J. Braz. Chem. Soc., Vol. 19, No. 3, S1-S13, 2008.
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0103 - 5053 $6.00+0.00

Eugenol and its Synthetic Analogues Inhibit Cell Growth of Human Cancer Cells (Part I)

H. Carrasco A.,*,[a] L. Espinoza C.,[b] V. Cardile,[c] C. Gallardo,[b] W. Cardona,[a] L. Lombardo,[c] K. Catalán M.,[b] M. Cuellar F.[e] and A. Russo[d]

[a]*Departamento de Ciencias Químicas, Universidad Andrés Bello, Campus Viña del Mar, Viña del Mar, Chile*

[b]*Departamento de Química, Universidad Técnica Federico. Santa Maria, Av. España N° 1680, Valparaiso, Chile*

[c]*Department of Physiological Sciences, University of Catania, V.le A. Doria 6, 95125, Catania, Italy*

[d]*Department of Biological Chemistry, Medical Chemistry and Molecular Biology, University of Catania, V.le A. Doria 6, 95125, Catania, Italy*

[e]*Facultad de Farmacia, Universidad de Valparaíso, Av. Gran Bretaña N° 1093, Valparaíso, Chile*

4-Allyl-2- methoxy-6-nitrophenol: In the pages S2-S4 we indicated the 1D & 2D NMR, HRMS, and IR spectra. IR spectra were recorded as thin film or KBr pellets in a Nicolet Impact 420 spectrometer. ν_{max} values are expressed in cm^{-1}. ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ solutions and referenced to the residual peak of $CHCl_3$ at δ 7.26 ppm and δ 77.00 ppm for ^1H and ^{13}C, respectively, on a Bruker Avance 400 Digital NMR spectrometer, operating at 400.1 MHz for ^1H and 100.6 MHz for ^{13}C. Chemical shifts are reported in δ ppm and coupling constants (*J*) are given in Hz. HRMS were recorder on a MAT 95XP, Thermo Finnigan spectrometer and represented at *m/z* (% rel. int.).

5-Allyl-3-nitrobenzene-1,2-diol: In the pages S5-S7 we indicated the 1D & 2D NMR, HRMS, and IR spectra. IR spectra were recorded as thin film or KBr pellets in a Nicolet Impact 420 spectrometer. ν_{max} values are expressed in cm^{-1}. ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ solutions and referenced to the residual peak of $CHCl_3$ at δ 7.26 ppm and δ 77.00 ppm for ^1H and ^{13}C, respectively, on a Bruker Avance 400 Digital NMR spectrometer, operating at 400.1 MHz for ^1H and 100.6 MHz for ^{13}C. Chemical shifts are reported in δ ppm and coupling constants (*J*) are given in Hz. HRMS were recorder on a MAT 95XP, Thermo Finnigan spectrometer and represented at *m/z* (% rel. int.).

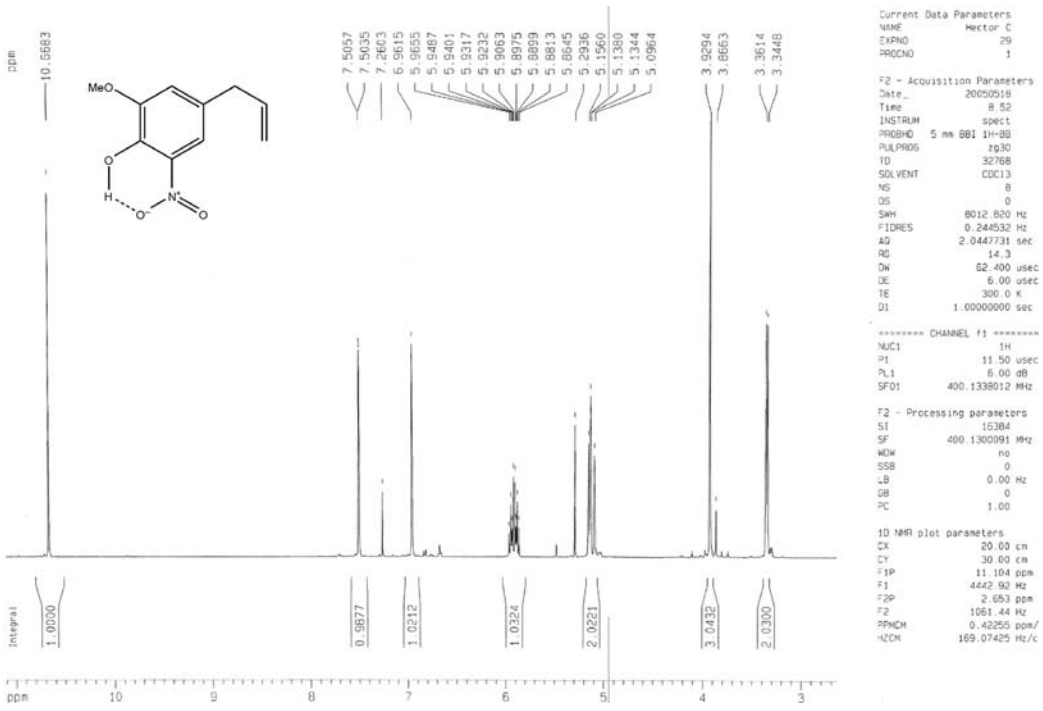
4-Allyl-2-methoxyphenyl acetate: In the pages S8-S9 we indicated the 1D & 2D NMR, HRMS, and IR spectra. IR spectra were recorded as thin film or KBr pellets in a Nicolet Impact 420 spectrometer. ν_{max} values are expressed in cm^{-1}. ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ solutions and referenced to the residual peak of $CHCl_3$ at δ 7.26 ppm and δ 77.00 ppm for ^1H and ^{13}C, respectively, on a Bruker Avance 400 Digital NMR spectrometer, operating at 400.1 MHz for ^1H and 100.6 MHz for ^{13}C. Chemical shifts are reported in δ ppm and coupling constants (*J*) are given in Hz. HRMS were recorder on a MAT 95XP, Thermo Finnigan spectrometer and represented at *m/z* (% rel. int.).

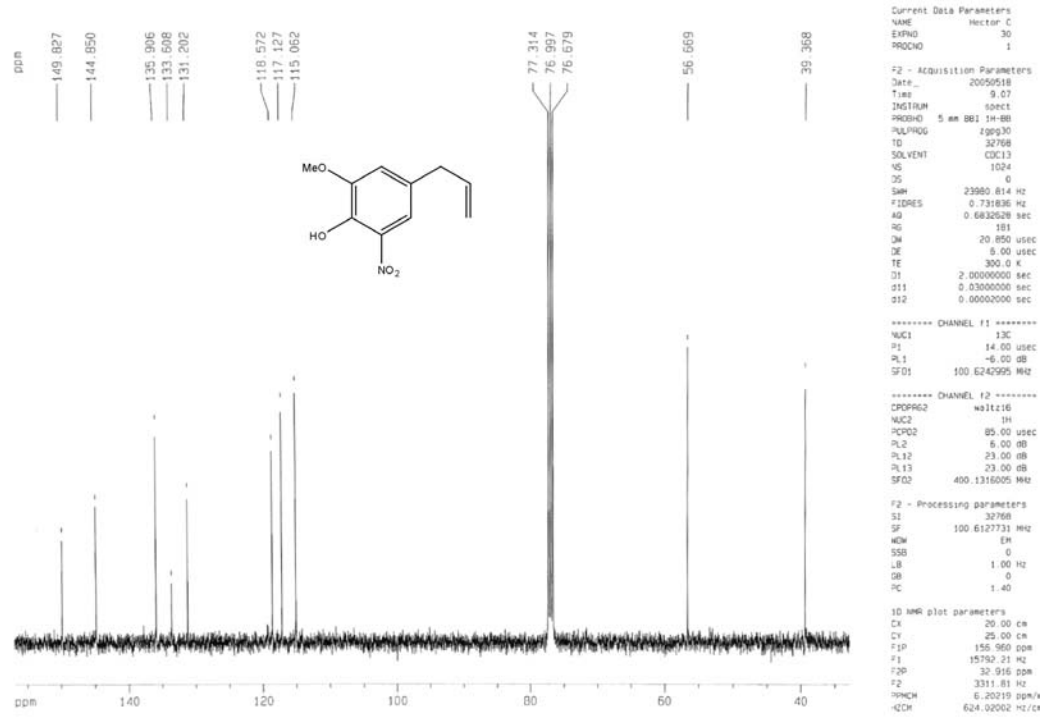
4-Allyl-2-methoxy-5-nitrophenyl acetate: In the pages S10-S11 we indicated the 1D & 2D NMR, HRMS, and IR spectra. IR spectra were recorded as thin film or KBr pellets in a Nicolet Impact 420 spectrometer. ν_{max} values are expressed in cm^{-1}. ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ solutions and referenced to the residual peak of $CHCl_3$ at δ 7.26 ppm and δ 77.00 ppm for ^1H and ^{13}C, respectively, on a Bruker Avance 400 Digital NMR spectrometer, operating at 400.1 MHz for ^1H and 100.6 MHz for ^{13}C. Chemical shifts are reported in δ ppm and coupling constants (*J*) are given in Hz. HRMS were recorder on a MAT 95XP, Thermo Finnigan spectrometer and represented at *m/z* (% rel. int.).

