

–Supporting Information for–

**Systematic comparison of sets of  $^{13}\text{C}$  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**

<sup>1</sup>H and <sup>13</sup>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<sub>2</sub>.

## **Experimental information for NMR spectra**

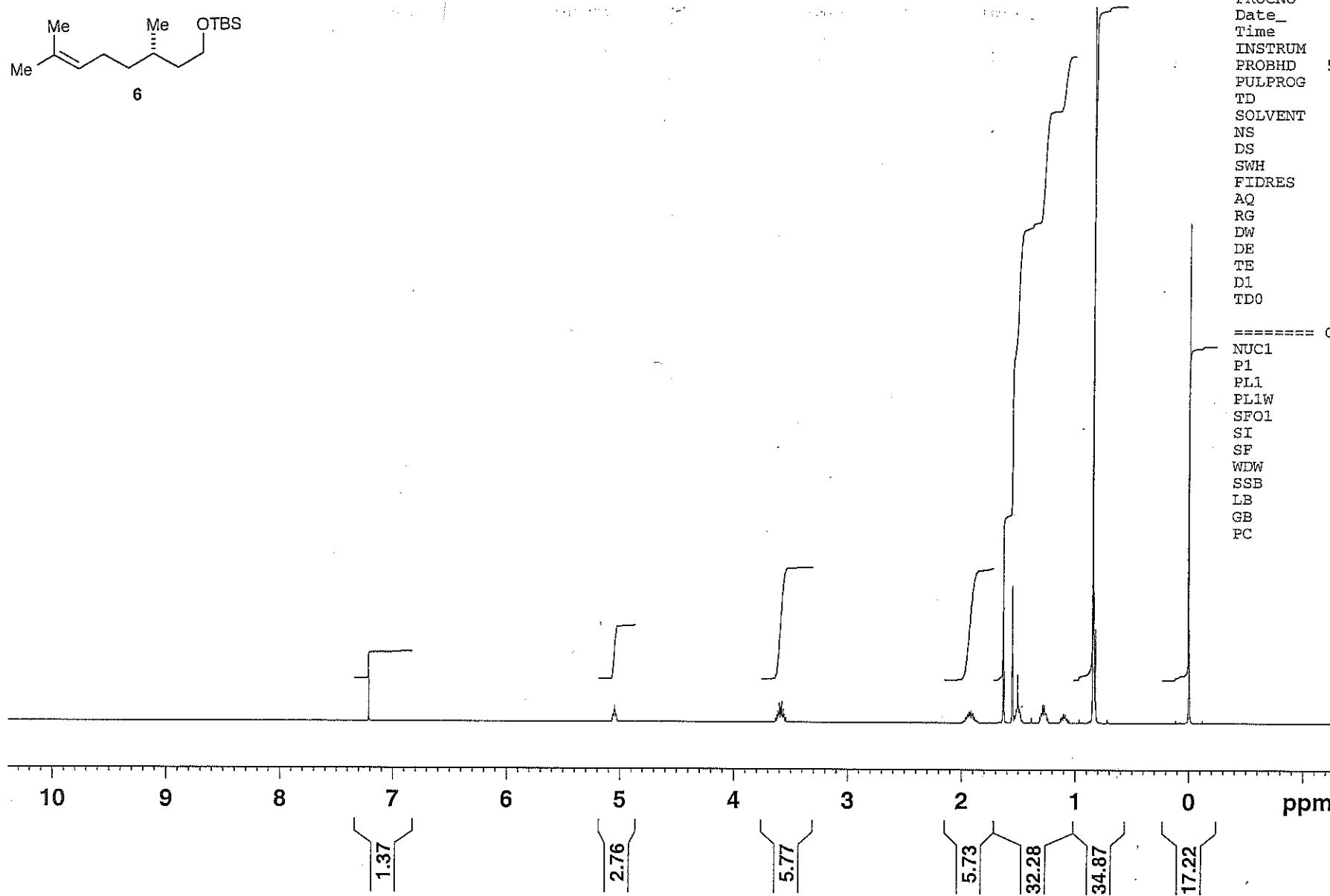
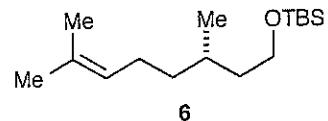
All the  $^{13}\text{C}$  NMR data that were used for the analysis were collected on a 700 MHz NMR spectrometer at  $^{13}\text{C}$  frequency of 176.03 MHz. The sample temperature was maintained at 293 or 298K at a precision of  $\pm 0.1\text{K}$  using a temperature controller. The samples were equilibrated 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. Traficante apodization function was used with a lb value of 0.4 Hz to improve resolution further. Line widths at half height of the  $^{13}\text{C}$  NMR peaks range from 0.7 to 1Hz. For samples 2 and 4,  $^{13}\text{C}$  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  $^{13}\text{C}$  NMR experiment is not necessarily the same as the temperature of the probe (the radiofrequency irradiation used for broadband  $^1\text{H}$  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  $\pm 1$  °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.

