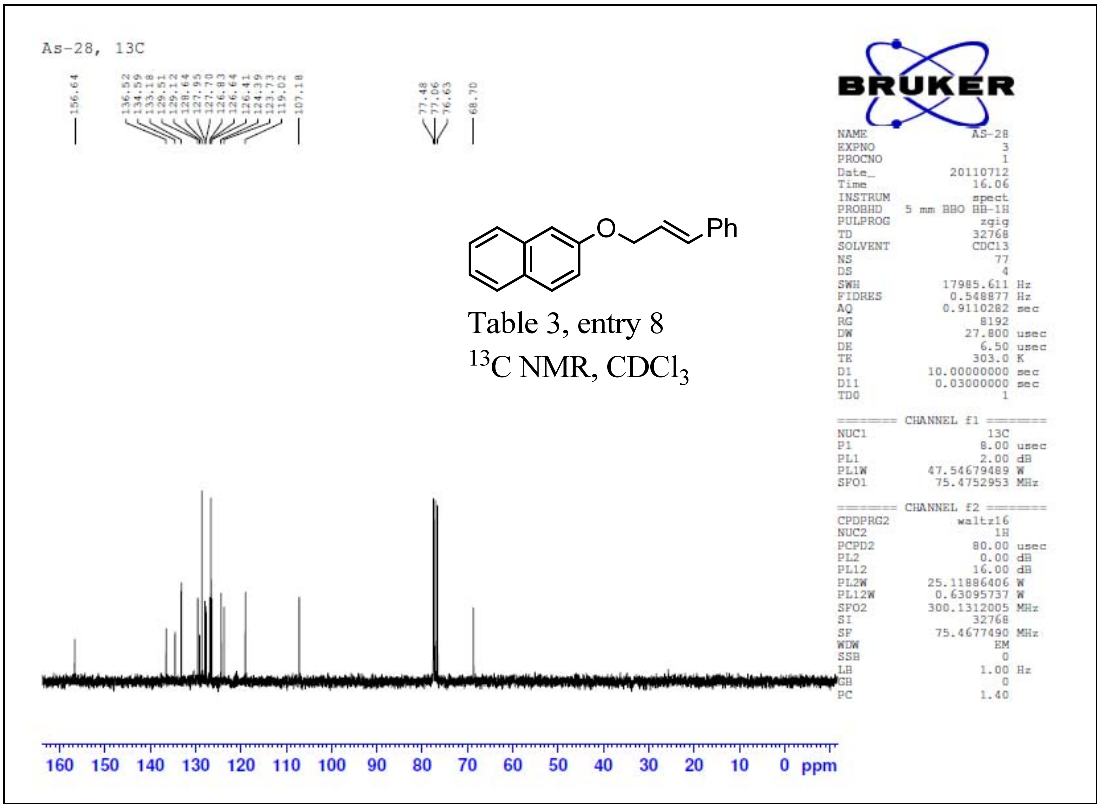

Table 3, entry 8
$^{13}C$ NMR, $CDCl_3$

```
NAME                AS-28
EXPNO                   3
PROCNO                  1
Date_            20110712
Time                16.06
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgig
TD                  32768
SOLVENT             CDC13
NS                     77
DS                      4
SWH             17985.611 Hz
FIDRES           0.548877 Hz
AQ              0.9110282 sec
RG                   8192
DW                 27.800 usec
DE                   6.50 usec
TE                  303.0 K
D1            10.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.00 usec
PL1                  2.00 dB
PL1W          47.54679489 W
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                16.00 dB
PL2W          25.11886406 W
PL12W          0.63095737 W