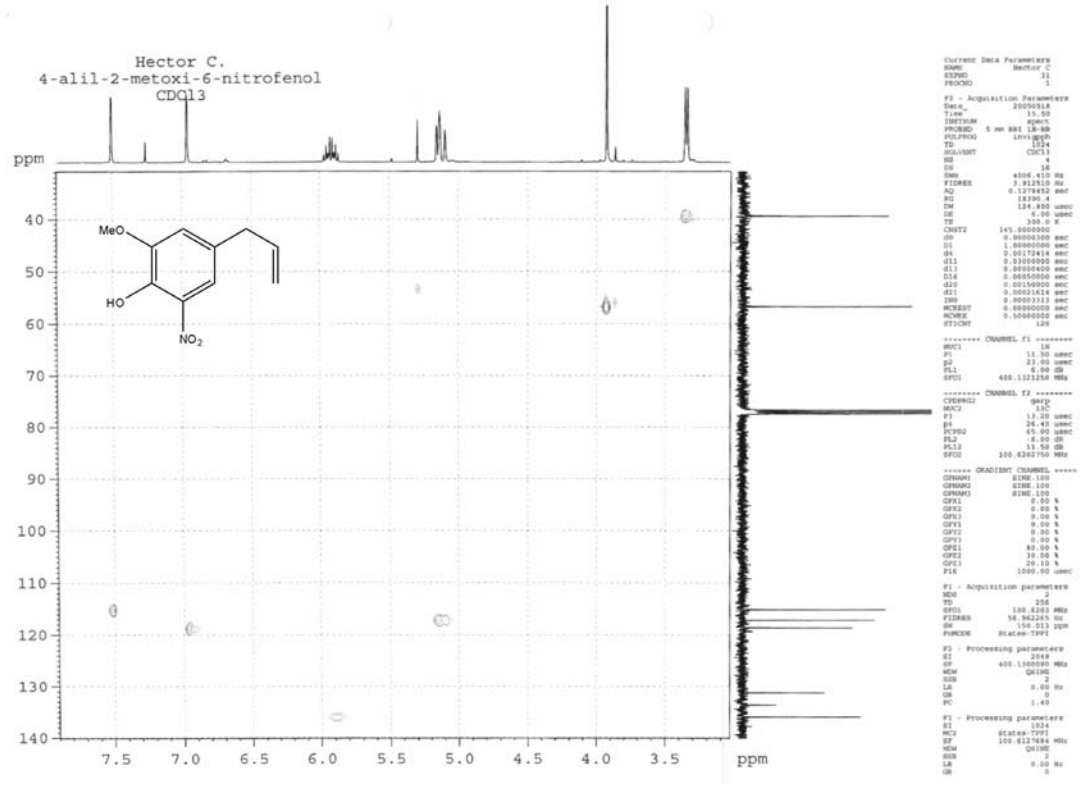
(E)-2-Methoxy-4-(prop-1-enyl) phenol: In the pages S12-S13 we indicated the 1D & 2D NMR, HRMS, and IR spectra. IR spectra were recorded as thin film or KBr pellets in a Nicolet Impact 420 spectrometer. ν_{max} values are expressed in cm^{-1}. ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ solutions and referenced to the

*e-mail: hcarrasco@unab.cl

residual peak of $CHCl_3$ at δ 7.26 ppm and δ 77.00 ppm for ^1H and ^{13}C, respectively, on a Bruker Avance 400 Digital NMR spectrometer, operating at 400.1 MHz for ^1H and 100.6 MHz for ^{13}C. Chemical shifts are reported in δ ppm and coupling constants (*J*) are given in Hz. HRMS were recorder on a MAT 95XP, Thermo Finnigan spectrometer and represented at *m/z* (% rel. int.).






Hector C.
4-alil-2-metoxi-6-nitrofenol
CDCl3
ppm
MeO
HO
NO2
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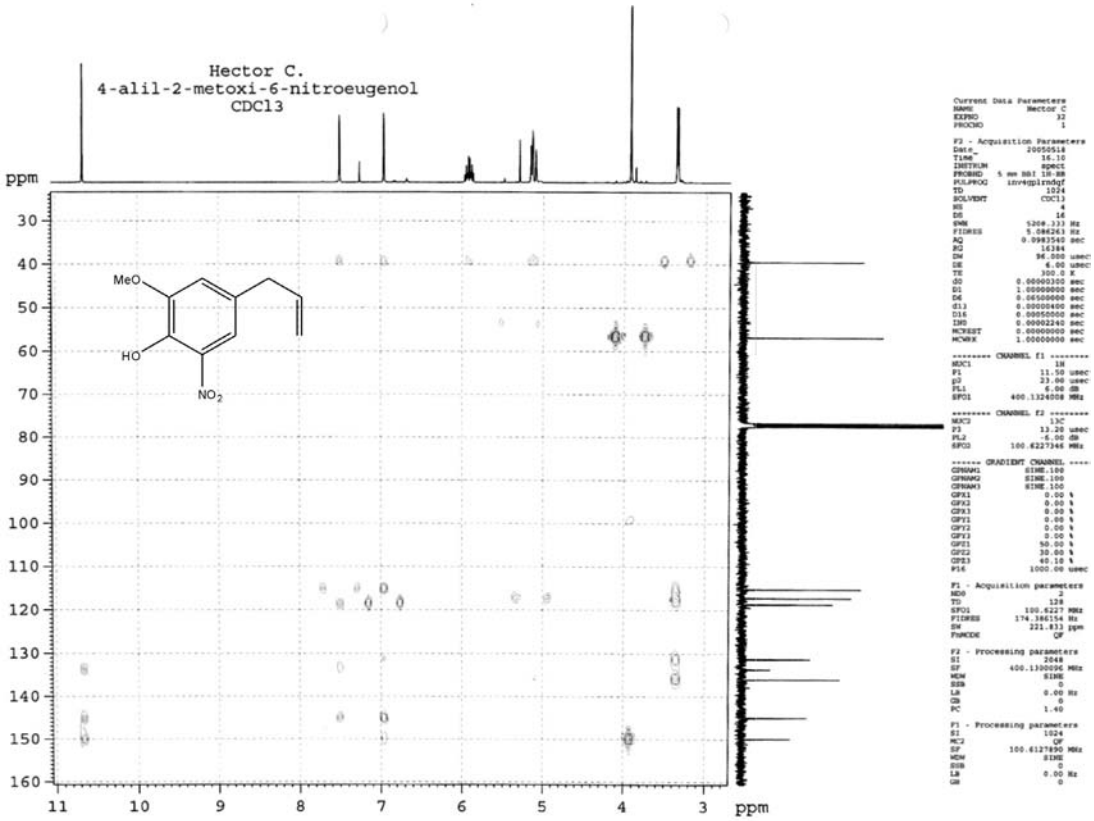
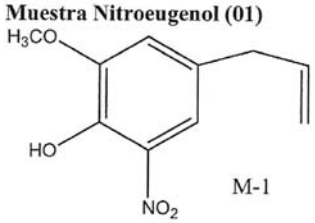
5.5
5.0
4.5
4.0
3.5
ppm


Hector C.
4-alil-2-metoxi-6-nitroeugenol
CDCl3
ppm
MeO
HO
NO2
11
10
9
8
7
6
5
4
3
ppm

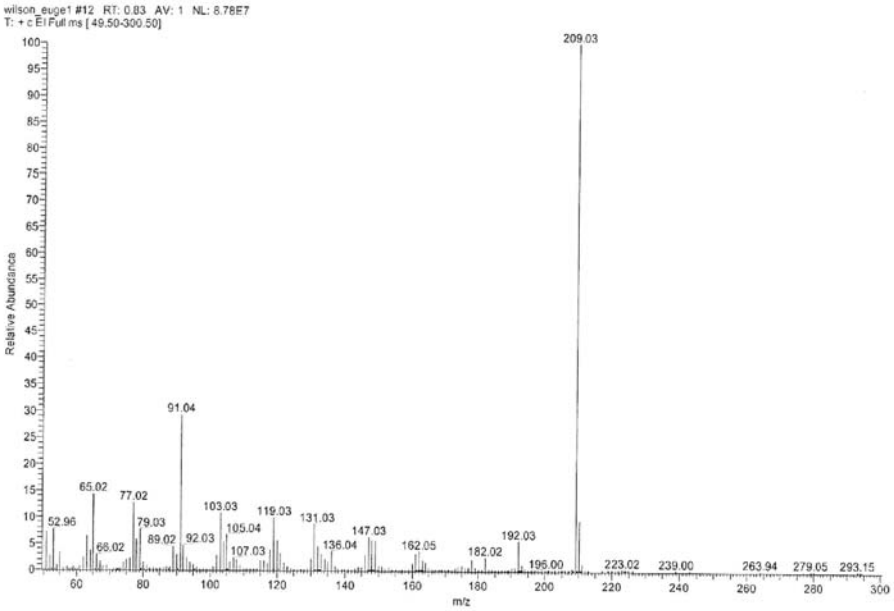
Muestra Nitroeugenol (01)