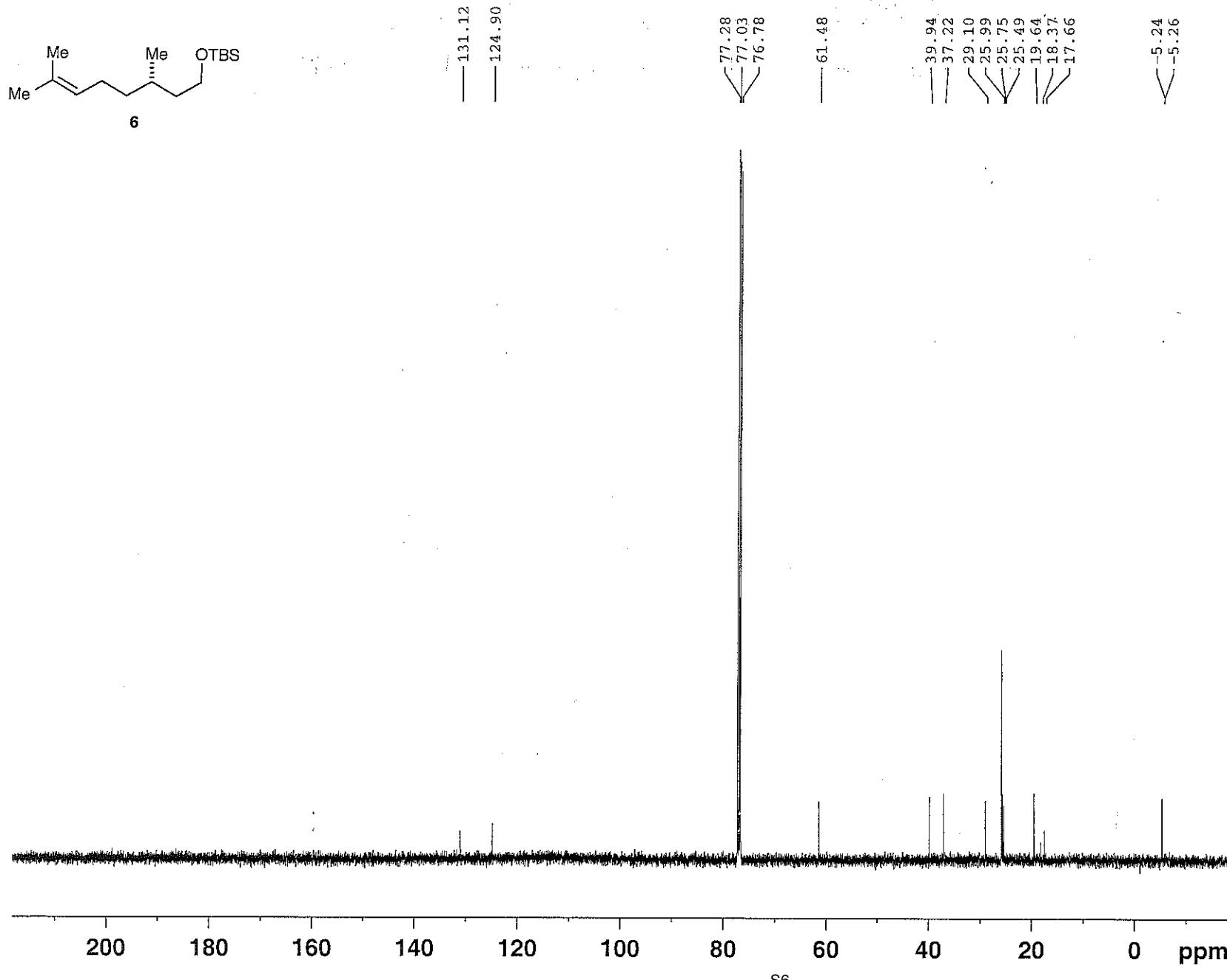
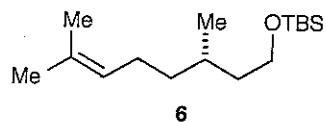
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