SFO2          300.1312005 MHz
SI                  32768
SF             75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

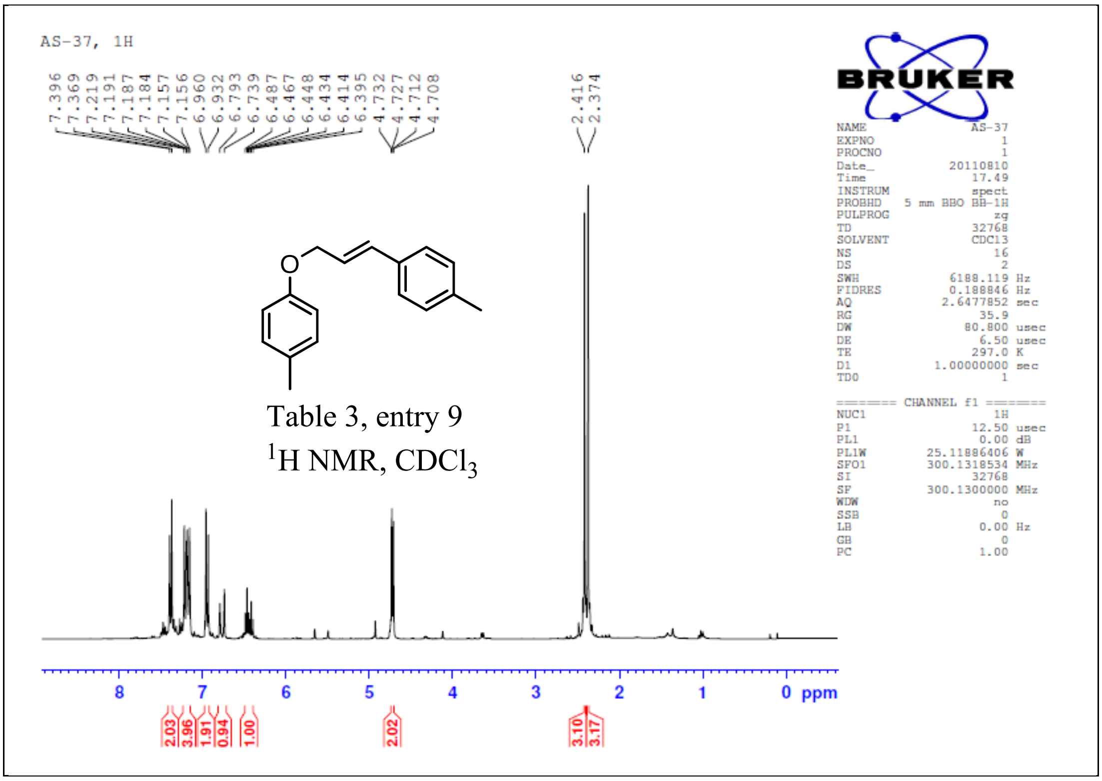

Table 3, entry 9
$^1$H NMR, $CDCl_3$

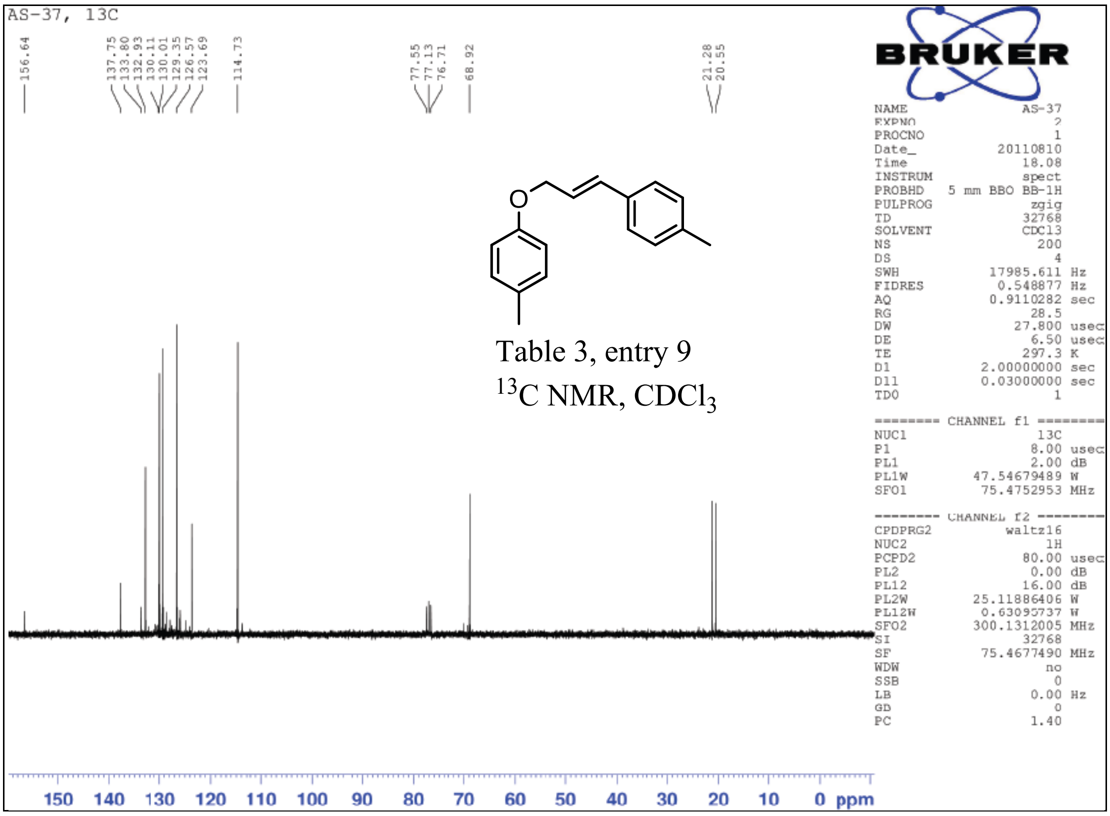

Table 3, entry 9
$^{13}$C NMR, $CDCl_3$

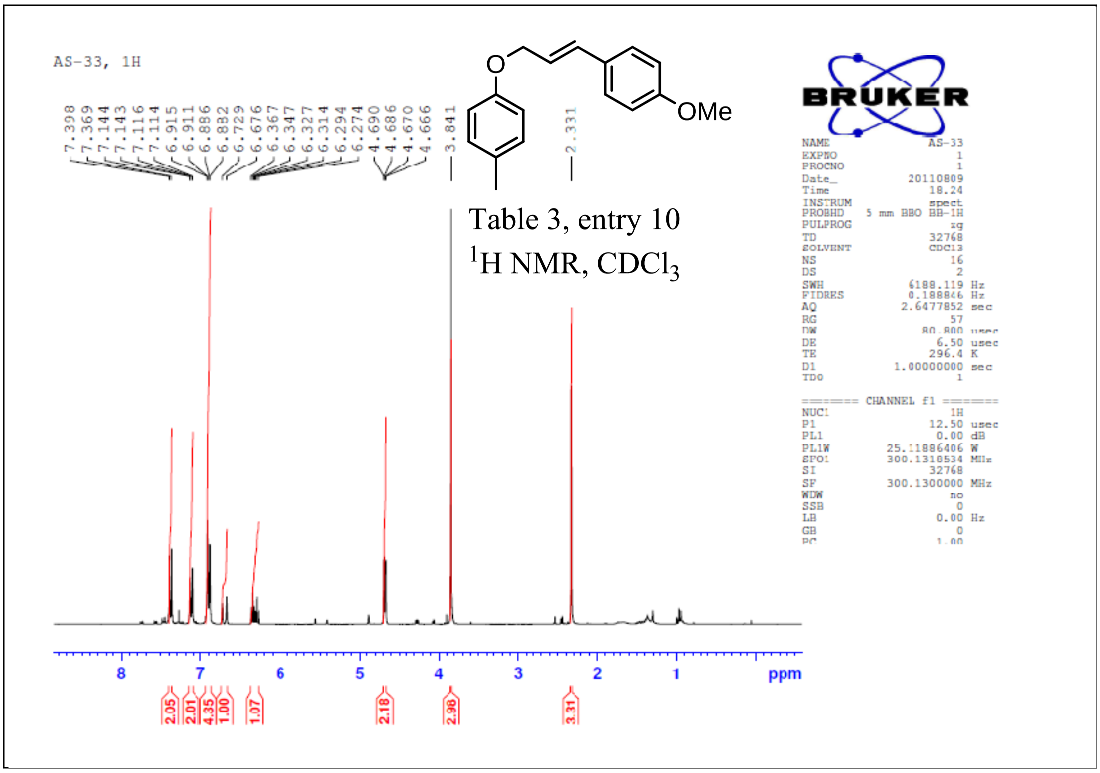

Table 3, entry 10
$^{1}$H NMR, $CDCl_3$

```
NAME            AS-33
EXPNO               1
PROCNO              1
Date_        20110809
Time            18.24
INSTRUM         spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg
TD              32768
SOLVENT         CDC13
NS                 16
DS                  2
SWH          6188.119 Hz
FIDRES       0.188846 Hz
AQ          2.6477852 sec
RG                 57
DW             80.800 usec
DE               6.50 usec
TE              296.4 K