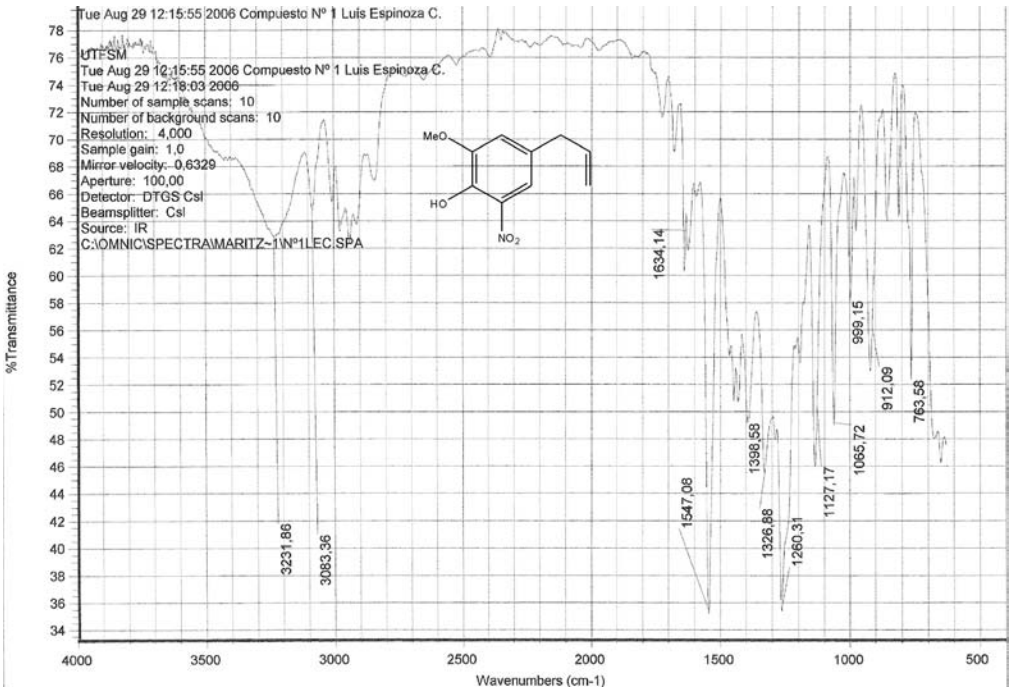


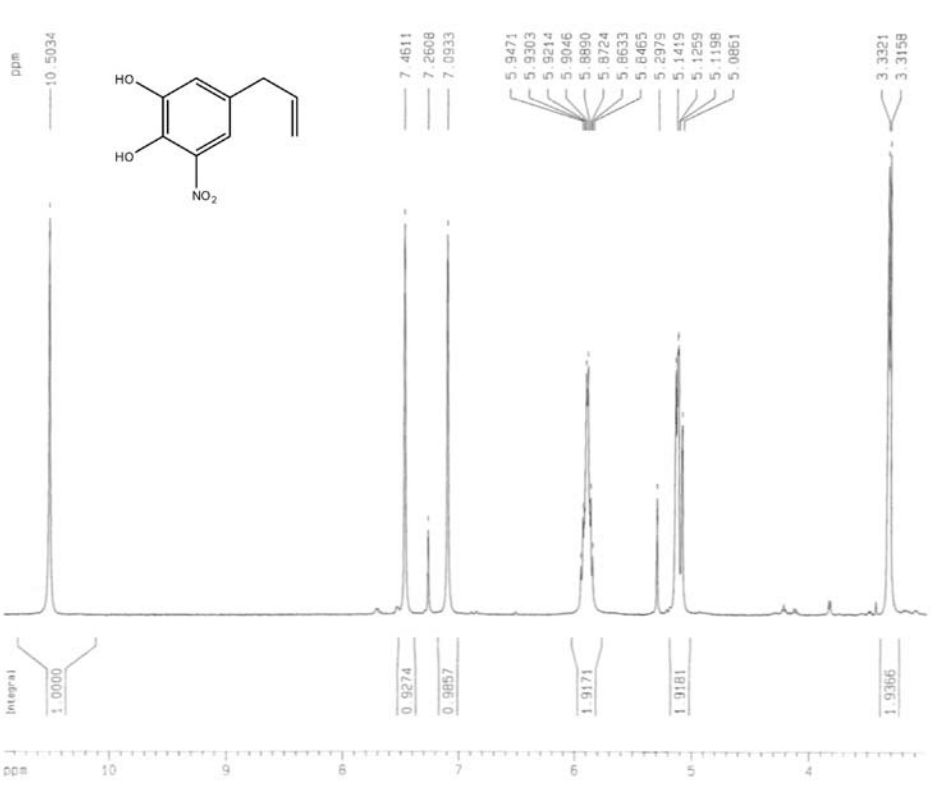
M-1

$C_{10}H_{11}NO_4$
Exact Mass: 209.06881
Mol. Wt.: 209.19868
C, 57.41; H, 5.30; N, 6.70; O, 30.59

Espectro impacto por electrones





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EXPNO                      35
PROCNO                      1

F2 - Acquisition Parameters
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Time                    5.13
INSTRUM                 spect
PROBHD   5 mm BBI 1H-BB
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                2.0447731 sec
RG                      14.3
DW                    62.400 usec
DE                     6.00 usec
TE                    300.0 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.50 usec
PL1                     6.00 dB
SFO1              400.1338012 MHz

F2 - Processing parameters
SI                         16384
SF                400.1300091 MHz
WDW                           no
SSB                            0
LB                      0.00 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                         20.00 cm
CY                         10.00 cm
F1P                        10.892 ppm
F1                       4358.37 Hz
F2P                        3.009 ppm
F2                       1203.81 Hz
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HZCM                   157.72789 Hz/cm
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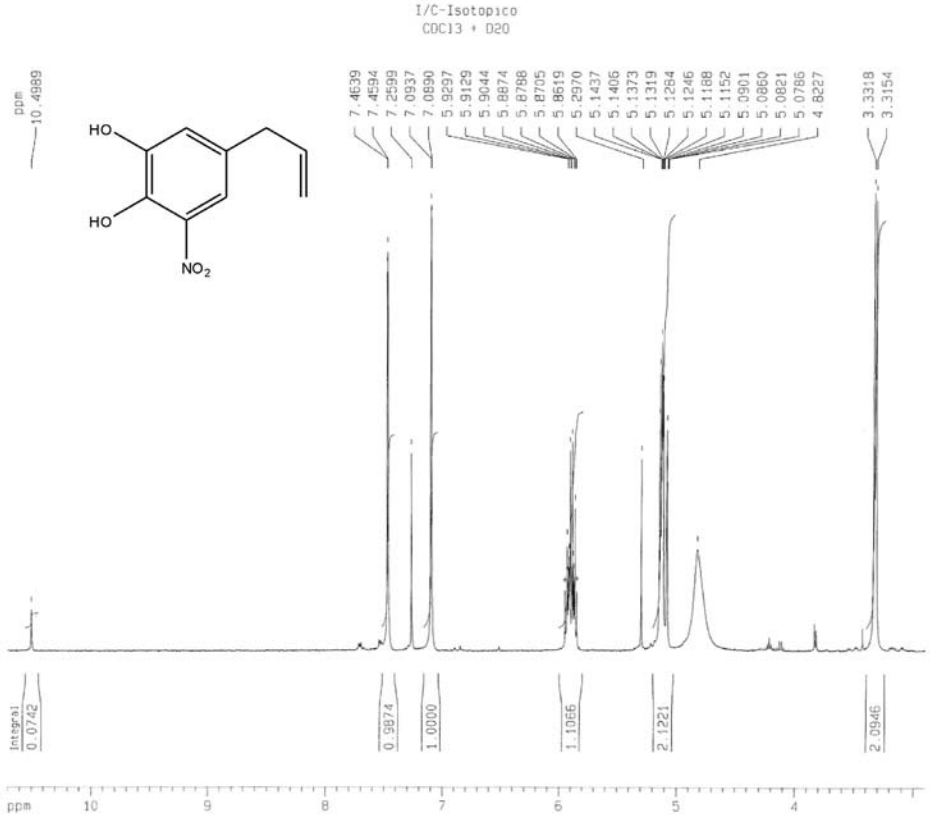


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EXPNO                      38
PROCNO                      1

F2 - Acquisition Parameters
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Time                    5.51
INSTRUM                 spect
PROBHD   5 mm BBI 1H-BB
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                2.0447731 sec
RG                      14.3
DW                    62.400 usec
DE                     6.00 usec
TE                    300.0 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.50 usec
PL1                     6.00 dB
SFO1              400.1338012 MHz