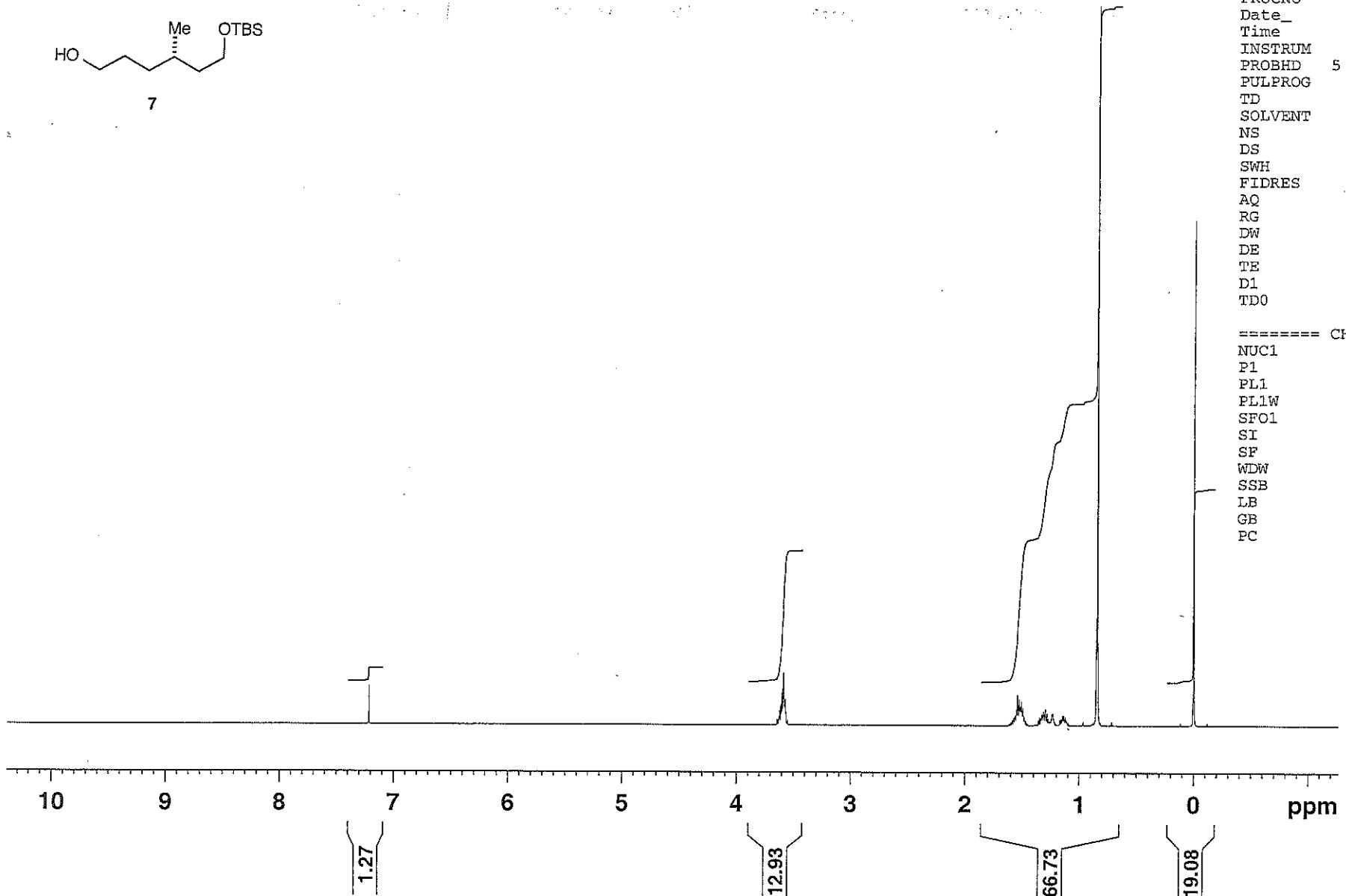
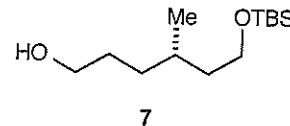
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