

–Supporting Information for–

**Systematic comparison of sets of ^{13}C NMR spectra that are potentially identical.
Confirmation of the configuration of a cuticular hydrocarbon from the cane beetle
*Antitrogus parvulus***

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General experimental procedures

^1H and ^{13}C NMR spectra were recorded with residual non-deuterated solvent as the internal standard. Coupling constants are rounded to the nearest 0.5 Hz. IR spectra were recorded on an FTIR as thin films produced by evaporation of a DCM solution on sodium chloride plates unless otherwise stated. Chemical ionisation (CI) in MS was performed using ammonia. Chromatography refers to flash column chromatography using silica gel (230-300 mesh).

Tetrahydrofuran (THF) was dried and distilled from sodium metal using benzophenone as an indicator under an atmosphere of nitrogen. Dichloromethane (DCM) was dried and distilled from calcium hydride under an atmosphere of nitrogen. Ether refers to diethyl ether, which was dried and distilled from sodium metal using benzophenone as an indicator under an atmosphere of nitrogen. Light petroleum refers to the fraction of petroleum ether distilled between 40–60 °C. Benzene and hexane were dried over sodium metal. Butyllithium (1.6 M in hexanes) was titrated against a solution of propan-2-ol in xylene with 2,2'-bipyridine as an indicator. Triethylamine and diisopropylamine were dried over potassium hydroxide pellets. Brine refers to saturated aqueous sodium chloride. Anhydrous cerium(III) chloride was prepared by heating the heptahydrate overnight at 80 °C under reduced pressure and was stored under an atmosphere of N_2 .

Experimental information for NMR spectra

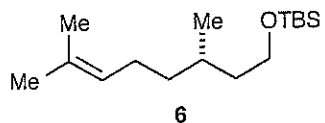
All the ^{13}C NMR data that were used for the analysis were collected on a 700 MHz NMR spectrometer at ^{13}C frequency of 176.03 MHz. The sample temperature was maintained at 293 or 298K at a precision of $\pm 0.1\text{K}$ using a temperature controller. The samples were equilibrated for about 30mins prior to acquisition. A narrow spectral width (SW) of about 94 ppm was used to improve resolution when the number of acquisition data points are kept the same. 32K data points (TD) were acquired, which were zero-filled to 128k (SI) before processing. Trafficante apodization function was used with a lb value of 0.4 Hz to improve resolution further. Line widths at half height of the ^{13}C NMR peaks range from 0.7 to 1Hz. For samples 2 and 4, ^{13}C NMR data was collected twice each (one week apart) at both 293 and 298K for reproducibility. They were reproducible to a level of about $\pm 1\text{ppb}$.

General procedure to estimate the sample temperature of a previously recorded spectrum.

The temperature of the sample in a ^{13}C NMR experiment is not necessarily the same as the temperature of the probe (the radiofrequency irradiation used for broadband ^1H decoupling will generally raise the temperature significantly), and the temperature of the probe is not necessarily the temperature indicated or set by the spectrometer hardware (calibration accuracy is rarely better than ± 1 °C). Sample temperature is therefore necessarily uncertain (unless independently measured), and some method for correcting the effects of uncontrolled differences in temperature between samples is needed.

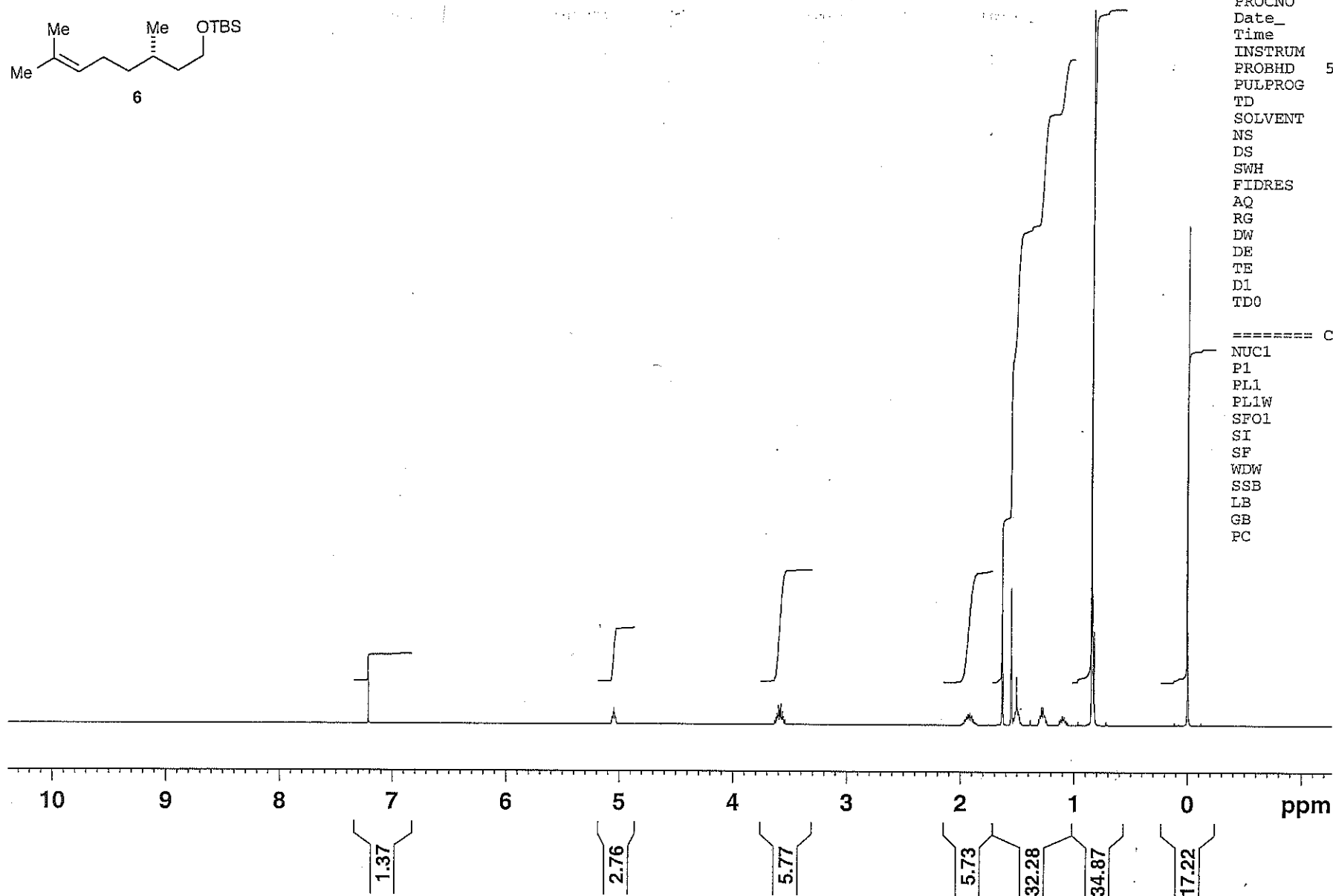
The procedure described here is for the case where the “same” resonances of the candidate samples match each other but not the natural product. The expectation is that the natural product spectrum was recorded at a different sample temperature. To identify this temperature, change the probe temperature of the synthetic samples by some small value (perhaps 3–5 K), then repeat the subtraction of the “same” group of resonances. If the absolute values of the subtraction values of S/R and the NP all get smaller, then temperature dependence is the problem and you changed the probe temperature in the right direction. If the absolute values of the subtraction values of S/R and the NP all get larger, then temperature dependence is again the problem, but you changed the probe temperature in the wrong direction. Temperature effects on chemical shifts are usually linear over small temperature changes, so a two-point line can now be plotted for each resonance and values of the natural product spectrum can be placed on the line to estimate the sample temperature. To confirm, record the spectra of the synthetic samples at the estimated temperature of the natural product sample. All the “same” values of NP will have zero difference or a small, constant difference (the calibration error) with S/R. Now you have learned the temperature of the natural product spectrum – or rather, the nominal temperature to which the probe in this spectrometer has to be set to obtain the same actual sample temperature as the NP sample.

HL102-006
mPROTON CDCl3 /opt/bruk500data/2010/Dec ejt 9

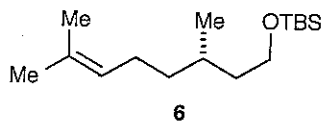


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TE 293.0 K
D1 1.00000000 sec
TD0 1

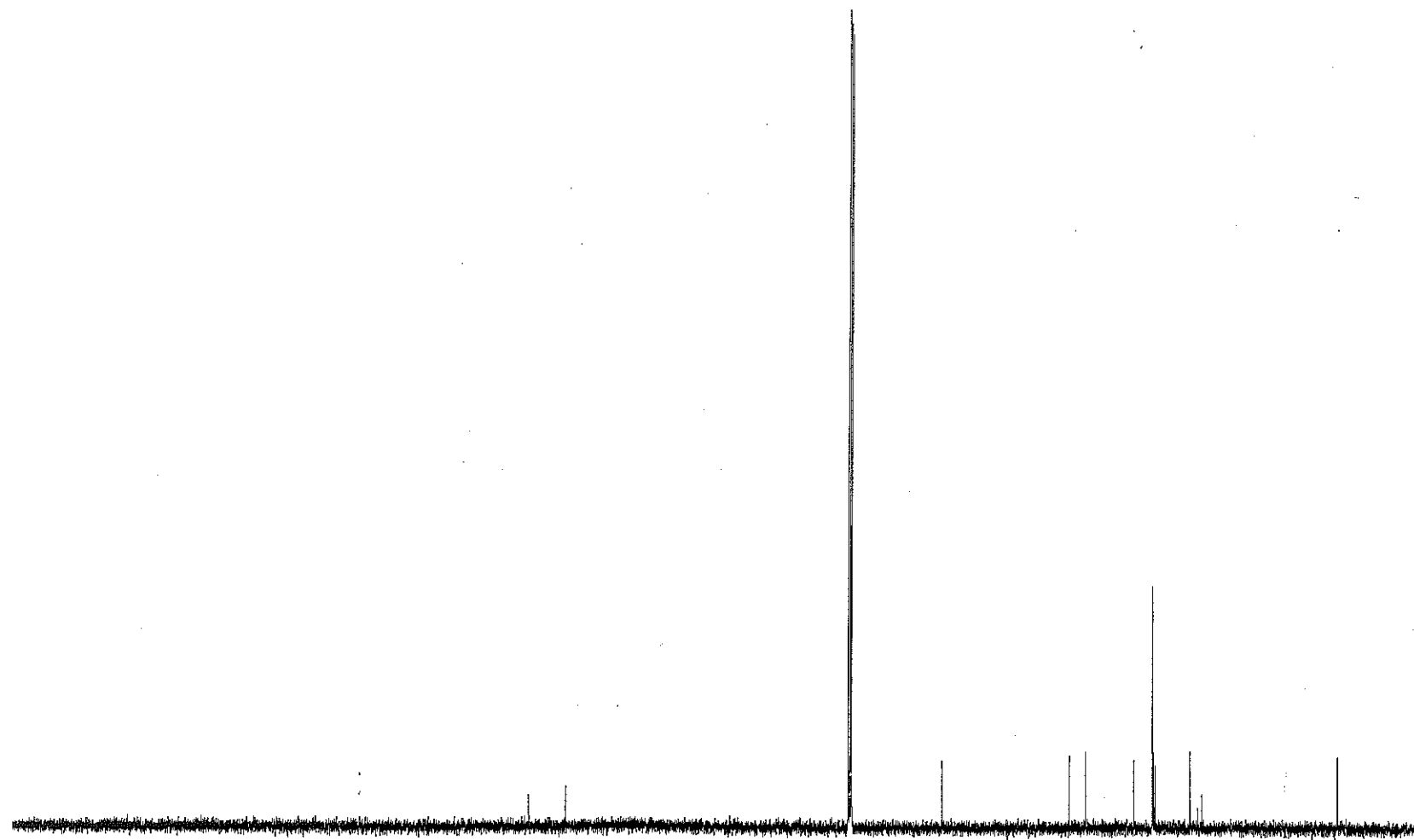
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



HL102-006
 mCARBON CDCl3 /opt/bruk500data/2010/Dec ejt 9



131.12
 124.90
 77.28
 77.03
 76.78
 61.48
 39.94
 37.22
 29.10
 25.99
 25.75
 25.49
 19.64
 18.37
 17.66
 -5.24
 -5.26



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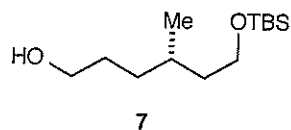
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PL13W     0.12841040 W
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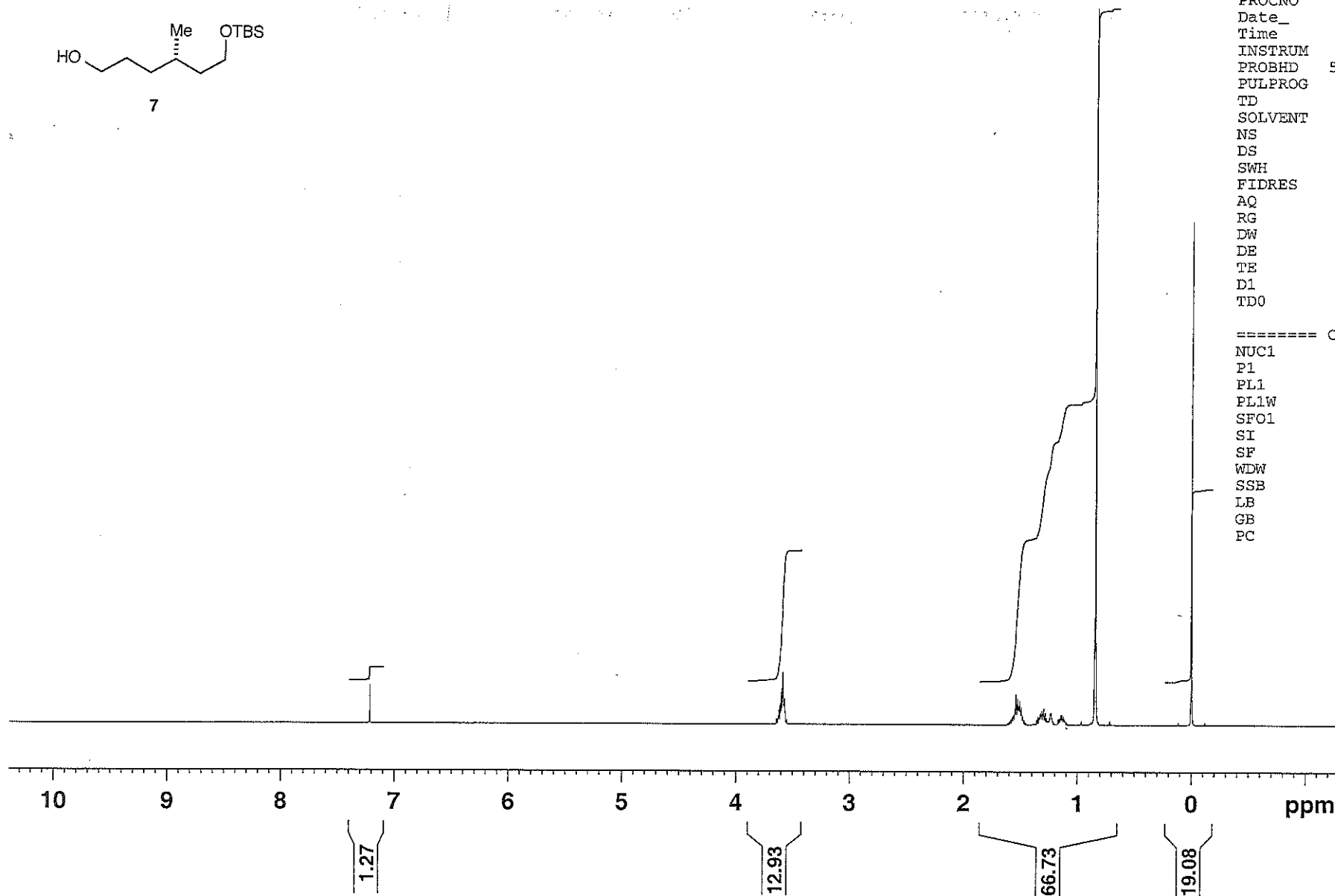
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HL102-007
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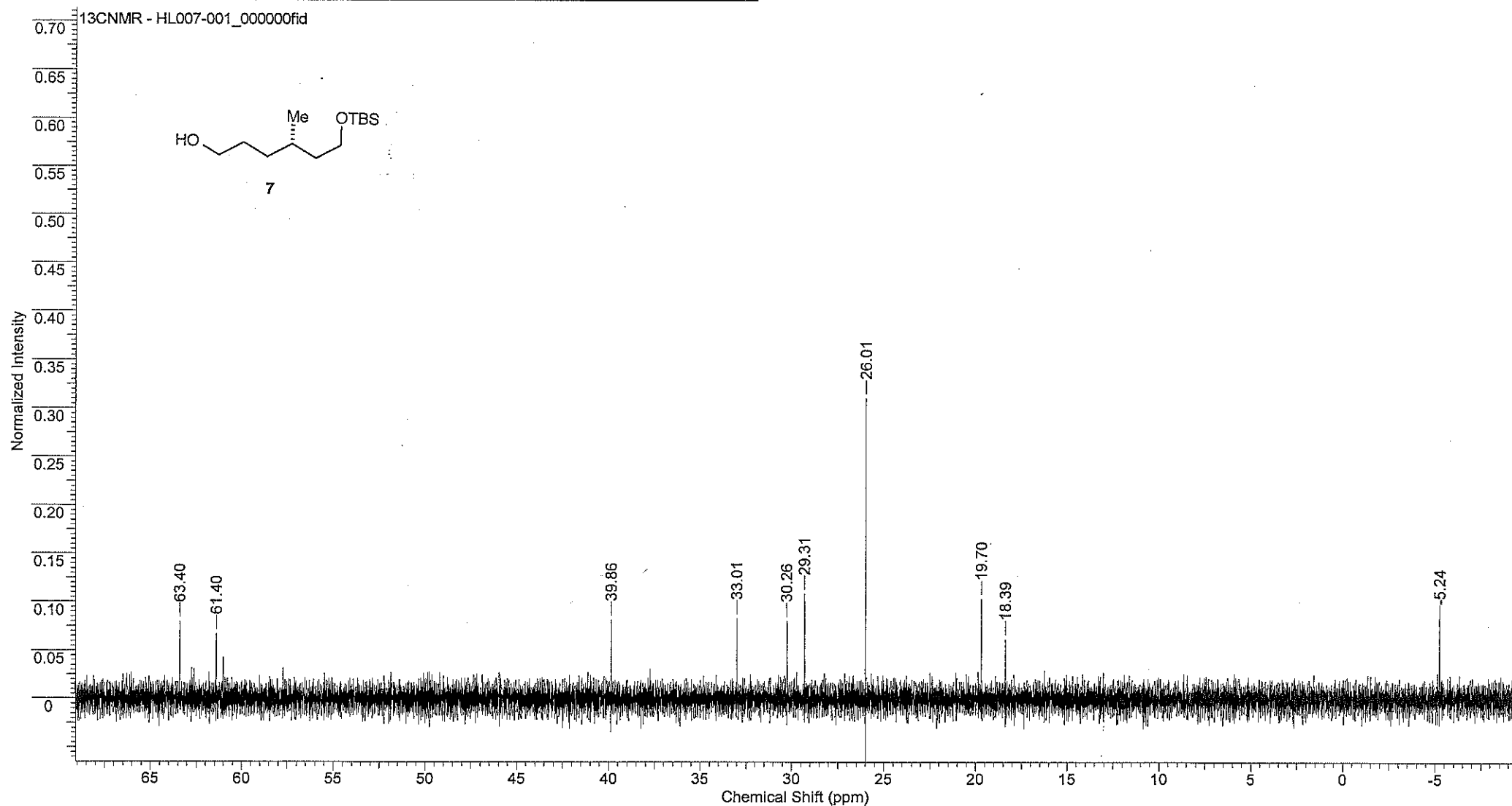


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AQ 3.1719923 sec
RG 161
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DE 13.38 usec
TE 293.0 K
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TD0 1

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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

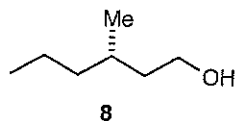


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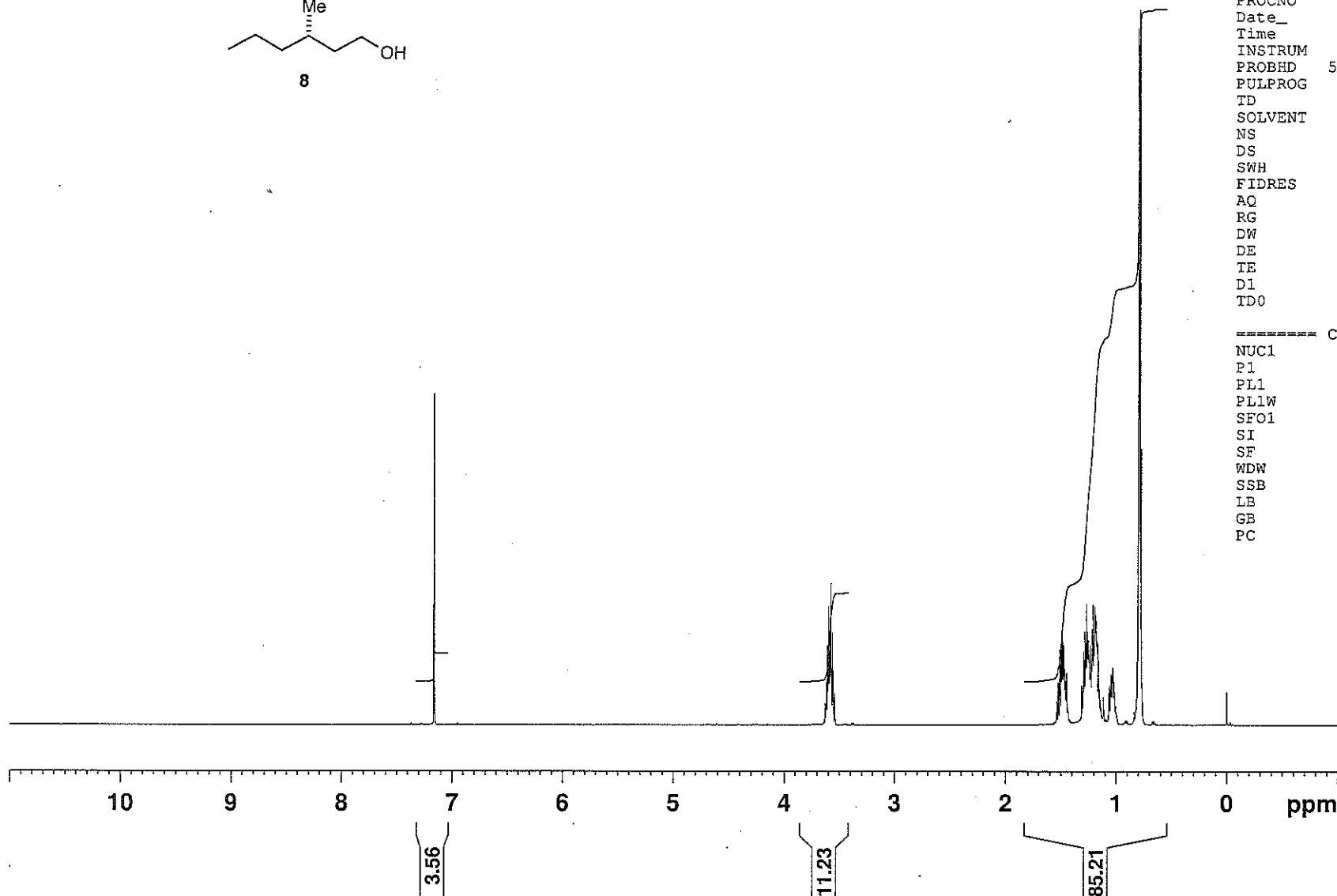
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HL046-001
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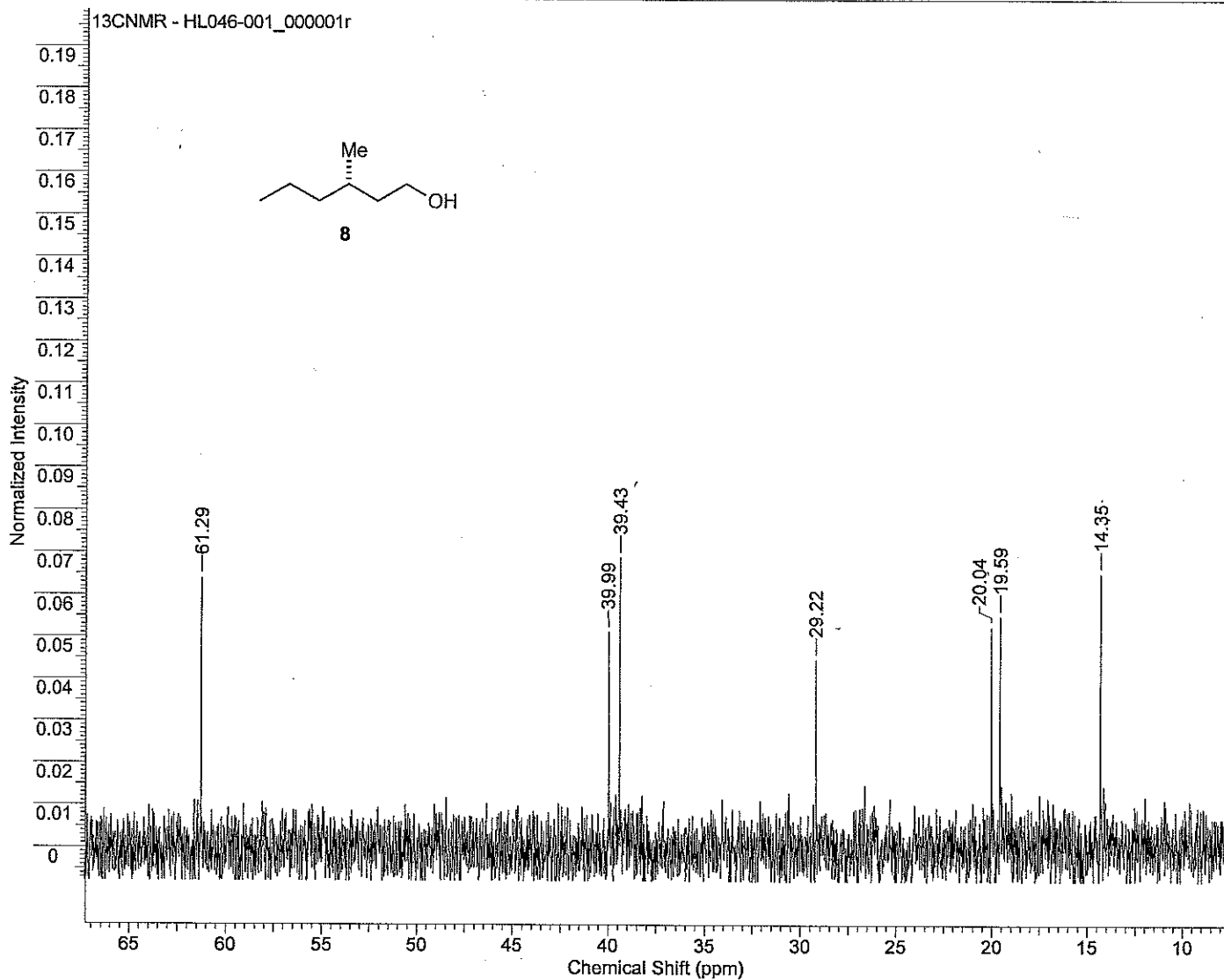


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D1 1.00000000 sec
TD0 1

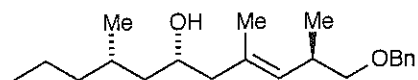
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SF 500.1300627 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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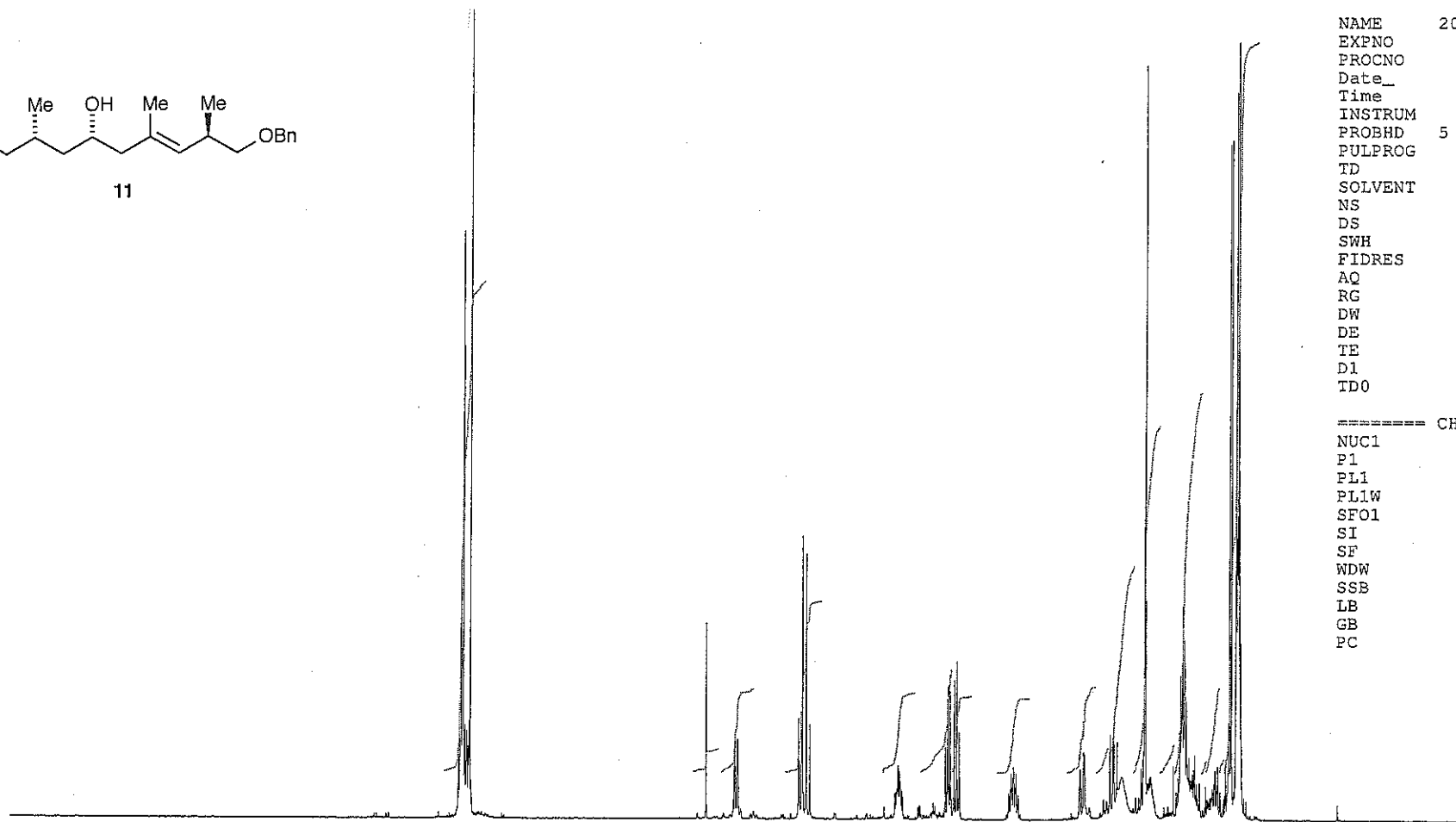
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11

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SWH 8264.463 Hz
FIDRES 0.126106 Hz
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RG 362
DW 60.500 usec
DE 9.40 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

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SFO1 400.1324710 MHz
SI 32768
SF 400.1300375 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm

16.19

0.75

2.76

5.67

2.62

3.40

2.52

2.46

2.88

0.84

6.90

11.50

0.94

12.61

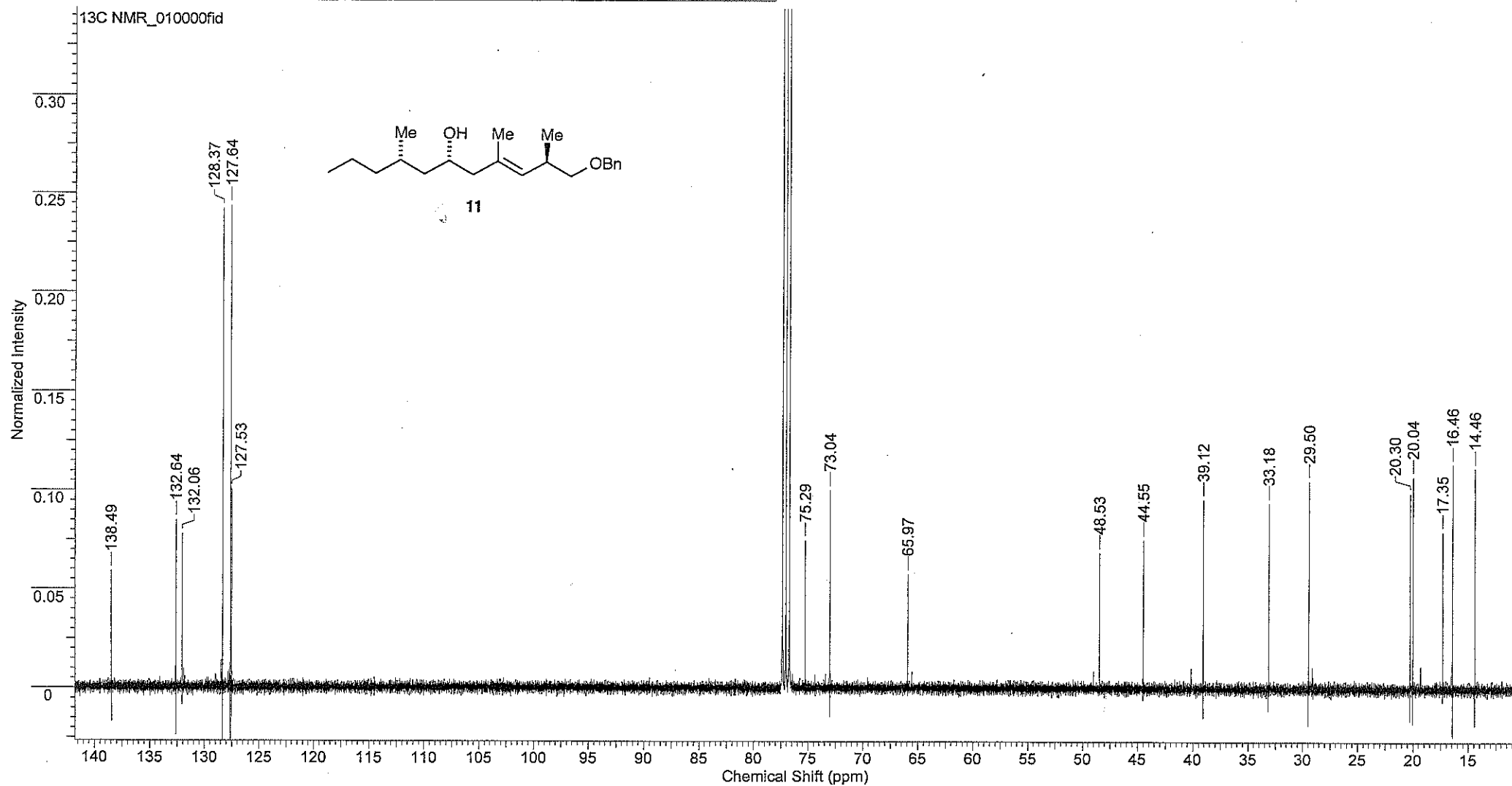
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2.83

