SUPPORTING INFORMATION

Oxygen Promoted Pd(II) Catalysis for the Coupling of Organoboron Compounds and Olefins

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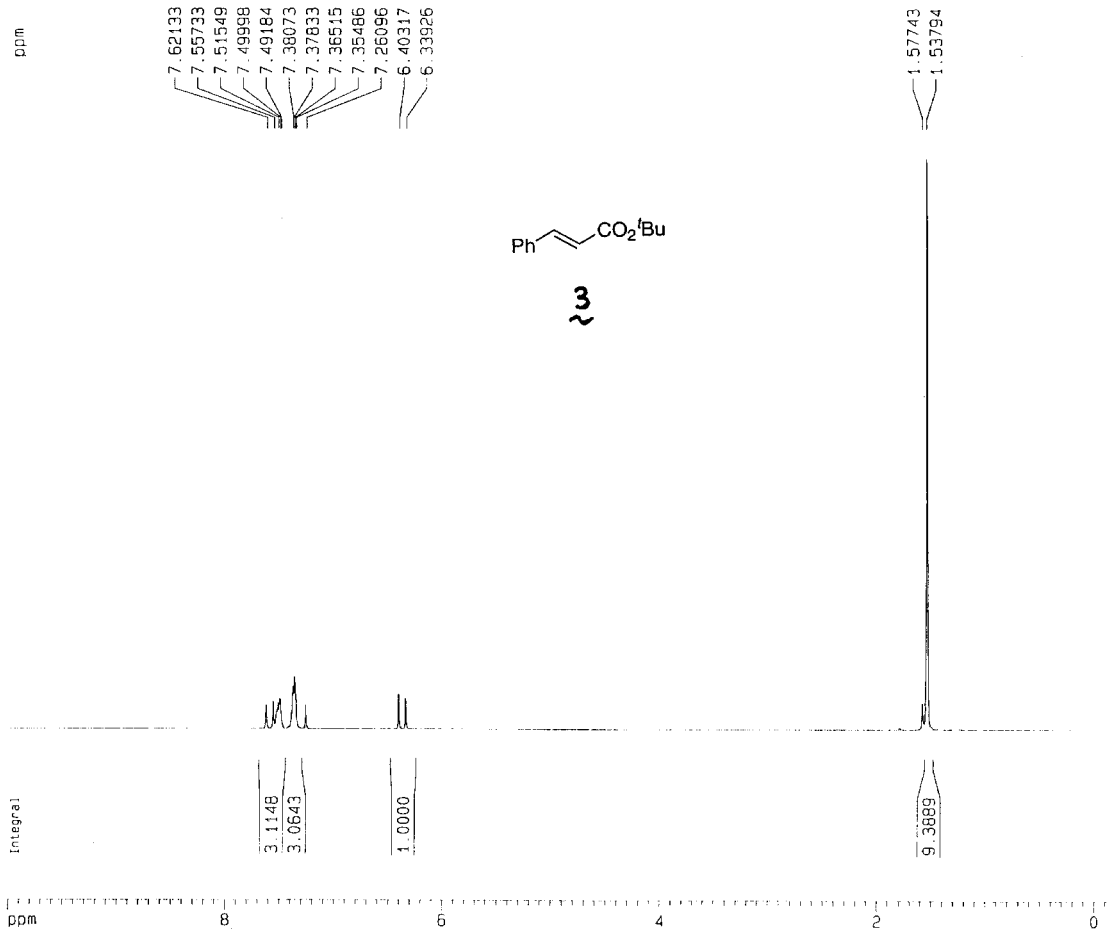
***Representative Experimental Procedure** :*

tert-Butyl acrylate **1** (64 mg, 0.5 mmol, 1 equiv.) was dissolved in DMF (2.5 mL, 0.2 M solution), and stirred at room temperature. To the clear solution, was added phenylboronic acid (74 mg, 0.6 mmol, 1.2 equiv.) followed by a single addition of Na_2CO_3 (106 mg, 1.0 mmol, 2 equiv.) and $Pd(OAc)_2$ (11 mg, 0.05 mmol, 0.1 equiv.). The reaction flask was fitted with an oxygen balloon, heated to 50 °C, and stirred for 3 h. The mixture was then diluted with ethyl acetate (20 mL), and washed with aqueous NaCl solution (3 X 10 mL). The organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated *in vacuo*, and subjected to flash chromatography (30 g of SiO_2). Elution with hexanes (100 mL), then 10:1 hexanes/EtOAc afforded *tert*-butyl *trans*-cinnamate (89 mg, 87%).