D1         1.00000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1               1H
P1              12.50 usec
PL1              0.00 dB
PL1W      25.11886406 W
SFO1      300.1318534 MHz
SI              32768
SF        300.1300000 MHz
WDW                no
SSB                 0
LB               0.00 Hz
GB                  0
PC               1.00
```

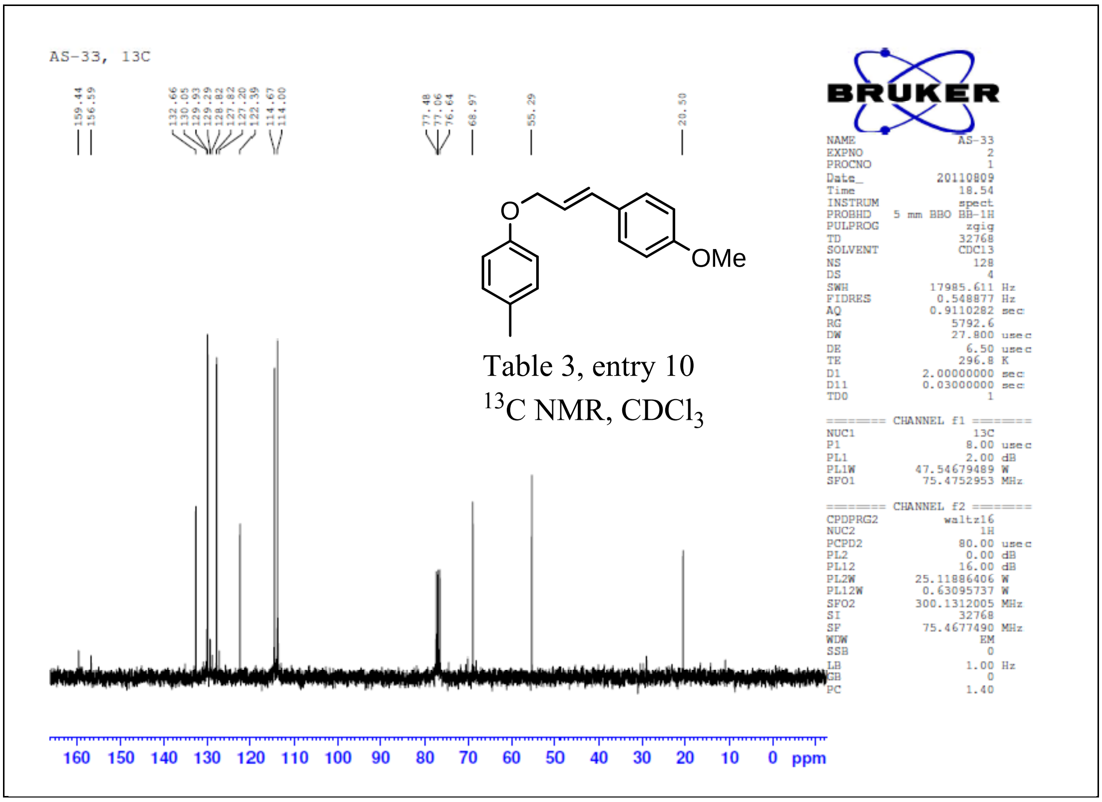

Table 3, entry 10
$^{13}$C NMR, $CDCl_3$

```
NAME            AS-33
EXPNO               2
PROCNO              1
Date_        20110809
Time            18.54
INSTRUM         spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgig
TD              32768
SOLVENT         CDC13
NS                128
DS                  4
SWH         17985.611 Hz
FIDRES       0.548877 Hz
AQ          0.9110282 sec
RG             5792.6
DW             27.800 usec
DE               6.50 usec