0.48

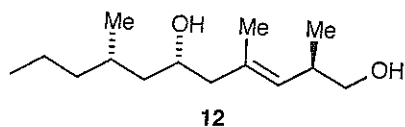
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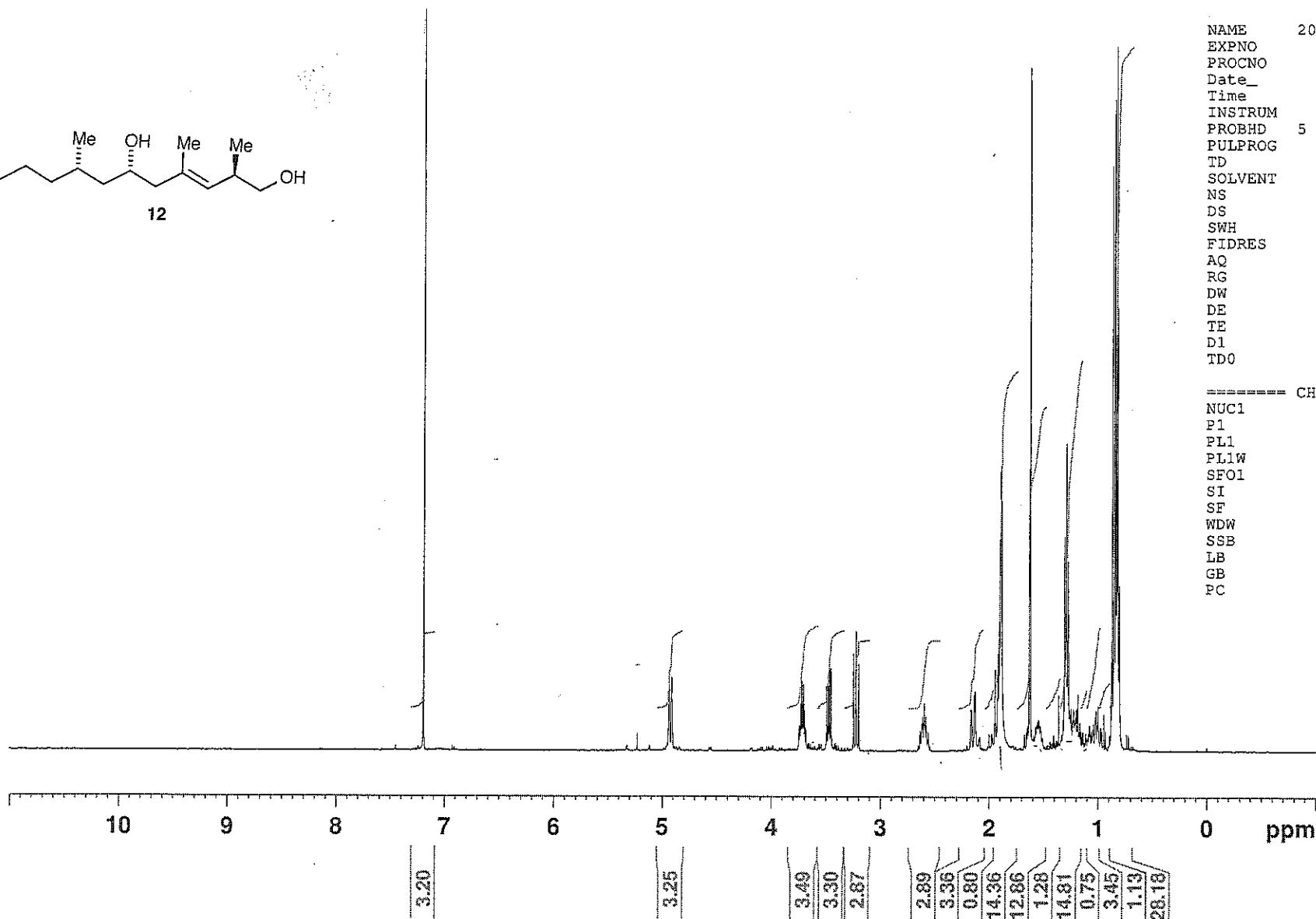
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HL089-001
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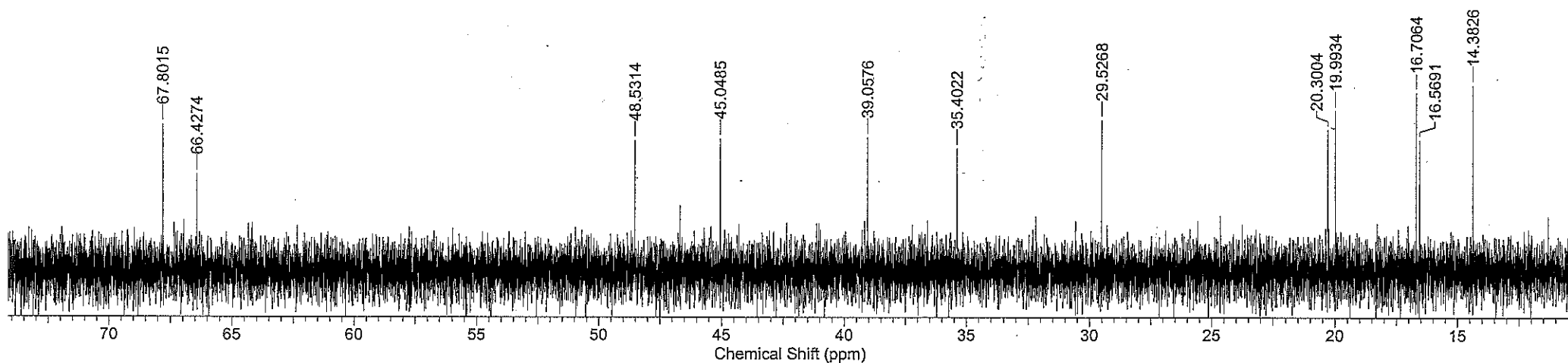
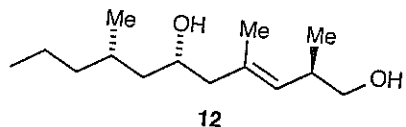
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SOLVENT CDCl3
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FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 362
DW 60.500 usec
DE 9.40 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1

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PL1 -3.60 dB
PL1W 17.83863831 W
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SI 32768
SF 400.1300364 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



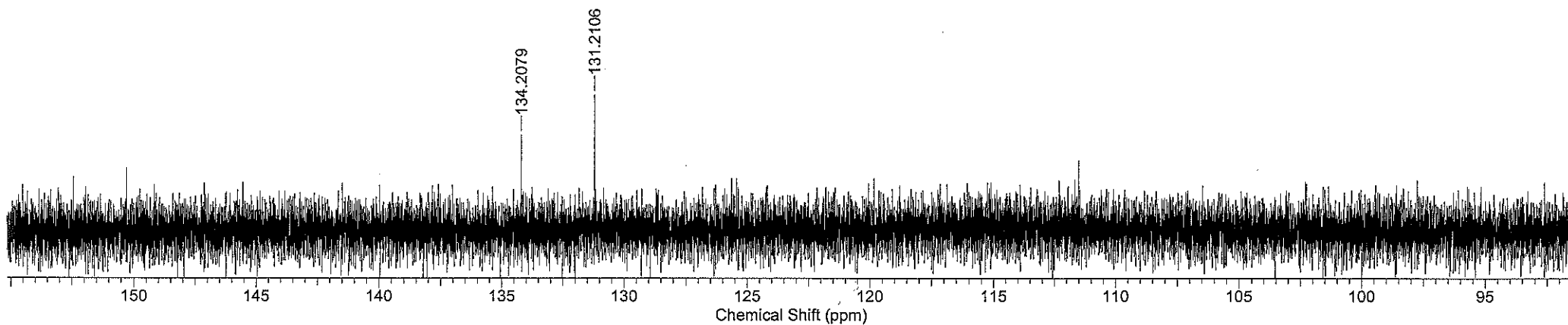
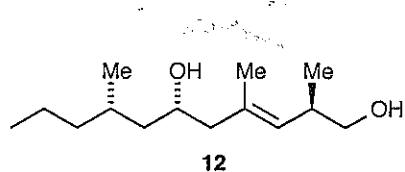
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ejt

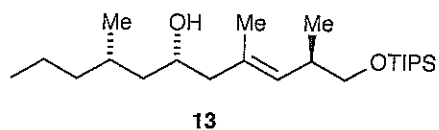


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ejt



HL102-012
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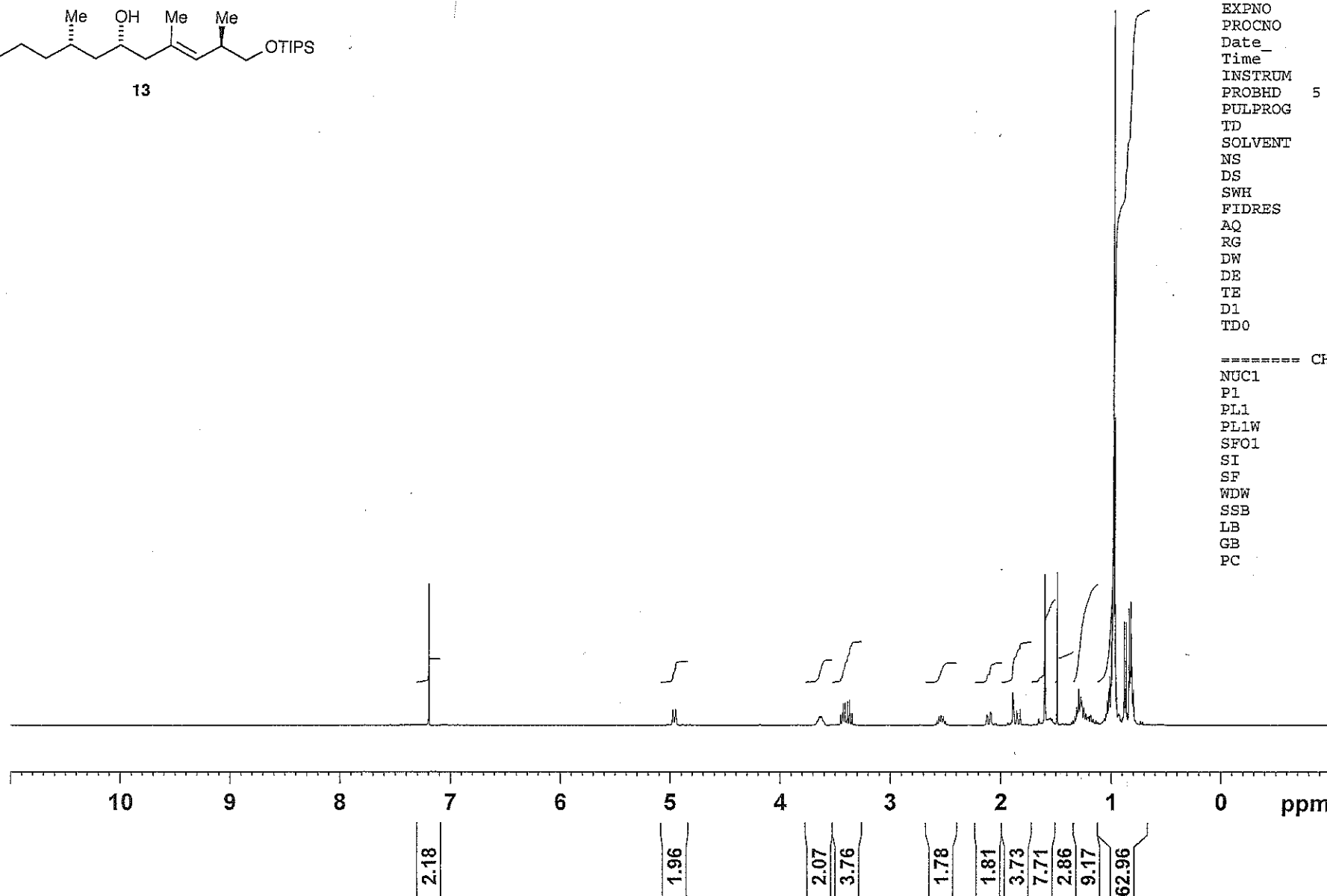


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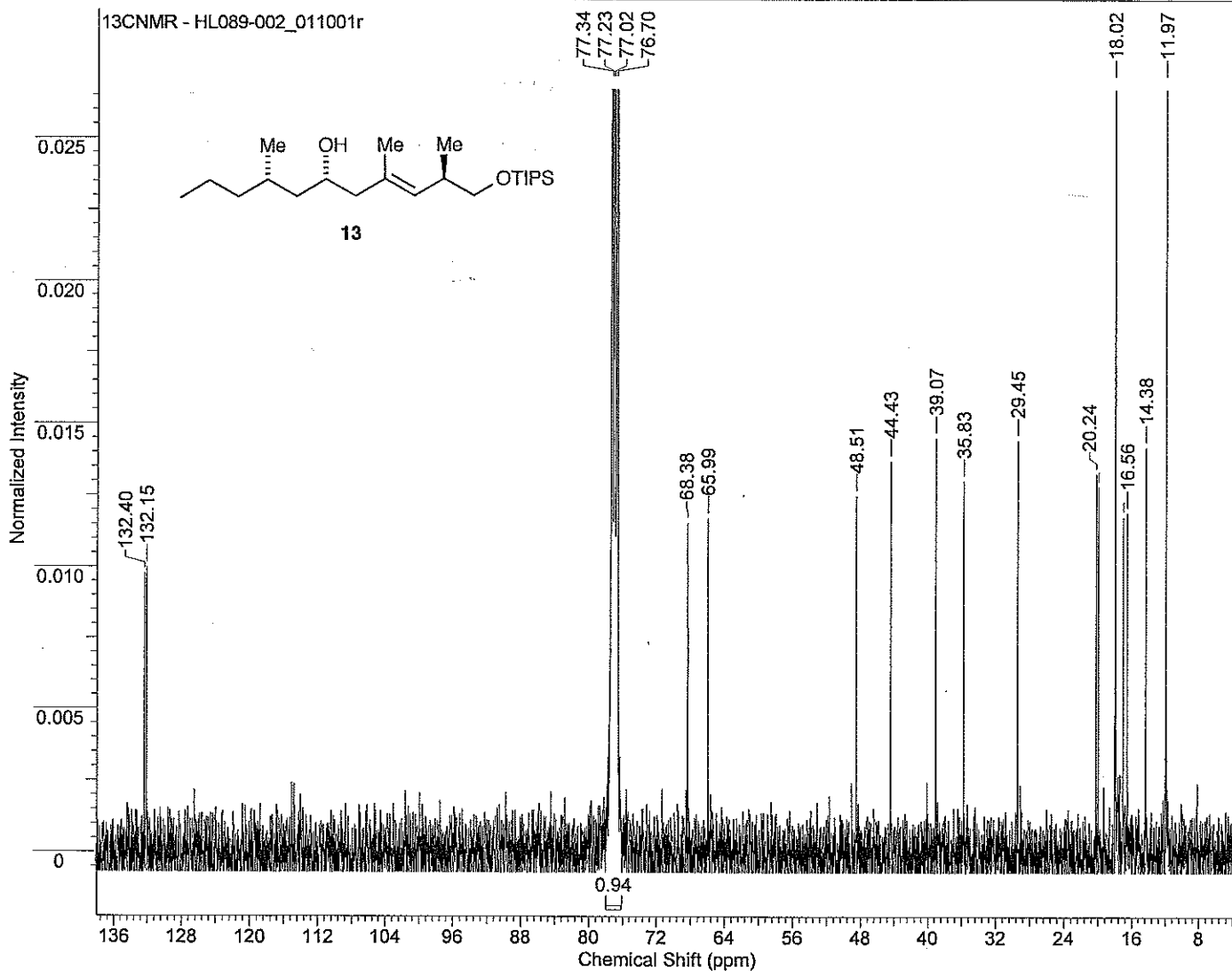
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FIDRES    0.126106 Hz
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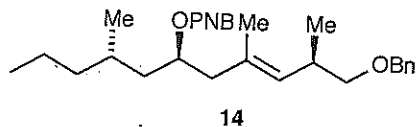
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PL1       -3.60 dB
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SI        32768
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WDW       EM
SSB       0
LB        0.30 Hz
GB        0
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| | | | |
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| Points Count | 32768 | Pulse Sequence | zgpg30 |
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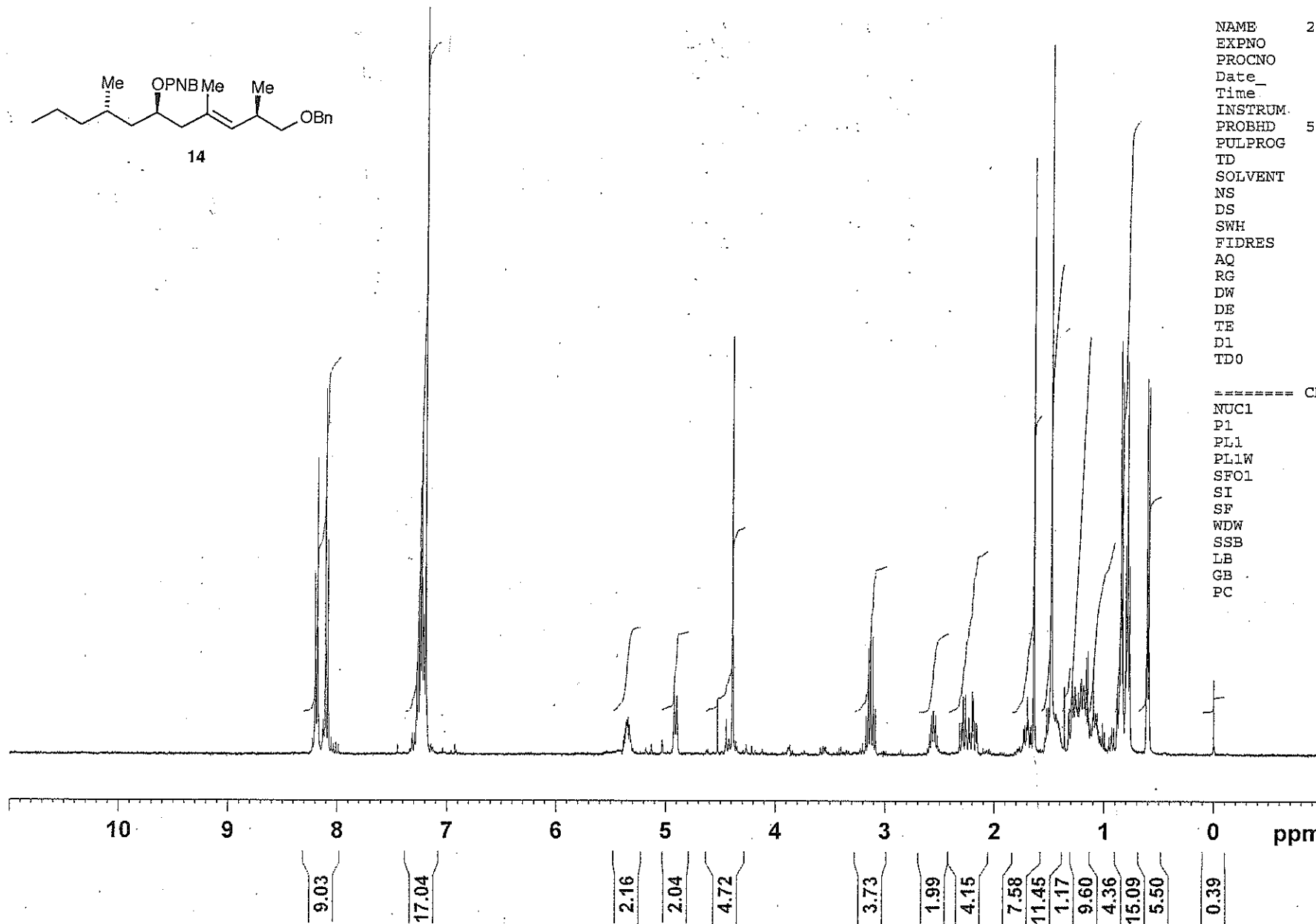


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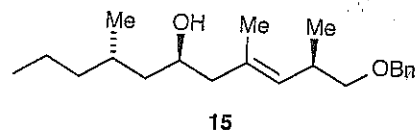
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FIDRES    0.126106 Hz
AQ        3.9649780 sec
RG         406
DW        60.500 usec
DE         9.40 usec
TE        294.0 K
D1        1.00000000 sec
TD0       1
  
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SF01      400.1324710 MHz
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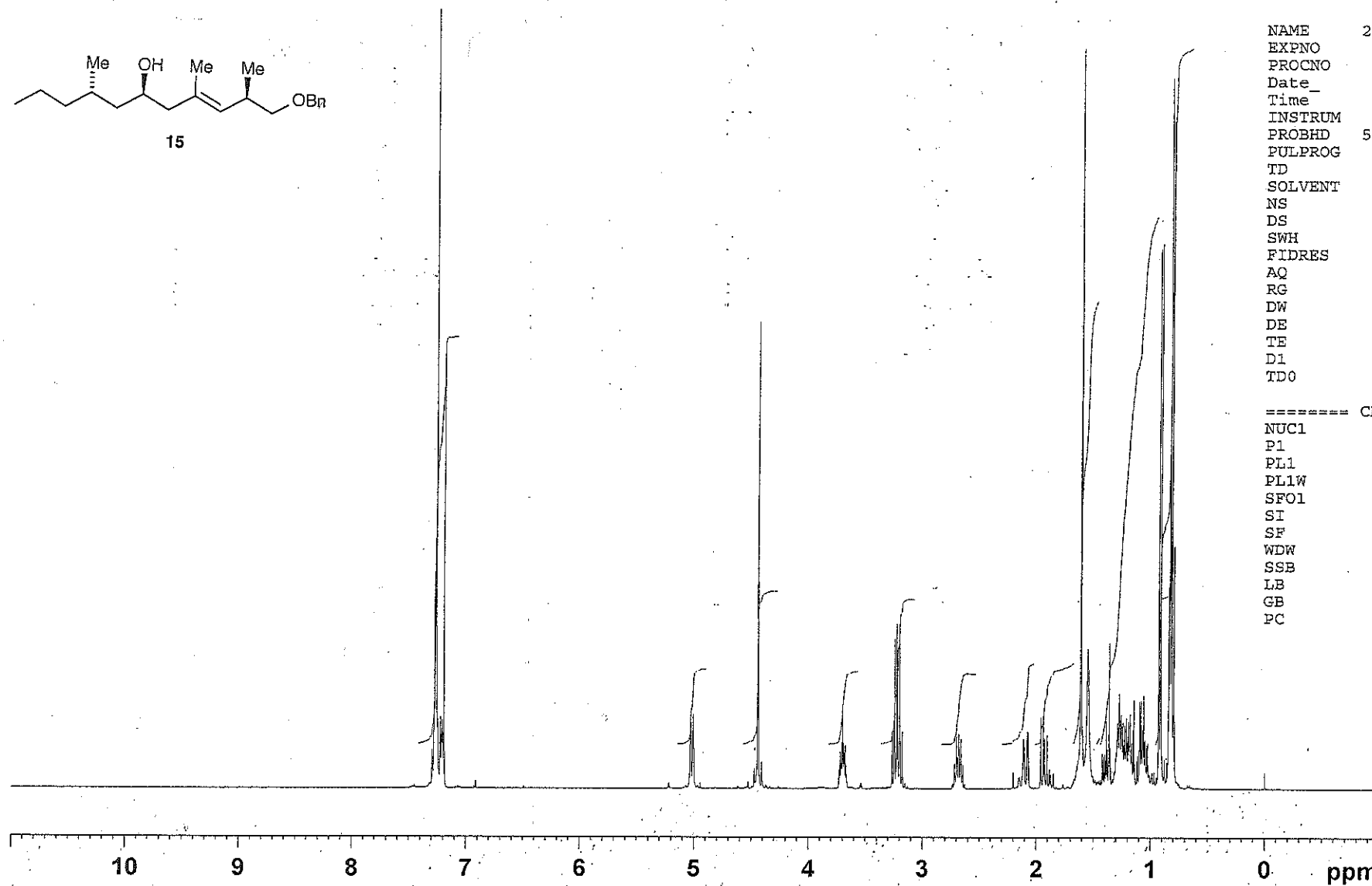


HL048-002
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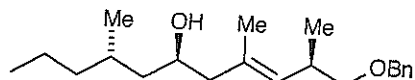


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SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 287
DW 60.500 usec
DE 9.40 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SF01 400.1324710 MHz
SI 32768
SF 400.1300374 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

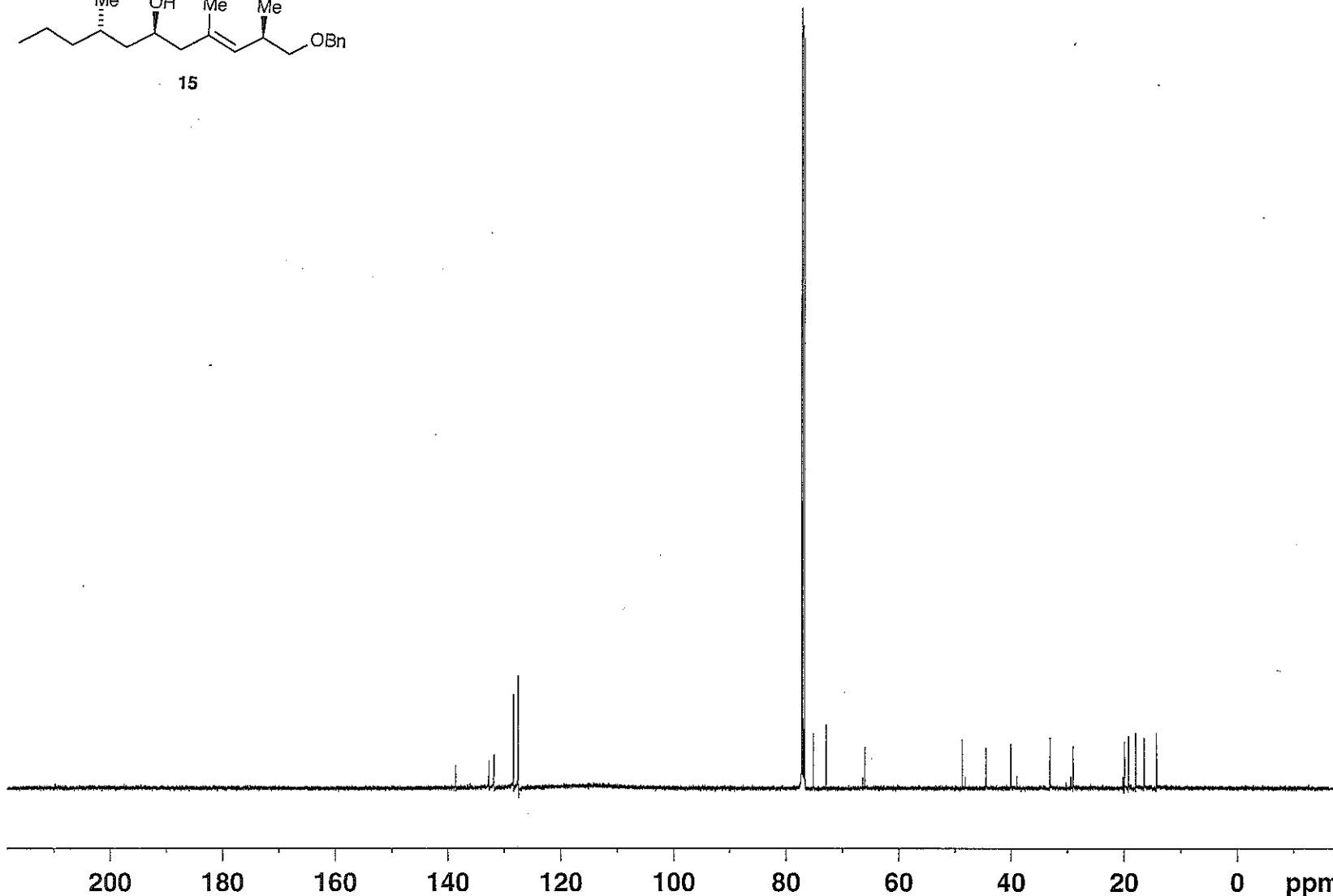


14.73
2.71
5.55
2.63
5.25
2.54
2.92
2.94
16.10
0.24
19.14
25.24



15

138.63
132.71
131.89
131.81
128.35
127.52
127.49
119.46
115.28
114.24
112.61
111.57
77.29
77.04
76.78
75.19
72.95
66.47
66.08
48.77
48.26
44.63
44.56
40.17
39.04
33.14
30.33
29.47
29.07
20.29
20.04
20.01
19.30
18.02
16.57
14.41
14.37

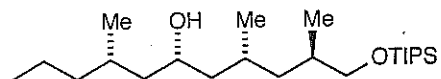


NAME 2009-10-30-ejt-9
EXPNO 10
PROCNO 1
Date_ 20091031
Time 0.11
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DW 16.800 usec
DE 32.21 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -4.20 dB
PL1W 218.02882385 W
SFO1 125.7703643 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.20 dB
PL12 23.99 dB
PL13 23.00 dB
PL2W 9.74092484 W
PL12W 0.10223514 W
PL13W 0.12841040 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

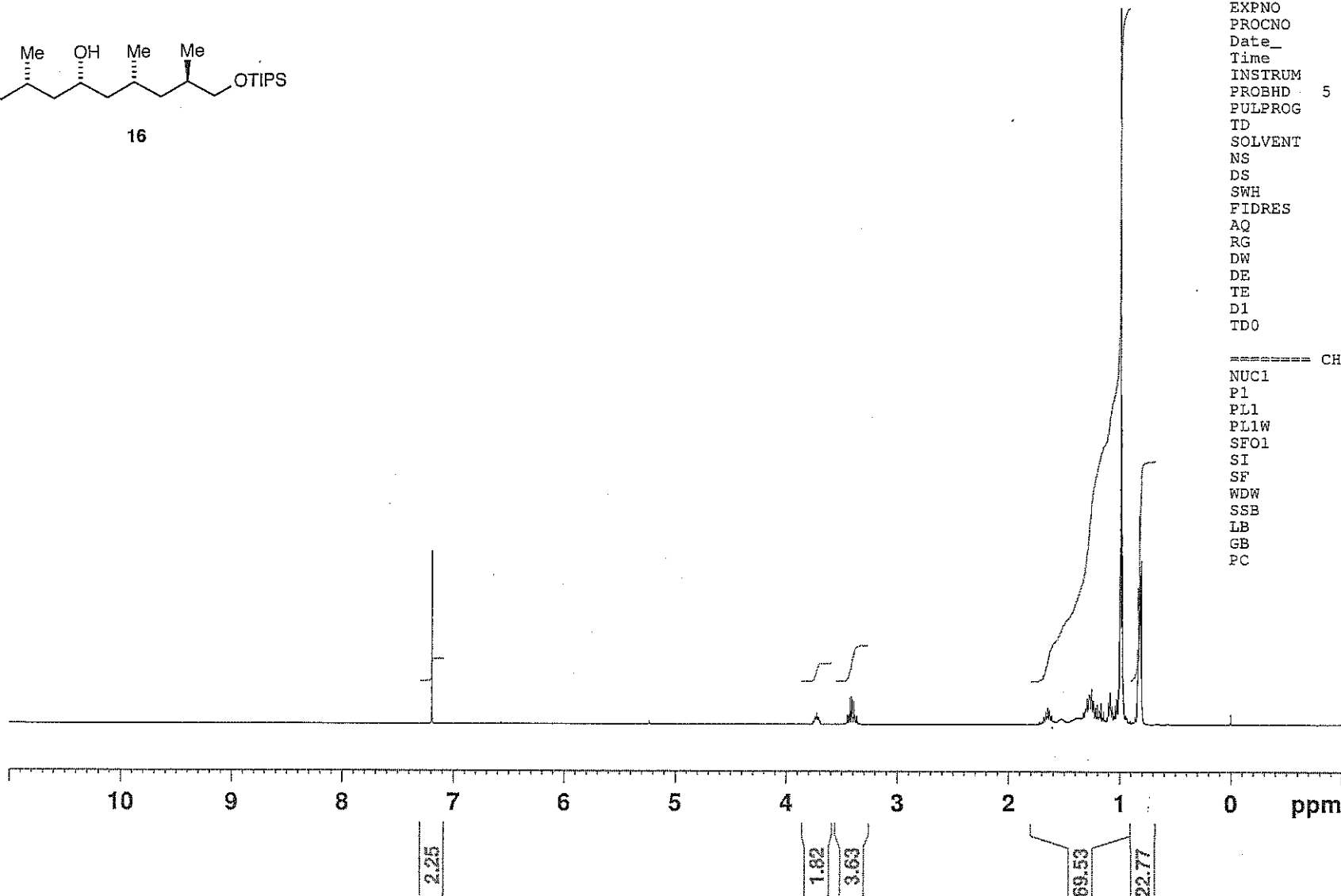
HL089-003
mPROTON CDCl3 {e:\bruk400data\2010\Jun} ejt 12



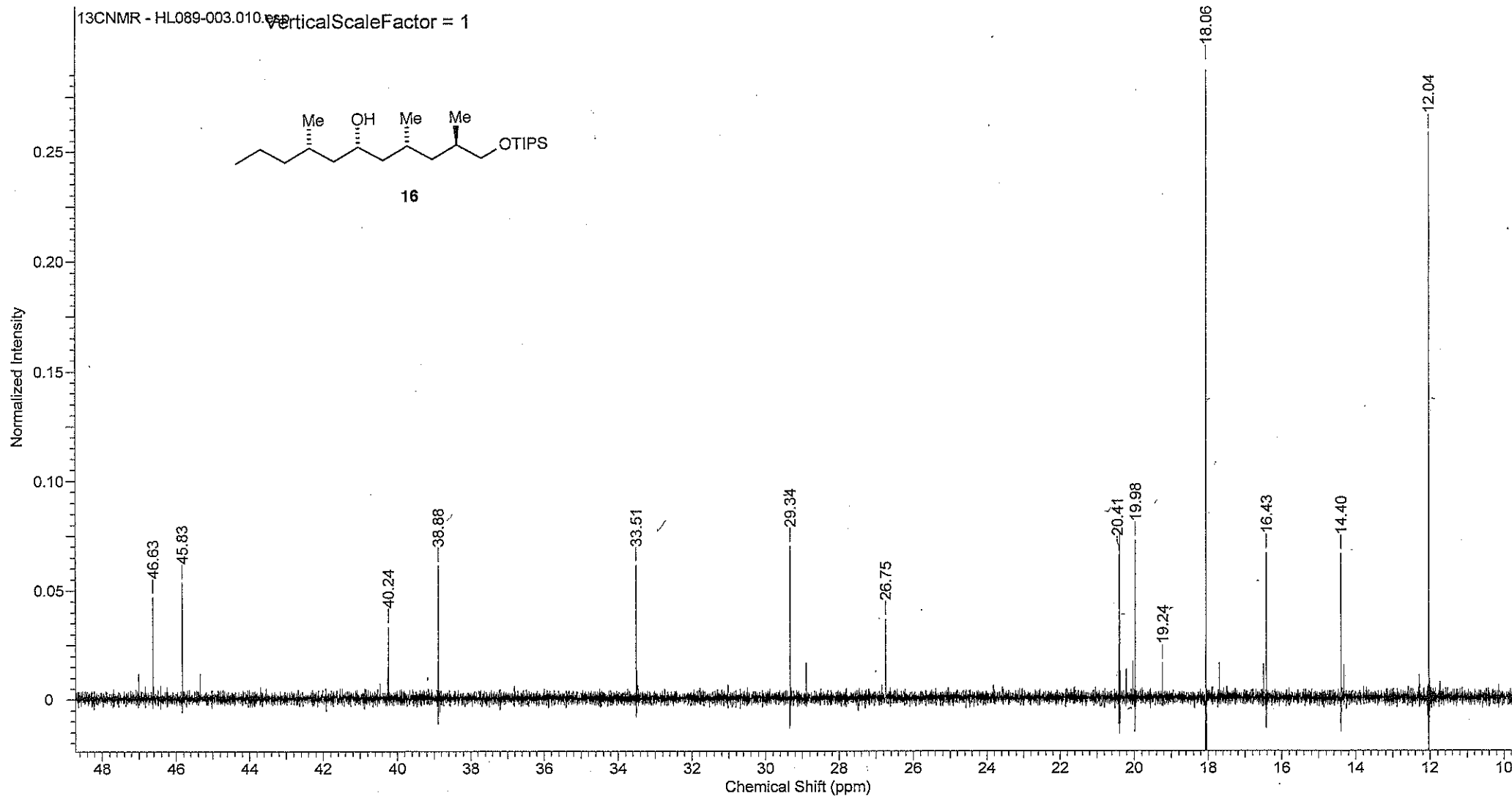
16

NAME 2010-06-04-ejt-12
EXPNO 10
PROCNO 1
Date_ 20100604
Time 15.39
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
ID 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 322
DW 60.500 usec
DE 9.40 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

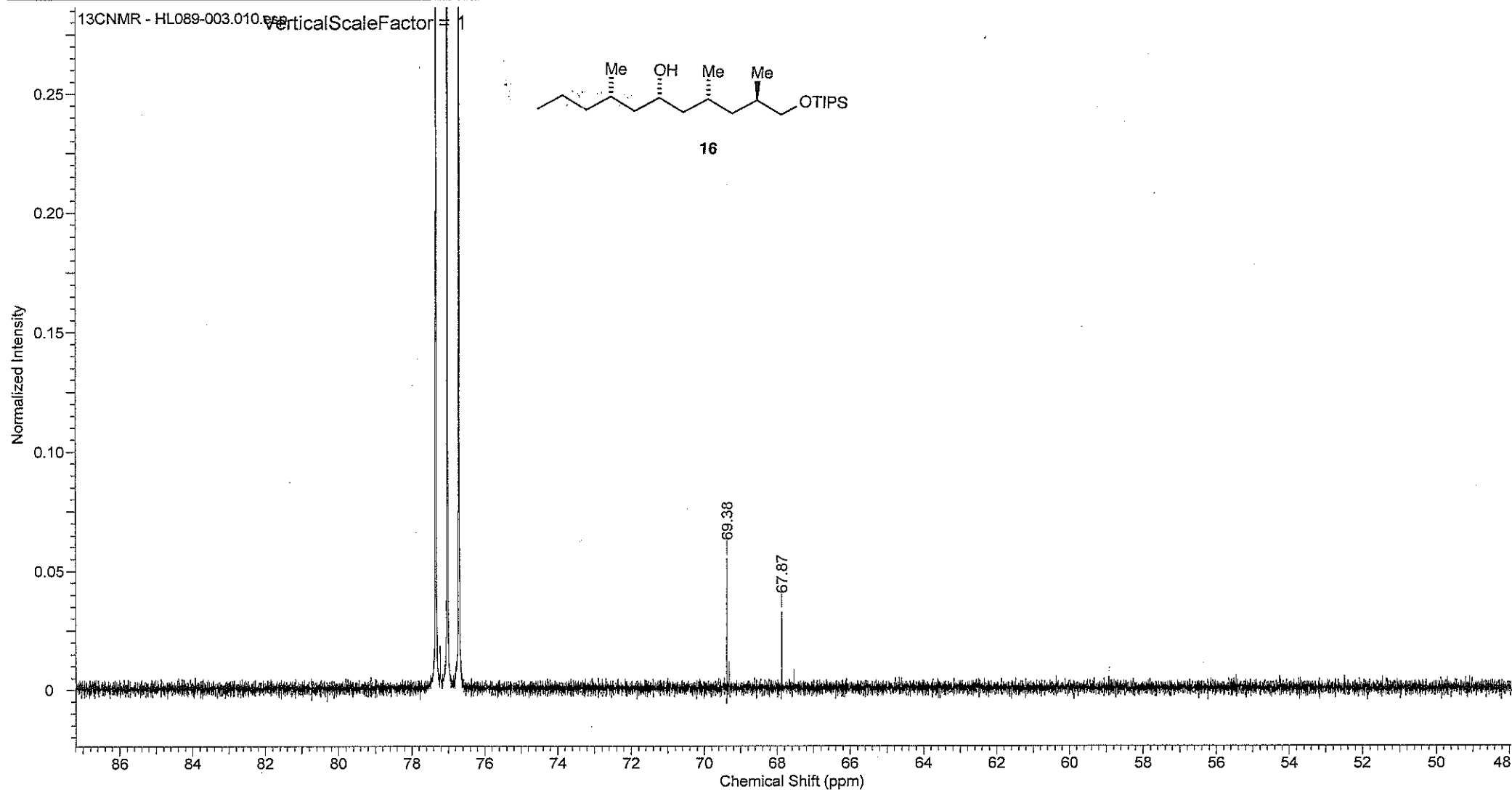
==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300368 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



