The Evolution of a Short and Stereocontrolled Synthesis of (+)-7,20-Diisocyanoadociane

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Supporting Information

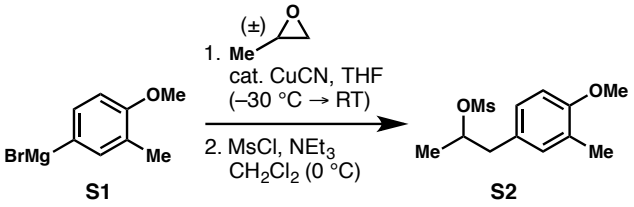
A. Table of Contents

B. General Experimental Details

All reactions were carried out under an argon atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. Argon balloons were the sole inert atmosphere used. Reactions run at an ambient temperature of 20–25 °C are designated as room temperature. Reactions that were performed open to air utilized solvent dispensed from a wash bottle or solvent bottle, and no precautions were taken to exclude water. Reactions that were performed open to air utilized solvent dispensed from a wash bottle or solvent bottle, and no precautions were taken to exclude water. Yields refer to chromatographically and spectroscopically homogeneous materials, unless otherwise stated. Dry tetrahydrofuran (THF) and dichloromethane (CH_2Cl_2) were obtained by passing commercially available formulations through activated alumina columns. Triethylamine (NEt_3) was purified by distillation from CaH_2. (±)-Propylene oxide was purified by distillation. Grignard reagents were titrated using salicylaldehyde phenylhydrazone in THF.

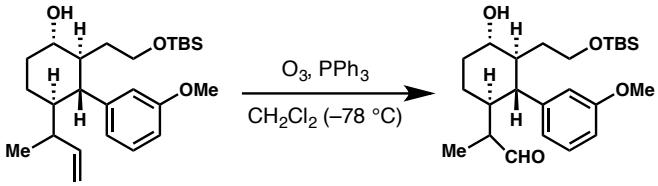
Thin layer chromatography was performed on 0.25 mm EMD glass-backed TLC plates impregnated with a fluorescent dye and visualized with UV light and $KMnO_4$ in K_2CO_3/NaOH/water. Forced flow (flash) chromatography was performed on EMD Silica 60, mesh 0.04-0.063 silica gel. NMR spectra were recorded on Bruker 500 MHz or 600 MHz instrument, obtained at 298 K unless otherwise noted and calibrated to residual undeuterated solvent as an internal reference. Chemical shifts are reported in ppm with the following abbreviations to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintuplet, sext = sextet, sep = septet, bs = broad signal, m = multiplet. All coupling constants are apparent *J* values measured at the indicated field strengths and reported in Hertz (Hz). FT-IR spectra were recorded on a Perkin-Elmer spectrum RX1 or Varian 640-IR spectrometer. High-resolution mass spectra (HRMS) were recorded on a Waters LCT Premier spectrometer using ESI-TOF (electrospray ionization-time of flight) or Waters GCT Premier spectrometer using GC-CI, as indicated. Melting points were measured on a MEL-TEMP II capillary apparatus and stand uncorrected.

C. Experimental Procedures and Characterization Data



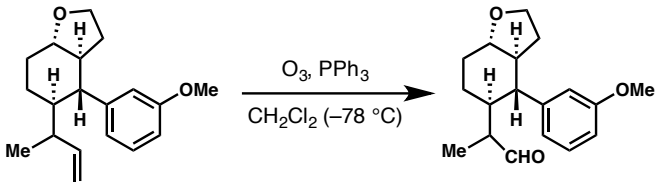
Mesylate S2: A 100 mL round bottom flask containing 720 mg (29.6 mmol) magnesium metal was flame-dried, layered with 5 mL THF, treated with a couple drops of dibromoethane and heated to 70 °C. A solution of 5.00 g (24.9 mmol) 4-bromo-2-methylanisole in 25 mL THF was added dropwise as to maintain a gentle reflux. After complete addition the reaction was stirred at 70 °C another hour then cooled to –30 °C. After the addition of 70 mg (0.80 mmol) CuCN and 2.0 mL (28.6 mmol) (rac)-propylene oxide the reaction was stirred for 1 hour with gradual warming to 0 °C, then stirred an additional half hour at room temperature. The reaction was quenched with 100 mL half sat. NH_4Cl and extracted with 100 mL EtOAc. The aqueous layer was separated and back extracted with 20 mL EtOAc. Both organic layers were combined, washed with 50 mL sat. NH_4Cl, 30 mL third sat. NH_4Cl, 20 mL brine, dried over $MgSO_4$, filtered and all volatiles removed in vacuo. The residue was used for the next without purification. To a 250 mL round bottom flask containing crude alcohol, was added 80 mL CH_2Cl_2 and 15 mL (108 mmol) NEt_3. After the dropwise addition of 3.0 mL (38.8 mmol) methanesulfonyl chloride at 0 °C, the reaction was stirred at 0 °C for 2 hours. To the stirring mixture was added 150 mL sat. $NaHCO_3$ and vigorous stirring continued without external cooling for 20 minutes. Layers were separated and the aqueous layer washed with 20 mL CH_2Cl_2. The organic layers were combined, washed with 40 mL brine, dried over $MgSO_4$, filtered and all volatiles removed in vacuo. The residue was purified by column chromatography (5:1 hexanes/EtOAc) then recrystallized from Et_2O/pentane to afford 5.24 g (81% over 2 steps) **S2** as white crystals (mp = 60–62 °C). ^{1}H NMR (500 MHz, $CDCl_3$ at 7.27 ppm) δ 7.03-6.98 (m, 2H), 6.77 (d, *J* = 8.1 Hz, 1H), 4.85 (ttd, *J* = 6.6, 6.4, 6.2 Hz, 1H), 3.82 (s, 3H), 2.91 (dd, *J* = 14.1, 8.0 Hz, 1H), 2.81 (dd, *J* = 14.0, 5.4 Hz, 1H), 2.54-2.52 (m, 3H), 2.18-2.16 (m, 3H), 1.46 (d, *J* = 6.2 Hz, 3H);

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$ at 77 ppm) δ 156.8, 131.8, 128.3, 127.7, 126.8, 109.9, 81.8, 55.3, 42.1, 37.8, 21.4, 16.2; IR (thin film) 2935, 2836, 1612, 1505, 1346, 1253, 1172 cm^{-1}; HRMS (ESI) calculated for $C_{12}H_{18}O_4S$ $[M+Na]^+$ 281.0833 found 281.0823.



62 **S3**

Alcohol S3: To a 1 dram vial containing 12 mg (0.029 mmol) **62** in 0.5 mL CH_2Cl_2 was bubbled O_3/O_2 at –78 °C until the solution turned blue. The flask was purged with O_2 until the blue color faded, then 9 mg (0.034 mmol) PPh_3 in 0.2 mL CH_2Cl_2 was added. Stirring was continued at –78 °C for 1 hour then the bath was removed. After 2 hours the contents were diluted with EtOAc, dried over $MgSO_4$, filtered and all volatiles removed in vacuo. The crude oil was purified by column chromatography (5:1 hexanes/EtOAc) to afford 8 mg (67%) **S3** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$ at 7.27 ppm) δ 9.47 (s, 0.5H), 9.40 (s, 0.5H), 7.21 (bs, 1H), 6.88-6.57 (m, 3H), 4.80 (bs, 1H), 3.81 (s, 1.5H), 3.80 (s, 1.5H), 3.61-3.58 (m, 1H), 3.39 (qd, J = 10.1, 3.7 Hz, 1H), 3.31-3.24 (m, 1H), 2.25-2.13 (m, 2H), 1.97-1.86 (m, 2H), 1.74-1.22 (m, 5H), 1.00 (d, J = 7.1 Hz, 1.5H), 1.01-0.89 (m, 1H), 0.95 (d, J = 7.1 Hz, 1.5H), 0.89 (s, 4.5H), 0.89 (s, 4.5H), 0.05 (s, 6H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$ at 77 ppm) δ 205.1, 203.9, 144.2, 144.1, 73.8, 73.8, 63.0, 55.2, 48.2, 47.8, 46.5, 35.1, 34.8, 34.4, 34.0, 26.8, 25.9, 24.6, 18.2, 10.9, 6.8, –5.5, –5.6; IR (thin film) 3410, 2929, 2857, 1721, 1599, 1464, 1256, 1081, 1047, 836, 778 cm^{-1}; HRMS (ESI) calculated for $C_{24}H_{40}O_4Si$ $[M+Na]^+$ 443.2594 found 443.2595.

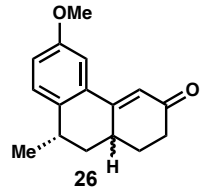


63 **S4**

To a 1 dram vial containing 73 mg (0.255 mmol) **63** in 2.5 mL CH_2Cl_2 was bubbled O_3/O_2 at –78 °C until the solution turned blue. The flask was purged with O_2 until the blue color faded, then 80 mg (0.305 mmol) PPh_3 was added. Stirring was continued at –78 °C for 2 hours then the bath was removed. After 6 hours the reaction was dried over $MgSO_4$, filtered and all volatiles removed in vacuo. The crude oil was purified by column chromatography (3:1→1:2 hexanes/EtOAc) to afford 65 mg (89%, with ~25% over oxidation) **S4** as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$ at 7.27 ppm) major δ 9.55 (s, 0.5H), 9.49 (s, 0.5H), 7.29-7.23 (m, 1H), 6.81-6.74 (m, 3H), 4.09 (s, 1H), 3.94-3.85 (m, 2H), 3.83 (s, 1.5H), 3.82 (s, 1.5H), 3.21 (dtd, J = 17.8, 10.5, 3.5 Hz, 1H), 2.56 (t, J = 10.9 Hz, 1H), 2.39-2.16 (m, 3H), 2.10-1.99 (m, 1H), 1.83-1.35 (m, 4H), 1.07 (d, J = 7.1 Hz, 1.5H), 1.00 (d, J = 7.1 Hz, 1.5H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$ at 77 ppm) δ 205.1, 204.1, 143.62, 143.59, 129.9, 129.84, 129.80, 111.8, 67.3, 67.2, 55.3, 55.2, 51.9, 51.7, 47.6, 47.0, 46.4, 42.2, 30.8, 30.4, 30.1, 29.9, 27.0, 24.8, 14.3, 11.3, 7.1; IR (thin film) 2936, 2879, 1720, 1600, 1485, 1262, 1158, 1045 cm^{-1}; HRMS (ESI) calculated for $C_{18}H_{24}O_3$ $[M+Na]^+$ 311.1623 found 311.1635.

D. Copies of NMR Spectra

1H spectrum



26

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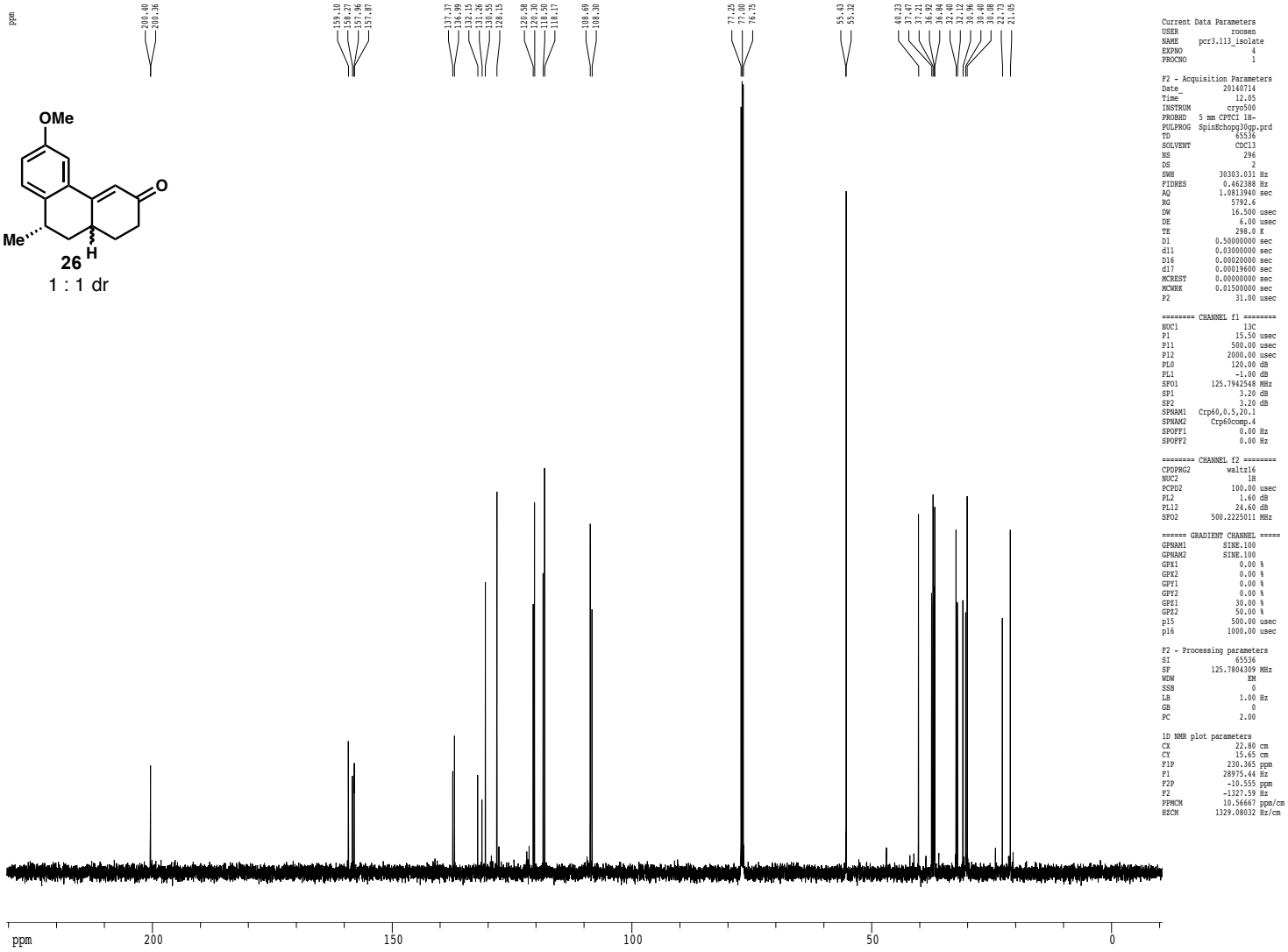
Z-restored spin-echo 13C spectrum with 1H decoupling



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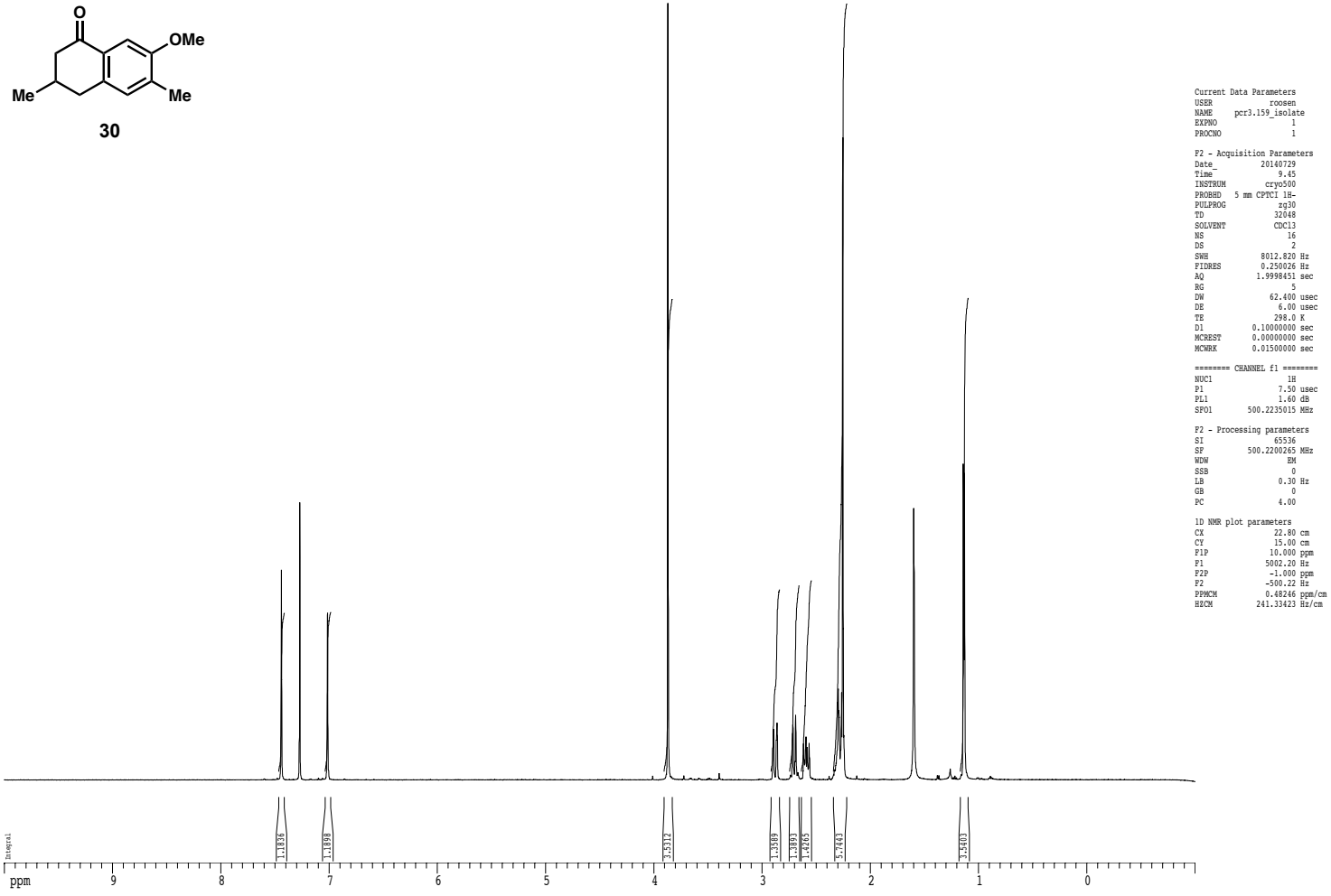
1H spectrum

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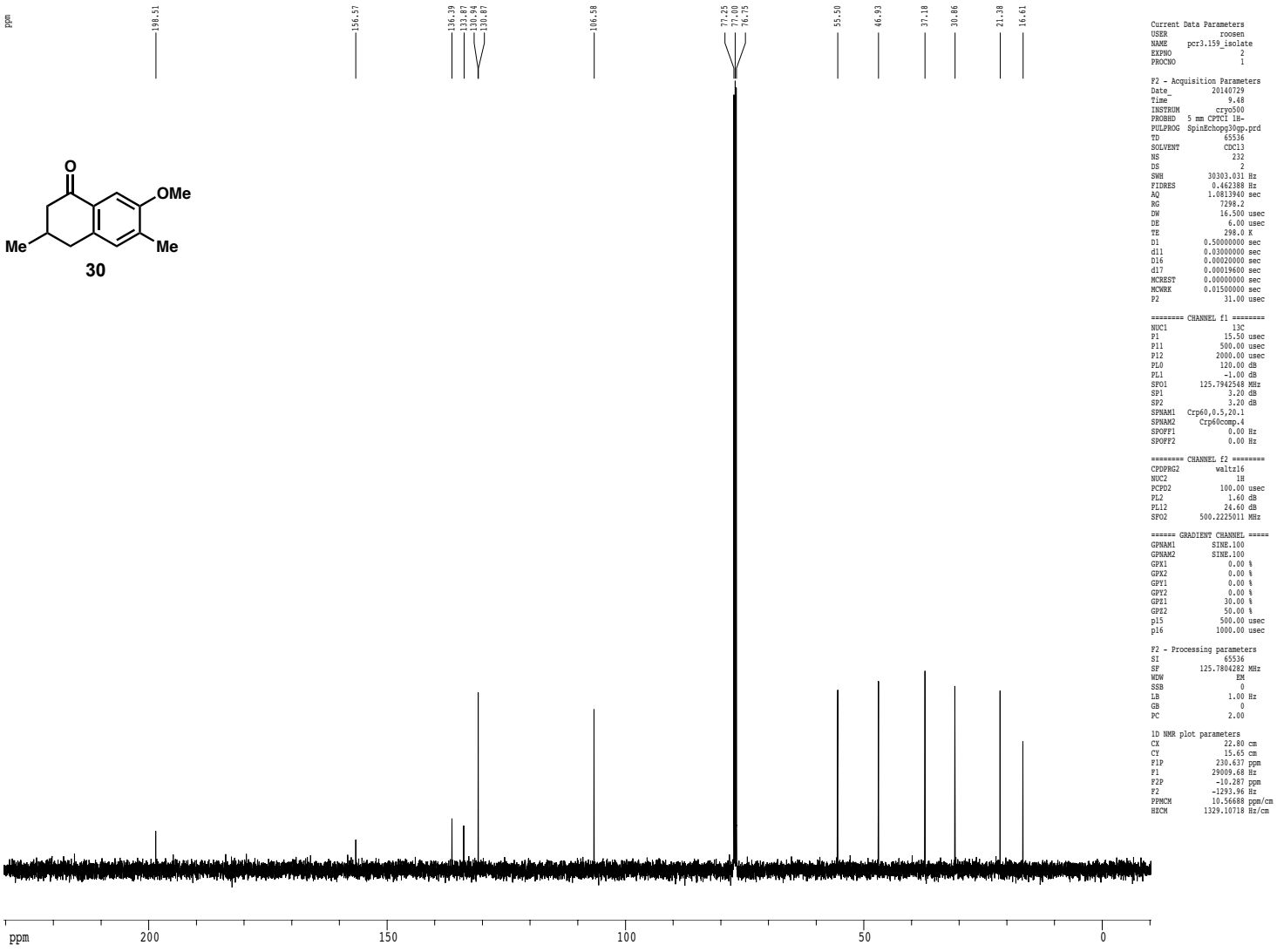
Z-restored spin-echo 13C spectrum with 1H decoupling