Current Data Parameters

NAME	proton
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	2
SWH	3063.726 Hz
FIDRES	0.093497 Hz
AQ	5.3477874 sec
RG	362
DW	163.200 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

========== CHANNEL f1 ========

NUC1	1H
P1	10.70 usec
PL1	0.00 dB
SFO1	250.1315008 MHz

F2 - Processing parameters

SI	16384
SF	250.1300072 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	10.000 ppm
F1	2501.30 Hz
F2P	-0.500 ppm
F2	-125.07 Hz
PPMCM	0.52500 ppm/cm
HZCM	131.31825 Hz/cm

Current Data Parameters
NAME carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 9.17
INSTRUM spect
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1116
DS 4
SWH 13227.514 Hz
FIDRES 0.403527 Hz
AQ 1.2386004 sec
RG 5160.6
DW 37.800 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

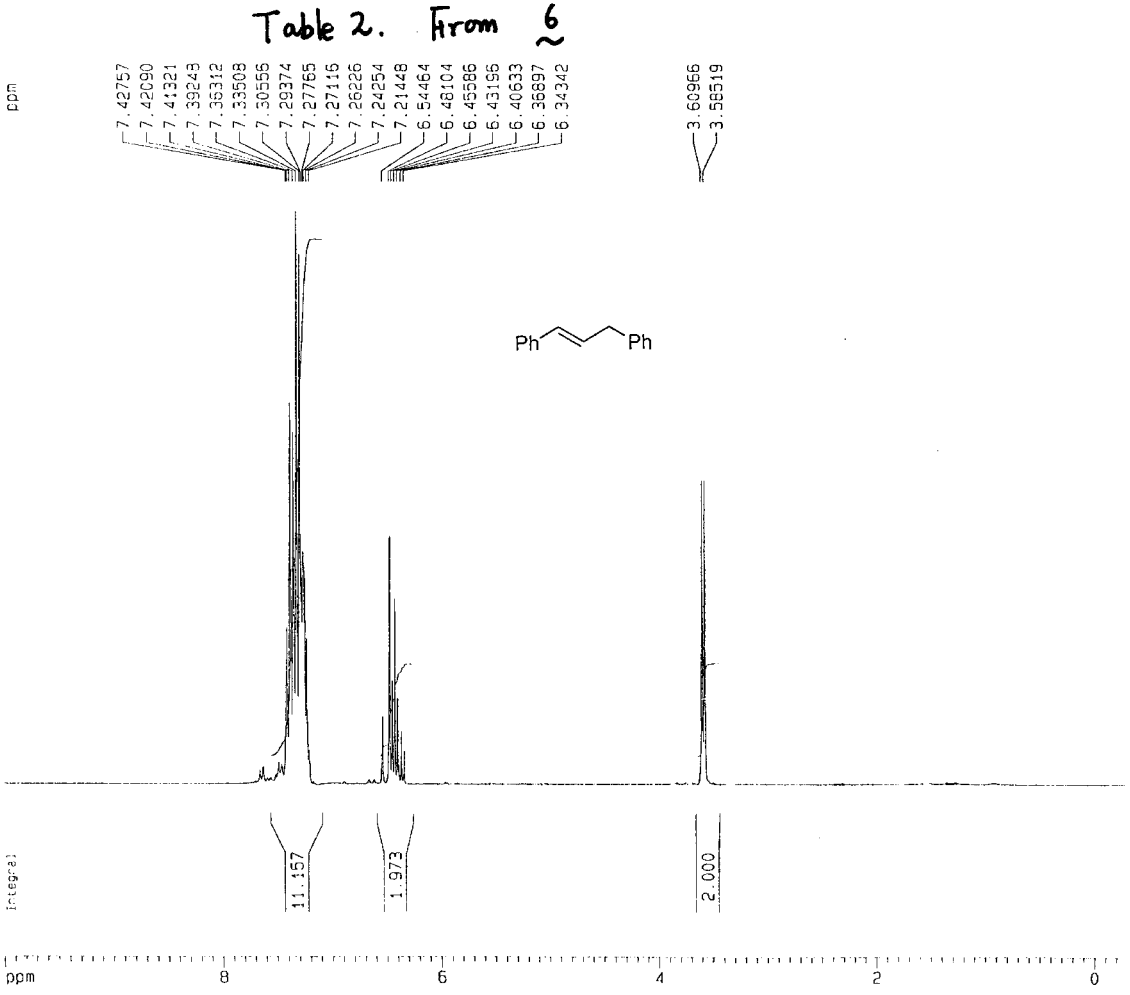
======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SF01 62.9015035 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 130.00 usec
PL2 3.00 dB
PL12 30.00 dB
PL13 32.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952429 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 215.000 ppm
F1 13522.48 Hz
F2P 5.000 ppm
F2 314.40 Hz
PPMCM 11.00000 ppm/cm
HZCM 691.86618 Hz/cm

Table 2. From 6



Current Data Parameters

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EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	6
DS	4
SWH	3132.832 Hz
FIDRES	0.095606 Hz
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RG	181
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DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