F2 - Processing parameters
SI                         16384
SF                400.1300096 MHz
WDW                           no
SSB                            0
LB                      0.00 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                         20.00 cm
CY                         10.00 cm
F1P                        10.700 ppm
F1                       4281.59 Hz
F2P                        2.905 ppm
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HZCM                   155.96432 Hz/cm
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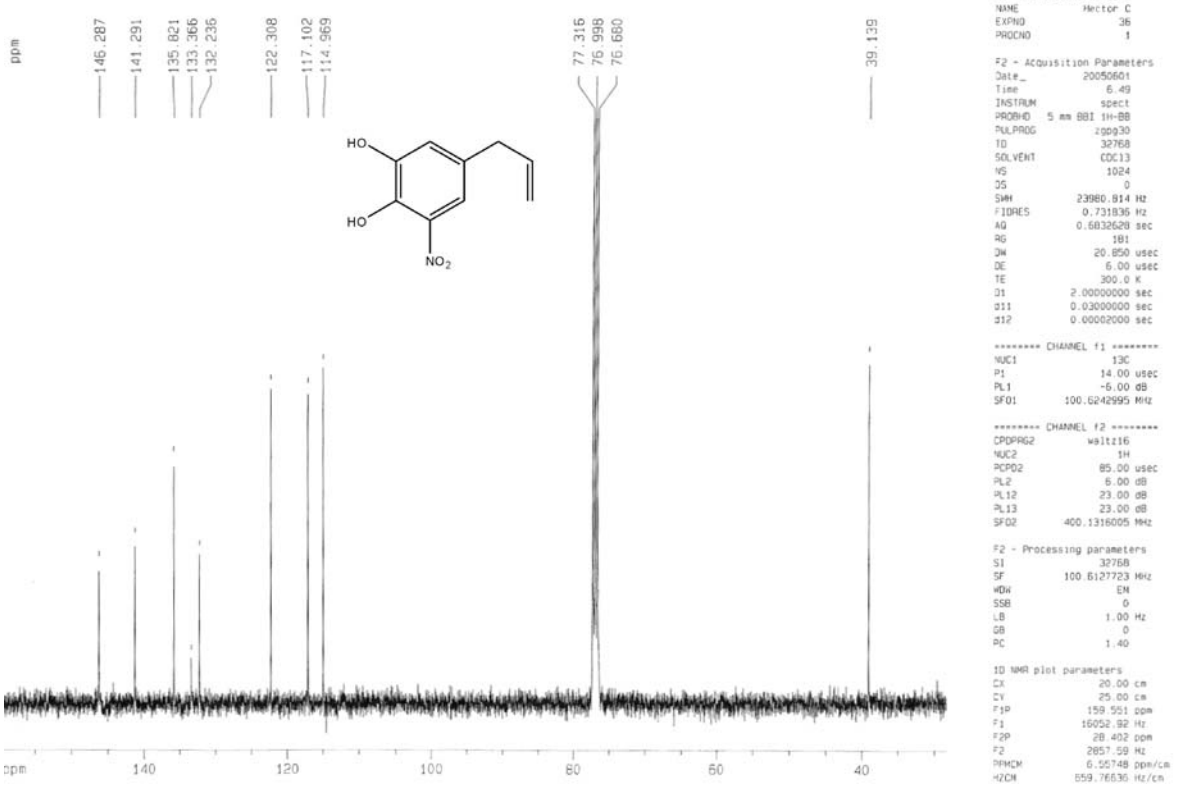


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Current Data Parameters
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EXPNO                 36
PROCNO                 1

F2 - Acquisition Parameters
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Time              6.49
INSTRUM           spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1024
DS                    0
SWH           23980.814 Hz
FIDRES        0.731836 Hz
AQ            0.6832620 sec
RG                  181
DW               20.850 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                14.00 usec
PL1               -6.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             85.00 usec
PL2               6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127723 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40

1D NMR plot parameters
CX                20.00 cm
CY                25.00 cm
F1P             159.551 ppm
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F2P              28.402 ppm
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HZCM          659.76636 Hz/cm
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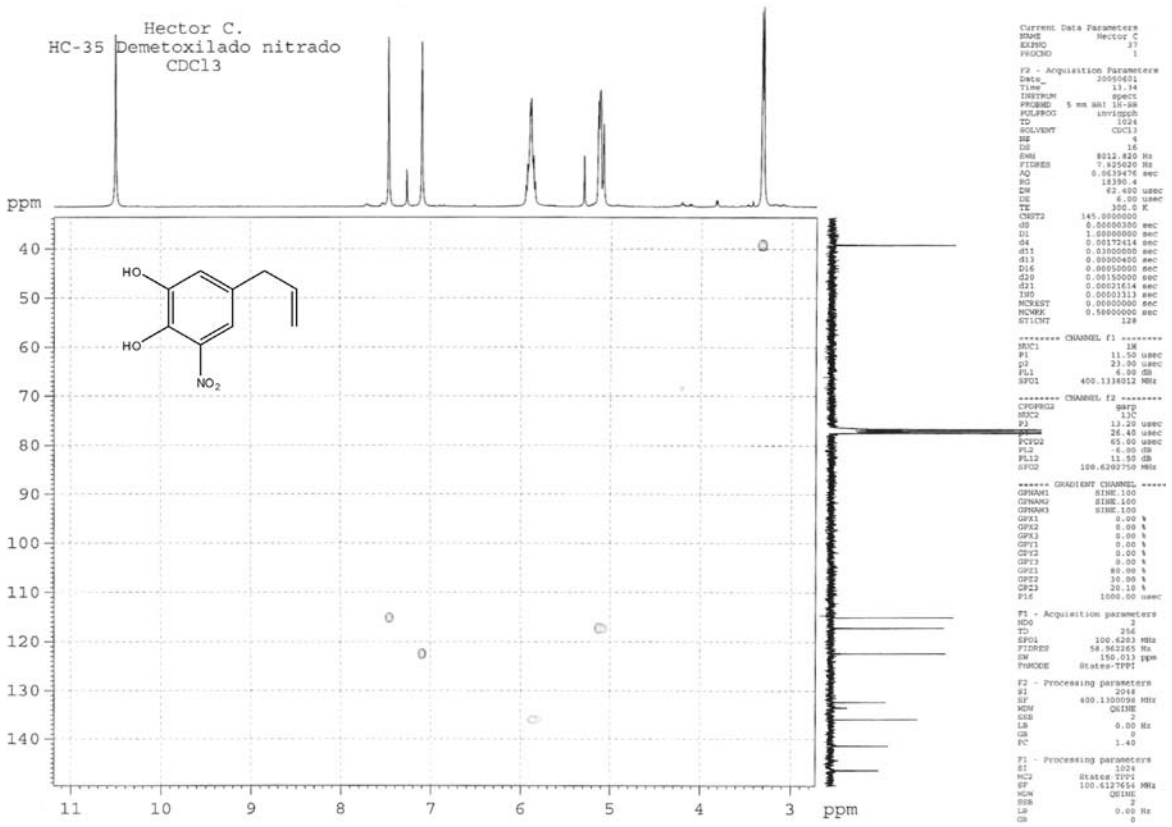


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Current Data Parameters
NAME            Hector C
EXPNO                 37
PROCNO                 1

F2 - Acquisition Parameters
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Time              13.34
INSTRUM           spect
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PULPROG       invigpph
TD                 1024
SOLVENT           CDCl3
NS                    4
DS                   16
SWH            8012.820 Hz
FIDRES         7.825620 Hz
AQ            0.0639476 sec
RG                18390.4
DW                62.400 usec
DE                6.00 usec
TE               300.0 K
CNST2        145.0000000
d0            0.00000300 sec
D1            1.00000000 sec
d4            0.00179214 sec
d11           0.03000000 sec
d13           0.00000400 sec
D16           0.00050000 sec
d20           0.00150000 sec
d21           0.00021614 sec
IN0           0.00003313 sec
MCREST        0.00000000 sec
MCWRK         0.50000000 sec
ST1CNT             128

======== CHANNEL f1 ========
NUC1                1H
P1                11.50 usec
p2                23.00 usec
PL1               6.00 dB
SFO1        400.1336012 MHz

======== CHANNEL f2 ========
CPDPRG2         garp
NUC2                13C
P3                13.20 usec
P4                26.40 usec
PCPD2             65.00 usec
PL2               -6.00 dB
PL12              11.50 dB
SFO2        100.6202750 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPX3                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPY3                0.00 %
GPZ1               80.00 %
GPZ2               30.00 %
GPZ3               20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
ND0                   2
TD                  256
SFO1        100.6203 MHz
FIDRES        58.962265 Hz
SW            159.013 ppm
FnMODE      States-TPPI

F2 - Processing parameters
SI                 2048
SF          400.1300096 MHz
WDW                QSINE
SSB                   2
LB                0.00 Hz
GB                    0
PC                1.40

F1 - Processing parameters
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MC2         States-TPPI
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SSB                   2
LB                0.00 Hz
GB                    0
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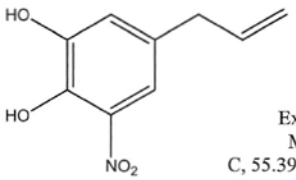
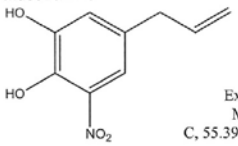


$C_9H_9NO_4$
Exact Mass: 195.05316
Mol. Wt.: 195.17210
C, 55.39; H, 4.65; N, 7.18; O, 32.79

