Supporting Information

Indium Tri(isopropoxide)-Catalyzed Selective Meerwein-Ponndorf-Verley Reduction of Aliphatic and Aromatic Aldehydes

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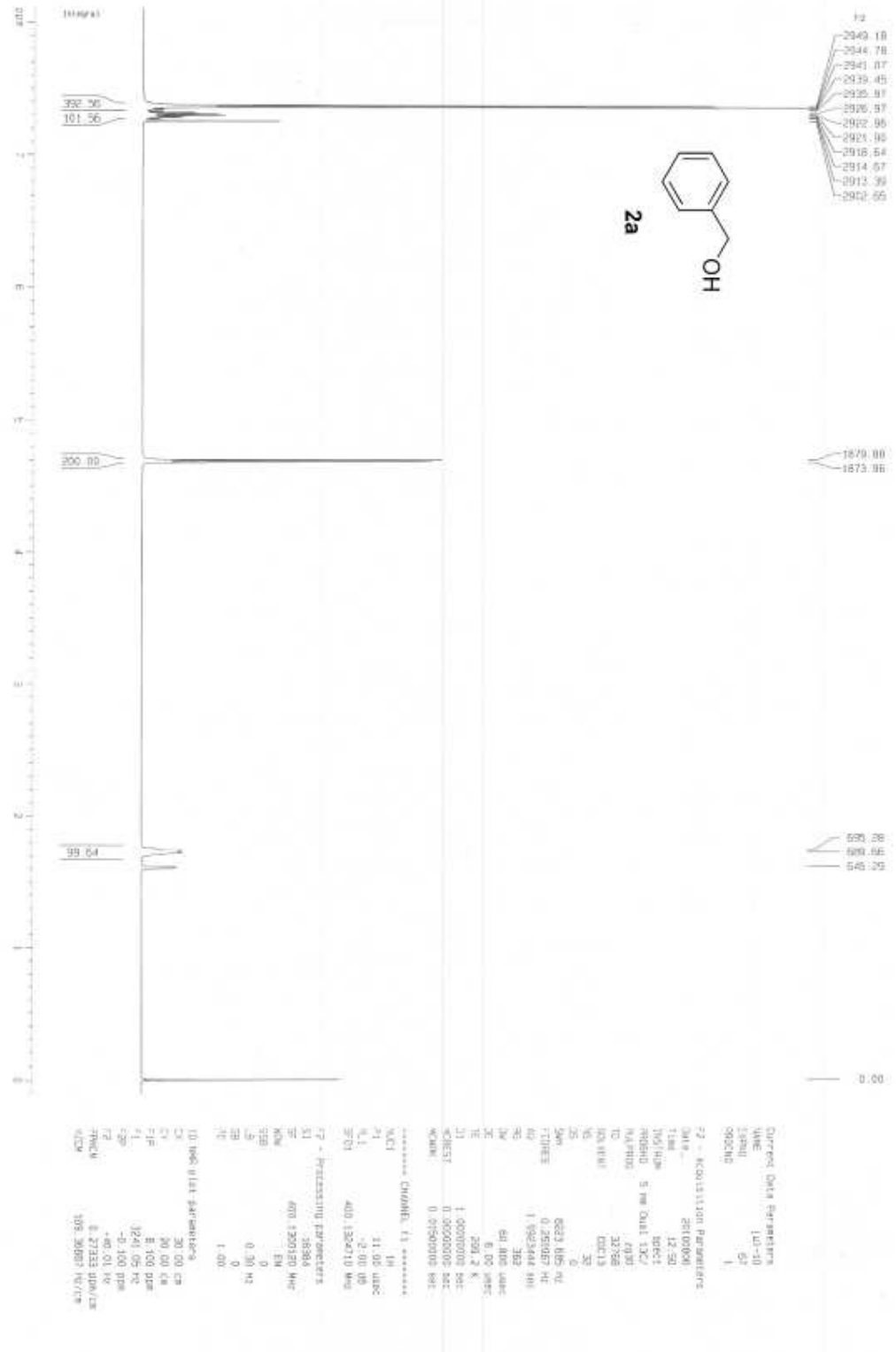
Table of Contents

1. General ····· **S2**

2. ^{1}H and ^{13}C NMR spectra of products ····· **S3 - S56**

Experimental Section

General: Reactions were carried out in oven-dried glassware under nitrogen atmosphere. All commercial reagents were used without purification, and all solvents were reaction grade. 2-Propanol was freshly distilled from calcium hydride. All reaction mixtures were stirred magnetically and were monitored by thin-layer chromatography using silica gel precoated glass plates, which were visualized with UV light and then developed using a solution of anisaldehyde. Flash column chromatography was carried out using silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. Deuterated chloroform was used as the NMR solvent. The chemical shift values (δ) are reported in parts per million relative to the residual signals of these solvents ($CDCl_3$: δ 7.24 for ^{1}H and δ 77.0 for ^{13}C). Infrared spectra were recorded on a FT-IR spectrometer using two sodium chloride plates.


2a
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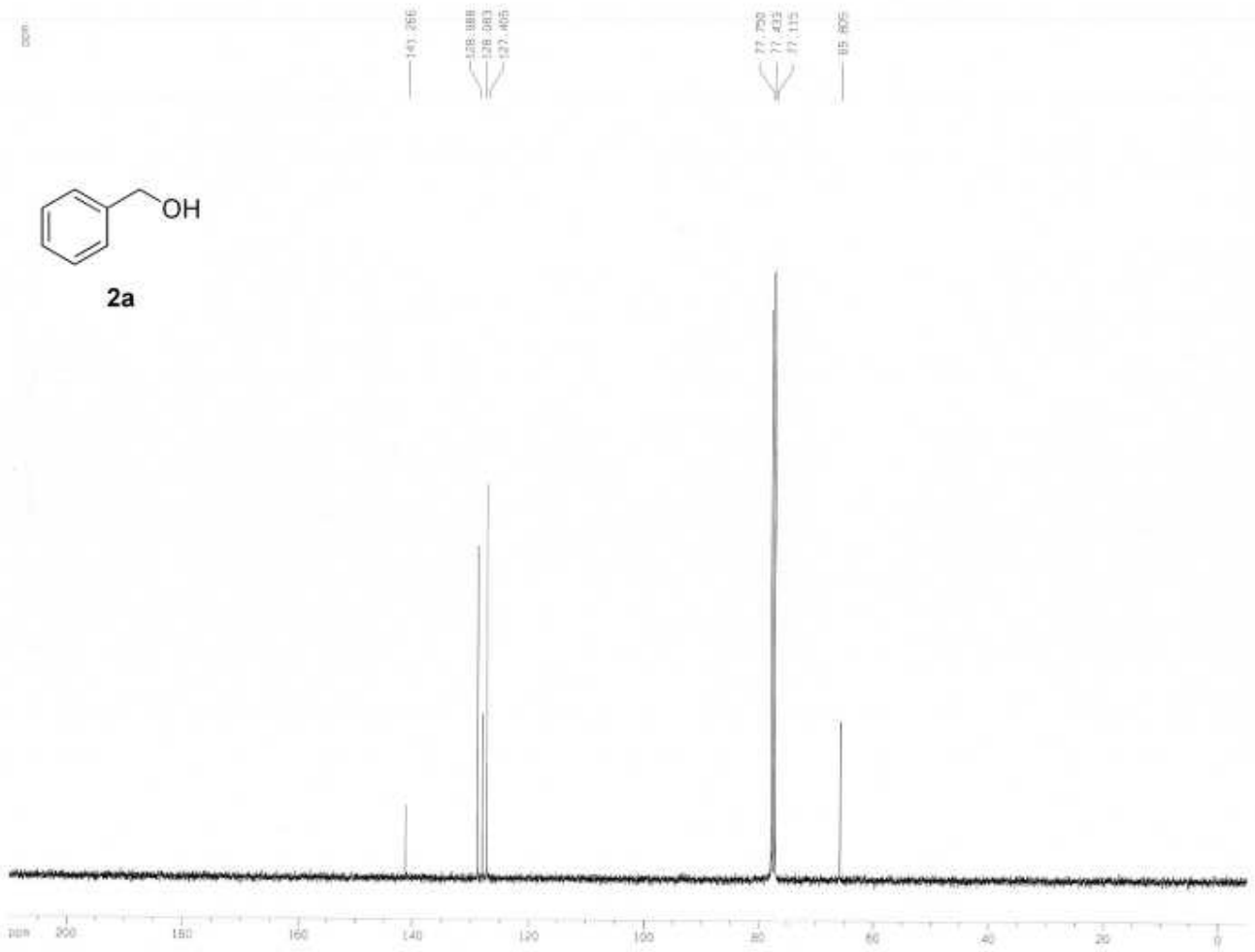


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PL1                    -1.00 dB
SFO1           100.6254358 MHz

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PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
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PC                      1.40

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CY                     15.00 cm
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F1                 21128.67 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.16667 ppm/cm
HZCM               721.05786 Hz/cm
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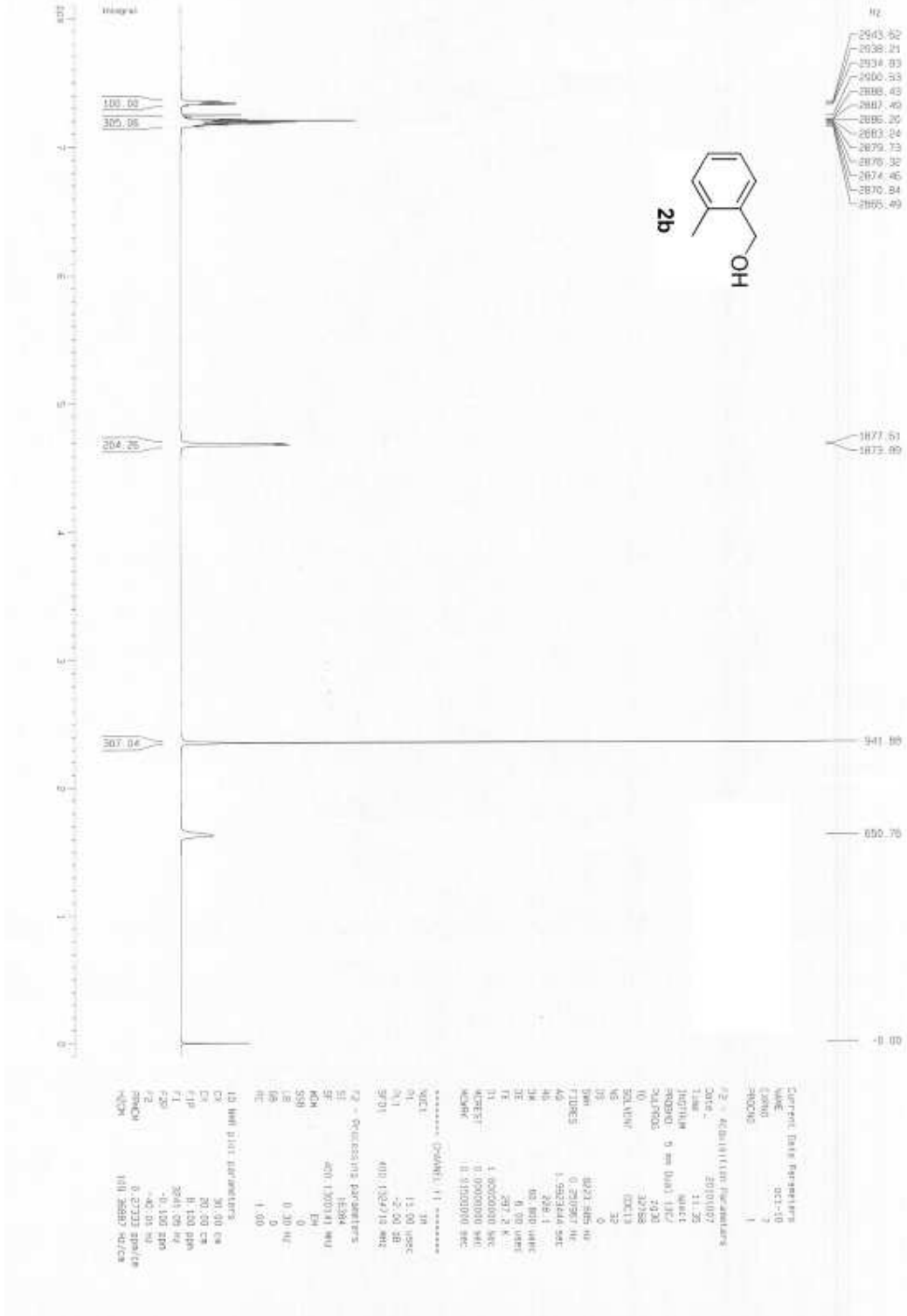
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2887.49
2886.20
2883.24
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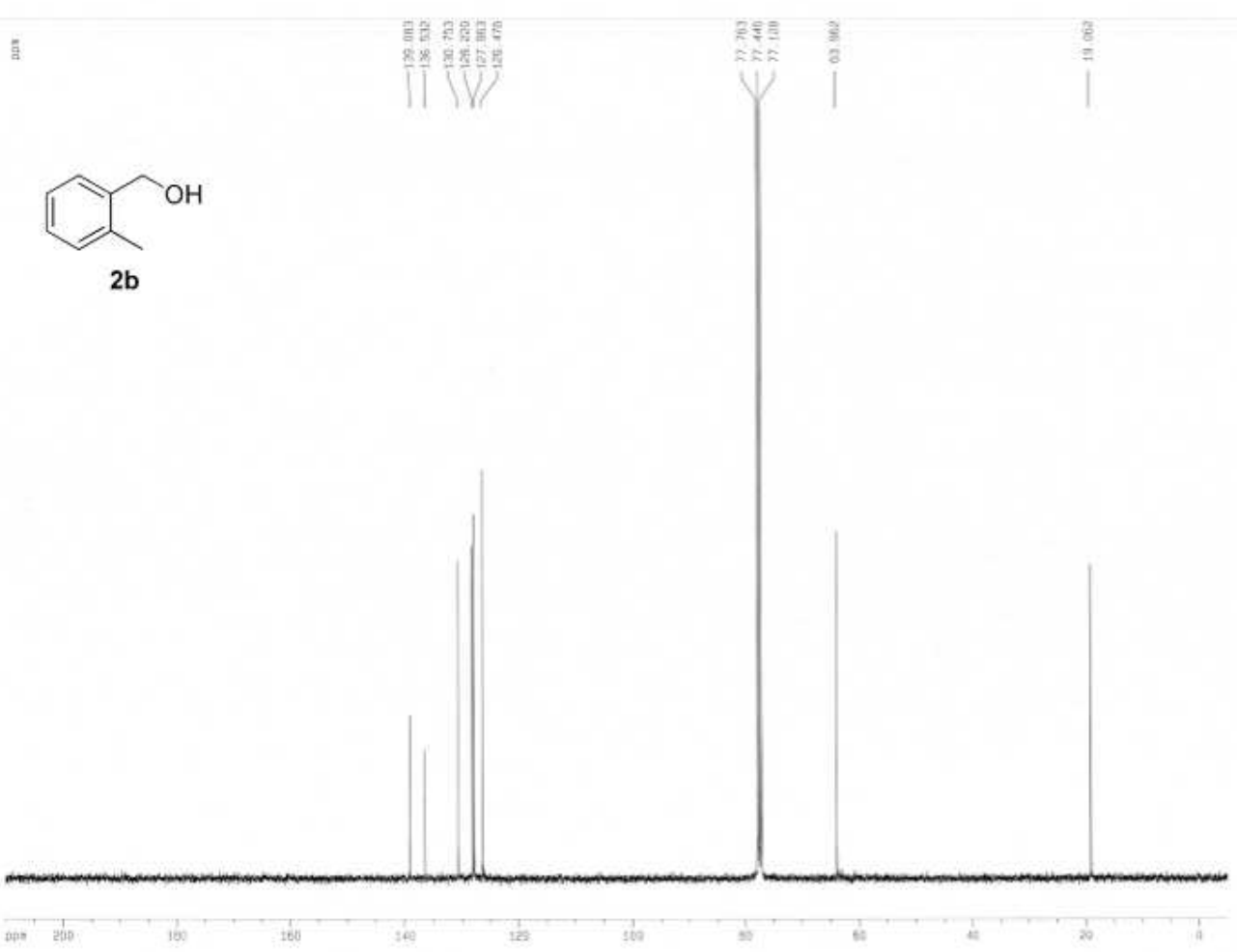


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FIDRES            0.485949 Hz
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DW                  15.700 usec
DE                   6.00 usec
TE                   298.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
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PL1                     -1.00 dB
SFO1            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2            400.1324708 MHz

F2 - Processing parameters
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1D NMR plot parameters
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F2P                     -5.000 ppm
F2                    -503.06 Hz
PPMCM                 7.16667 ppm/cm
HZCM                721.05786 Hz/cm
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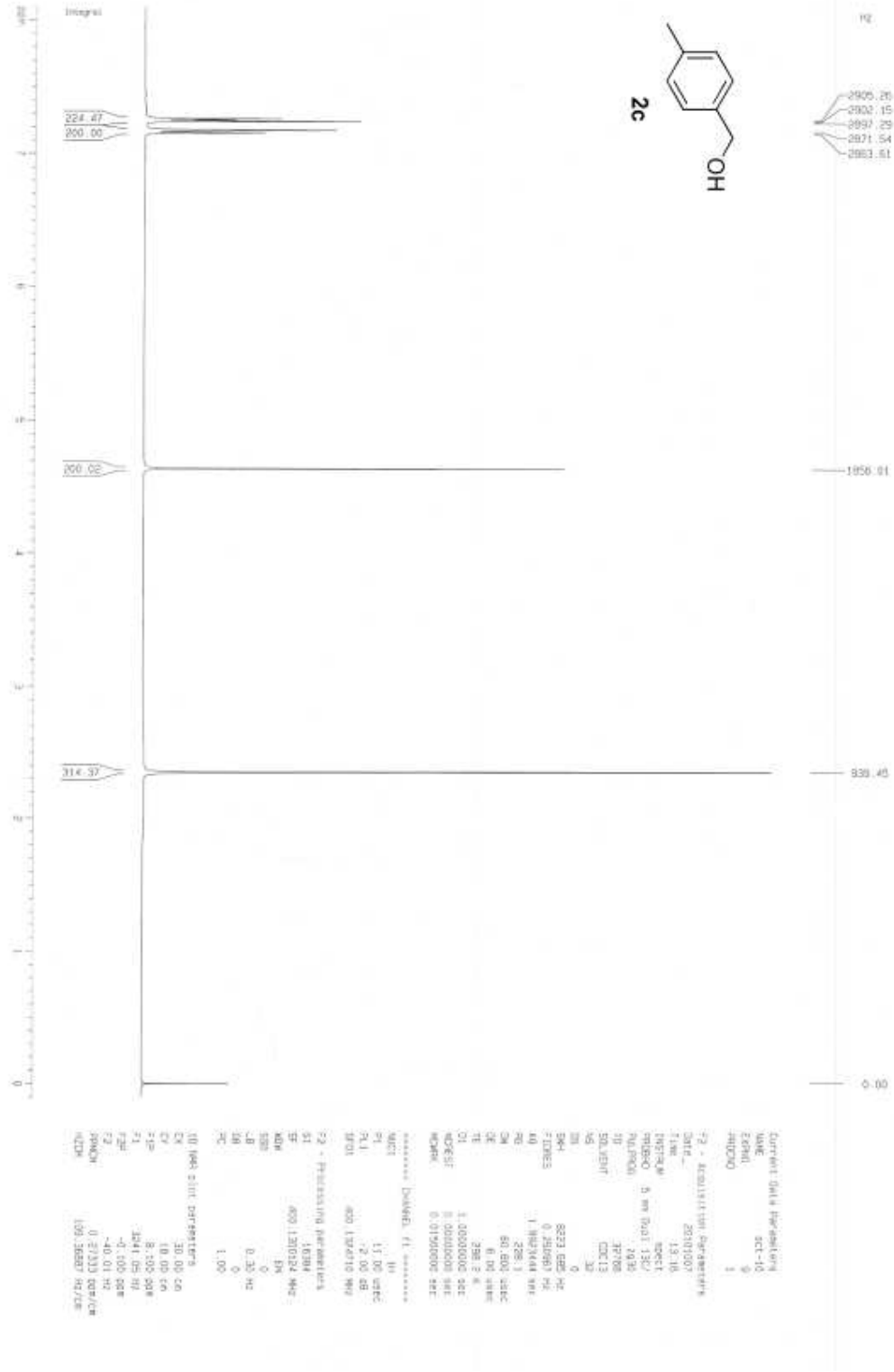
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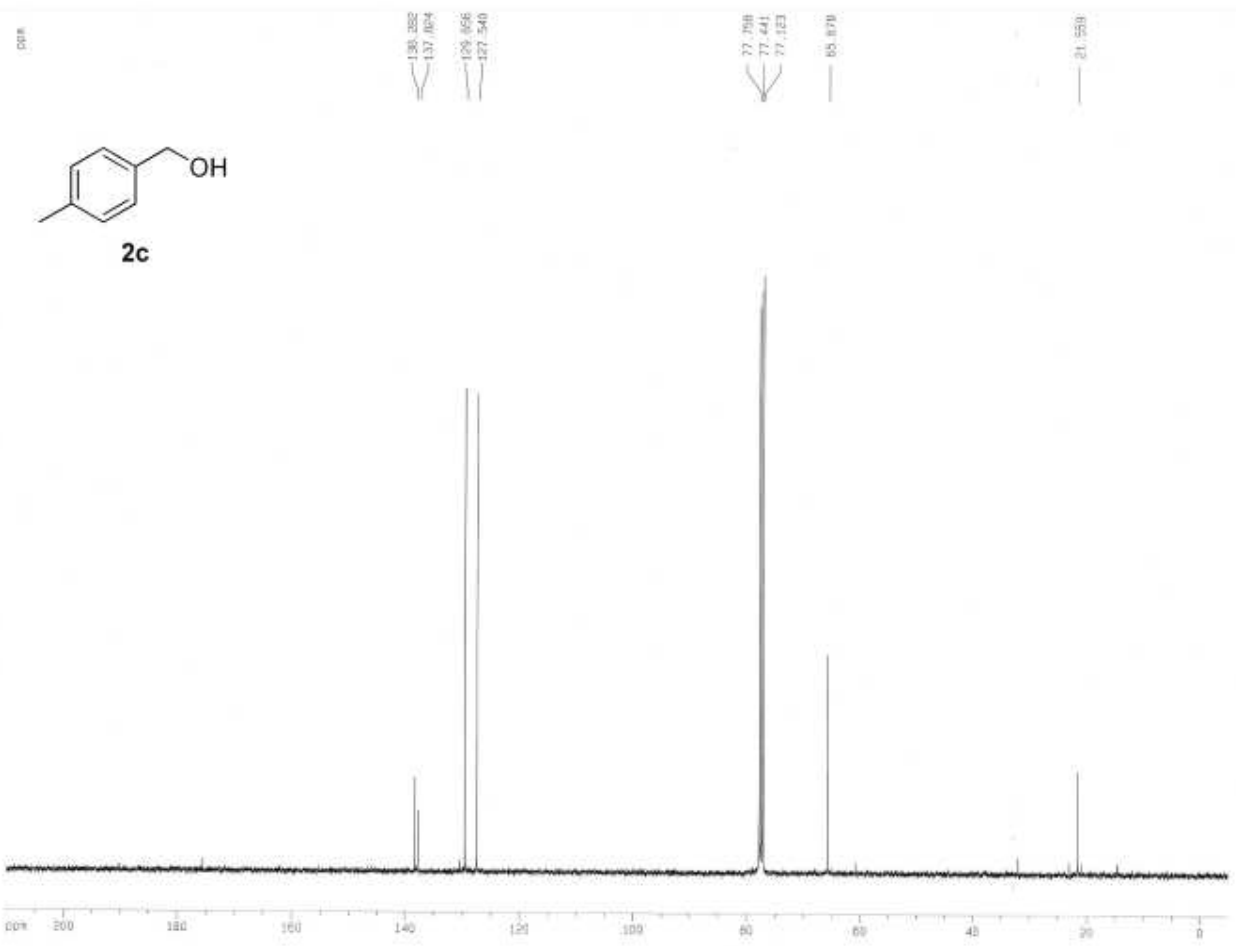