========== CHANNEL f1 ========

NUC1	1H
P1	6.50 usec
PL1	3.00 dB
SFO1	250.1315008 MHz

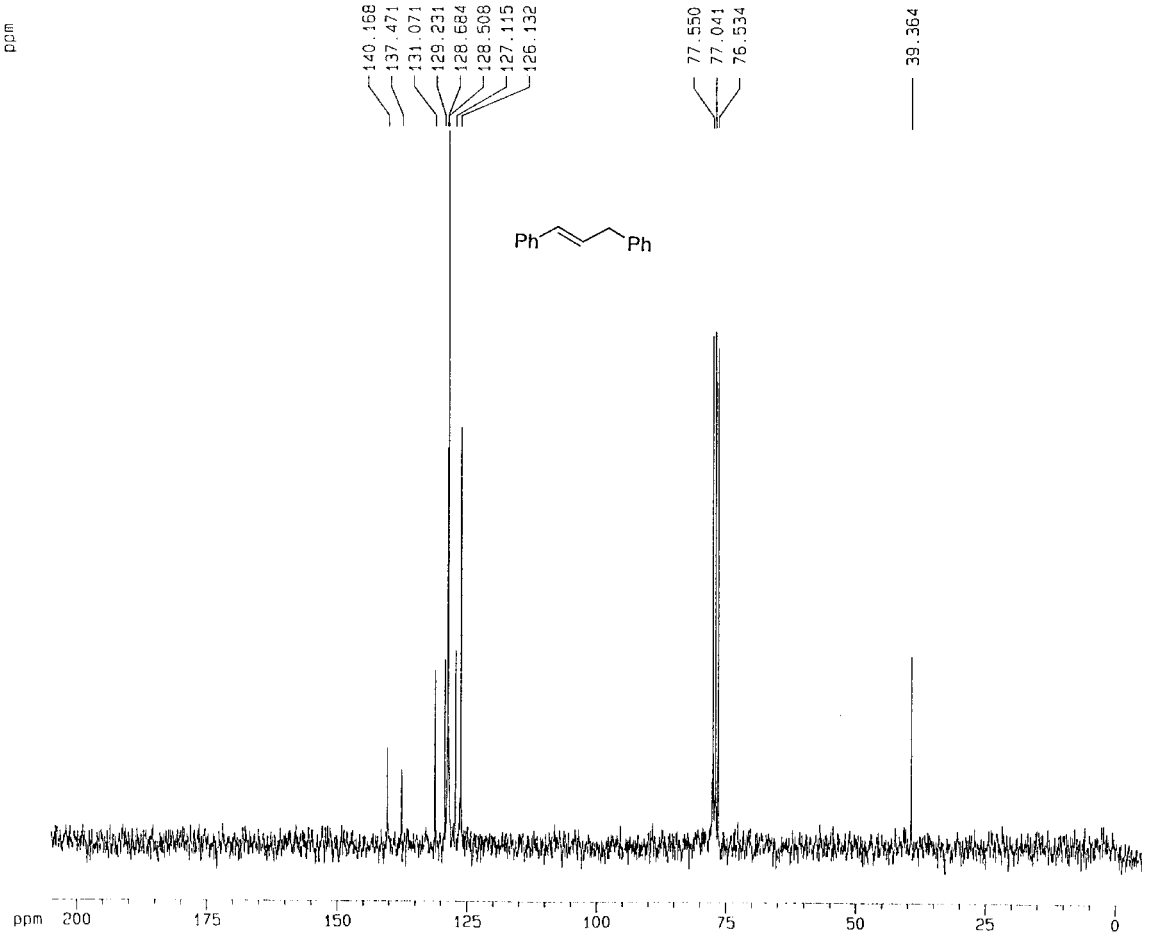
F2 - Processing parameters

SI	16384
SF	250.1300072 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	10.000 ppm
F1	2501.30 Hz
F2P	-0.500 ppm
F2	-125.07 Hz
PPMCM	0.52500 ppm/cm
HZCM	131.31825 Hz/cm

Table 2. From 6

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Current Data Parameters
NAME                  carbon
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
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PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      320
DS                        4
SWH               13227.514 Hz
FIDRES             0.403672 Hz
AQ                 1.2386804 sec
RG                     8192
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DE                    6.00 usec
TE                   300.0 K
D1                3.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec

========== CHANNEL f1 ==========
NUC1                      13C
P1                      12.50 usec
PL1                      0.00 dB
SFO1              62.9015035 MHz

========== CHANNEL f2 ==========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  130.00 usec
PL2                      3.00 dB
PL12                    30.00 dB
PL13                    32.00 dB
SFO2             250.1310005 MHz