TE              296.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1              13C
P1               8.00 usec
PL1              2.00 dB
PL1W      47.54679489 W
SFO1       75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2       waltz16
NUC2               1H
PCPD2           80.00 usec
PL2              0.00 dB
PL12            16.00 dB
PL2W      25.11886406 W
PL12W      0.63095737 W
SFO2      300.1312005 MHz
SI              32768
SF         75.4677490 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

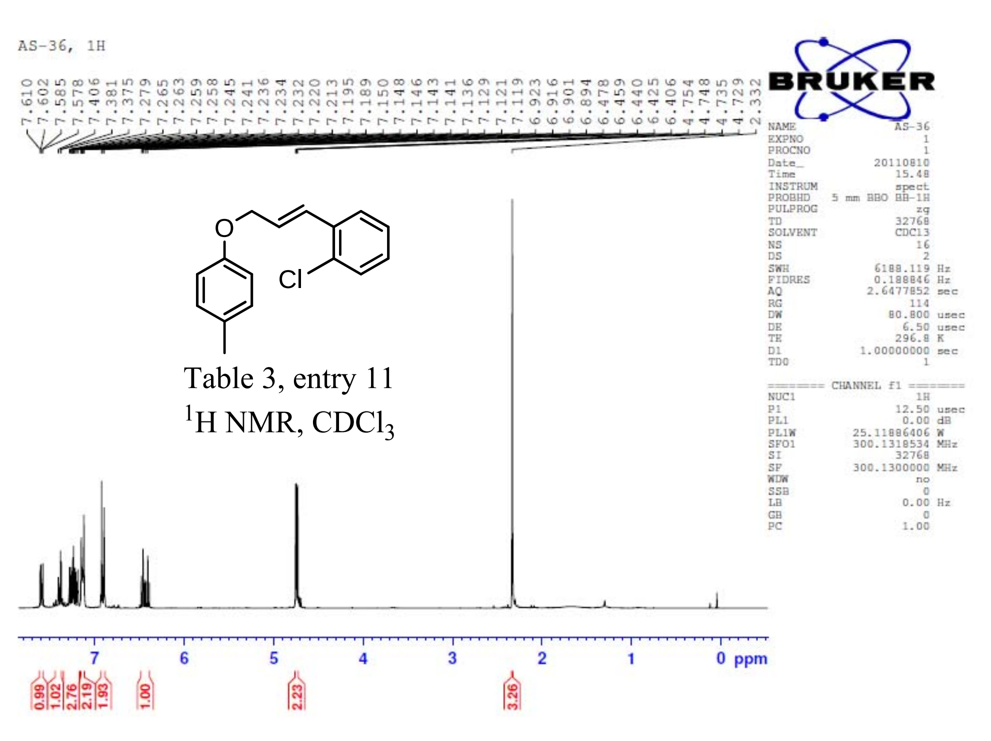

Table 3, entry 11
$^1$H NMR, $CDCl_3$

```
NAME             AS-36
EXPNO                1
PROCNO               1
Date_         20110810
Time             15.48
INSTRUM          spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           6188.119 Hz
FIDRES        0.188846 Hz
AQ           2.6477852 sec
RG                 114