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NS                       1195
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RG                    3648.1
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DE                    6.00 usec
TE                   298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89999998 sec
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MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   16.00 dB
PL13                   20.00 dB
SFO2            400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127290 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    15.00 cm
F1P                  210.000 ppm
F1                 21128.67 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.16687 ppm/cm
HZCM               721.05786 Hz/cm
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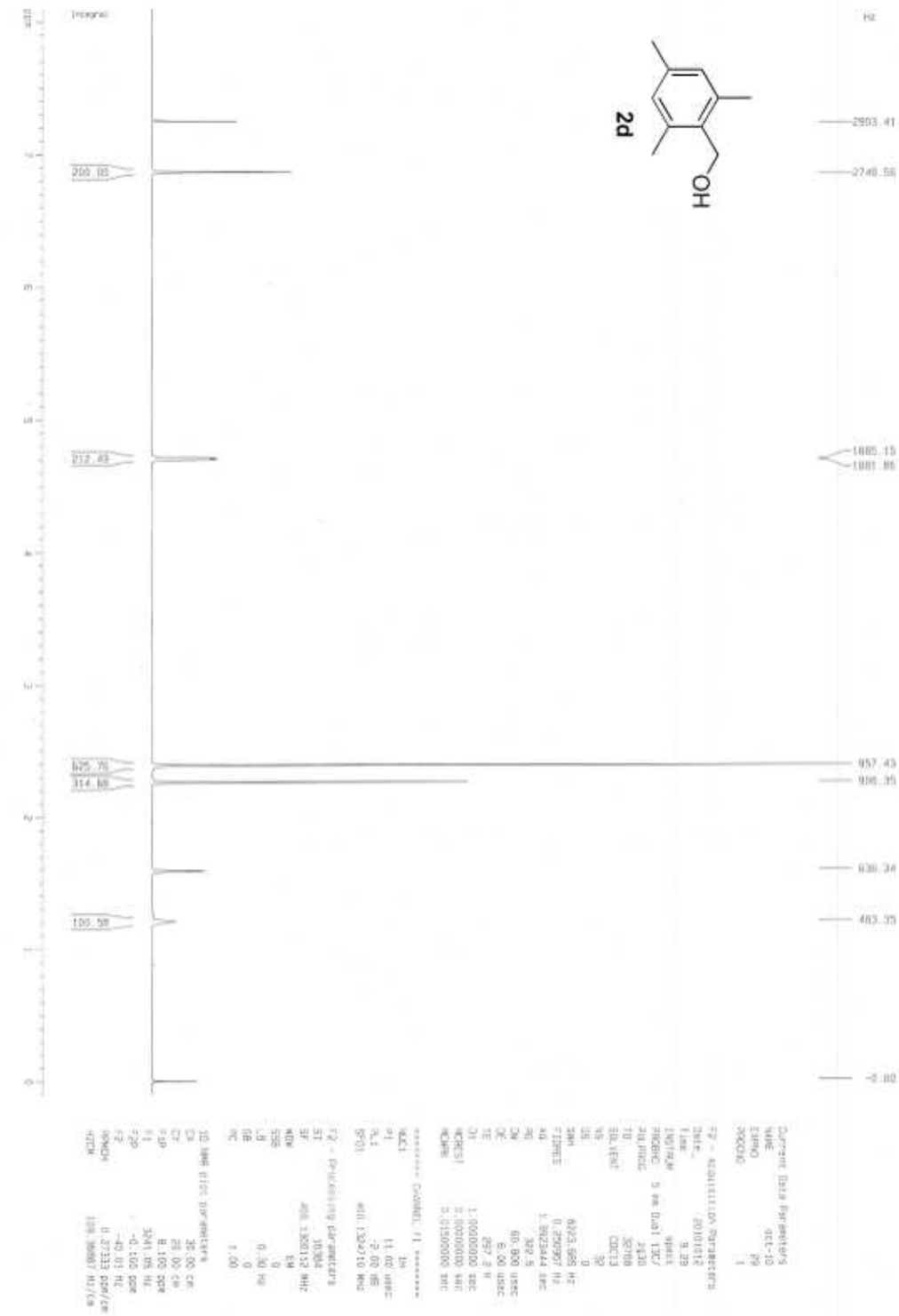
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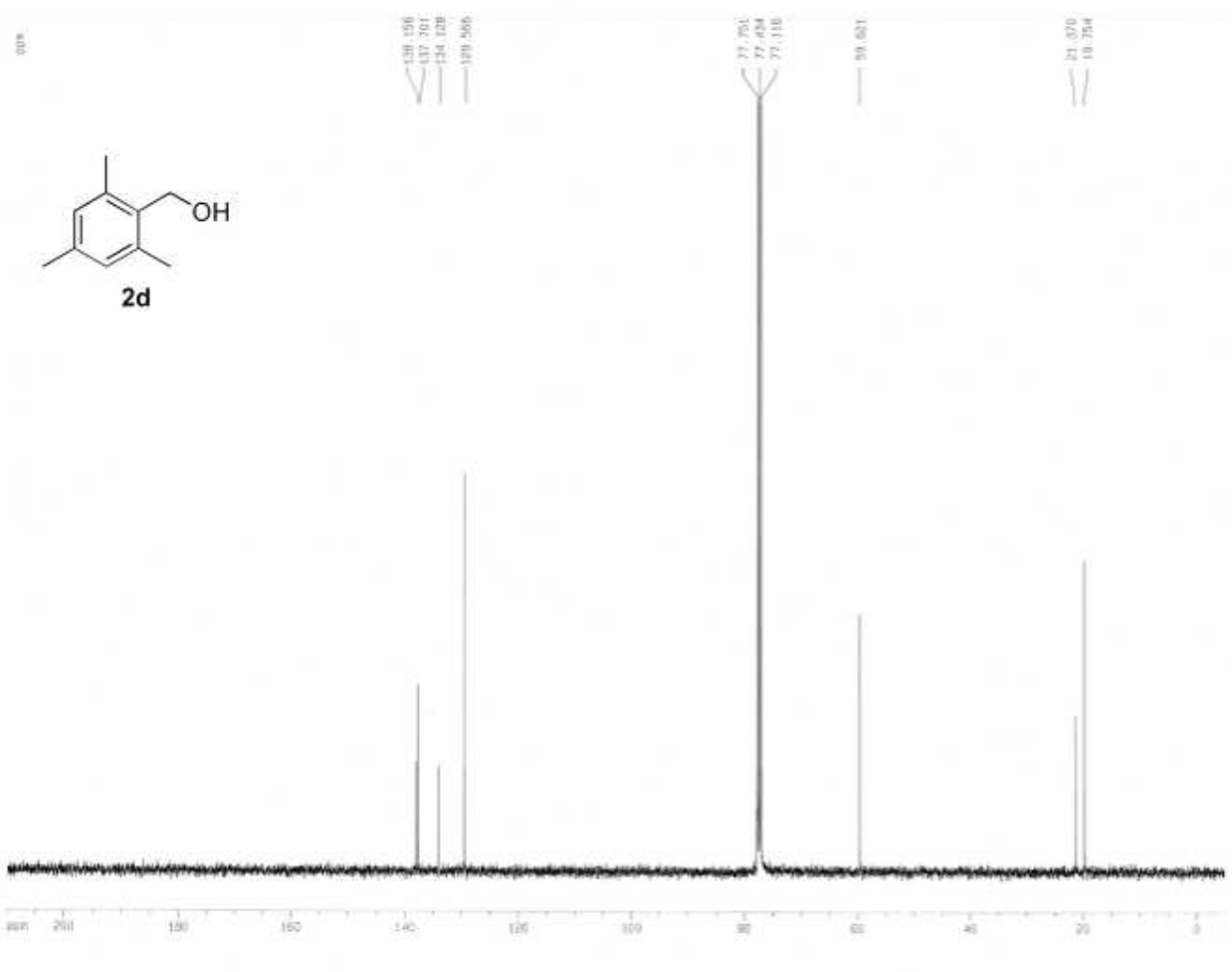


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PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1523
DS                       2
SWH              31847.133 Hz
FIDRES           0.485949 Hz
AQ               1.0289652 sec
RG                  3849.1
DW                 15.700 usec
DE                  6.00 usec
TE                 297.2 K
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D11             0.03000000 sec
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MCREST          0.00000000 sec
MCWRK           0.01500000 sec

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P1                   10.50 usec
PL1                  -1.00 dB
SFO1          100.6254308 MHz

======== CHANNEL f2 ========
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NUC2                    1H
PCPD2                105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2          400.1324708 MHz

F2 - Processing parameters
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SF            100.6127290 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                   35.00 cm
CY                   14.00 cm
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F1                 21128.67 Hz
F2P                 -5.000 ppm
F2                 -503.06 Hz
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HZCM               721.05786 Hz/cm
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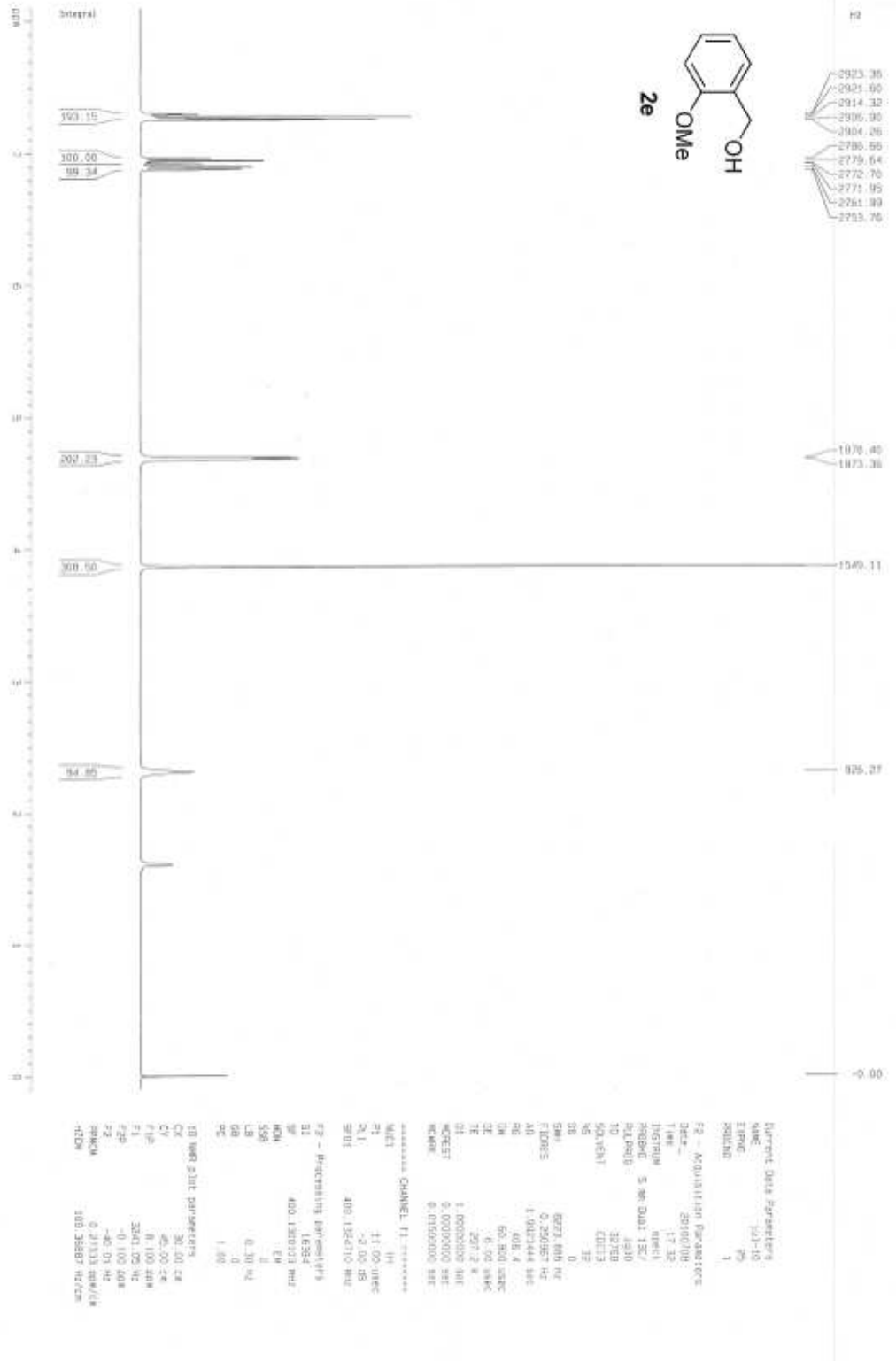
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2914.32
2906.90
2904.26
2786.66
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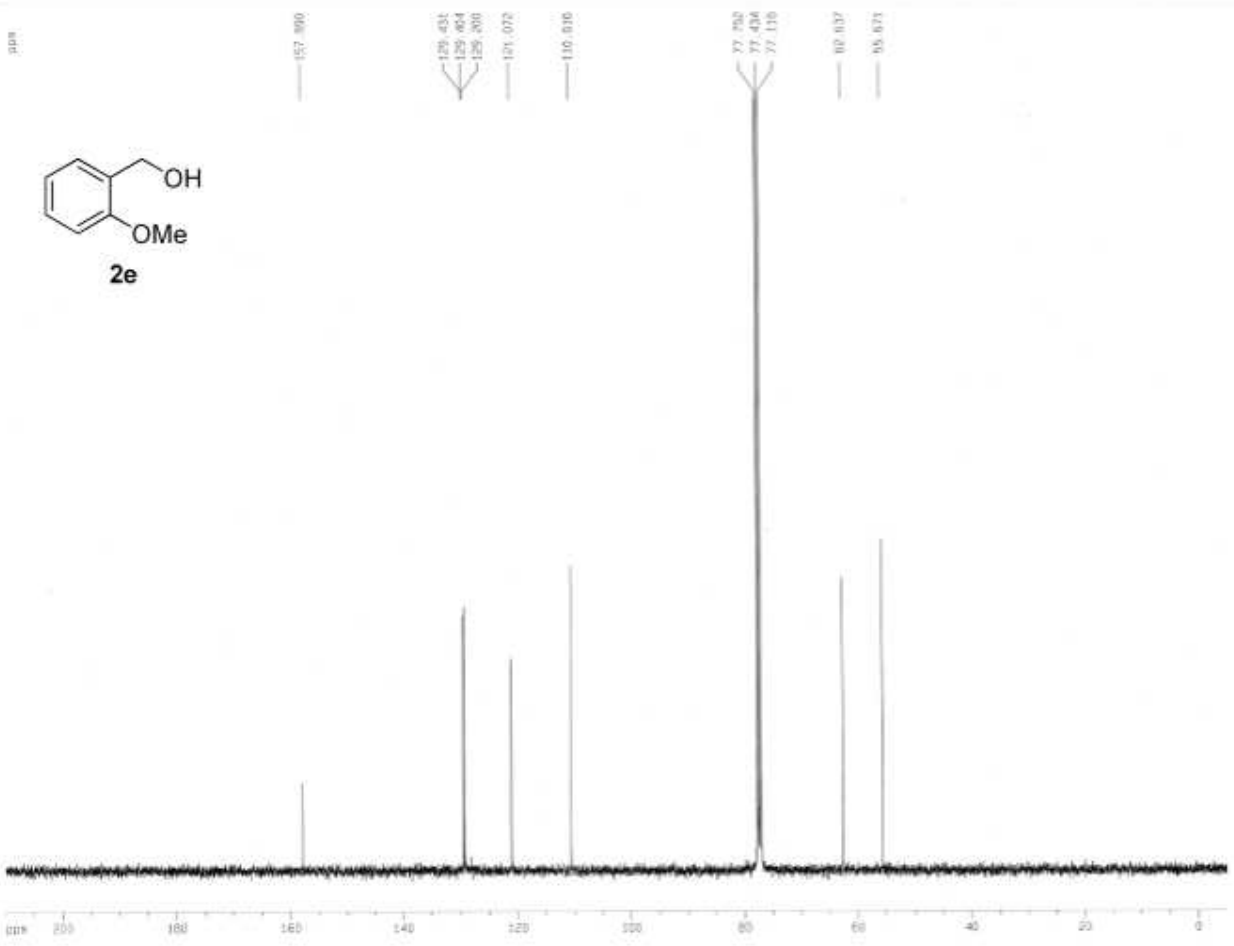


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DS                         2
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FIDRES             0.486049 Hz
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RG                     228.1
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DE                     6.00 usec
TE                    297.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
DECPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2             400.1324709 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127290 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     30.00 cm
CY                     34.00 cm
F1P                  210.000 ppm
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F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.16667 ppm/cm
HZCM               721.05766 Hz/cm
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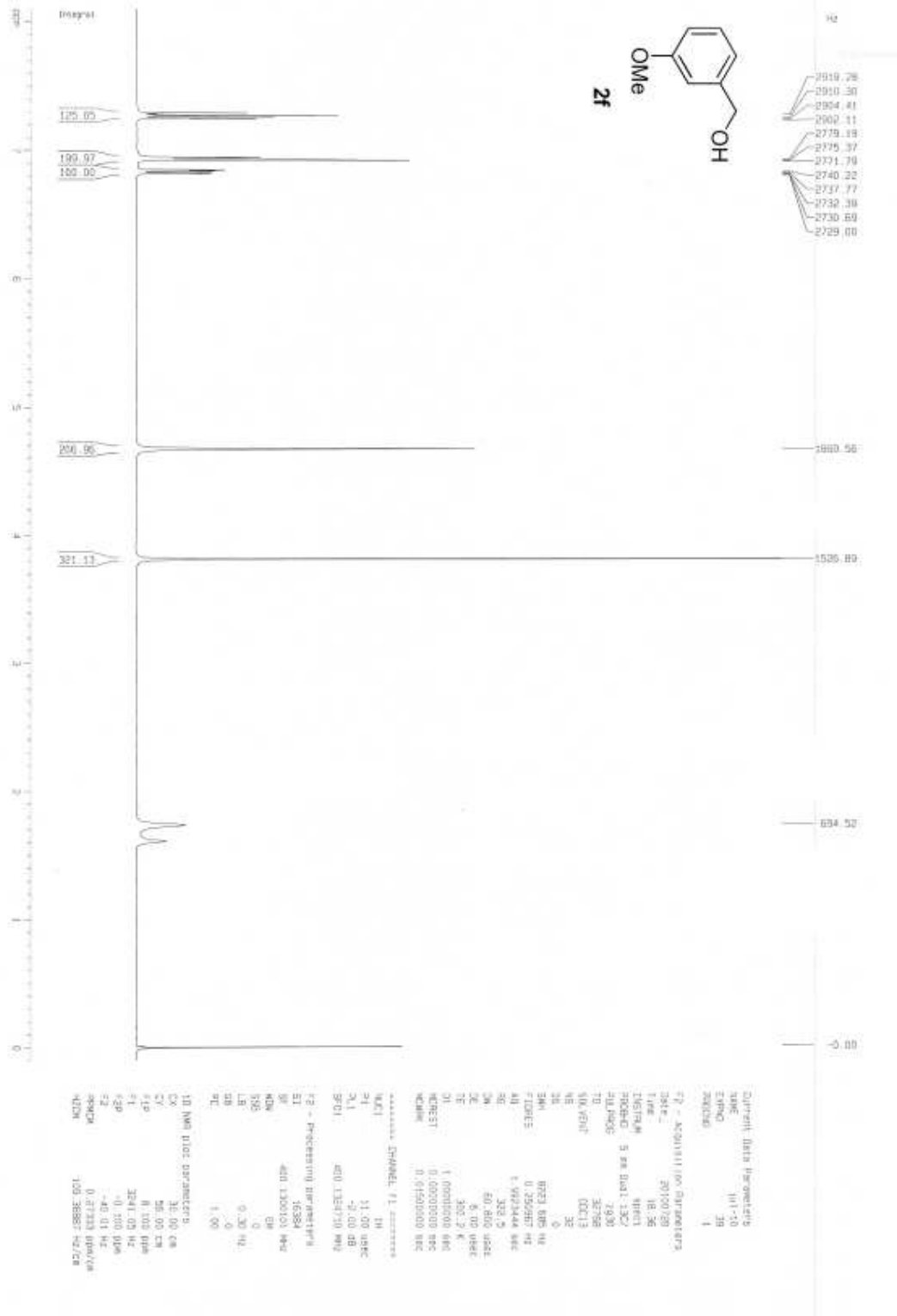
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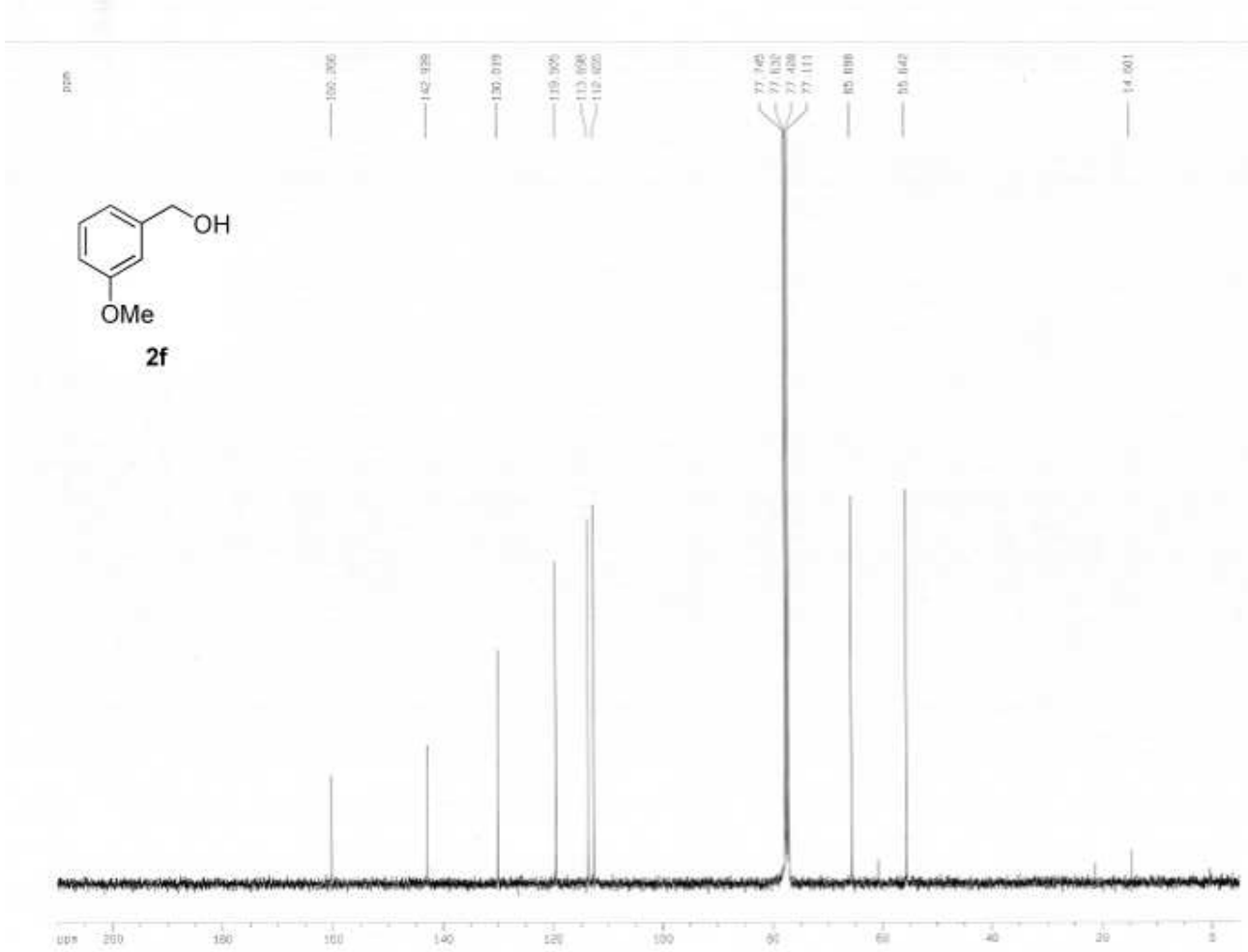
OH
2f

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TD                      65536
SOLVENT                 CDCl3
NS                       2048
DS                          4
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289852 sec
RG                        181
DW                    15.700 usec
DE                     6.00 usec
TE                    298.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
HCREST             0.00000000 sec
HCWAM              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1               100.6254998 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2               400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127290 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                        30.00 cm
CY                        34.00 cm
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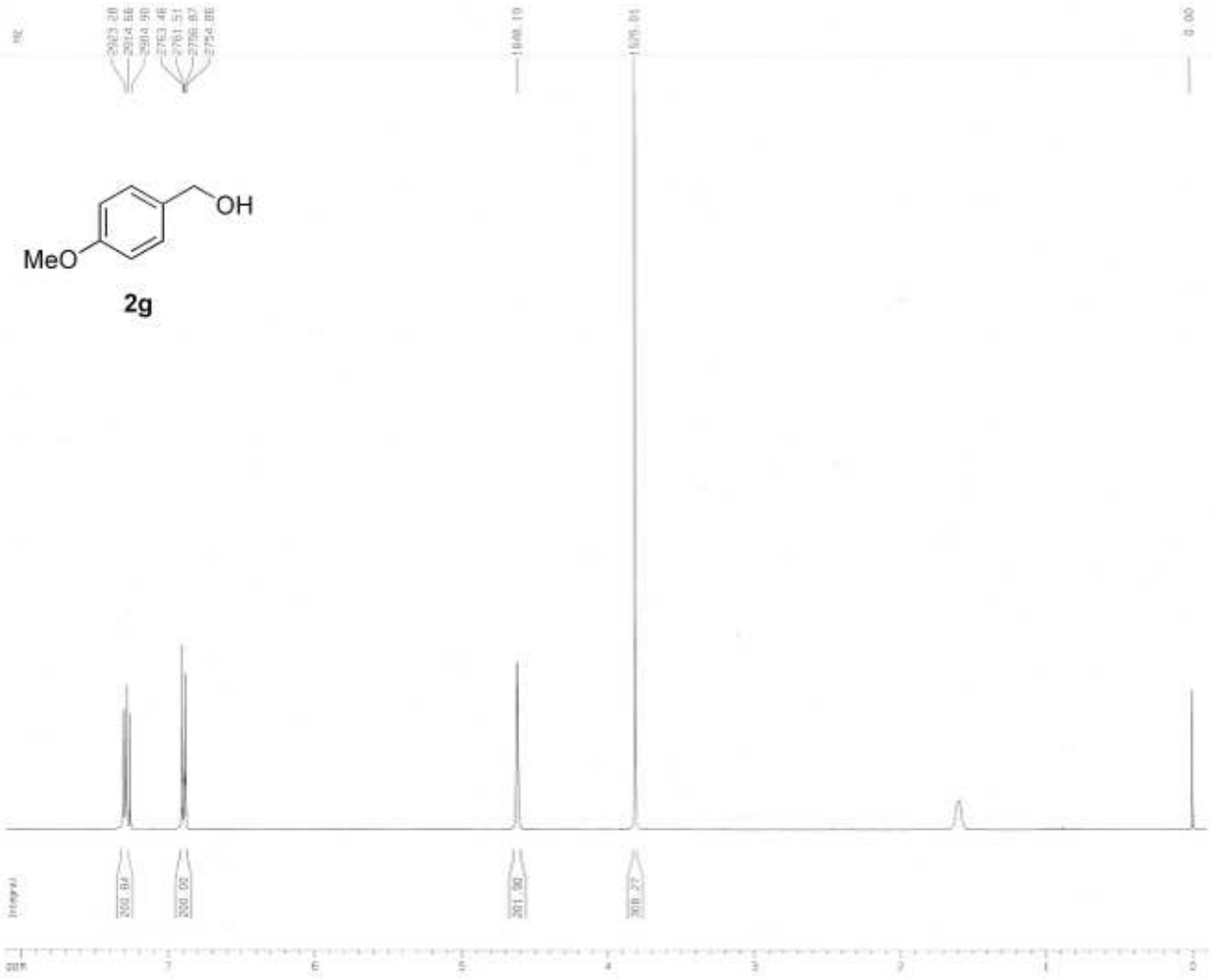

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SOLVENT CDCl3
NS 16
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FIDRES 0.250967 Hz
AQ 1.9923448 sec
RG 362
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DE 6.00 usec
TE 297.2 K
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MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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PL1 -2.00 dB
SFO1 400.1324710 MHz