Muestra W-3

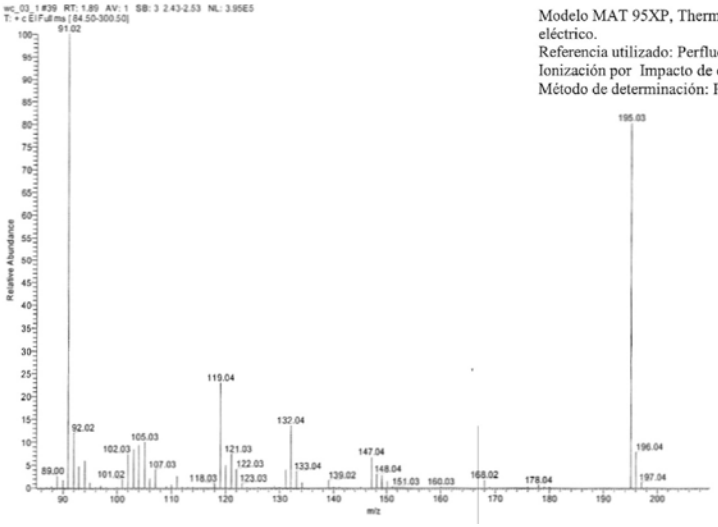


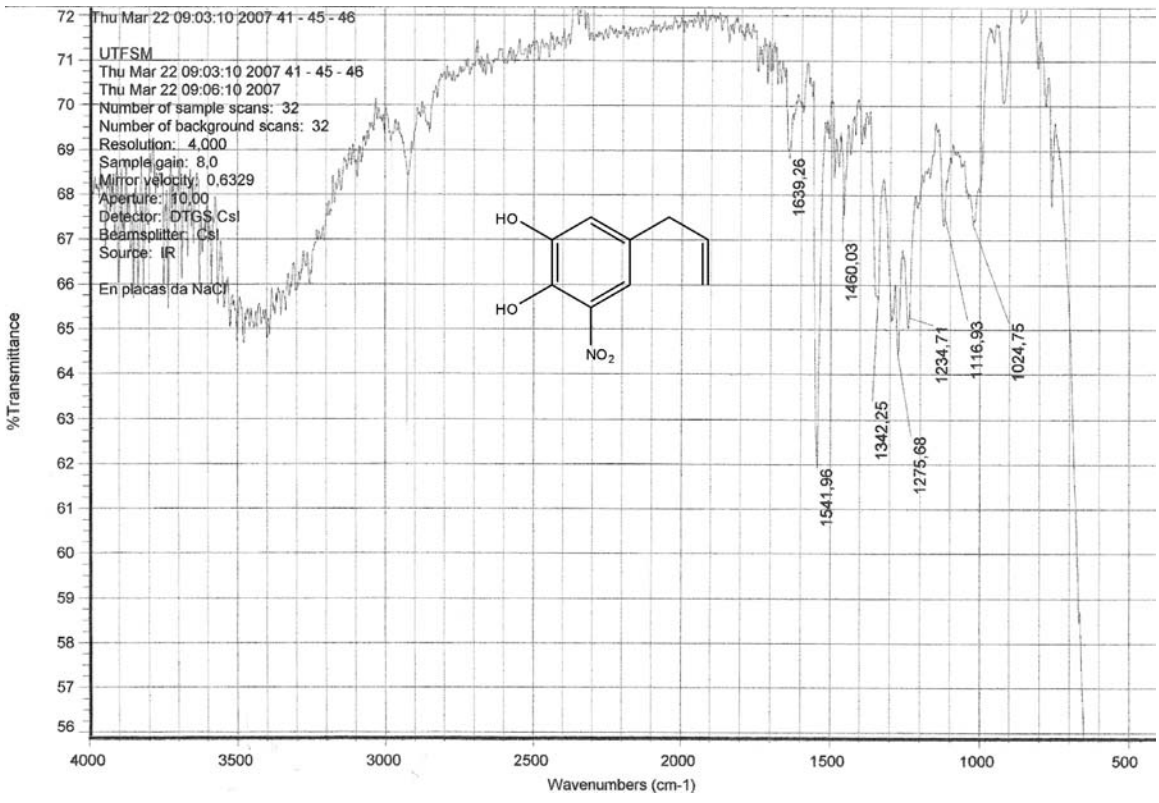
$C_9H_9NO_4$
Exact Mass: 195.05316
Mol. Wt.: 195.17210
C, 55.39; H, 4.65; N, 7.18; O, 32.79

Compuesto	Formula	Masa Exacta Calculada	Masa experimental	Error / ppm
W-3	$C_9H_9NO_4$	195.05316	195.05241	3.8

Especificaciones del espectrómetro de masas:

Modelo MAT 95XP, Thermo Finnigan. Analizador de doble enfoque, sector magnético y eléctrico.
Referencia utilizado: Perfluoroterbutil amina (FC43).
Ionización por Impacto de electrones, EI.
Método de determinación: Peak-matching



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PROCNO                       1

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Time                    4.17
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PULPROG                 zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  2.0447731 sec
RG                      574.7
DW                     62.400 usec
DE                      6.00 usec
TE                     300.0 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      11.50 usec
PL1                      6.00 dB
SFO1             400.1338012 MHz

F2 - Processing parameters
SI                      16384
SF                400.1300091 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      12.00 cm
F1P                      8.051 ppm
F1                    3221.60 Hz
F2P                      2.024 ppm
F2                     810.02 Hz
PPMCM                 0.30135 ppm/cm
HZCM                120.57881 Hz/cm
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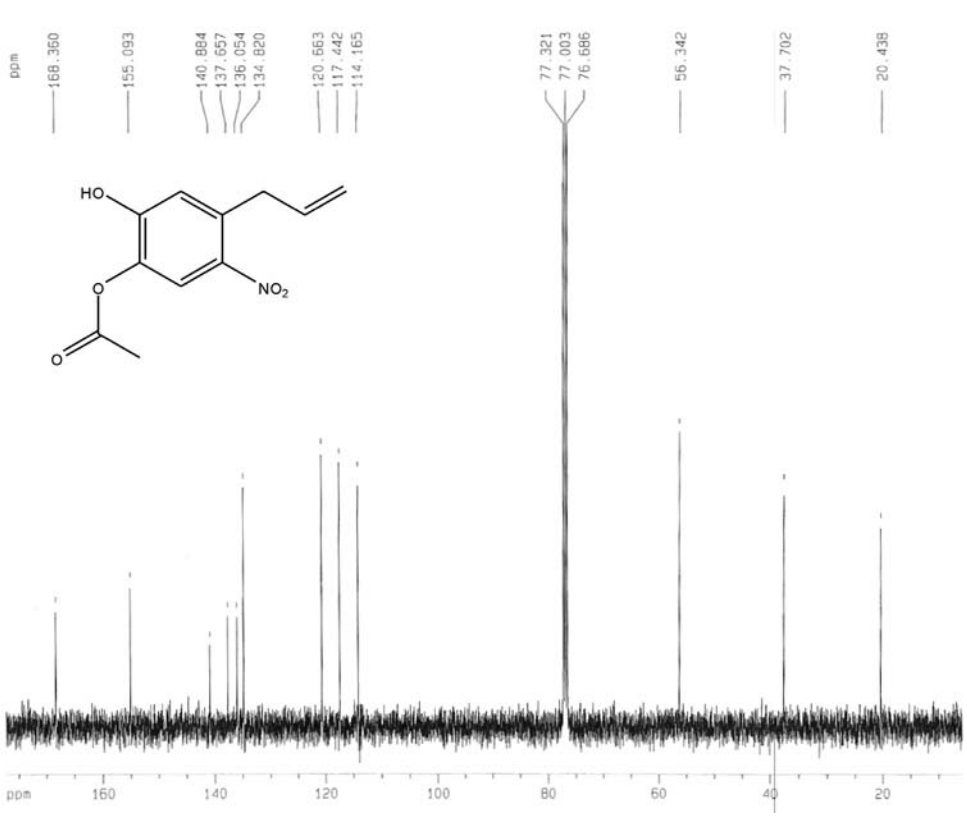


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Current Data Parameters
NAME                  Hector C
EXPNO                       42
PROCNO                       1