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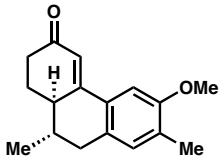

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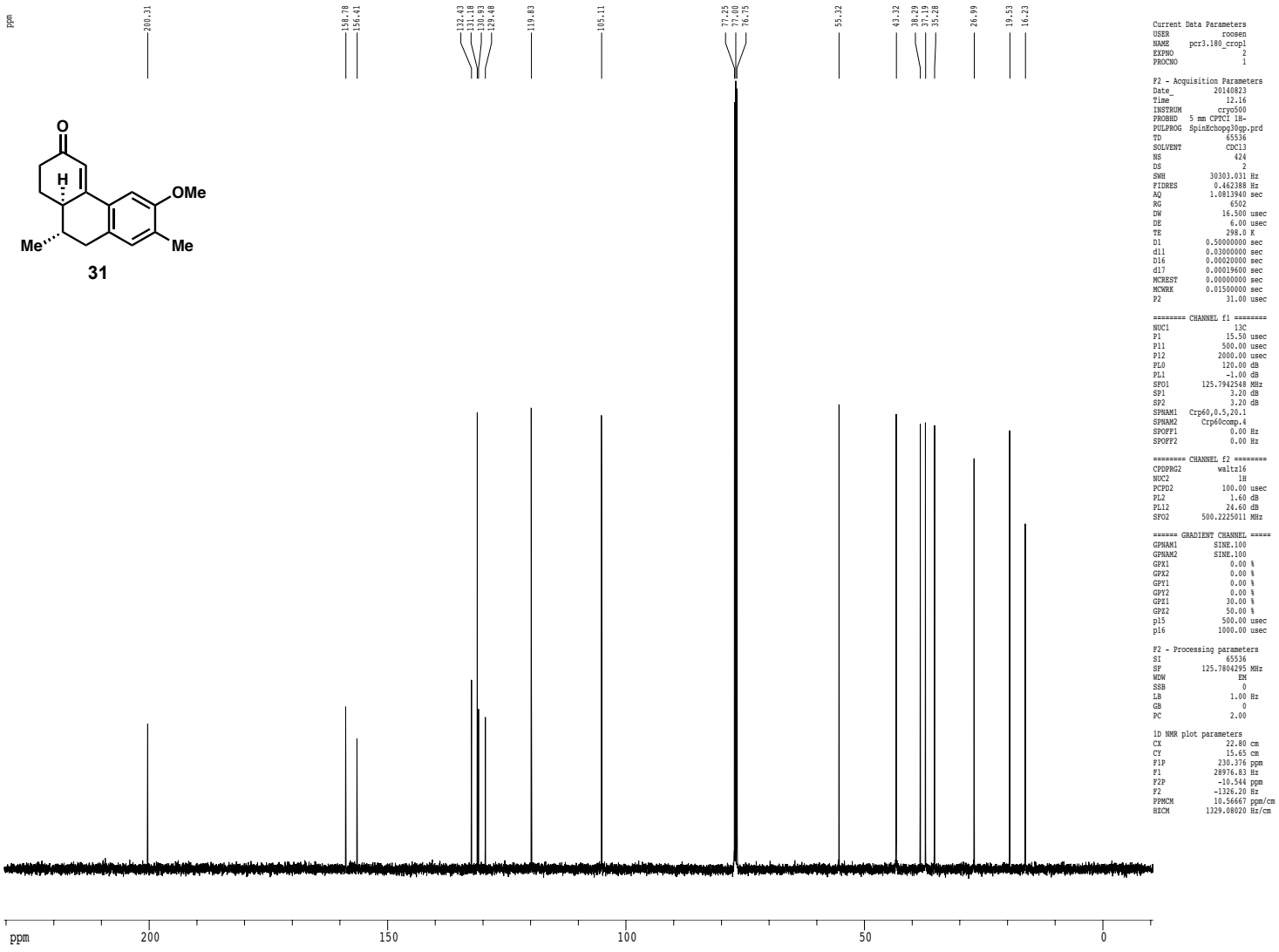
Z-restored spin-echo 13C spectrum with 1H decoupling

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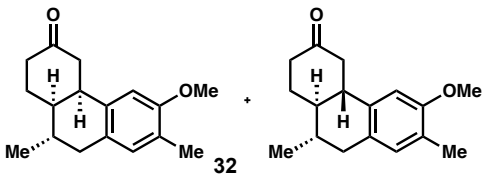
1H spectrum



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======== CHANNEL f1 ========
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CY 10.00 cm
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F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
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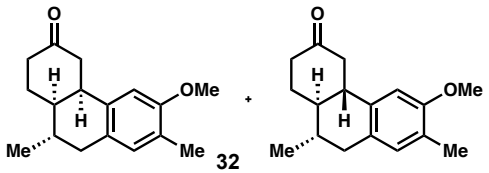
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



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DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                31.00 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                15.50 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

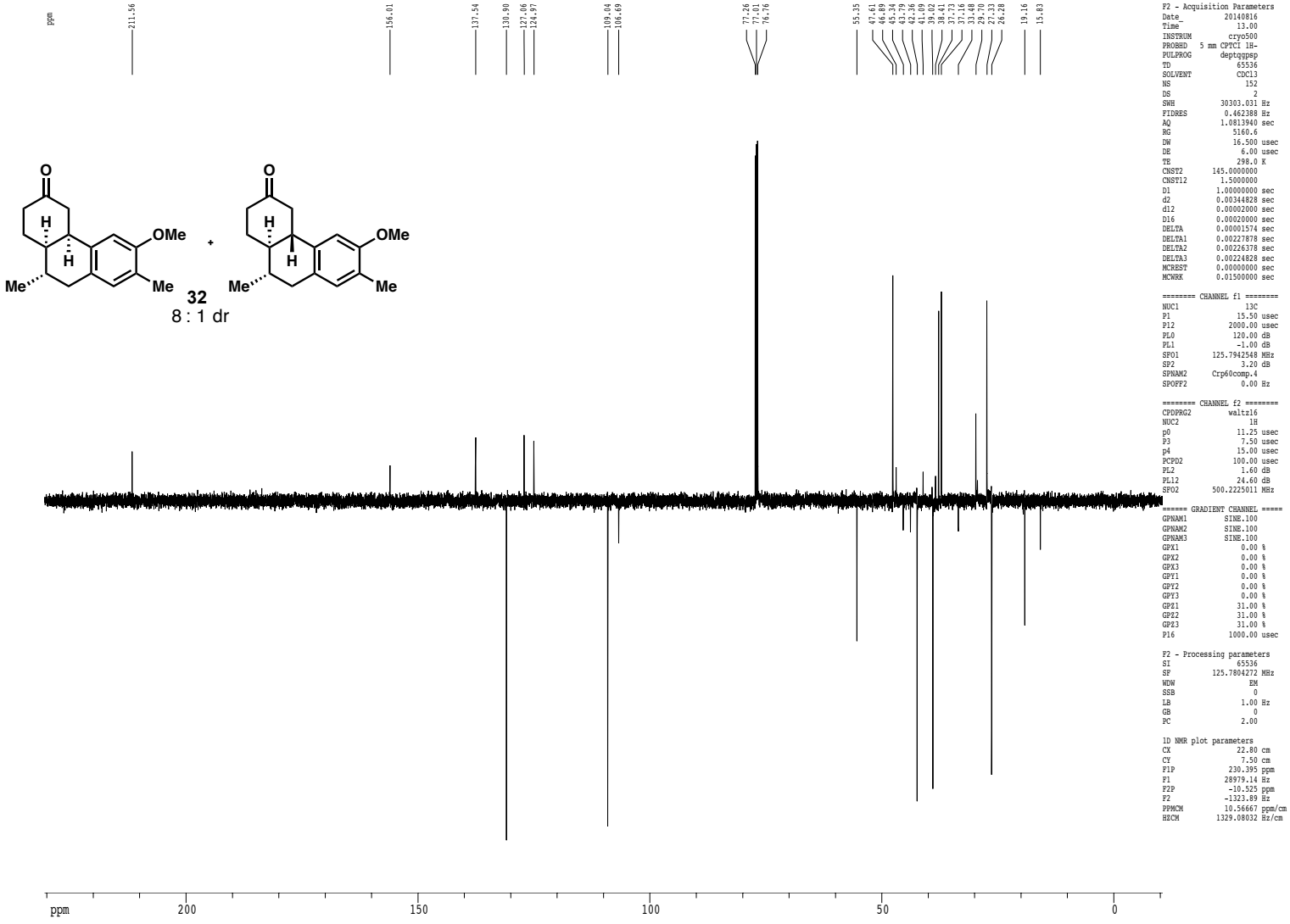
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804286 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.384 ppm
F1                28977.75 Hz
F2P               -10.536 ppm
F2                -1325.28 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

deptq 13C spectrum with 1H decoupling (CH & CH3 one way up; C, CH2 and solvent the other)




```
Current Data Parameters
USER                roosen
NAME      pcr3.185_isolate
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_           20140816
Time               13.00
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG       deptqgpsp
TD                65536
SOLVENT           CDCl3
NS                  152
DS                    2
SWH           30303.031 Hz
FIDRES        0.462388 Hz
AQ            1.0813940 sec
RG               5160.6
DW               16.500 usec
DE                6.00 usec
TE                298.0 K
CNST2       145.0000000
CNST12        1.5000000
D1            1.00000000 sec
d2            0.00344828 sec
d12           0.00002000 sec
D16           0.00020000 sec
DELTA         0.00001574 sec
DELTA1        0.00227878 sec
DELTA2        0.00226378 sec
DELTA3        0.00224828 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

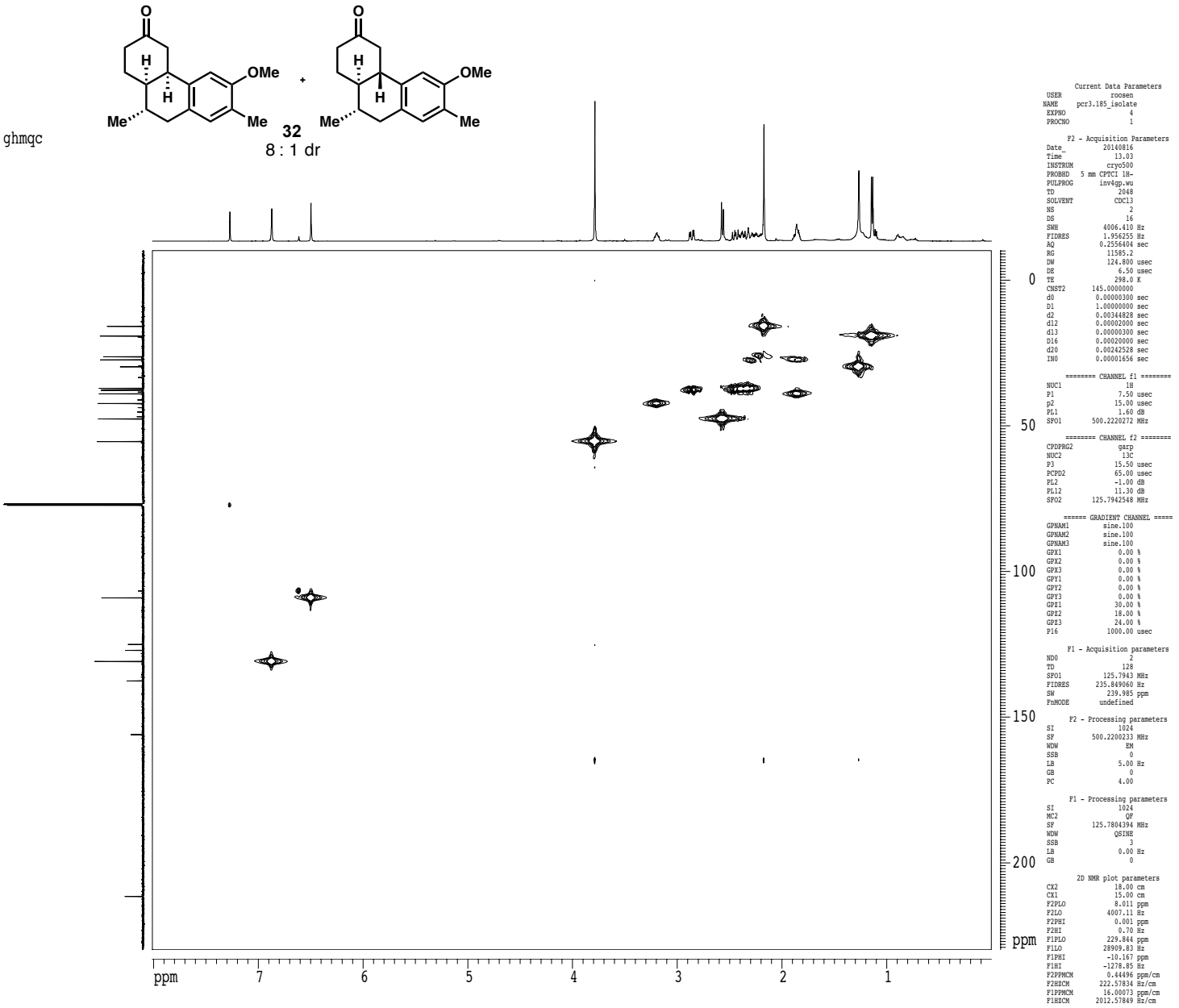
======== CHANNEL f1 ========
NUC1                13C
P1                15.50 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942548 MHz
SP2               1.20 dB
SPNAM2       Crp60comp.4
SPOFF2            0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
p0                11.25 usec
P3                 7.50 usec
p4                15.00 usec
PCPD2            100.00 usec
PL2               1.60 dB
PL12             24.60 dB
SFO2         500.2225011 MHz

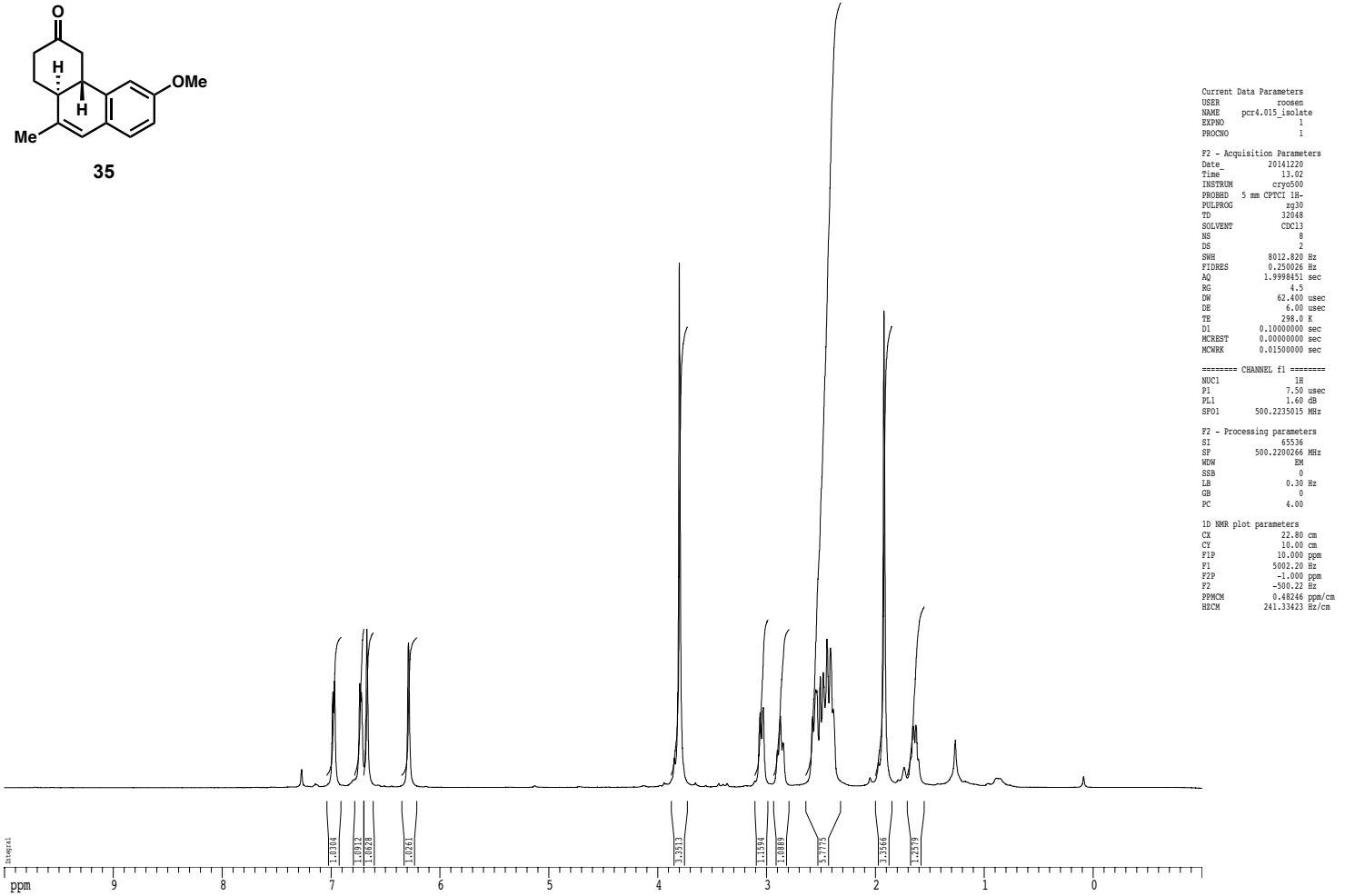
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPX1              0.00 %
GPX2              0.00 %
GPX3              0.00 %
GPY1              0.00 %
GPY2              0.00 %
GPY3              0.00 %
GPZ1             31.00 %
GPZ2             31.00 %
GPZ3             31.00 %
P16            1000.00 usec

F2 - Processing parameters
SI                65536
SF           125.7804272 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                 7.50 cm
F1P              230.395 ppm
F1              28979.14 Hz
F2P               -10.525 ppm
F2              -1323.89 Hz
PPMCM           10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```


ghmqc
32
8 : 1 dr
OMe
Me
ppm
Current Data Parameters
USER roosen
NAME pcr3.185_isolate
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140816
Time 13.03
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG inv4gp.wu
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2556404 sec
RG 11585.2
DW 124.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000300 sec
D16 0.00020000 sec
d20 0.00242528 sec
IN0 0.00001656 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p2 15.00 usec
PL1 1.60 dB
SFO1 500.2220272 MHz
======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 15.50 usec
PCPD2 65.00 usec
PL2 -1.00 dB
PL12 11.30 dB
SFO2 125.7942548 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 30.00 %
GPZ2 18.00 %
GPZ3 24.00 %
P16 1000.00 usec
F1 - Acquisition parameters
ND0 2
TD 128
SFO1 125.7943 MHz
FIDRES 235.849060 Hz
SW 239.985 ppm
FnMODE undefined
F2 - Processing parameters
SI 1024
SF 500.2200233 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 4.00
F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7804394 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 8.011 ppm
F2LO 4007.11 Hz
F2PHI 0.001 ppm
F2HI 0.70 Hz
F1PLO 229.844 ppm
F1LO 28909.83 Hz
F1PHI -10.167 ppm
F1HI -1278.85 Hz
F2PPMCM 0.44496 ppm/cm
F2HZCM 222.57834 Hz/cm
F1PPMCM 16.00073 ppm/cm
F1HZCM 2012.57849 Hz/cm

1H spectrum




```
Current Data Parameters
USER                roosen
NAME      pcr4.015_isolate
EXPNO                   1
PROCNO                  1