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CY 20.00 cm
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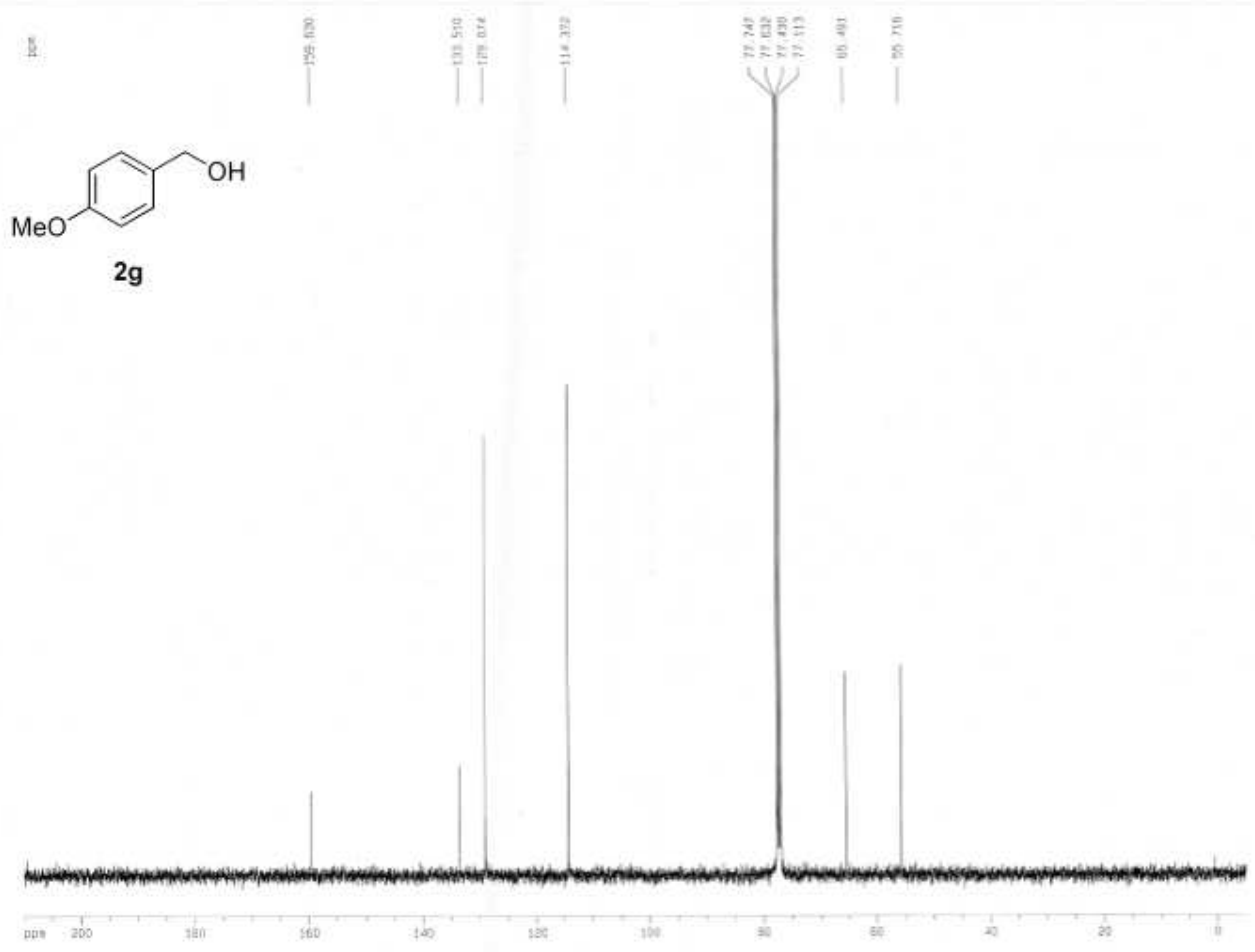
HZCM 109.36887 Hz/cm

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PROCNO                     1

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FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                   297.2 K
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d11               0.03000000 sec
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MCWRK             0.01500000 sec

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PL1                    -1.00 dB
SFO1             100.6254958 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
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SF                100.6127290 MHz
WDW                          EM
SSB                           0
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GB                            0
PC                         1.40

1D NMR plot parameters
CX                        30.00 cm
CY                        34.00 cm
F1P                     210.000 ppm
F1                    21128.67 Hz
F2P                      -5.000 ppm
F2                     -503.06 Hz
PPMCM                  7.16667 ppm/cm
HZCM                 721.05786 Hz/cm
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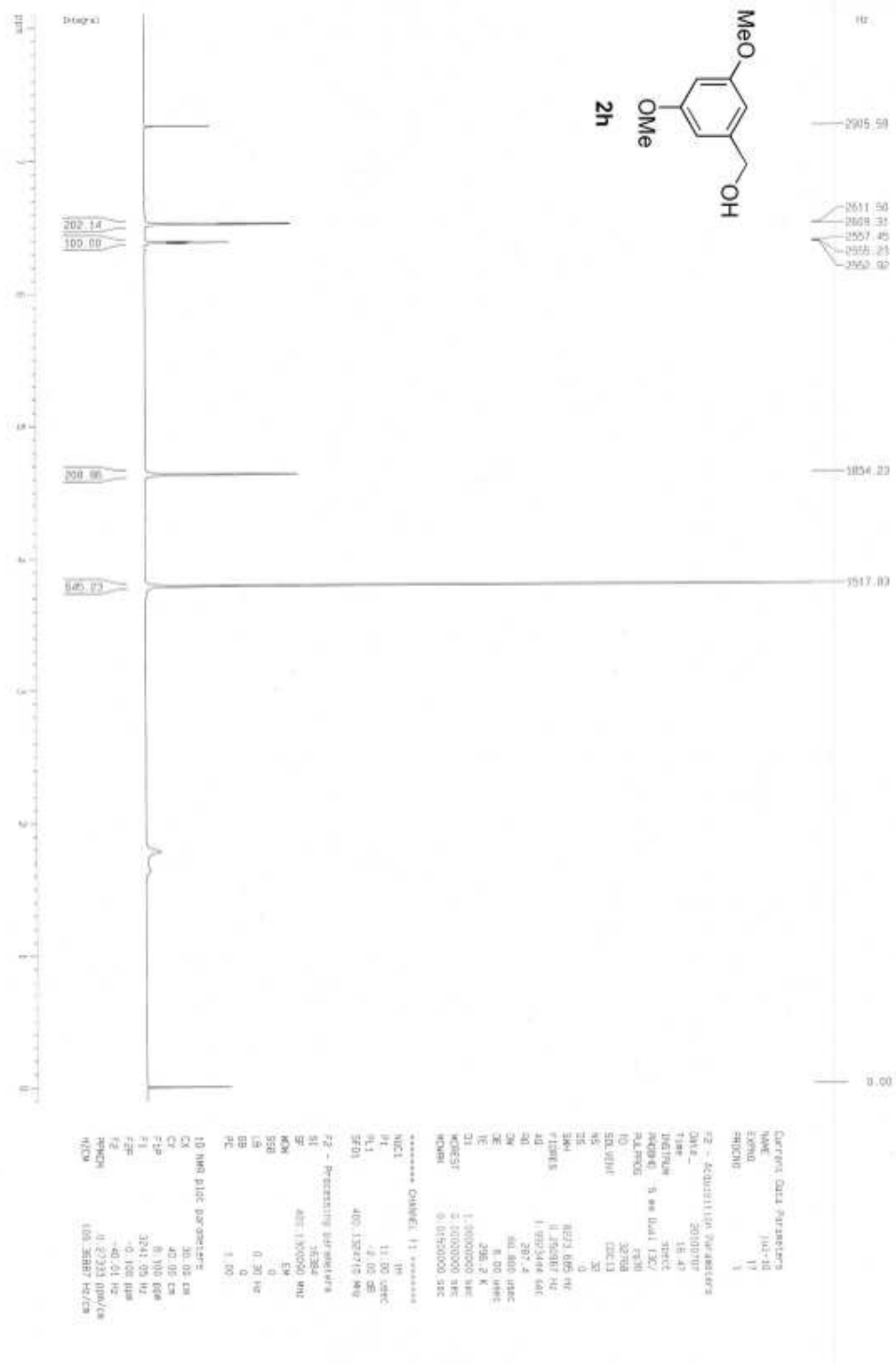
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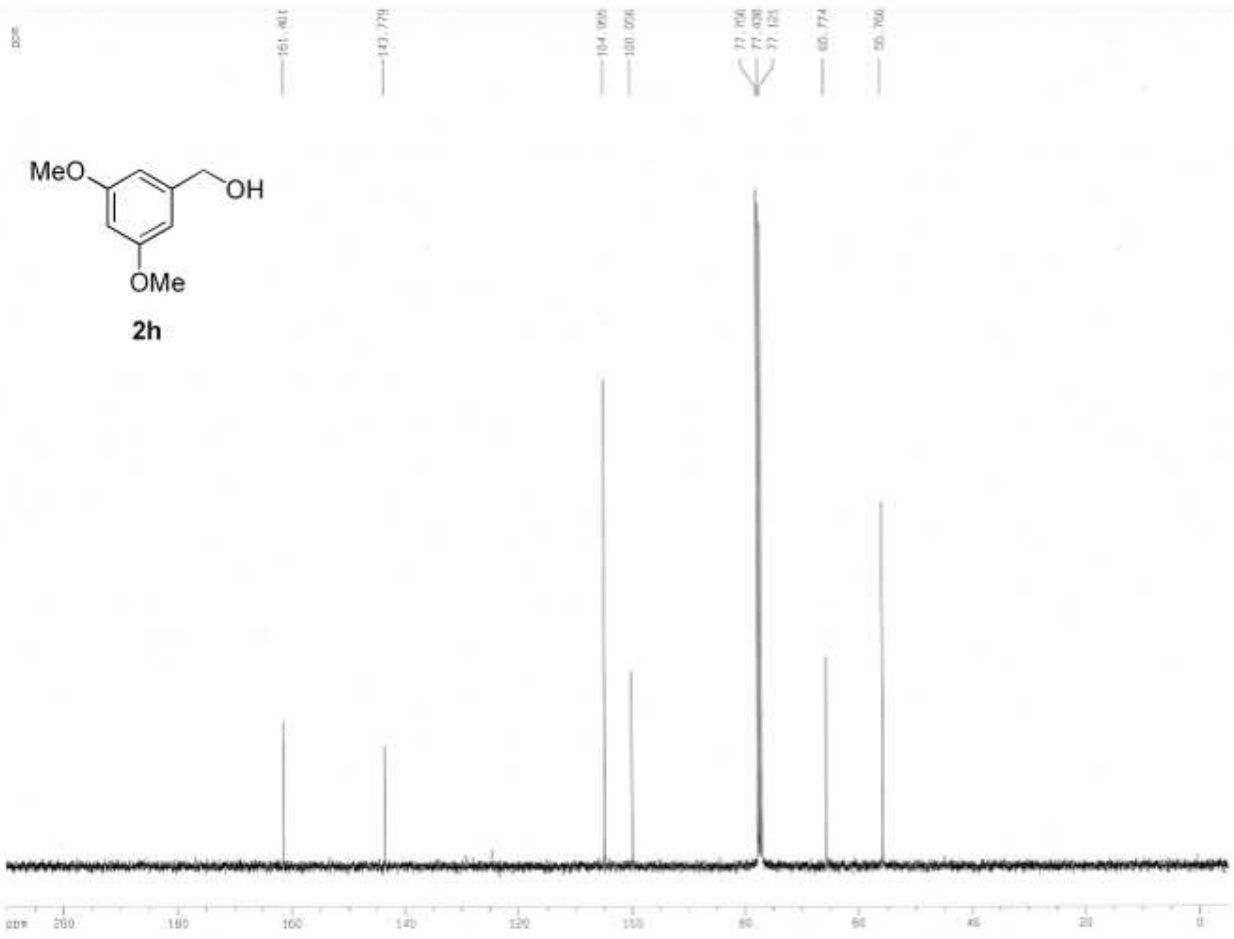
2555.23
2552.92
1854.23
1517.83
0.00
202.14
100.00
208.86
645.23
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F2P
F2
PHMCM
NZCW

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PROCNO                     1

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TD                    65536
SOLVENT                CDCl3
NS                       553
DS                         2
SWH               31847.133 Hz
FIDRES                0.485948 Hz
AQ                1.0288652 sec
RG                     143.7
DW                    15.700 usec
DE                     6.00 usec
TE                    296.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      13.50 usec
PL1                     -1.00 dB
SFO1            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    16.00 dB
PL13                    20.00 dB
SFO2            400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127290 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     30.00 cm
CY                     17.00 cm
F1P                  210.000 ppm
F1                 21128.67 Hz
F2P                   -5.000 ppm
F2                  -503.08 Hz
PPMCM                7.15667 ppm/cm
HZCM               721.05786 Hz/cm
```

2i
OH
Integral
Hz
2585.12
2745.01
2743.78
2719.51
2717.51
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2705.71
2378.15
1626.56
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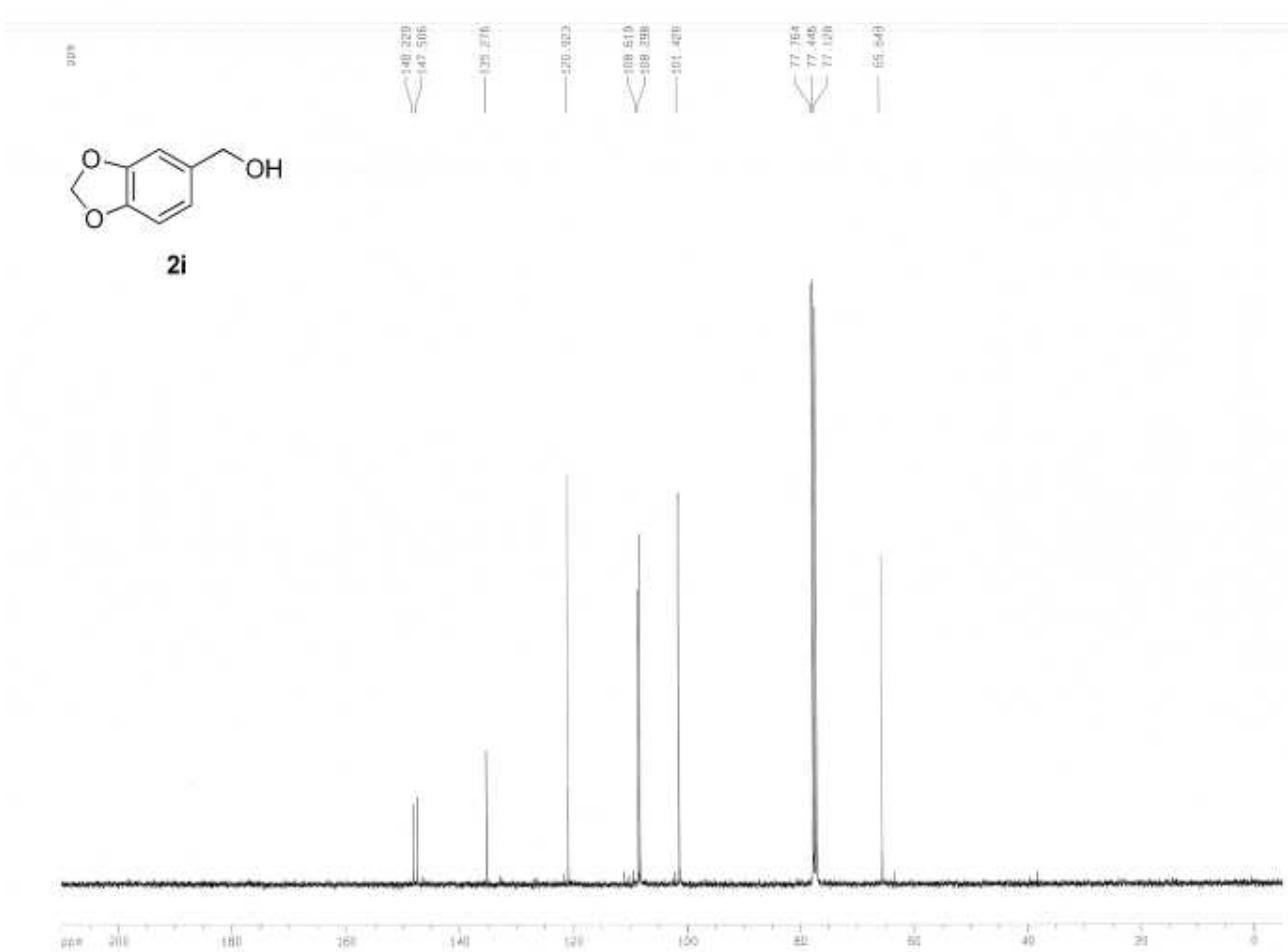
100.00
192.76
103.51
206.15
201.90

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PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1069
DS                        2
SWH               31847.133 Hz
FIDRES            0.485849 Hz
AQ                1.0288652 sec
RG                   3649.1
DW                  15.700 usec
DE                   6.00 usec
TE                  298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.50 usec
PL1                   -1.00 dB
SFO1          100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                105.00 usec
PL2                   -2.00 dB
PL12                  18.00 dB
PL13                  20.00 dB
SFO2          400.1324708 MHz

F2 - Processing parameters
SI                      32768
SF            100.6127290 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    15.00 cm
F1P                 210.000 ppm
F1                21128.67 Hz
F2P                  -5.000 ppm
F2                 -503.06 Hz
PPMCM              7.15667 ppm/cm
HZCM             721.05786 Hz/cm
```
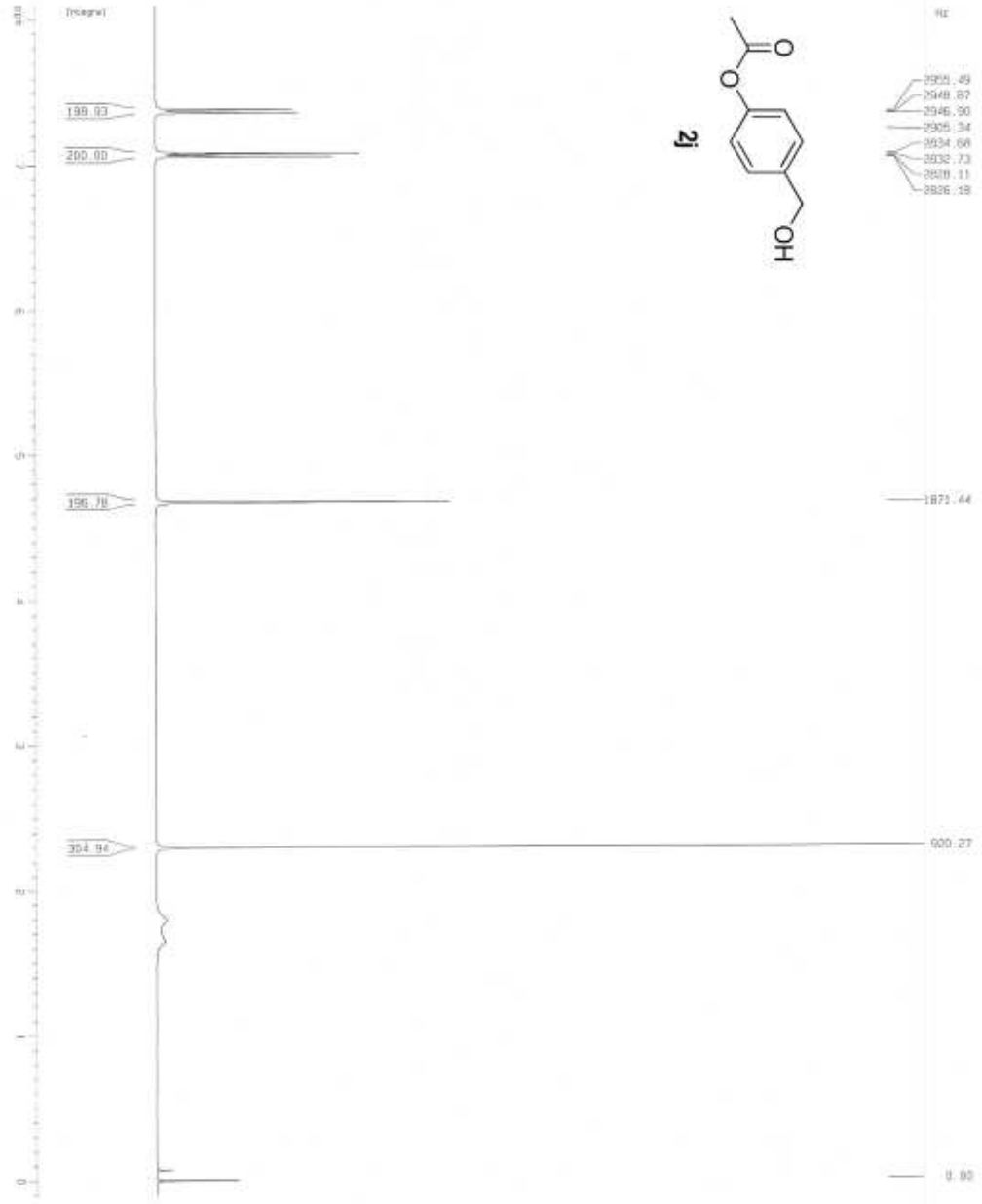
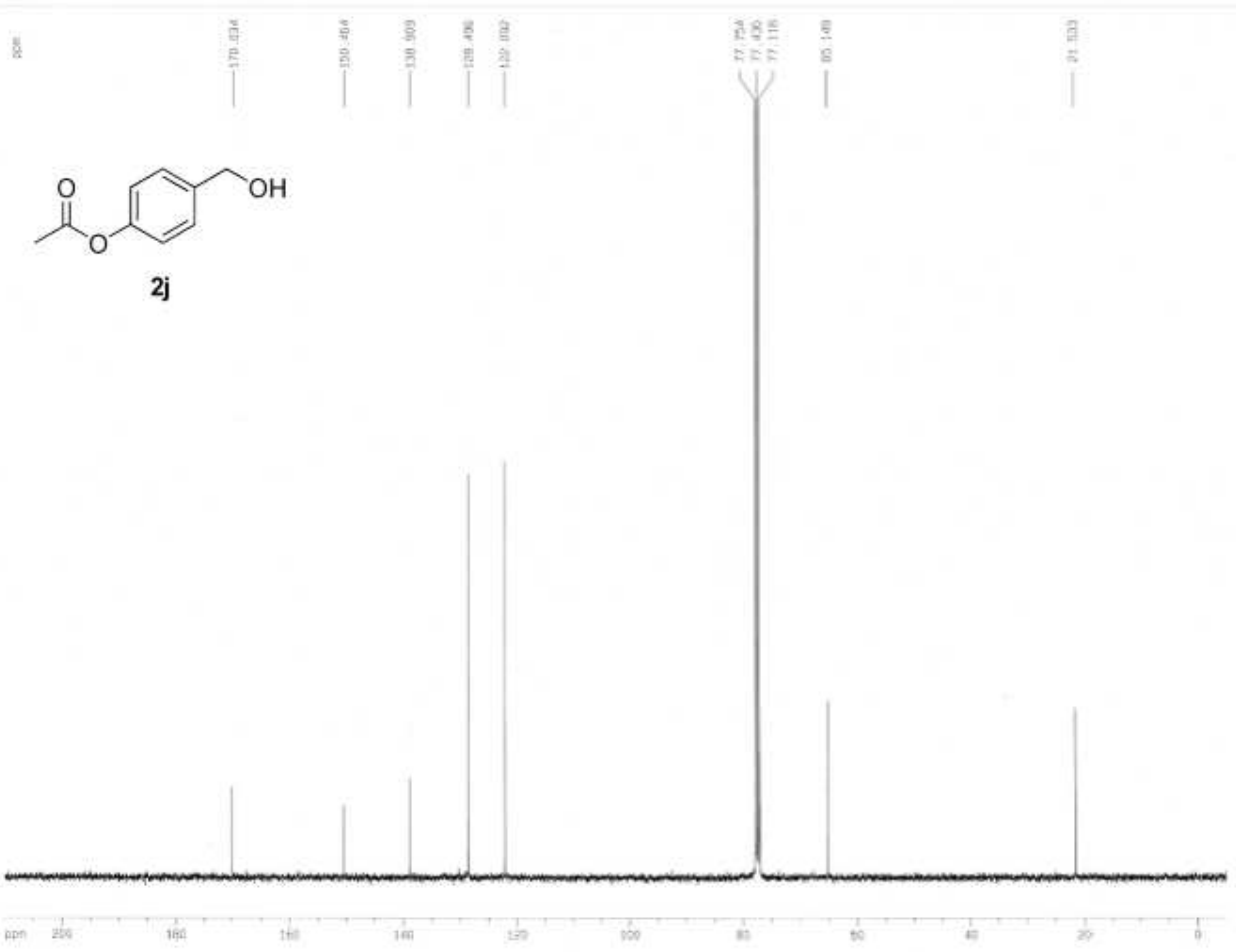
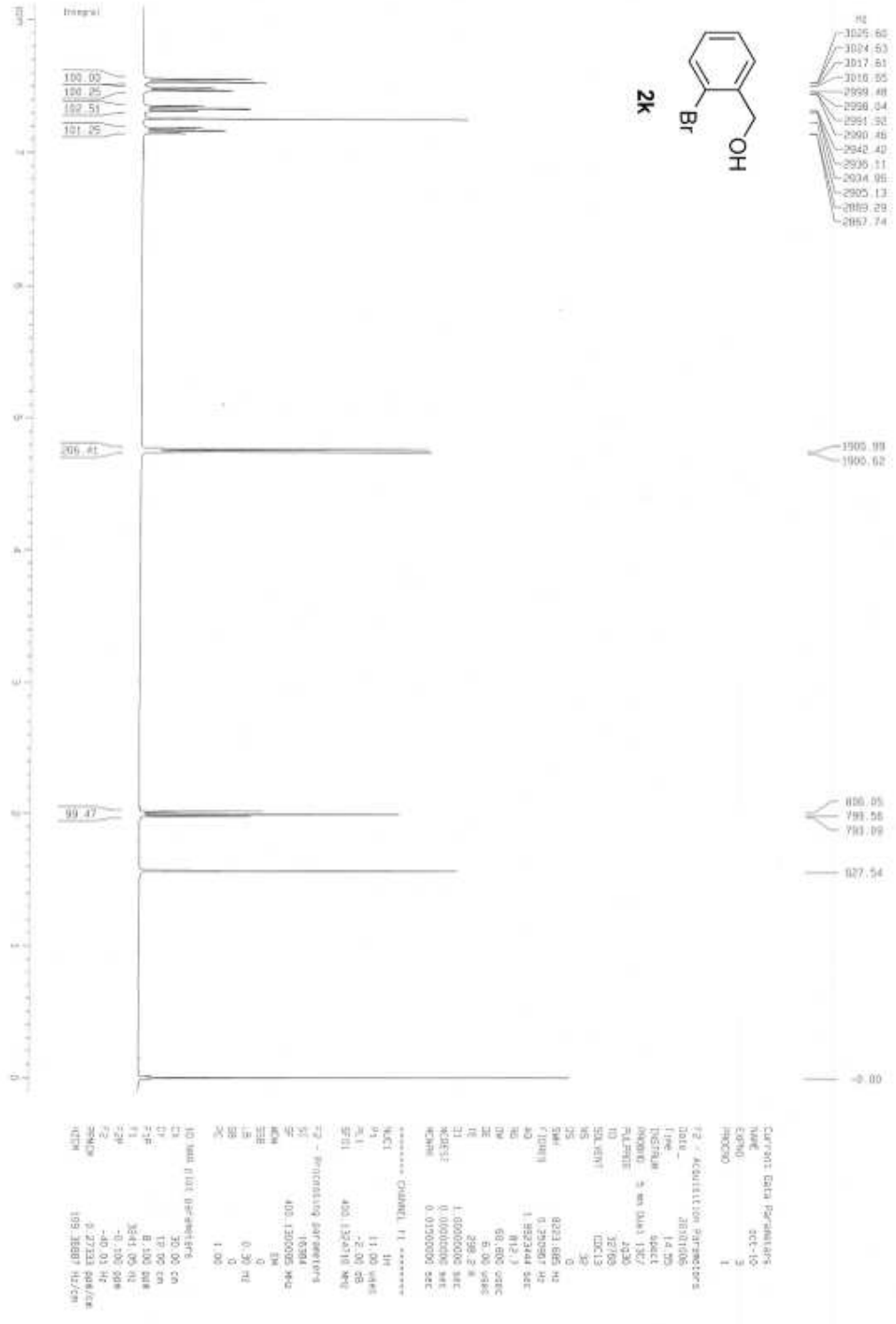
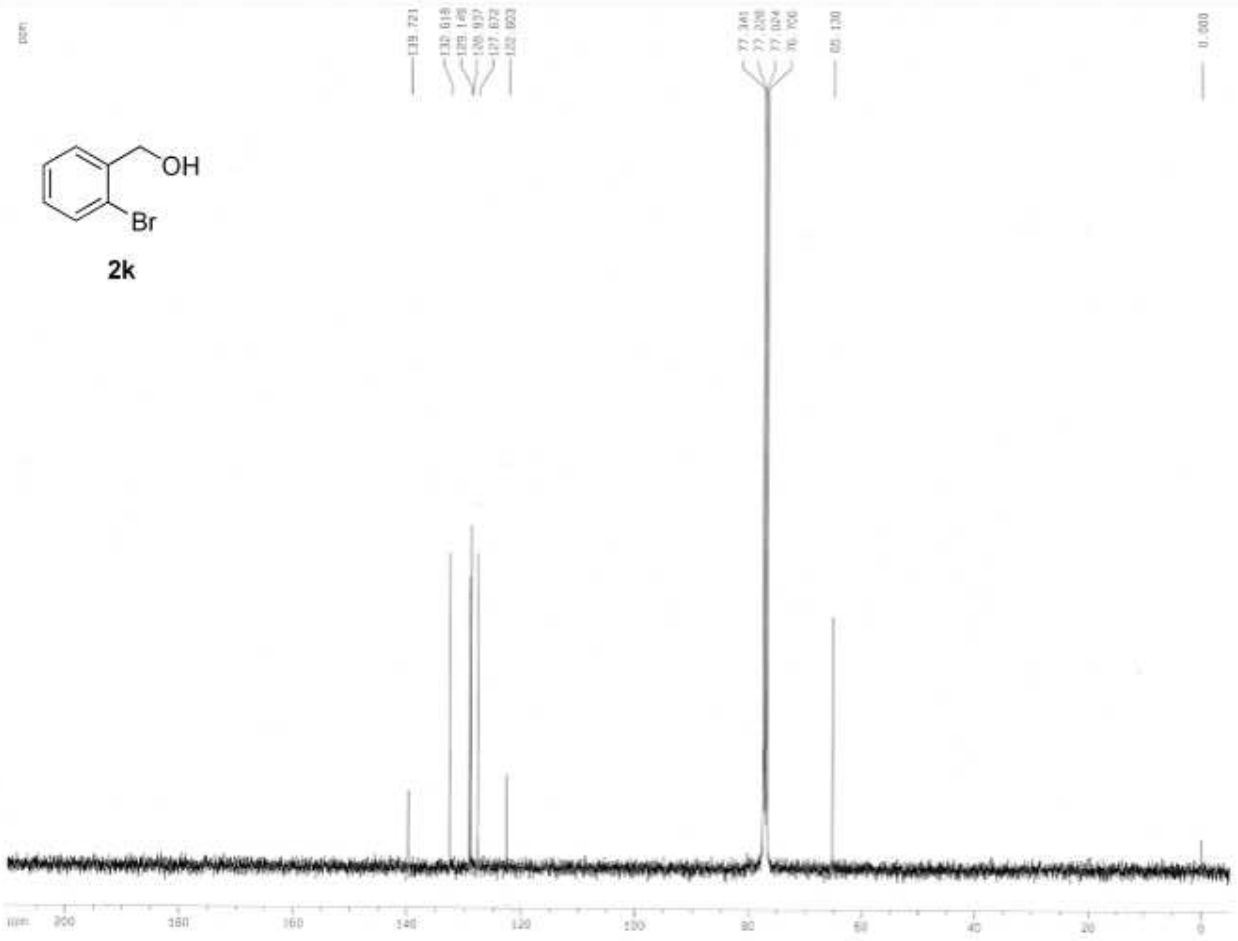