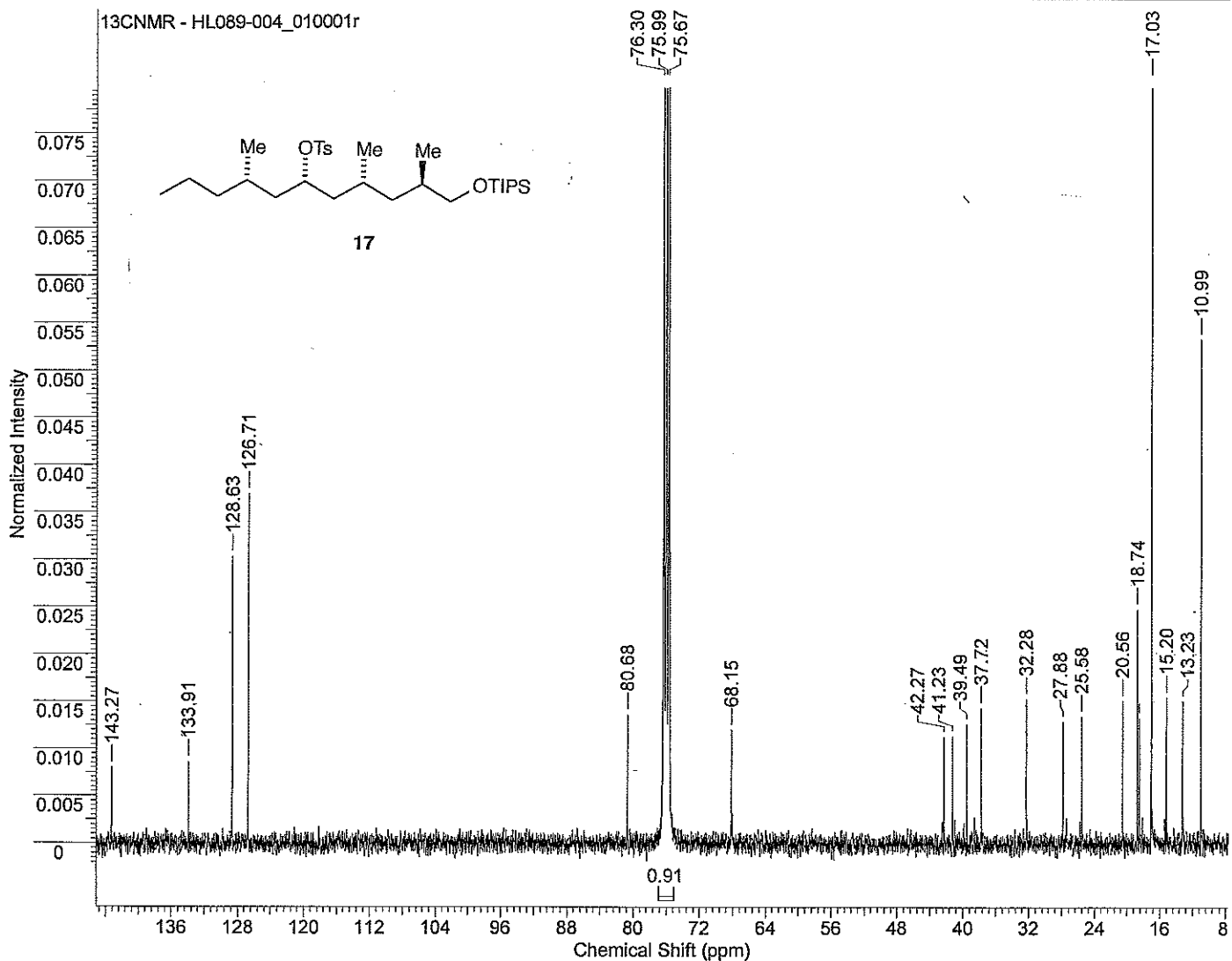
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|------------------------|--|-----------------------|--|------------------------|---------------|
| Acquisition Time (sec) | 1.3631 | Comment | H. Liu 0610-012 HL089-003 mCARBON CDCl3 (E:\bruk400service_data\2010\Jun} Administrator 45 | | |
| Date | 08 Jun 2010 08:00:16 | Date Stamp | 08 Jun 2010 08:00:16 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-013\13CNMR - HL089-003\10\fid | | | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C | Number of Transients | 14336 |
| Origin | AV400_S | Original Points Count | 32768 | Owner | Administrator |
| Points Count | 262144 | Pulse Sequence | zgpg30 | Receiver Gain | 2050.00 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 24038.37 | Temperature (degree C) | 26.100 |



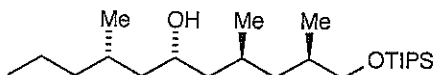
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|------------------------|--|-----------------------|--|------------------------|---------------|
| Acquisition Time (sec) | 1.3631 | Comment | H. Liu 0610-012 HL089-003 mCARBON CDCl3 (E:\bruk400service_data\2010\Jun) Administrator 45 | | |
| Date | 08 Jun 2010 08:00:16 | Date Stamp | 08 Jun 2010 08:00:16 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-013\13CNMR - HL089-003\10\fid | | | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C | Number of Transients | 14336 |
| Origin | AV400_S | Original Points Count | 32768 | Owner | Administrator |
| Points Count | 262144 | Pulse Sequence | zgpg30 | Receiver Gain | 2050.00 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 24038.37 | Temperature (degree C) | 26.100 |



| | | | |
|------------------------|---|------------------------|----------------------|
| Acquisition Time (sec) | 1.3631 | | |
| Comment | H.Liu 0610-016 HL0089-004 mCARBON CDCl3 {E:\bruk400service_data\2010\Jun} Administrator 53 | | |
| Date | 10 Jun 2010 07:00:16 | Date Stamp | 10 Jun 2010 07:00:16 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL089 - LHS synthesis\HL089-004\13CNMR - HL089-004_010001r | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C |
| Number of Transients | 17408 | Origin | AV400 S |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 9960.0313 |
| Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 26.000 |



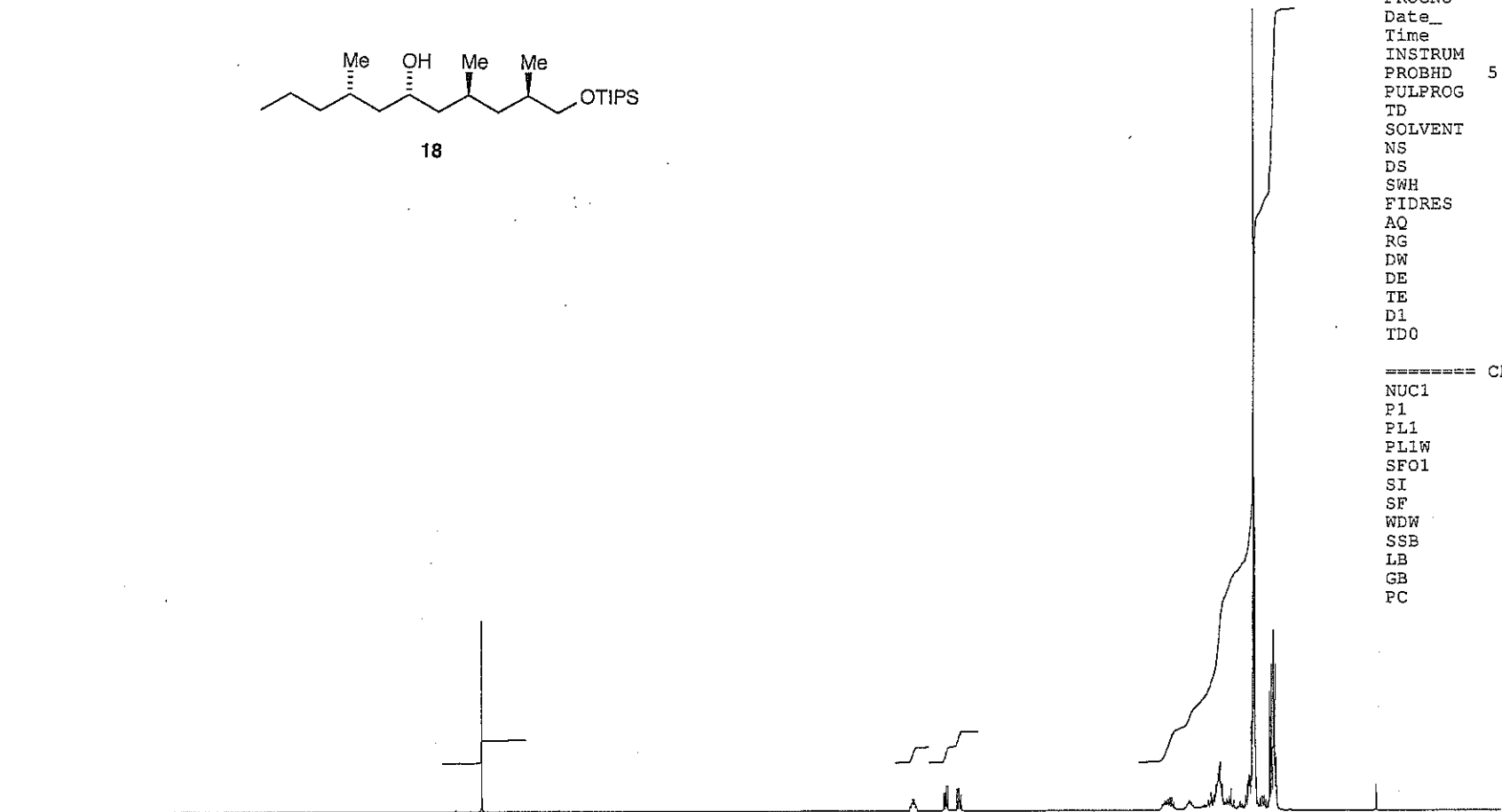
HL055-002
mPROTON CDCI3 /opt/bruk500data/2009/Dec ejt 38



18

NAME 2009-12-04-ejt-38
EXPNO 10
PROCNO 1
Date_ 20091204
Time 10.30
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCI3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 362
DW 48.400 usec
DE 13.38 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SF01 500.1330885 MHz
SI 32768
SF 500.1300474 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm

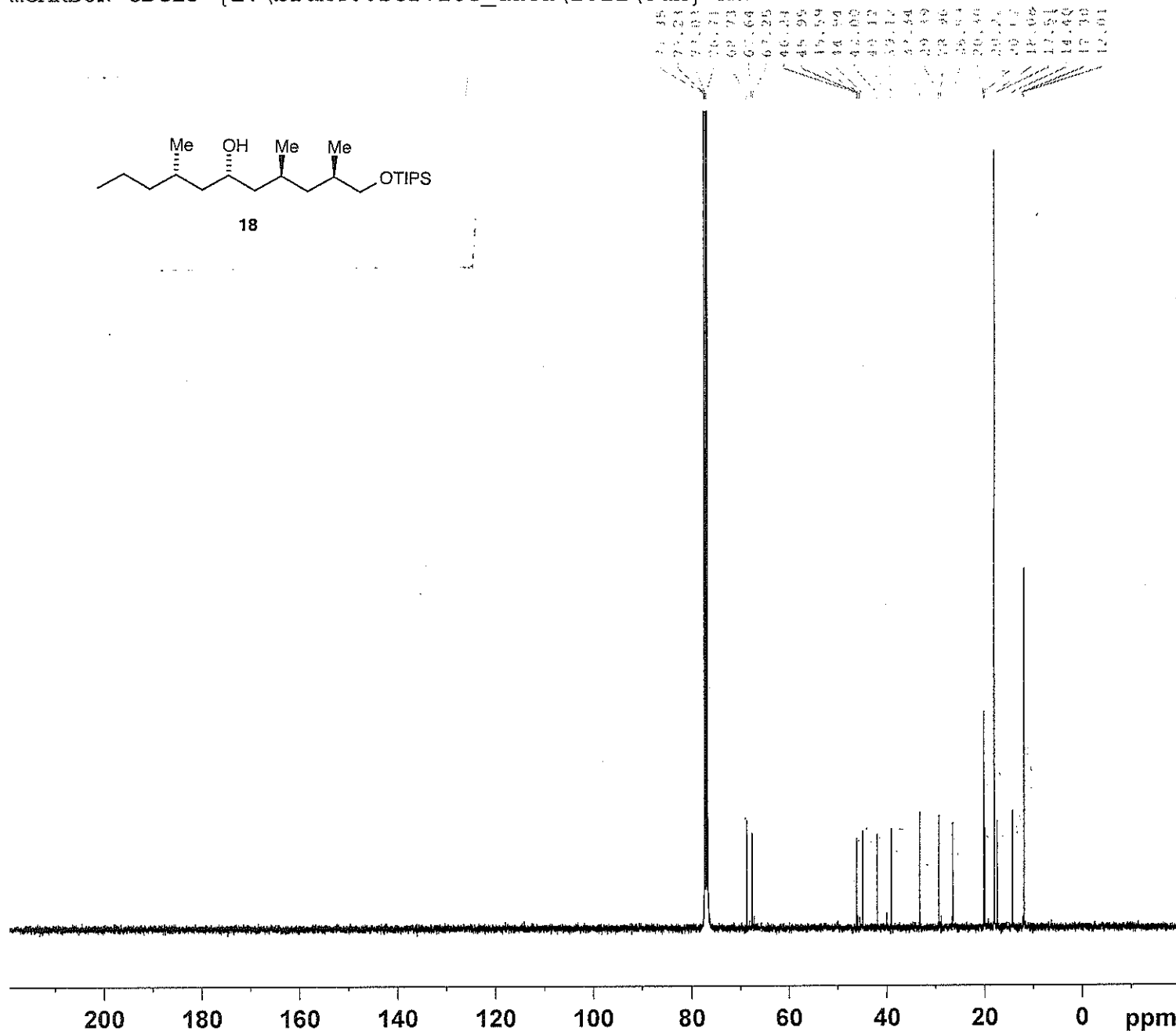
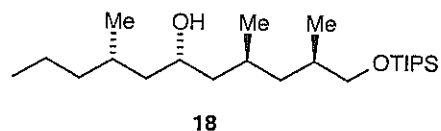
2.84

1.86
3.78

91.52

H liu HL055-002 . 0611-006

mCARBON CDC13 {E:\bruk400service_data\2011\Jun} Administrator 8

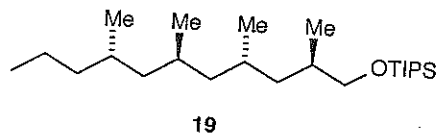


NAME 2011-06-10-Administrator-8
EXPNO 11
PROCNO 1
Date_ 20110612
Time 21.18
INSTRUM AV400 S
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 33.91046524 W
SFO1 100.6479773 MHz

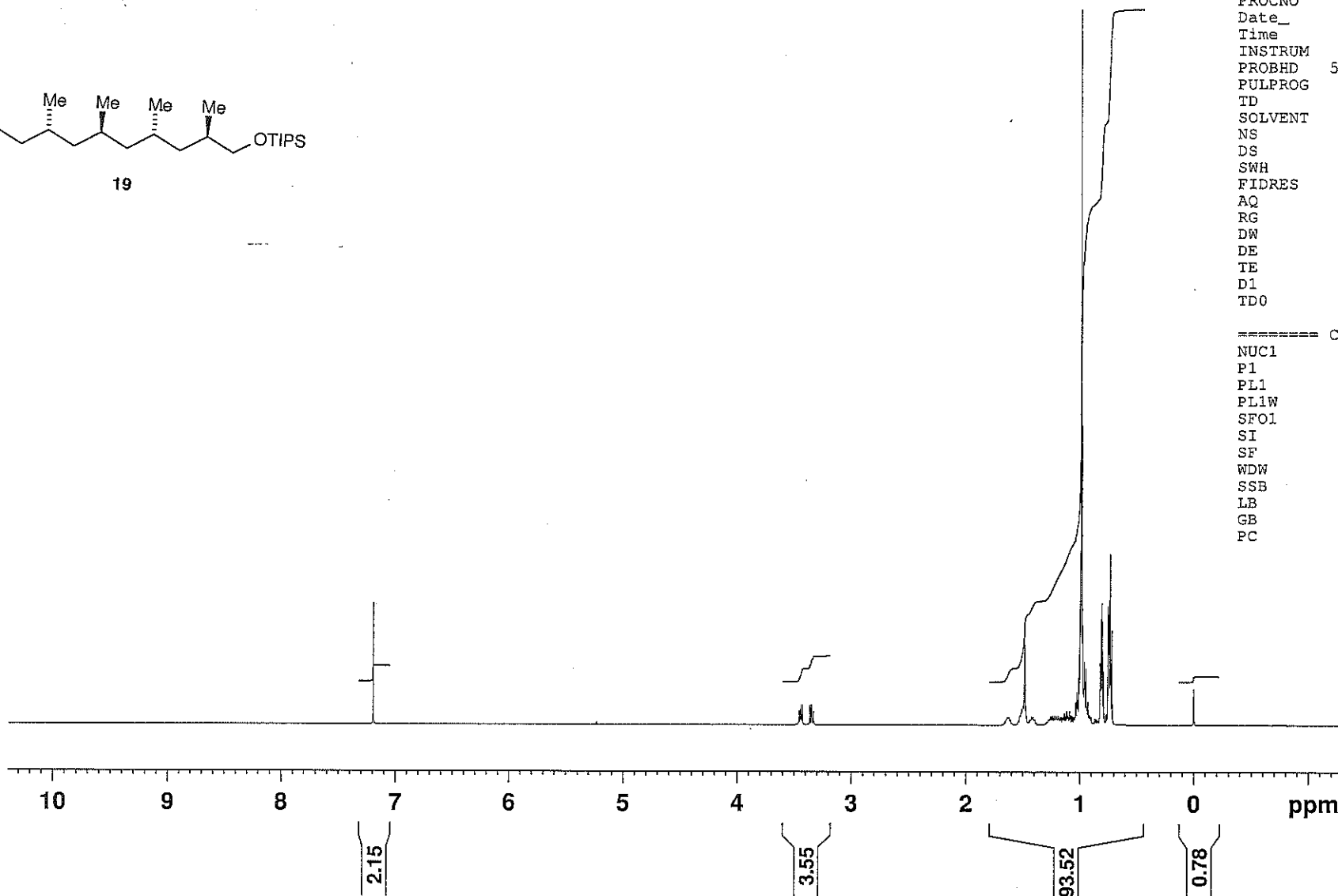
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 18.98951721 W
PL12W 0.24406971 W
PL13W 0.13137537 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379140 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HL089-005
mPROTON CDCl3 /opt/bruk500data/2010/Jun ejt 18

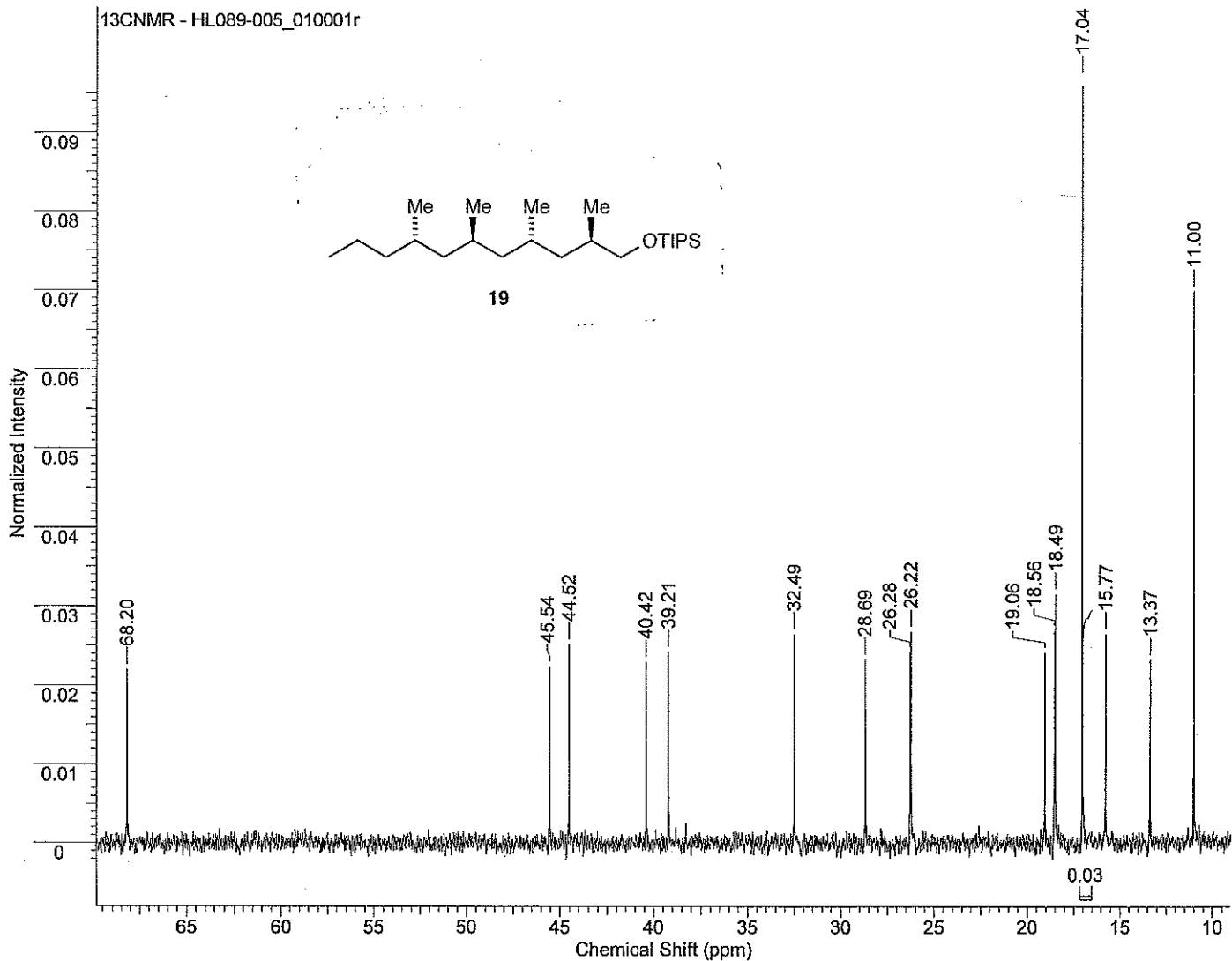


NAME 2010-06-15-ejt-18
EXPNO 10
PROCNO 1
Date_ 20100615
Time 9.33
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 287
DW 48.400 usec
DE 13.38 usec
TE 294.2 K
D1 1.0000000 sec
TD0 1

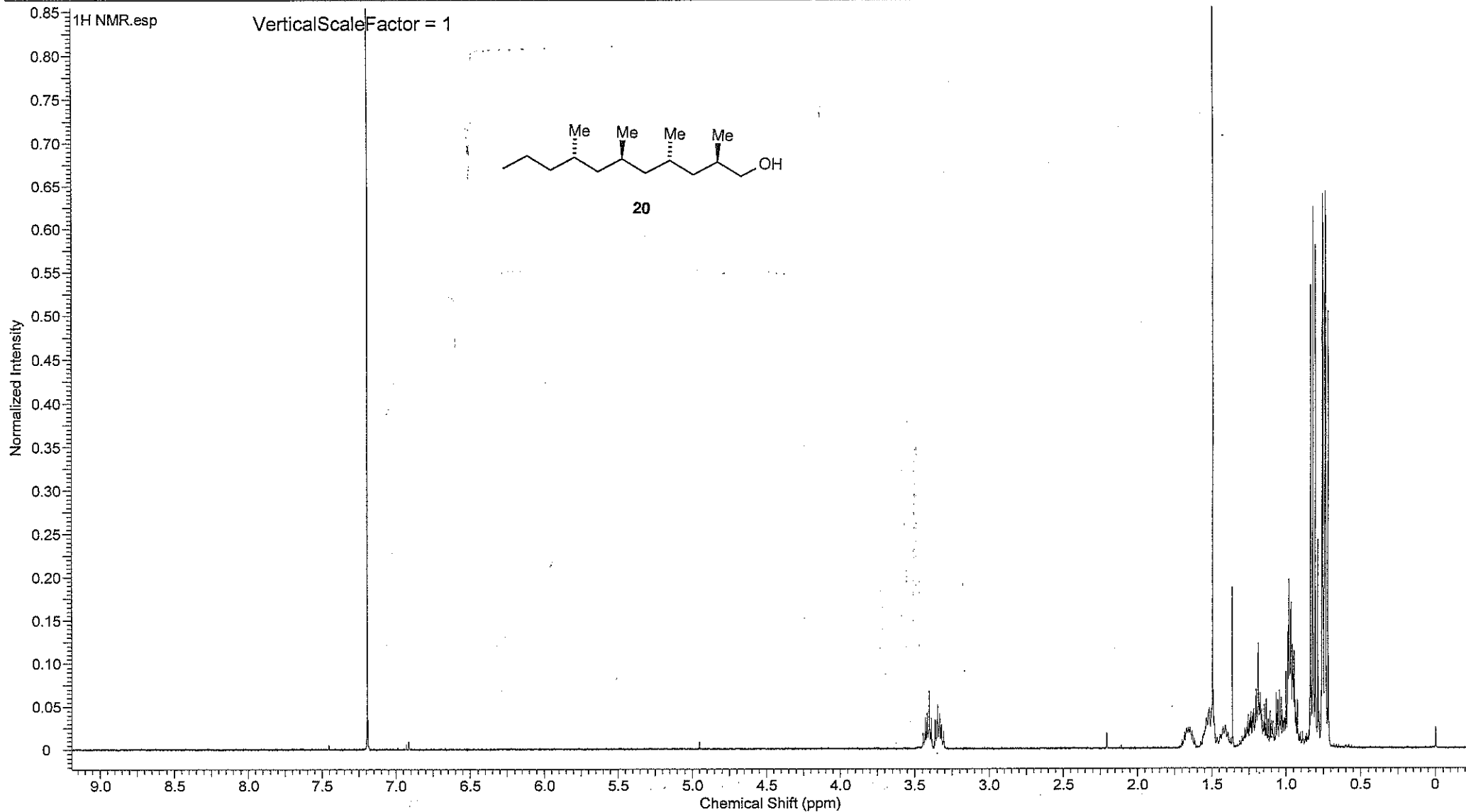
==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300474 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



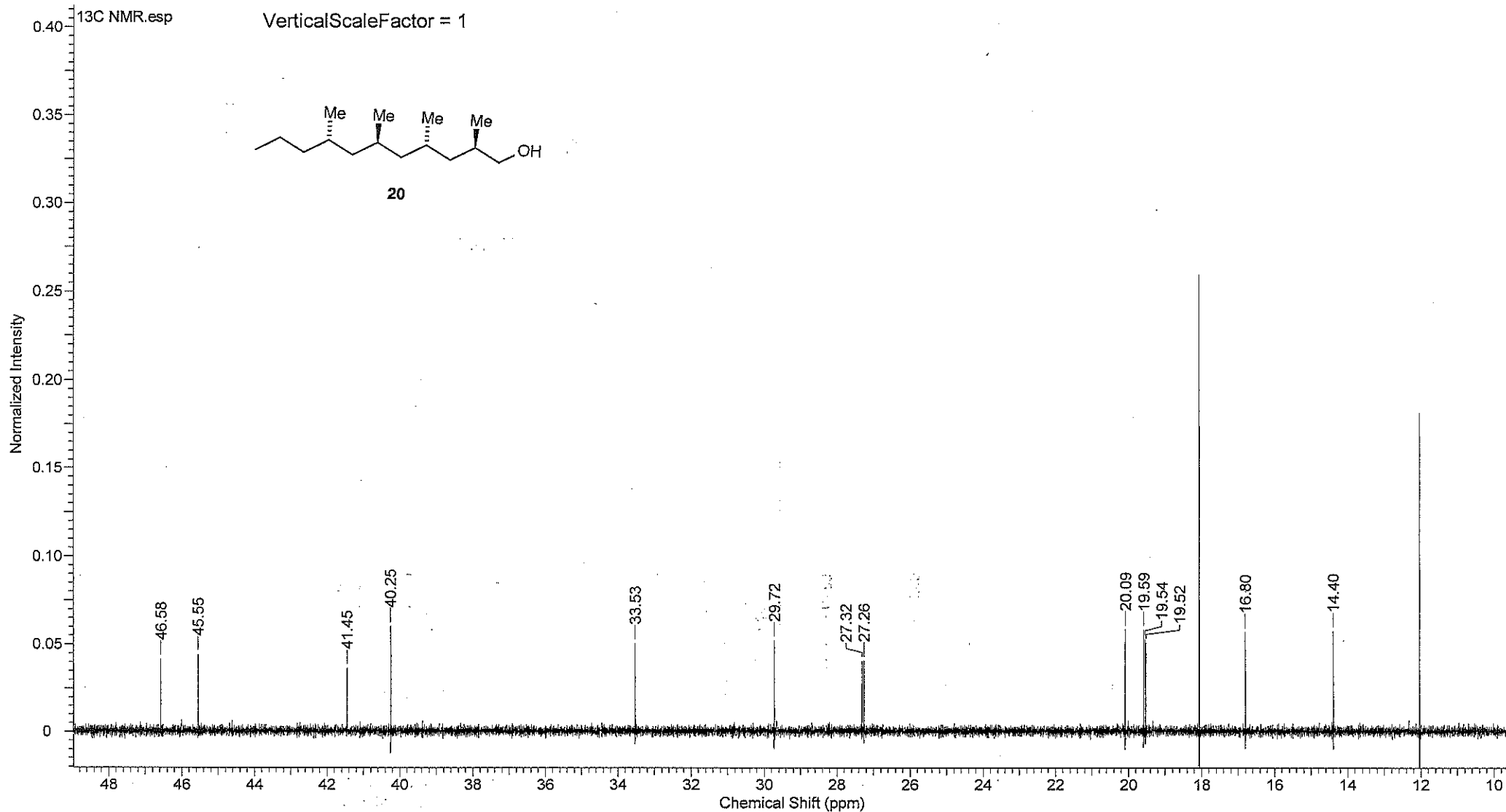
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|-------------------------------|---|-------------------------------|----------------------|
| Acquisition Time (sec) | 1.3631 | | |
| Comment | H. Liu 0610-022 HL089-005 mCARBON CDCl3 {E:\bruk400service_data\2010\Jun} Administrator 22 | | |
| Date | 16 Jun 2010 07:13:04 | Date Stamp | 16 Jun 2010 07:13:04 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL089 - LHS synthesis\HL089-005\13CNMR - HL089-005_010001r | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C |
| Number of Transients | 11264 | Origin | AV400 S |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 9960.1025 |
| Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 24.900 |



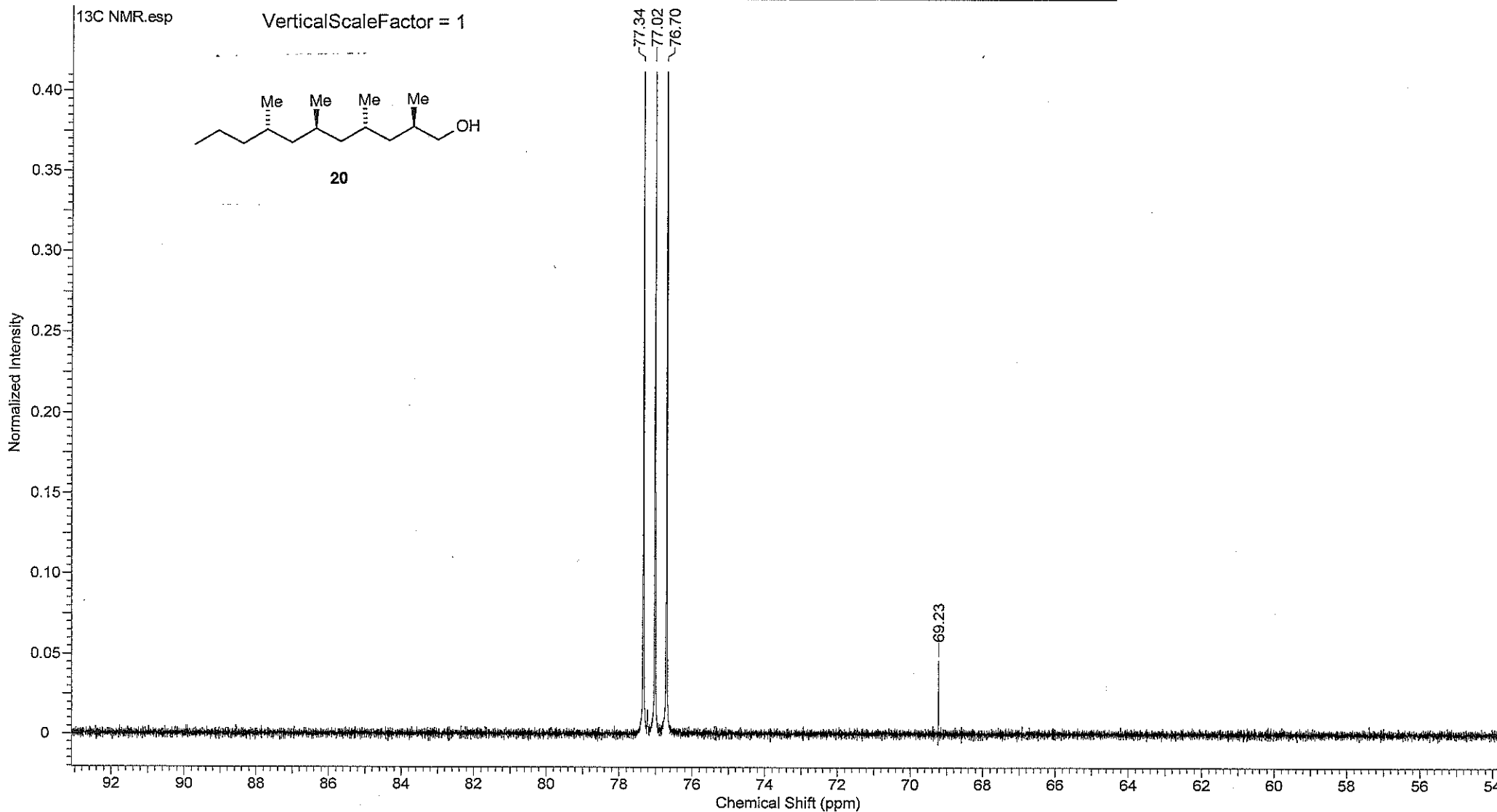
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|------------------------|----------------------|-------------------|---|------------------------|--------------|----------------------|-----------|
| Acquisition Time (sec) | 3.9649 | Comment | HL102-016 mPROTON CDCl3 (e:\bruk400data\2011\Jan) ejt 57 | | Date | 30 Jan 2011 20:07:28 | |
| Date Stamp | 30 Jan 2011 20:07:28 | File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-016\1H NMR\fid | | | | |
| Frequency (MHz) | 400.13 | Nucleus | 1H | Number of Transients | 16 | Origin | AV400 |
| Original Points Count | 32768 | Owner | Administrator | Points Count | 32768 | Pulse Sequence | zg30b |
| Receiver Gain | 362.00 | SW(cyclical) (Hz) | 8264.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 2434.2427 |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 8264.21 | Temperature (degree C) | 19.100 | | |



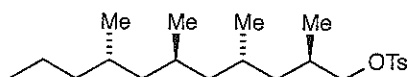
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|------------------------|--|-------------------|---|------------------------|--------------|
| Acquisition Time (sec) | 1.3631 | Comment | H Liu 0111-019 HL102-016 mCARBON CDCl3 (E:\bruk400service_data\2011\Feb) Administrator 60 | | |
| Date | 02 Feb 2011 07:13:04 | Date Stamp | 02 Feb 2011 07:13:04 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-016\13C NMR\fid | | | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C | Number of Transients | 16384 |
| Original Points Count | 32768 | Owner | Administrator | Points Count | 262144 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 24038.37 | Temperature (degree C) | 25.400 |
| | | | | Origin | AV400_S |
| | | | | Pulse Sequence | zgpg30 |
| | | | | Spectrum Offset (Hz) | 10063.3350 |



| | | | | | |
|------------------------|--|-------------------|---|------------------------|--------------|
| Acquisition Time (sec) | 1.3631 | Comment | H Liu 0111-019 HI102-016 mCARBON CDCl3 (E:\bruk400service_data\2011\Feb) Administrator 60 | | |
| Date | 02 Feb 2011 07:13:04 | Date Stamp | 02 Feb 2011 07:13:04 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-016\13C NMR\fid | | | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C | Number of Transients | 16384 |
| Original Points Count | 32768 | Owner | Administrator | Points Count | 262144 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 24038.37 | Temperature (degree C) | 25.400 |
| | | | | Origin | AV400 S |
| | | | | Pulse Sequence | zpgpg30 |
| | | | | Spectrum Offset (Hz) | 10063.3350 |