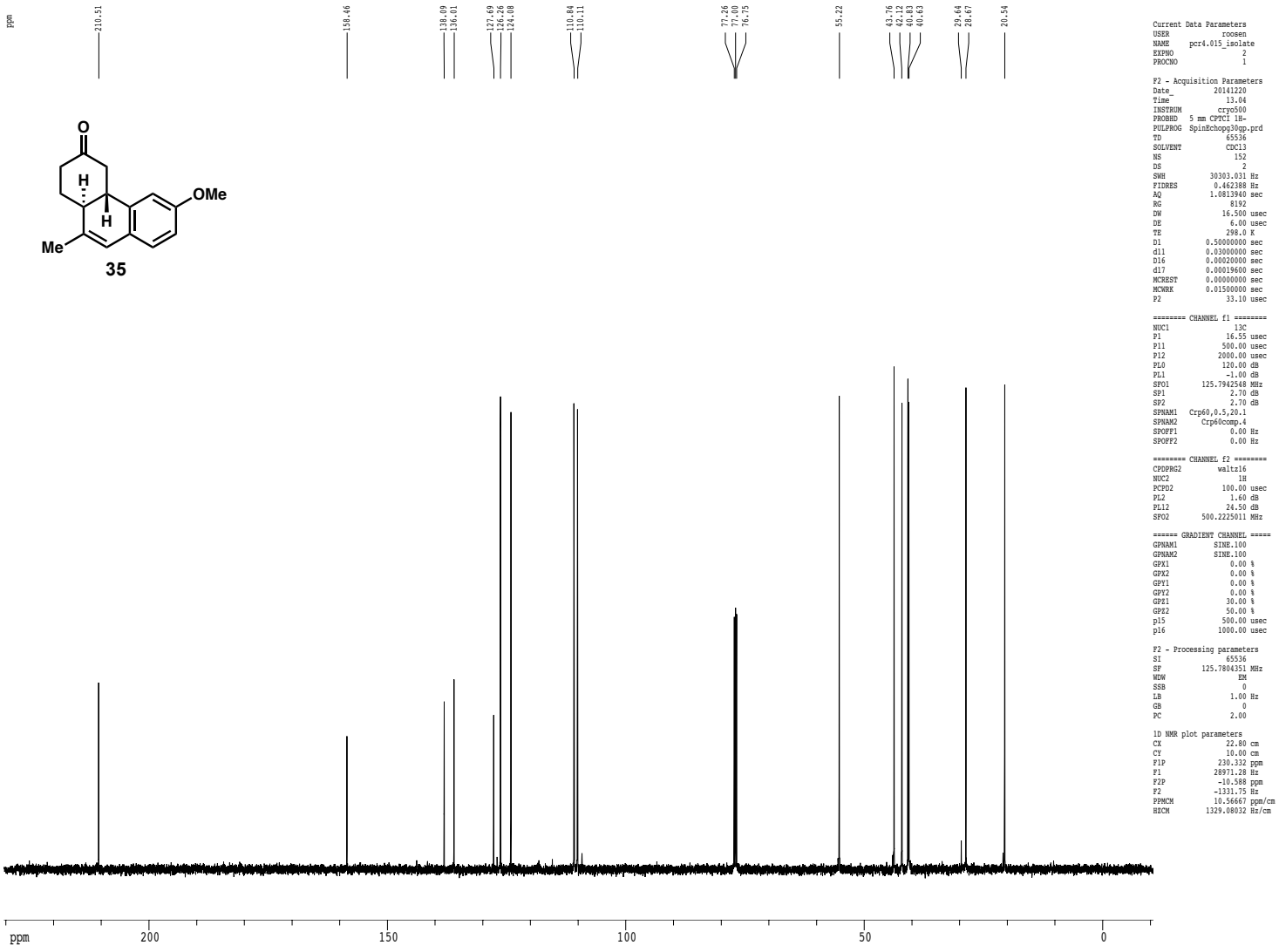
F2 - Acquisition Parameters
Date_           20141220
Time               12.02
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32048
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250026 Hz
AQ              1.9998451 sec
RG                   4.5
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1        500.2235015 MHz

F2 - Processing parameters
SI                 65536
SF          500.2200266 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 10.00 cm
F1P               10.000 ppm
F1              5002.20 Hz
F2P               -1.000 ppm
F2              -500.22 Hz
PPMCM           0.48246 ppm/cm
HZCM          241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.015_isolate
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20141220
Time                13.04
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    152
DS                      2
SWH           30303.031 Hz
FIDRES        0.462388 Hz
AQ            1.08113940 sec
RG                   8192
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1        125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

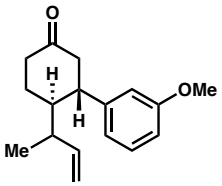
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF          125.7804351 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 10.00 cm
F1P              230.332 ppm
F1               28971.28 Hz
F2P              -10.588 ppm
F2               -1331.75 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



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```
Current Data Parameters
USER                roosen
NAME      pcr4.115_77-80
EXPNO                    1
PROCNO                   1

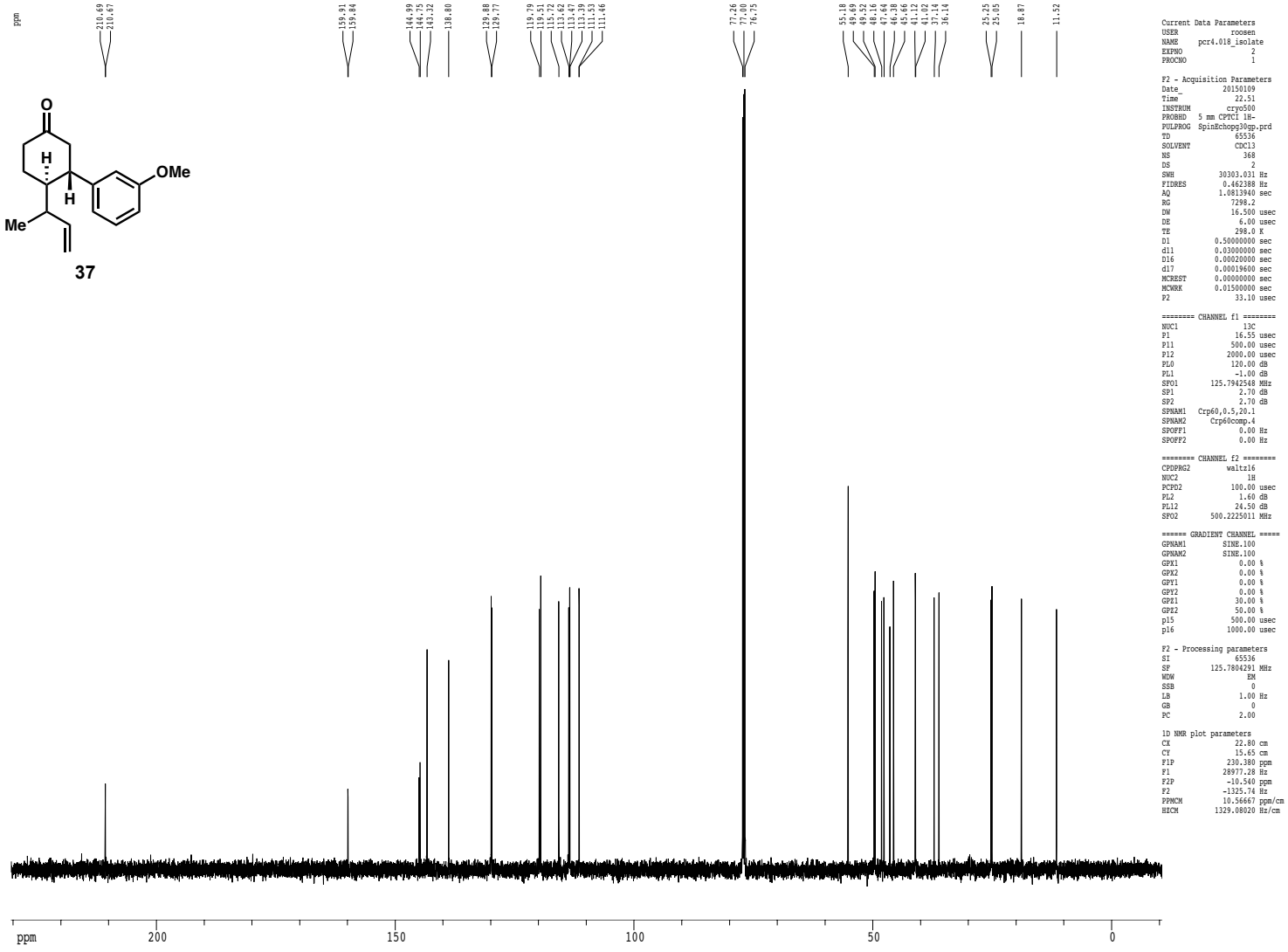
F2 - Acquisition Parameters
Date_           20150417
Time               12.43
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32048
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250026 Hz
AQ              1.9998451 sec
RG                   5.7
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                 7.50 usec
PL1                1.60 dB
SFO1        500.2235015 MHz

F2 - Processing parameters
SI                 65536
SF          500.2200265 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P              10.000 ppm
F1             5002.20 Hz
F2P              -1.000 ppm
F2             -500.22 Hz
PPMCM          0.48246 ppm/cm
HZCM         241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.018_isolate
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150109
Time                22.51
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    368
DS                      2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1        125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

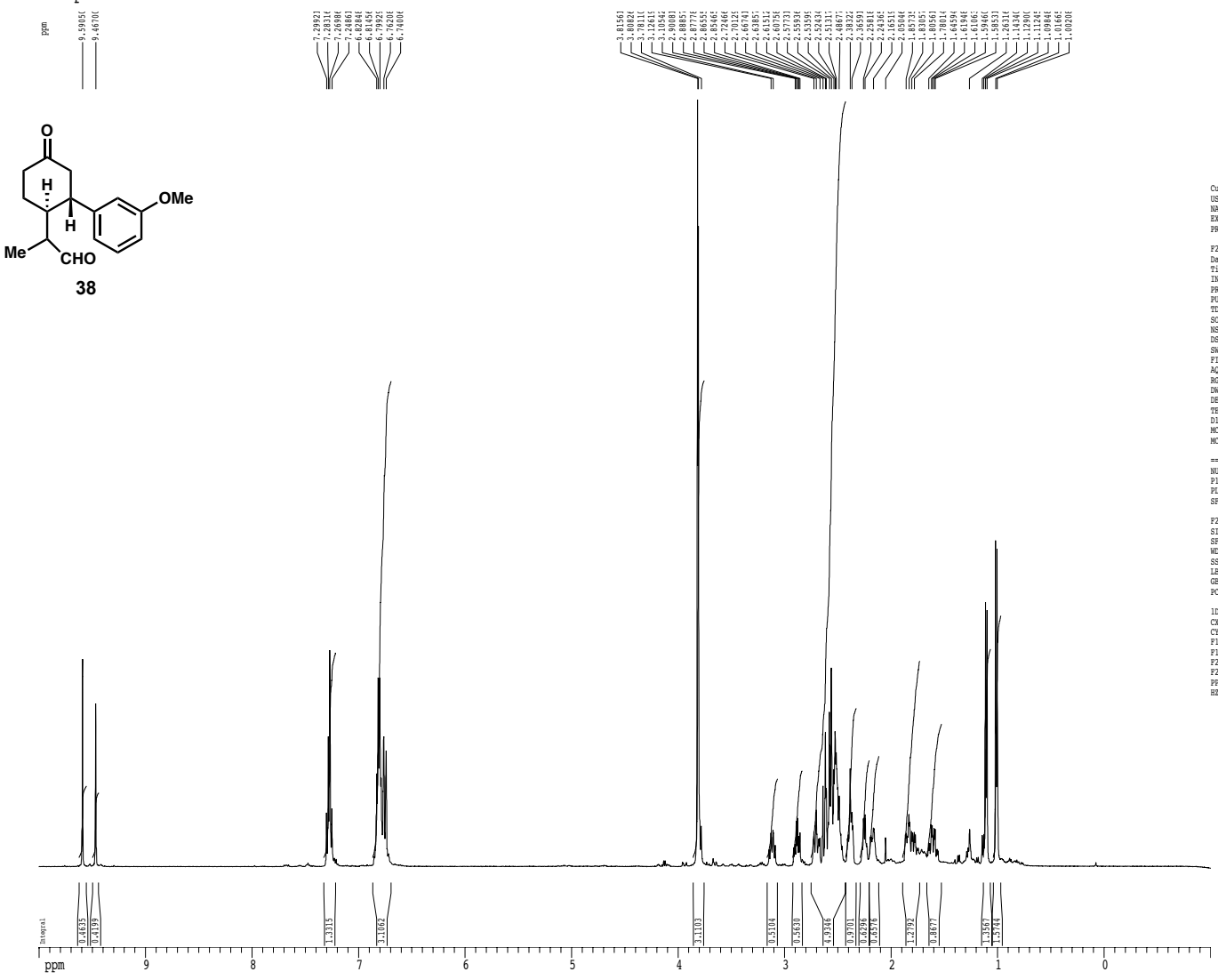
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                   65536
SF          125.7804291 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P               230.380 ppm
F1                28977.28 Hz
F2P                -10.540 ppm
F2                -1325.74 Hz
PPMCM             10.56667 ppm/cm
HZCM          1329.08020 Hz/cm
```

1H spectrum



Current Data Parameters
USER roosen
NAME pcr4.014_isolate
EXPNO 1
PROCNO 1

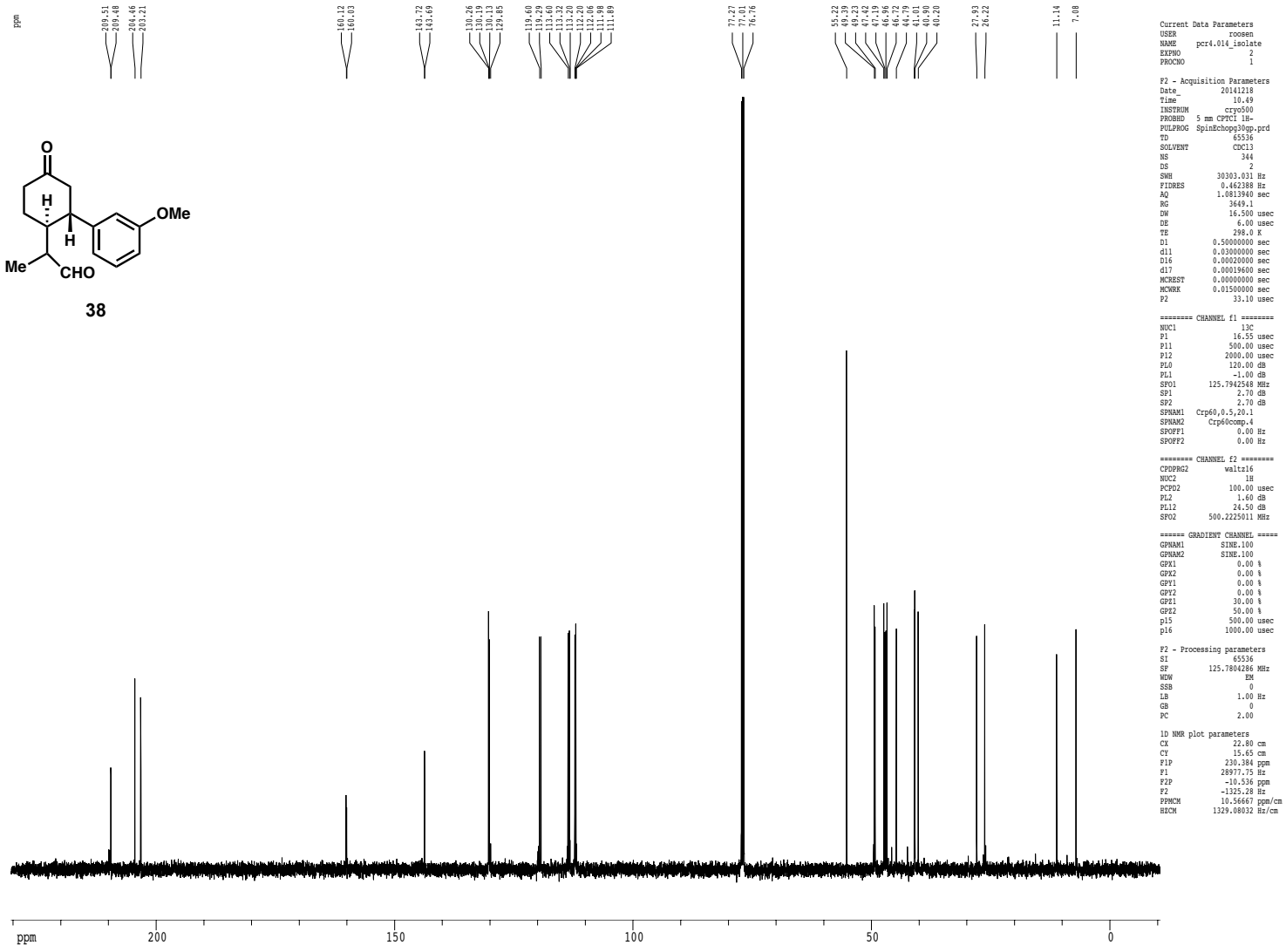
F2 - Acquisition Parameters
Date_ 20141218
Time 10.47
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.014_isolate
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20141218
Time              10.49
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                65536
SOLVENT           CDCl3
NS                  344
DS                    2
SWH           30303.031 Hz
FIDRES        0.462388 Hz
AQ            1.0813940 sec
RG              3649.1
DW               16.500 usec
DE                6.00 usec
TE               298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                13C
P1                16.55 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1        125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

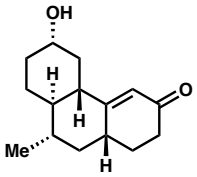
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF          125.7804286 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.384 ppm
F1                28977.75 Hz
F2P               -10.536 ppm
F2                -1325.28 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



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Current Data Parameters
USER roosen
NAME pcr4.024_isolate
EXPNO 1
PROCNO 1

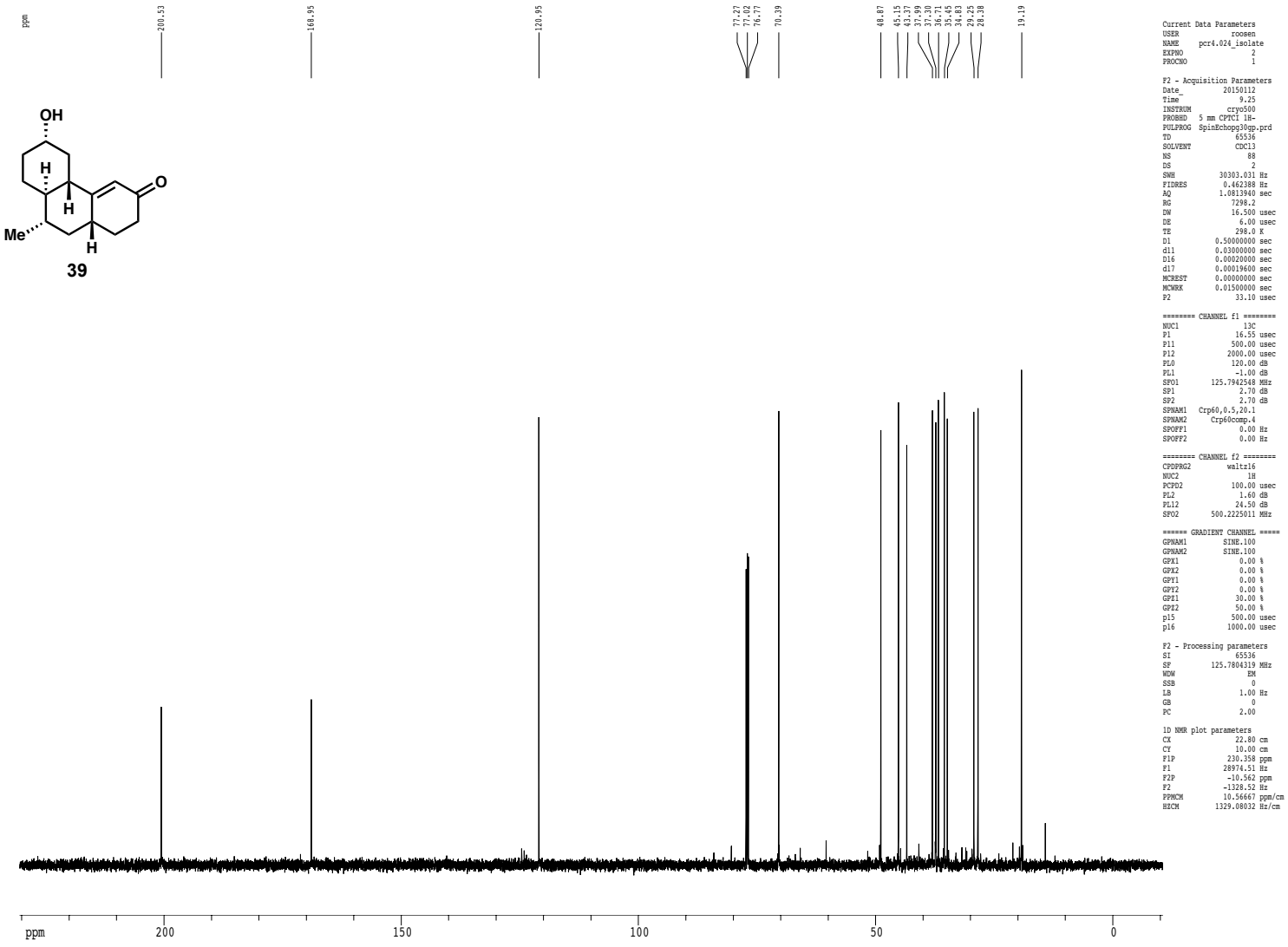
F2 - Acquisition Parameters
Date_ 20150112
Time 9.23
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200262 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.024_isolate
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150112
Time                   9.25
INSTRUM             cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT               CDCl3
NS                       88
DS                        2
SWH              30303.031 Hz
FIDRES            0.462388 Hz
AQ                1.0813940 sec
RG                   7298.2
DW                  16.500 usec
DE                   6.00 usec
TE                  298.0 K
D1              0.50000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

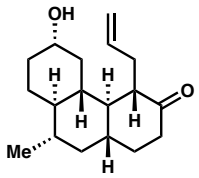
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                    65536
SF            125.7804319 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   10.00 cm
F1P               230.358 ppm
F1                28974.51 Hz
F2P                -10.562 ppm
F2                -1328.52 Hz
PPMCM             10.56667 ppm/cm
HZCM           1329.08032 Hz/cm
```

1H spectrum



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```
Current Data Parameters
USER                roosen
NAME       pcr4.083_monoallyl
EXPNO                    1
PROCNO                   1