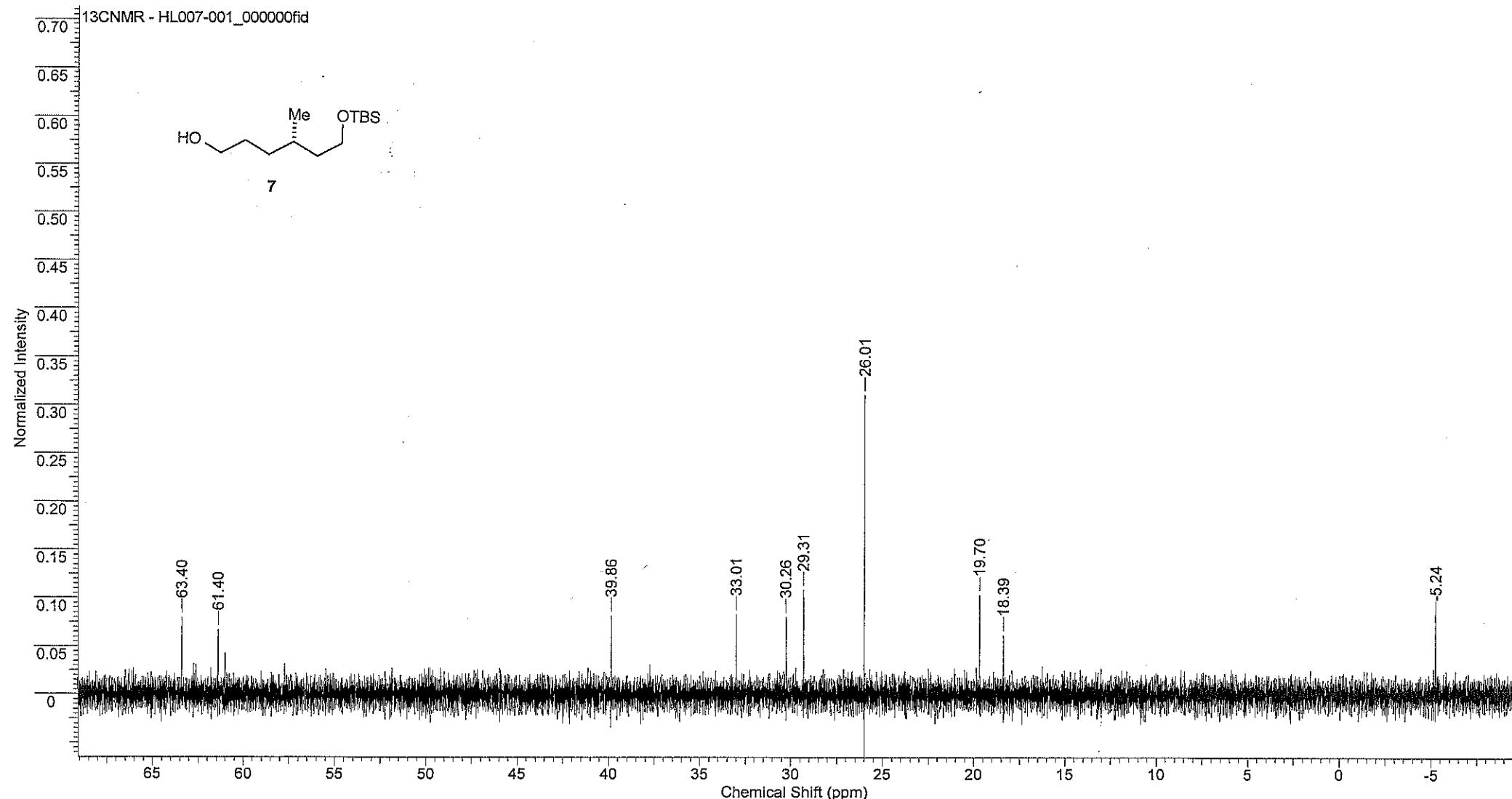
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