DW              80.800 usec
DE                6.50 usec
TE               296.8 K
D1          1.00000000 sec
TD0                  1

======= CHANNEL f1 =======
NUC1                1H
P1               12.50 usec
PL1               0.00 dB
PL1W       25.11886406 W
SFO1       300.1318534 MHz
SI               32768
SF         300.1300000 MHz
WDW                 no
SSB                  0
LB                0.00 Hz
GB                   0
PC                1.00
```

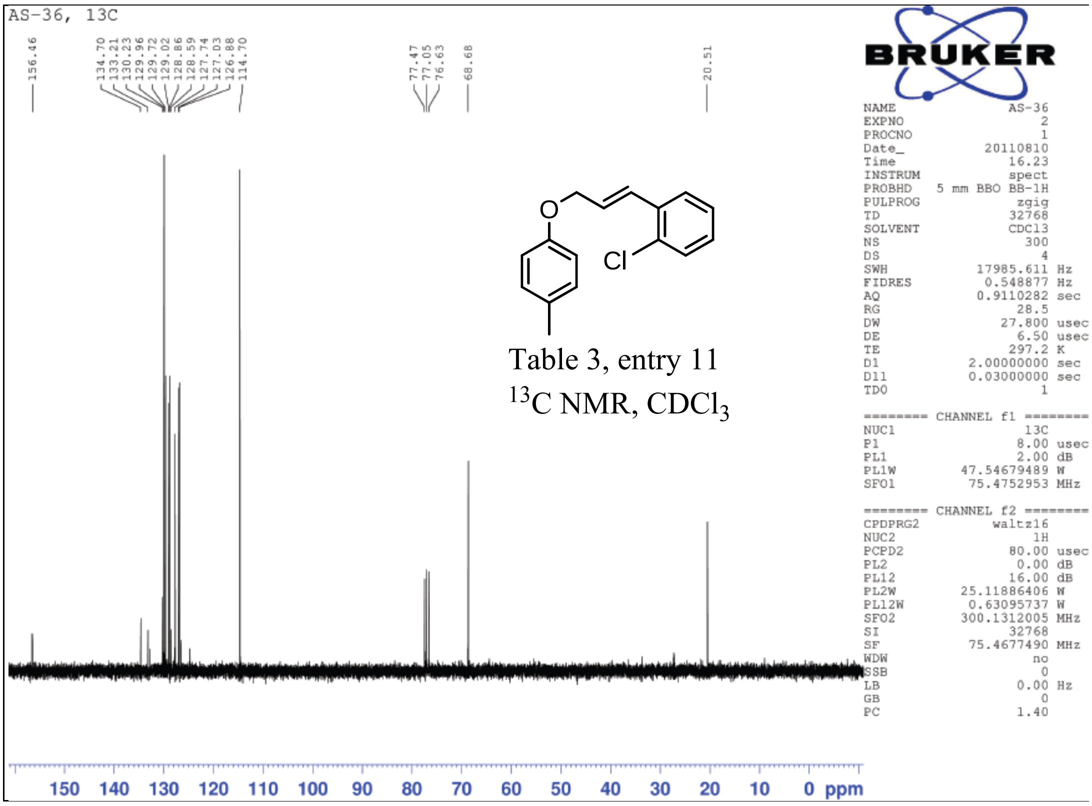

Table 3, entry 11
$^{13}$C NMR, $CDCl_3$

```
NAME             AS-36
EXPNO                2
PROCNO               1
Date_         20110810
Time             16.23
INSTRUM          spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgig
TD               32768
SOLVENT          CDCl3
NS                 300
DS                   4
SWH          17985.611 Hz