F2 - Processing parameters
SI                        32768
SF                62.8952425 MHz
WDW                          EM
SSB                           0
LB                       3.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                       20.00 cm
F1P                     215.000 ppm
F1                    13522.48 Hz
F2P                      -5.000 ppm
F2                     -314.48 Hz
PPMCM                 11.00000 ppm/cm
HZCM                691.84766 Hz/cm
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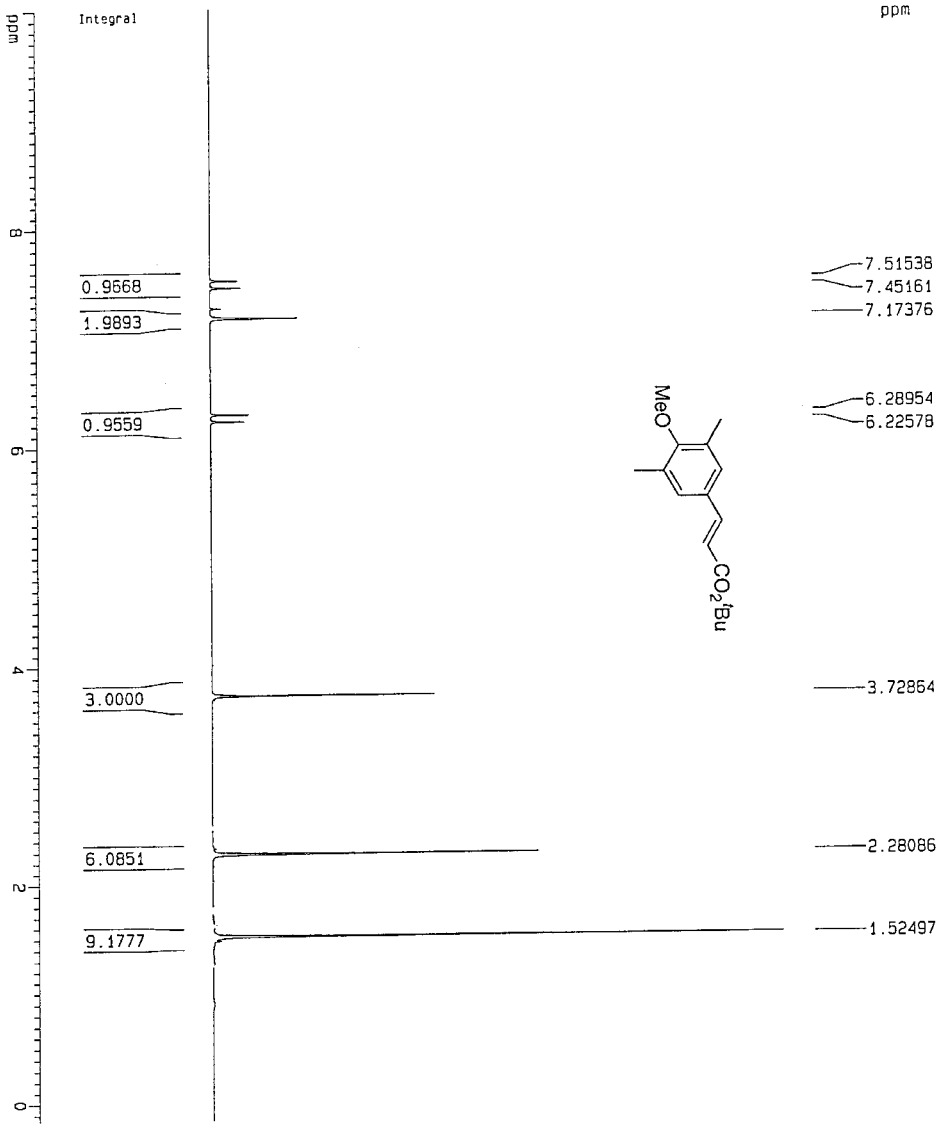
Table 3. from 11 ~

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NAME                  proton
EXPNO                      1
PROCNO                     1

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INSTRUM               spect
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PULPROG              zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              3003.726 Hz
FIDRES           0.091697 Hz
AQ               5.3477874 sec
RG                     128
DW               163.200 usec
DE                 6.00 usec
TE                 300.0 K
D1               1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.70 usec
PL1                 0.00 dB
SFO1         250.1315008 MHz

F2 - Processing parameters
SI                    16384
SF           250.1300072 MHz
WDW                      EM
SSB                       0
LB                  0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                   20.00 cm
F1P                10.000 ppm
F1                2501.30 Hz
F2P                -0.500 ppm
F2                -125.07 Hz
PPMCM             0.52500 ppm/cm
HZCM             131.31825 Hz/cm
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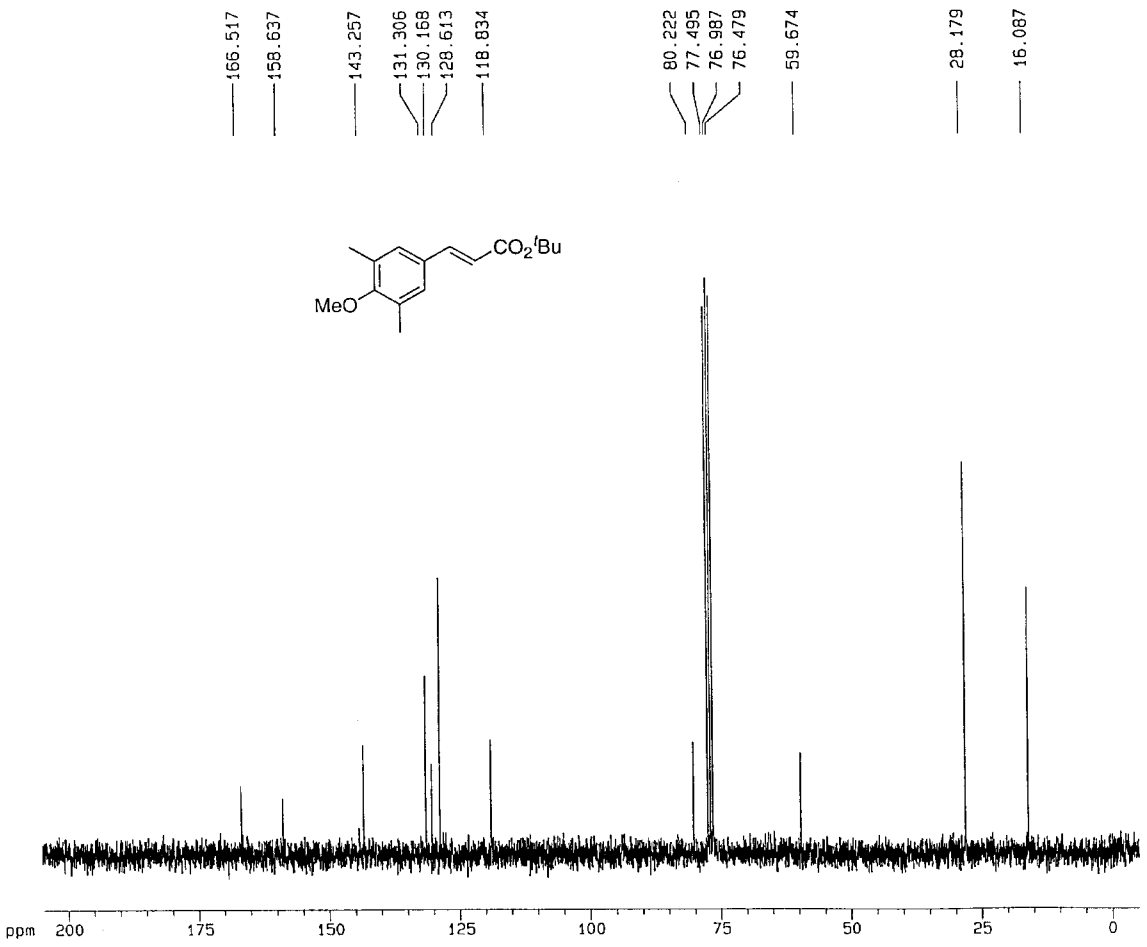
Table 3. From 11