F2 - Acquisition Parameters
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Time                    4.23
INSTRUM                 spect
PROBHD   5 mm BBI 1H-BB
PULPROG                 zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        512
DS                          0
SWH                23980.814 Hz
FIDRES              0.731836 Hz
AQ                  0.6832628 sec
RG                        181
DW                     20.850 usec
DE                      6.00 usec
TE                     300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                      14.00 usec
PL1                      -6.00 dB
SFO1             100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   85.00 usec
PL2                      6.00 dB
PL12                    23.00 dB
PL13                    23.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF                100.6127731 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
CY                      25.00 cm
F1P                   177.300 ppm
F1                  17838.65 Hz
F2P                     5.988 ppm
F2                     602.44 Hz
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HZCM                861.81055 Hz/cm
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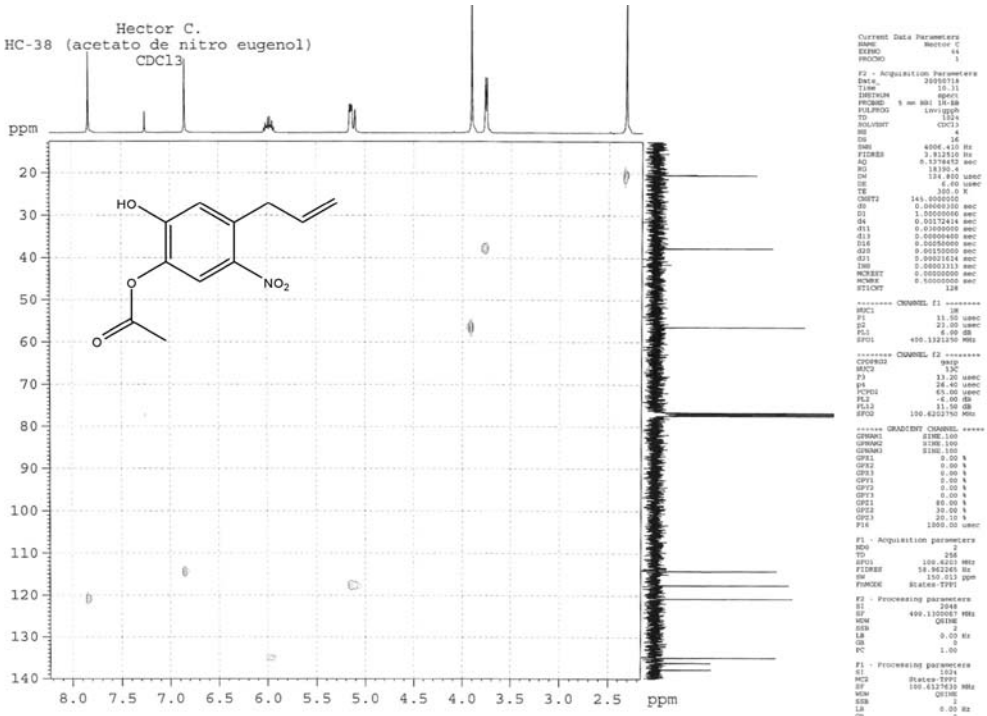
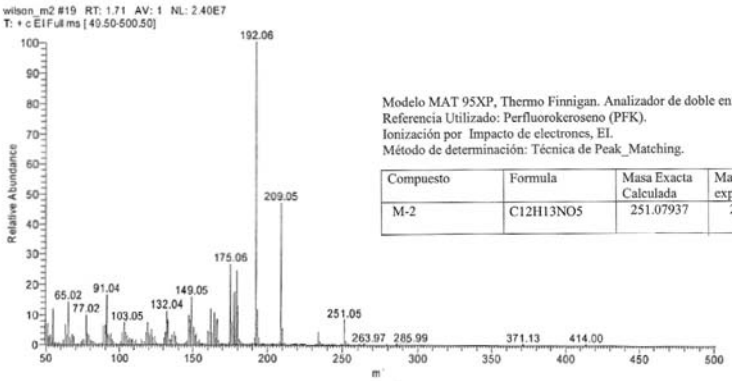
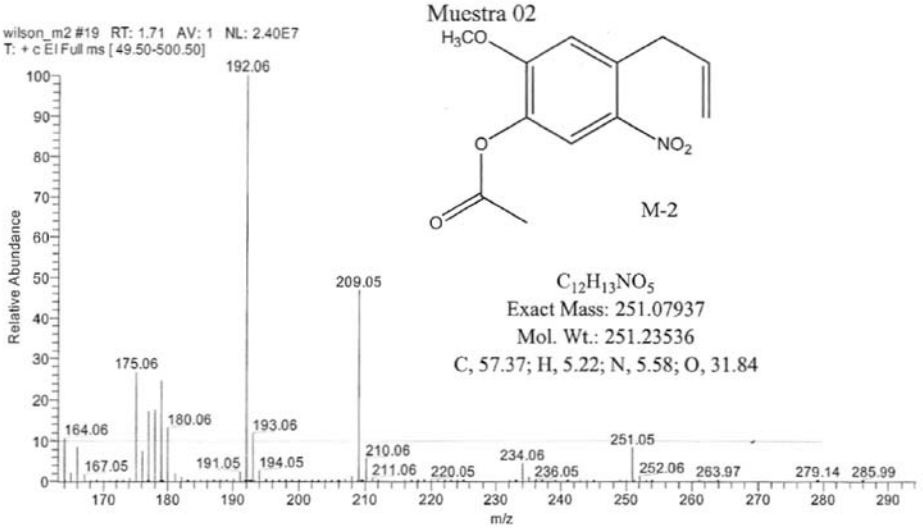




Modelo MAT 95XP, Thermo Finnigan. Analizador de doble enfoque, sector magnético y eléctrico.
Referencia Utilizado: Perfluorokeroseno (PFK).
Ionización por Impacto de electrones, EI.
Método de determinación: Técnica de Peak_Matching.

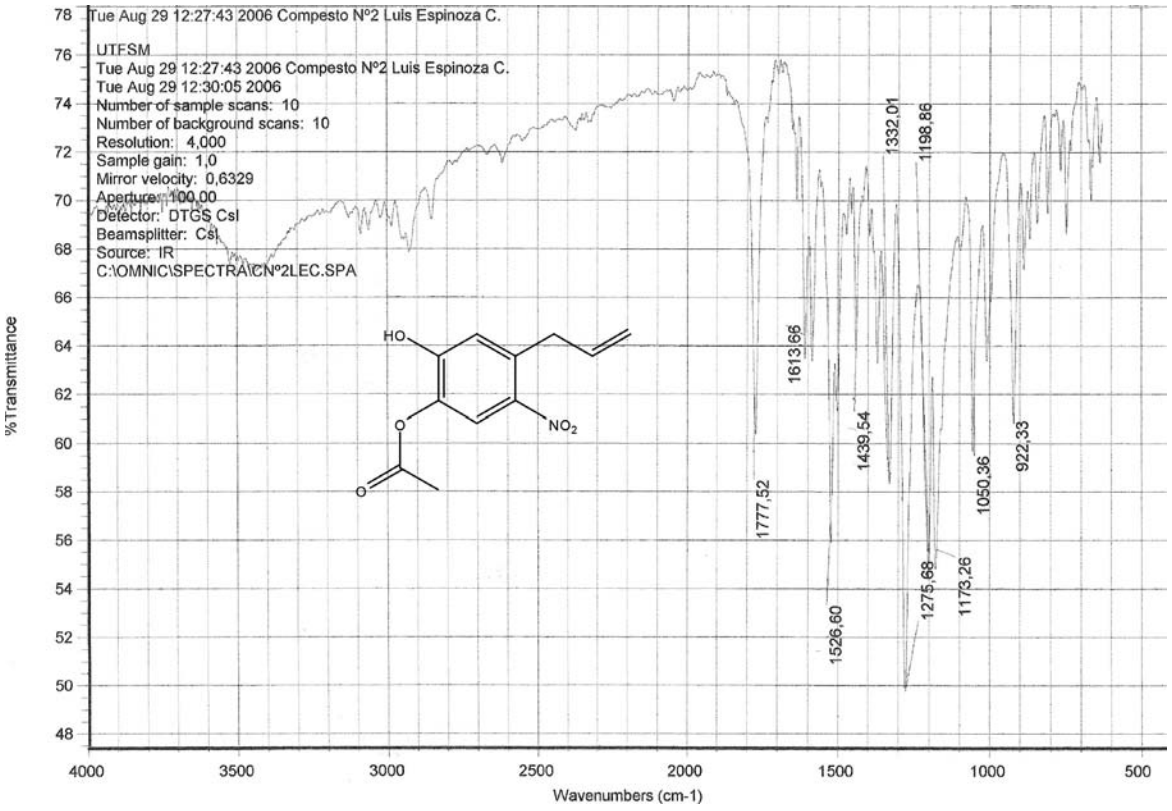
Compuesto	Formula	Masa Exacta Calculada	Masa experimental	Error / ppm
M-2	C12H13NO5	251.07937	251.07273	26.5

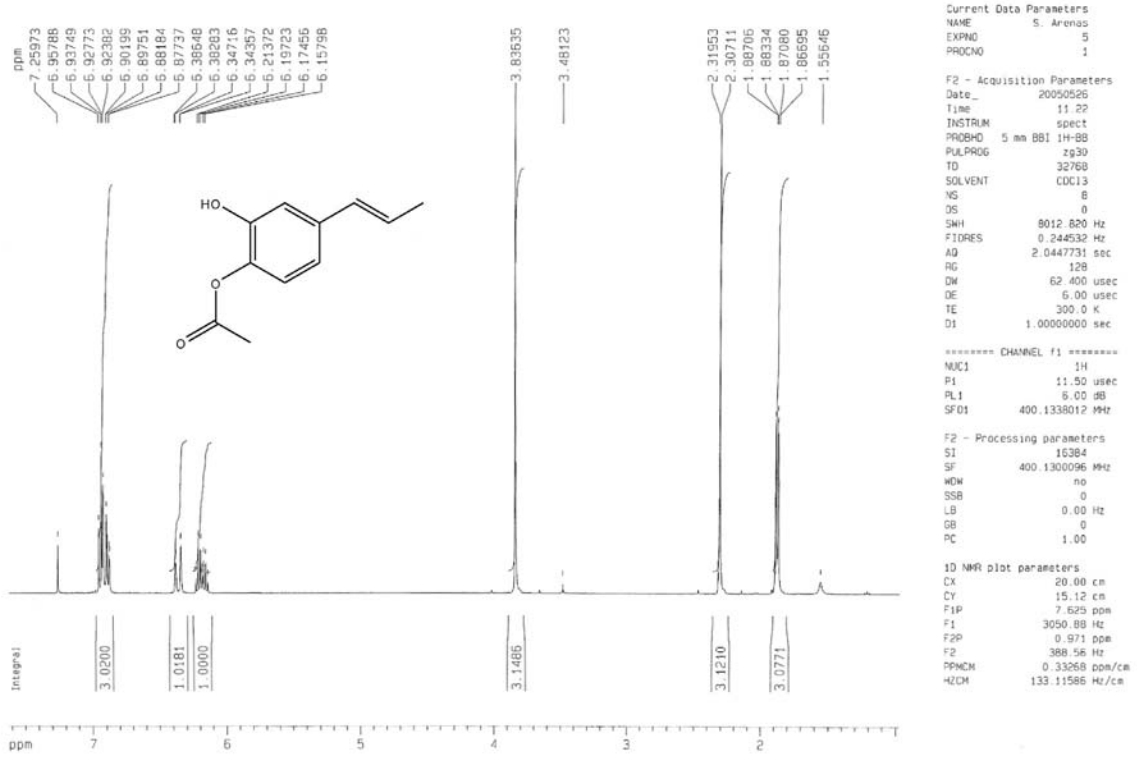


Muestra 02

M-2

$C_{12}H_{13}NO_5$
Exact Mass: 251.07937
Mol. Wt.: 251.23536
C, 57.37; H, 5.22; N, 5.58; O, 31.84