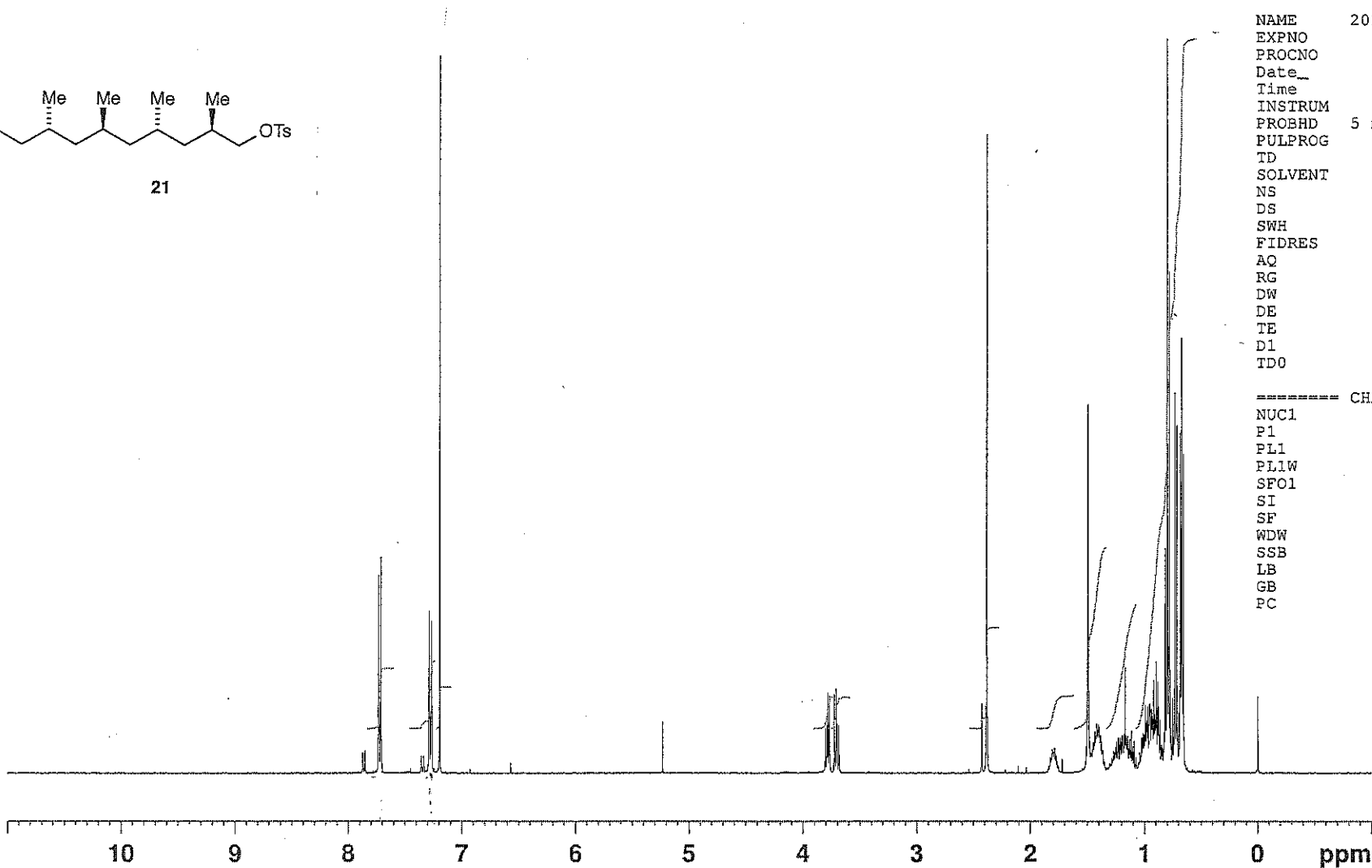
HL099-002
mPROTON CDCI3 {e:\bruk400data\2010\Nov} ejt 16



21

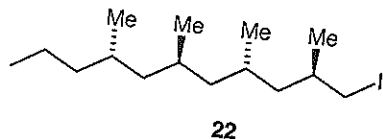
NAME 2010-11-19-ejt-16
EXPNO 10
PROCNO 1
Date_ 20101119
Time 16.01
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCI3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 362
DW 60.500 usec
DE 9.40 usec
TE 293.4 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PLLW 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300366 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



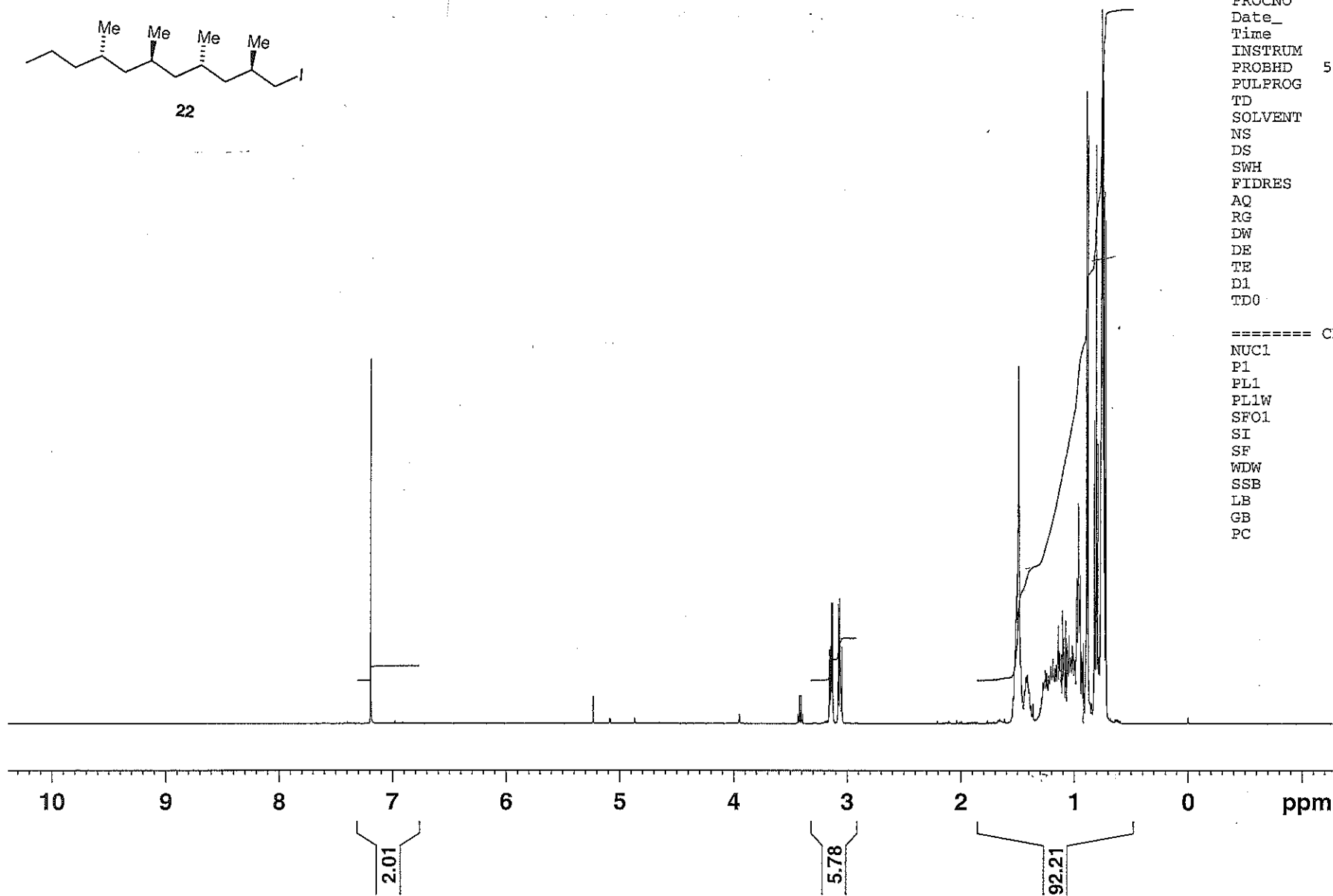
4.43
4.96
3.04
2.32
2.27
7.43
2.41
13.35
9.08
50.72

HL101-003
mPROTON CDCl3 /opt/bruk500data/2010/Dec ejt 34

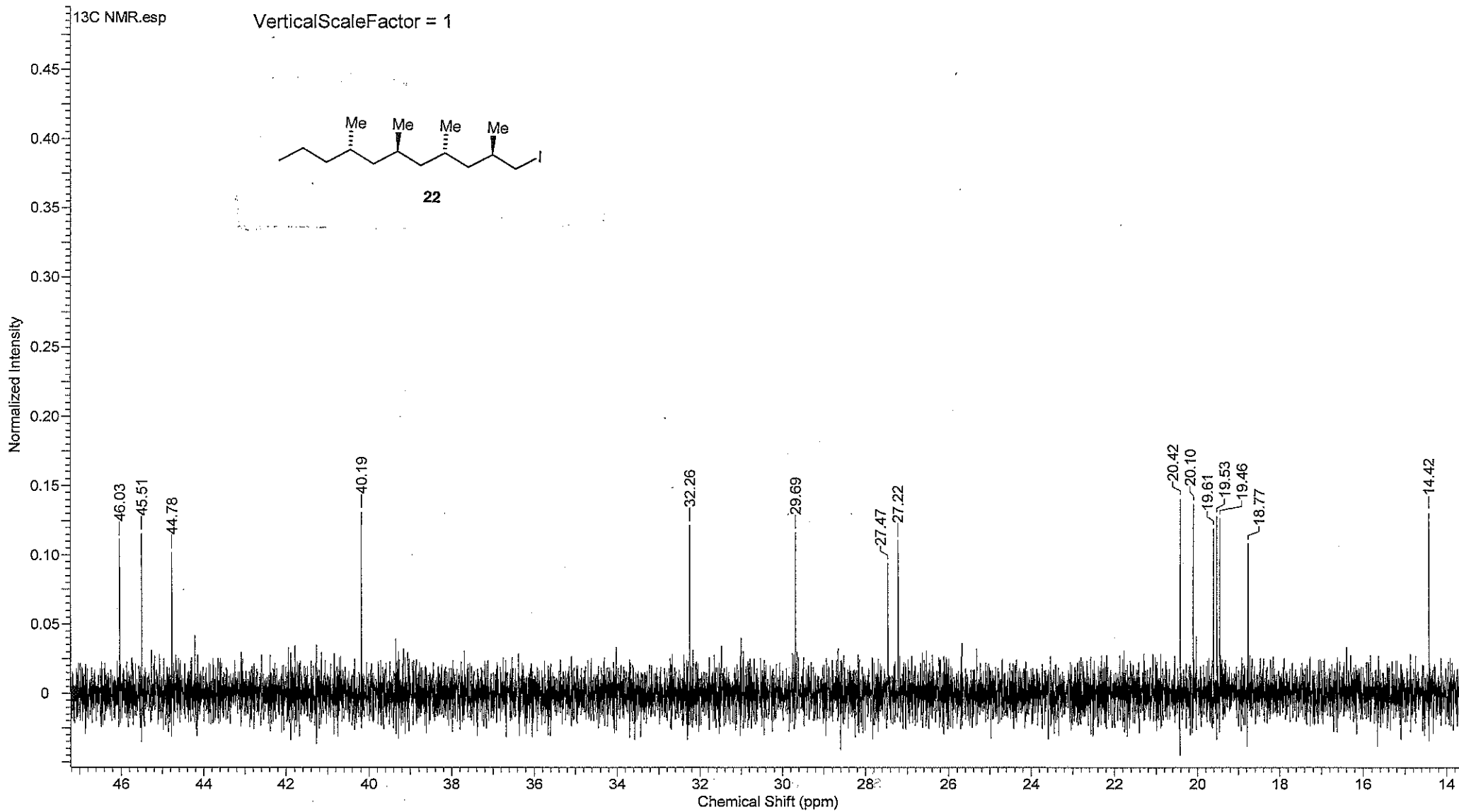


NAME 2010-12-07-ejt-34
EXPNO 10
PROCNO 1
Date_ 20101207
Time 9.28
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 287
DW 48.400 usec
DE 13.38 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1

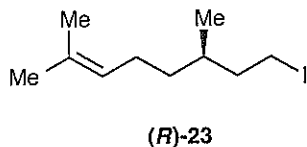
===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300469 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



| | | | | | | | |
|------------------------|----------------------|-------------------|--|------------------------|--------------|----------------------|------------|
| Acquisition Time (sec) | 1.1010 | Comment | HL101-003 mCARBON CDCl3 /opt/bruk500data/2010/Dec ejt 34 | | Date | 07 Dec 2010 09:42:24 | |
| Date Stamp | 07 Dec 2010 09:42:24 | File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-018\13C NMR\fid | | | | |
| Frequency (MHz) | 125.76 | Nucleus | 13C | Number of Transients | 256 | Origin | spect |
| Original Points Count | 32768 | Owner | vnmr1 | Points Count | 262144 | Pulse Sequence | zgpg30 |
| Receiver Gain | 512.00 | SW(cyclical) (Hz) | 29761.90 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 12575.3066 |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 29761.79 | Temperature (degree C) | 19.803 | | |

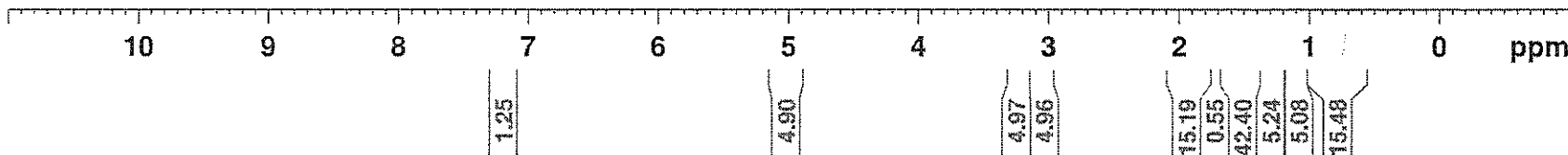
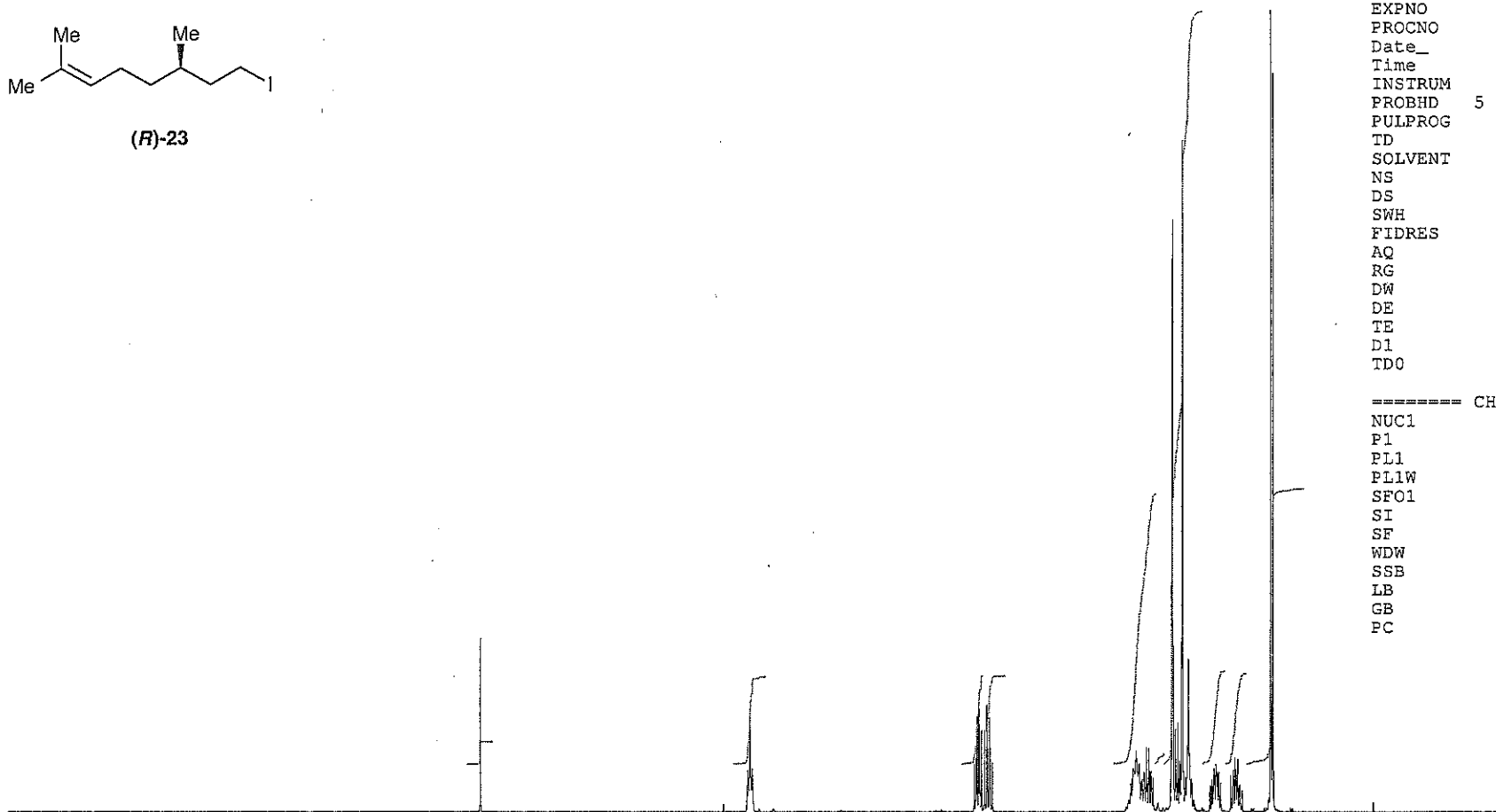


HL092-002
mPROTON CDCl3 {e:\bruk400data\2010\Aug} ejt 40

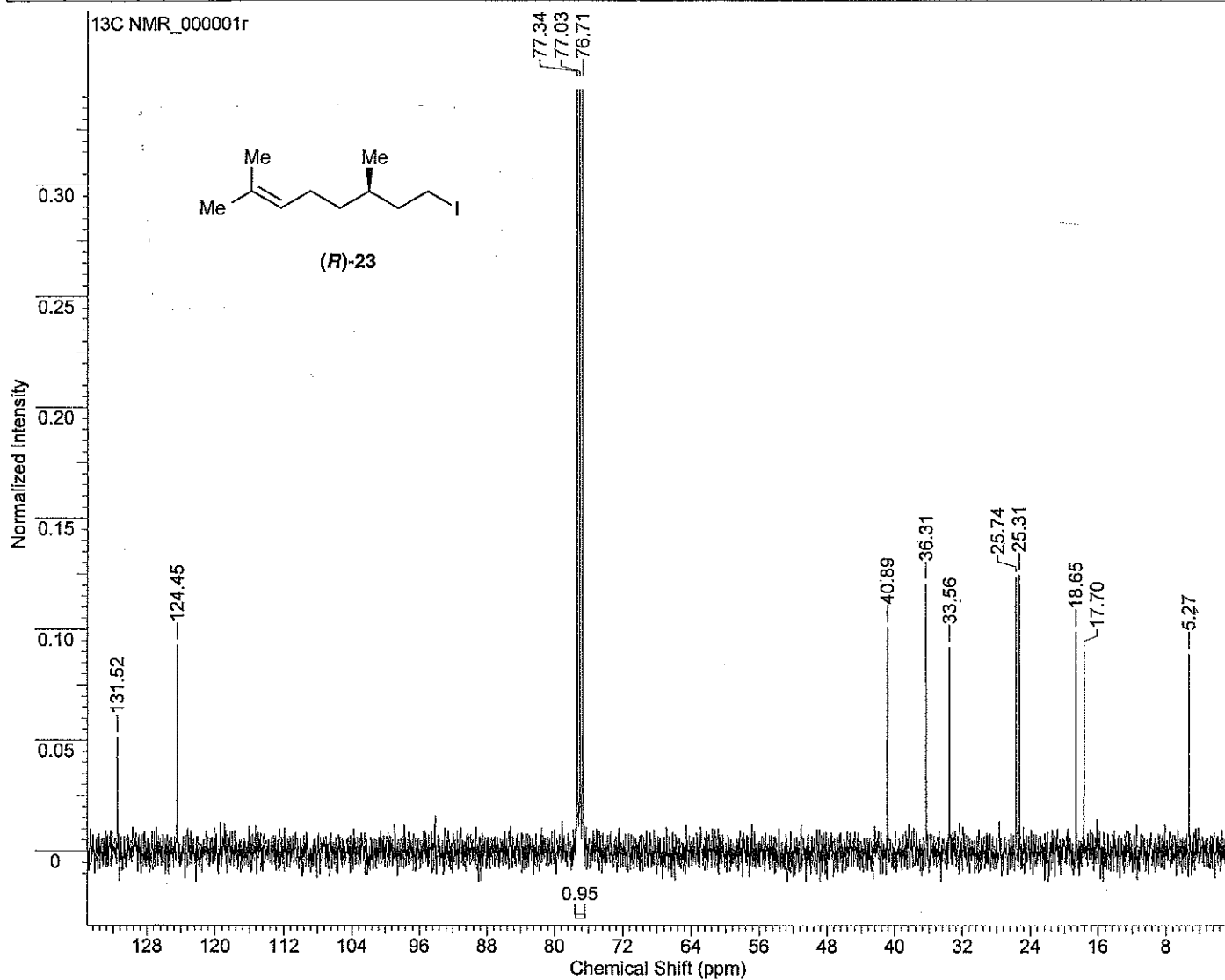


NAME 2010-08-12-ejt-40
EXPNO 10
PROCNO 1
Date_ 20100812
Time 15.16
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 256
DW 60.500 usec
DE 9.40 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

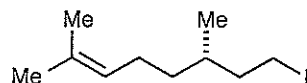
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300367 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



| | | | |
|------------------------|---|------------------------|--|
| Acquisition Time (sec) | 1.0835 | Comment | HL092-002 mCARBON CDCl3 {e:\bruk400data\2010\Aug} ejt 40 |
| Date | 12 Aug 2010 14:30:24 | Date Stamp | 12 Aug 2010 14:30:24 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL092 - (R)-citronellol iodonation\HL092-002\13C NMR_000001r | | |
| Frequency (MHz) | 100.61 | Nucleus | 13C |
| Number of Transients | 256 | Origin | AV400 |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 512.00 | SW(cyclical) (Hz) | 30241.94 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 11335.2197 |
| Sweep Width (Hz) | 30241.01 | Temperature (degree C) | 21.500 |



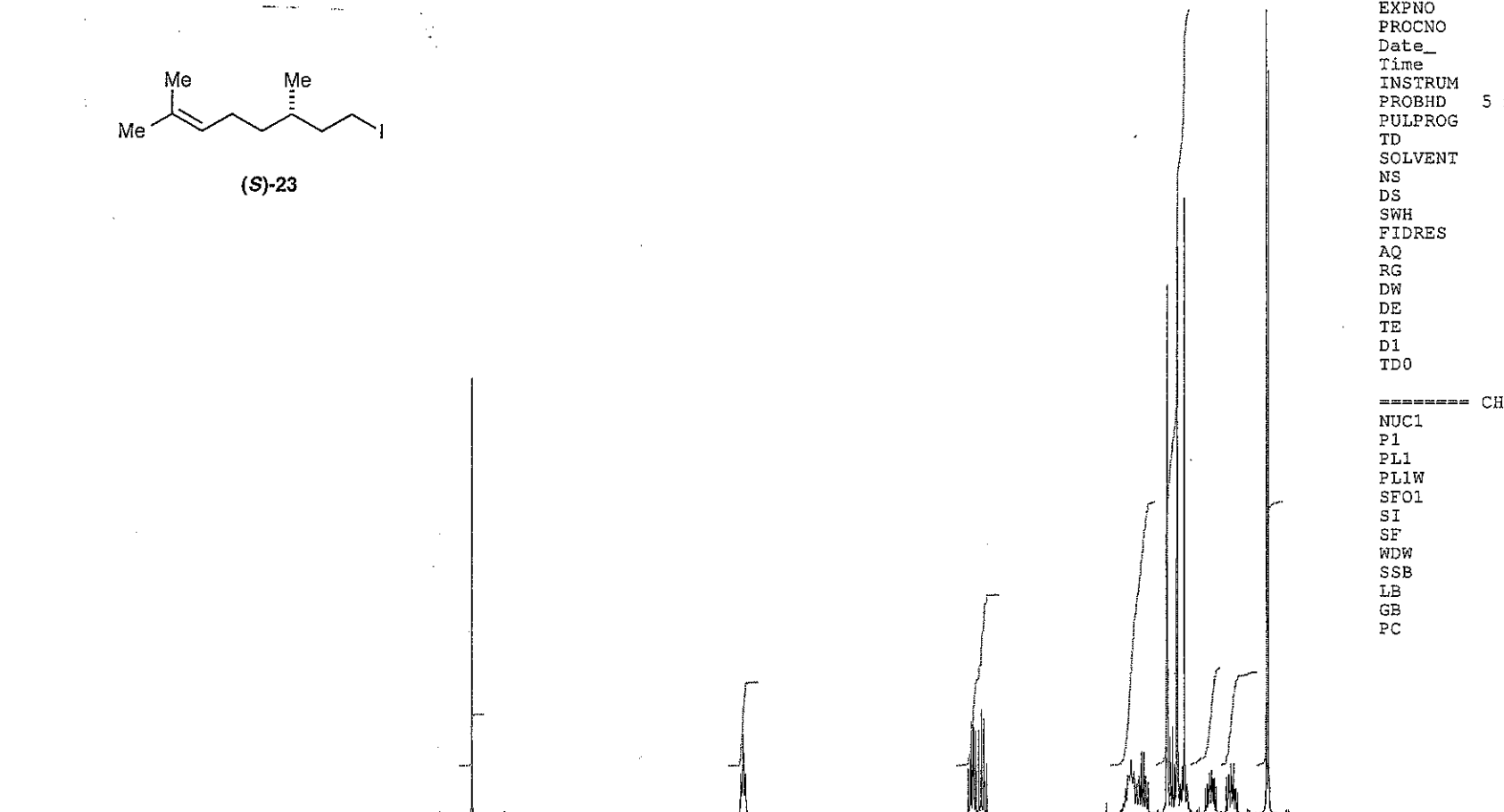
HL102-029
mPROTON CDCl3 {e:\bruk400data\2011\Feb} ejt 8



(S)-23

NAME 2011-02-09-ejt-8
EXPNO 10
PROCNO 1
Date_ 20110209
Time 15.57
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 406
DW 60.500 usec
DE 9.40 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm

2.88

4.70

9.61

14.82

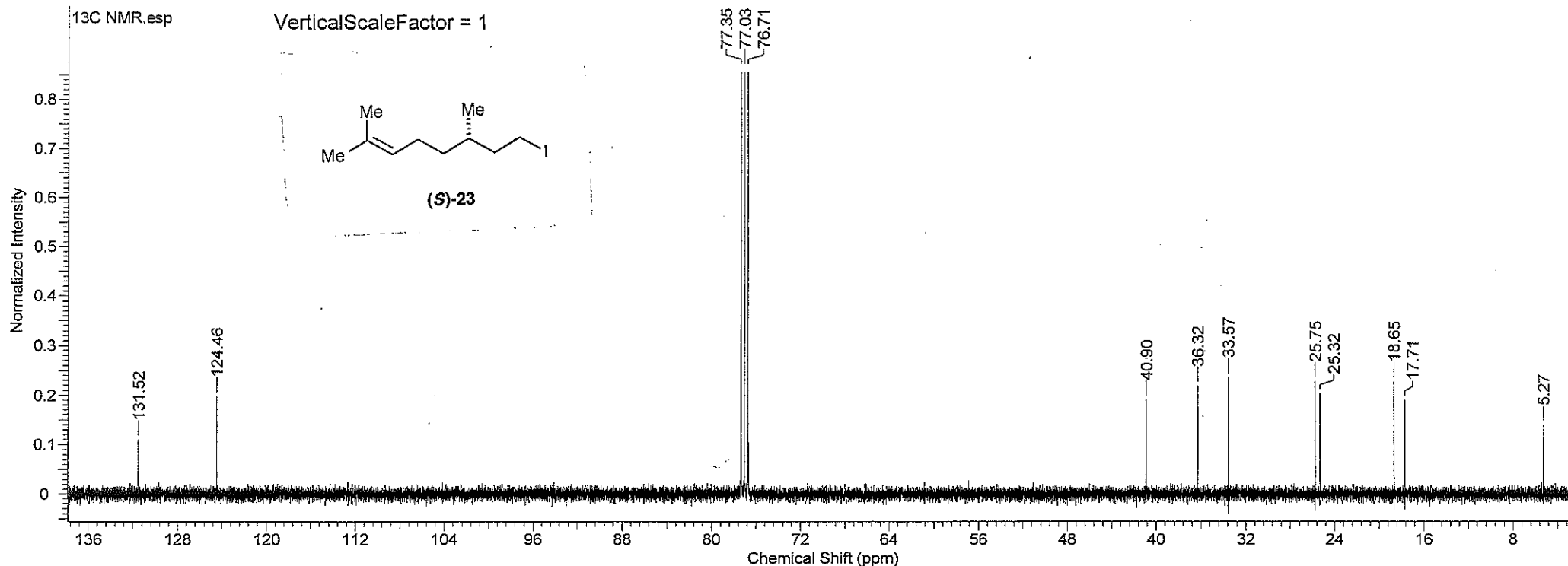
42.42

5.51

5.26

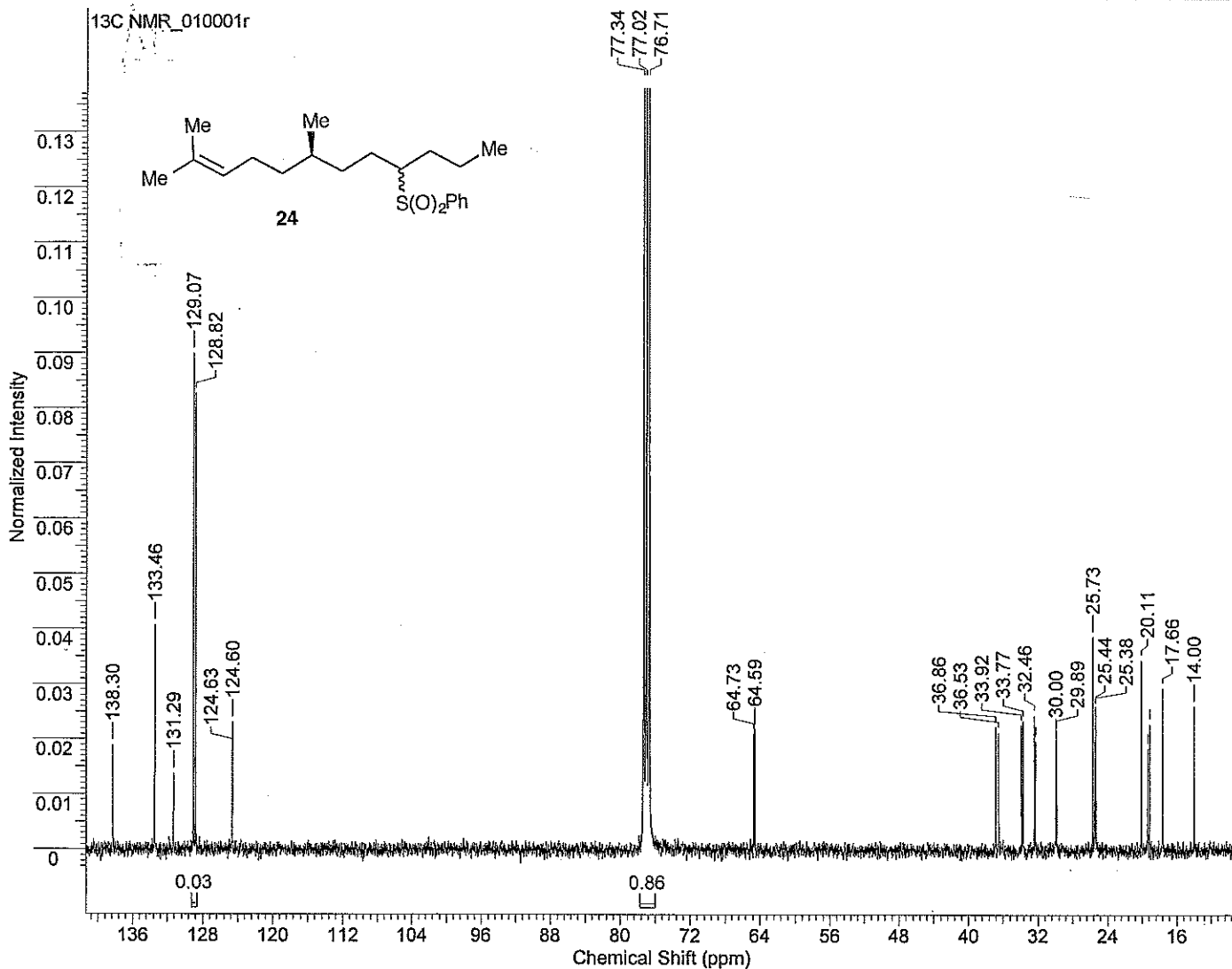
14.80

| | | | | | |
|------------------------|--|------------------------|--|----------------------|----------------------|
| Acquisition Time (sec) | 1.0835 | Comment | HL092-002 mCARBON CDCI3 {e:\bruk400data\2010\Aug} ejt 40 | Date | 12 Aug 2010 15:30:24 |
| Date Stamp | 12 Aug 2010 15:30:24 | | | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL092 - (R)-citronellol iodination\HL092-002\13C NMR\fid | | | Frequency (MHz) | 100.61 |
| Nucleus | 13C | Number of Transients | 256 | Origin | AV400 |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 |
| SW(cyclical) (Hz) | 30241.94 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 11335.2197 |
| Sweep Width (Hz) | 30241.91 | Temperature (degree C) | 21.500 | Spectrum Type | STANDARD |

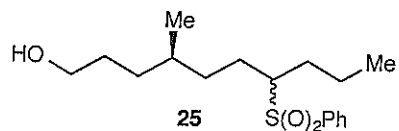


| No. | (ppm) | (Hz) | Height | No. | (ppm) | (Hz) | Height | No. | (ppm) | (Hz) | Height | No. | (ppm) | (Hz) | Height |
|-----|-------|--------|--------|-----|-------|--------|--------|-----|-------|--------|--------|-----|--------|---------|--------|
| 1 | 5.27 | 530.4 | 0.1409 | 4 | 25.32 | 2547.3 | 0.2051 | 7 | 36.32 | 3654.1 | 0.2199 | 10 | 77.03 | 7750.4 | 1.0000 |
| 2 | 17.71 | 1781.6 | 0.1915 | 5 | 25.75 | 2590.9 | 0.2289 | 8 | 40.90 | 4114.8 | 0.1921 | 11 | 77.35 | 7782.3 | 0.9641 |
| 3 | 18.65 | 1876.9 | 0.2289 | 6 | 33.57 | 3377.4 | 0.2367 | 9 | 76.71 | 7718.5 | 0.9622 | 12 | 124.46 | 12522.4 | 0.1974 |
| | | | | | | | | | | | | 13 | 131.52 | 13232.4 | 0.1103 |

| | | | |
|------------------------|---|------------------------|----------------------|
| Acquisition Time (sec) | 1.3631 | | |
| Comment | Leo 0910-040 HL093-001 mCARBON CDCl3 {E:\bruk400service_data\2010\Sep} Administrator 56 | | |
| Date | 20 Sep 2010 10:57:04 | Date Stamp | 20 Sep 2010 10:57:04 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL093 - Sulfone alkylation\HL093-001\13C NMR_010001r | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C |
| Number of Transients | 10240 | Origin | AV400 S |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 23.600 |