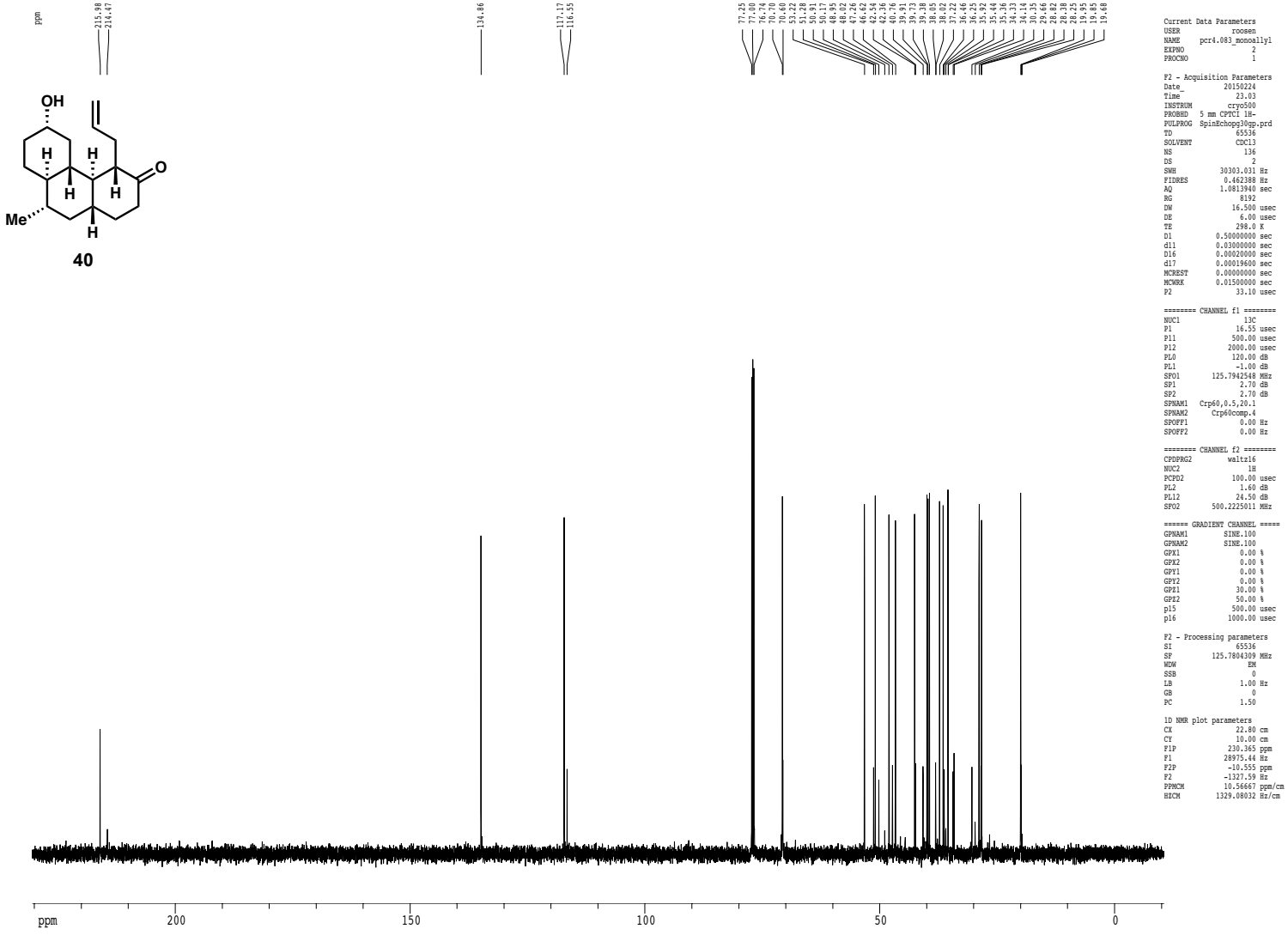
F2 - Acquisition Parameters
Date_             20150224
Time                23.01
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32048
SOLVENT             CDCl3
NS                     8
DS                     2
SWH              8012.820 Hz
FIDRES           0.250026 Hz
AQ               1.9998451 sec
RG                   3.6
DW                 62.400 usec
DE                  6.00 usec
TE                 298.0 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1         500.2235015 MHz

F2 - Processing parameters
SI                  65536
SF           500.2200268 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P               10.000 ppm
F1                5002.20 Hz
F2P                -1.000 ppm
F2                -500.22 Hz
PPMCM             0.48246 ppm/cm
HZCM            241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.083_monoallyl
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150224
Time                23.03
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    136
DS                      2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                   8192
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1        125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

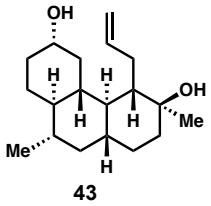
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                   65536
SF          125.7804309 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                  1.50

1D NMR plot parameters
CX                  22.80 cm
CY                  10.00 cm
F1P              230.365 ppm
F1               28975.44 Hz
F2P               -10.555 ppm
F2               -1327.59 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



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Current Data Parameters
USER roosen
NAME pcr4.086_major
EXPNO 1
PROCNO 1

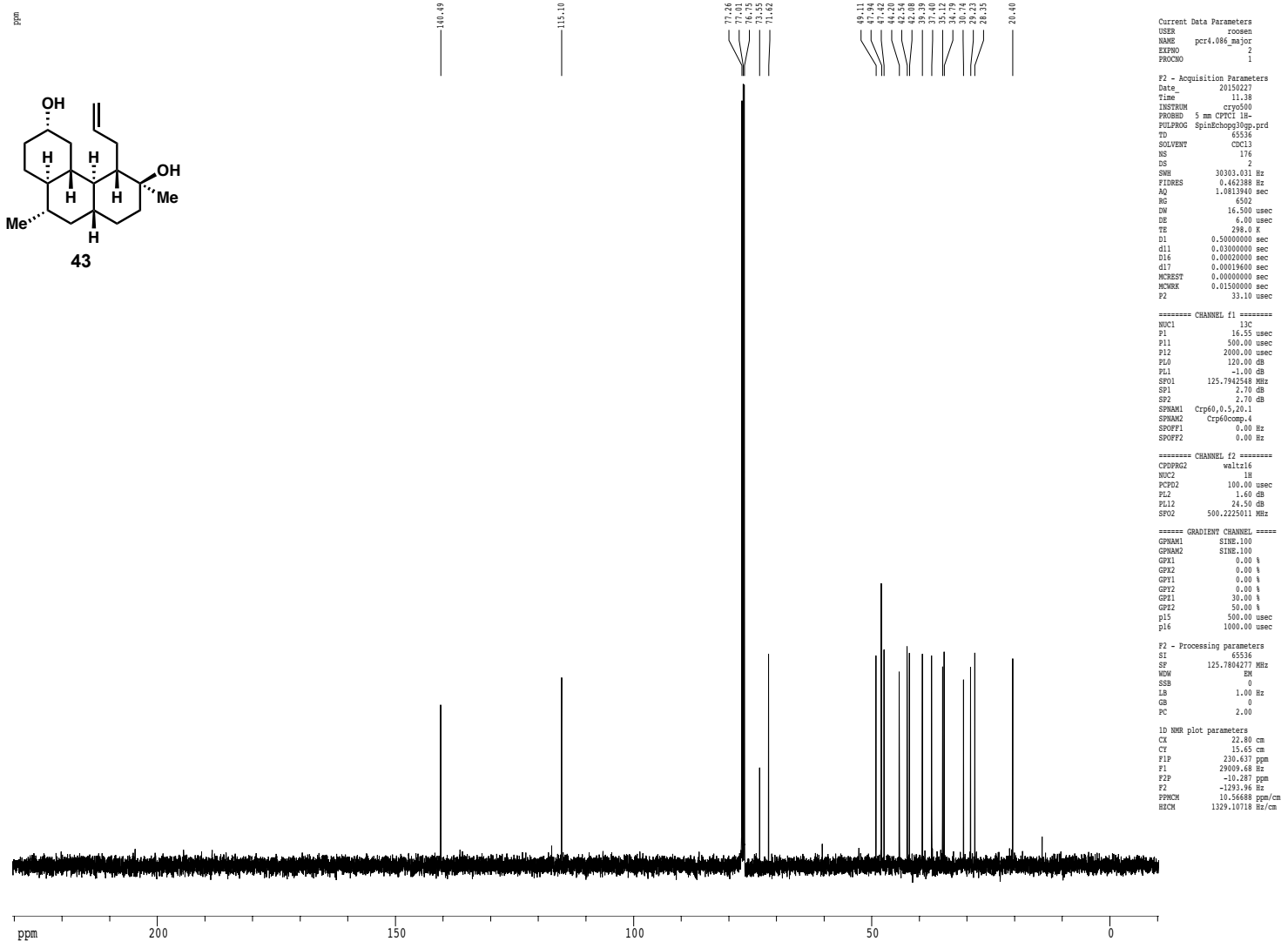
F2 - Acquisition Parameters
Date_ 20150328
Time 15.50
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200265 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.086_major
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150227
Time                 11.38
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     176
DS                       2
SWH            30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                    6502
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

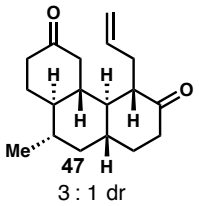
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                   65536
SF           125.7804277 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P               230.637 ppm
F1                29009.68 Hz
F2P                -10.287 ppm
F2                -1293.96 Hz
PPMCM            10.56688 ppm/cm
HZCM          1329.10718 Hz/cm
```

1H spectrum



3 : 1 dr


```
Current Data Parameters
USER                roosen
NAME      pcr4.048_isolate
EXPNO                   1
PROCNO                  1

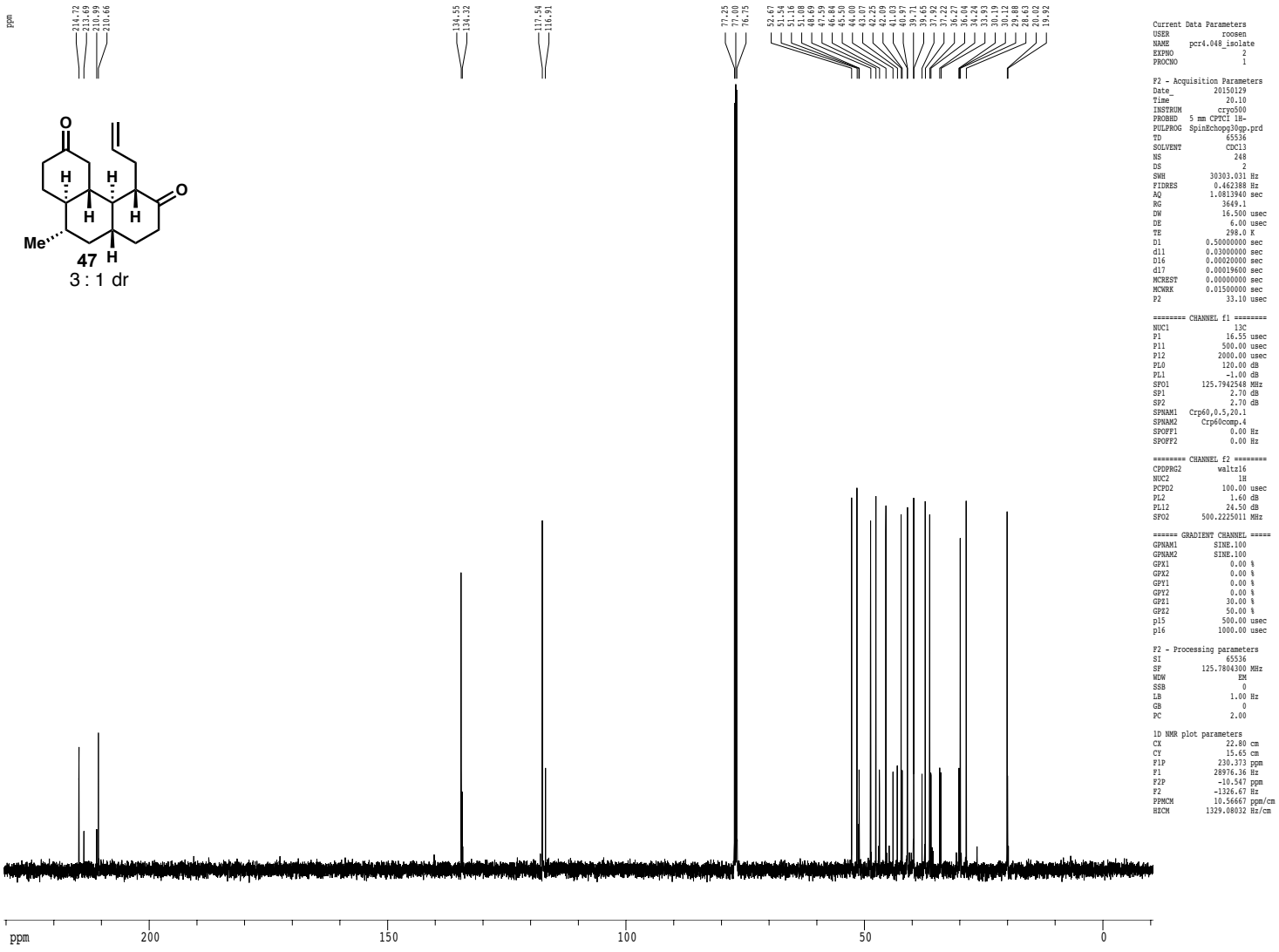
F2 - Acquisition Parameters
Date_            20150129
Time                20.04
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32048
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250026 Hz
AQ              1.9998451 sec
RG                     5
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                  1.60 dB
SFO1         500.2235015 MHz

F2 - Processing parameters
SI                 65536
SF           500.2200268 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P               10.000 ppm
F1              5002.20 Hz
F2P               -1.000 ppm
F2              -500.22 Hz
PPMCM           0.48246 ppm/cm
HZCM          241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.048_isolate
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20150129
Time              20.10
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                65536
SOLVENT           CDCl3
NS                  248
DS                    2
SWH           30303.031 Hz
FIDRES        0.462388 Hz
AQ            1.0813940 sec
RG               3649.1
DW              16.500 usec
DE               6.00 usec
TE              298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2              33.10 usec

======== CHANNEL f1 ========
NUC1                13C
P1               16.55 usec
P11             500.00 usec
P12            2000.00 usec
PL0             120.00 dB
PL1              -1.00 dB
SFO1        125.7942548 MHz
SP1              2.70 dB
SP2              2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

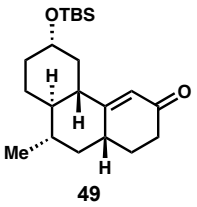
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           100.00 usec
PL2              1.60 dB
PL12            24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15              500.00 usec
p16             1000.00 usec

F2 - Processing parameters
SI                 65536
SF          125.7804300 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.65 cm
F1P              230.373 ppm
F1              28976.36 Hz
F2P              -10.547 ppm
F2              -1326.67 Hz
PPMCM           10.56667 ppm/cm
HZCM         1329.08032 Hz/cm
```

1H spectrum



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```
Current Data Parameters
USER                roosen
NAME      pcr4.269_isolate
EXPNO                   1
PROCNO                  1

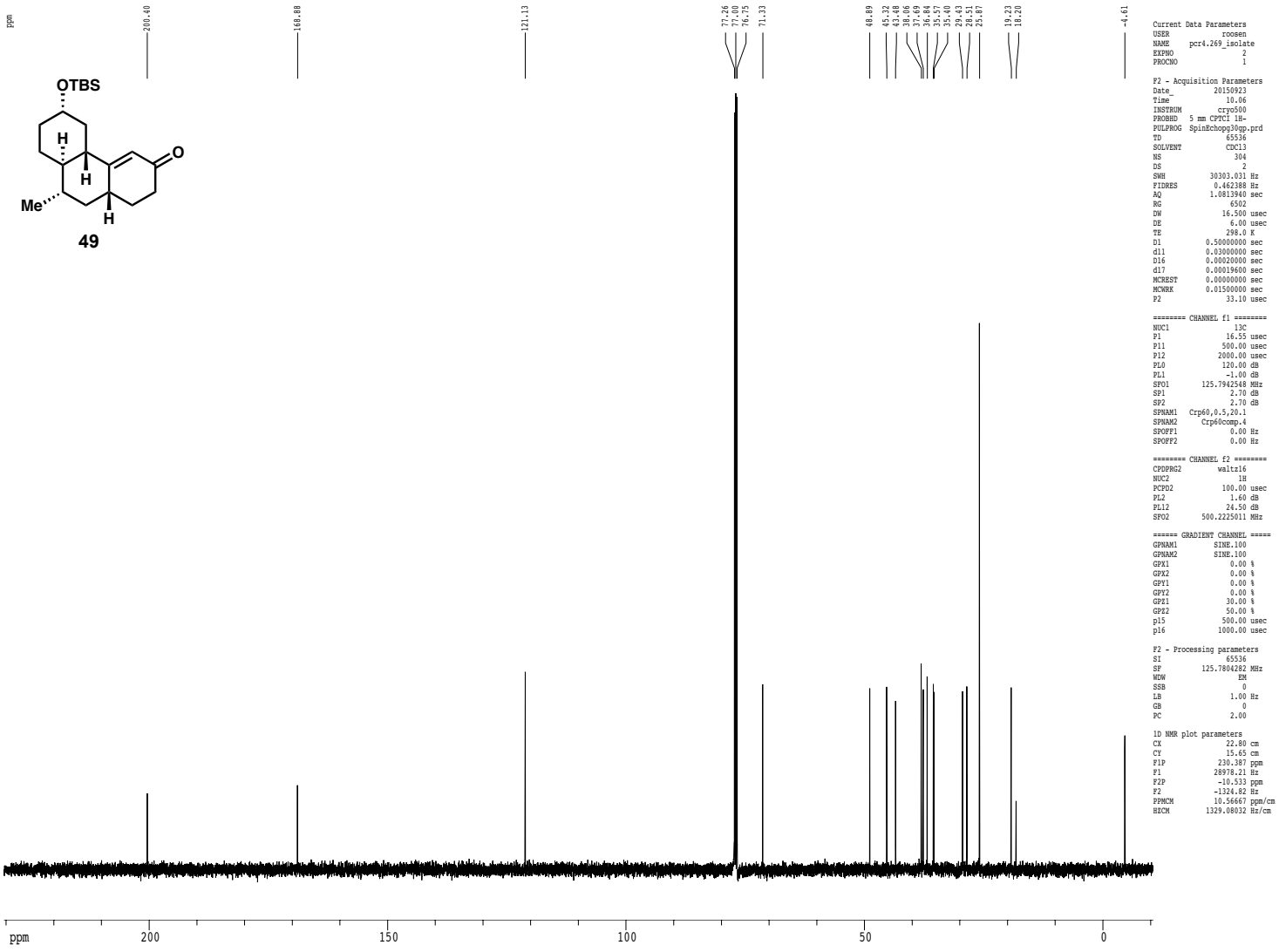
F2 - Acquisition Parameters
Date_            20150923
Time                10.04
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  32048
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.250026 Hz
AQ               1.9998451 sec
RG                    6.3
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1         500.2235015 MHz

F2 - Processing parameters
SI                  65536
SF           500.2200266 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                10.000 ppm
F1                 5002.20 Hz
F2P                -1.000 ppm
F2                 -500.22 Hz
PPMCM            0.48246 ppm/cm
HZCM           241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.269_isolate
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150923
Time                10.06
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    304
DS                      2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.08113940 sec
RG                   6502
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1        125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

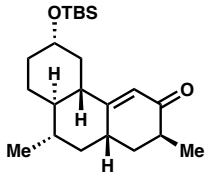
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF          125.7804282 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.65 cm
F1P              230.387 ppm
F1               28978.21 Hz
F2P               -10.533 ppm
F2               -1324.82 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



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```
Current Data Parameters
USER                roosen
NAME      pcr4.289_isolate
EXPNO                   1
PROCNO                  1

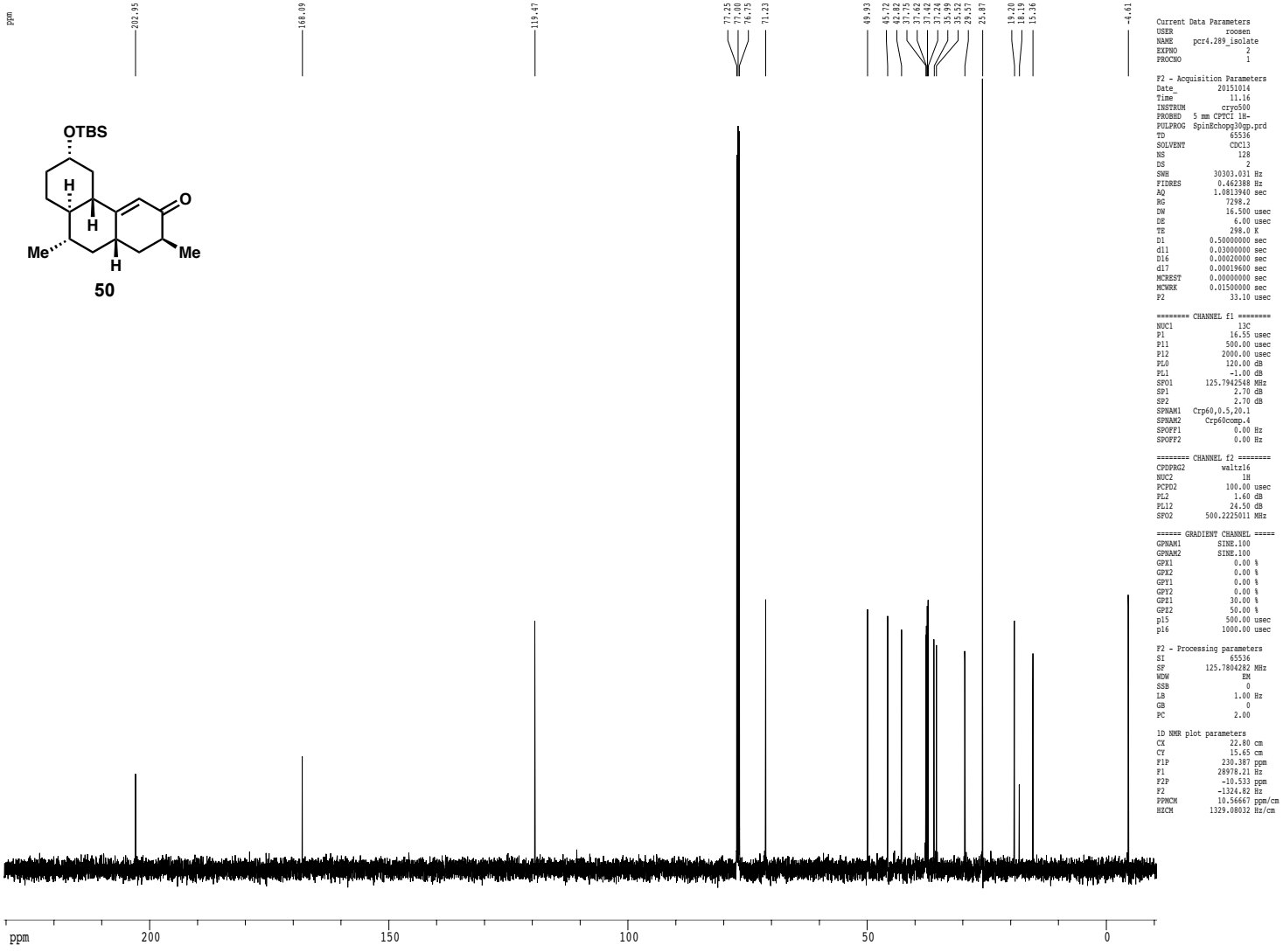
F2 - Acquisition Parameters
Date_           20151014
Time               11.15
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32048
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250026 Hz
AQ              1.9998451 sec
RG                  10.1
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                  1.60 dB
SFO1        500.2235015 MHz

F2 - Processing parameters
SI                 65536
SF          500.2200265 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P               10.000 ppm
F1              5002.20 Hz
F2P               -1.000 ppm
F2              -500.22 Hz
PPMCM           0.48246 ppm/cm
HZCM          241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.289_isolate
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20151014
Time                11.16
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.08113940 sec
RG                 7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

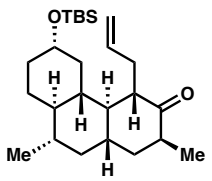
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                    65536
SF           125.7804282 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P               230.387 ppm
F1                28978.21 Hz
F2P                -10.533 ppm
F2                -1324.82 Hz
PPMCM             10.56667 ppm/cm
HZCM           1329.08032 Hz/cm
```