2i
OH
O
O
199.93
200.00
196.78
304.94
1871.44
920.27
0.00
2955.49
2948.87
2946.90
2905.34
2834.66
2832.73
2828.11
2826.18

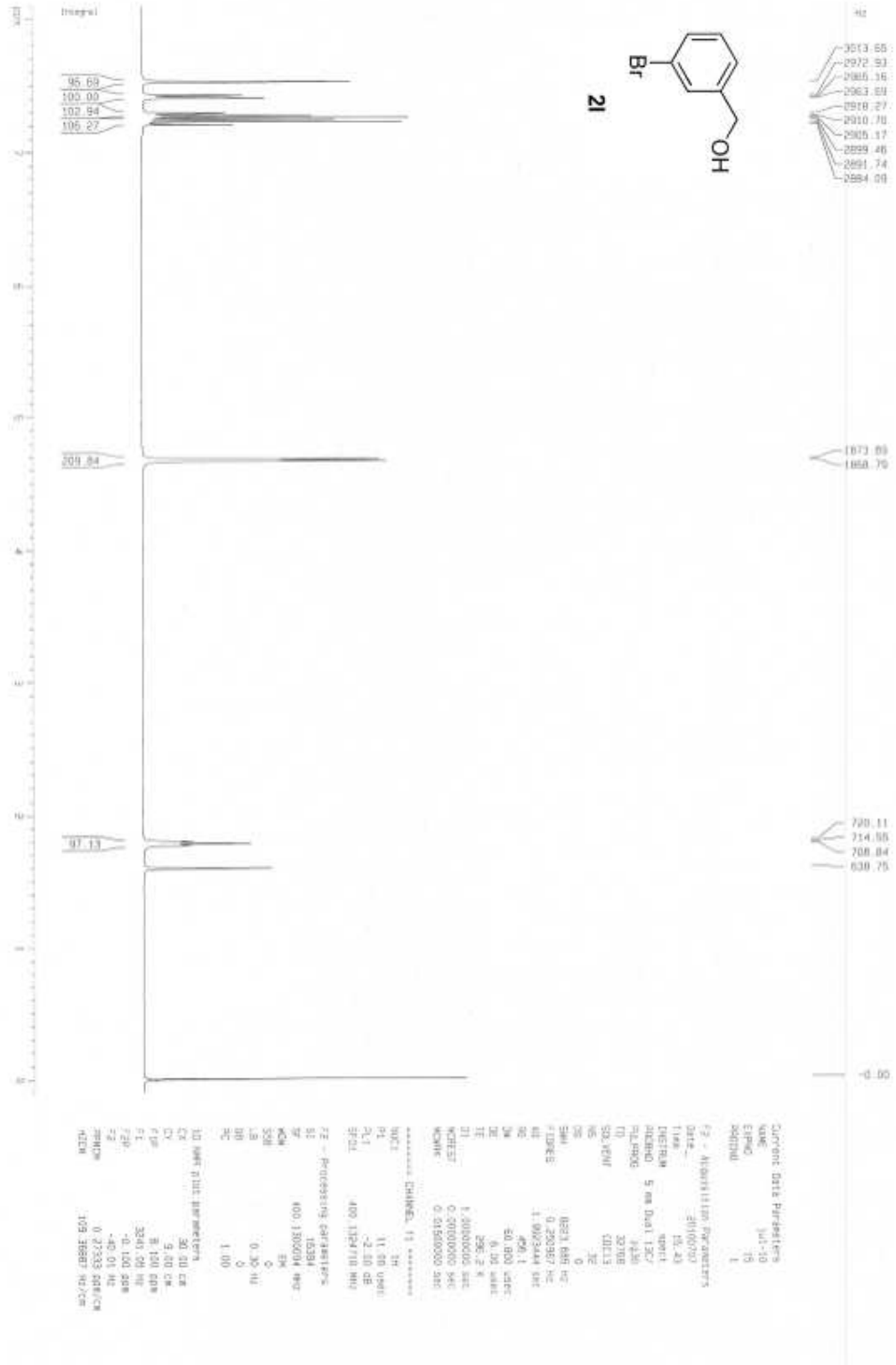


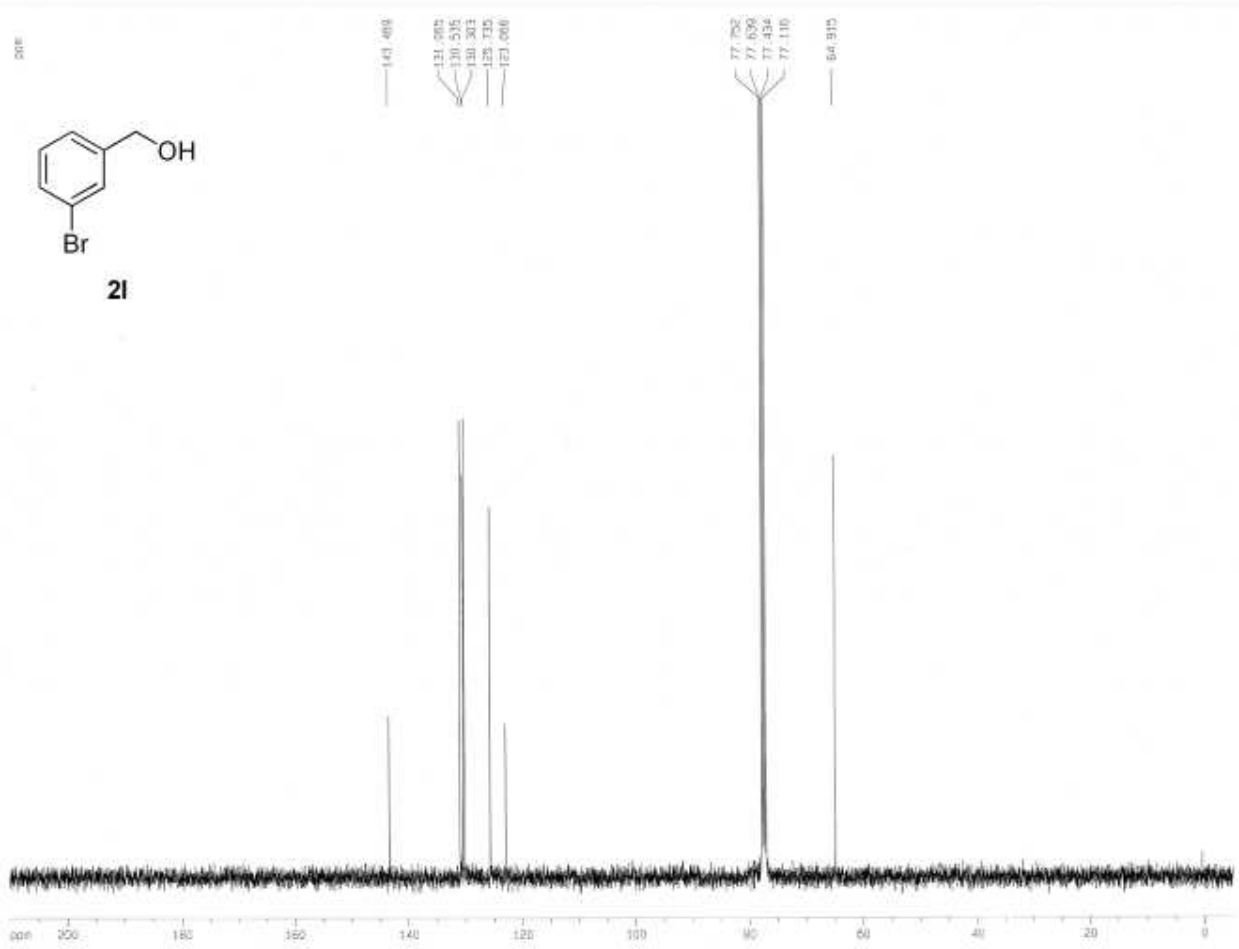

```
Current Data Parameters
NAME                  jul-10
EXPNO                     50
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100727
Time                   16.20
INSTRUM                spect
PROBHD     5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1639
DS                         2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                   298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz15
NUC2                        1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127290 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      30.00 cm
CY                      23.00 cm
F1P                   210.000 ppm
F1                  21138.67 Hz
F2P                    -5.000 ppm
F2                   -503.06 Hz
PPMCM                 7.10667 ppm/cm
HZCM                721.05786 Hz/cm
```


2k
Br
OH
100.00
100.25
102.51
101.25
206.41
99.47
3025.60
3024.53
3017.61
3016.55
2999.48
2998.04
2991.32
2990.46
2942.40
2935.11
2934.06
2905.13
2889.29
2857.74
1905.99
1900.62
806.05
799.58
793.09
827.54
-0.00

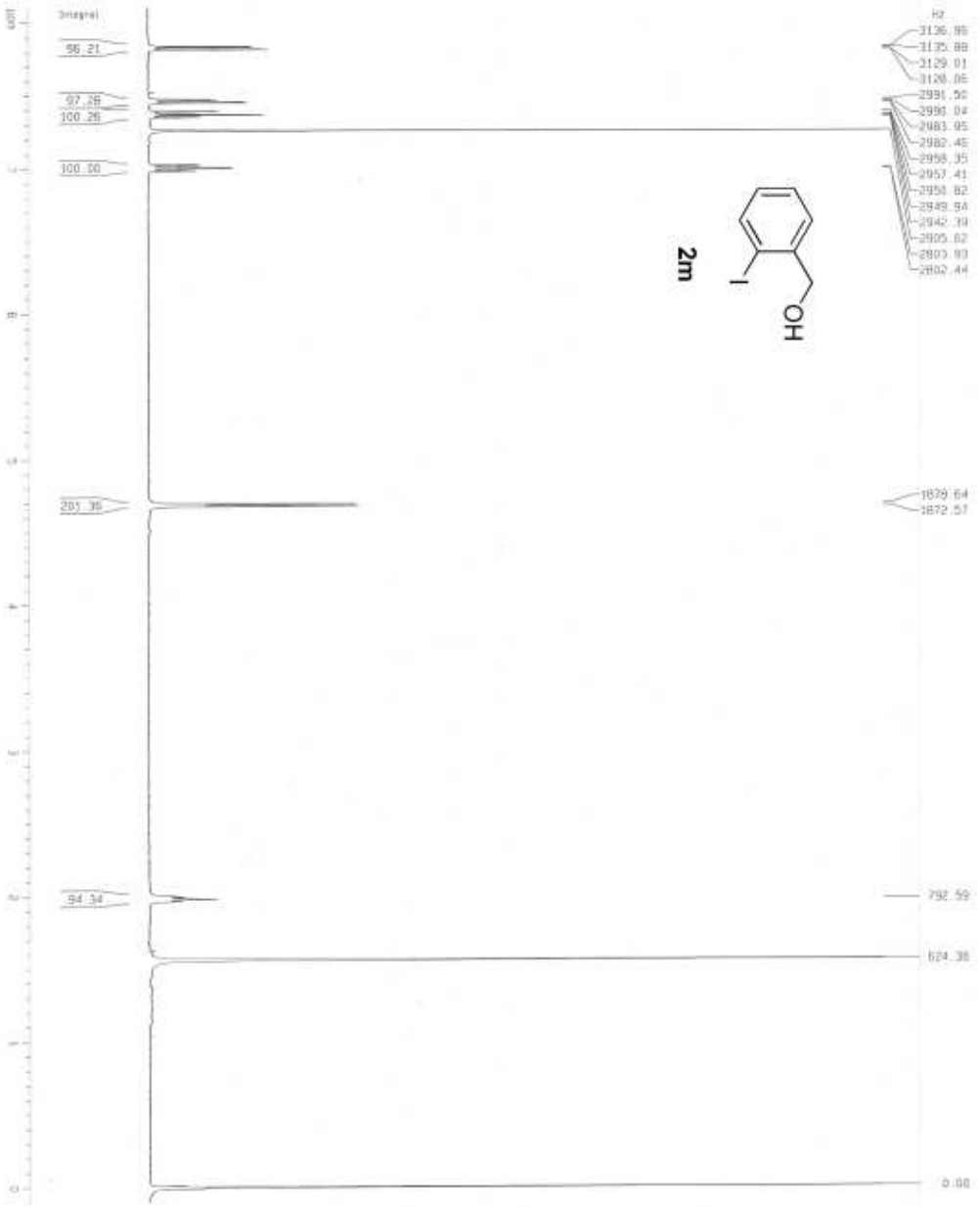


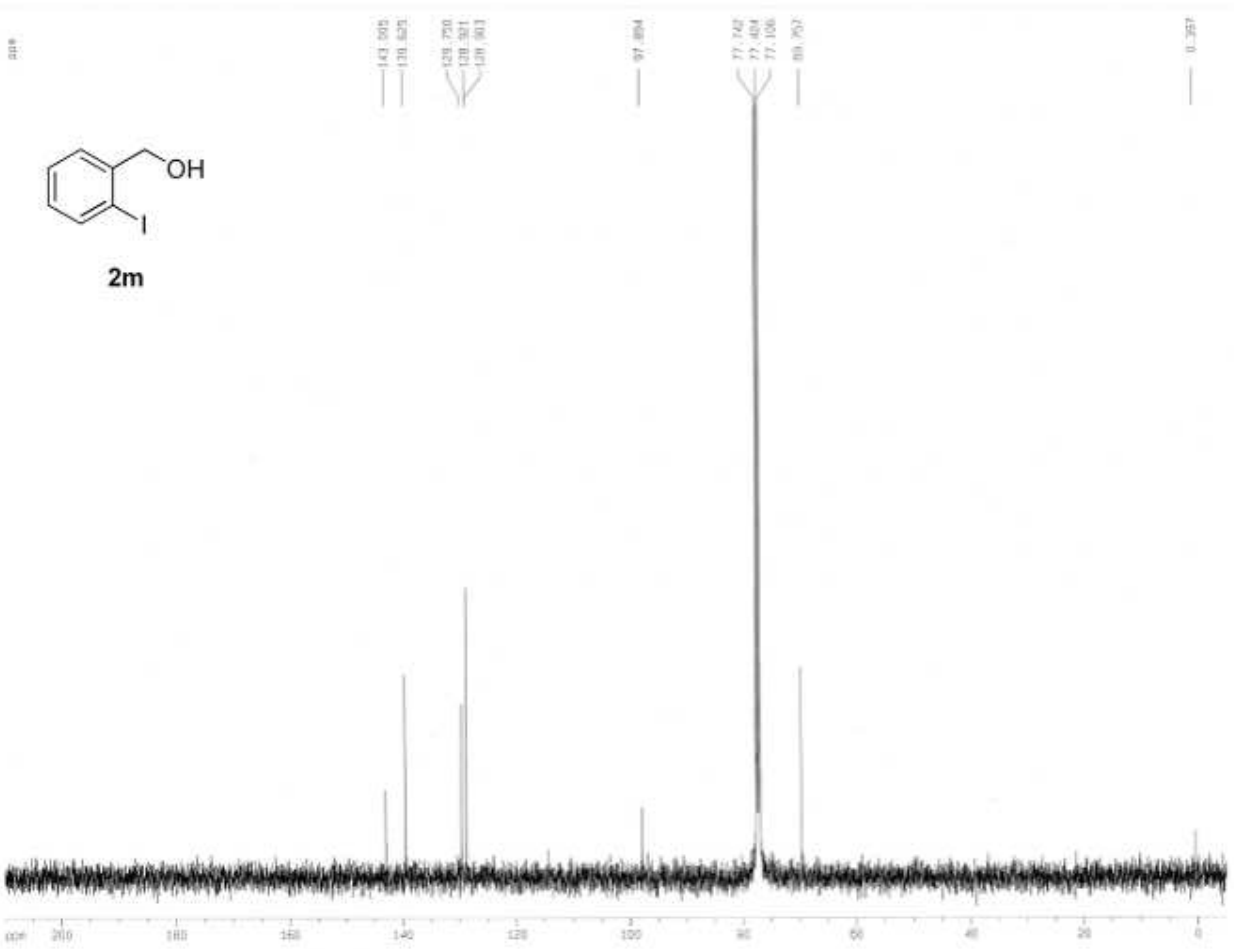

```
Current Data Parameters
NAME                  oct-10
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_              20101006
Time                   15.32
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1366
DS                         2
SWH               31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                   298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
DELTA             1.89999998 sec
MDRES2            0.00000000 sec
MDWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127690 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      30.00 cm
CY                      67.00 cm
F1P                   210.000 ppm
F1                   21128.68 Hz
F2P                    -5.000 ppm
F2                    -503.06 Hz
PPMCM                 7.18860 ppm/cm
HZCM                 721.05817 Hz/cm
```


Br
OH
2l
95.69
100.00
102.94
106.27
209.84
97.13
3013.65
2972.93
2965.16
2963.59
2918.27
2910.70
2905.17
2899.46
2891.74
2884.08
1873.89
1868.70
720.11
714.56
708.84
638.75
-0.00

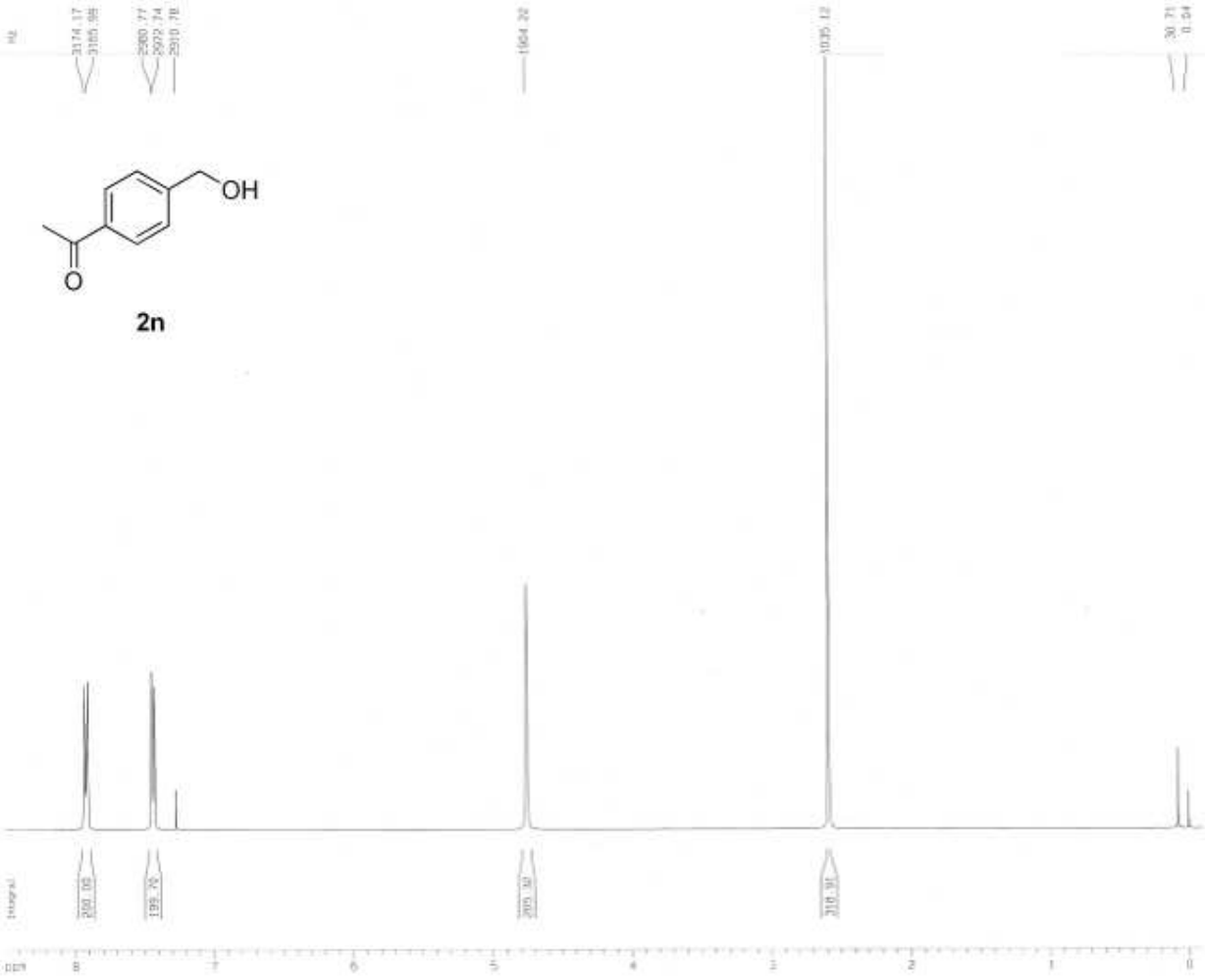



```
Current Data Parameters
NAME                  jul-10
EXPNO                     16
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100707
Time                   15.48
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1035
DS                         2
SWH                31847.133 Hz
FIDRES              0.485940 Hz
AQ                  1.0289652 sec
RG                     3649.1
DW                    15.700 usec
DE                     6.00 usec
TE                     298.2 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1               100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2               400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127290 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                     30.00 cm
CY                     45.00 cm
F1P                   210.000 ppm
F1                  21128.67 Hz
F2P                    -5.000 ppm
F2                   -503.06 Hz
PPMCM                7.16667 ppm/cm
HZCM               721.05786 Hz/cm
```