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Current Data Parameters
NAME                  carbon
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
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Time                   11.14
INSTRUM                spect
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PULPROG              zgpg30
TD                     32768
SOLVENT                CDCl3
NS                       550
DS                         4
SWH               13227.514 Hz
FIDRES             0.403672 Hz
AQ                 1.2386804 sec
RG                      6502
DW                   37.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                3.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec

========== CHANNEL f1 ==========
NUC1                      13C
P1                     12.50 usec
PL1                     0.00 dB
SFO1              62.9015035 MHz

========== CHANNEL f2 ==========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 130.00 usec
PL2                     3.00 dB
PL12                   30.00 dB
PL13                   32.00 dB
SFO2             250.1310005 MHz

F2 - Processing parameters
SI                        32768
SF                62.0952425 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                        20.00 cm
F1P                      215.000 ppm
F1                     13522.48 Hz
F2P                       -5.000 ppm
F2                      -314.48 Hz
PPMCM                  11.00000 ppm/cm
HZCM                 691.84766 Hz/cm
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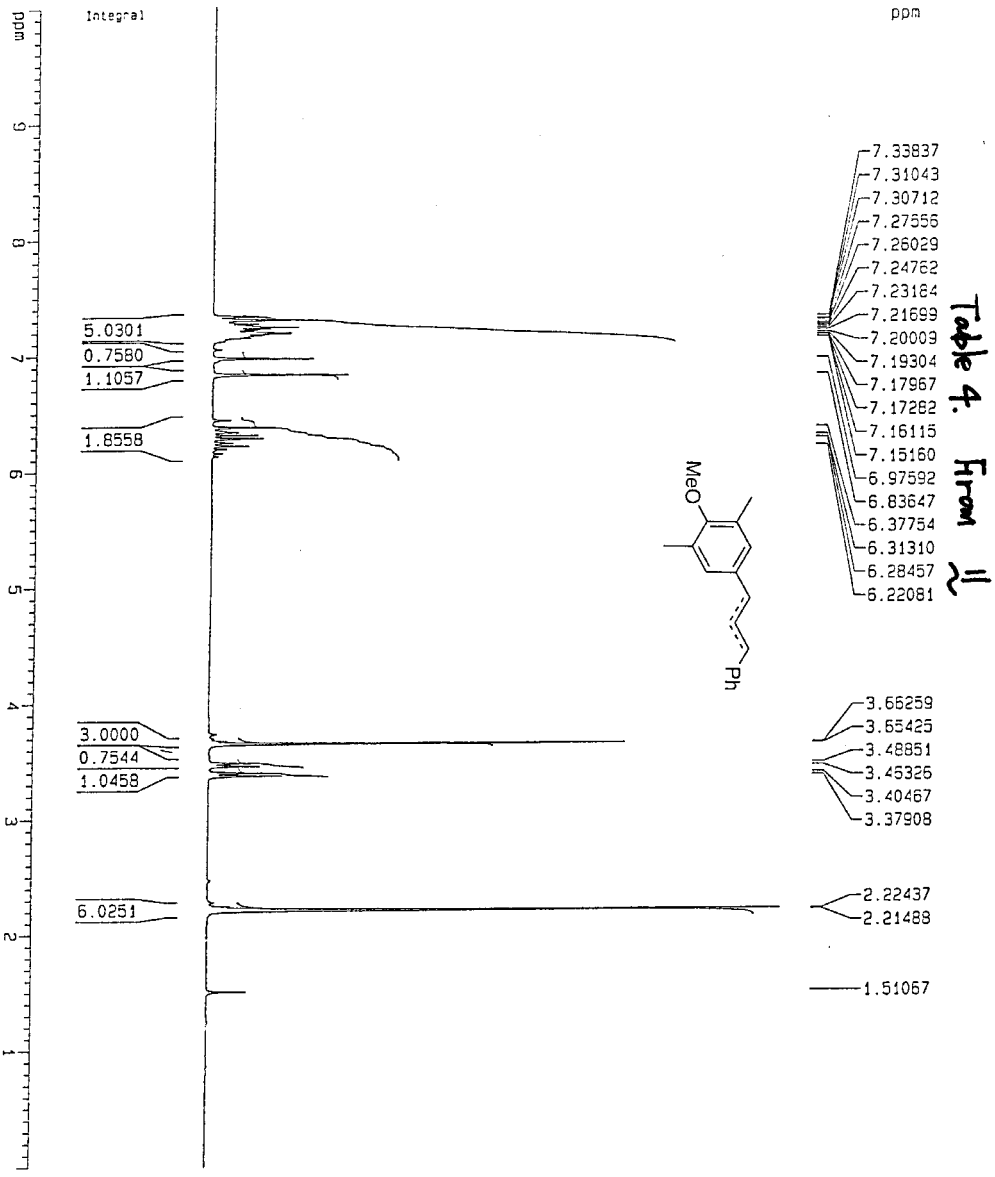