HL093-002
 mPROTON CDCl3 /opt/bruk500data/2010/Sep ejt 15

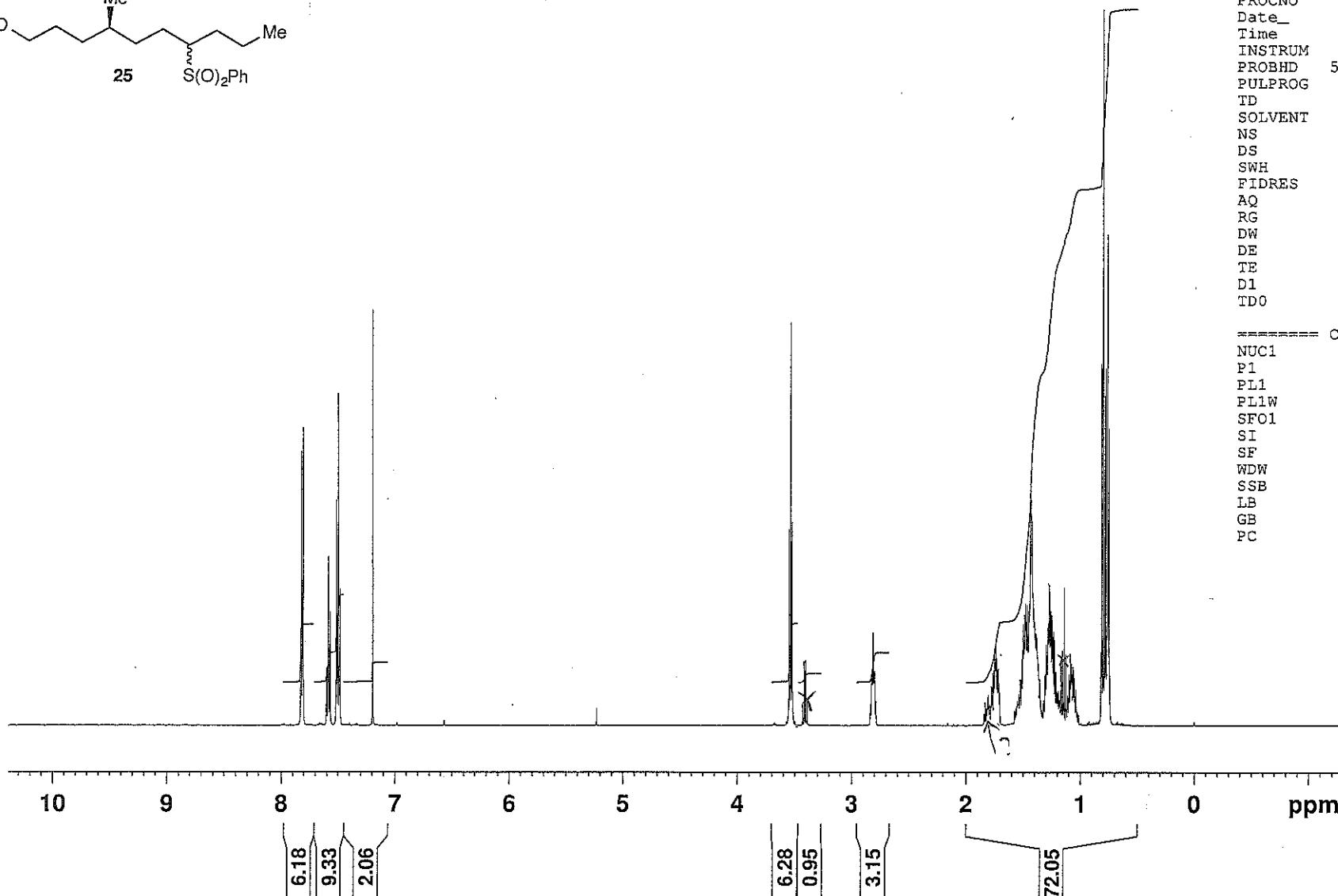


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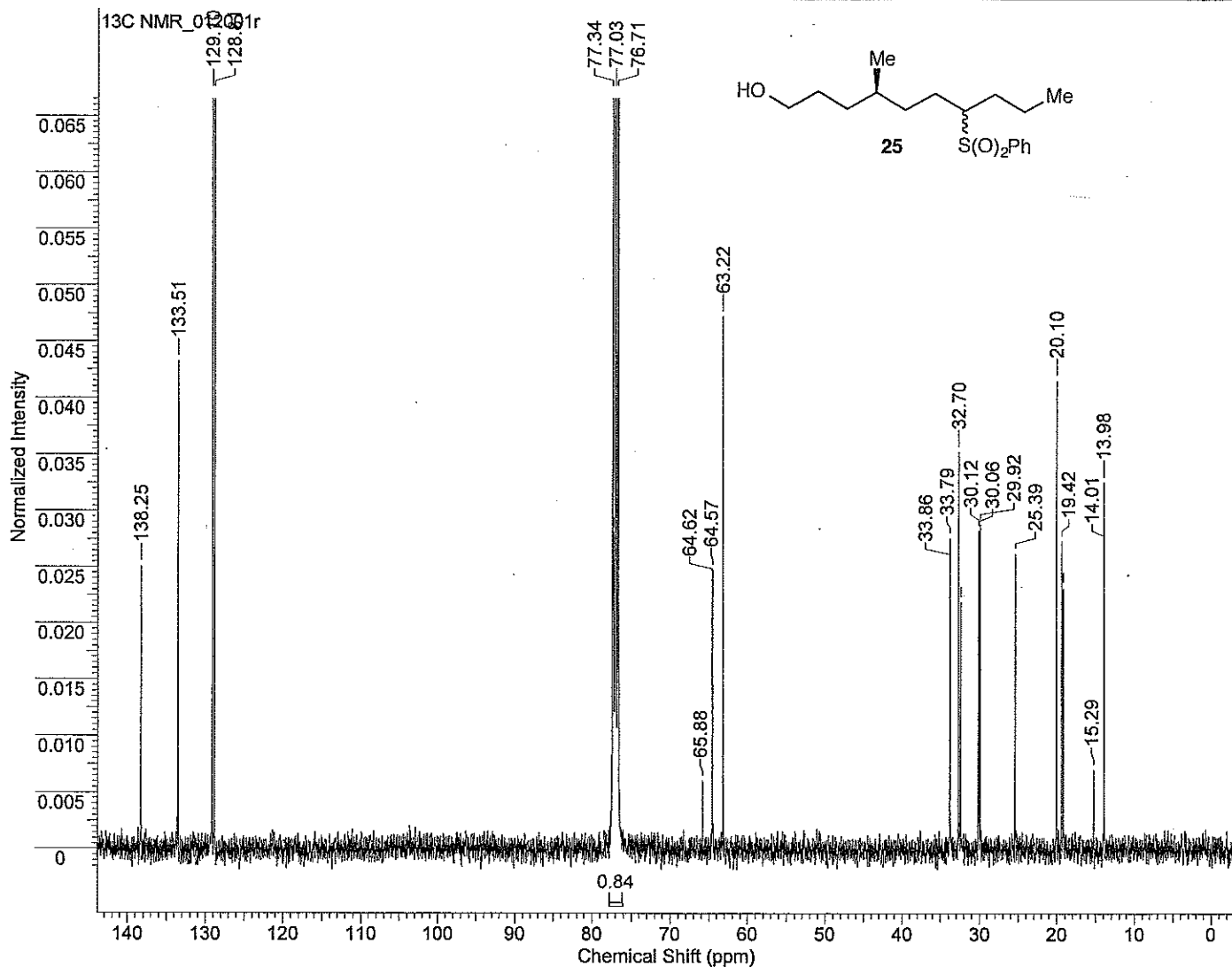
NAME      2010-09-20-ejt-15
EXPNO     10
PROCNO    1
Date_     20100920
Time      12.16
INSTRUM   spect
PROBHD    5 mm TXI 1H/D-
PULPROG   zg30b
TD         65536
SOLVENT   CDCl3
NS         16
DS         0
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ         3.1719923 sec
RG         322
DW         48.400 usec
DE         13.38 usec
TE         294.3 K
D1         1.00000000 sec
TDO        1
  
```

```

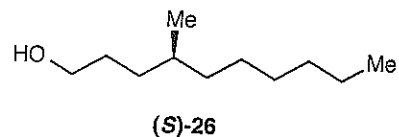
===== CHANNEL f1 =====
NUC1      1H
P1         8.20 usec
PL1        3.25 dB
PL1W       12.12272263 W
SF01      500.1330885 MHz
SI         32768
SF         500.1300463 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```



| | | | |
|------------------------|---|------------------------|----------------------|
| Acquisition Time (sec) | 1.3631 | | |
| Comment | Leo 0910-043 HL093-002 mCARBON CDCI3 (E:\bruk400service_data\2010\Sep) Administrator 8 | | |
| Date | 22 Sep 2010 14:17:36 | Date Stamp | 22 Sep 2010 14:17:36 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL093 - Sulfone alkylation\HL093-002\13C NMR_012001r | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C |
| Number of Transients | 12000 | Origin | AV400_S |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 23.600 |

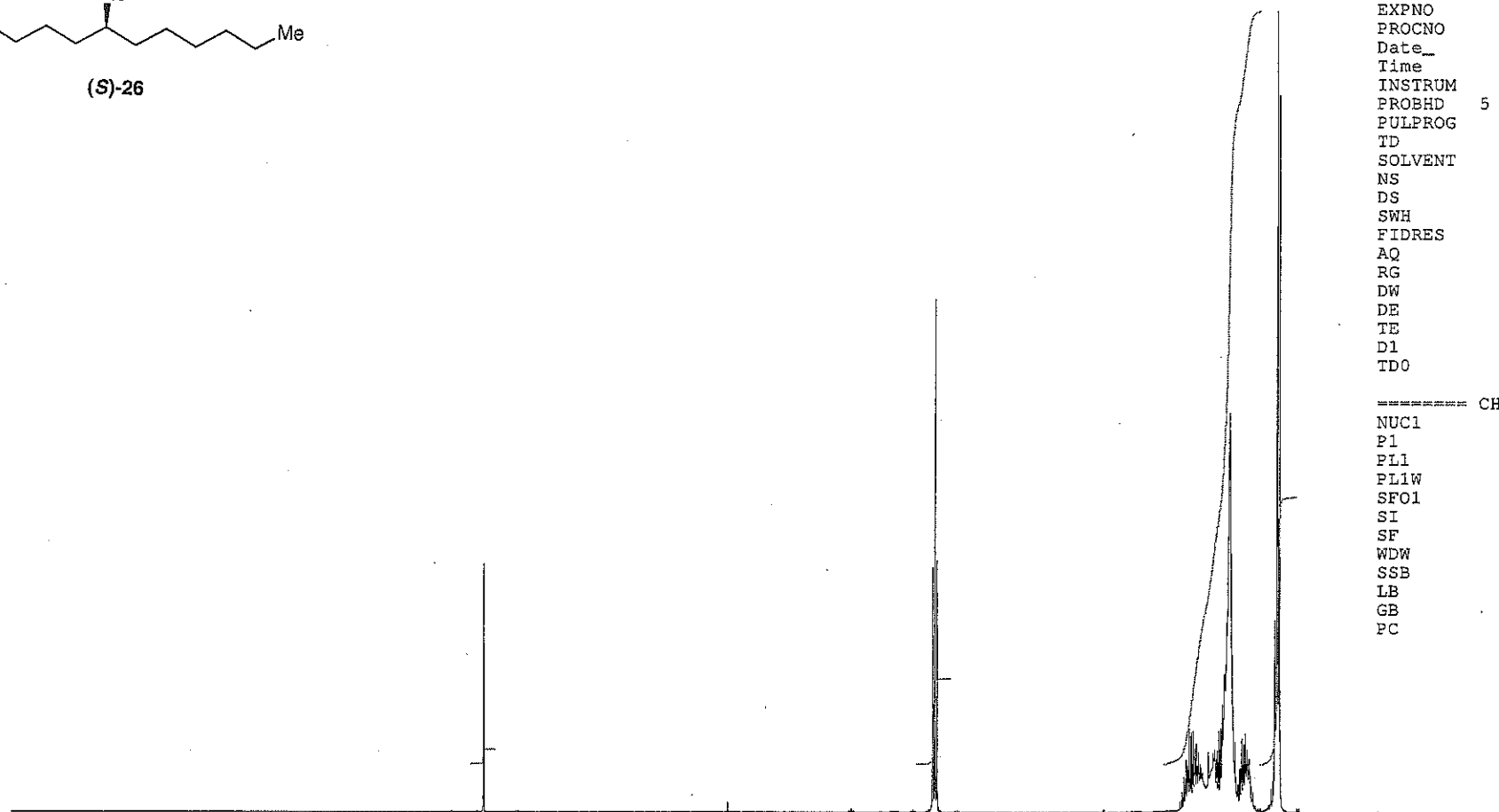


HL094-001
mPROTON CDCl3 {e:\bruk400data\2010\Sep} ejt 54



NAME 2010-09-23-ejt-54
EXPNO 10
PROCNO 1
Date_ 20100923
Time 17.25
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 256
DW 60.500 usec
DE 9.40 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300361 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm

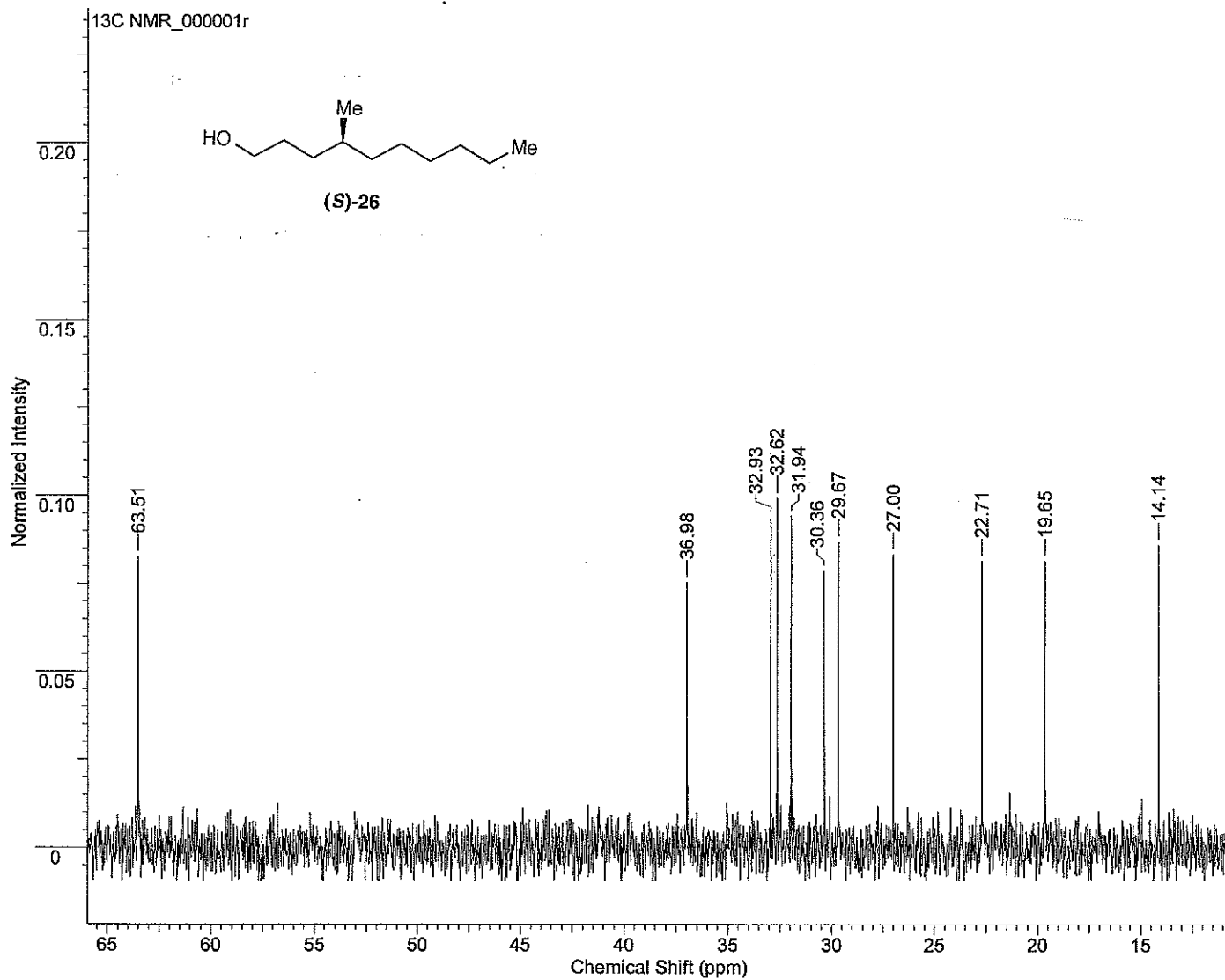
1.25

7.63

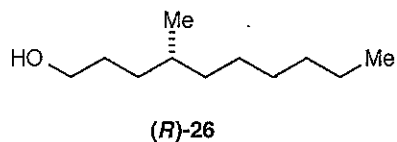
67.18

23.93

| | | | |
|-------------------------------|---|-------------------------------|--|
| Acquisition Time (sec) | 1.0835 | Comment | HL094-001 mCARBON CDCl3 {e:\bruk400data\2010\Sep} ejt 50 |
| Date | 23 Sep 2010 13:05:04 | Date Stamp | 23 Sep 2010 13:05:04 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL094 - Dithiane formation\HL094-001\13C NMR_000001r | | |
| Frequency (MHz) | 100.61 | Nucleus | 13C |
| Number of Transients | 256 | Origin | AV400 |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 512.00 | SW(cyclical) (Hz) | 30241.94 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 11335.2197 |
| Sweep Width (Hz) | 30241.01 | Temperature (degree C) | 21.300 |

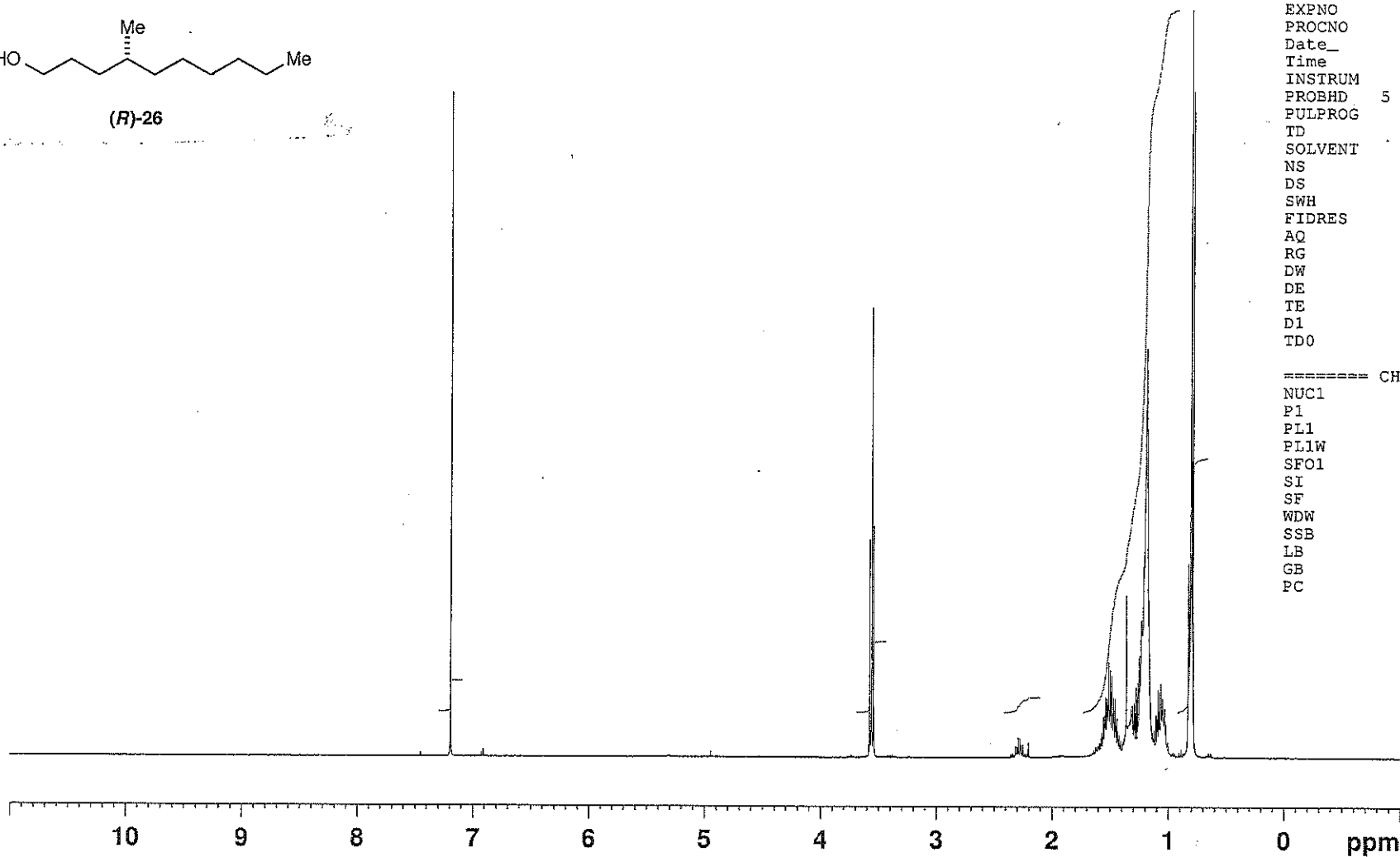


HL102-032
mPROTON CDCl3 {e:\bruk400data\2011\Feb} ejt 45

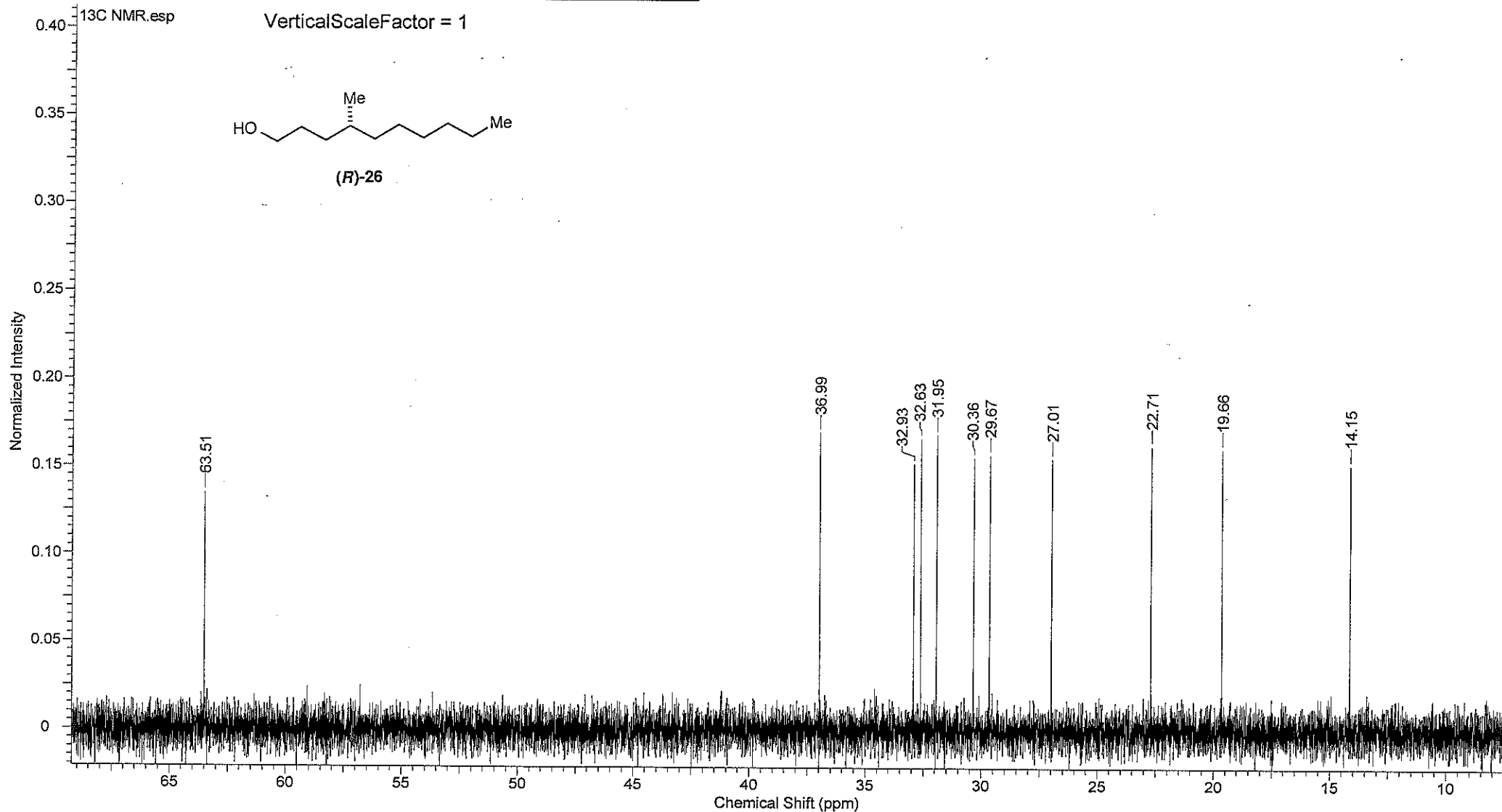


NAME 2011-02-25-ejt-45
EXPNO 10
PROCNO 1
Date_ 20110225
Time 10.32
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 406
DW 60.500 usec
DE 9.40 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

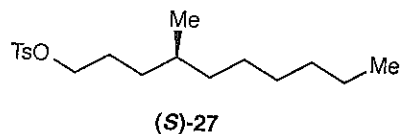
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300366 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



| | | | | | |
|------------------------|--|------------------------|--|----------------------|----------------------|
| Acquisition Time (sec) | 1.0835 | Comment | HL094-001 mCARBON CDCl3 (e:\bruk400data\2010\Sep) eit 50 | Date | 23 Sep 2010 14:05:04 |
| Date Stamp | 23 Sep 2010 14:05:04 | | | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL094 - Dithiane formation\HL094-001\13C NMR\fid | | | Frequency (MHz) | 100.61 |
| Nucleus | 13C | Number of Transients | 256 | Origin | AV400 |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 |
| SW(cyclical) (Hz) | 30241.94 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 11335.2197 |
| Sweep Width (Hz) | 30241.91 | Temperature (degree C) | 21.300 | Spectrum Type | STANDARD |

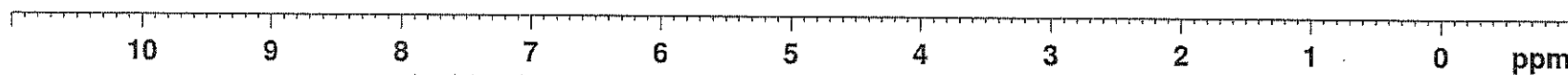
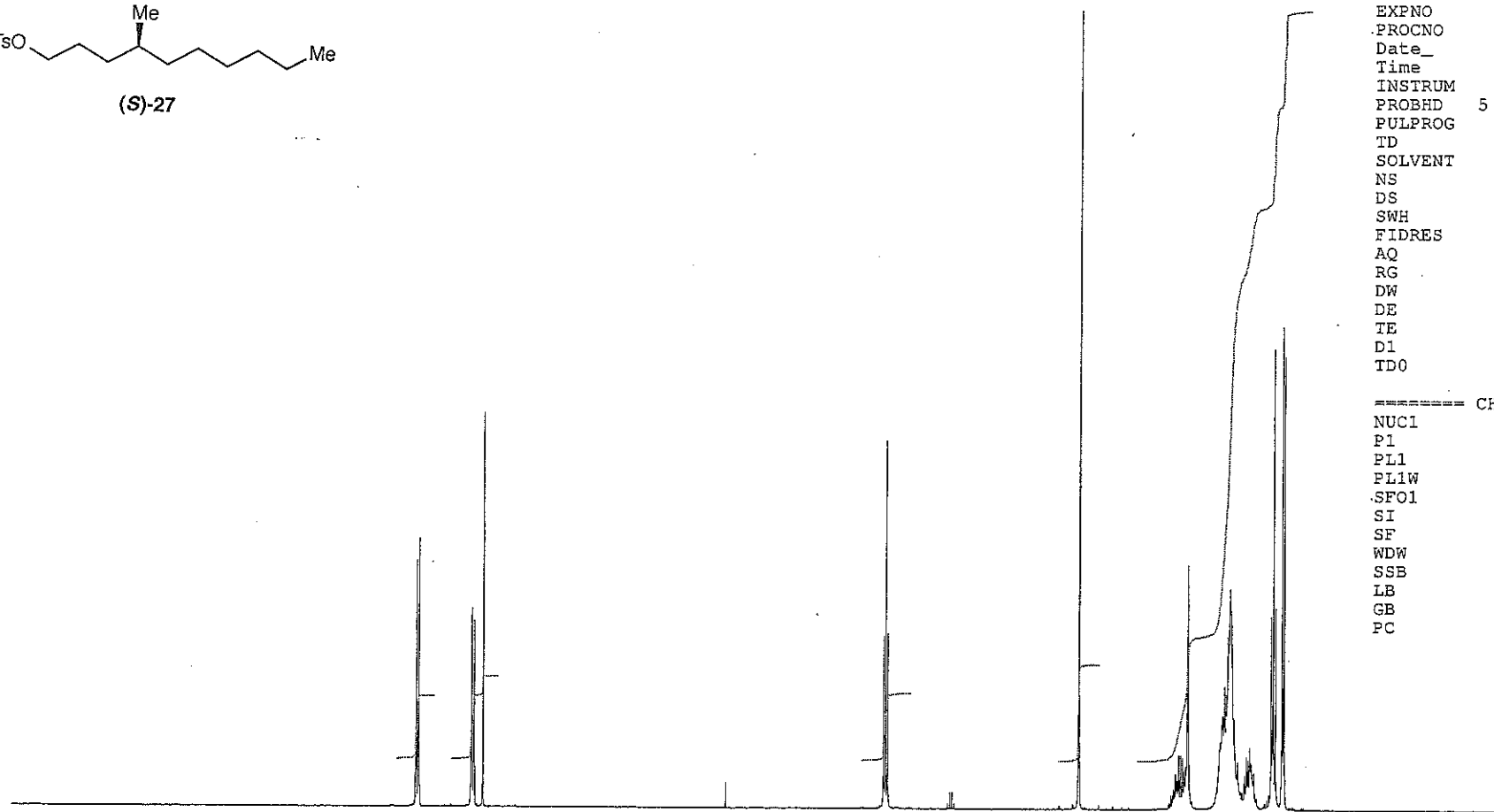


HL098-001
mPROTONnight CDCl3 {e:\bruk400data\2010\Nov} ejt 12



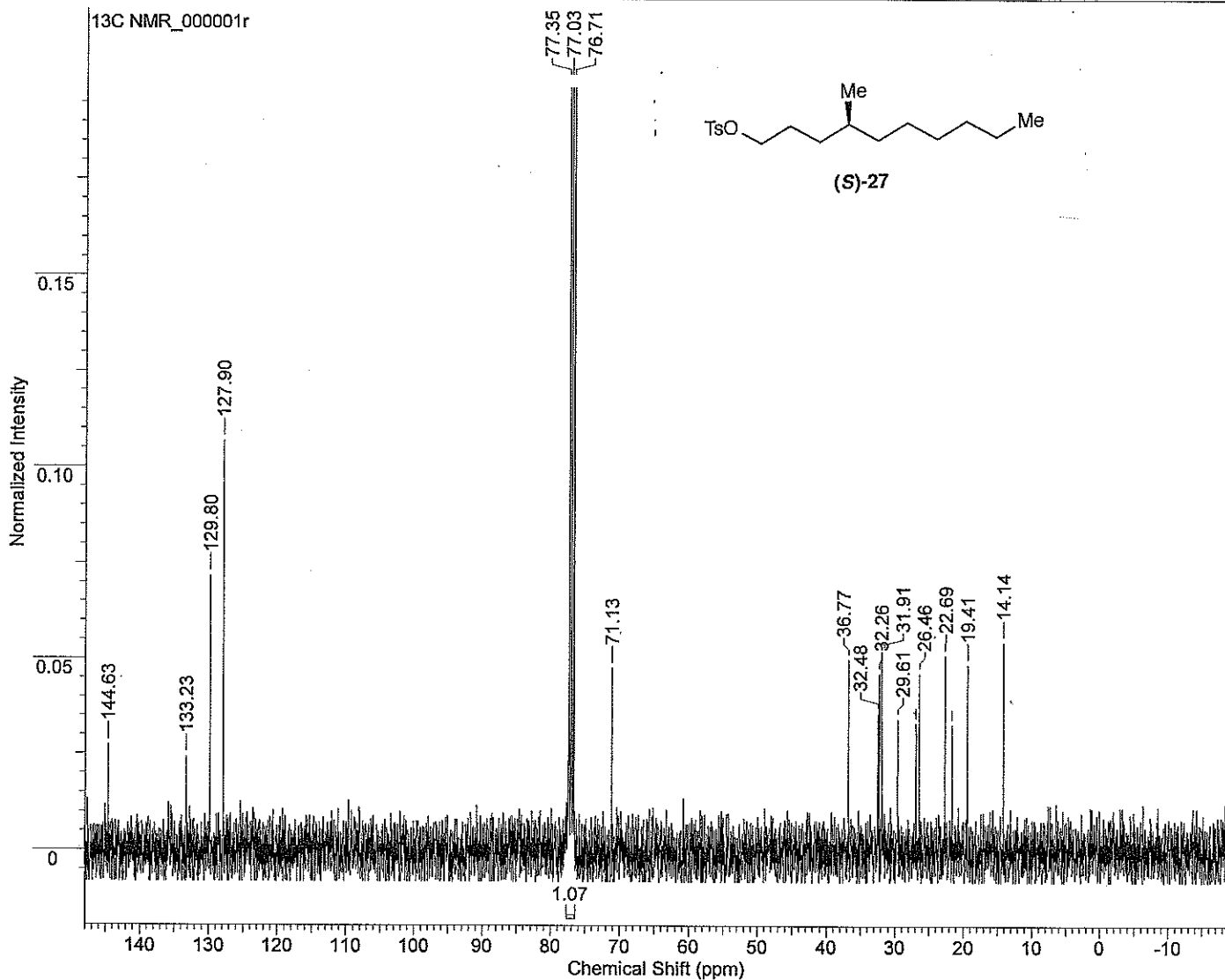
NAME 2010-11-16-ejt-12
EXPNO 10
PROCNO 1
Date_ 20101117
Time 4.53
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 406
DW 60.500 usec
DE 9.40 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

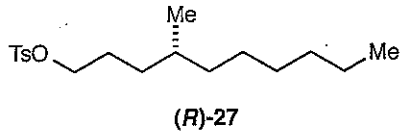
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300364 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



5.87 7.81 6.34 9.14 70.85

| | | | |
|------------------------|--|------------------------|---|
| Acquisition Time (sec) | 1.0835 | Comment | HL098-001 mCARBONnight CDCI3 {e:\bruk400data\2010\Nov} ejt 12 |
| Date | 17 Nov 2010 05:07:12 | Date Stamp | 17 Nov 2010 05:07:12 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL098 - RHS sulfone synthesis\HL098-001\13C NMR_000001r | | |
| Frequency (MHz) | 100.61 | Nucleus | 13C |
| Number of Transients | 256 | Origin | AV400 |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 512.00 | SW(cyclical) (Hz) | 30241.94 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 11335.2197 |
| Sweep Width (Hz) | 30241.01 | Temperature (degree C) | 20.600 |



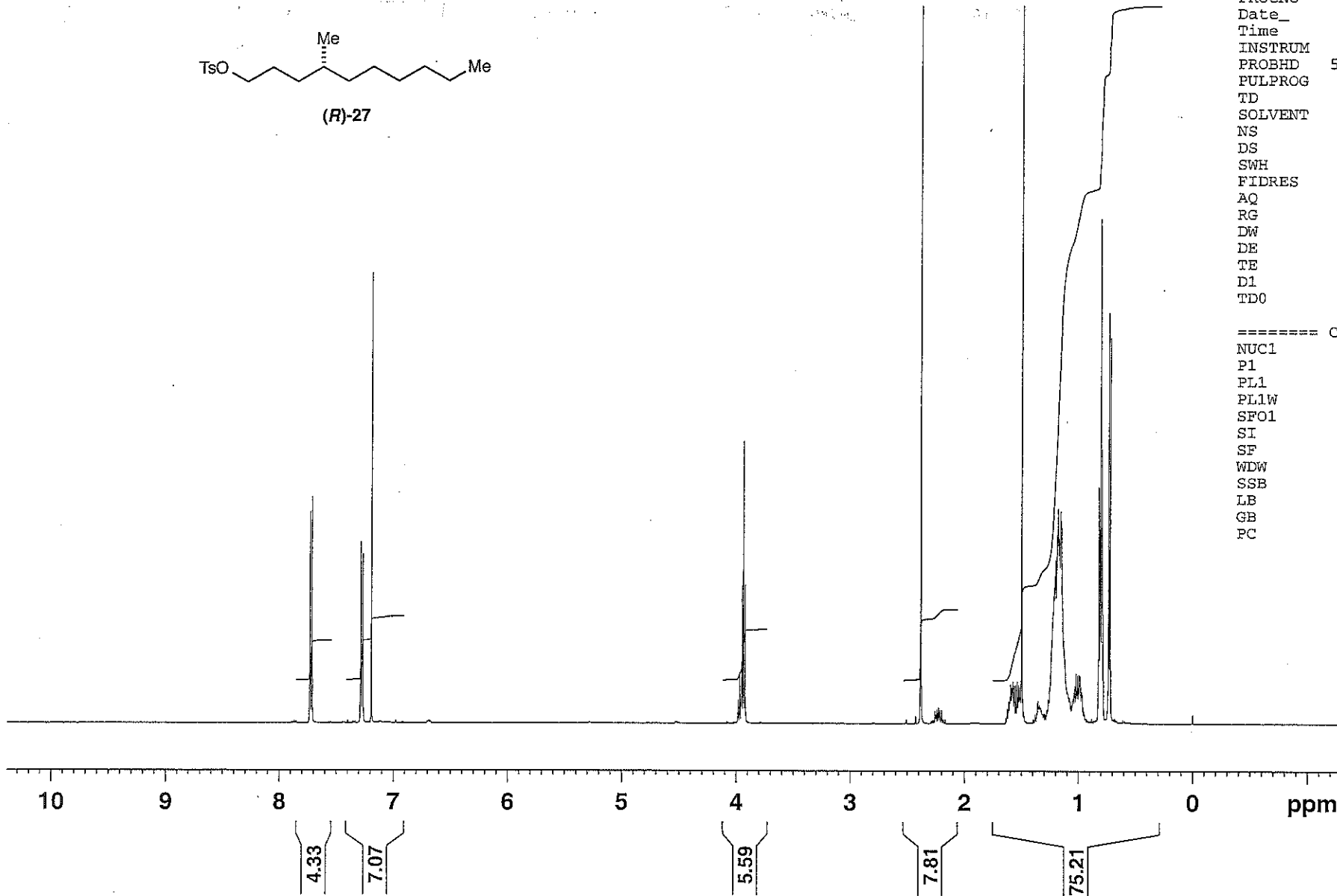


```

NAME      2011-02-28-ejt-1
EXPNO     10
PROCNO    1
Date_     20110228
Time      11.15
INSTRUM   spect
PROBHD    5 mm TXI 1H/D-
PULPROG   zg30b
TD        65536
SOLVENT   CDCl3
NS        16
DS        0
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1719923 sec
RG        322
DW        48.400 usec
DE        13.38 usec
TE        290.6 K
D1        1.00000000 sec
TD0       1
  