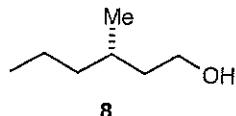
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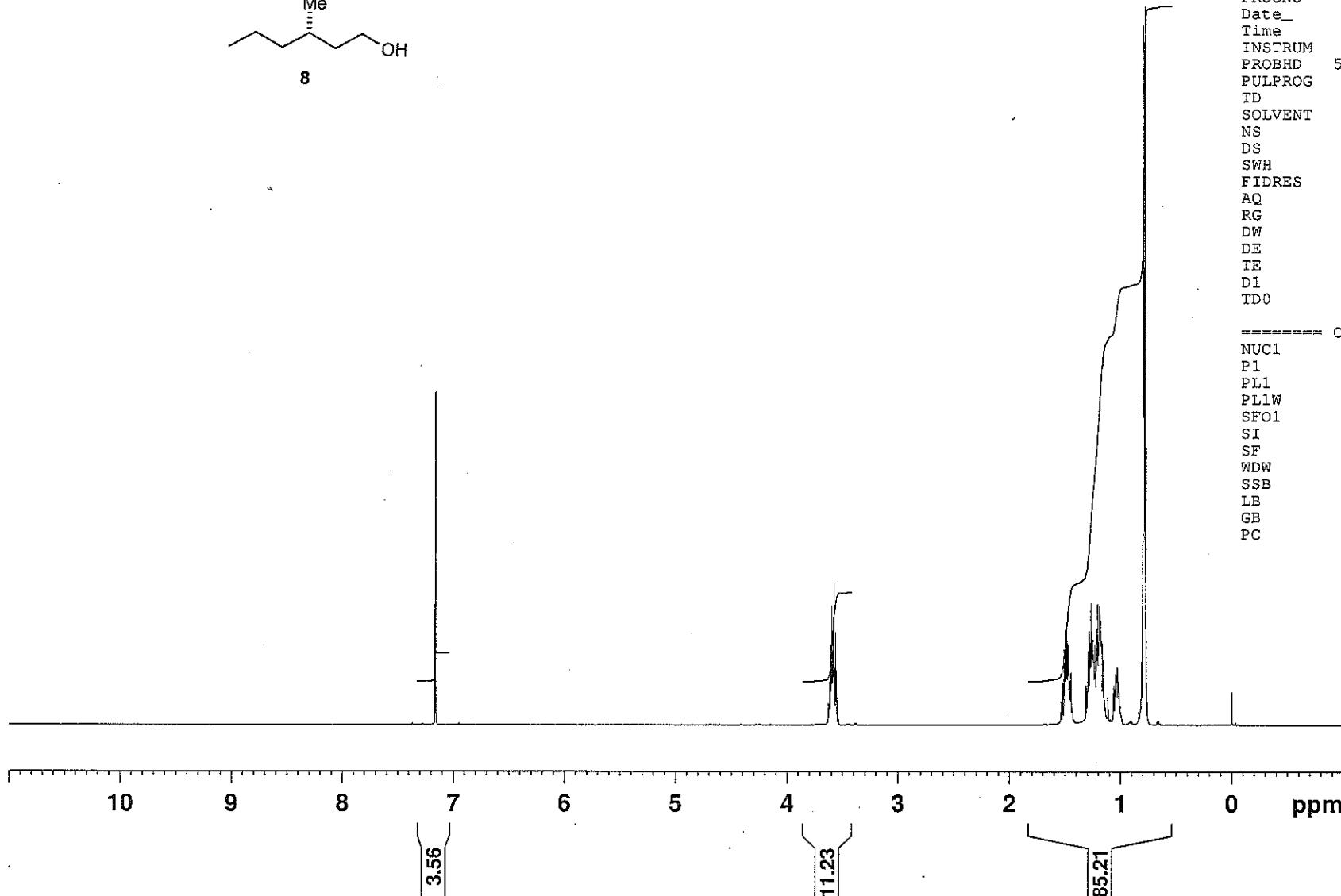