Table 4. From 11 ~

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Current Data Parameters
NAME                  proton
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
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Time                   15.24
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PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                         6
DS                         4
SWH               3132.032 Hz
FIDRES            0.095606 Hz
AQ                5.2230226 sec
RG                     203.2
DW                159.600 usec
DE                  6.00 usec
TE                  300.0 K
D1                1.00000000 sec

========== CHANNEL f1 ==========
NUC1                       1H
P1                       7.72 usec
PL1                      3.00 dB
SFO1           250.1315000 MHz

F2 - Processing parameters
SI                        16384
SF             250.1300242 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
F1P                   10.000 ppm
F1                   2501.30 Hz
F2P                   0.000 ppm
F2                      0.00 Hz
PPMCM              0.50000 ppm/cm
HZCM             125.06501 Hz/cm
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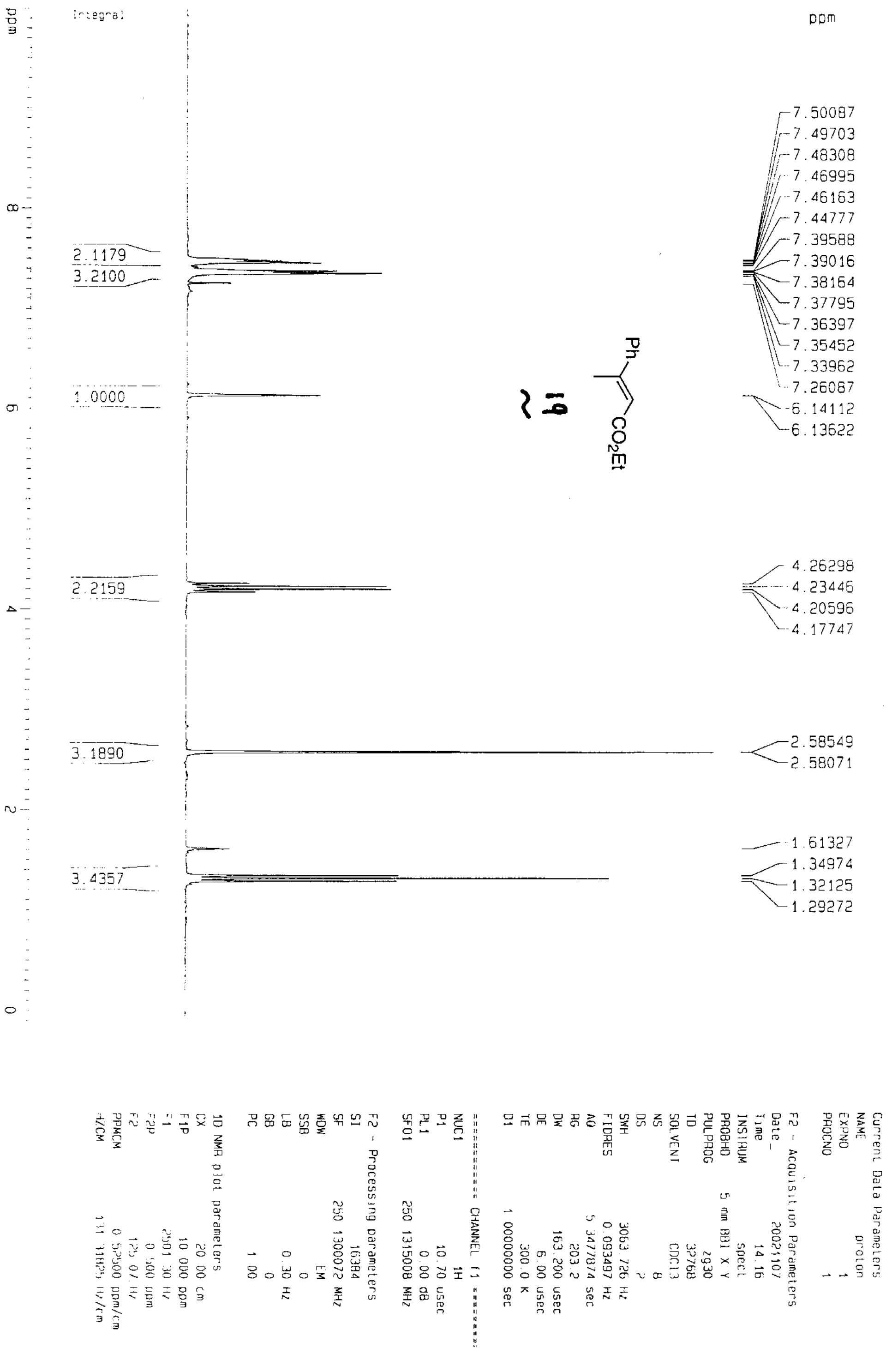
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7.46163
7.44777
7.39588
7.39016
7.38164
7.37795
7.36397
7.35452
7.33962
7.26087
6.14112
6.13622
4.26298
4.23446
4.20596
4.17747
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1.32125
1.29272
Ph
CO_2Et
19
Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
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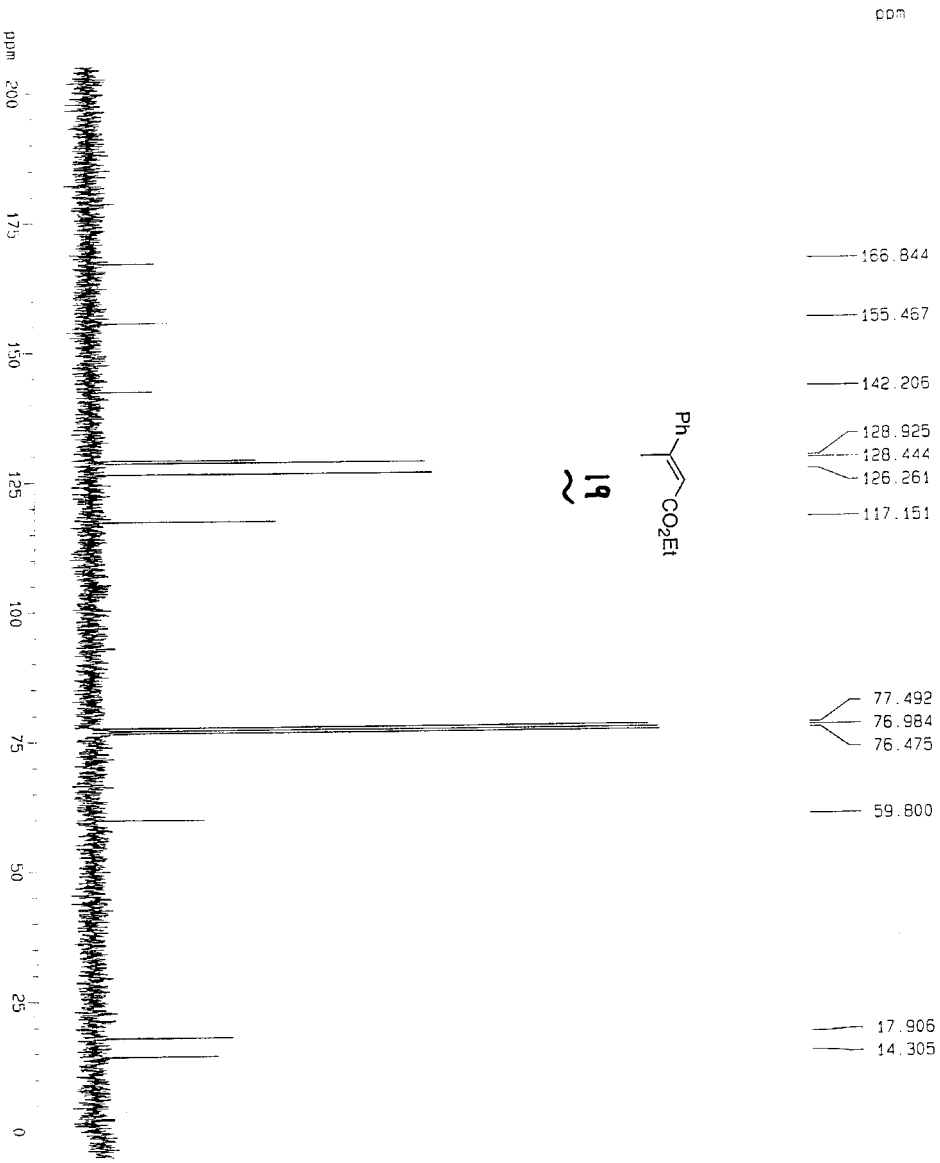
Time 14.16
INSTRUM spect
PROBHD 5 mm BBI X Y
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 3063.726 Hz
FIDRES 0.093497 Hz
AQ 5.3477874 sec
RG 203.2
DW 163.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
============ CHANNEL f1 ============
NUC1 1H
P1 10.70 usec
PL1 0.00 dB
SFO1 250.1315008 MHz
F2 - Processing parameters
SI 16384
SF 250.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 2501.30 Hz
F2P 0.500 ppm
PPMCM 0.52500 ppm/cm