```

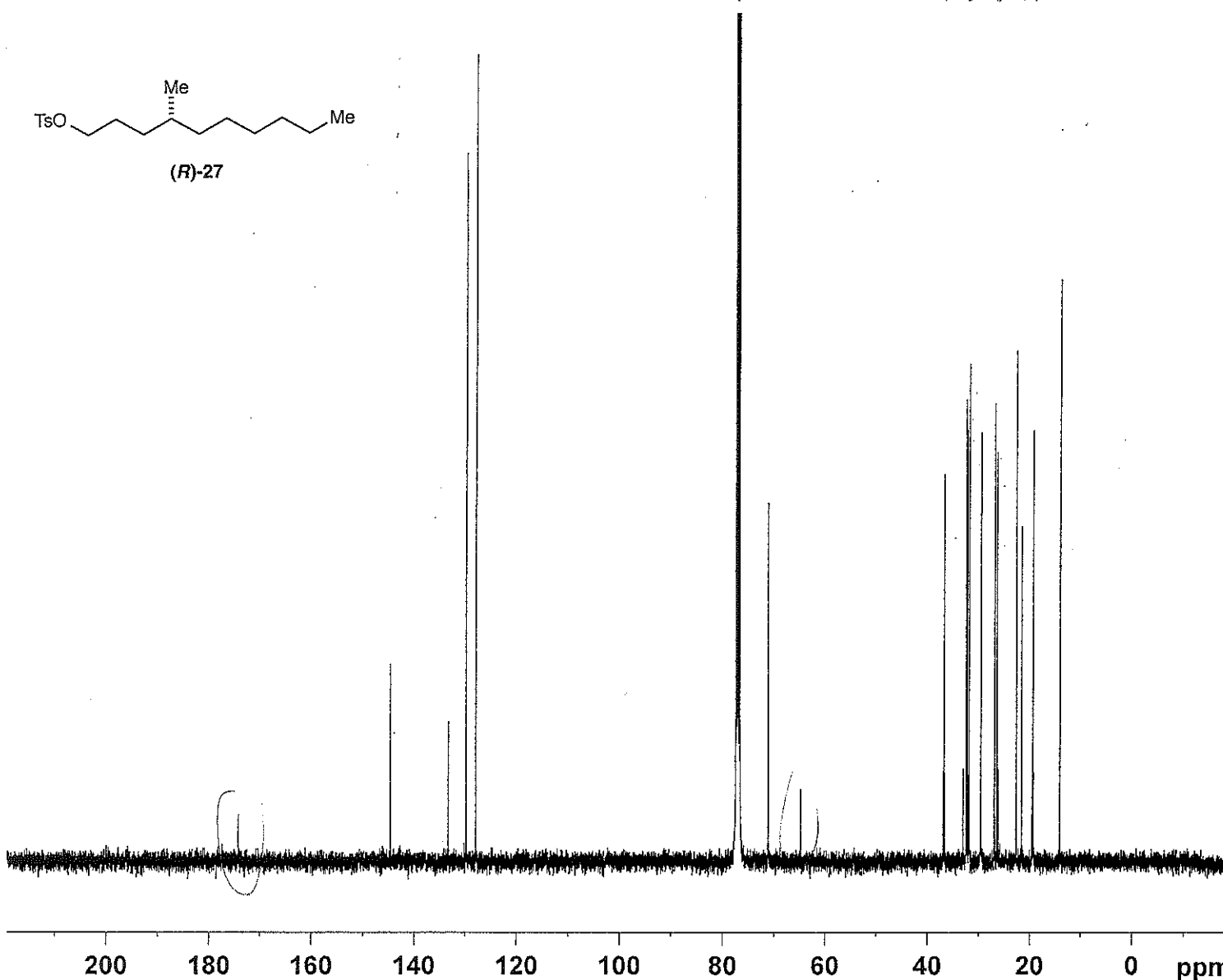
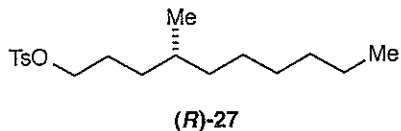
```

===== CHANNEL f1 =====
NUC1      1H
P1        8.20 usec
PL1       3.25 dB
PL1W      12.12272263 W
SFO1      500.1330885 MHz
SI        32768
SF        500.1300466 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



H. Liu
0211-035
HL102-033

mCARBON CDCl3 {E:\bruk400service_data\2011\Mar} Administrator-36

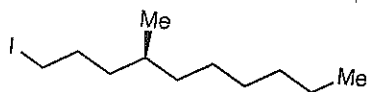


NAME 2011-03-07-Administrator-36
EXPNO 10
PROCNO 1
Date 20110307
Time 15.37
INSTRUM AV400 S
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 17408
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 33.91046524 W
SFO1 100.6479773 MHz

===== CHANNEL f2 =====
CFDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL2W 18.98951721 W
PL12W 0.24406971 W
PL13W 0.13137537 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379140 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

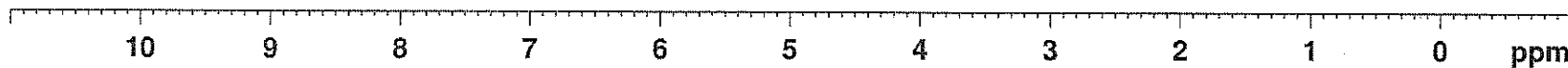
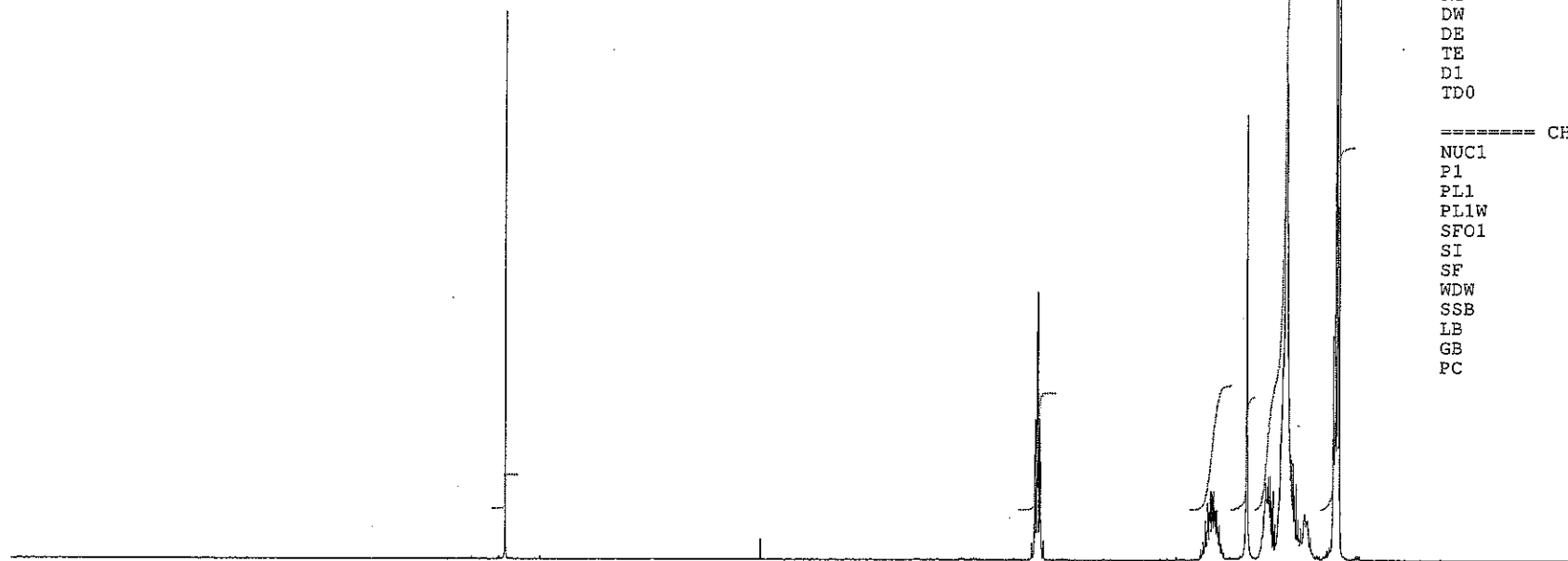
HL094-002
mPROTON CDCl3 {e:\bruk400data\2010\Sep} ejt 10



(S)-28

NAME 2010-09-27-ejt-10
EXPNO 10
PROCNO 1
Date_ 20100927
Time 10.29
INSTRUM AV400
PROBHD 5 mm PABBO BE-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 322
DW 60.500 usec
DE 9.40 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300368 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.16

7.57

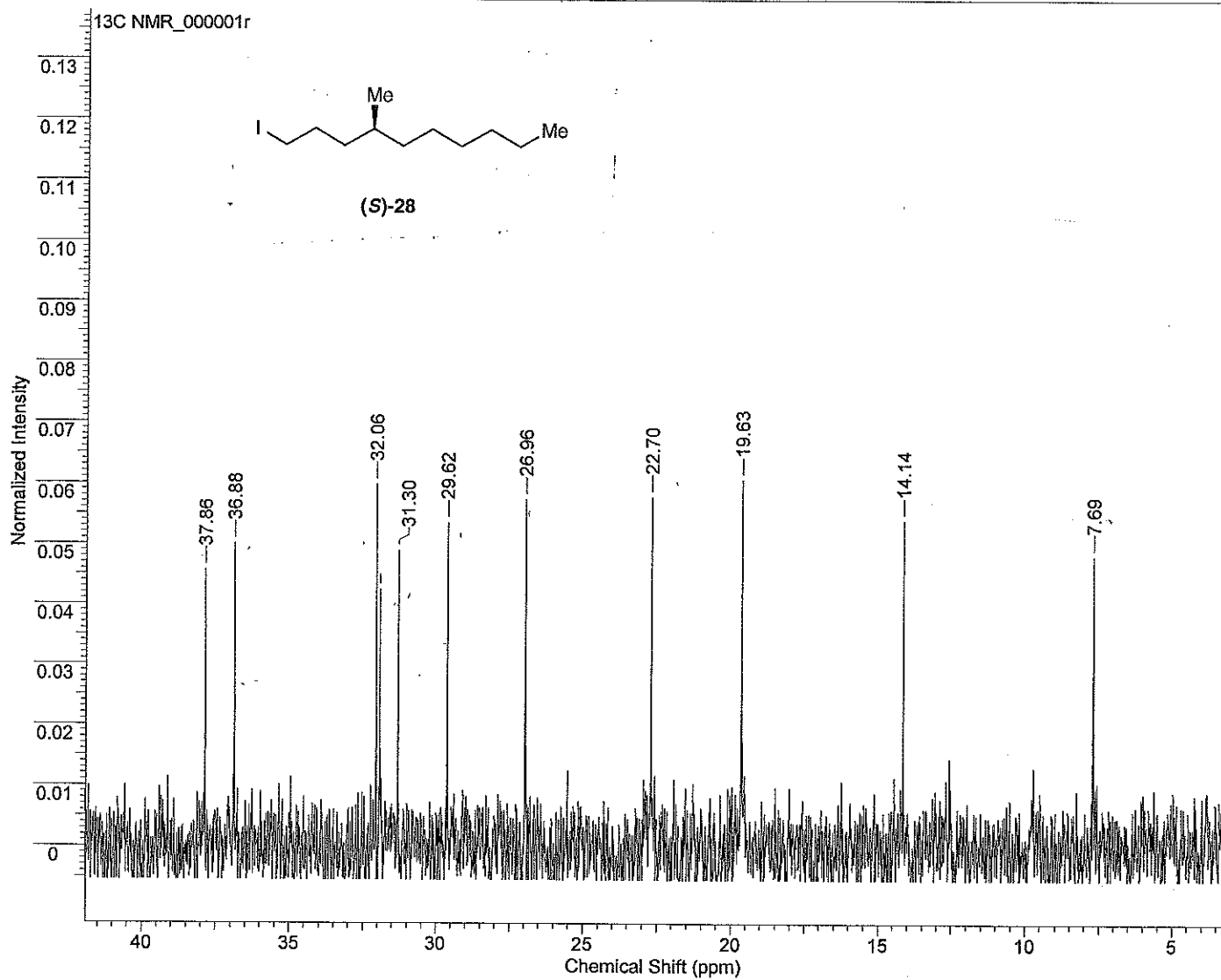
8.11

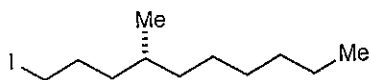
7.35

51.25

23.55

| | | | |
|------------------------|---|------------------------|--|
| Acquisition Time (sec) | 1.0835 | Comment | HL094-002 mCARBON CDCl3 (e:\bruk400data\2010\Sep) ejt 10 |
| Date | 27 Sep 2010 09:44:32 | Date Stamp | 27 Sep 2010 09:44:32 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL094 - Dithiane formation\HL094-002\13C NMR_000001r | | |
| Frequency (MHz) | 100.61 | Nucleus | 13C |
| Number of Transients | 256 | Origin | AV400 |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 512.00 | SW(cyclical) (Hz) | 30241.94 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 11335.2197 |
| Sweep Width (Hz) | 30241.01 | Temperature (degree C) | 21.600 |

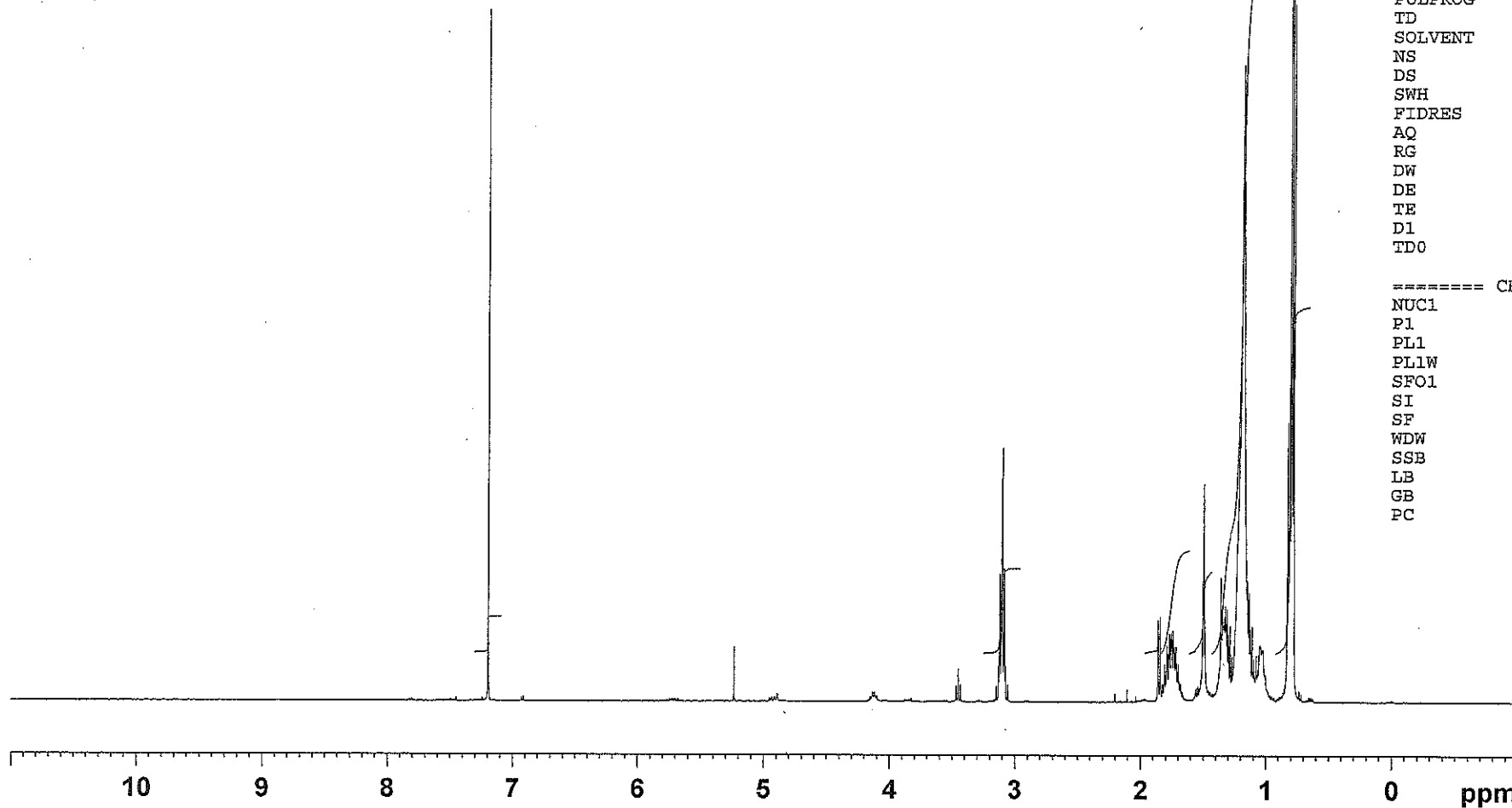




(R)-28

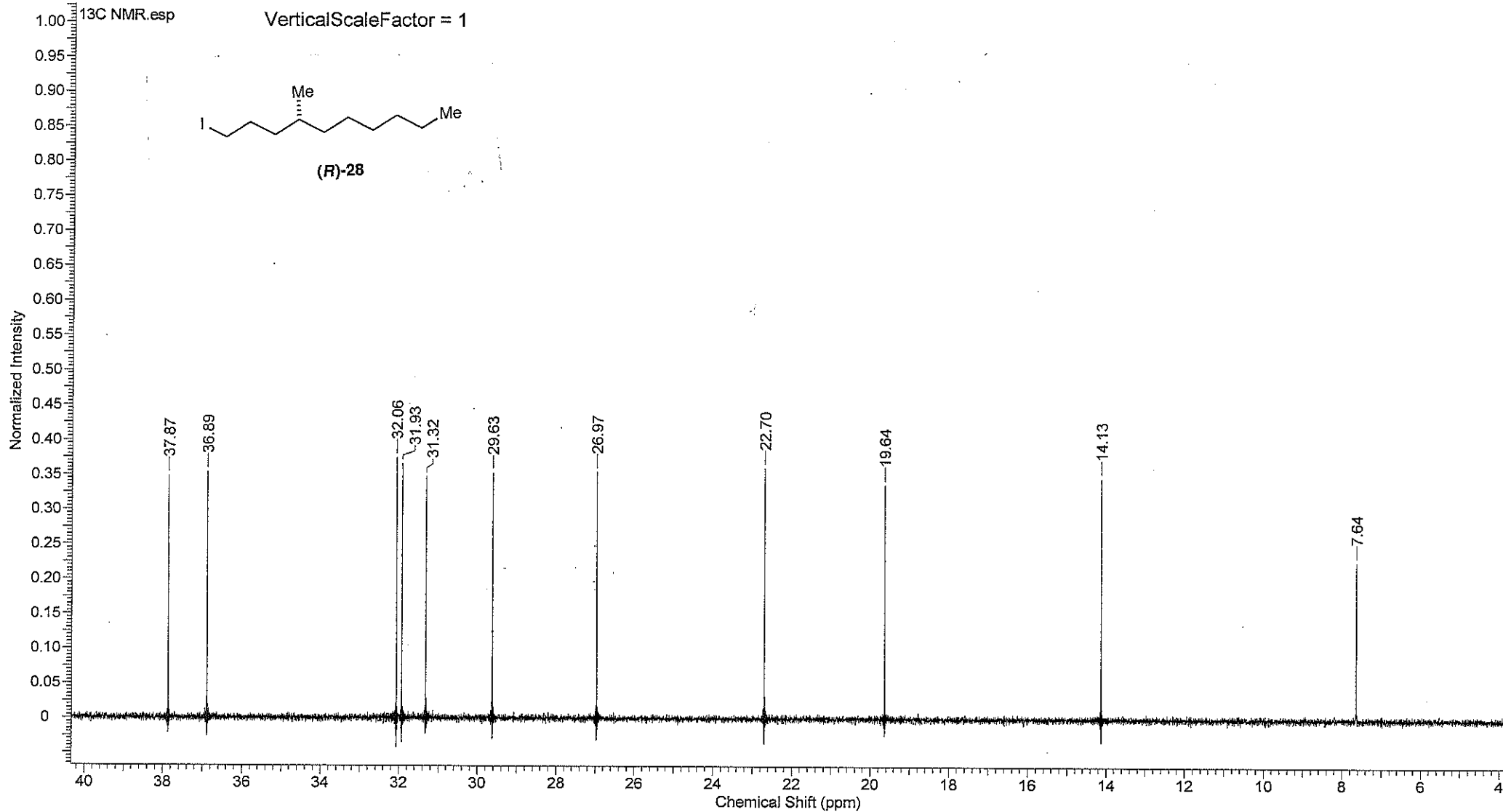
NAME 2010-12-03-ejt-22
EXPNO 20
PROCNO 1
Date_ 20101203
Time 14.50
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 322
DW 60.500 usec
DE 9.40 usec
TE 290.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300362 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

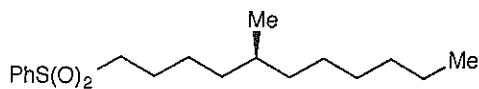


2.46
5.83
1.66
7.10
5.66
53.25
24.04

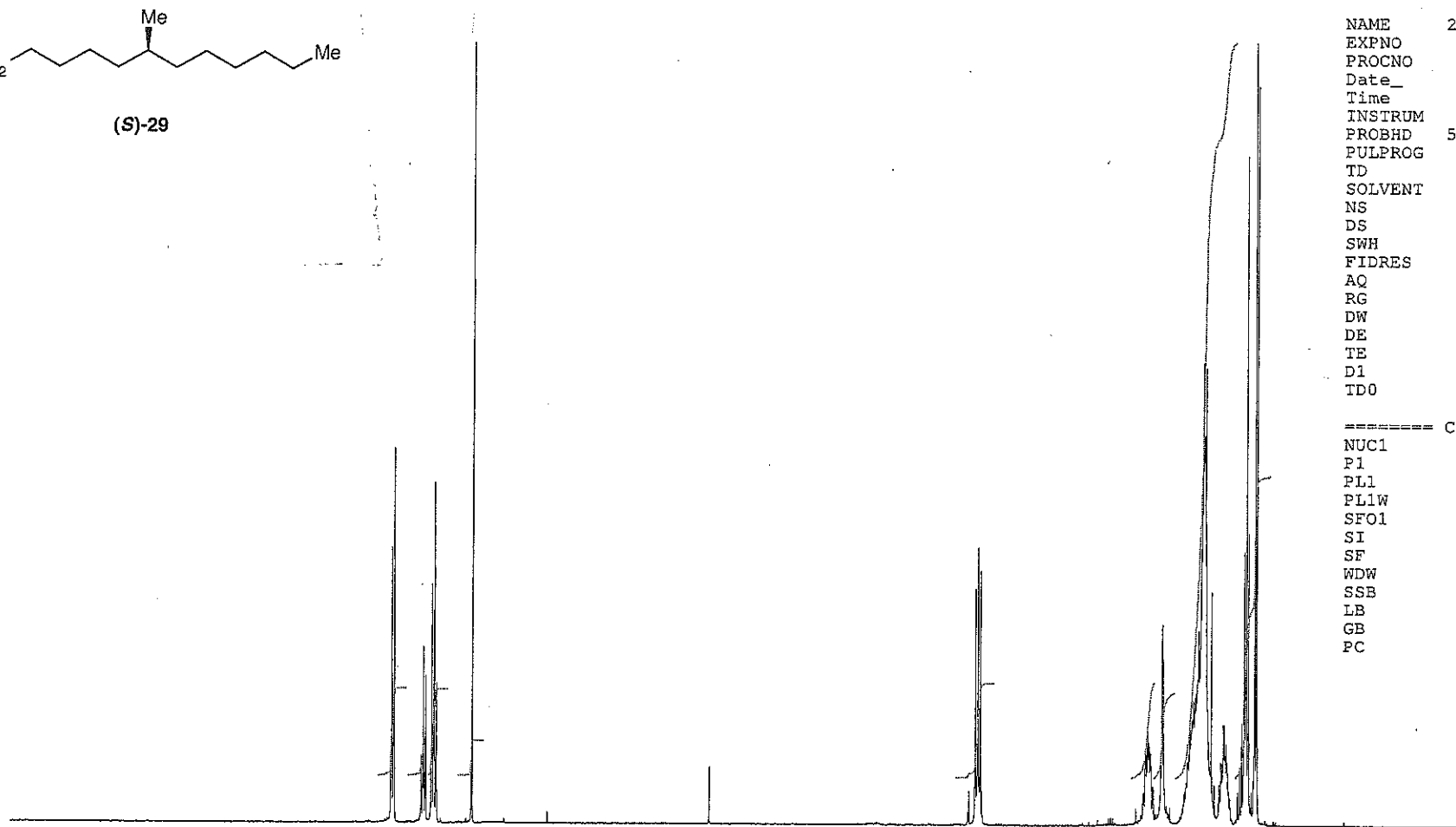
| | | | | | |
|------------------------|---|------------------------|---|----------------------|------------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 1110-056 HL098-002 mCARBON CDCl3 {E:\bruk400service_data\2010\Nov} Administrator 36 | | |
| Date | 22 Nov 2010 13:30:40 | Date Stamp | 22 Nov 2010 13:30:40 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL098 - RHS sulfone synthesis\HL098-002\13C NMR\fid | | | Frequency (MHz) | 100.64 |
| Nucleus | 13C | Number of Transients | 2364 | Origin | AV400_S |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24038.44 | Temperature (degree C) | 24.500 | Spectrum Type | STANDARD |



HL098-003
mPROTON CDCl3 {e:\bruk400data\2010\Nov} ejt 7



(S)-29



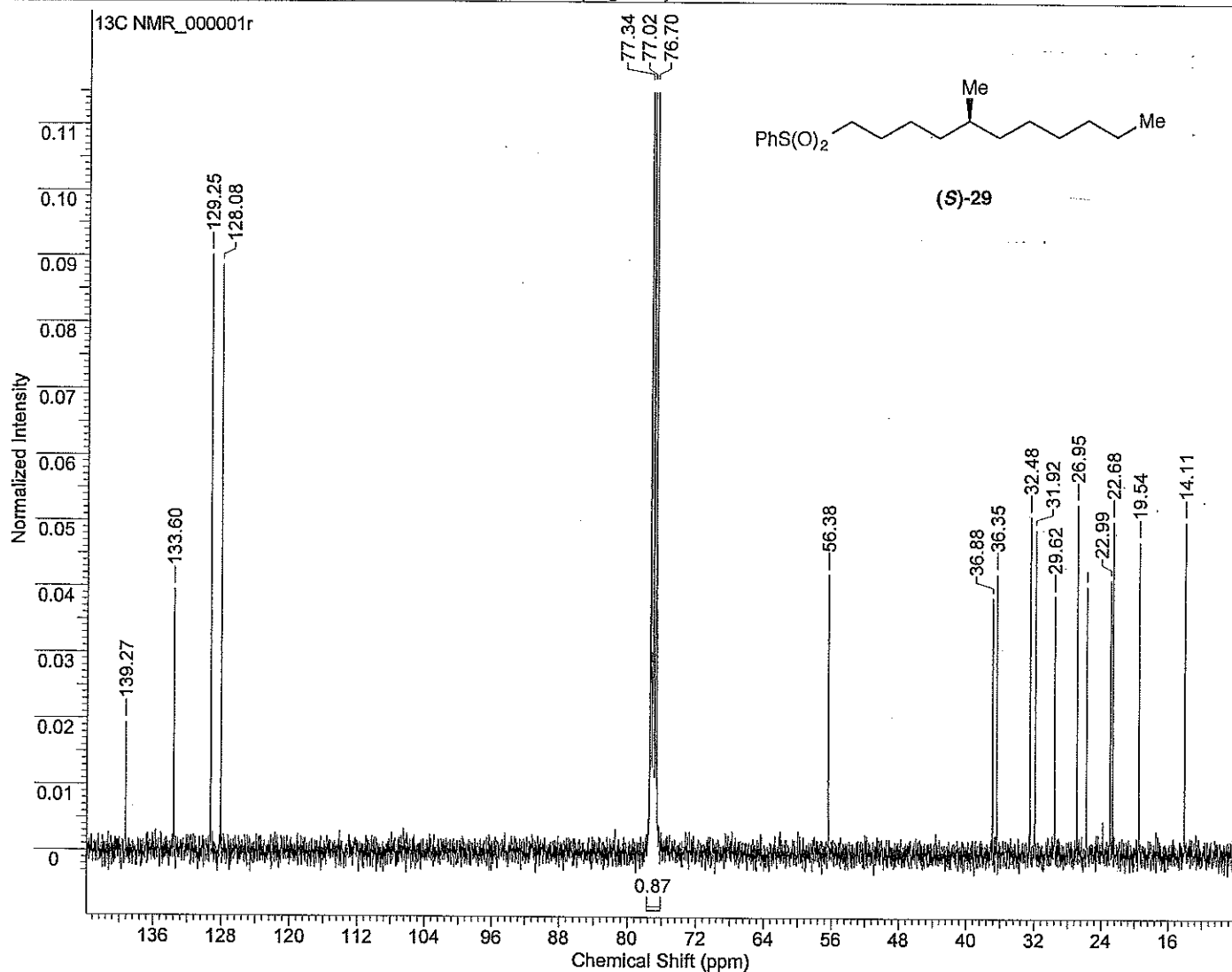
NAME 2010-11-17-ejt-7
EXPNO 10
PROCNO 1
Date_ 20101117
Time 15.33
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 322
DW 60.500 usec
DE 9.40 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300363 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 9 8 7 6 5 4 3 2 1 0 ppm

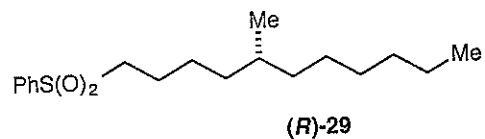
5.58
2.90
5.51
2.25
6.01
6.09
5.45
46.94
19.26

| | | | |
|------------------------|--|------------------------|----------------------|
| Acquisition Time (sec) | 1.3631 | | |
| Comment | Leo 1110-055 HL098-003 mCARBON CDCl3 (E:\bruk400service_data\2010\Nov\ Administrator 18 | | |
| Date | 19 Nov 2010 08:36:16 | Date Stamp | 19 Nov 2010 08:36:16 |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL098 - RHS sulfone synthesis\HL098-003\13C NMR_000001r | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C |
| Number of Transients | 4096 | Origin | AV400 S |
| Original Points Count | 32768 | Owner | Administrator |
| Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 |
| Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 25.100 |



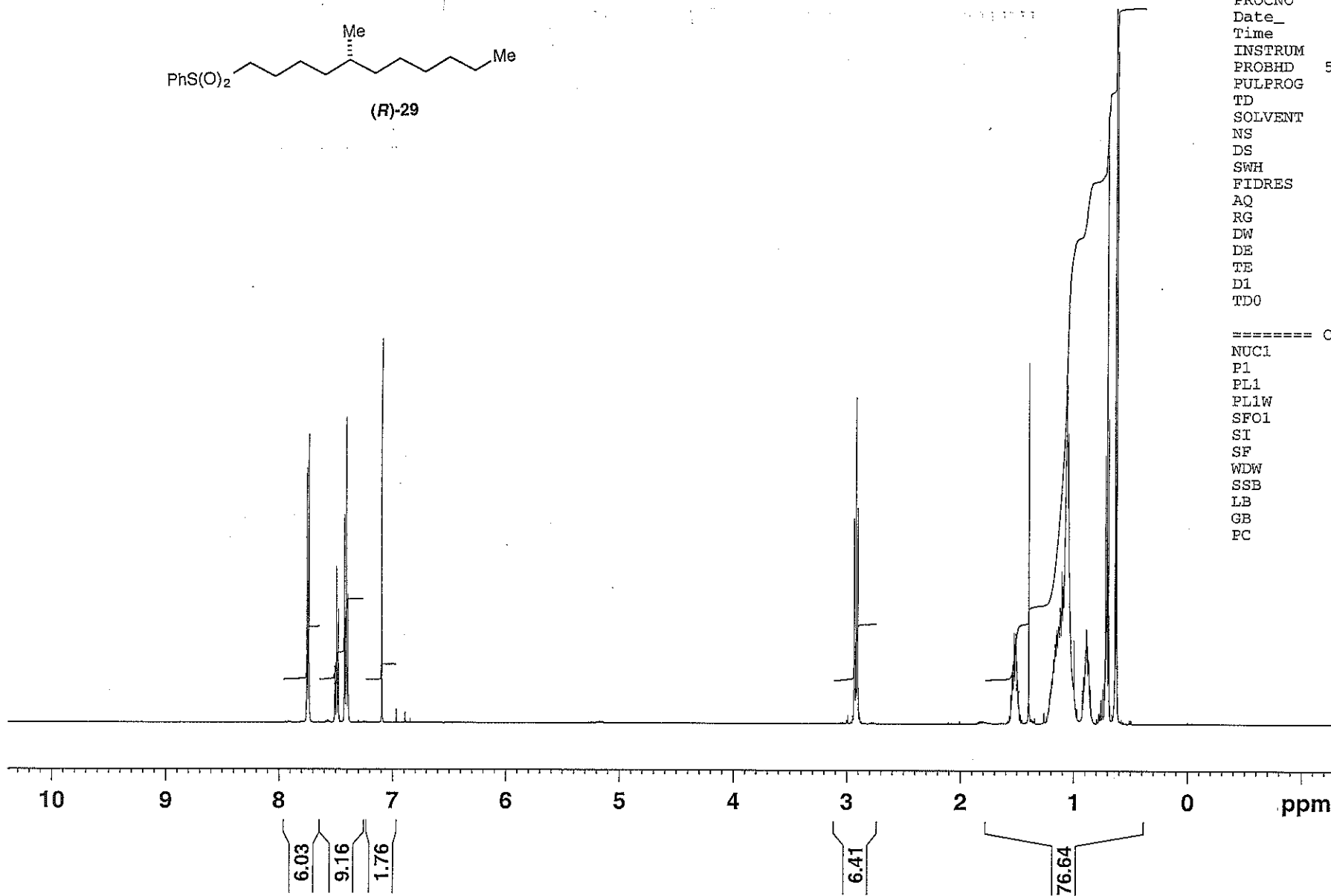
HL102-035

mPROTON CDCl3 /opt/bruk500data/2011/Jan ejt 1

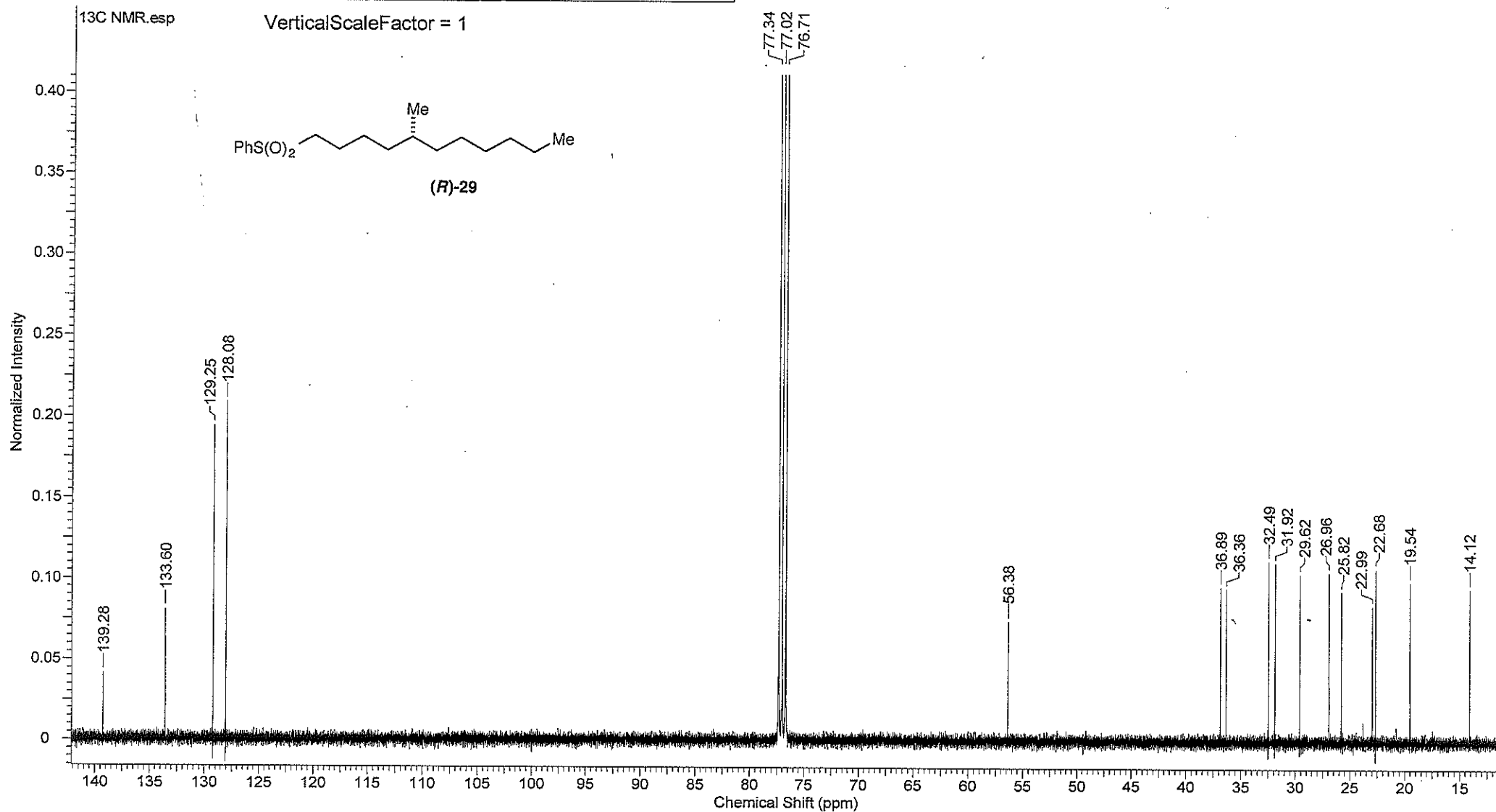


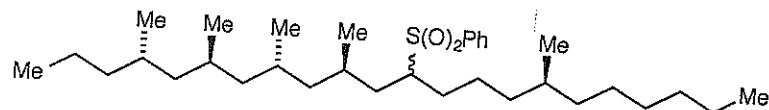
NAME 2011-01-31-ejt-1
EXPNO 10
PROCNO 1
Date_ 20110131
Time 10.49
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 228
DW 48.400 usec
DE 13.38 usec
TE 293.2 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300954 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

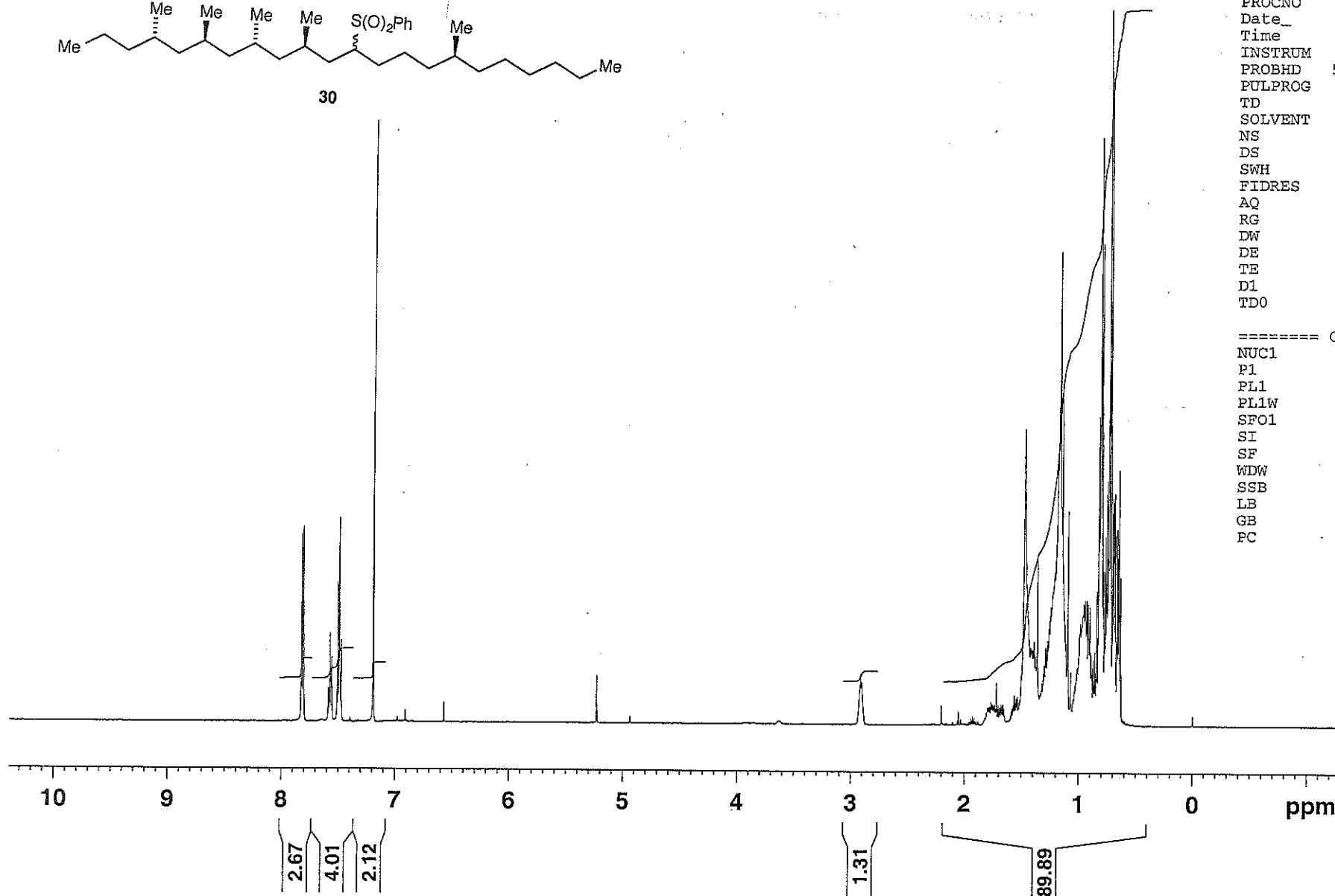


| | | | | | |
|------------------------|---|------------------------|---|----------------------|------------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 1110-055 HL098-003 mCARBON CDCl3 (E:\bruk400service_data\2010\Nov) Administrator 18 | | |
| Date | 19 Nov 2010 08:36:16 | Date Stamp | 19 Nov 2010 08:36:16 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL098 - RHS sulfone synthesis\HL098-003\13C NMR\fid | | | Frequency (MHz) | 100.64 |
| Nucleus | 13C | Number of Transients | 4096 | Origin | AV400_S |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24038.44 | Temperature (degree C) | 25.100 | Spectrum Type | STANDARD |