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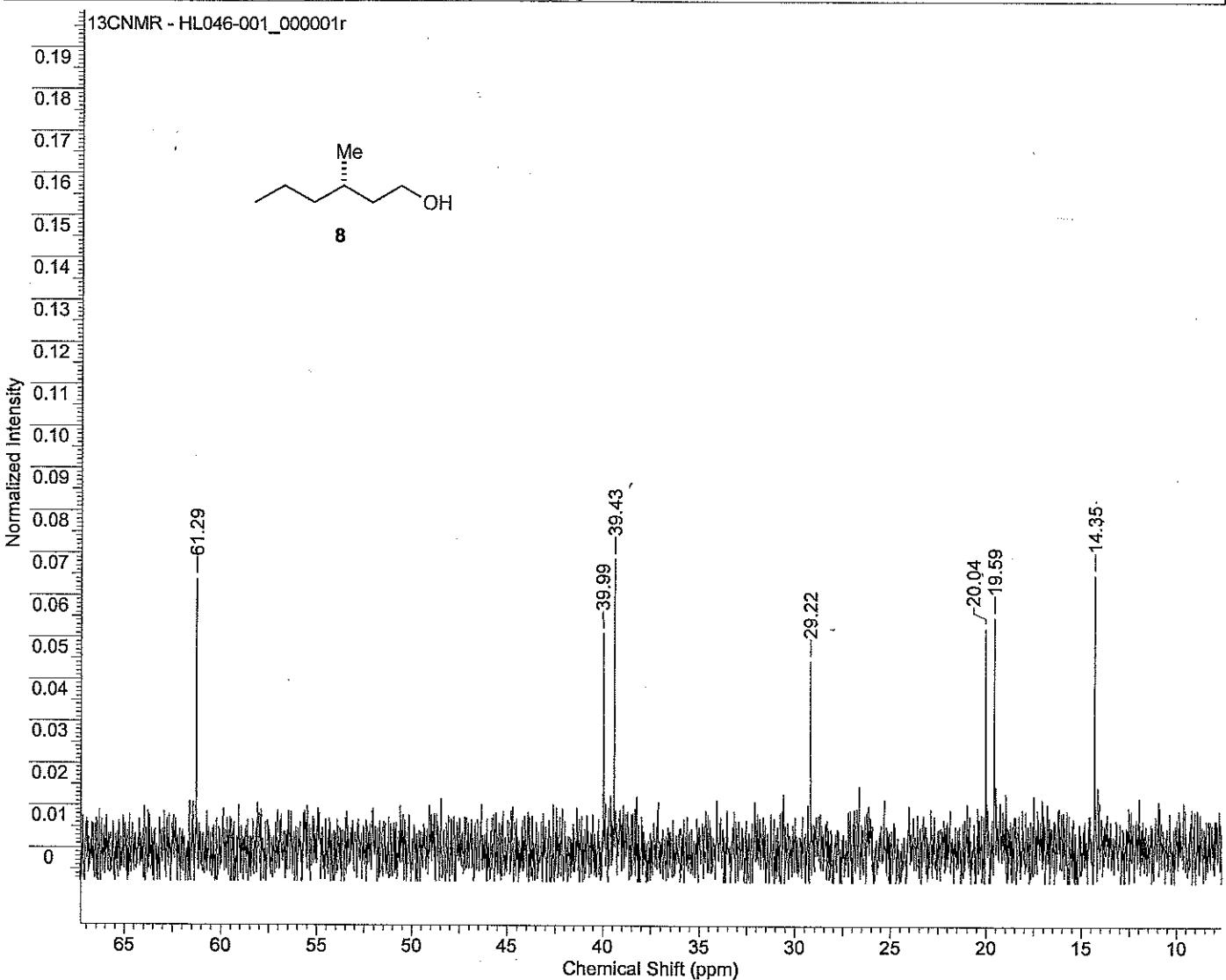