1H spectrum



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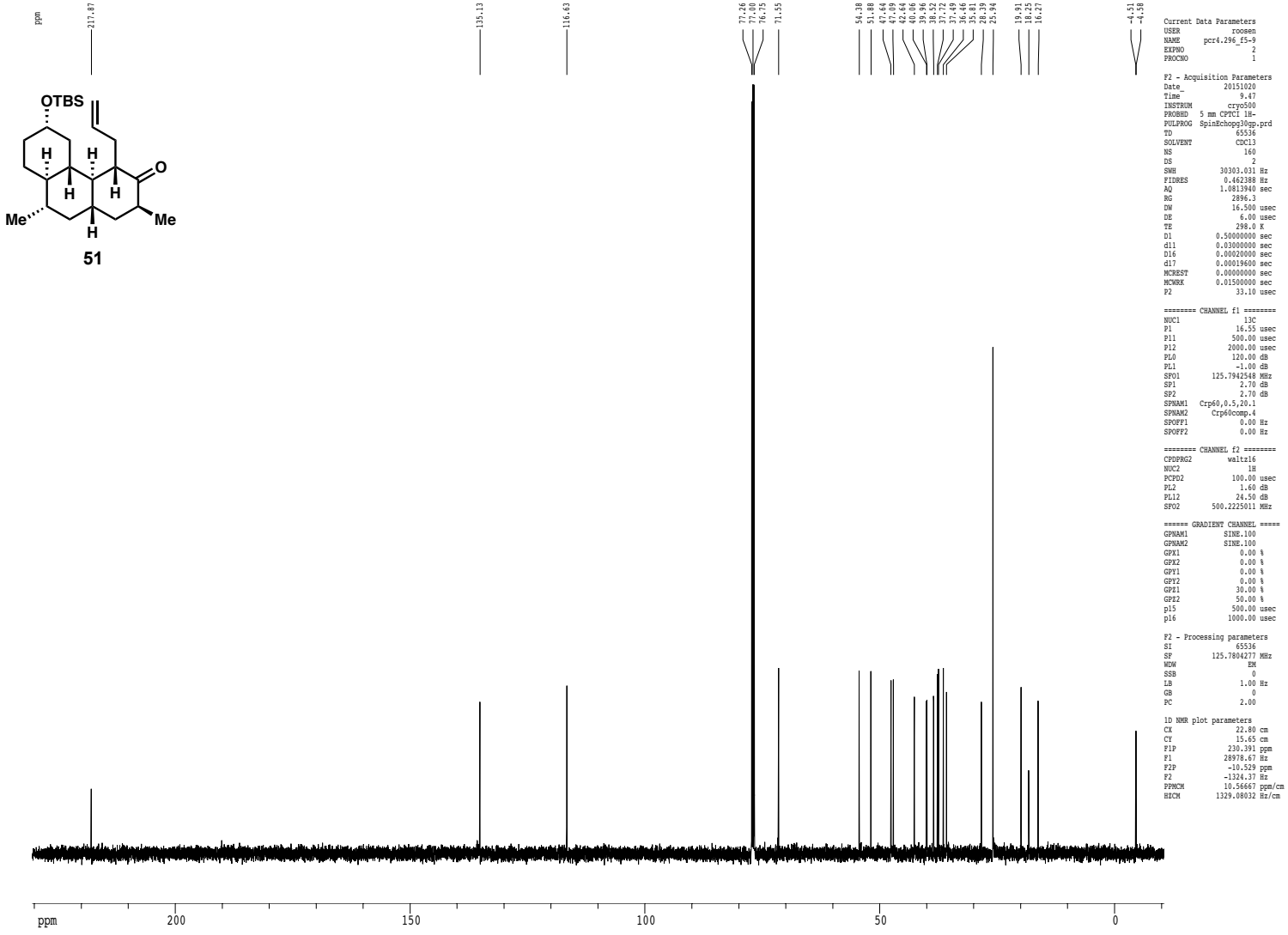
Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME       pcr4.296_f5-9
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20151020
Time                9.47
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    160
DS                      2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                2896.3
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1        125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

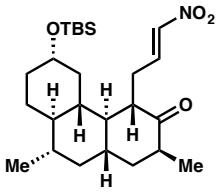
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF          125.7804277 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.391 ppm
F1               28978.67 Hz
F2P               -10.529 ppm
F2               -1324.37 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



52

Current Data Parameters
USER roosen
NAME pcr5.011_f5-8
EXPNO 1
PROCNO 1

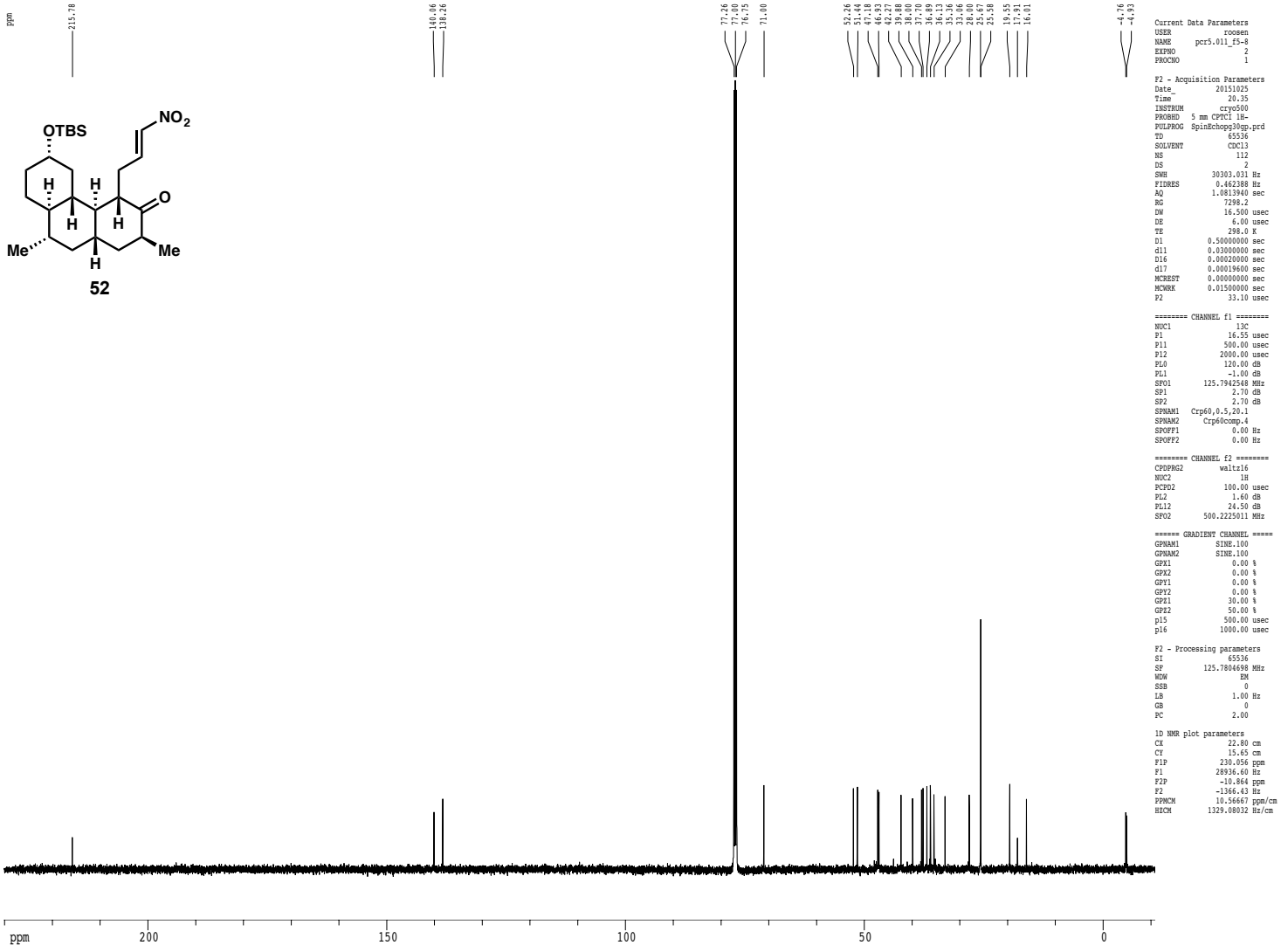
F2 - Acquisition Parameters
Date_ 20151025
Time 20.33
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 5.7
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

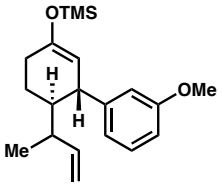
F2 - Processing parameters
SI 65536
SF 500.2200266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



1H spectrum



57

Current Data Parameters
USER roosen
NAME pcr4.205_isolate_c6H6
EXPNO 1
PROCNO 1

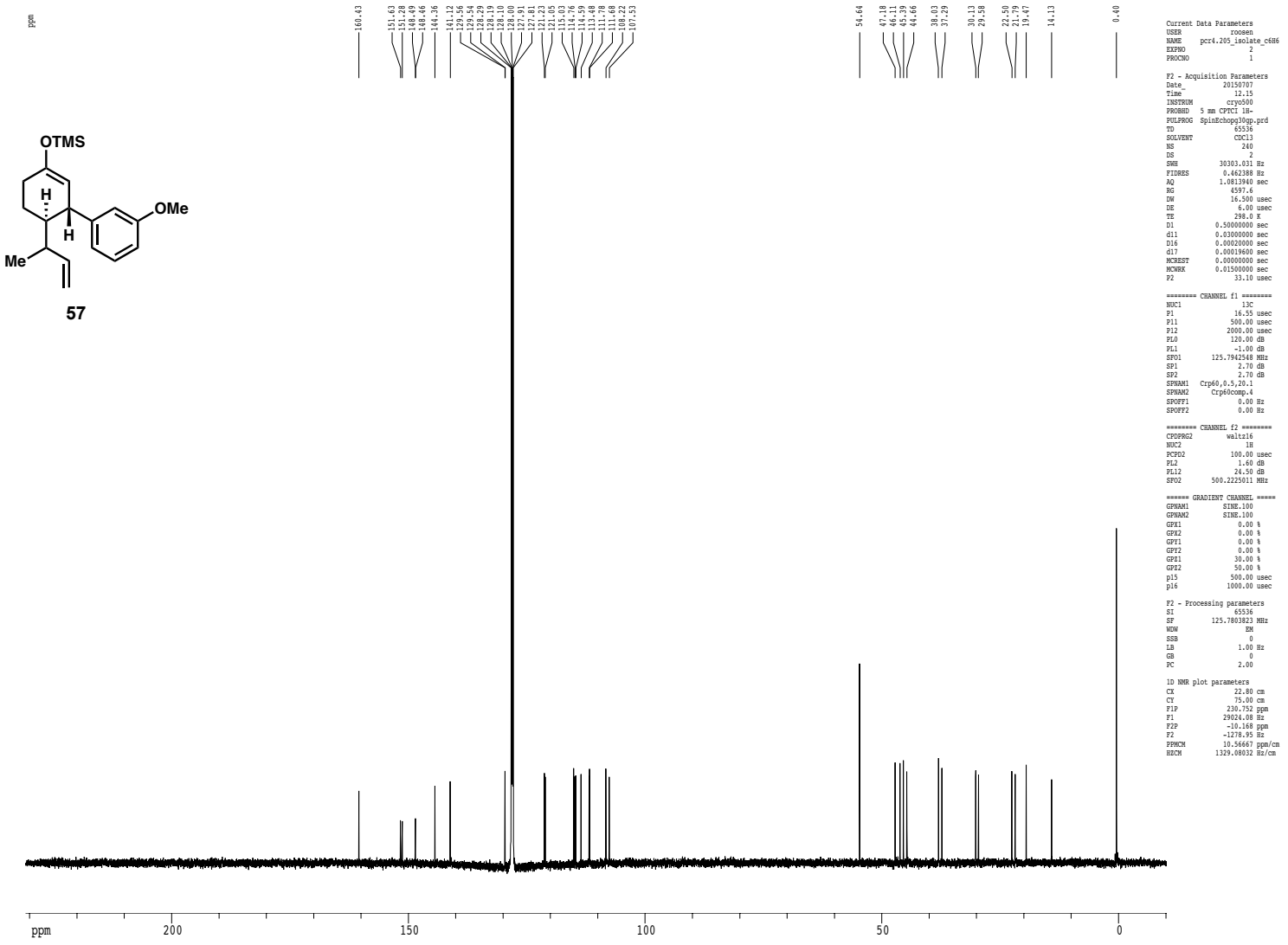
F2 - Acquisition Parameters
Date_ 20150707
Time 12.13
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT C6D6
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 5.7
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33421 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.205_isolate_c6H6
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150707
Time                12.15
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    240
DS                      2
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                 4597.6
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1         125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1   Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

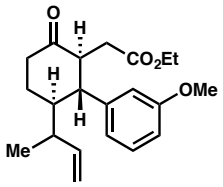
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7803823 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 75.00 cm
F1P              230.752 ppm
F1               29024.08 Hz
F2P              -10.168 ppm
F2               -1278.95 Hz
PPMCM           10.56667 ppm/cm
HZCM         1329.08032 Hz/cm
```

1H spectrum



58

Current Data Parameters
USER roosen
NAME pcr4.188_isolate
EXPNO 2
PROCNO 1

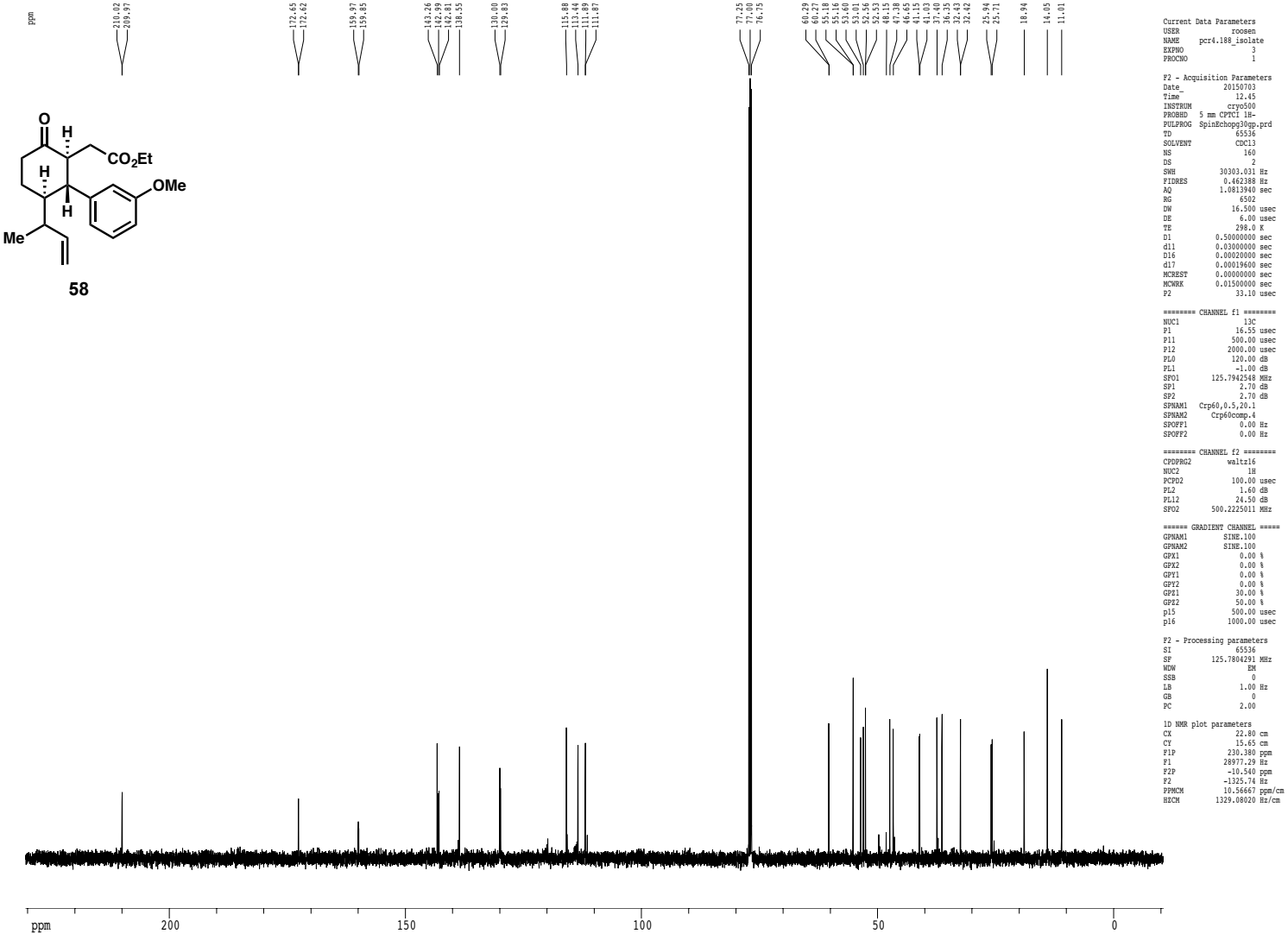
F2 - Acquisition Parameters
Date_ 20150703
Time 12.43
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 6.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200265 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



58

```
Current Data Parameters
USER                roosen
NAME      pcr4.188_isolate
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150703
Time                 12.45
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     160
DS                       2
SWH            30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.08113940 sec
RG                    6502
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                16.55 usec
P11              500.00 usec
P12             2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