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Current Data Parameters
NAME          S. Arenas
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20050526
Time              11.22
INSTRUM           spect
PROBHD  5 mm BBI 1H-BB
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            2.0447731 sec
RG                 128
DW              62.400 usec
DE               6.00 usec
TE              300.0 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                11.50 usec
PL1               6.00 dB
SF01        400.1338012 MHz

F2 - Processing parameters
SI                16384
SF          400.1300096 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                15.12 cm
F1P               7.625 ppm
F1              3050.88 Hz
F2P               0.971 ppm
F2               388.56 Hz
PPMCM          0.33268 ppm/cm
HZCM          133.11586 Hz/cm
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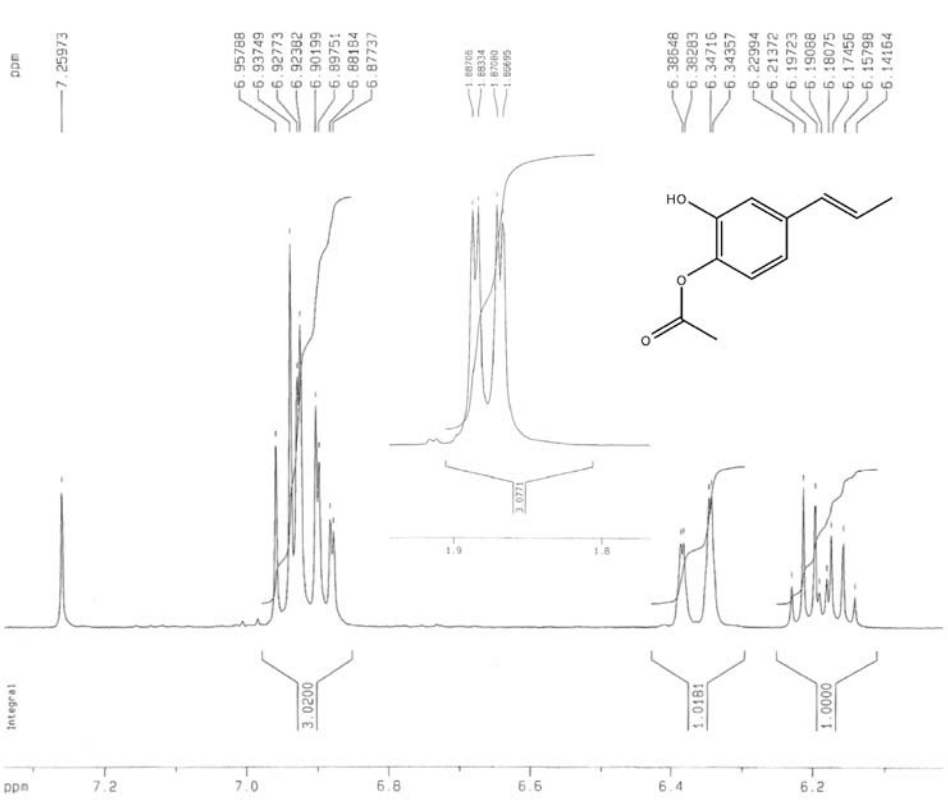


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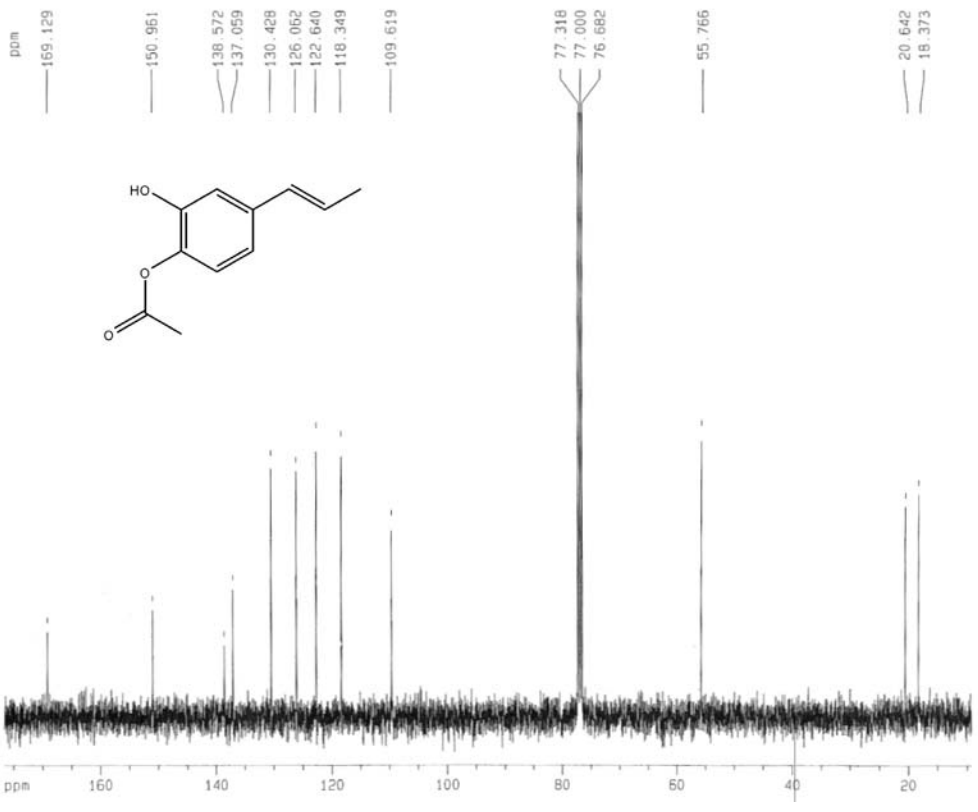
Current Data Parameters
NAME                  S. Arenas
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20050526
Time                      11.22
INSTRUM                   spect
PROBHD    5 mm BBI 1H-BB
PULPROG                    zg30
TD                        32768
SOLVENT                   CDCl3
NS                            8
DS                            0
SWH                  8012.820 Hz
FIDRES               0.244532 Hz
AQ                   2.0447731 sec
RG                          128
DW                     62.400 usec
DE                      6.00 usec
TE                     300.0 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                     11.50 usec
PL1                     6.00 dB
SF01               400.1338012 MHz

F2 - Processing parameters
SI                        16384
SF                 400.1300096 MHz
WDW                          no
SSB                           0
LB                     0.00 Hz
GB                            0
PC                         1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       40.00 cm
F1P                       7.341 ppm
F1                     2937.17 Hz
F2P                       6.019 ppm
F2                     2408.32 Hz
PPMCM                 0.06609 ppm/cm
HZCM                 26.44268 Hz/cm
```




```
Current Data Parameters
NAME                  S. Arenas
EXPNO                         6
PROCNO                        1