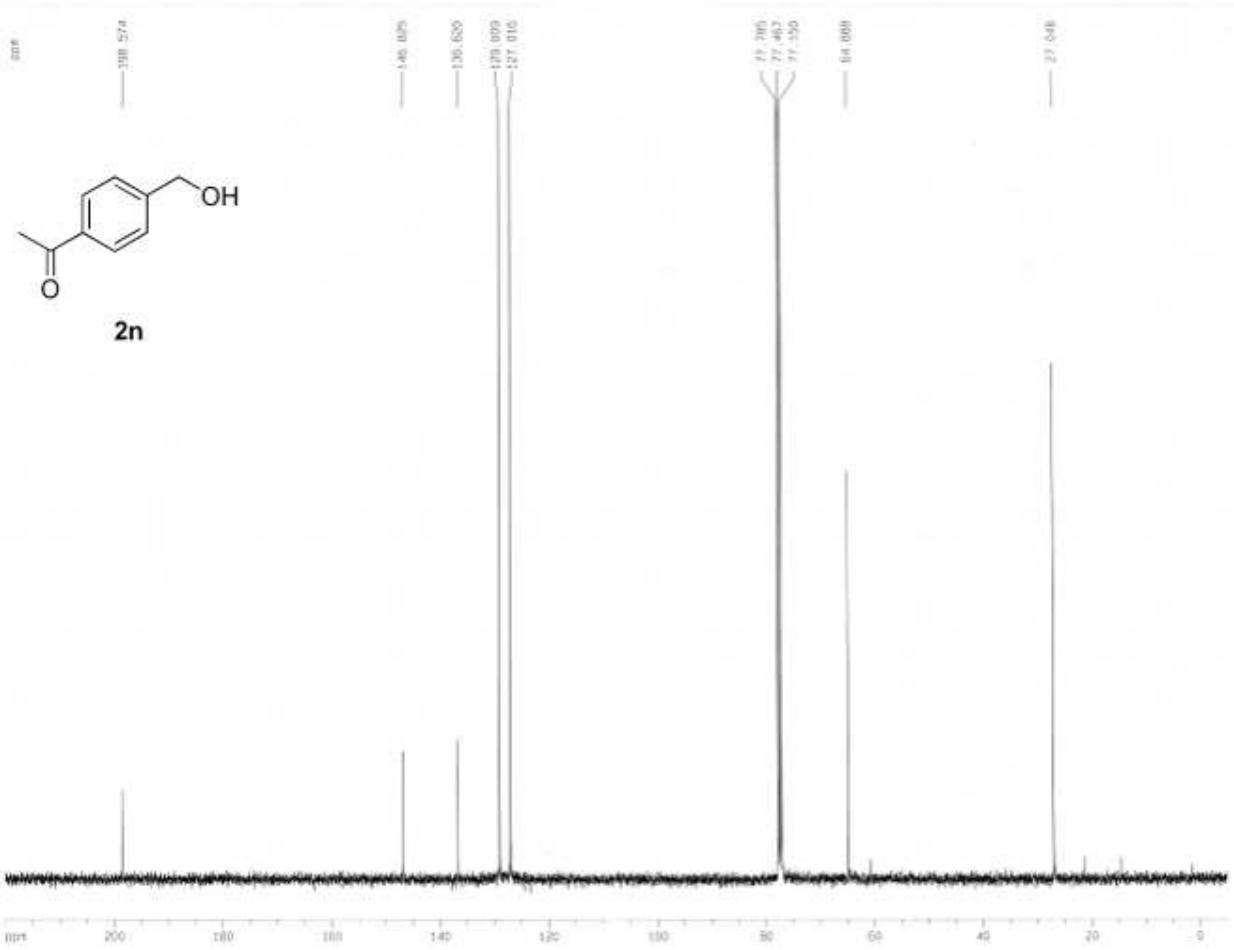

2m
I
OH



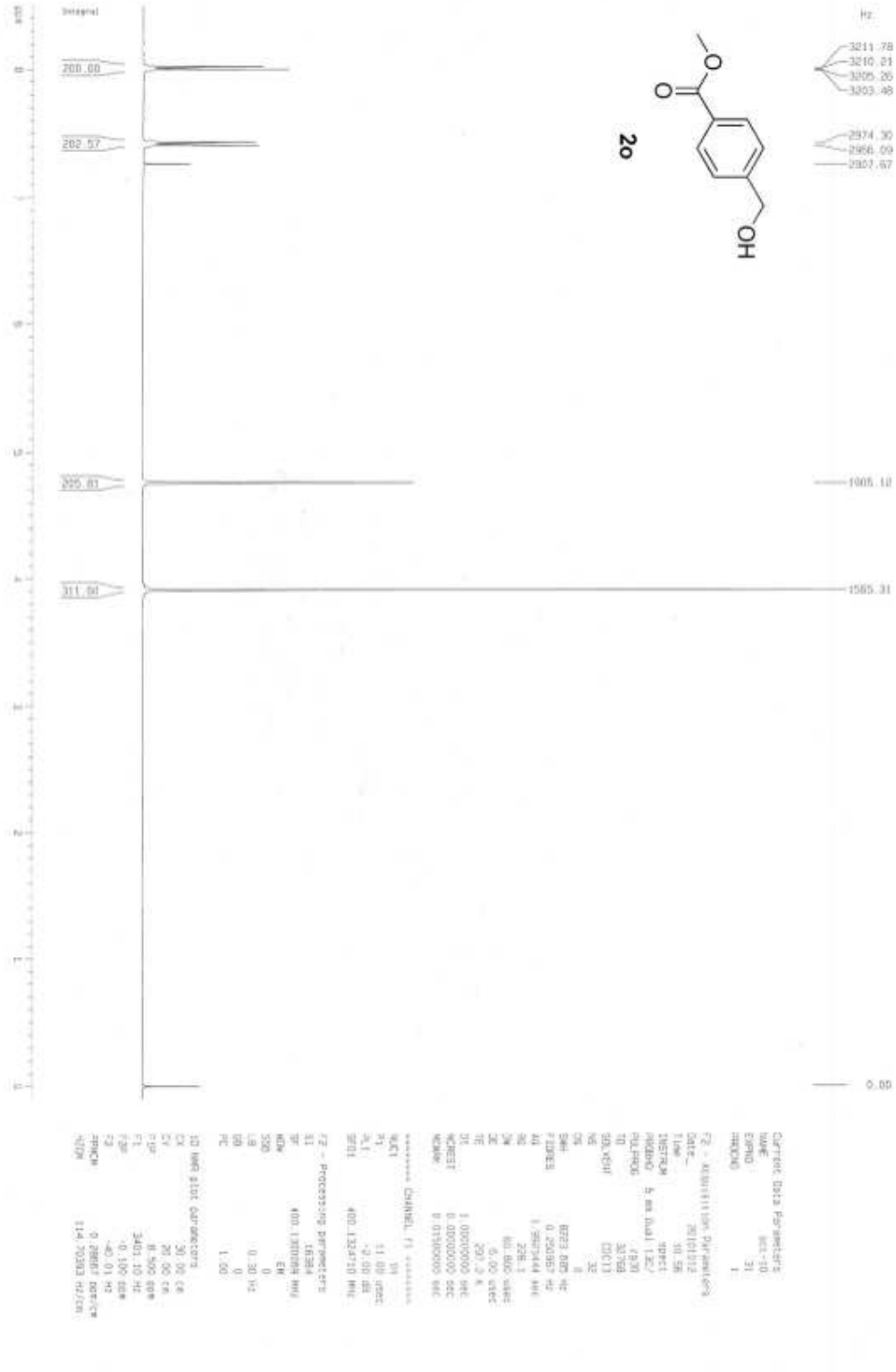

```
Current Data Parameters
NAME                  jul-10
EXPNO                     54
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100729
Time                  13.03
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      2048
DS                         2
SWH               31847.133 Hz
FIDRES                0.485949 Hz
AQ                1.0288652 sec
RG                     2896.3
DW                   15.700 usec
DE                    6.00 usec
TE                    296.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89999998 sec
PCREST             0.00000000 sec
PCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2             400.1324709 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127290 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      30.00 cm
CY                      90.00 cm
F1P                   210.000 ppm
F1                  21128.87 Hz
F2P                    -5.000 ppm
F2                   -503.06 Hz
PPMCM                7.16667 ppm/cm
HZCM               721.05786 Hz/cm
```

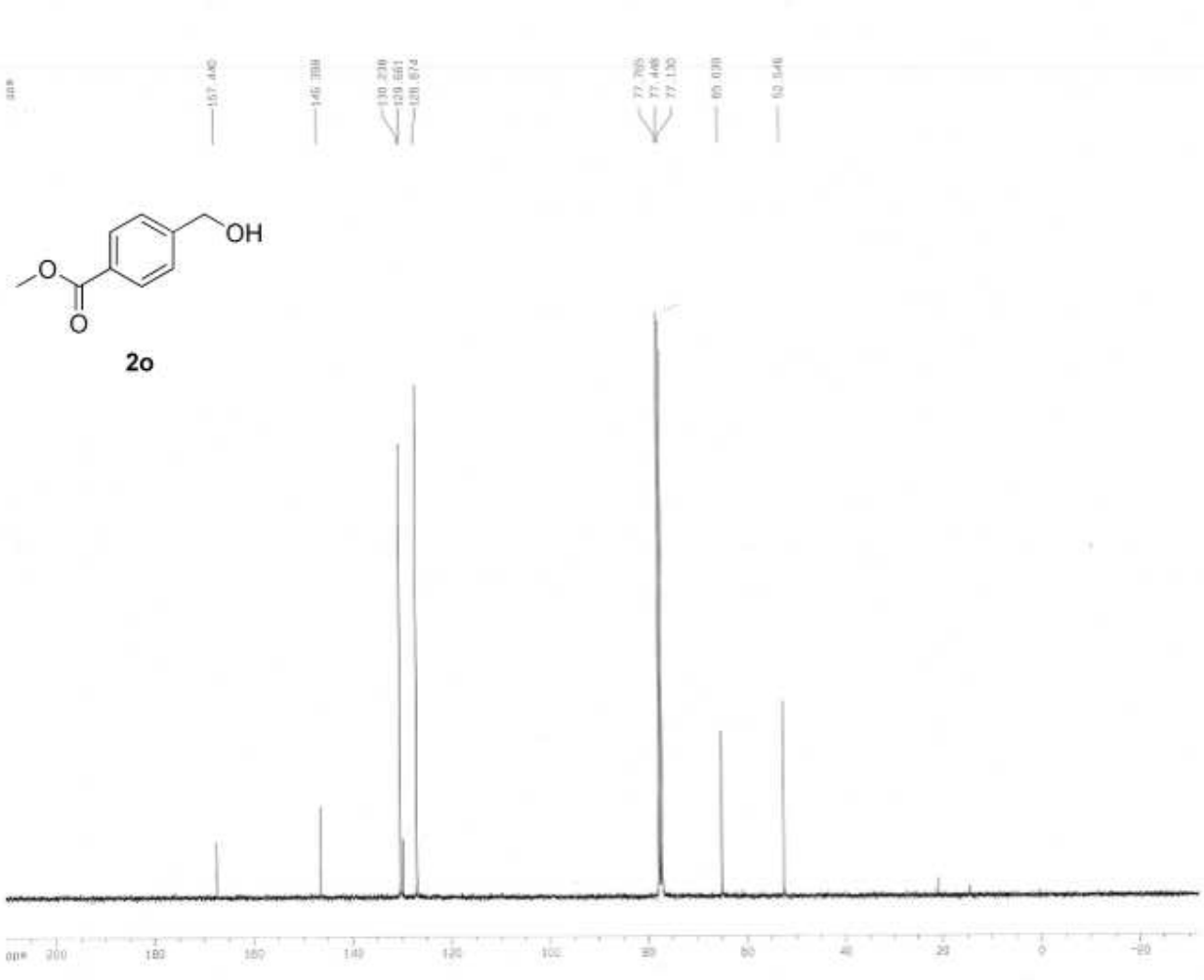



```
Current Data Parameters
NAME                  jul-10
EXPNO                     47
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100727
Time                   15.08
INSTRUM                spect
PROBHD    5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT                CDCl3
NS                        20
DS                         0
SWH               8223.685 Hz
FIDRES               0.250867 Hz
AQ                1.9923444 sec
RG                     161.3
DW                    60.800 usec
DE                     6.00 usec
TE                    298.2 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF              400.1300035 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     30.00 cm
CY                     20.00 cm
F1P                    8.500 ppm
F1                  3401.10 Hz
F2P                   -0.100 ppm
F2                    -40.01 Hz
PPMCM               0.38667 ppm/cm
HZCM               154.70393 Hz/cm
```



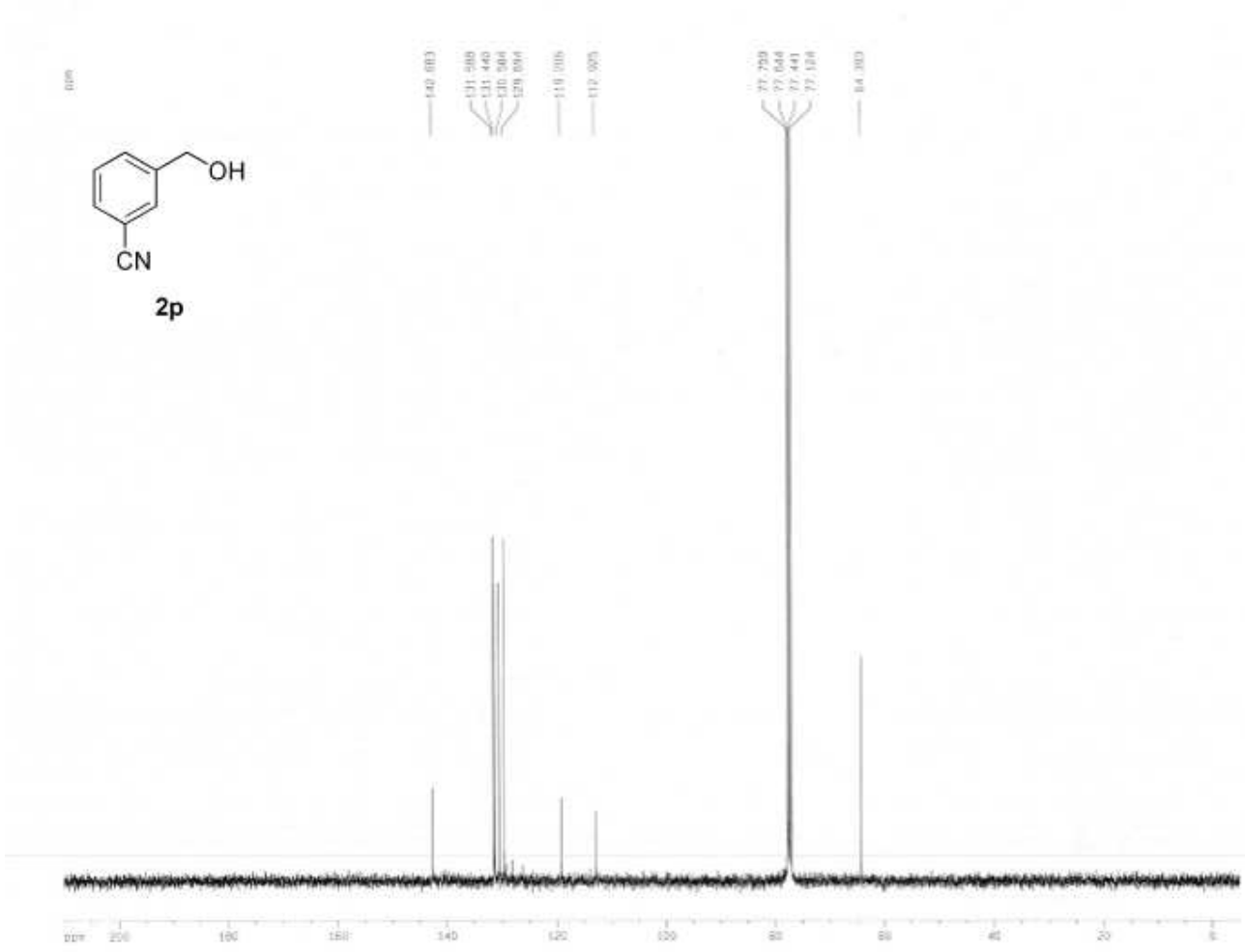

```
Current Data Parameters
NAME                  jul-10
EXPNO                     48
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100727
Time                   15.26
INSTRUM                spect
PROBHD     5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       900
DS                         2
SWH               31847.133 Hz
FIDRES             0.485948 Hz
AQ                 1.0289652 sec
RG                     203.2
DW                    15.700 usec
DE                     6.00 usec
TE                     298.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.05000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    16.00 dB
PL13                    20.00 dB
SFO2              400.1324705 MHz

F2 - Processing parameters
SI                       32768
SF                100.6127290 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                     30.00 cm
CY                     35.00 cm
F1P                  220.000 ppm
F1                  22134.80 Hz
F2P                   -5.000 ppm
F2                   -503.06 Hz
PPMCM                7.50000 ppm/cm
HZCM               754.59548 Hz/cm
```


Integral
200.00
202.57
295.81
311.91
Hz
3211.78
3210.21
3205.26
3203.48
2974.30
2966.09
2957.67
1905.12
1565.31
0.00
2o
O
O
OH

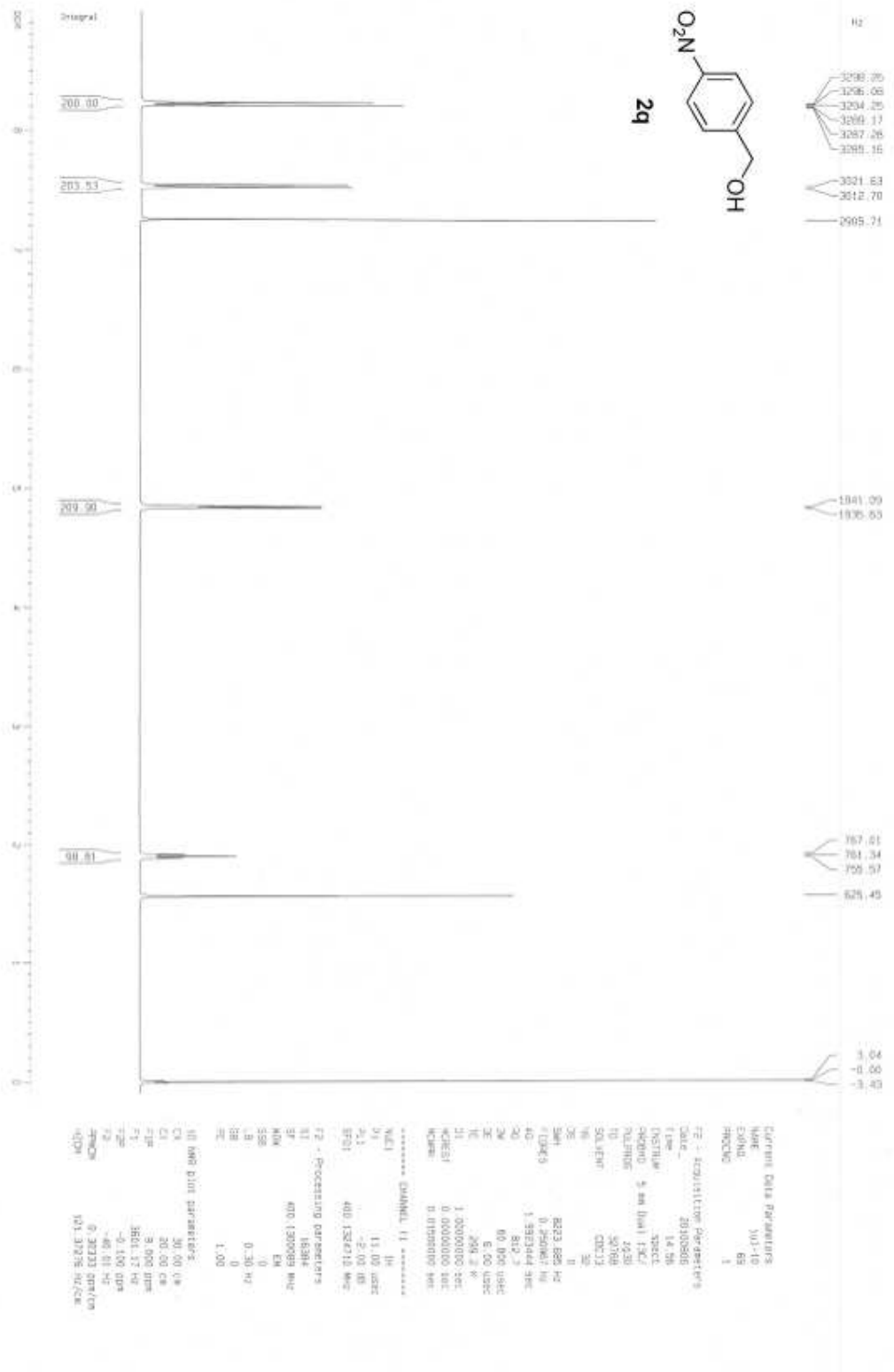


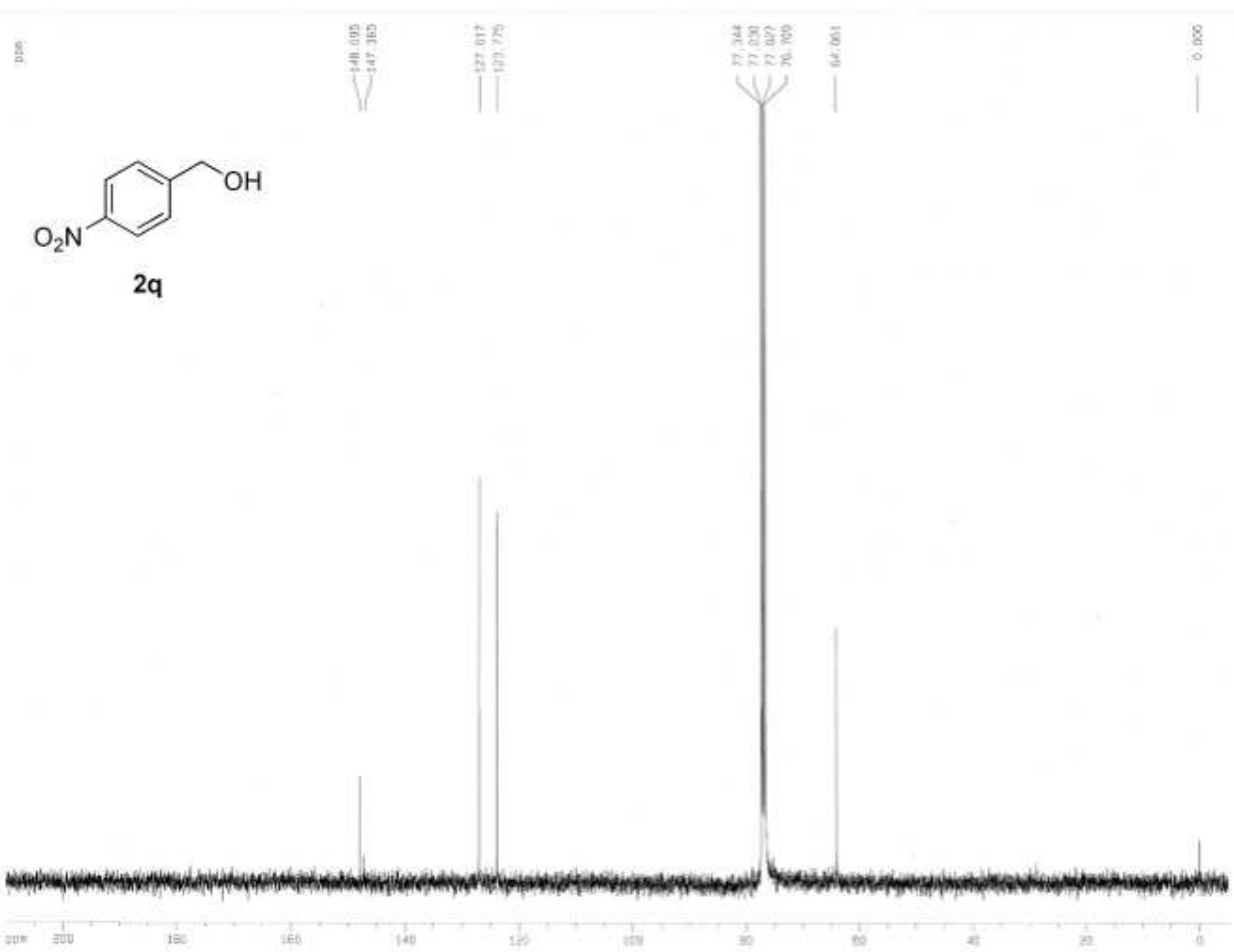

```
Current Data Parameters
NAME                  oct-10
EXPNO                     32
PROCNO                     1

F2 - Acquisition Parameters
Date_              20101012
Time                   13.43
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1432
DS                         2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                   297.2 K
D1                2.00000000 sec
D11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF                100.6127290 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       30.00 cm
CY                       15.00 cm
F1P                    210.000 ppm
F1                   21128.68 Hz
F2P                    -31.973 ppm
F2                   -3216.79 Hz
PPMCM                 6.96573 ppm/cm
HZCM                 811.51556 Hz/cm
```

Integral
94.98
197.67
100.00
100.04
100.03
CN
OH
2p
Hz
3072.61
3045.59
3037.90
3028.31
2996.44
2988.72
2981.00
2907.58
1951.01
828.53
658.57
0.00