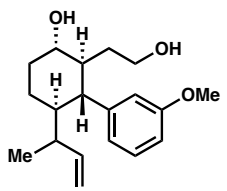
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                   65536
SF           125.7804291 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P               230.380 ppm
F1                28977.29 Hz
F2P                -10.540 ppm
F2                -1325.74 Hz
PPMCM             10.56667 ppm/cm
HZCM          1329.08020 Hz/cm
```

1H spectrum



60

Current Data Parameters
USER roosen
NAME pcr4.276_isolate
EXPNO 1
PROCNO 1

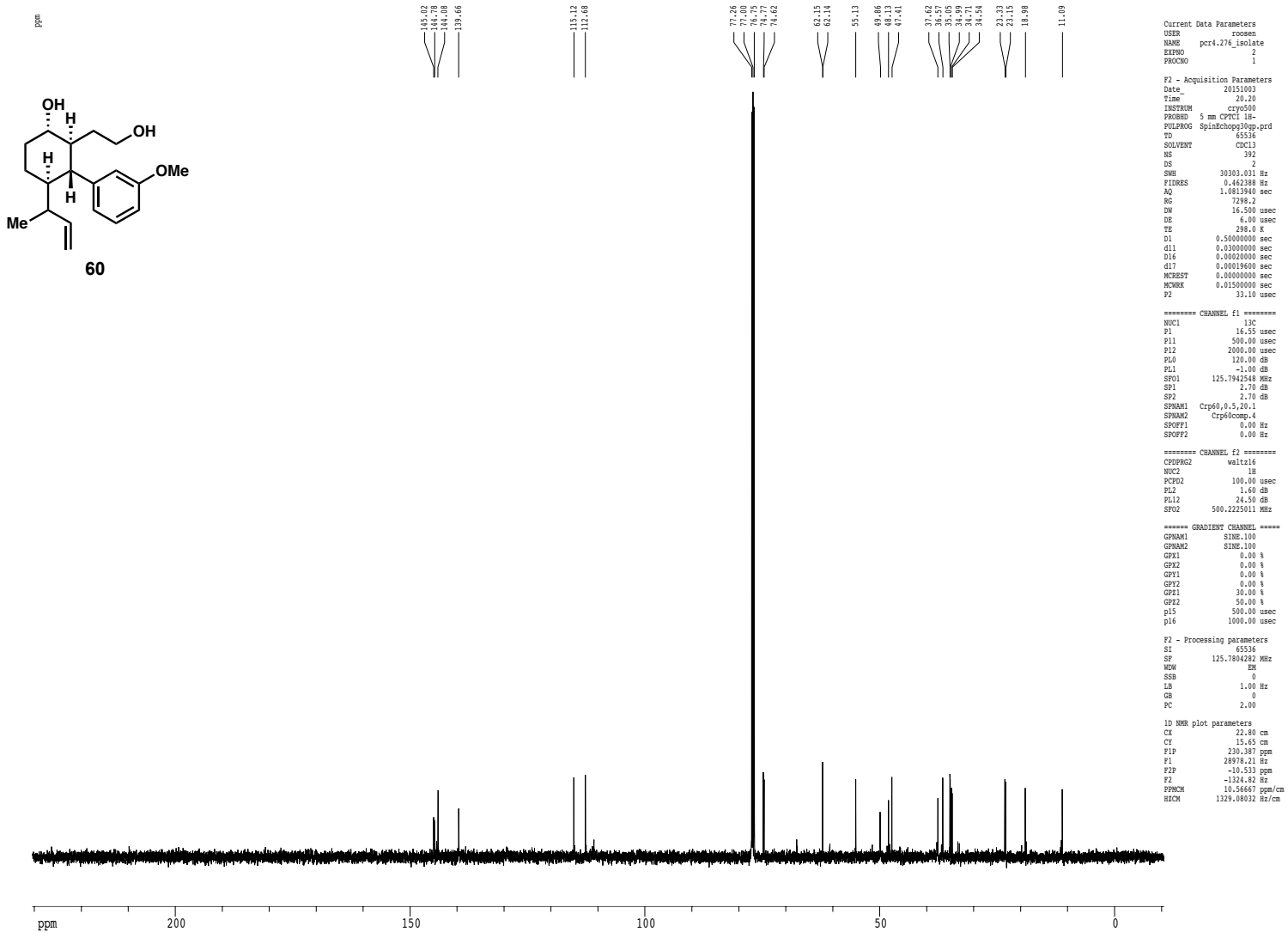
F2 - Acquisition Parameters
Date_ 20151003
Time 20.17
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 9
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

F2 - Processing parameters
SI 65536
SF 500.2200267 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.276_isolate
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20151003
Time              20.20
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                65536
SOLVENT           CDCl3
NS                  392
DS                    2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                7298.2
DW               16.500 usec
DE                6.00 usec
TE                298.0 K
D1            0.50000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2               33.10 usec

======== CHANNEL f1 ========
NUC1                13C
P1                16.55 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1        125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

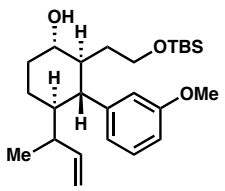
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2        500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF          125.7804282 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.387 ppm
F1                28978.21 Hz
F2P               -10.533 ppm
F2                -1324.82 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



62

Current Data Parameters
USER roosen
NAME pcr4.215_isolate
EXPNO 3
PROCNO 1

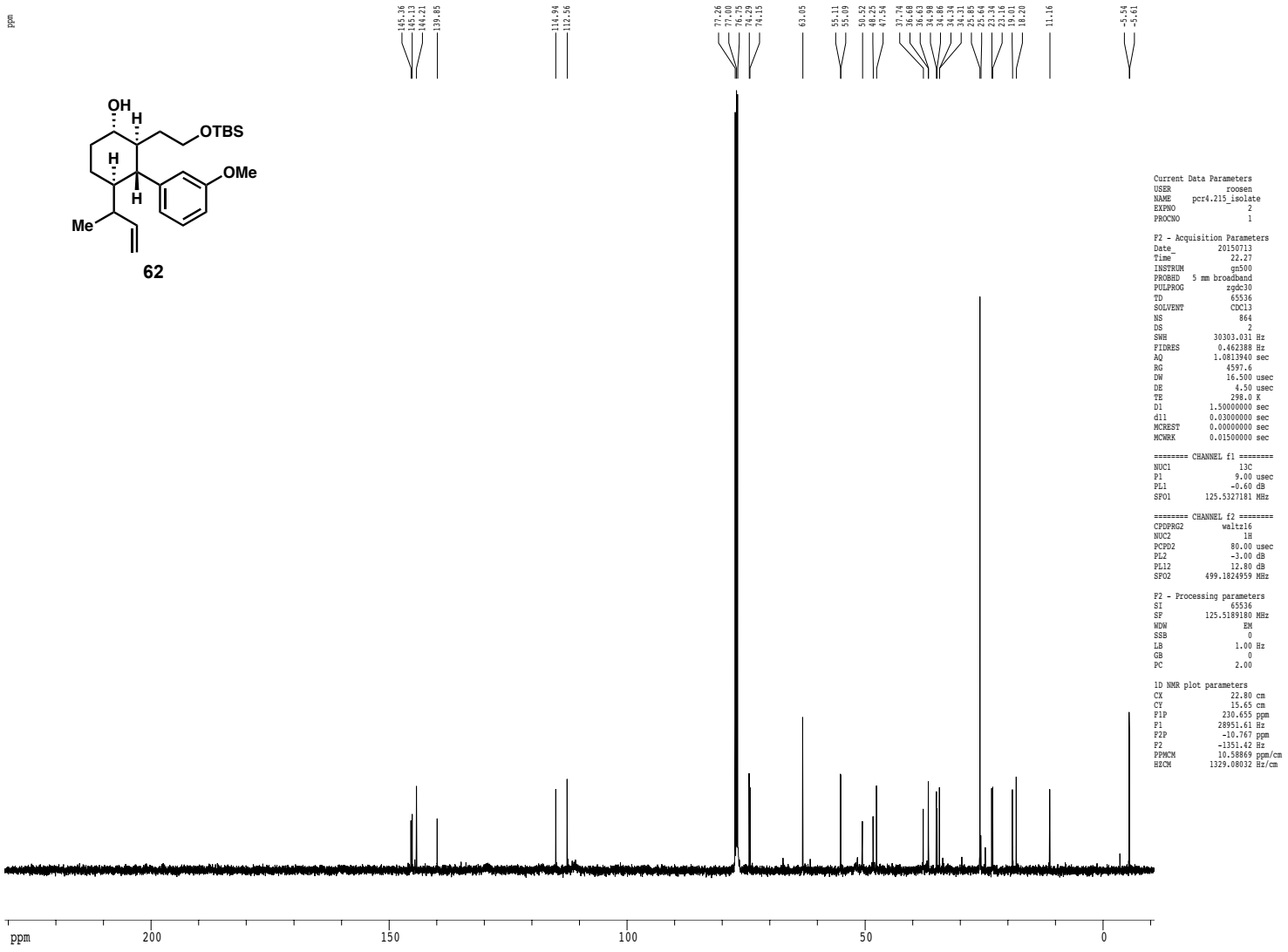
F2 - Acquisition Parameters
Date_ 20150713
Time 22.23
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 32048
SOLVENT CDCl3T
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 80.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -5.80 dB
SFO1 499.1834943 MHz

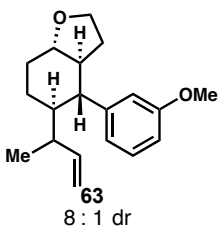
F2 - Processing parameters
SI 65536
SF 499.1800225 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 4991.80 Hz
F2P -1.000 ppm
F2 -499.18 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.83247 Hz/cm

13C spectrum with 1H decoupling



1H spectrum



63

8 : 1 dr


```
Current Data Parameters
USER                roosen
NAME      pcr4.222_isolate
EXPNO                   1
PROCNO                  1

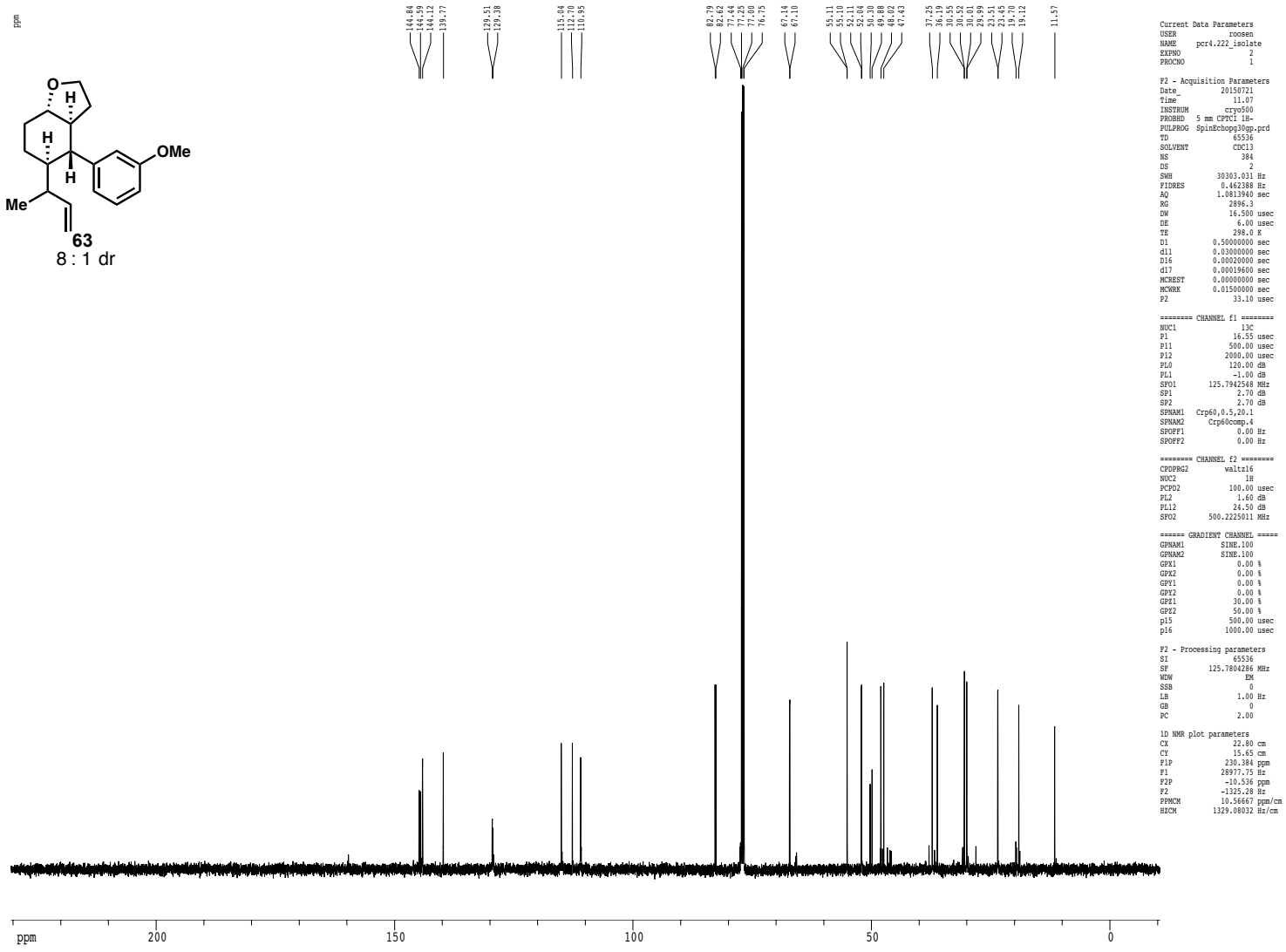
F2 - Acquisition Parameters
Date_           20150721
Time               11.05
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32048
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250026 Hz
AQ              1.9998451 sec
RG                   7.1
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                  1.60 dB
SFO1         500.2235015 MHz

F2 - Processing parameters
SI                   65536
SF           500.2200267 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                10.000 ppm
F1               5002.20 Hz
F2P                -1.000 ppm
F2               -500.22 Hz
PPMCM            0.48246 ppm/cm
HZCM           241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                 roosen
NAME      pcr4.222_isolate
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150721
Time                11.07
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    384
DS                      2
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                2896.3
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                16.55 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