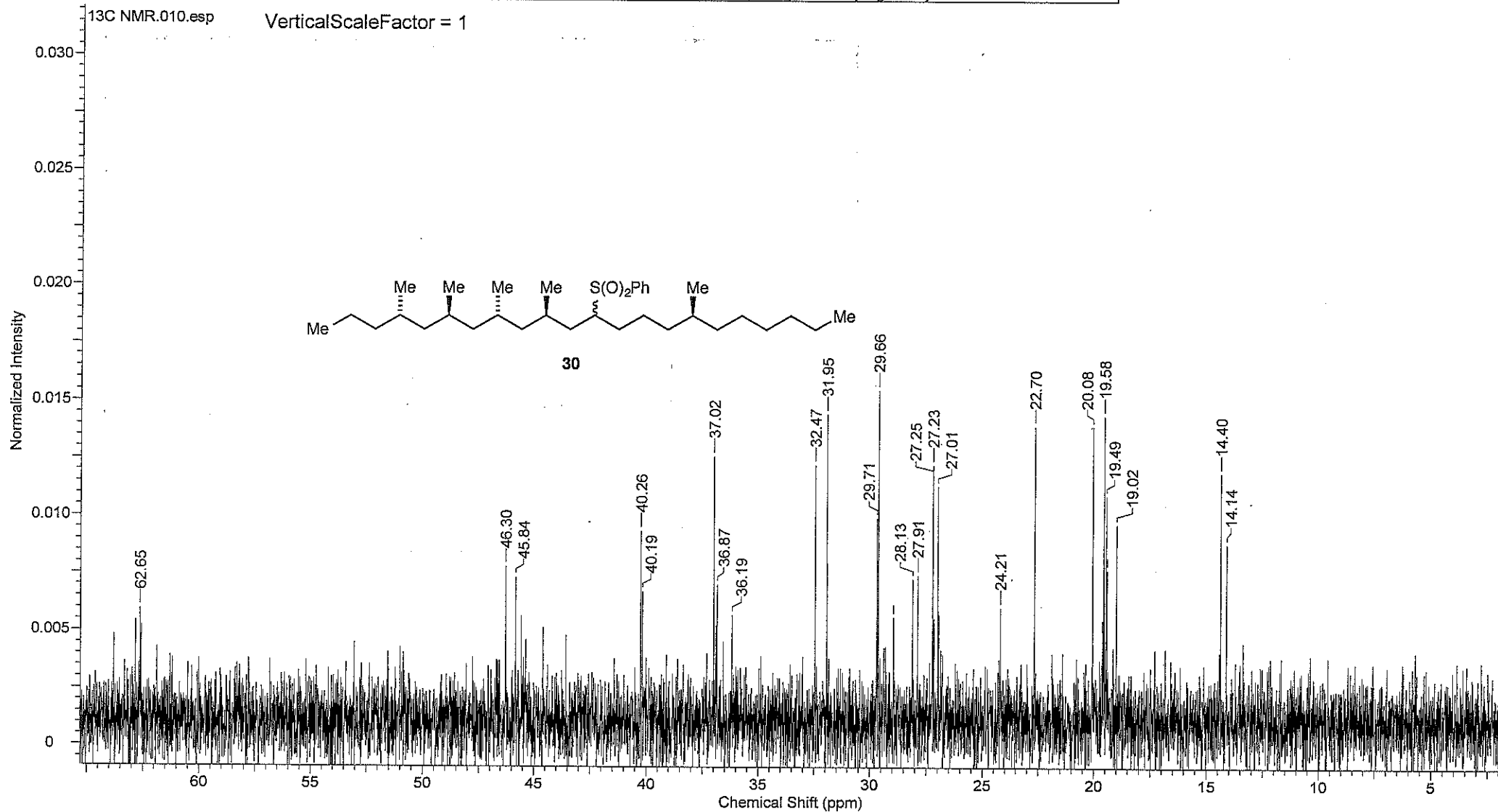
30



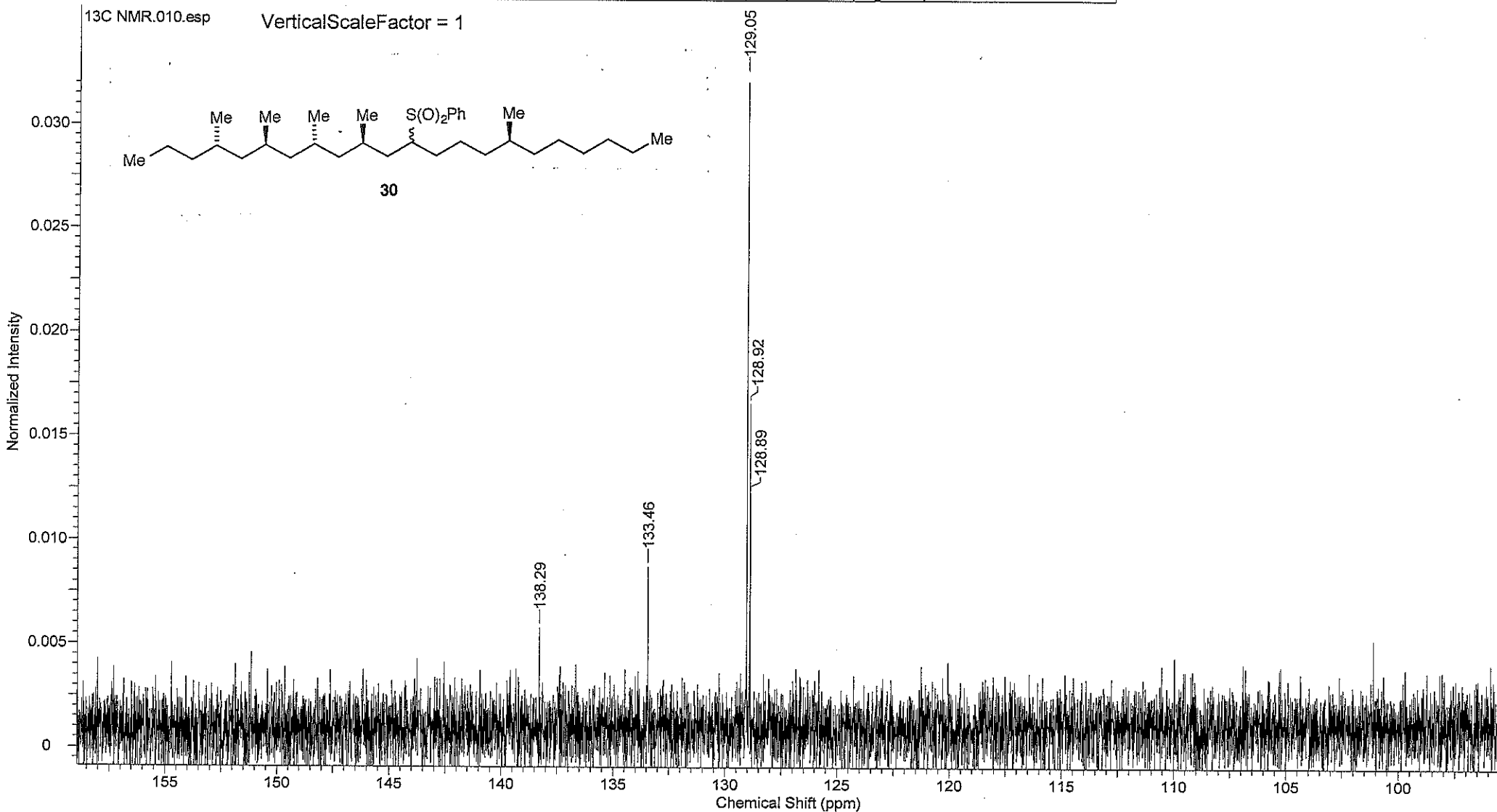
NAME 2010-11-22-ejt-12
EXPNO 10
PROCNO 1
Date_ 20101122
Time 12.10
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 322
DW 48.400 usec
DE 13.38 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SF01 500.1330885 MHz
SI 32768
SF 500.1300479 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

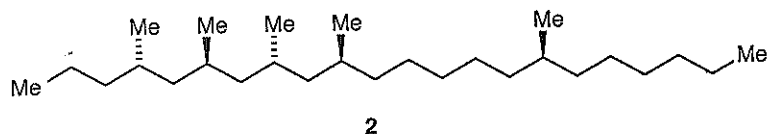
| | | | | | |
|------------------------|---|-------------------|---|------------------------|--------------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 1110-062 HL099-004 mCARBON CDCl3 (E:\bruk400service_data\2010\Nov) Administrator 38 | | |
| Date | 23 Nov 2010 08:12:48 | Date Stamp | 23 Nov 2010 08:12:48 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-027\13C NMR\10\fid | | | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C | Number of Transients | 12288 |
| Original Points Count | 32768 | Owner | Administrator | Points Count | 32768 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 25.500 |
| | | | | Origin | AV400_S |
| | | | | Pulse Sequence | zpgq30 |
| | | | | Spectrum Offset (Hz) | 10063.3350 |



| | | | | | |
|------------------------|---|-------------------|---|------------------------|--------------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 1110-062 HL099-004 mCARBON CDCl3 (E:\bruk400service_data\2010\Nov) Administrator 38 | | |
| Date | 23 Nov 2010 08:12:48 | Date Stamp | 23 Nov 2010 08:12:48 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-027\13C NMR\10\fid | | | | |
| Frequency (MHz) | 100.64 | Nucleus | 13C | Number of Transients | 12288 |
| Original Points Count | 32768 | Owner | Administrator | Points Count | 32768 |
| Receiver Gain | 2050.00 | SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 24037.73 | Temperature (degree C) | 25.500 |
| | | | | Origin | AV400_S |
| | | | | Pulse Sequence | zgpg30 |
| | | | | Spectrum Offset (Hz) | 10063.3350 |

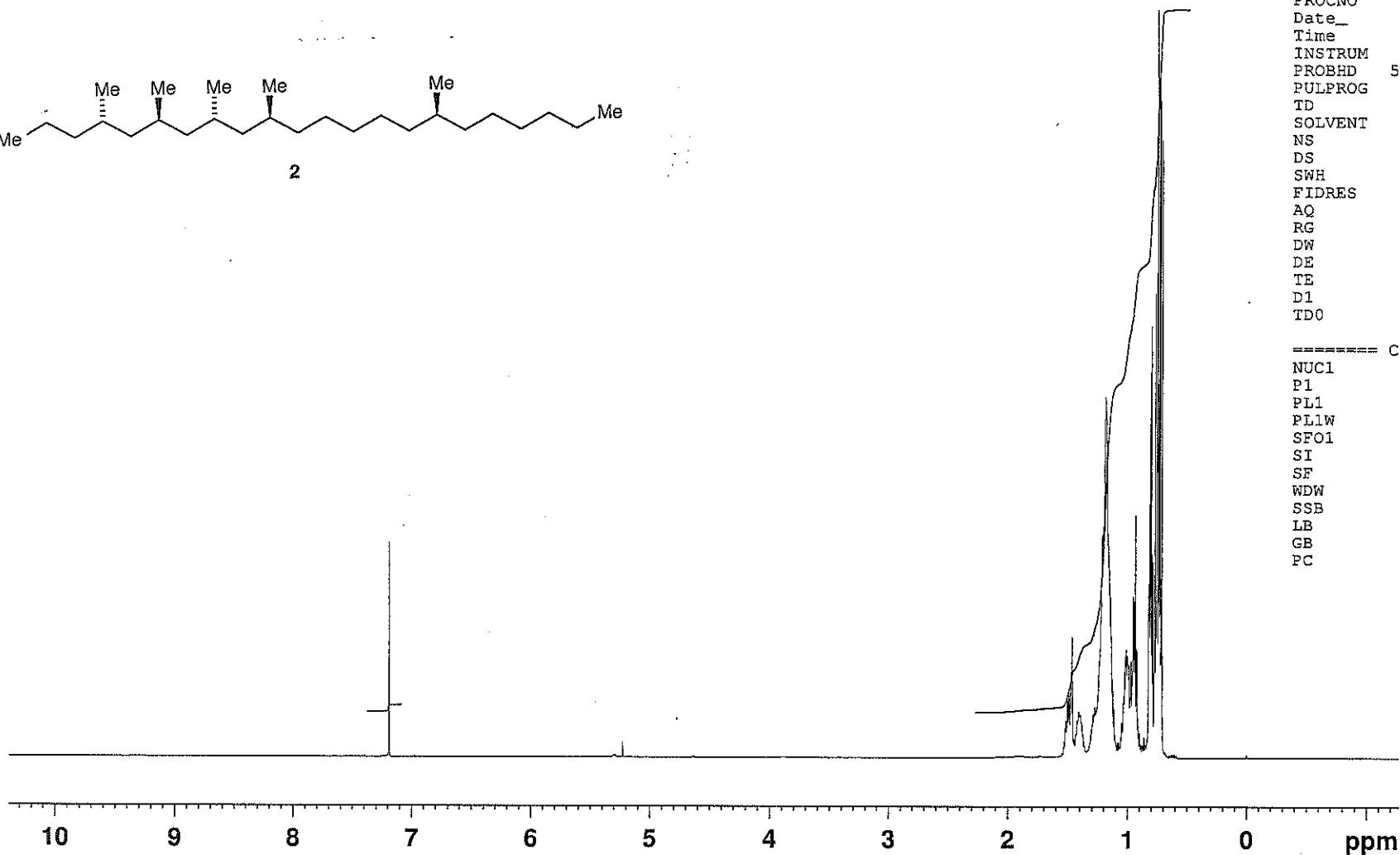


HL099-005
mPROTON CDCl3 /opt/bruk500data/2010/Nov ejt 39

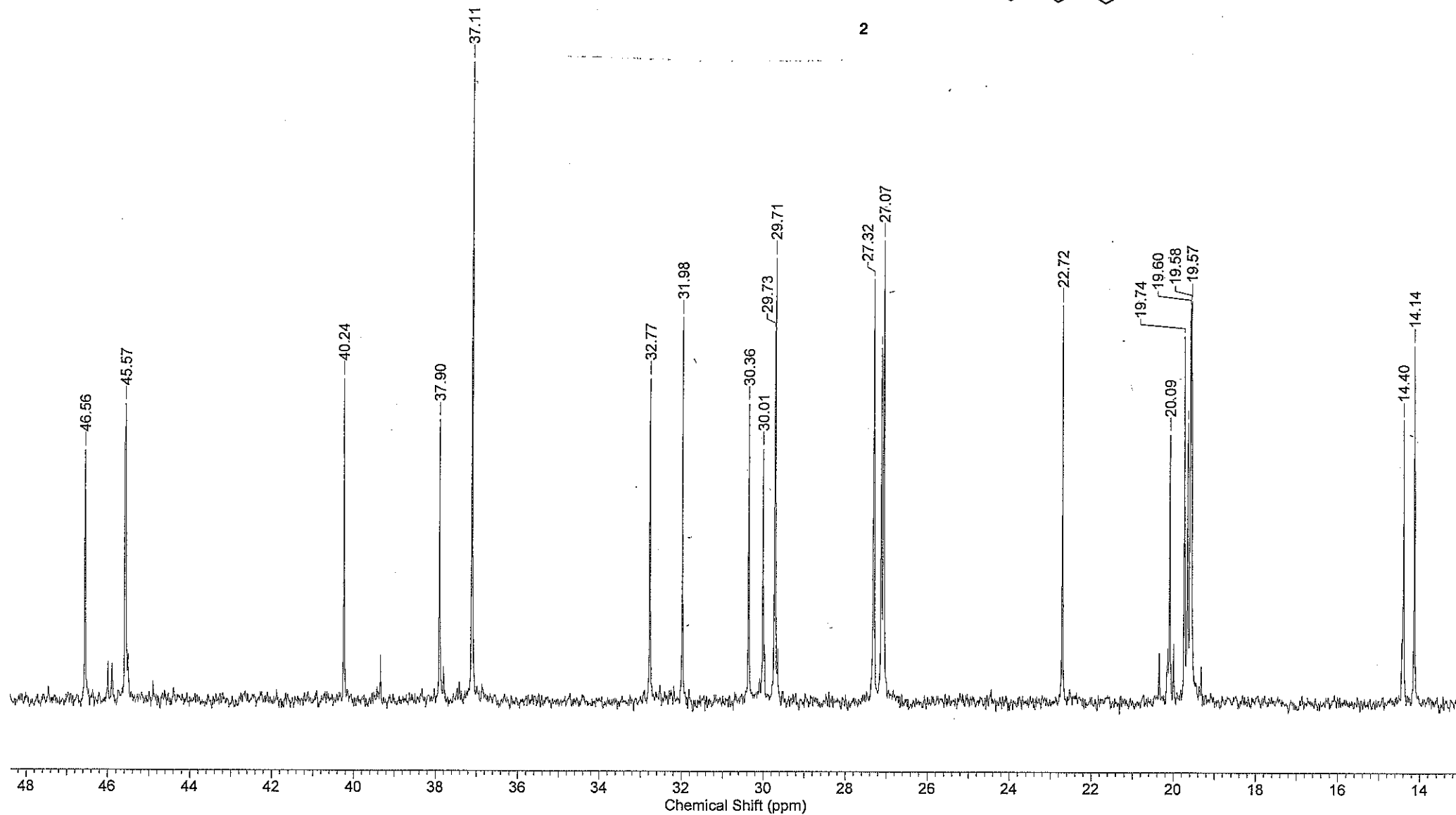
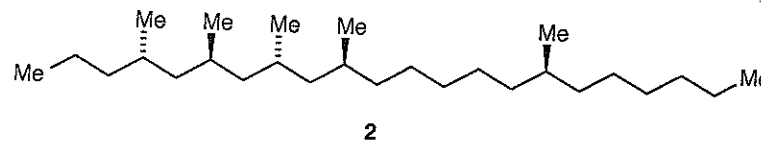


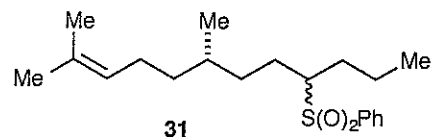
NAME 2010-11-23-ejt-39
EXPNO 10
PROCNO 1
Date_ 20101124
Time 2.43
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 13.38 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300486 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



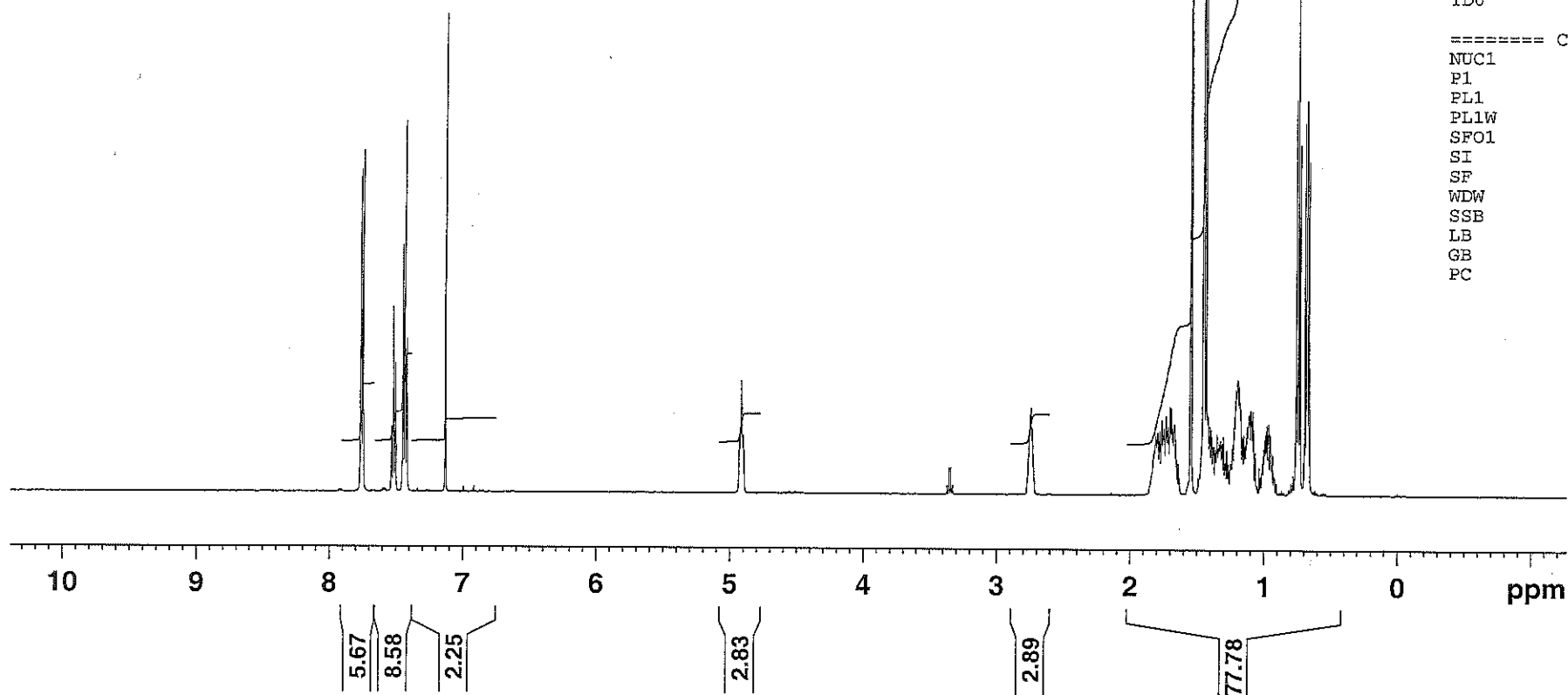
2010-11-25-Administrator-52.010.001.1r.esp



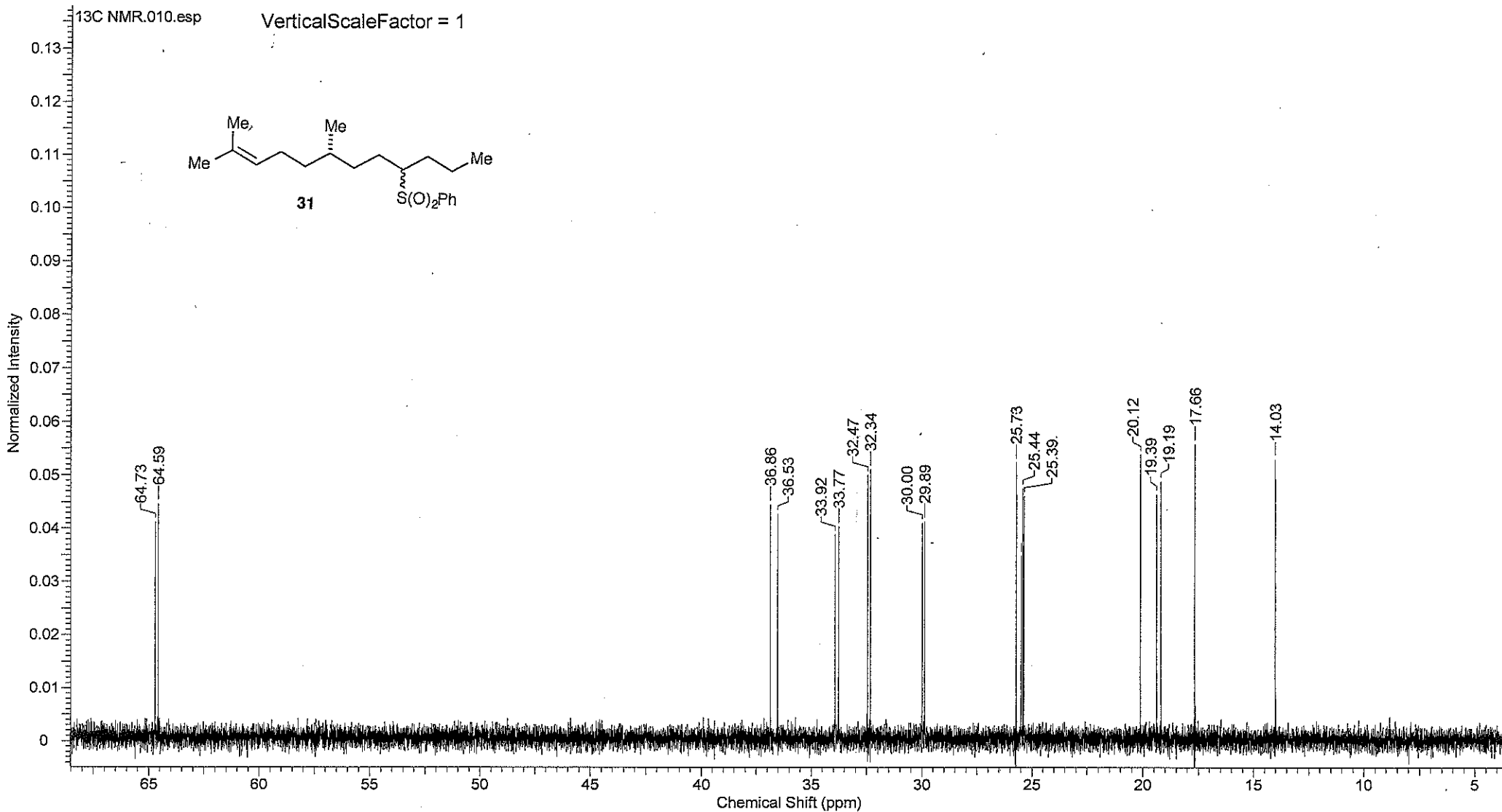


NAME 2011-02-15-ejt-8
EXPNO 10
PROCNO 1
Date_ 20110215
Time 16.17
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 287
DW 48.400 usec
DE 13.38 usec
TE 293.2 K
D1 1.0000000 sec
TD0 1

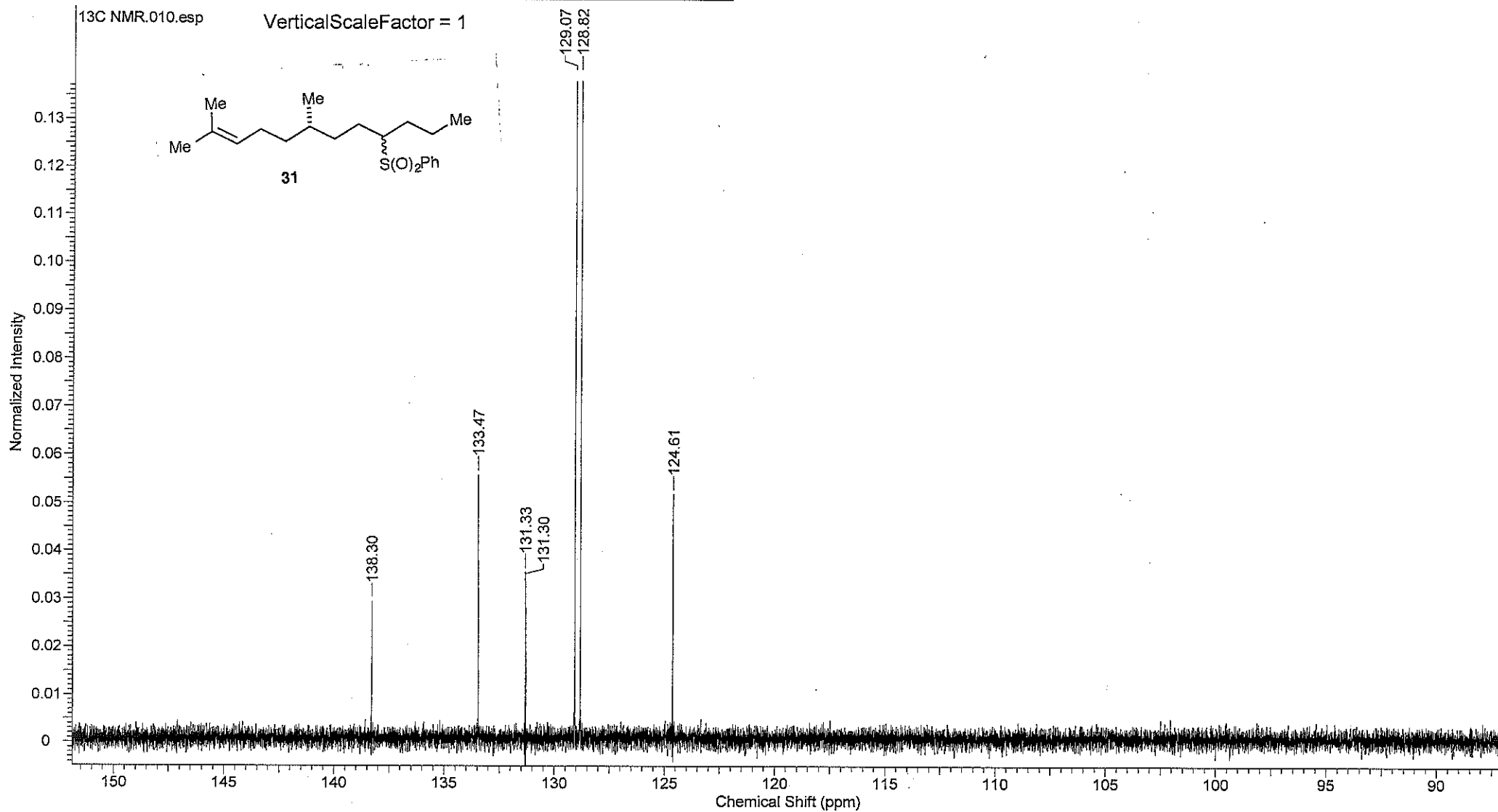
==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300773 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



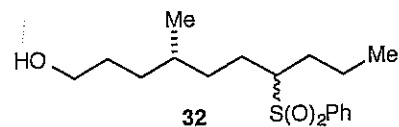
| | | | | | | | |
|------------------------|---|------------------------|---|----------------------|-----------------|-----------------------|----------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 0910-040 HL093-001 mCARBON CDCI3 (E:\bruk400service_data\2010\Sep) Administrator 56 | | | | |
| Date | 20 Sep 2010 11:57:04 | Date Stamp | 20 Sep 2010 11:57:04 | | | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL093 - Sulfone alkylation\HL093-001\13C NMR\10\fid | | | | Frequency (MHz) | 100.64 | |
| Nucleus | 13C | Number of Transients | 10240 | Origin | AV400_S | Original Points Count | 32768 |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 | Receiver Gain | 2050.00 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 | Spectrum Type | STANDARD |
| Sweep Width (Hz) | 24038.44 | Temperature (degree C) | 23.600 | | | | |



| | | | | | |
|------------------------|---|------------------------|---|----------------------|------------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 0910-040 HL093-001 mCARBON CDCl3 {E:\bruk400service_data\2010\Sep} Administrator 56 | | |
| Date | 20 Sep 2010 11:57:04 | Date Stamp | 20 Sep 2010 11:57:04 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL093 - Sulfone alkylation\HL093-001\13C NMR\10\fid | | | Frequency (MHz) | 100.64 |
| Nucleus | 13C | Number of Transients | 10240 | Origin | AV400_S |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24038.44 | Temperature (degree C) | 23.600 | Spectrum Type | STANDARD |

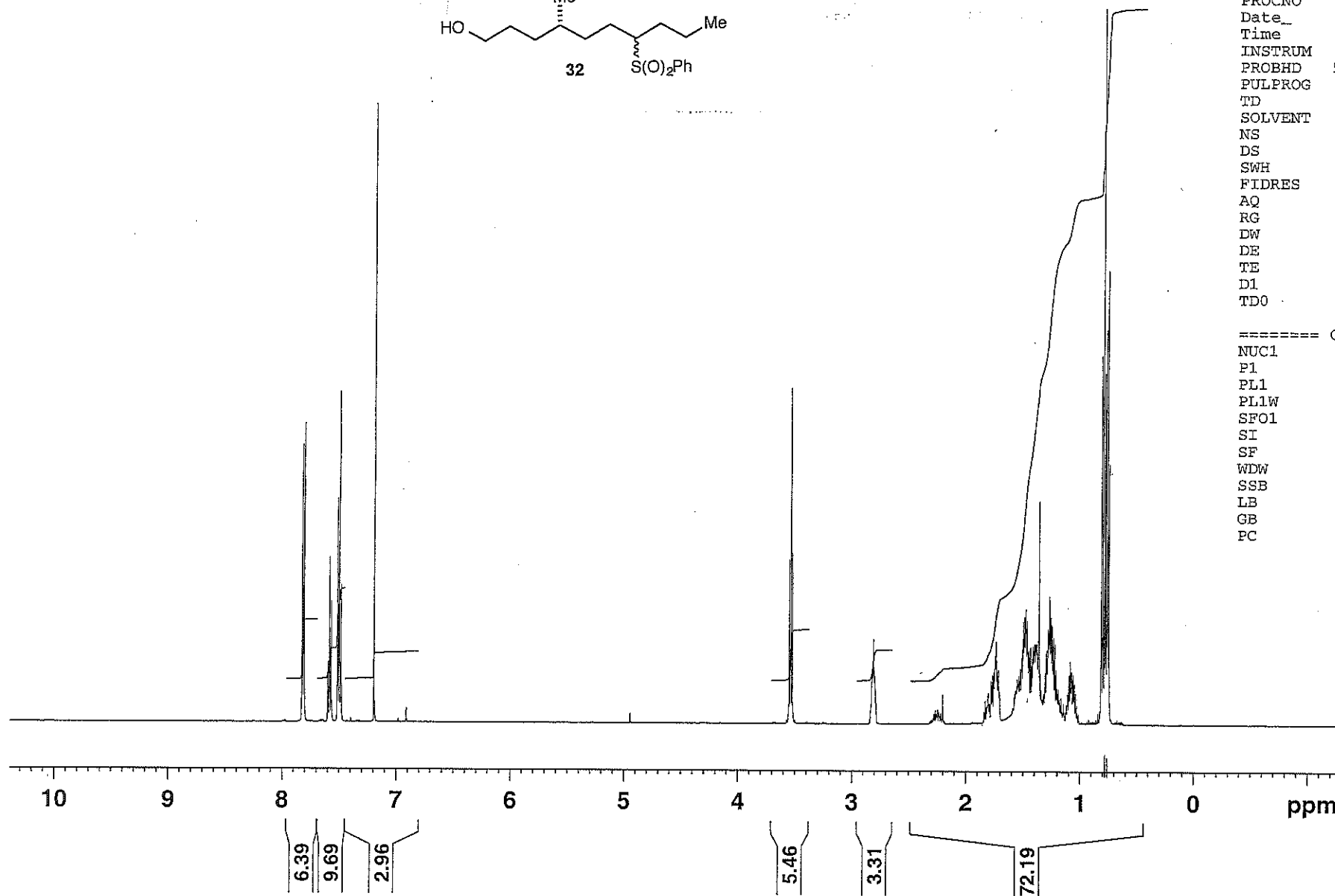


HL102-031
mPROTON CDCl3 /opt/bruk500data/2011/Feb ejt 5

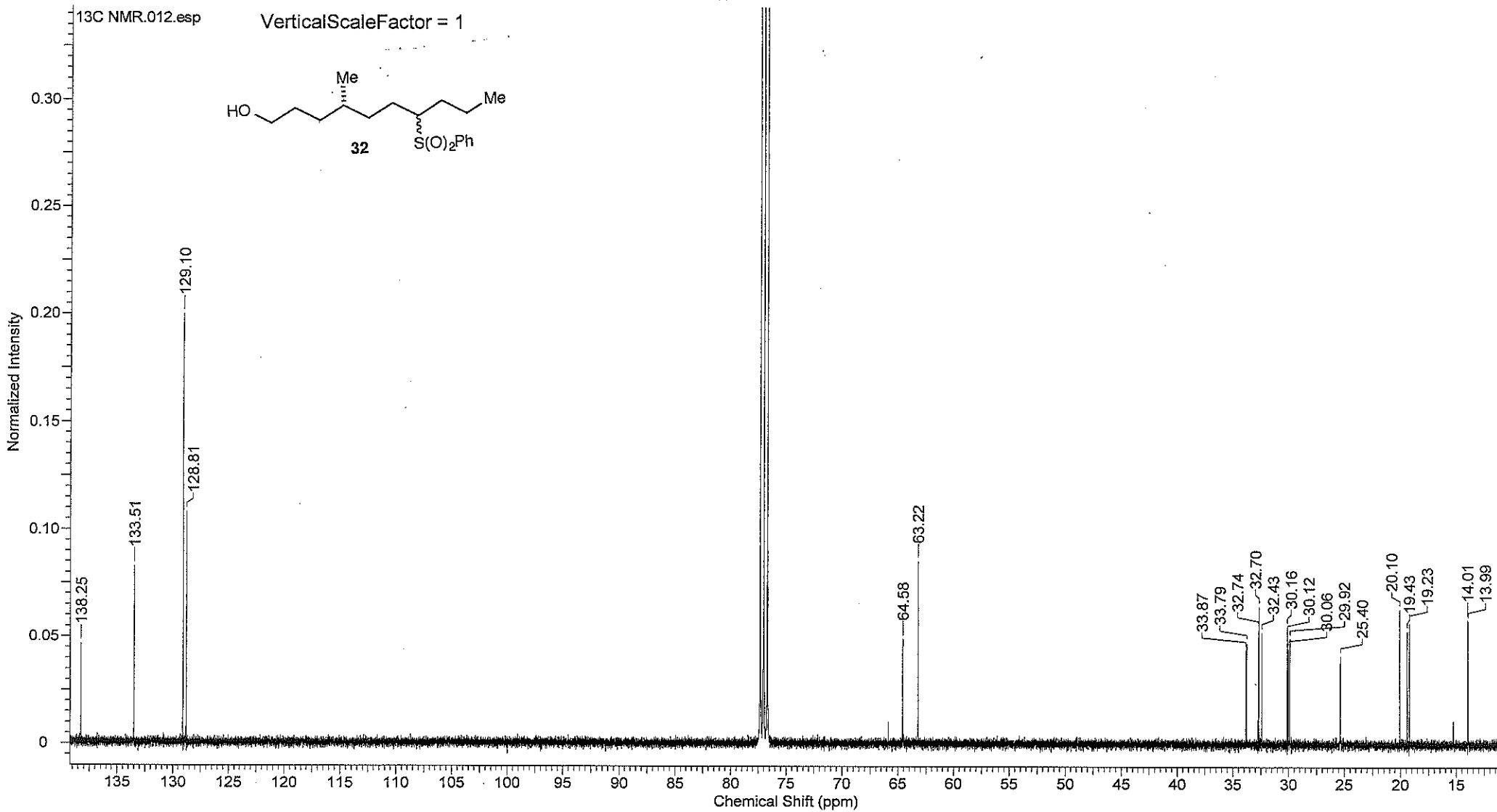


NAME 2011-02-23-ejt-5
EXPNO 10
PROCNO 1
Date_ 20110223
Time 9.31
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 322
DW 48.400 usec
DE 13.38 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

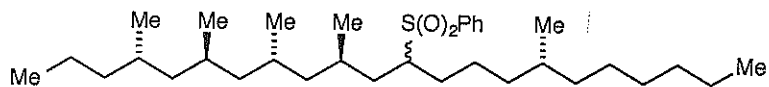
==== CHANNEL f1 =====
NUC1 1H
P1 8.20 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300469 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



| | | | | | |
|------------------------|---|------------------------|--|----------------------|------------|
| Acquisition Time (sec) | 1.3631 | Comment | Leo 0910-043 HI093-002 mCARBON CDCl3 {E:\bruk400service_data\2010\Sep} Administrator 8 | | |
| Date | 22 Sep 2010 15:17:36 | Date Stamp | 22 Sep 2010 15:17:36 | | |
| File Name | C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL093 - Sulfone alkylation\HL093-002\13C NMR\12\fid | | | Frequency (MHz) | 100.64 |
| Nucleus | 13C | Number of Transients | 12000 | Origin | AV400_S |