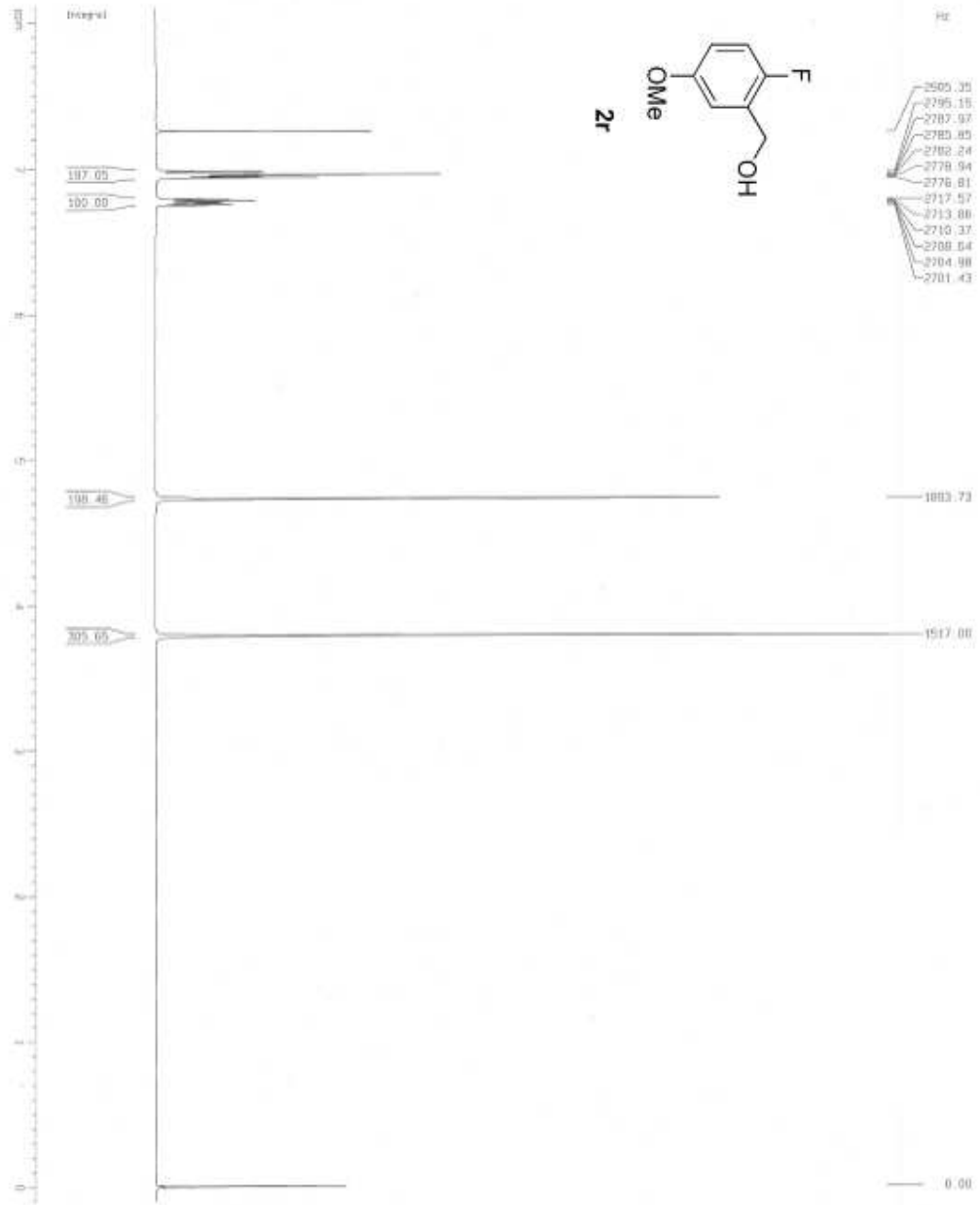



```
Current Data Parameters
NAME                  ju1-10
EXPNO                     52
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100720
Time                   11.08
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       2
SWH              31847.133 Hz
FIDRES           0.485949 Hz
AQ               1.0289852 sec
RG                     114
DW                 15.700 usec
DE                  6.00 usec
TE                 295.2 K
D1              2.00000000 sec
D11             0.03000000 sec
DELTA           1.89998998 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1          100.6254958 MHz

======== CHANNEL f2 ========
DPRGF2              waltz16
NUC2                    1H
PCPD2              105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2          400.1324709 MHz

F2 - Processing parameters
SI                     32768
SF            100.6127290 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   30.00 cm
F1P                 210.000 ppm
F1                 21128.67 Hz
F2P                  -5.000 ppm
F2                 -503.06 Hz
PPMCM              7.18667 ppm/cm
HZCM             721.05786 Hz/cm
```

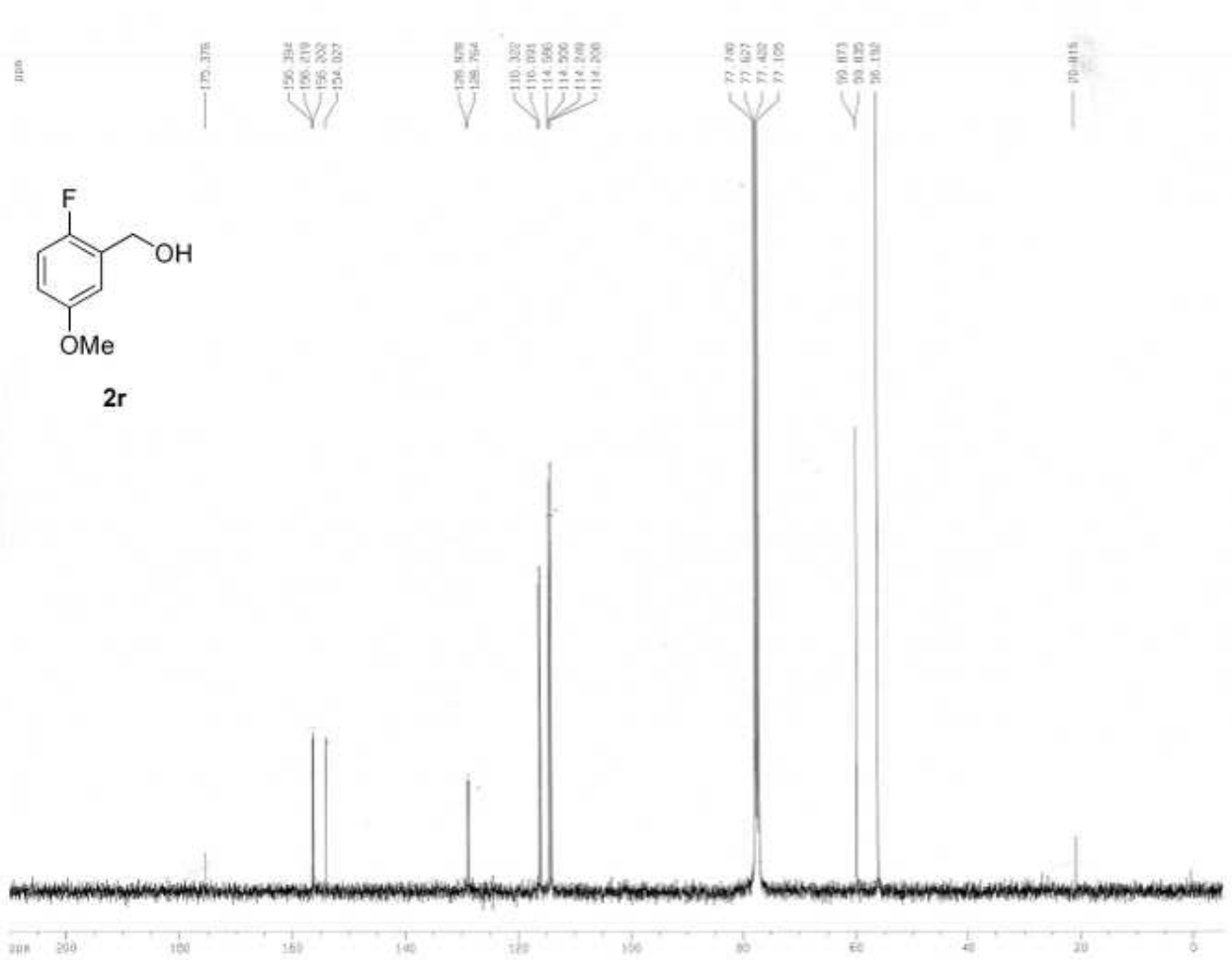

2q
O2N
OH
Integral
200.00
203.53
209.90
98.81
3298.25
3296.06
3294.25
3289.17
3287.26
3285.16
3021.63
3012.70
2905.71
1841.09
1835.63
767.01
761.34
755.57
625.45
3.04
-0.00
-3.43



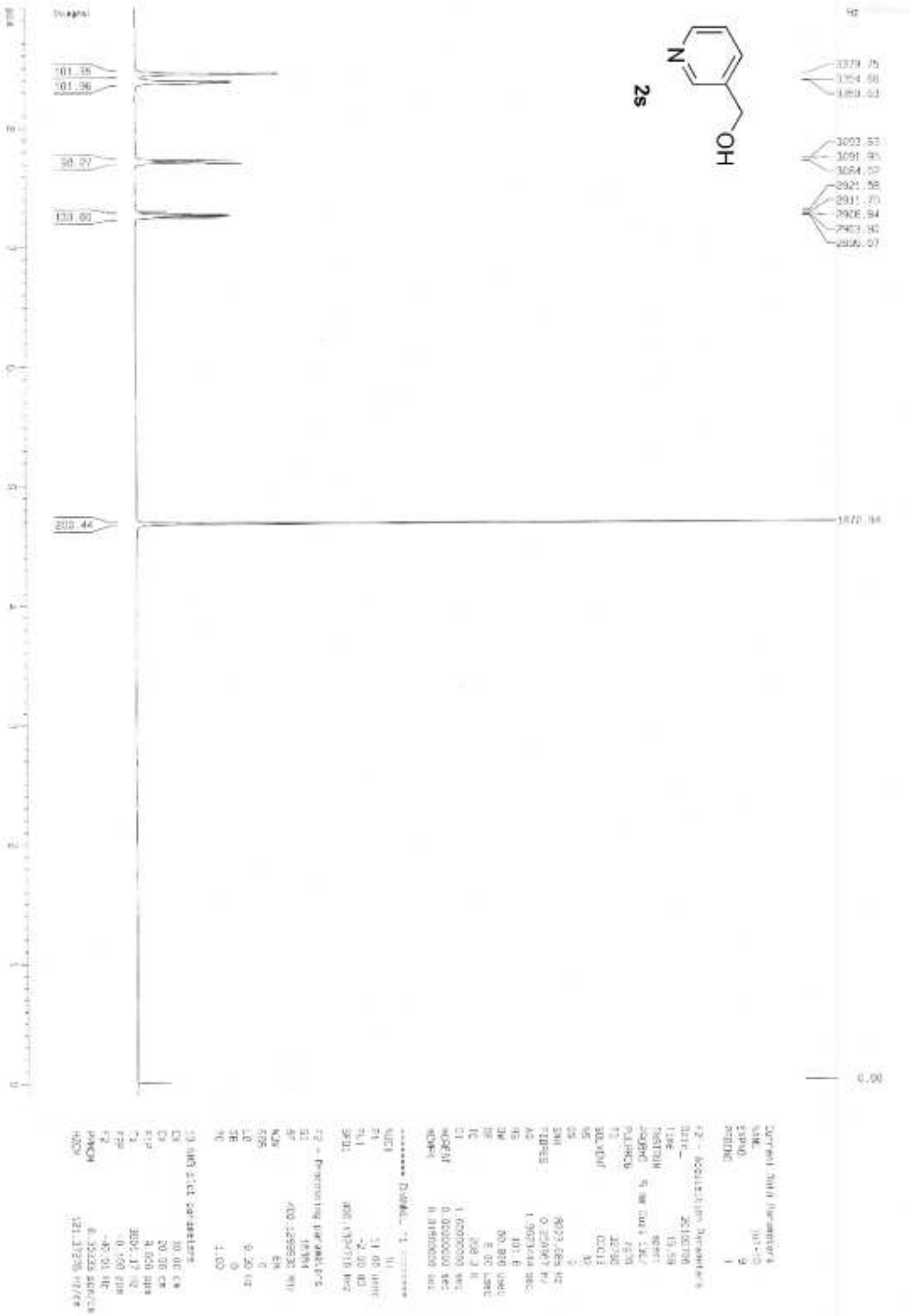

```
Current Data Parameters
NAME                  (u)-10
EXPNO                     70
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100606
Time                   15.14
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgdc30
TD                       65536
SOLVENT                  CDCl3
NS                        4096
DS                           2
SWH                31847.133 Hz
FIDRES              0.485949 Hz
AQ                  1.0289952 sec
RG                     3649.1
DW                    15.700 usec
DE                     6.00 usec
TE                     299.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
DELTA               1.89999998 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127682 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                        30.00 cm
CY                        19.00 cm
F1P                     210.000 ppm
F1                    21128.56 Hz
F2P                      -5.000 ppm
F2                     -503.06 Hz
PPMCM                  7.16667 ppm/cm
HZCM                  721.05817 Hz/cm
```

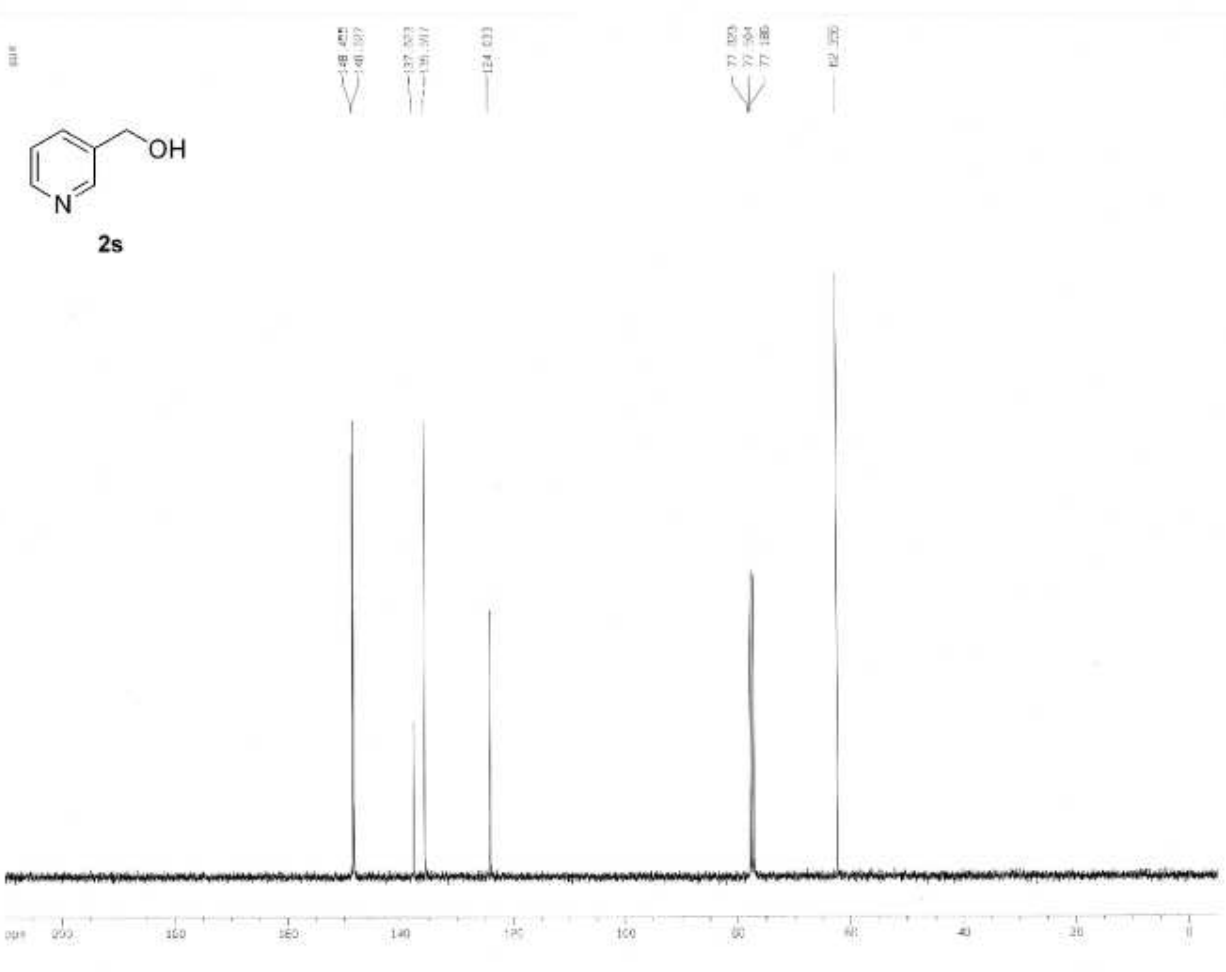


Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm PABBO BB/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F2P
PPM
HZ
PPMCM
HZCM




```
Current Data Parameters
NAME                  acc-10
EXPNO                    124
PROCNO                     1

F2 - Acquisition Parameters
Date_              20101222
Time                   17.46
INSTRUM                spect
PROBHD     5 mm Dual 13C/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      5834
DS                         2
SWH                31847.133 Hz
FIDRES             0.485849 Hz
AQ                 1.0289652 sec
RG                       181
DW                  15.700 usec
DE                   6.00 usec
TE                  298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89969998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1               100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2               400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127290 MHz
WDW                          EM
SSB                           0
LB                       1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                       30.00 cm
CY                       20.00 cm
F1P                    210.000 ppm
F1                   21128.67 Hz
F2P                     -5.000 ppm
F2                    -503.05 Hz
PPMCM                 7.16667 ppm/cm
HZCM                721.05786 Hz/cm
```


2s
N
OH
101.35
101.96
98.27
133.00
203.44
3379.75
3354.66
3353.53
3093.53
3091.95
3084.52
2921.58
2911.70
2906.94
2903.92
2906.07
1872.94
0.00



Current Data Parameters
NAME jul-10
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100706
Time 16.04
INSTRM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 130
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 1290.2
DW 15.700 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000300 sec
D16 0.00100000 sec

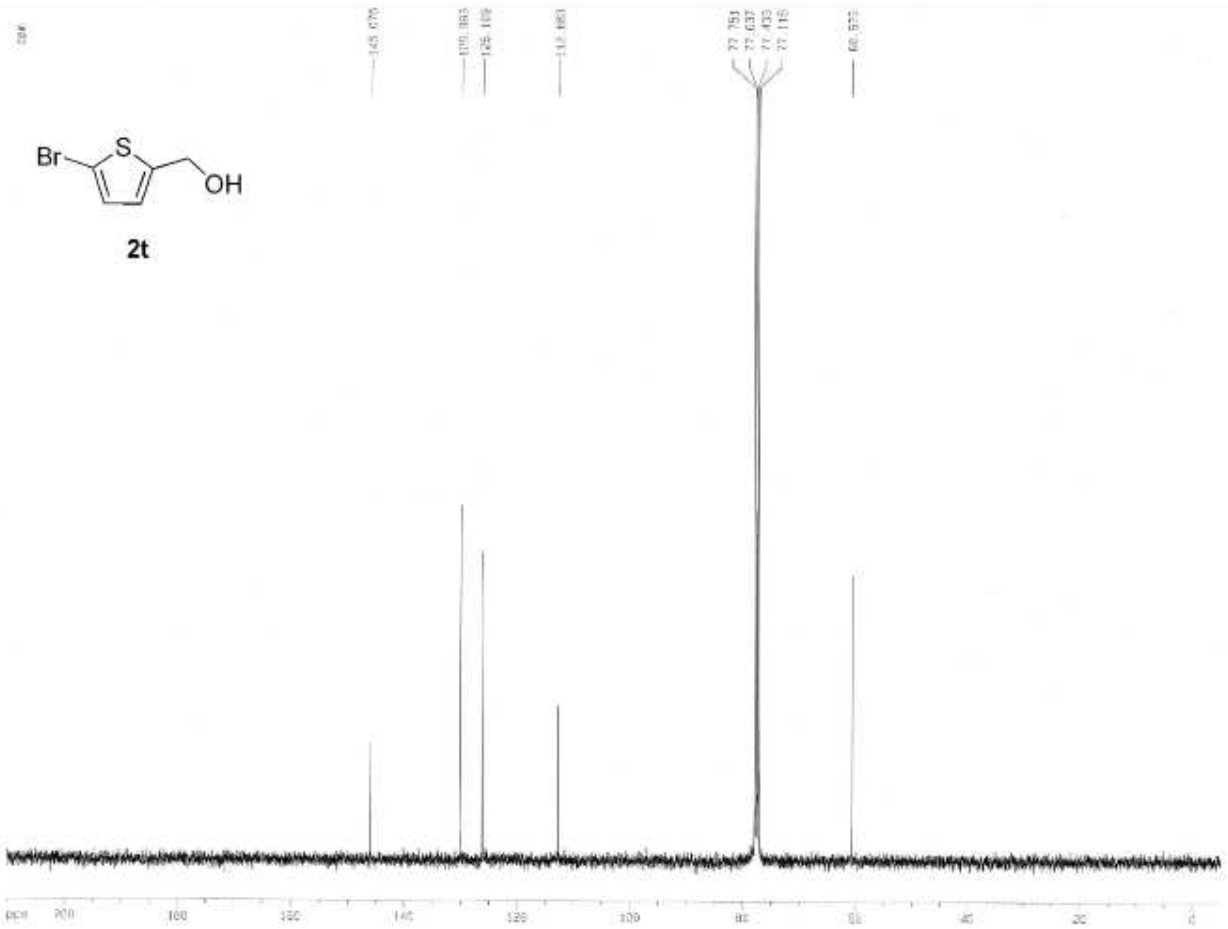
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 210.000 ppm
F1 21130.67 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.10057 ppm/cm
HZCM 714.00786 Hz/cm

Br
S
OH
2t



Current Data Parameters
NAME 2ct-10
EXPNO 6
PROCNO 1

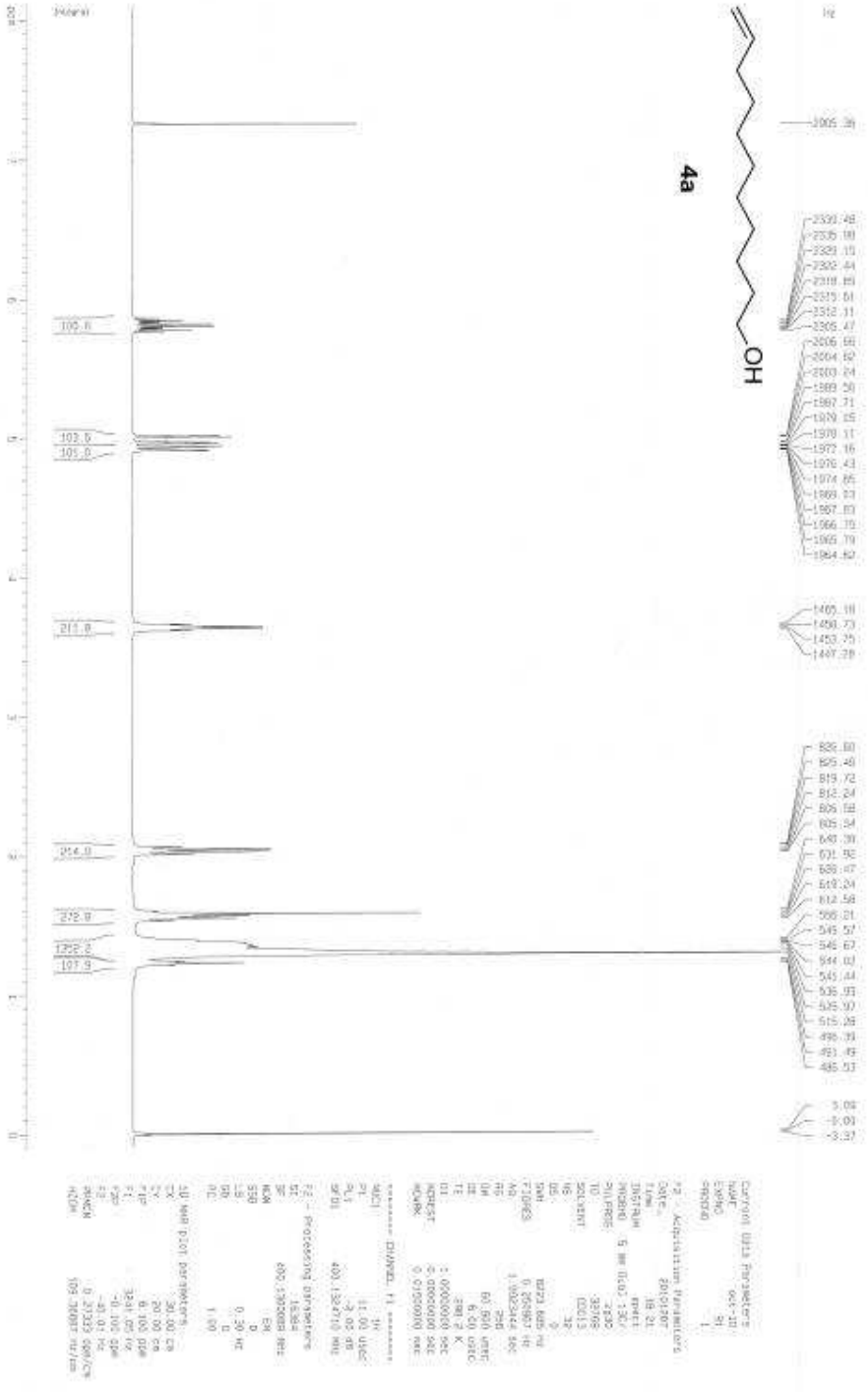
F2 - Acquisition Parameters
Date_ 20181007
Time 10.40
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1167
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289050 sec
RG 3645.1
DW 15.700 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.09000000 sec
MCWRK 0.01500000 sec