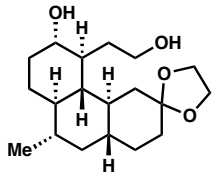
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                   65536
SF           125.7804286 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P               230.384 ppm
F1                28977.75 Hz
F2P                -10.536 ppm
F2                -1325.28 Hz
PPMCM             10.56667 ppm/cm
HZCM           1329.08032 Hz/cm
```

Parameter		Value
1	Title	pcr5.024_isolate.1.fid
2	Comment	1H spectrum
3	Origin	Bruker Analytik GmbH
4	Owner	nmrprd
5	Site	
6	Instrument	cryo500
7	Author	
8	Solvent	CDCl3
9	Temperature	298.0
10	Pulse Sequence	zg30
11	Experiment	1D
12	Probe	5 mm CPTCI 1H-13C/ 15N/ 2H Z-GRD Z44881/ 0020
13	Number of Scans	8
14	Receiver Gain	7.1
15	Relaxation Delay	0.1000
16	Pulse Width	7.5000
17	Presaturation Frequency	
18	Acquisition Time	1.9998
19	Acquisition Date	2015-10-29T19:33:56
20	Modification Date	2021-12-07T23:12:16
21	Class	
22	Spectrometer Frequency	500.22
23	Spectral Width	8012.8
24	Lowest Frequency	-536.7
25	Nucleus	1H
26	Acquired Size	16024
27	Spectral Size	65536
28	Digital Resolution	0.12



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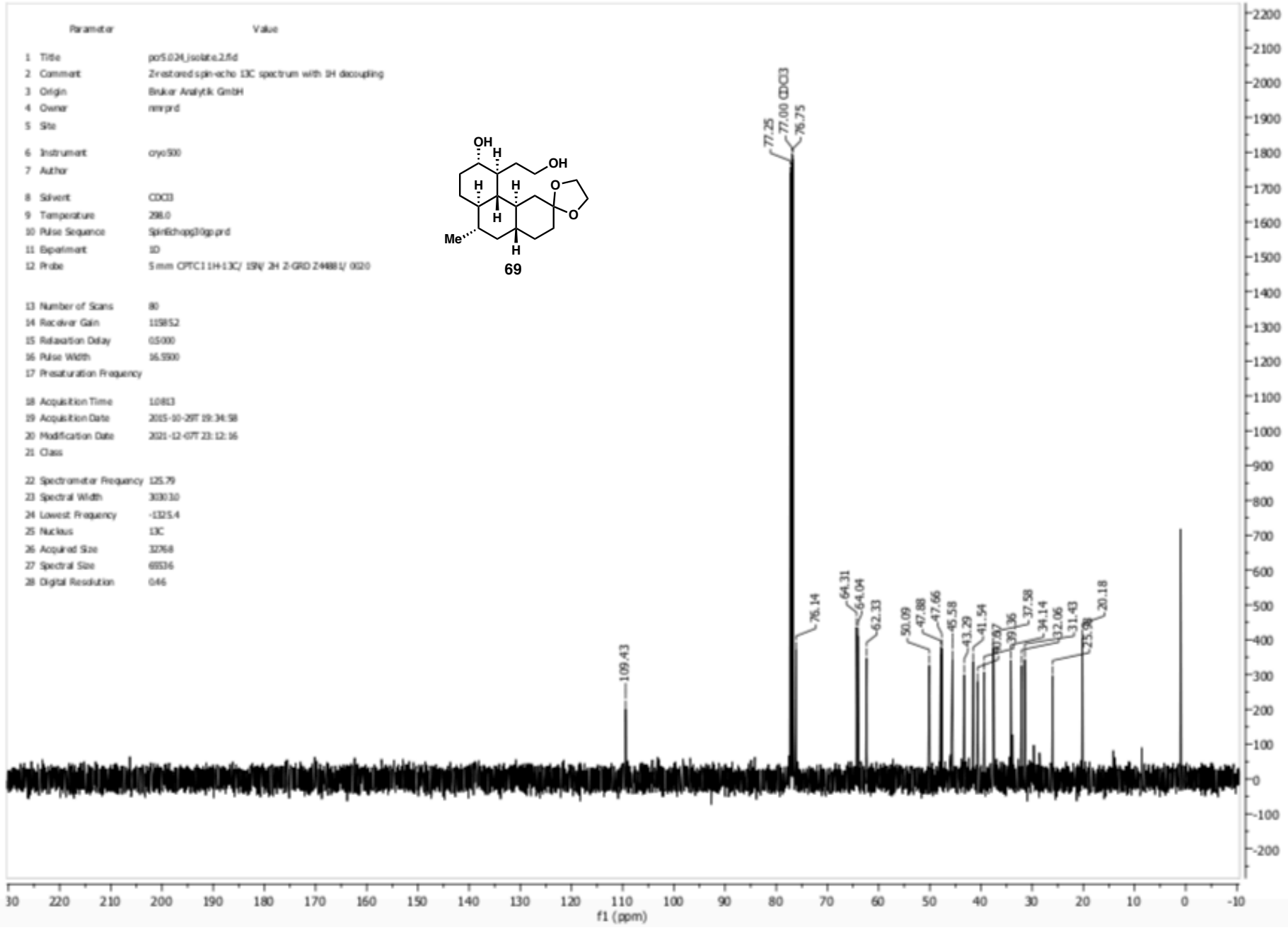
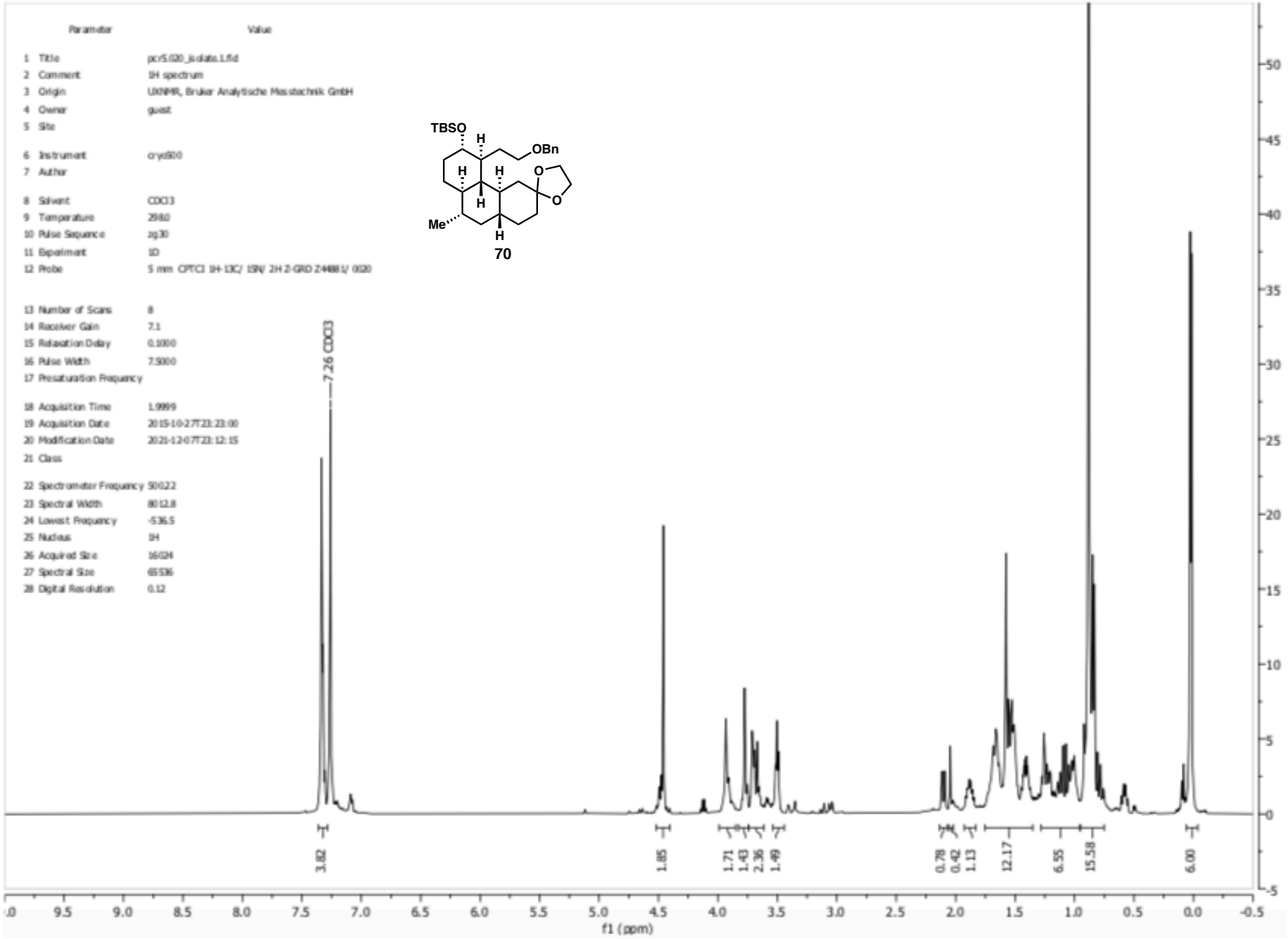
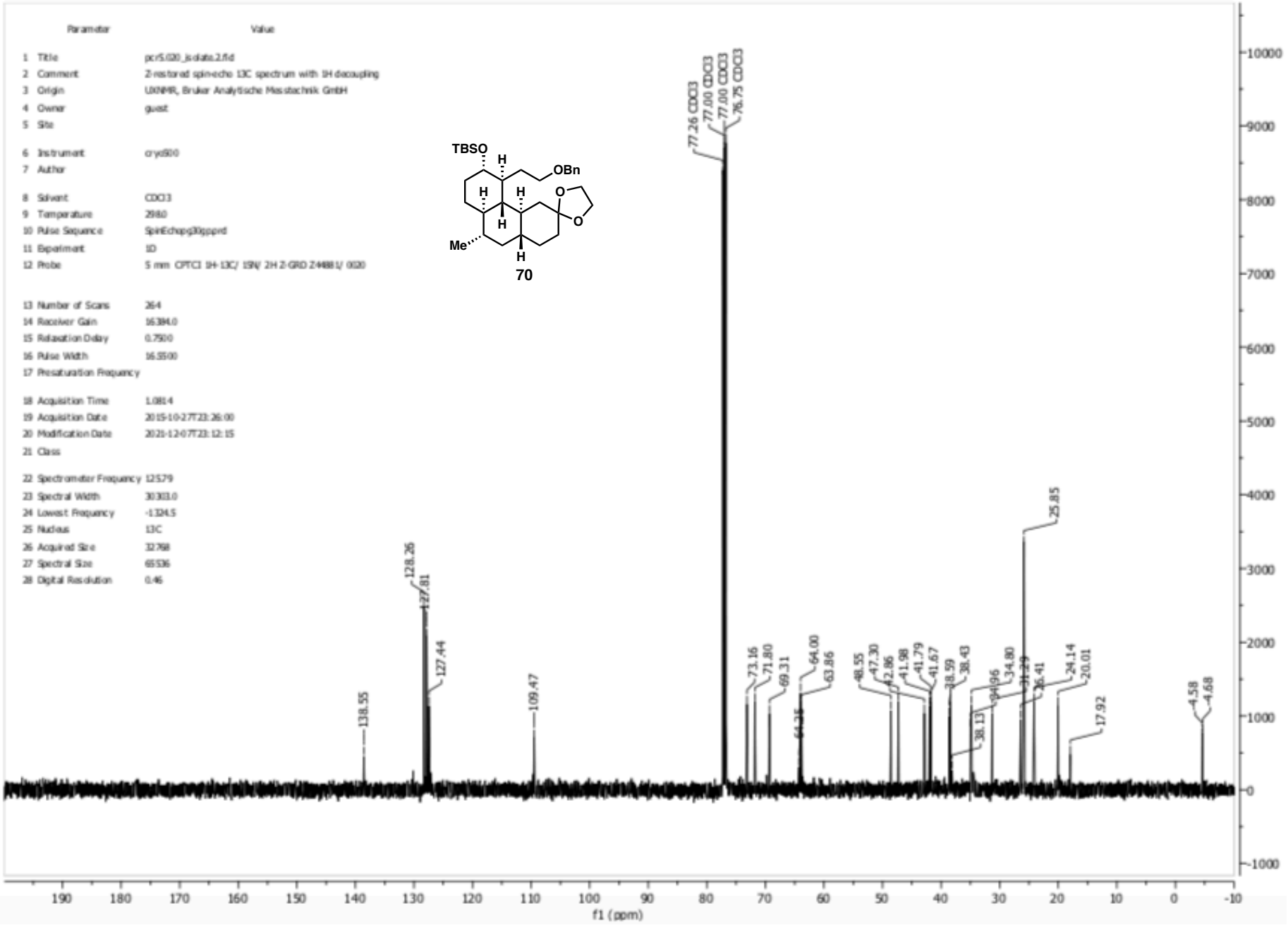
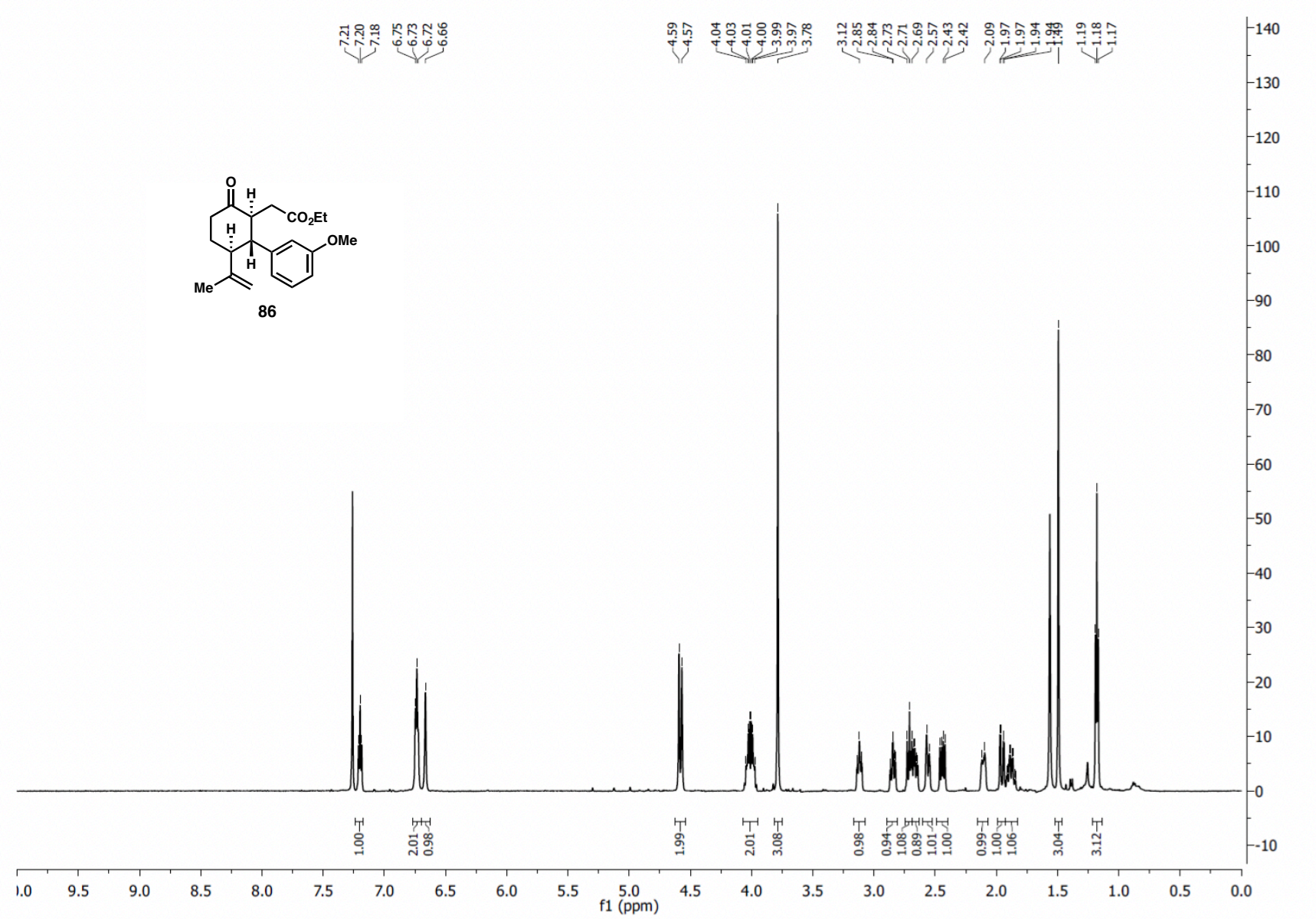
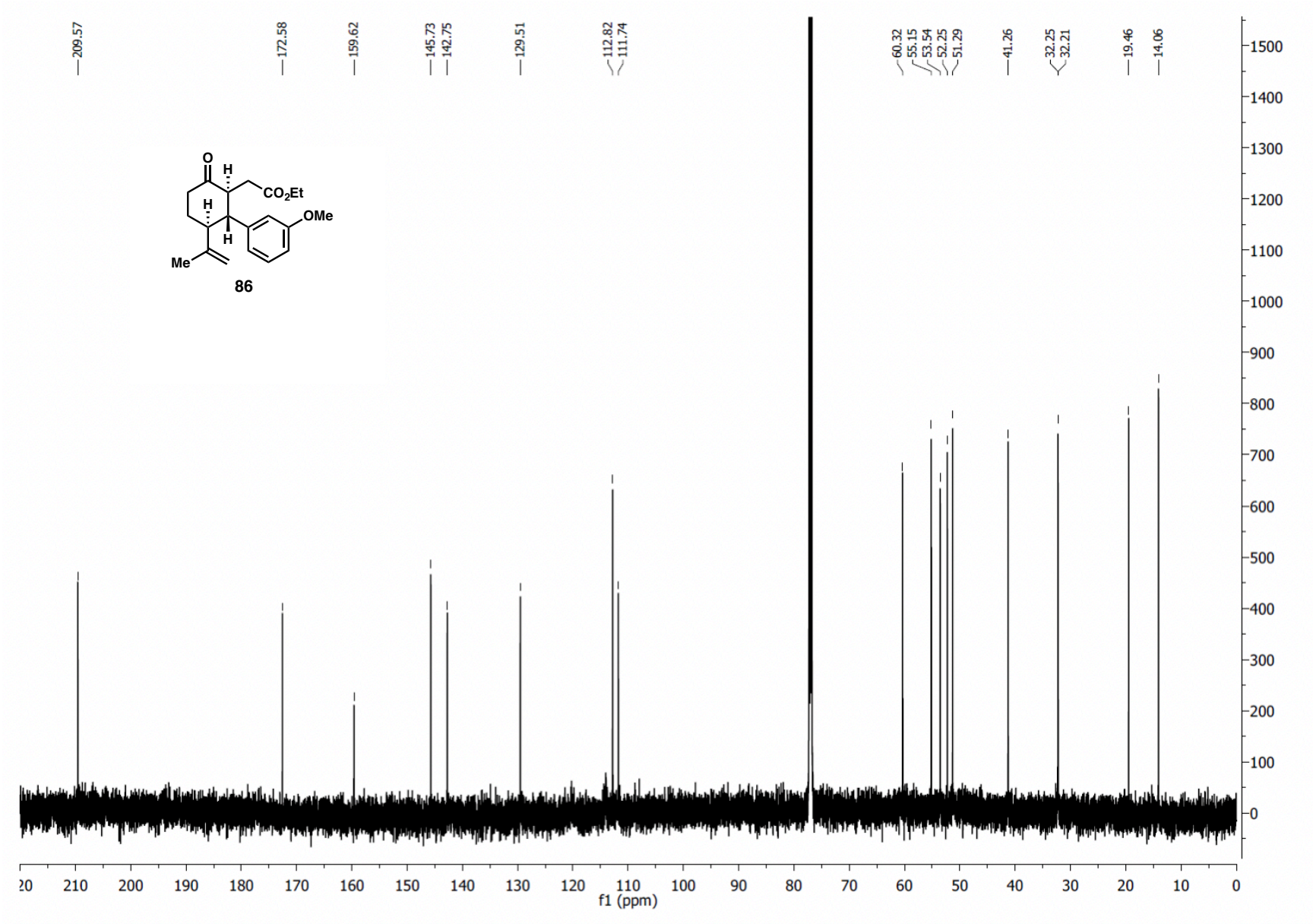
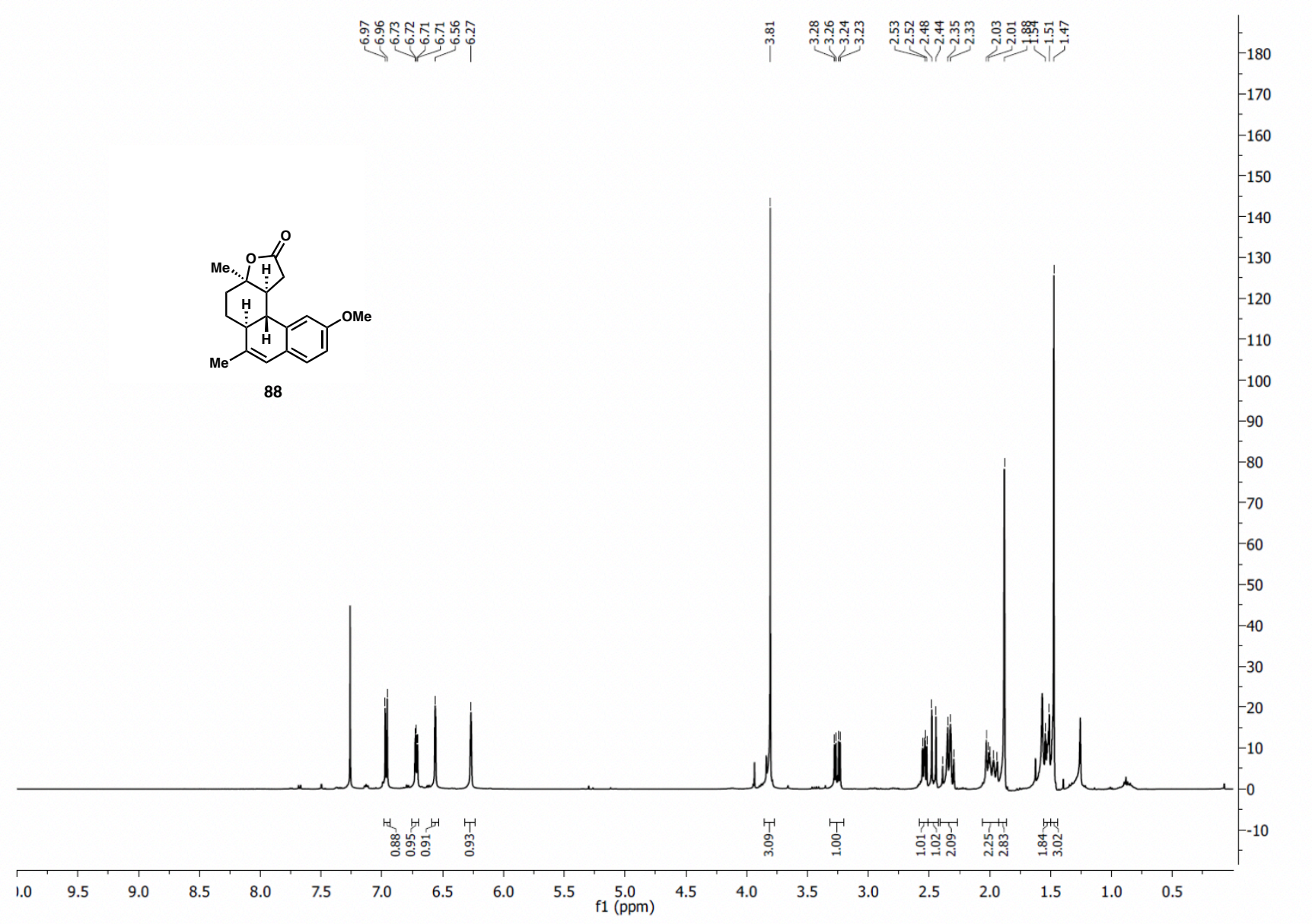

Parameter Value
1 Title po5.024_isolate.2.fid
2 Comment Zn-restored spin-echo 13C spectrum with 1H decoupling
3 Origin Bruker Analytik GmbH
4 Owner nmrprd
5 Site
6 Instrument cryo500
7 Author
8 Solvent CDCl3
9 Temperature 298.0
10 Pulse Sequence Spin6chopp30gp.prd
11 Experiment 1D
12 Probe 5 mm CPTC1 1H-13C/ 15N/ 2H Z-GRD Z44881/ 0020
13 Number of Scans 80
14 Receiver Gain 115852
15 Relaxation Delay 0.5000
16 Pulse Width 16.5500
17 Presaturation Frequency
18 Acquisition Time 1.0813
19 Acquisition Date 2015-10-29T 19:34:58
20 Modification Date 2021-12-07T 23:12:16
21 Class
22 Spectrometer Frequency 125.79
23 Spectral Width 30303.0
24 Lowest Frequency -1325.4
25 Nucleus 13C
26 Acquired Size 32768
27 Spectral Size 65536
28 Digital Resolution 0.46
OH
H
OH
H
H
O
H
O
Me
H
69
77.25
77.00 CDCl3
76.75
109.43
76.14
64.31
64.04
62.33
50.09
47.88
47.66
45.58
43.29
41.54
39.36
37.58
34.14
32.06
31.43
25.38
20.18
f1 (ppm)

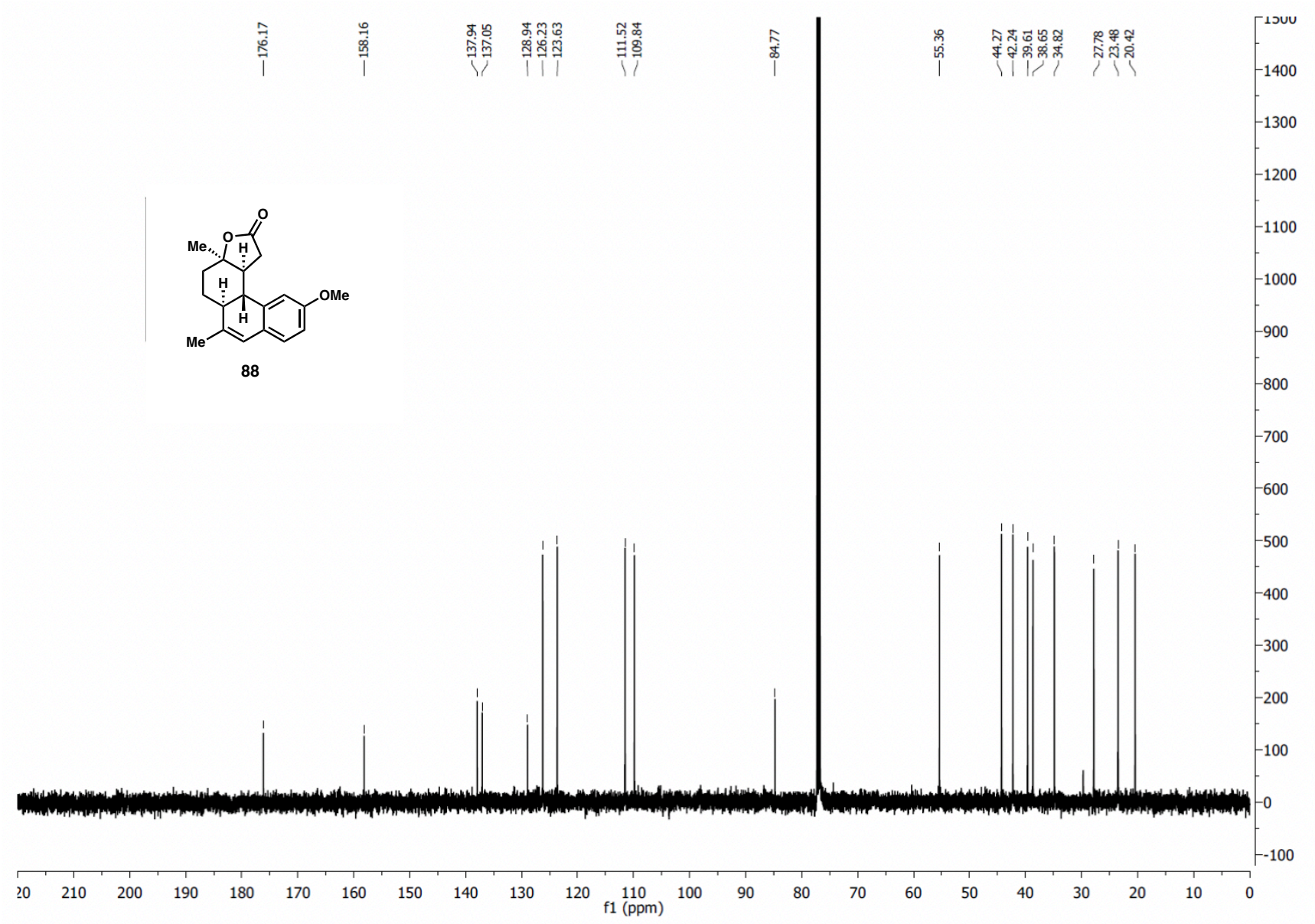

Parameter Value
1 Title pcr5.020_isolate.1.fid
2 Comment 1H spectrum
3 Origin UXNMR, Bruker Analytische Messtechnik GmbH
4 Owner guest
5 Site
6 Instrument cryo500
7 Author
8 Solvent CDCl3
9 Temperature 298.0
10 Pulse Sequence zg30
11 Experiment 1D
12 Probe 5 mm CPTCI 1H-13C/ 15N/ 2H Z-GRD Z44881/ 0020
13 Number of Scans 8
14 Receiver Gain 7.1
15 Relaxation Delay 0.1000
16 Pulse Width 7.5000
17 Presaturation Frequency
18 Acquisition Time 1.9999
19 Acquisition Date 2015-10-27T23:23:00
20 Modification Date 2021-12-07T23:12:15
21 Class
22 Spectrometer Frequency 500.22
23 Spectral Width 8012.8
24 Lowest Frequency -536.5
25 Nucleus 1H
26 Acquired Size 16024
27 Spectral Size 65536
28 Digital Resolution 0.12
TBSO
H
OBn
H
H
O
O
H
Me
H
70
7.26 CDCl3
3.82
1.85
1.71
1.43
2.36
1.49
0.78
0.42
1.13
12.17
6.55
15.58
6.00
f1 (ppm)

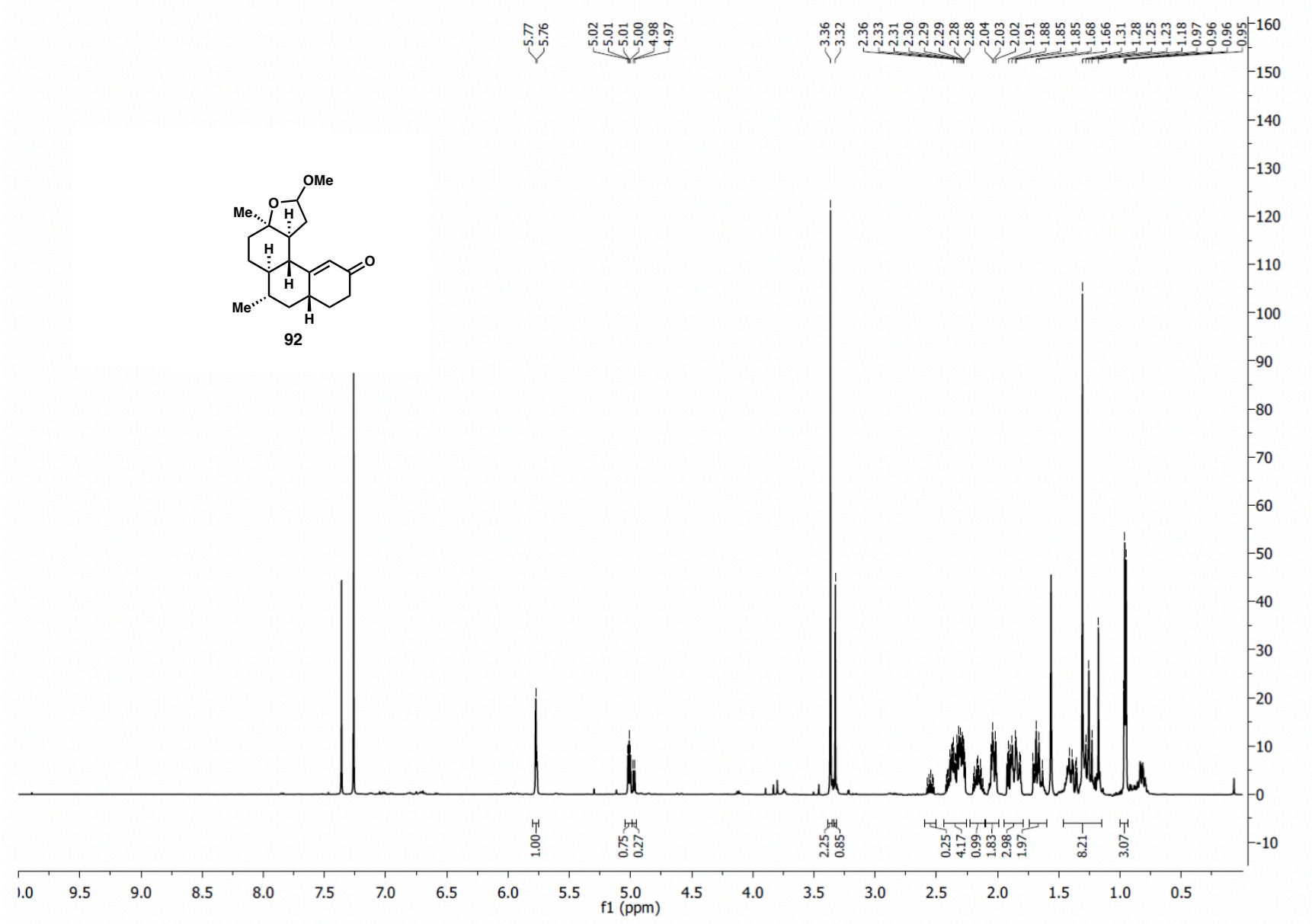

Parameter Value
1 Title pcr5.020_isolate.2.fid
2 Comment 2-restored spin-echo 13C spectrum with 1H decoupling
3 Origin UNMR, Bruker Analytische Messtechnik GmbH
4 Owner guest
5 Site
6 Instrument cryo500
7 Author
8 Solvent CDCl3
9 Temperature 298.0
10 Pulse Sequence SpinEchopg30gppnd
11 Experiment 1D
12 Probe 5 mm CPTCI 1H-13C/ 15N/ 2H Z-GRD Z44881/ 0020
13 Number of Scans 264
14 Receiver Gain 16384.0
15 Relaxation Delay 0.7500
16 Pulse Width 16.3500
17 Presaturation Frequency
18 Acquisition Time 1.0814
19 Acquisition Date 2015-10-27T23:26:00
20 Modification Date 2021-12-07T23:12:15
21 Class
22 Spectrometer Frequency 125.79
23 Spectral Width 30303.0
24 Lowest Frequency -1324.5
25 Nucleus 13C
26 Acquired Size 32768
27 Spectral Size 65536
28 Digital Resolution 0.46
TBSO
H
OBn
H
H
O
O
H
Me
H
70
77.26 CDCl3
77.00 CDCl3
77.00 CDCl3
76.75 CDCl3
128.26
127.81
127.44
138.55
109.47
73.16
71.80
69.31
64.00
63.86
64.35
48.55
47.30
42.86
41.98
41.79
41.67
38.59
38.43
38.13
34.80
34.96
31.29
26.41
25.85
24.14
20.01
17.92
4.58
4.68
f1 (ppm)

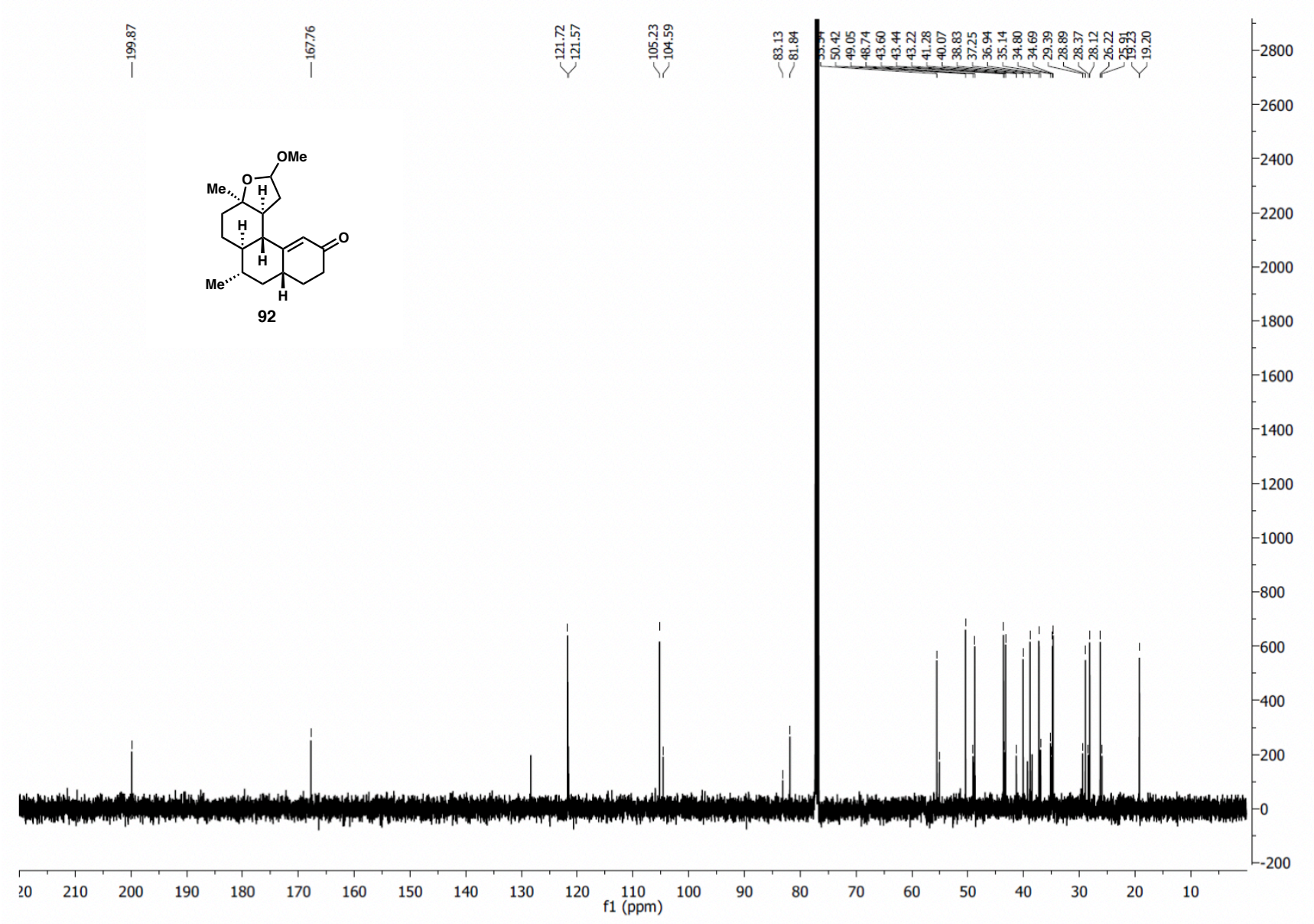

7.21
7.20
7.18
6.75
6.73
6.72
6.66
4.59
4.57
4.04
4.03
4.01
4.00
3.99
3.97
3.78
3.12
2.85
2.84
2.73
2.71
2.69
2.57
2.43
2.42
2.09
1.97
1.97
1.94
1.19
1.18
1.17
O
H
CO2Et
H
OMe
H
Me
86
1.00
2.01
0.98
1.99
2.01
3.08
0.98
0.94
1.08
0.89
1.01
1.00
0.99
1.00
1.06
3.04
3.12
f1 (ppm)


209.57
172.58
159.62
145.73
142.75
129.51
112.82
111.74
60.32
55.15
53.54
52.25
51.29
41.26
32.25
32.21
19.46
14.06
O
H
CO2Et
H
OMe
H
Me
86
f1 (ppm)

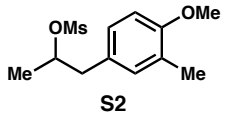

6.97
6.96
6.73
6.72
6.71
6.71
6.56
6.27
3.81
3.28
3.26
3.24
3.23
2.53
2.52
2.48
2.44
2.35
2.33
2.03
2.01
1.88
1.54
1.51
1.47
O
O
Me
H
H
H
OMe
Me
88
0.88
0.95
0.91
0.93
3.09
1.00
1.01
1.02
2.09
2.25
2.83
1.84
3.02
f1 (ppm)


176.17
158.16
137.94
137.05
128.94
126.23
123.63
111.52
109.84
84.77
55.36
44.27
42.24
39.61
38.65
34.82
27.78
23.48
20.42
O
O
Me
H
H
H
OMe
Me
88
f1 (ppm)


OMe
O
Me
H
H
H
O
Me
H
92
f1 (ppm)


199.87
167.76
121.72
121.57
105.23
104.59
83.13
81.84
50.42
49.05
48.74
43.60
43.44
43.22
41.28
40.07
38.83
37.25
36.94
35.14
34.80
34.69
29.39
28.89
28.37
28.12
26.22
19.23
19.20
OMe
O
Me
H
H
H
O
Me
H
92
f1 (ppm)

1H spectrum



S2