| Owner | Administrator | Points Count | 1048576 | Pulse Sequence | zgpg30 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10063.3350 |
| Sweep Width (Hz) | 24038.44 | Temperature (degree C) | 23.600 | Spectrum Type | STANDARD |



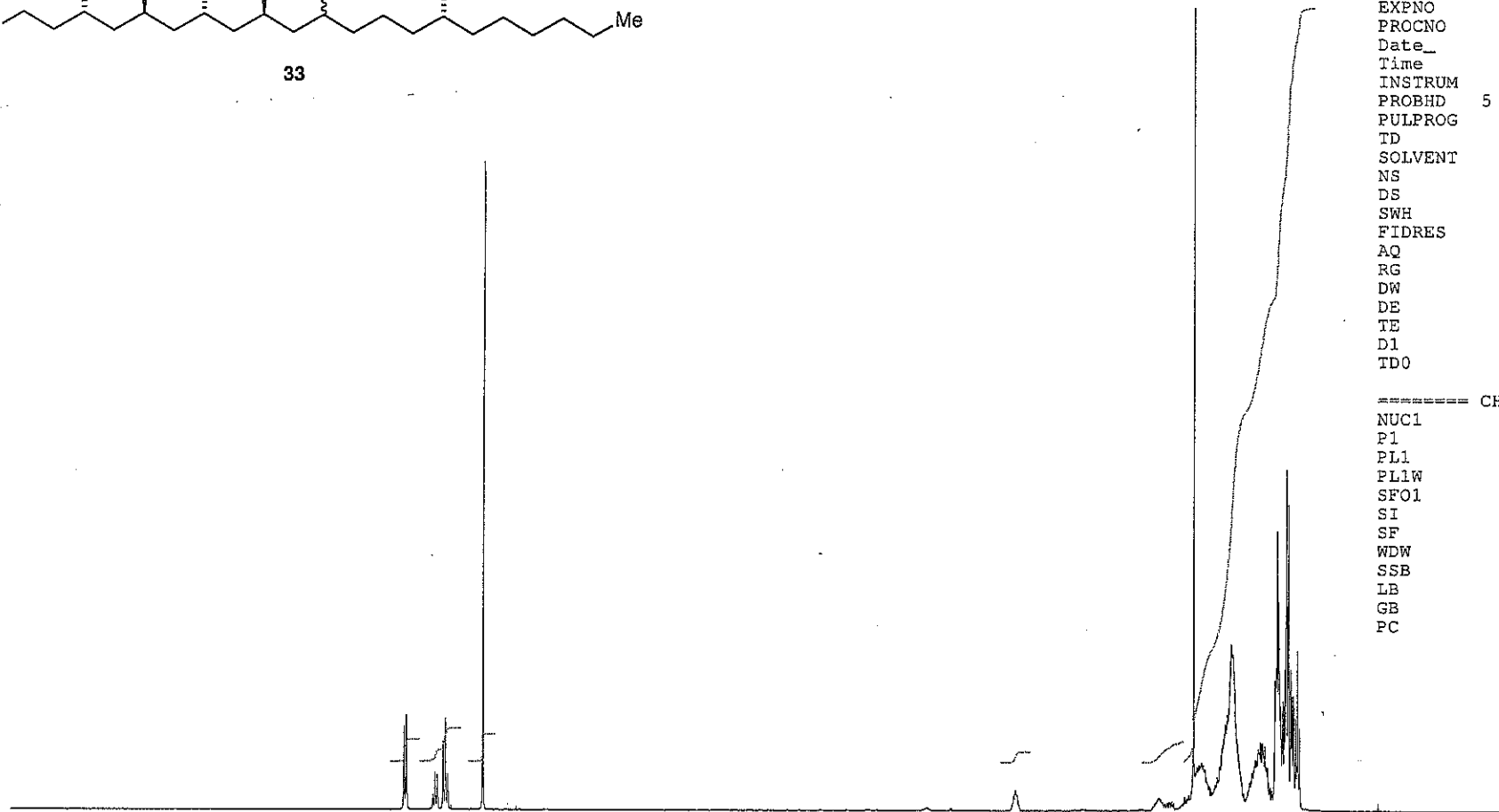
HL102-036
mPROTON CDCl3 {e:\bruk400data\2011\Feb} ejt 60



33

NAME 2011-02-03-ejt-60
EXPNO 10
PROCNO 1
Date_ 20110203
Time 9.24
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 362
DW 60.500 usec
DE 9.40 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

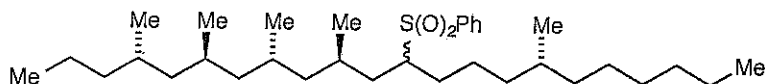
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300364 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm

2.49 3.78 3.11 1.17 2.51 96.94

H. Liu
 0211-003
 HL102-036
 mCARBON CDC13



33

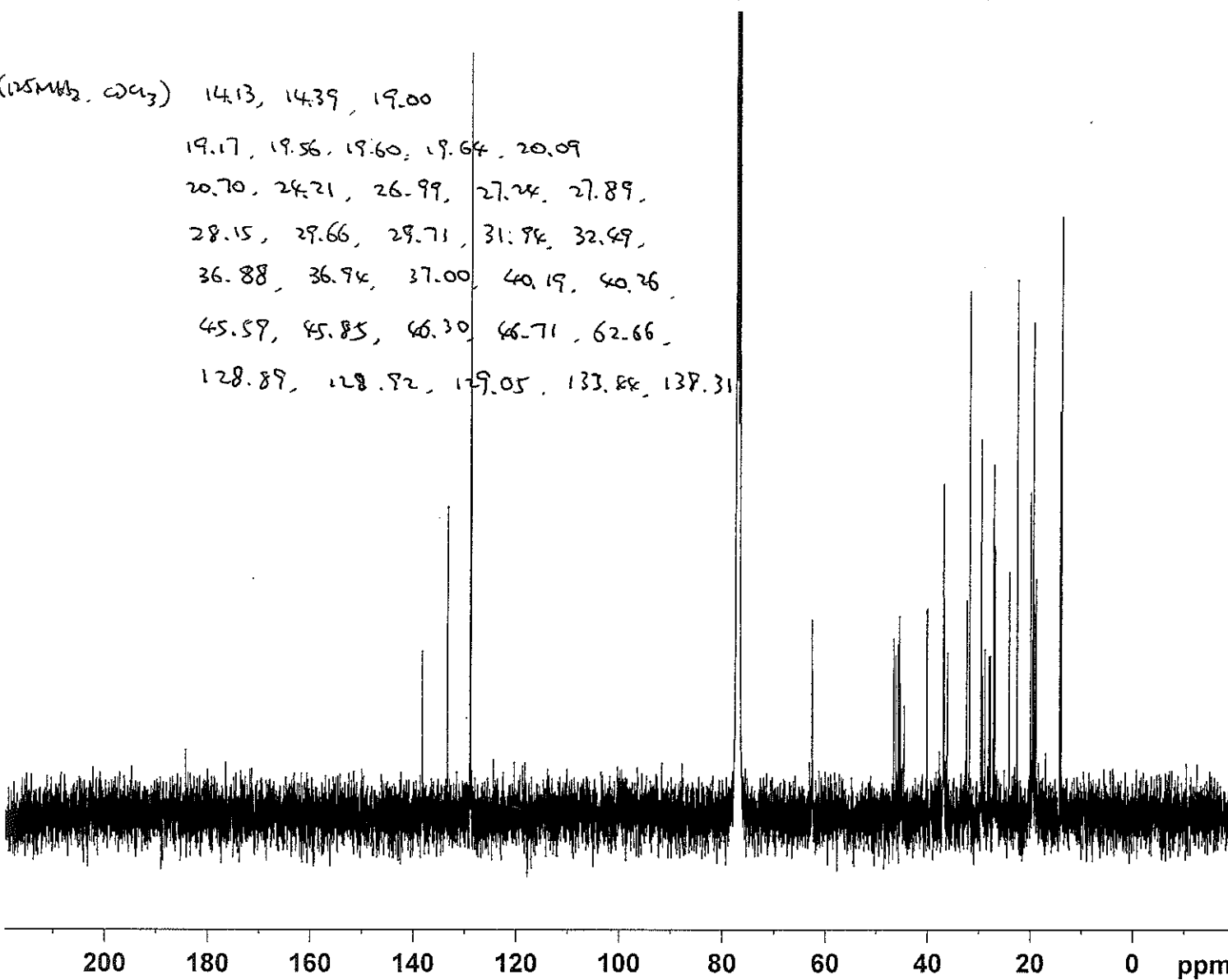
{E:\bruk400service_data\2011\Feb\ Administrator-18



2011-02-03-Administrator-18
 NAME
 EXPNO 10
 PROCNO 1
 Date_ 20110203
 Time_ 14.50
 INSTRUM AV400_S
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 16000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

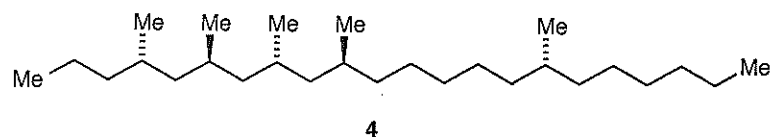
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 0.00 dB
 PL1W 33.91046524 W
 SFO1 100.6479773 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -3.60 dB
 PL12 15.31 dB
 PL13 18.00 dB
 PL2W 18.98951721 W
 PL12W 0.24406971 W
 PL13W 0.13137537 W
 SFO2 400.2316009 MHz
 SI 32768
 SF 100.6379140 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



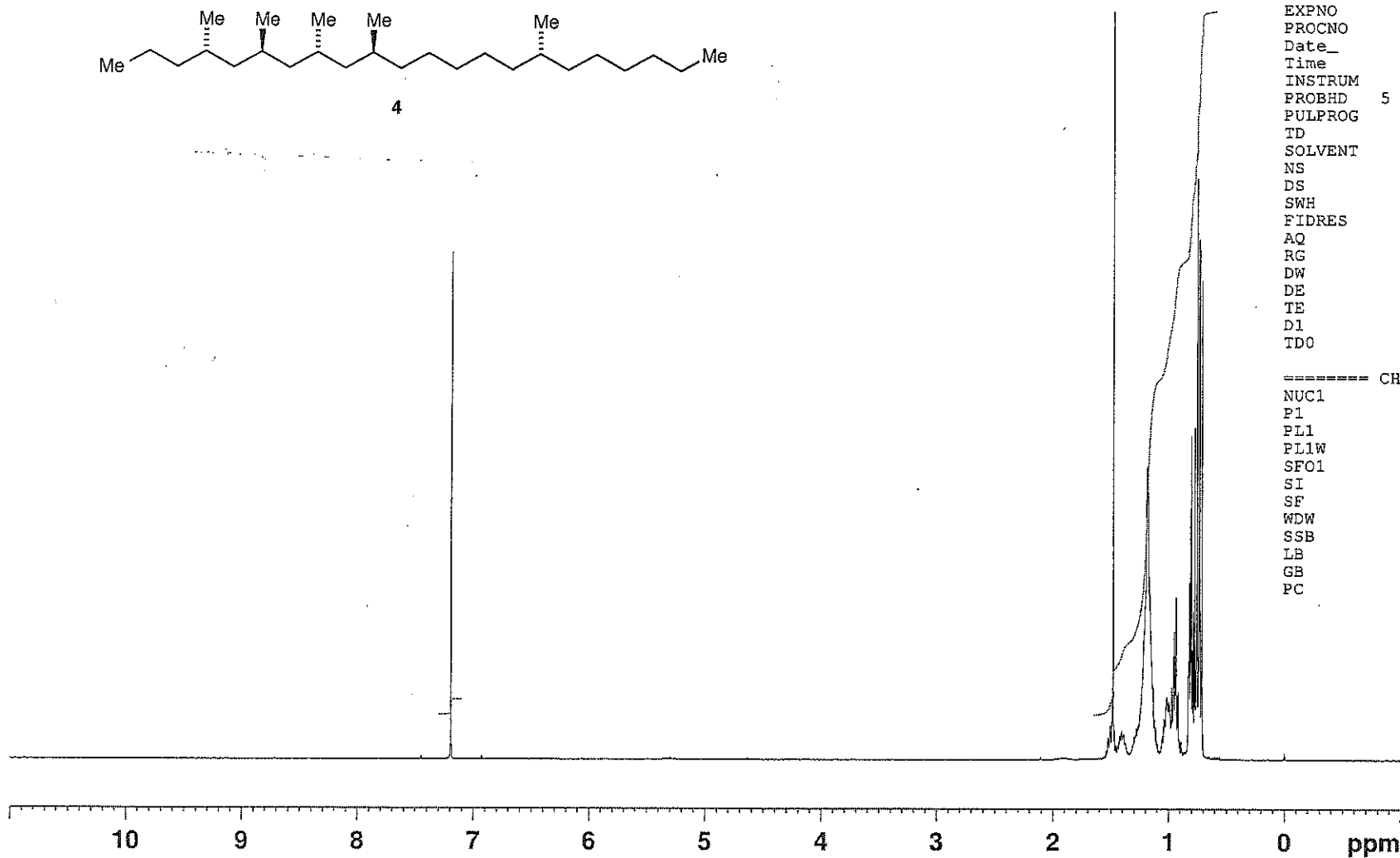
δ (125 MHz, CDCl₃) 14.13, 14.39, 19.00
 19.17, 19.56, 19.60, 19.64, 20.09
 20.70, 24.21, 26.99, 27.24, 27.89,
 28.15, 29.66, 29.71, 31.94, 32.49,
 36.88, 36.94, 37.00, 40.19, 40.26,
 45.59, 45.85, 46.30, 46.71, 62.66,
 128.89, 128.92, 129.05, 133.84, 138.31

HL101-006a
mPROTON CDCl3 {e:\bruk400data\2011\Feb} ejt 24

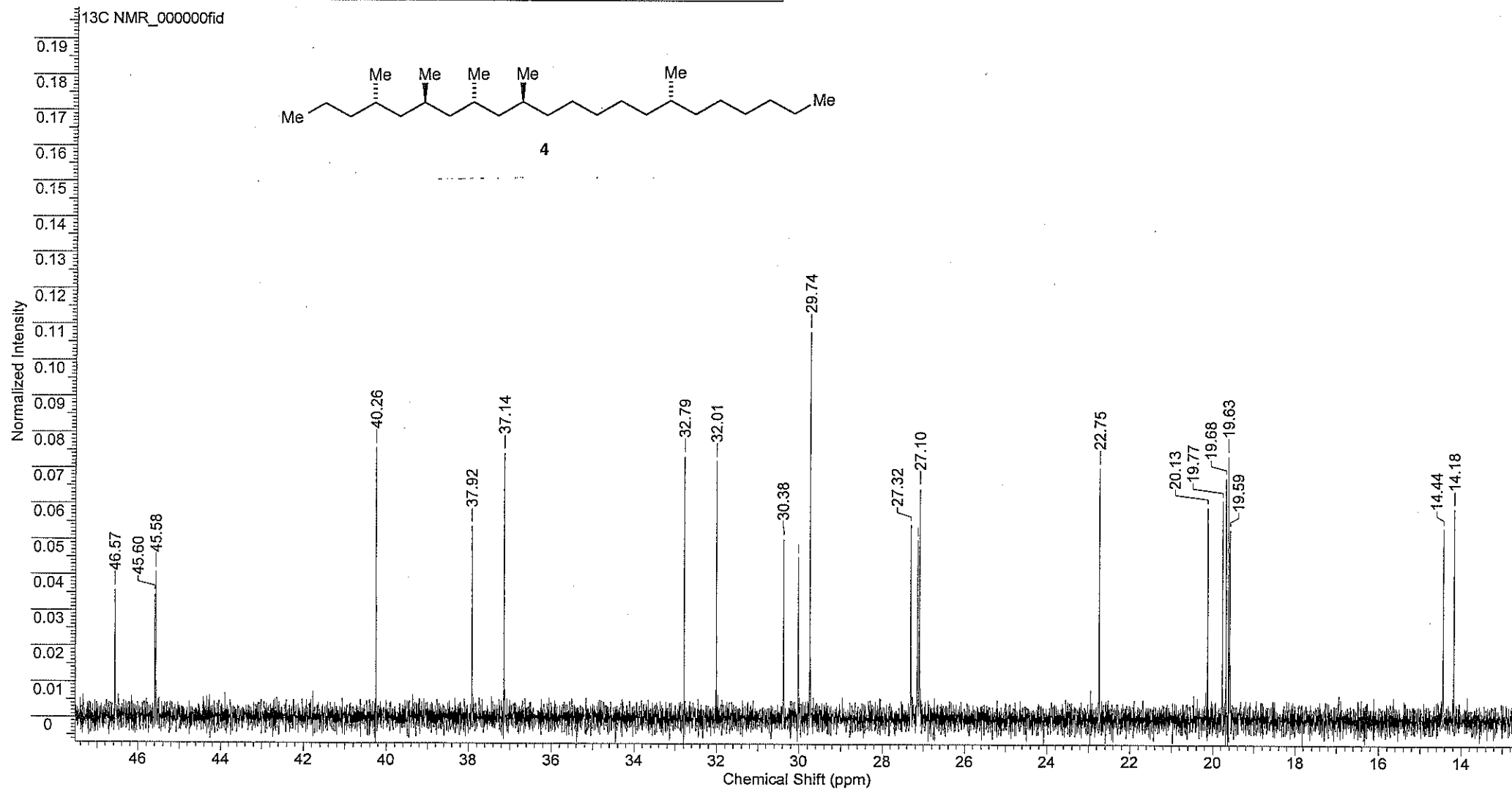


NAME 2011-02-04-ejt-24
EXPNO 10
PROCNO 1
Date_ 20110204
Time 14.46
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 362
DW 60.500 usec
DE 9.40 usec
TE 292.9 K
D1 1.00000000 sec
TDC 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300367 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



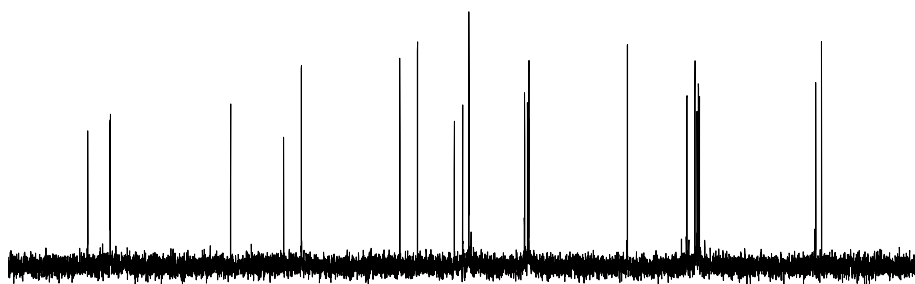
| | | | | | |
|------------------------|---|---|---|----------------------|---------------|
| Acquisition Time (sec) | 1.3631 | Comment | H. Liu 0211-009 HL101-006a mCARBON CDCl3 {E:\bruk400service_data\2011\Feb} Administrator 54 | | |
| Date | 13 Feb 2011 11:18:24 | Date Stamp | 13 Feb 2011 11:18:24 | | |
| File Name | E:\Postgraduate Database\Experiment Database\Experiment 101-150\HL101 - Natural | Product diastereomer synthesis\HL101-006a\13C NMR\13C NMR_000000fid | | | |
| Frequency (MHz) | 100.65 | Nucleus | 13C | Number of Transients | 12288 |
| Origin | AV400_S | Original Points Count | 32768 | Owner | Administrator |
| Points Count | 131072 | Pulse Sequence | zgpg30 | Receiver Gain | 2050.00 |
| SW(cyclical) (Hz) | 24038.46 | Solvent | CHLOROFORM-d | Spectrum Offset (Hz) | 10065.5420 |
| Sweep Width (Hz) | 24038.28 | Temperature (degree C) | 22.500 | | |



E:\Postgraduate Database\Experiment Database\Experiment 101-150\HL101 - Natural Product diastereomer synthesis\HL101-006a\13C NMR\13C NMR_000000fid

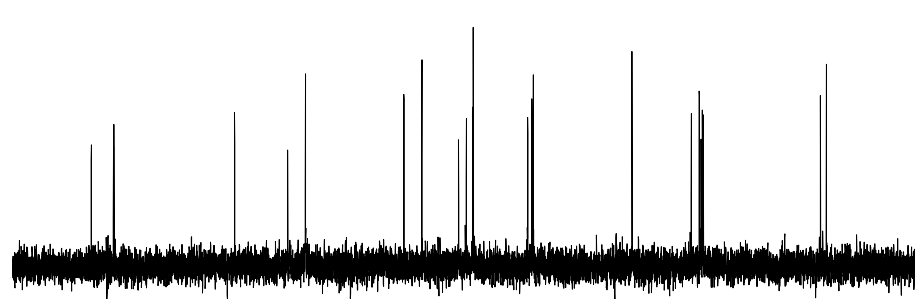
46.5057
 45.5251
 45.5084
 40.2022
 37.8688
 37.0859
 37.0795
 32.7401
 31.9614
 30.3366
 29.9641
 29.6975
 29.6805
 27.2409
 27.2354
 27.1081
 27.0643
 27.0450
 22.7028
 20.0772
 19.7233
 19.6310
 19.5696
 19.5388
 19.5230
 14.3959
 14.1389

A1 (2 at 293 K)



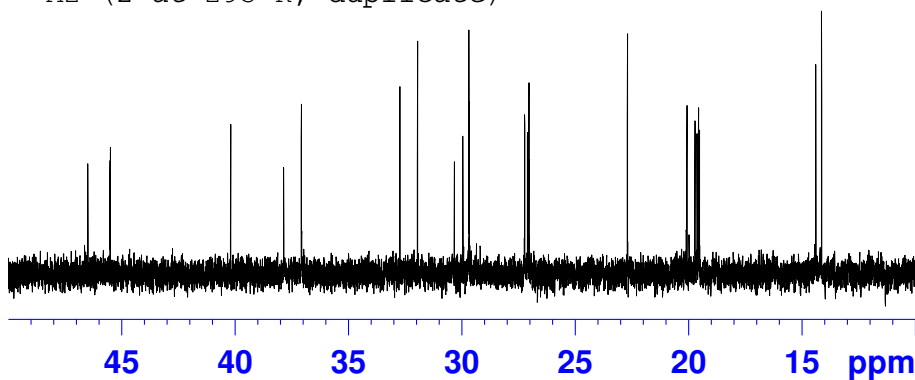
46.5411
 45.5642
 45.5470
 40.2204
 37.8820
 37.0968
 37.0913
 32.7535
 31.9608
 30.3427
 29.9988
 29.7143
 29.6953
 27.2977
 27.2922
 27.1091
 27.0629
 27.0477
 22.6970
 20.0768
 19.7266
 19.6481
 19.5874
 19.5660
 19.5507
 14.3836
 14.1192

A3 (2 at 298 K)



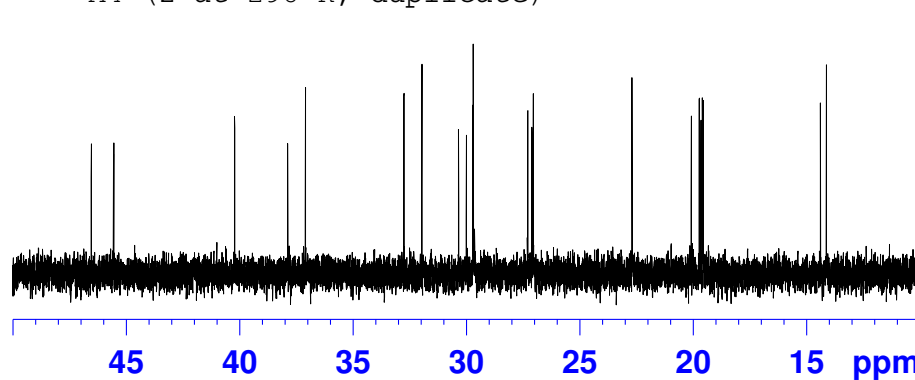
46.5038
 45.5233
 45.5065
 40.2003
 37.8665
 37.0836
 37.0776
 32.7381
 31.9595
 30.3344
 29.9621
 29.6956
 29.6786
 27.2387
 27.2334
 27.1061
 27.0622
 27.0432
 22.7011
 20.0753
 19.7213
 19.6289
 19.5676
 19.5363
 19.5209
 14.3941
 14.1372

A2 (2 at 293 K, duplicate)



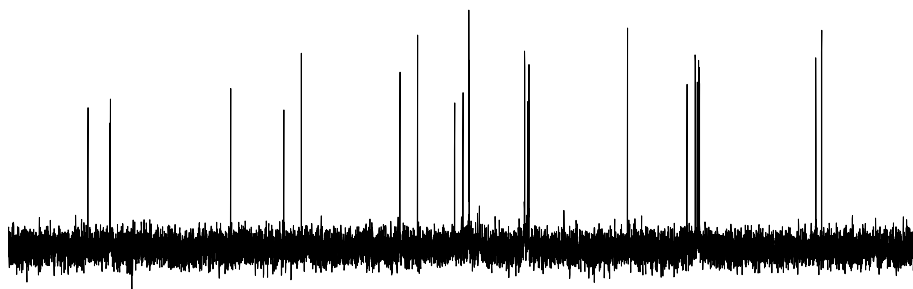
46.5404
 45.5633
 45.5463
 40.2199
 37.8814
 37.0965
 37.0910
 32.7530
 31.9605
 30.3422
 29.9983
 29.7135
 29.6951
 27.2971
 27.2913
 27.1088
 27.0629
 27.0476
 22.6969
 20.0767
 19.7263
 19.6477
 19.5871
 19.5655
 19.5502
 14.3834
 14.1195

A4 (2 at 298 K, duplicate)



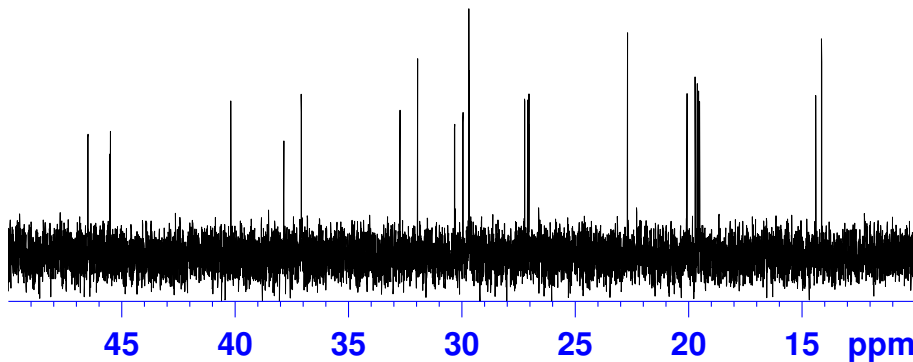
46.4975
 45.5304
 45.5050
 40.1959
 37.8574
 37.0855
 37.0772
 32.7330
 31.9555
 30.3228
 29.9552
 29.6915
 29.6755
 27.2359
 27.2302
 27.0971
 27.0573
 27.0414
 22.6980
 20.0720
 19.7112
 19.6208
 19.5649
 19.5348
 19.5182
 14.3916
 14.1347

B1 (4 at 293 K)



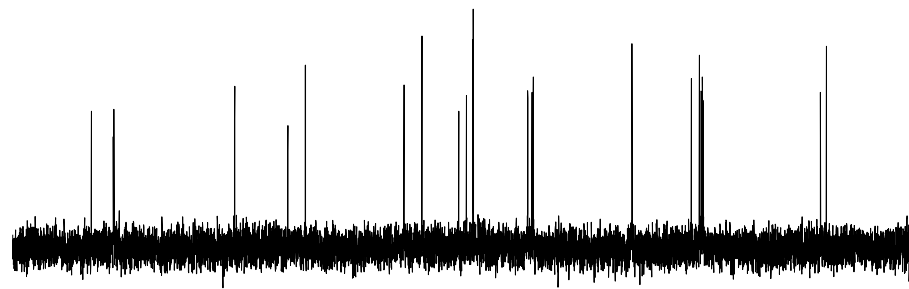
46.4994
 45.5330
 45.5066
 40.1982
 37.8594
 37.0871
 37.0794
 32.7348
 31.9573
 30.3243
 29.9569
 29.6936
 29.6773
 27.2381
 27.2322
 27.0989
 27.0586
 27.0433
 22.6996
 20.0737
 19.7130
 19.6225
 19.5668
 19.5362
 19.5199
 14.3933
 14.1361

B2 (4 at 293 K, duplicate)



46.5362
 45.5723
 45.5465
 40.2179
 37.8753
 37.1003
 37.0922
 32.7498
 31.9587
 30.3324
 29.9932
 29.7125
 29.6937
 27.2970
 27.2901
 27.1025
 27.0606
 27.0481
 22.6961
 20.0756
 19.7187
 19.6419
 19.5863
 19.5655
 19.5495
 14.3831
 14.1192

B3 (4 at 298 K)



46.5366
 45.5728
 45.5471
 40.2180
 37.8751
 37.1005
 37.0923
 32.7499
 31.9585
 30.3324
 29.9937
 29.7129
 29.6932
 27.2974
 27.2908
 27.1022
 27.0602
 27.0478
 22.6958
 20.0755
 19.7184
 19.6417
 19.5862
 19.5657
 19.5496
 14.3828
 14.1187

B4 (4 at 298 K, duplicate)