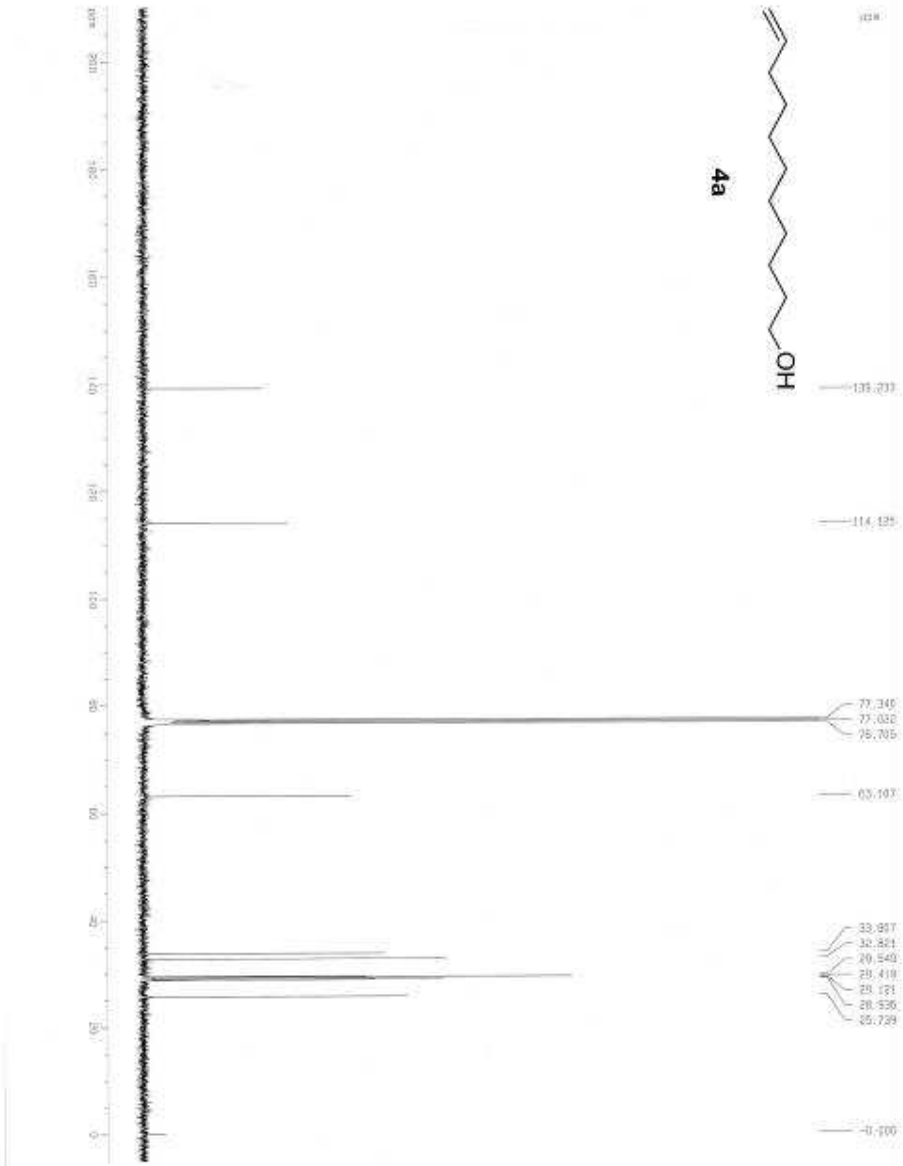
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 +1.00 dB
SFO1 100.6256359 MHz

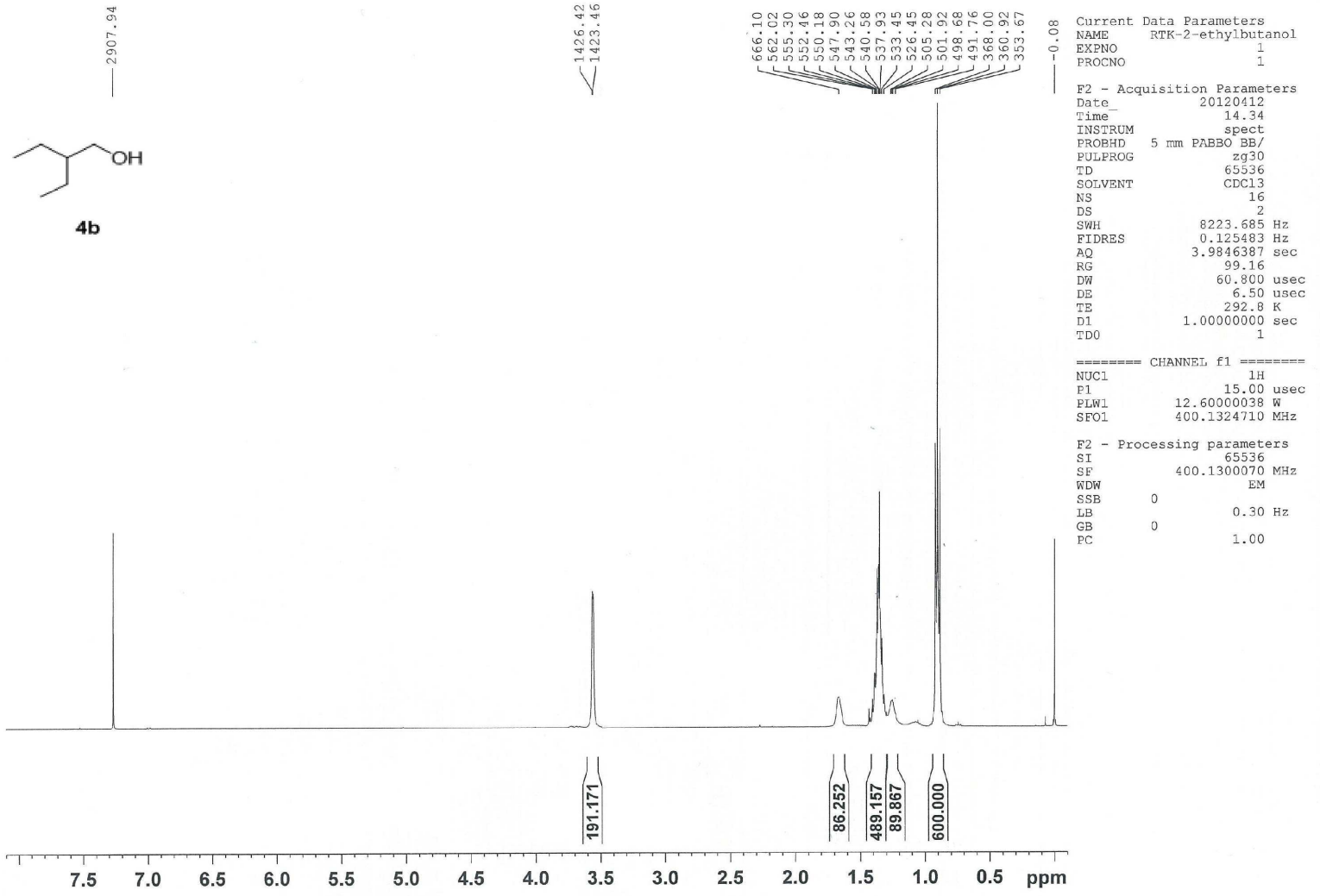
======== CHANNEL f2 ========
DECOUPLE waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324709 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

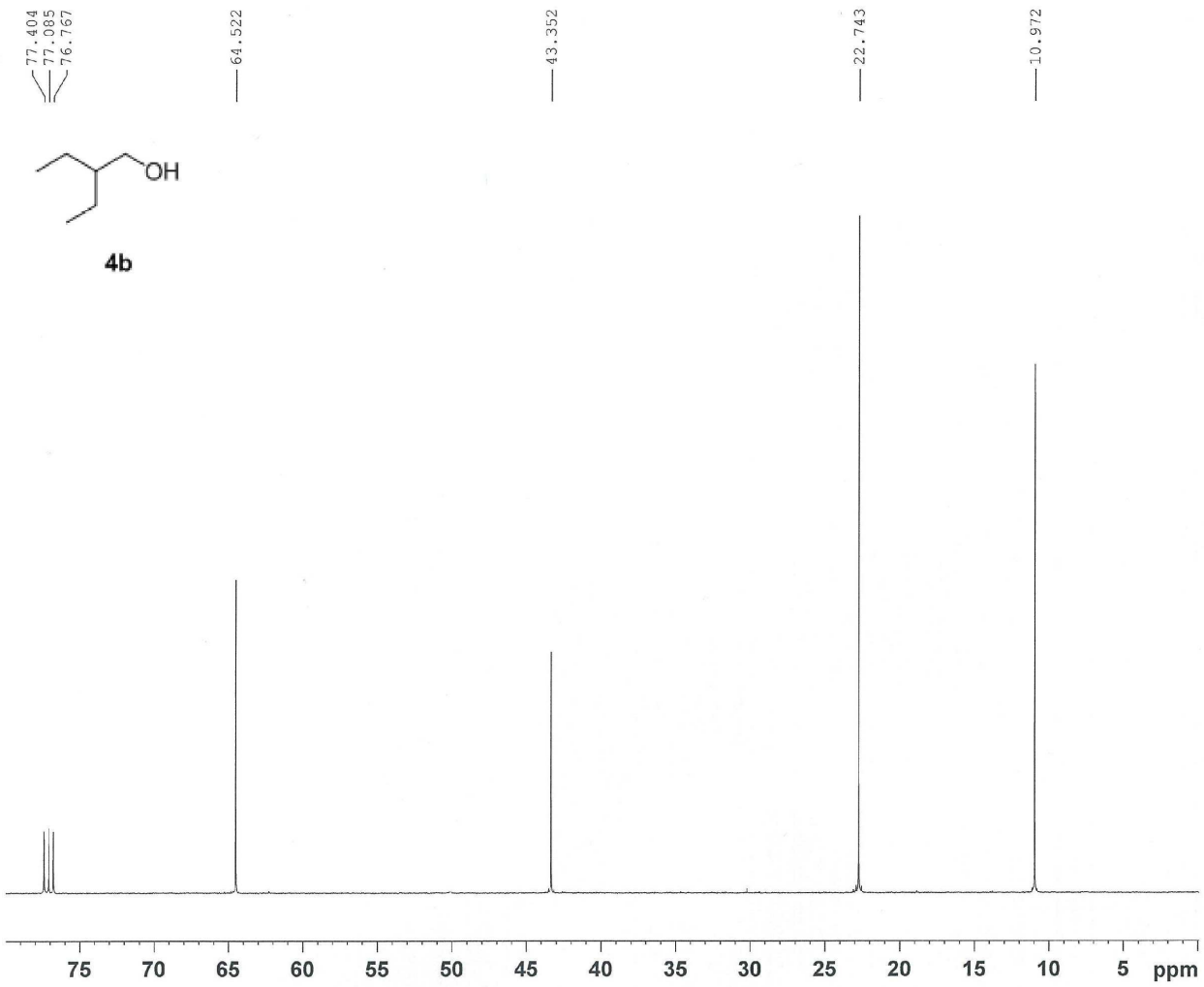
1D NMR plot parameters
CX 30.00 cm
CY 24.00 cm
F1P 210.000 ppm
F1 21139.67 Hz
F2P -8.500 ppm
F2 -853.08 Hz
PPMCM 7.16667 ppm/cm
HZCM 721.05788 Hz/cm


4a
OH

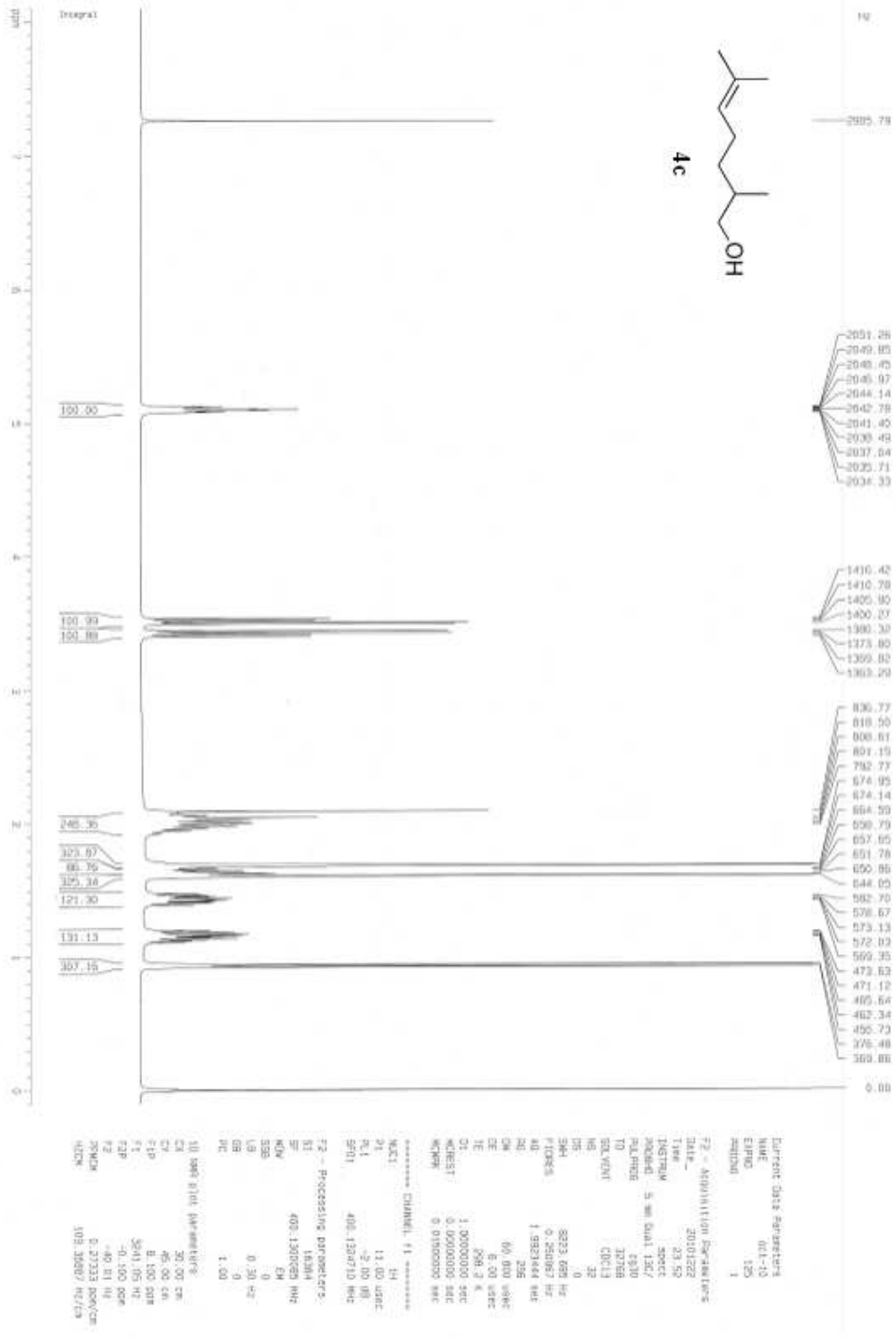

4a
OH
135.233
114.125
77.340
77.032
76.705
63.107
33.857
32.821
29.540
29.419
29.131
28.536
25.739
0.000

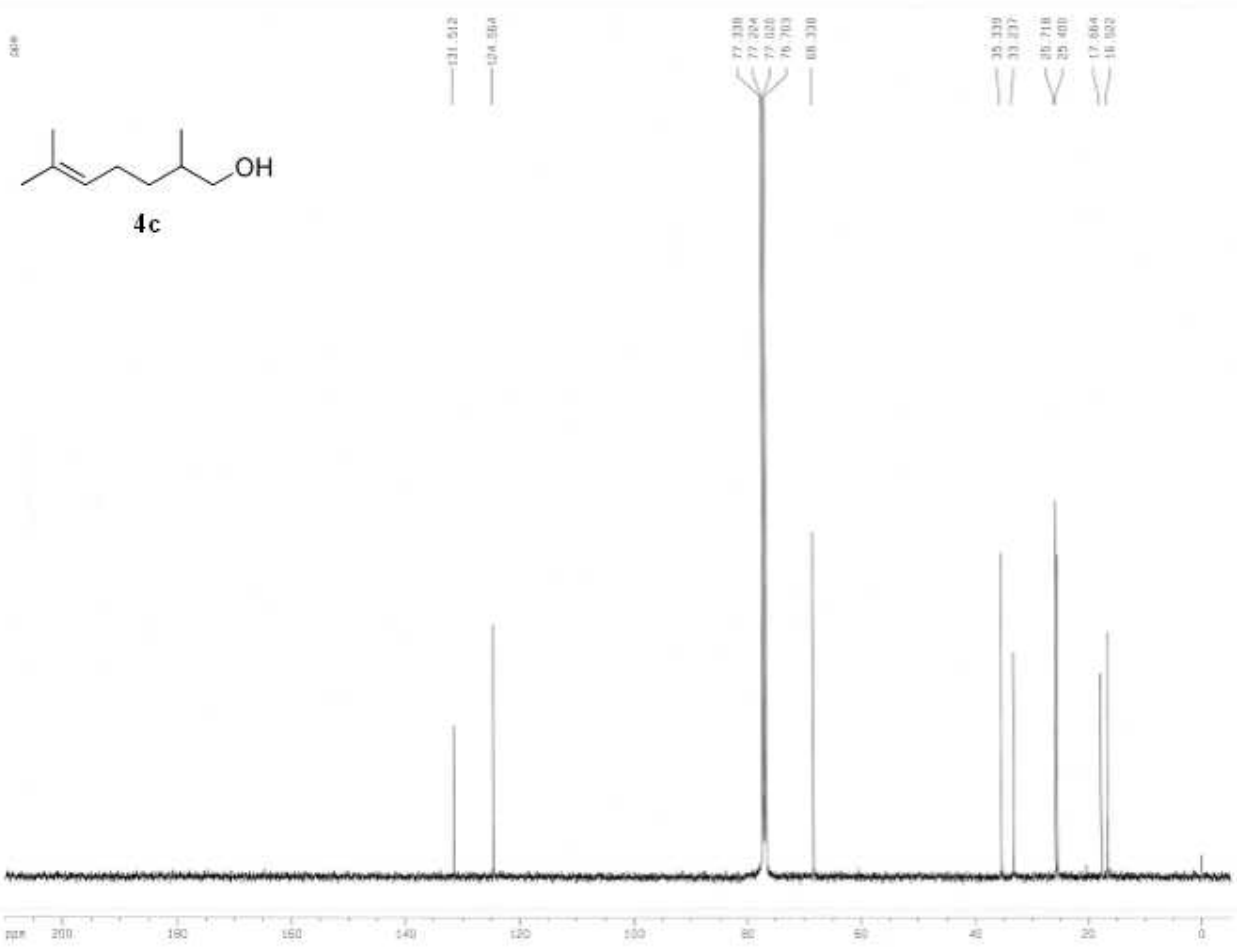



```
Current Data Parameters
NAME      RTK-2-ethylbutanol
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120412
Time                   14.34
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                     99.16
DW                    60.800 usec
DE                     6.50 usec
TE                    292.8 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1           12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF             400.1300070 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```



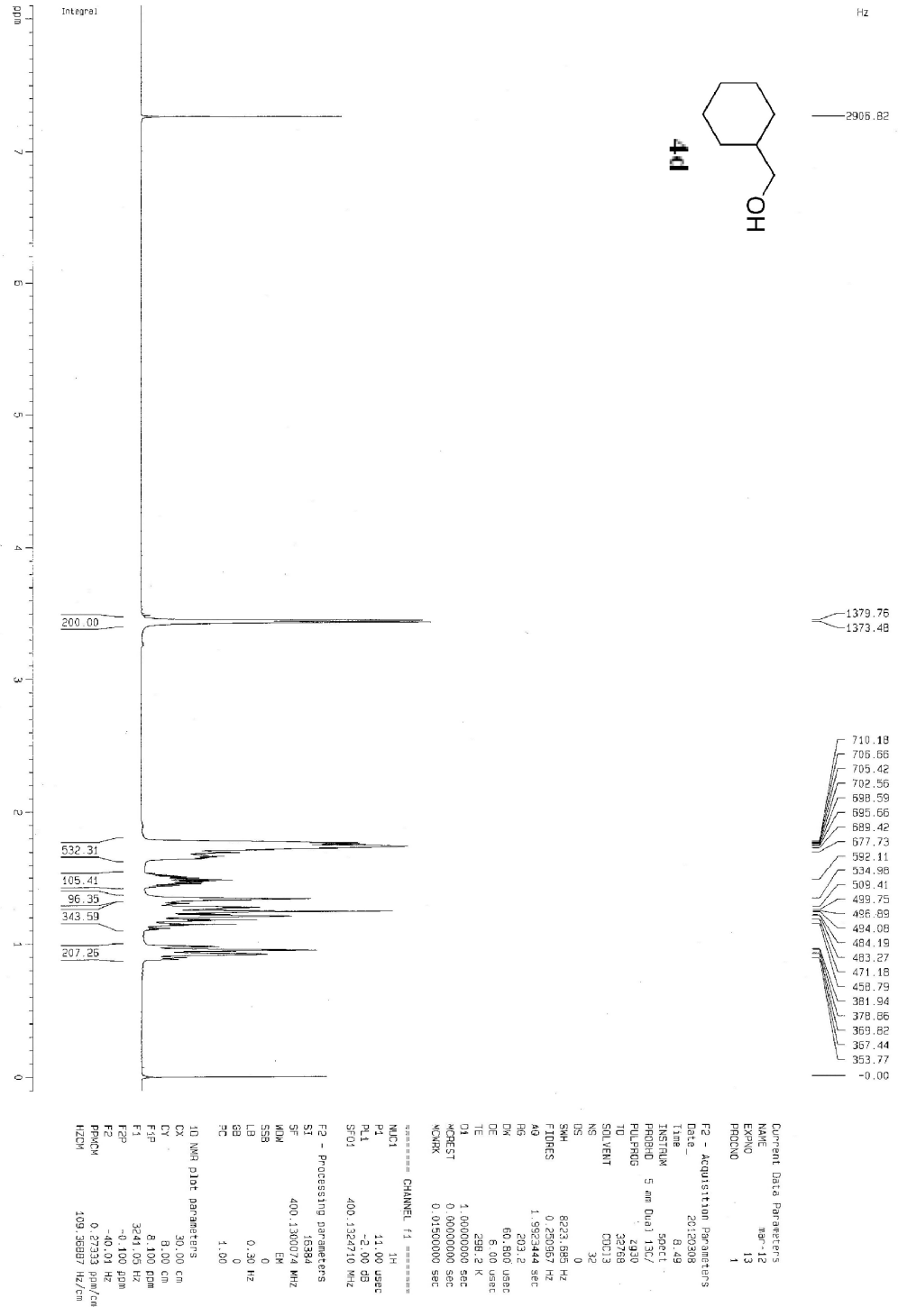

```
Current Data Parameters
NAME      RTK-2ethylbutanol
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120418
Time                 16.11
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                 186.53
DW                 20.800 usec
DE                  6.50 usec
TE                 292.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.98 usec
PLW1         52.09999847 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PLW2         12.60000038 W
PLW12         0.34999999 W
PLW13         0.28349999 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