Current Data Parameters
NAME
EXPNO 1
PROCNO 1

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Time 20 39
INSTRUM spect
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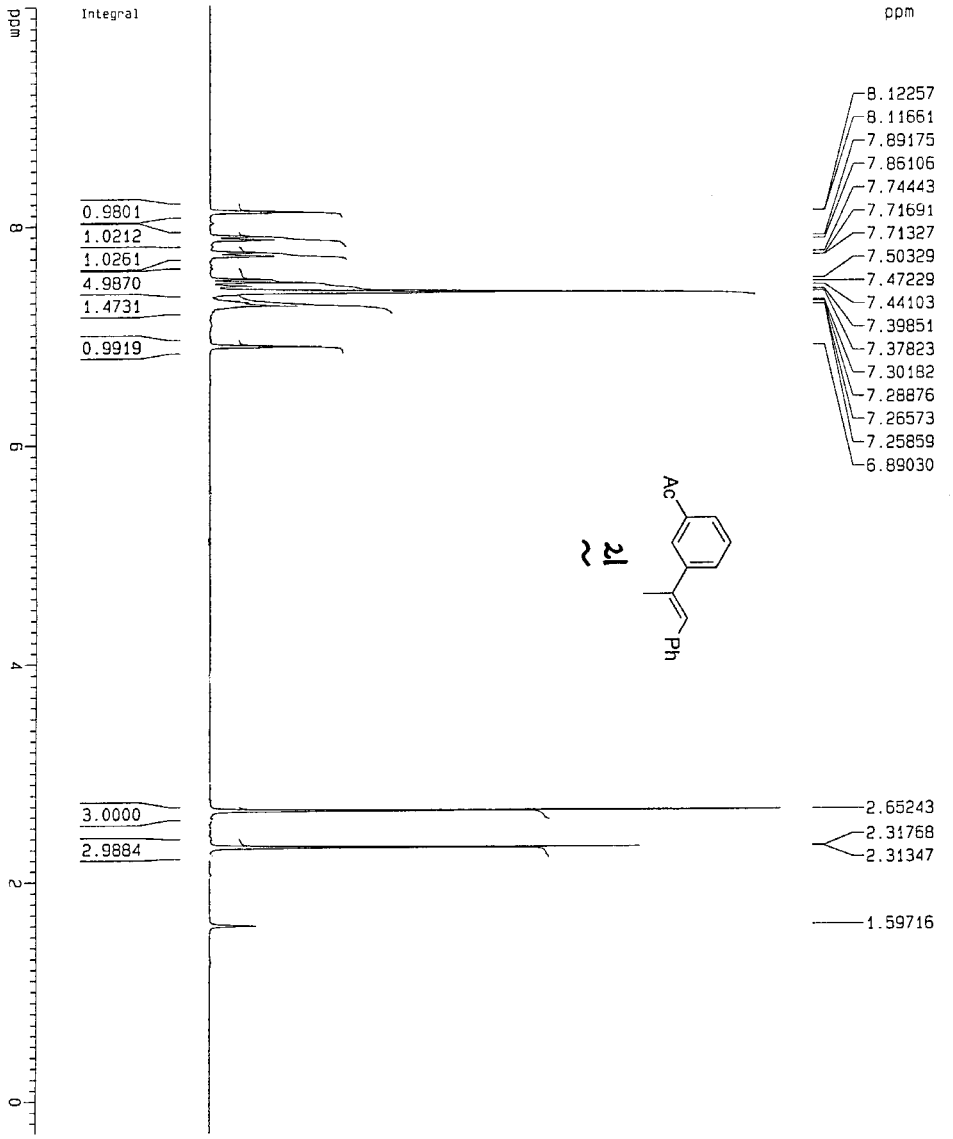
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 466
DS 4
SWH 13227.514 Hz
FIDRES 0.403672 Hz
AQ 1.2386804 sec
RG 5160.6
DW 37.800 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

CHANNEL f1
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SFO1 62.9015035 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 130.00 usec
PL2 1.00 dB
PL12 30.00 dB
PL13 32.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952425 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 200.000 ppm
F1 12562.48 Hz
F2P -1.000 ppm
F2 -114.48 Hz
PPMCM 11.00000 ppm/cm
HZCM 1691.86768 Hz/cm

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Current Data Parameters
NAME                  proton
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20021123
Time                   13.56
INSTRUM                spect
PROBHD     5 mm BBI X Y
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        6
DS                        4
SWH               3132.832 Hz
FIDRES            0.095606 Hz
AQ                5.2298226 sec
RG                      362
DW                159.600 usec
DE                6.00 usec
TE                   300.0 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                      6.50 usec
PL1                     3.00 dB
SFO1           250.1315008 MHz

F2 - Processing parameters
SI                       16384
SF             250.1300072 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                       20.00 cm
F1P                    10.000 ppm
F1                   2501.30 Hz
F2P                   -0.500 ppm
F2                   -125.07 Hz
PPMCM                0.52500 ppm/cm
HZCM               131.31825 Hz/cm
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Current Data Parameters
NAME carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021101
Time 15.02
INSTRUM spect
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PULPROG zgdc30
TD 32768
SOLVENT CDCl3
NS 909
DS 4
SWH 13227.514 Hz
FIDRES 0.403672 Hz
AQ 1.2386804 sec
RG 5160.6
DW 37.800 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

========== CHANNEL f1 ==========
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SFO1 62.9015035 MHz

========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 130.00 usec
PL2 3.00 dB
PL12 32.00 dB
PL13 32.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952425 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 215.000 ppm
F1 13522.40 Hz
F2P 15.000 ppm
F2 314.48 Hz
PPMCM 11.00000 ppm/cm
HZCM 691.84766 Hz/cm