```
Current Data Parameters
USER              roosen
NAME      pcr3.140_isolate
EXPNO                   1
PROCNO                  1

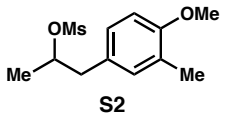
F2 - Acquisition Parameters
Date_           20140707
Time              23.02
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG            zg30
TD                32048
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.250026 Hz
AQ             1.9998451 sec
RG                    5
DW               62.400 usec
DE                6.00 usec
TE                298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                7.50 usec
PL1               1.60 dB
SFO1       500.2235015 MHz

F2 - Processing parameters
SI                65536
SF         500.2200266 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P             10.000 ppm
F1              5002.20 Hz
F2P             -1.000 ppm
F2              -500.22 Hz
PPMCM          0.48246 ppm/cm
HZCM          241.33423 Hz/cm
```

Z-restored spin-echo 13C spectrum with 1H decoupling



S2


```
Current Data Parameters
USER                roosen
NAME          pcr3.140_isolate
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20140707
Time                23.04
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    304
DS                      2
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                   3251
DW                 16.500 usec
DE                  6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                  31.00 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                  15.50 usec
P11                500.00 usec
P12               2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

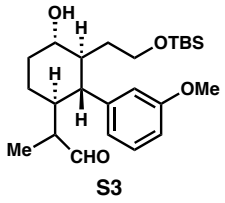
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            125.7804286 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.384 ppm
F1                28977.75 Hz
F2P               -10.536 ppm
F2               -1325.28 Hz
PPMCM            10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



S3

Current Data Parameters
USER roosen
NAME pcr4.217_isolate
EXPNO 1
PROCNO 1

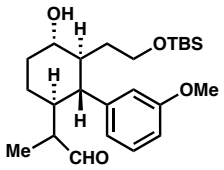
F2 - Acquisition Parameters
Date_ 20150715
Time 14.59
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 32048
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250026 Hz
AQ 1.9998451 sec
RG 8
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz

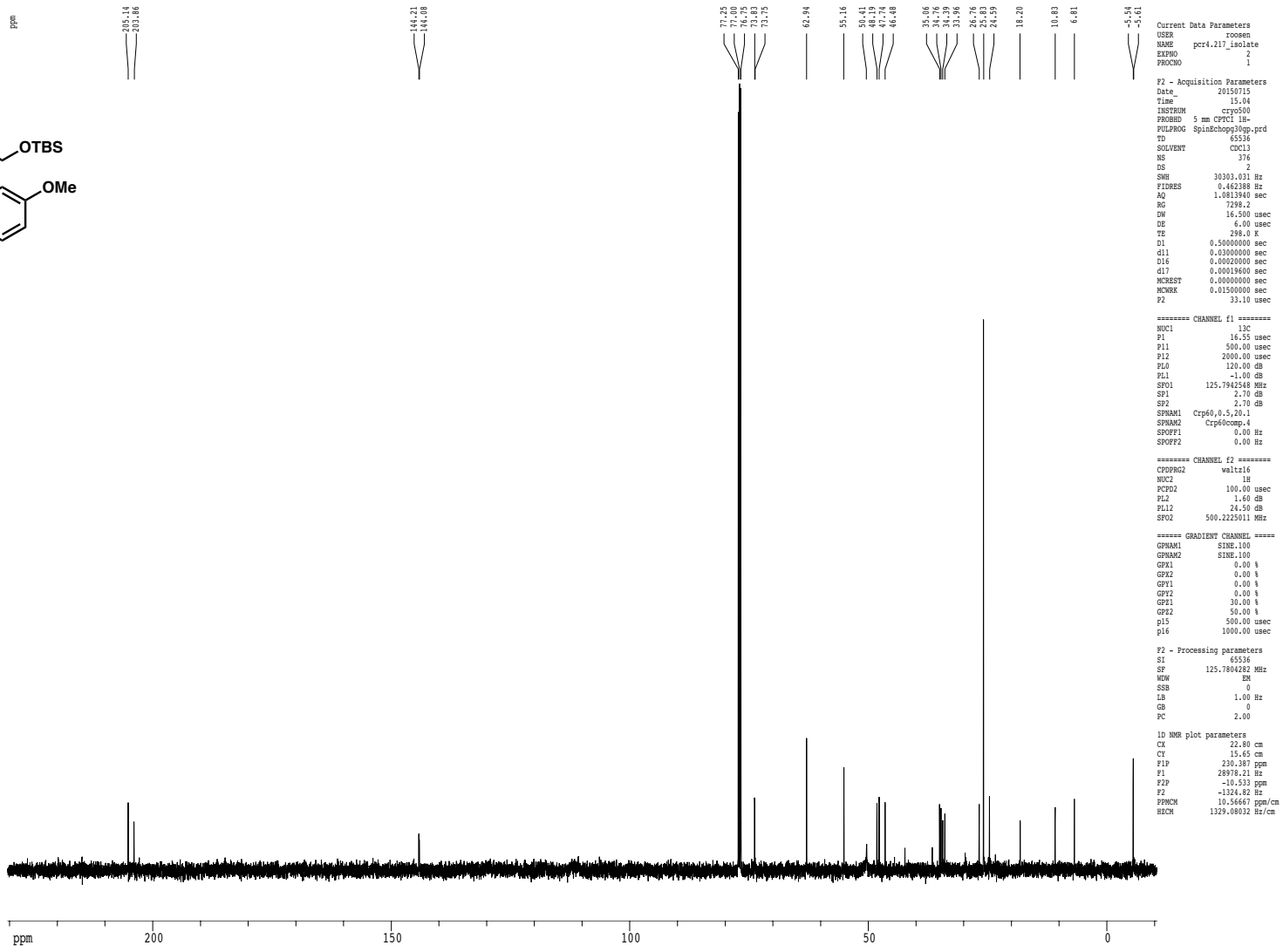
F2 - Processing parameters
SI 65536
SF 500.2200269 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5002.20 Hz
F2P -1.000 ppm
F2 -500.22 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



S3




```
Current Data Parameters
USER                roosen
NAME      pcr4.217_isolate
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20150715
Time                15.04
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    376
DS                      2
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

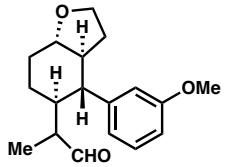
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804282 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

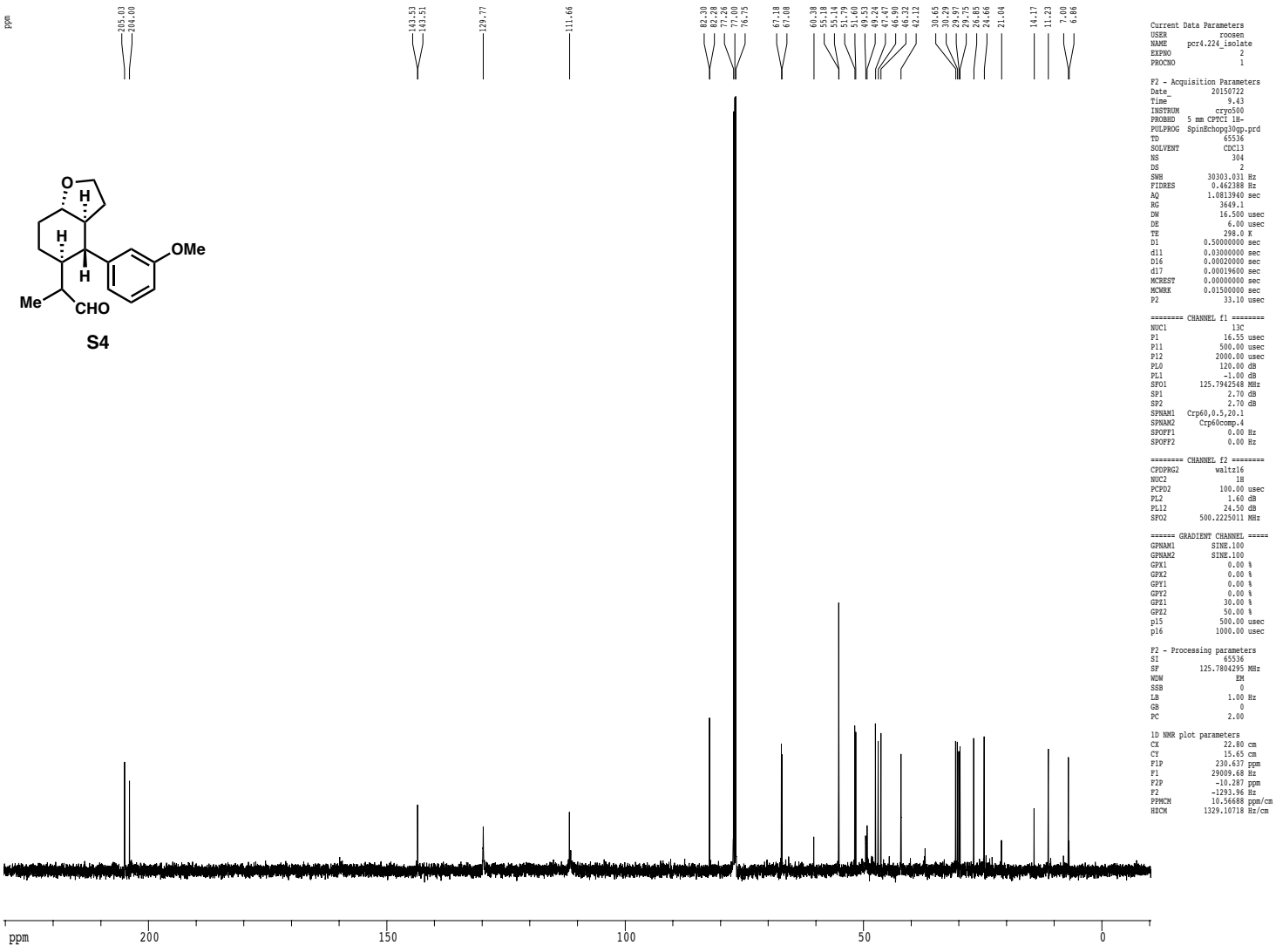
1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.387 ppm
F1              28978.21 Hz
F2P               -10.533 ppm
F2              -1324.82 Hz
PPMCM           10.56667 ppm/cm
HZCM          1329.08032 Hz/cm
```

1H spectrum



S4

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                roosen
NAME      pcr4.224_isolate
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150722
Time                9.43
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    304
DS                      2
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                 3649.1
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.50000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804295 MHz
WDW                    EM
SSB                     0
LB                  1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               230.637 ppm
F1               29009.68 Hz
F2P               -10.287 ppm
F2               -1293.96 Hz
PPMCM           10.56688 ppm/cm
HZCM          1329.10718 Hz/cm
```