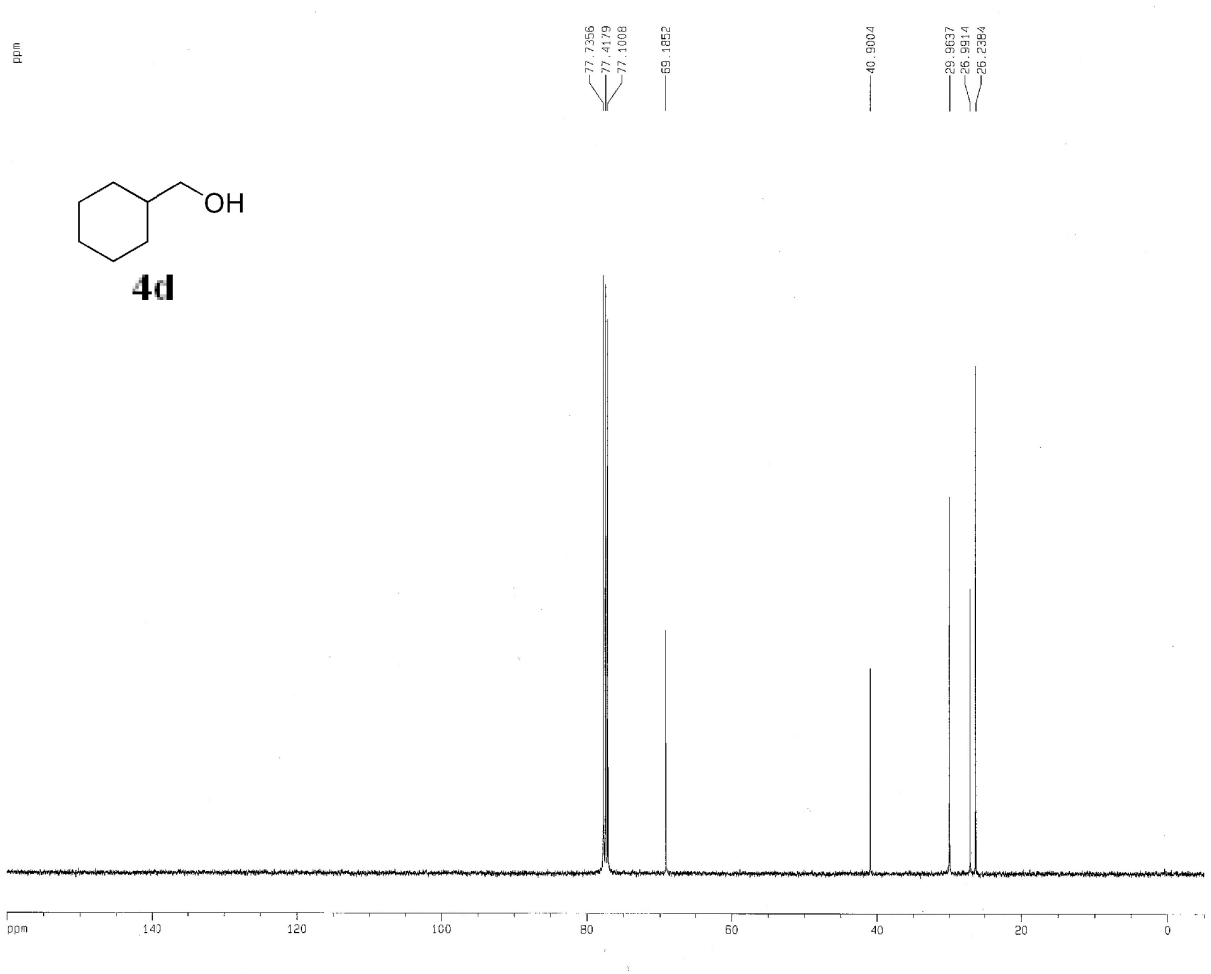

4c
OH



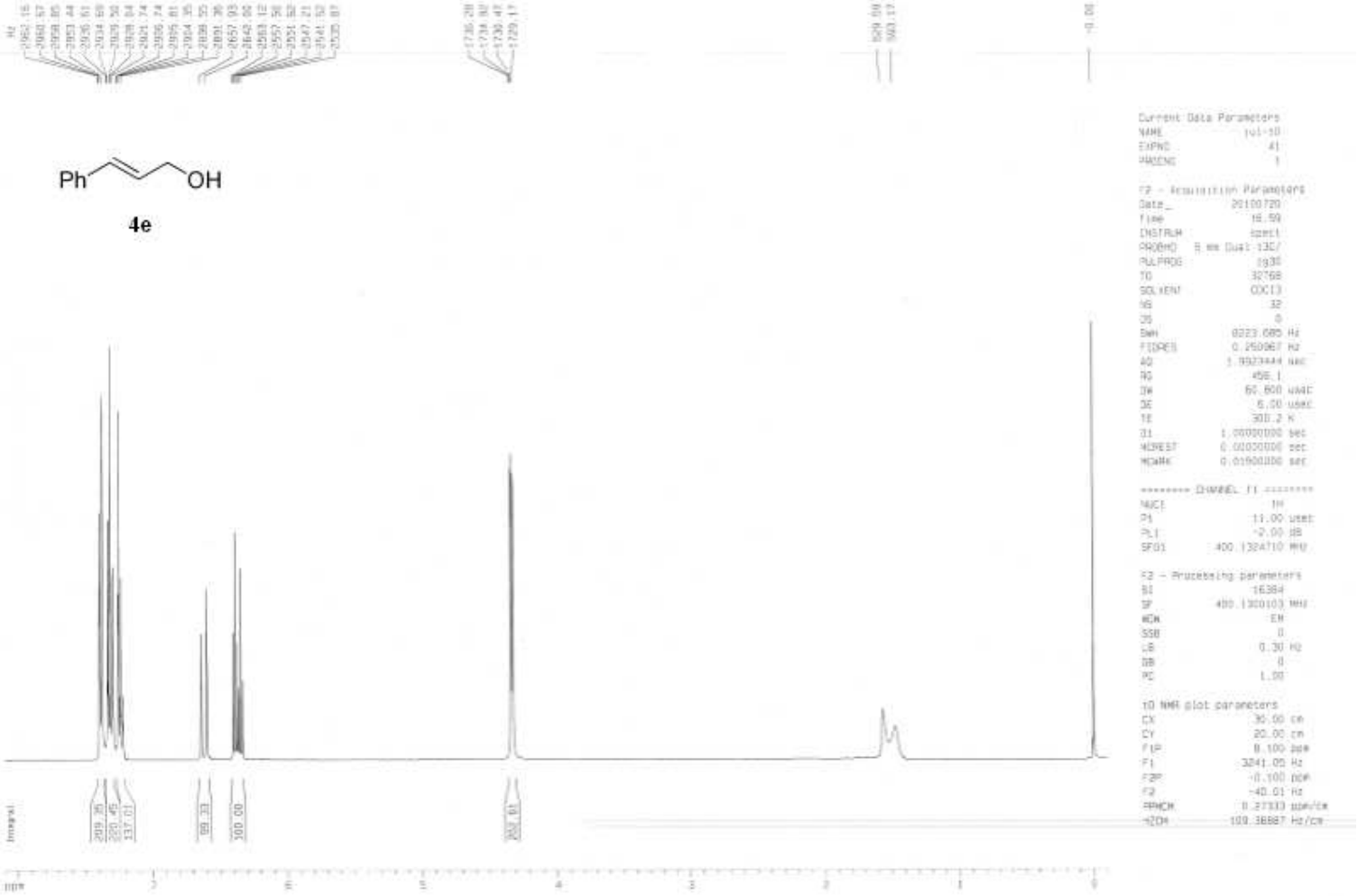
4c

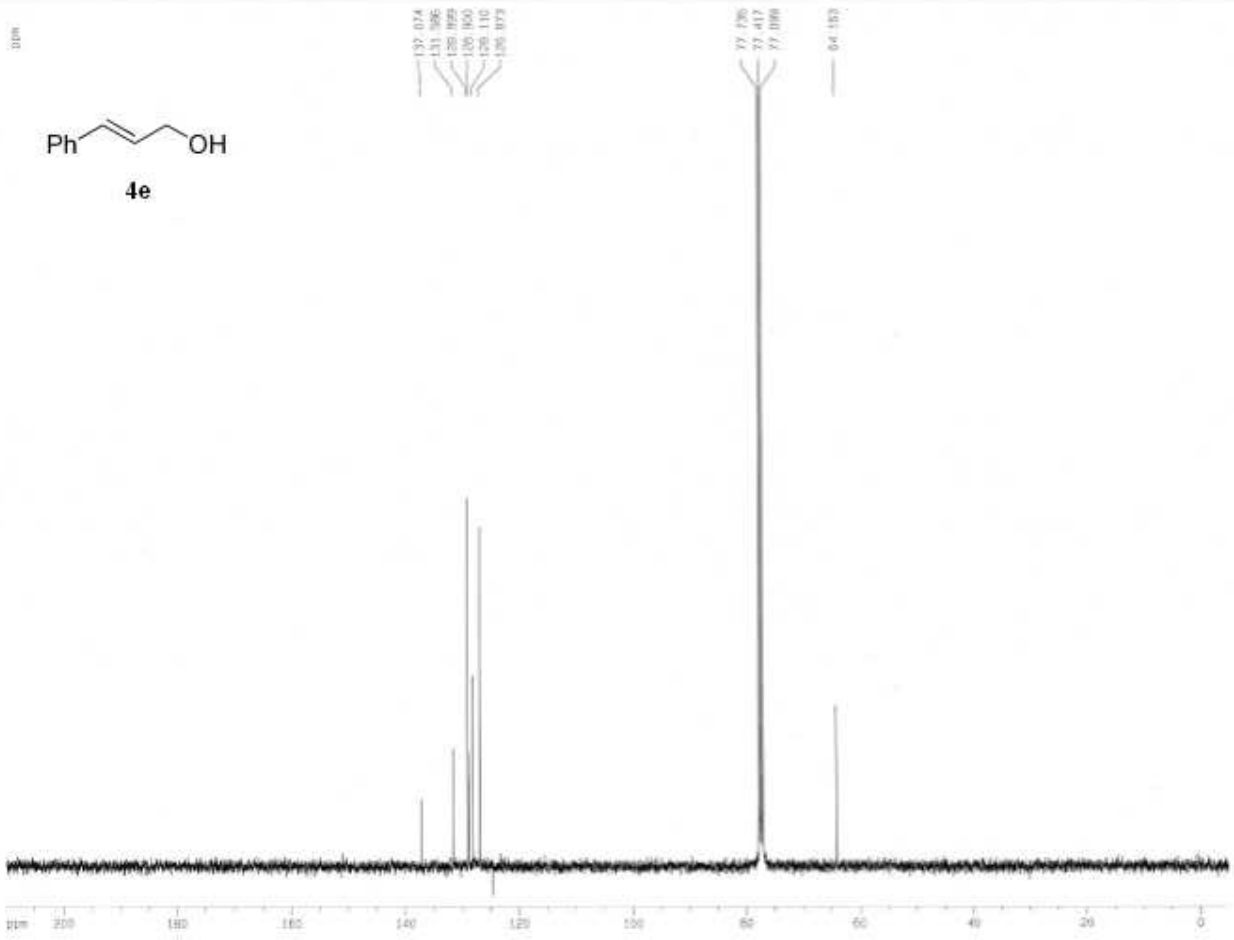
```
Current Data Parameters
NAME                  dcl-10
EXPNO                    120
PROCNO                     1

F2 - Acquisition Parameters
Date_              20101223
Time                   4.18
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    5120
DS                       2
SWH                31847.133 Hz
FIDRES             0.485849 Hz
AQ                 1.0289652 sec
RG                      181
DW                  15.700 usec
DE                   6.00 usec
TE                  298.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1           100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2           400.1324708 MHz

F2 - Processing parameters
SI                      32768
SF              100.6127607 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   45.00 cm
F1P                 250.000 ppm
F1                  25128.68 Hz
F2P                  -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.16667 ppm/cm
HZCM               721.05817 Hz/cm
```


Integral
Hz
ppm
2906.82
1379.76
1373.48
200.00
532.31
105.41
96.35
343.59
207.25
710.18
706.66
705.42
702.56
698.59
695.66
689.42
677.73
592.11
534.98
509.41
499.75
496.89
494.08
484.19
483.27
471.18
458.79
381.94
378.86
369.82
367.44
353.77
-0.00
OH
Current Data Parameters
NAME mar-12
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120308
Time 8.49
INSTRUM 5mm Dual 13C/
PROBHD
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250957 Hz
AQ 1.9923444 sec
RG 203.2
DW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 8.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm




```
Current Data Parameters
NAME                  mar-12
EXPNO                     14
PROCNO                     1

F2 - Acquisition Parameters
Date_              20120308
Time                  10.18
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2048
DS                       2
SWH              31847.133 Hz
FIDRES           0.485948 Hz
AQ               1.0289652 sec
RG                 3649.1
DW                  15.700 usec
DE                   6.00 usec
TE                  298.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.50 usec
PL1                 -1.00 dB
SFO1          100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              105.00 usec
PL2                 -2.00 dB
PL12                18.00 dB
PL13                20.00 dB
SFO2          400.1324708 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127290 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   15.00 cm
F1P                160.000 ppm
F1                16098.04 Hz
F2P                 -5.000 ppm
F2                 -503.06 Hz
PPMCM               5.50000 ppm/cm
HZCM              553.37006 Hz/cm
```


Ph
OH
4e
Current Data Parameters
NAME jul-10
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100720
Time 16.59
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 456.1
DW 60.800 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
MCREST 0.00050000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.38887 Hz/cm
Integral
209.35
220.45
137.01
99.33
100.00
303.61
ppm



Current Data Parameters
NAME jul-10
EXPNO 42
PROCNO 1

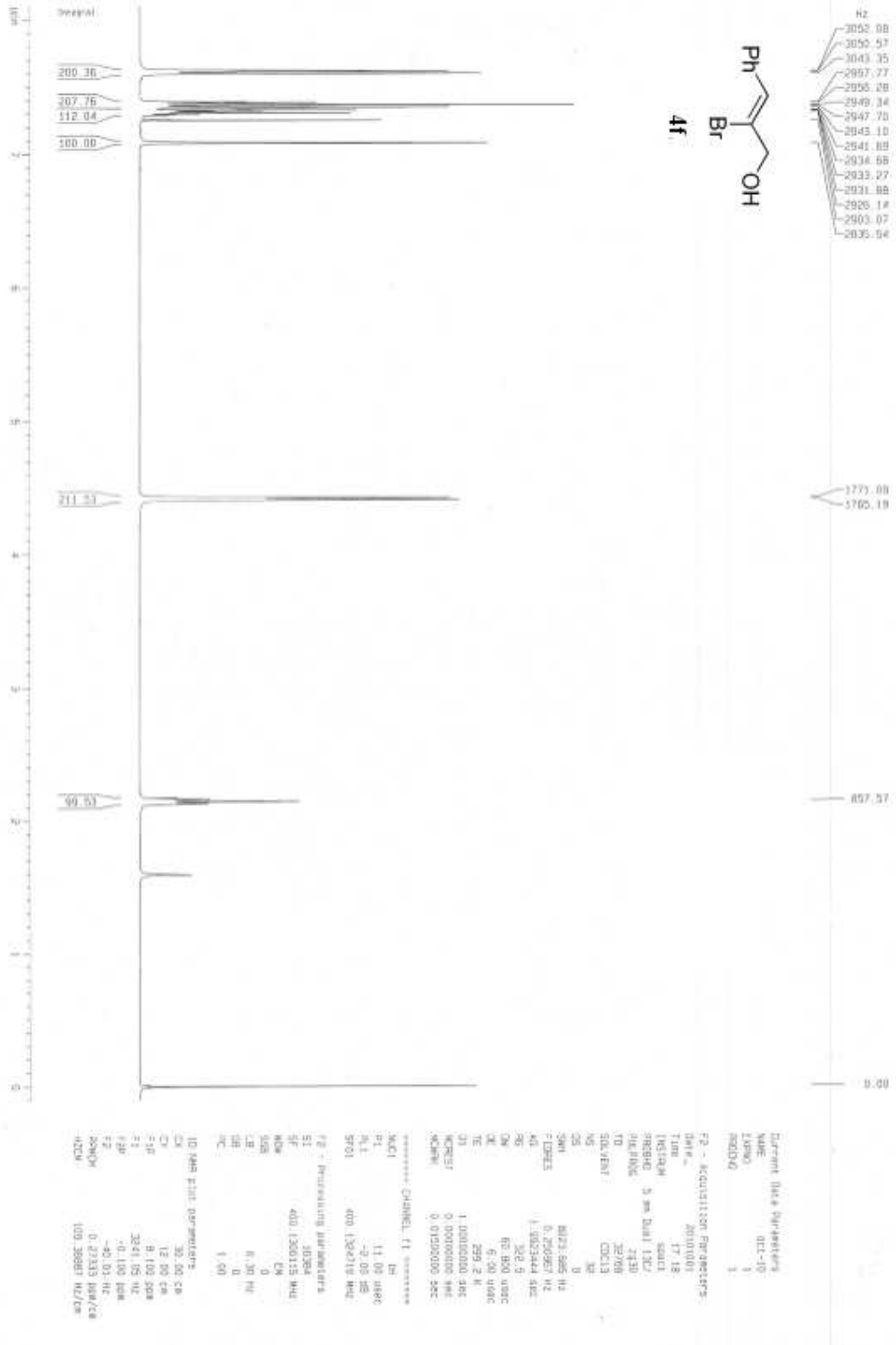
F2 - Acquisition Parameters
Date_ 20100720
Time 17.13
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1552
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 114
DW 15.700 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

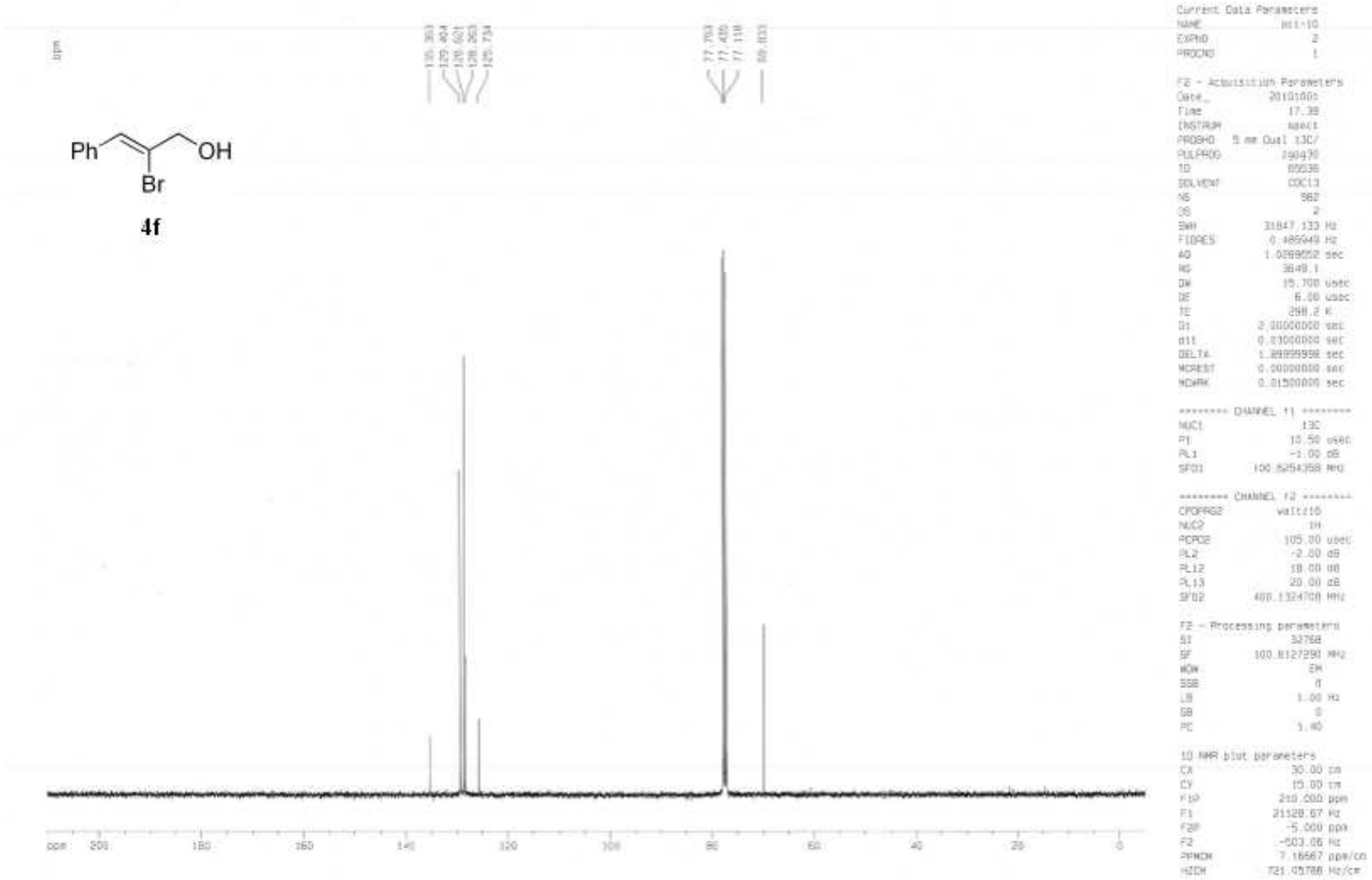
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz

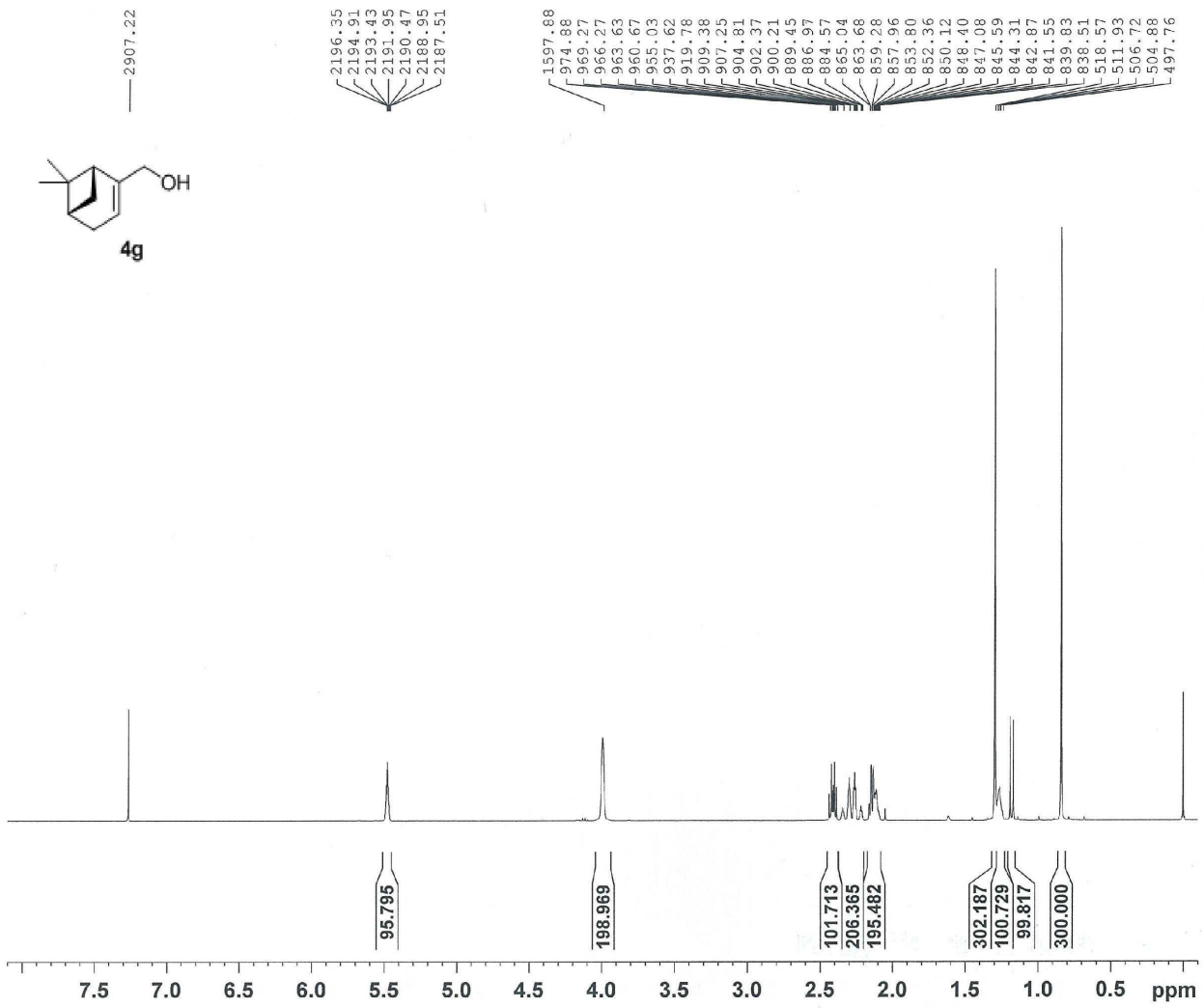
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

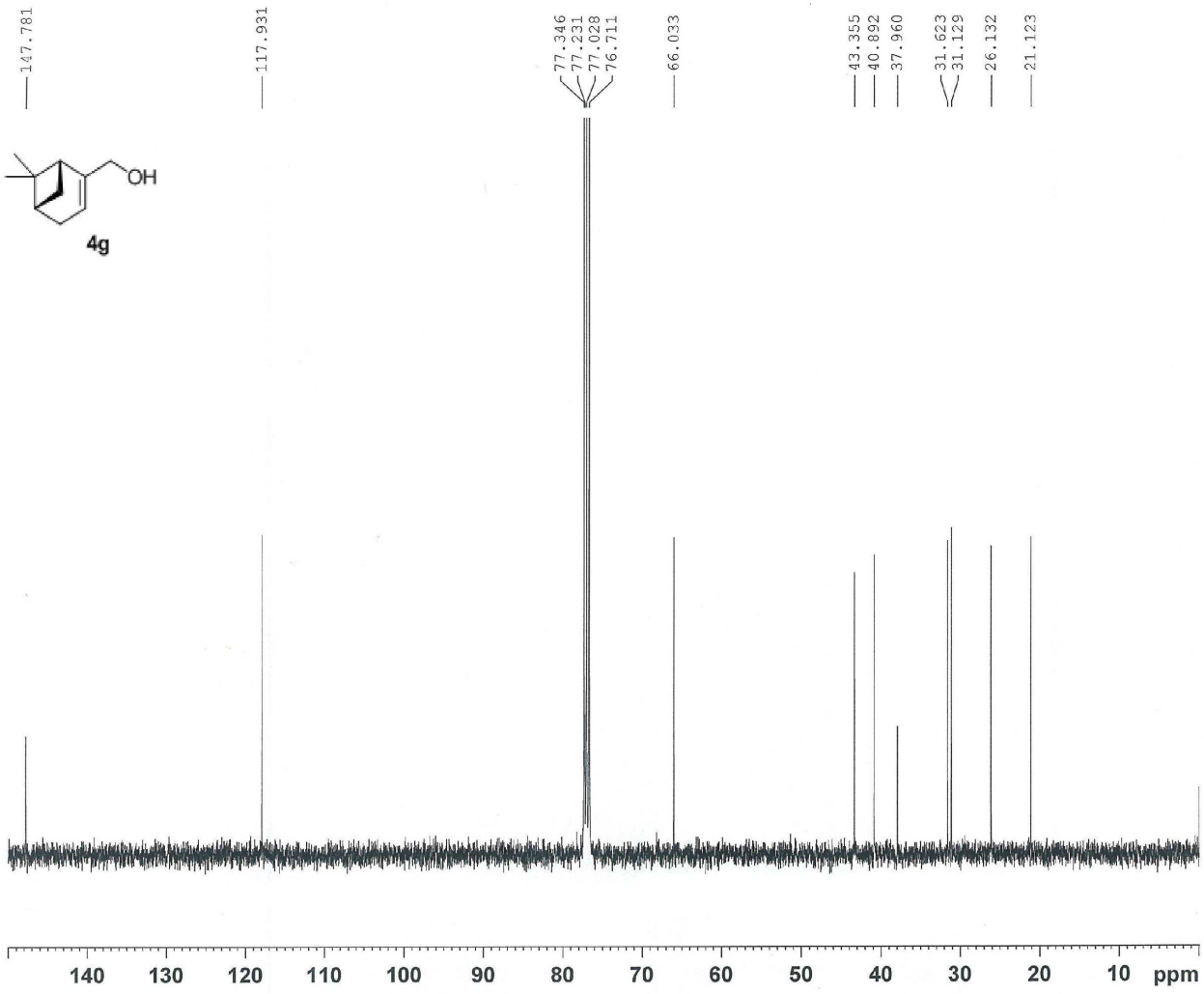
1D NMR plot parameters
CX 30.00 cm
CY 34.00 cm
F1P 210.000 ppm
F1 21128.57 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.16667 ppm/cm
HZCM 721.05795 Hz/cm


Ph
Br
OH
4f


Ph
OH
Br
4f
ppm
200
180
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME mit-10
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101001
Time 17.39
INSTRUM spect
PROBHD 5 mm Qual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 982
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0288552 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 210.000 ppm
F1 21128.67 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.16667 ppm/cm
HZCM 721.05788 Hz/cm




```
Current Data Parameters
NAME                  RTK-861
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120418
Time                  14.44
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                    99.16
DW                   60.800 usec
DE                    6.50 usec
TE                   291.4 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PLW1           12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF             400.1300077 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```




```
Current Data Parameters
NAME                  RTK-856
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120416
Time                   22.39
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   292.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.98 usec
PLW1             52.09999847 W
SFO1            100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127690 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```