FIDRES        0.548877 Hz
AQ           0.9110282 sec
RG                28.5
DW              27.800 usec
DE                6.50 usec
TE               297.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1                8.00 usec
PL1               2.00 dB
PL1W       47.54679489 W
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               0.00 dB
PL12             16.00 dB
PL2W       25.11886406 W
PL12W       0.63095737 W
SFO2       300.1312005 MHz
SI               32768
SF          75.4677490 MHz
WDW                 no
SSB                  0
LB                0.00 Hz
GB                   0
PC                1.40
```

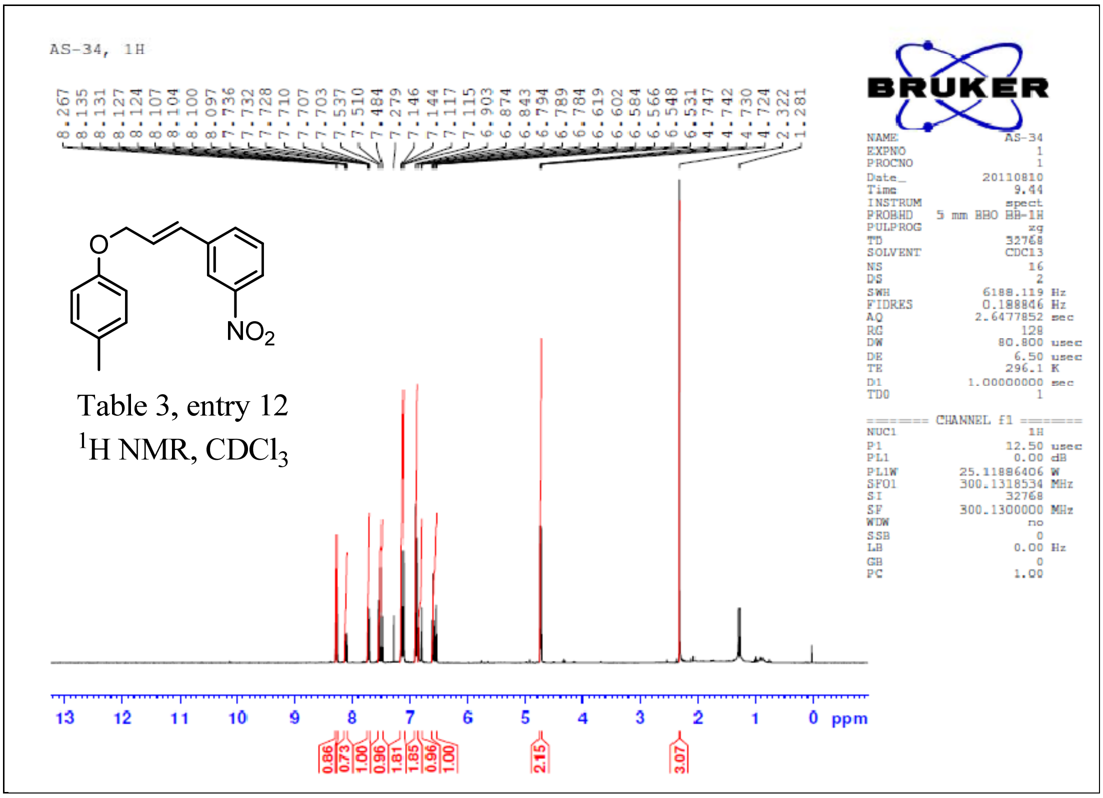

Table 3, entry 12
$^1$H NMR, $CDCl_3$

```
NAME                 AS-34
EXPNO                    1
PROCNO                   1
Date_             20110810
Time                  9.44