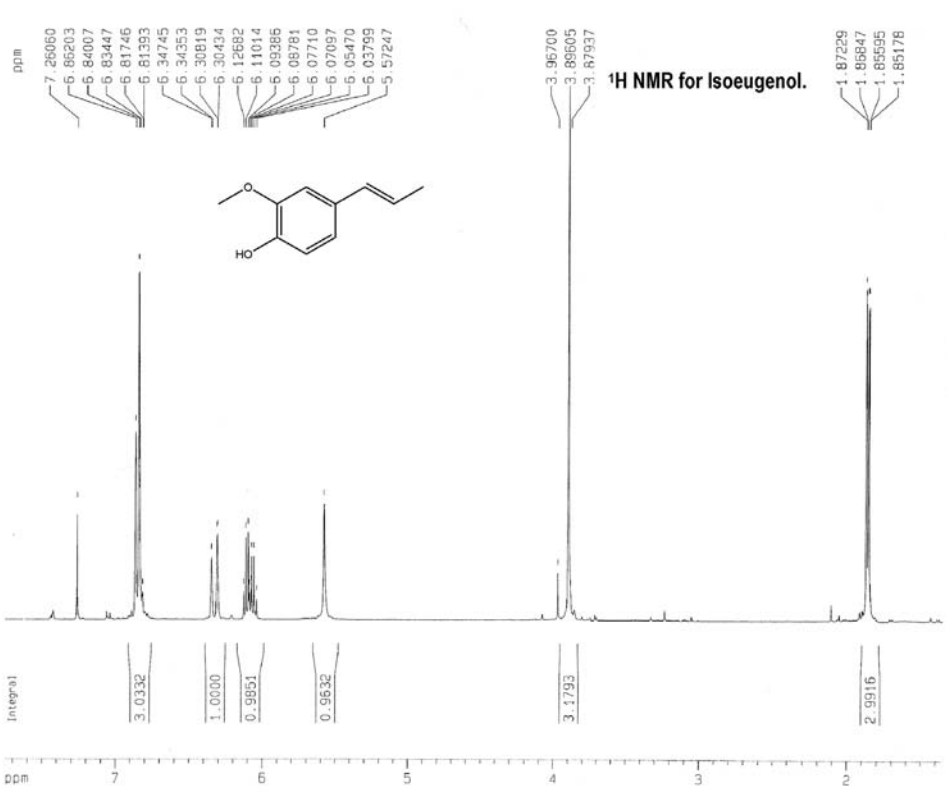
F2 - Acquisition Parameters
Date_                  20050526
Time                      11.30
INSTRUM                   spect
PROBHD    5 mm BBI 1H-BB
PULPROG                 zgpg30
TD                        32768
SOLVENT                   CDCl3
NS                          512
DS                            0
SWH                 23980.814 Hz
FIDRES               0.731836 Hz
AQ                   0.6832628 sec
RG                          181
DW                     20.850 usec
DE                      6.00 usec
TE                     300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                     14.00 usec
PL1                    -6.00 dB
SF01               100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                  85.00 usec
PL2                     6.00 dB
PL12                   23.00 dB
PL13                   23.00 dB
SF02               400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127723 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                       20.00 cm
CY                       25.00 cm
F1P                     176.564 ppm
F1                     17764.55 Hz
F2P                       9.239 ppm
F2                     929.53 Hz
PPMCM                 8.36624 ppm/cm
HZCM                 841.75079 Hz/cm
```



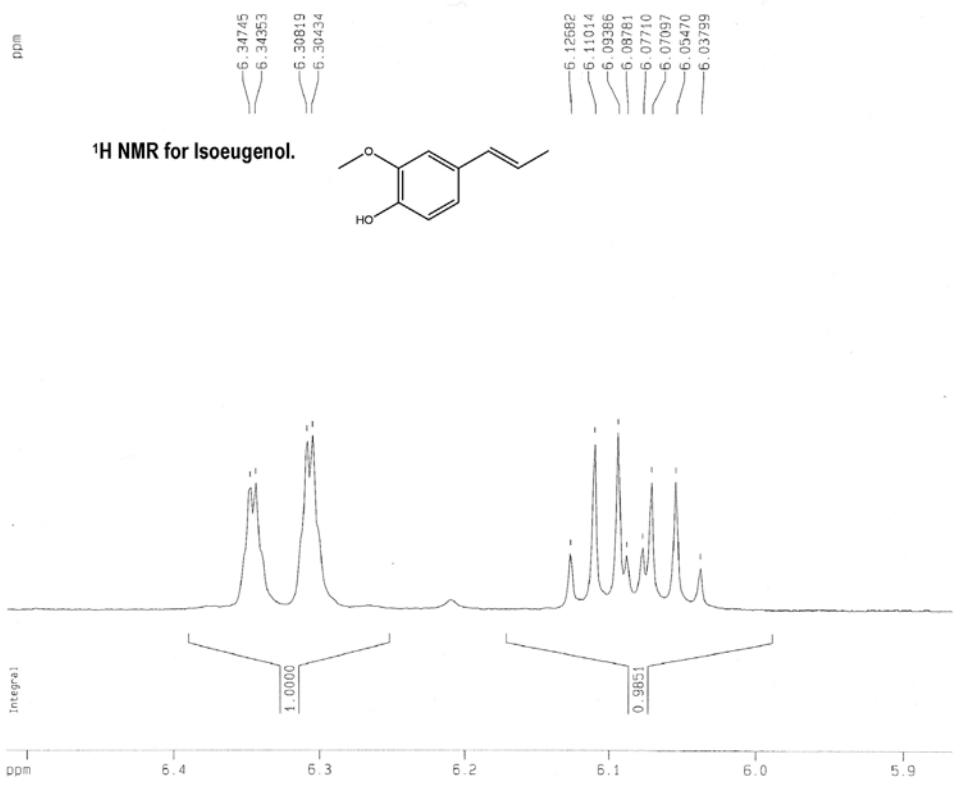

```
Current Data Parameters
NAME            S. Arenas
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050610
Time                6.21
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              2.0447731 sec
RG                  14.3
DW                62.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.50 usec
PL1                 6.00 dB
SFO1          400.1338012 MHz

F2 - Processing parameters
SI                 16384
SF            400.1300091 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 25.00 cm
F1P                 7.752 ppm
F1                3101.69 Hz
F2P                 1.353 ppm
F2                 541.26 Hz
PPMCM           0.31995 ppm/cm
HZCM          128.02173 Hz/cm
```



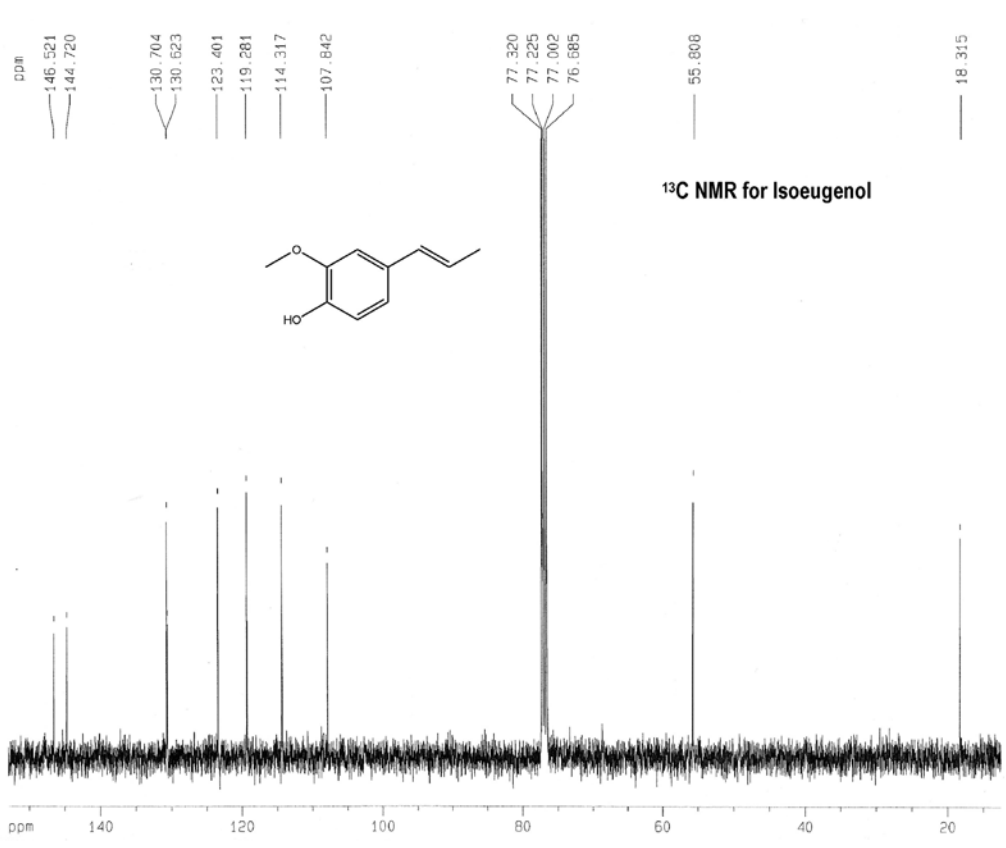

```
Current Data Parameters
NAME            S. Arenas
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050610
Time                6.21
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              2.0447731 sec
RG                  14.3
DW                62.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.50 usec
PL1                 6.00 dB
SFO1          400.1338012 MHz

F2 - Processing parameters
SI                 16384
SF            400.1300091 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 50.00 cm
F1P                 6.514 ppm
F1                2606.45 Hz
F2P                 5.866 ppm
F2                2347.30 Hz
PPMCM           0.03238 ppm/cm
HZCM          12.95759 Hz/cm
```




```
Current Data Parameters
NAME                  S. Arenas
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_               20050610
Time                     6.27
INSTRUM                  spect
PROBHD     5 mm BBI 1H-BB
PULPROG                zgpg30
TD                      32768
SOLVENT                  CDCl3
NS                         512
DS                           0
SWH                23980.814 Hz
FIDRES              0.731836 Hz
AQ                  0.6832628 sec
RG                         181
DW                    20.850 usec
DE                     6.00 usec
TE                     300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
d12               0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                    14.00 usec
PL1                    -6.00 dB
SFO1              100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                 85.00 usec
PL2                    6.00 dB
PL12                  23.00 dB
PL13                  23.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                100.6127723 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       20.00 cm
CY                       25.00 cm
F1P                     152.957 ppm
F1                    15389.42 Hz
F2P                      12.584 ppm
F2                     1266.10 Hz
PPMCM                  7.01865 ppm/cm
HZCM                 706.16589 Hz/cm
```