INSTRUM              spect
PROBHD     5 mm BBO BB-1H
PULPROG                 zg
TD                   32768
SOLVENT              CDC13
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES            0.188846 Hz
AQ               2.6477852 sec
RG                     128
DW                  80.800 usec
DE                    6.50 usec
TE                   296.1 K
D1              1.00000000 sec
TD0                      1

======= CHANNEL f1 =======
NUC1                    1H
P1                   12.50 usec
PL1                   0.00 dB
PL1W           25.11886406 W
SFO1           300.1318534 MHz
SI                   32768
SF             300.1300000 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

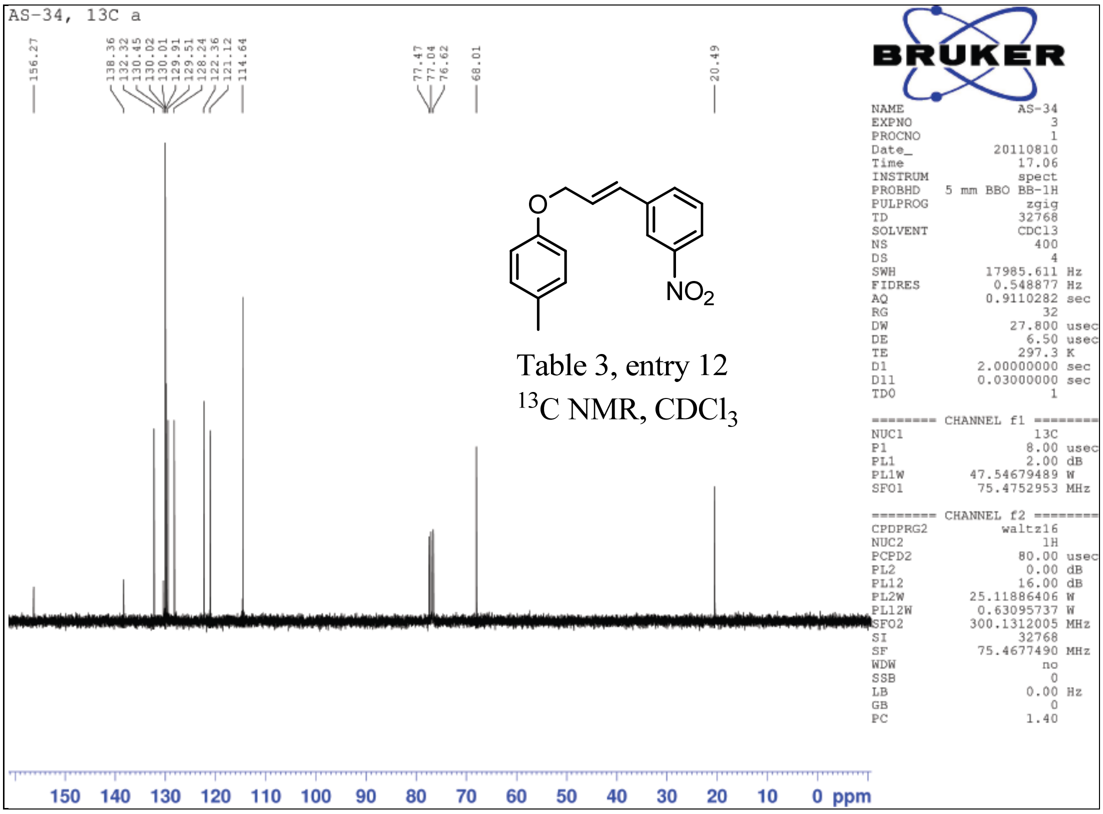

Table 3, entry 12
$^{13}$C NMR, $CDCl_3$

```
NAME                 AS-34
EXPNO                    3
PROCNO                   1
Date_             20110810
Time                 17.06
INSTRUM              spect
PROBHD     5 mm BBO BB-1H
PULPROG               zgig
TD                   32768
SOLVENT              CDC13
NS                     400
DS                       4
SWH              17985.611 Hz
FIDRES            0.548877 Hz
AQ               0.9110282 sec
RG                      32
DW                  27.800 usec
DE                    6.50 usec
TE                   297.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    8.00 usec
PL1                   2.00 dB
PL1W           47.54679489 W
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 16.00 dB
PL2W           25.11886406 W
PL12W           0.63095737 W
SFO2           300.1312005 MHz
SI                   32768
SF              75.4677490 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
```