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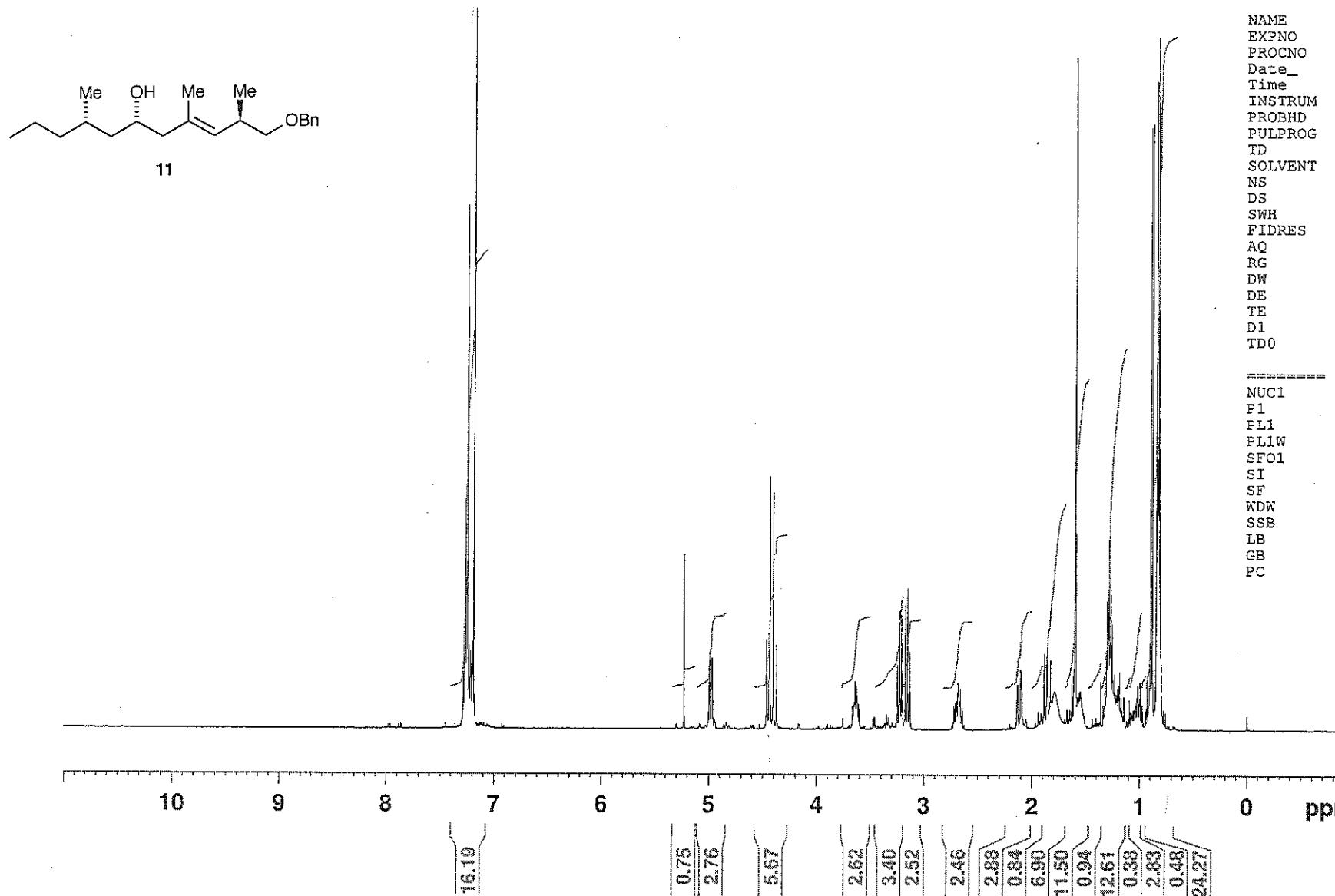
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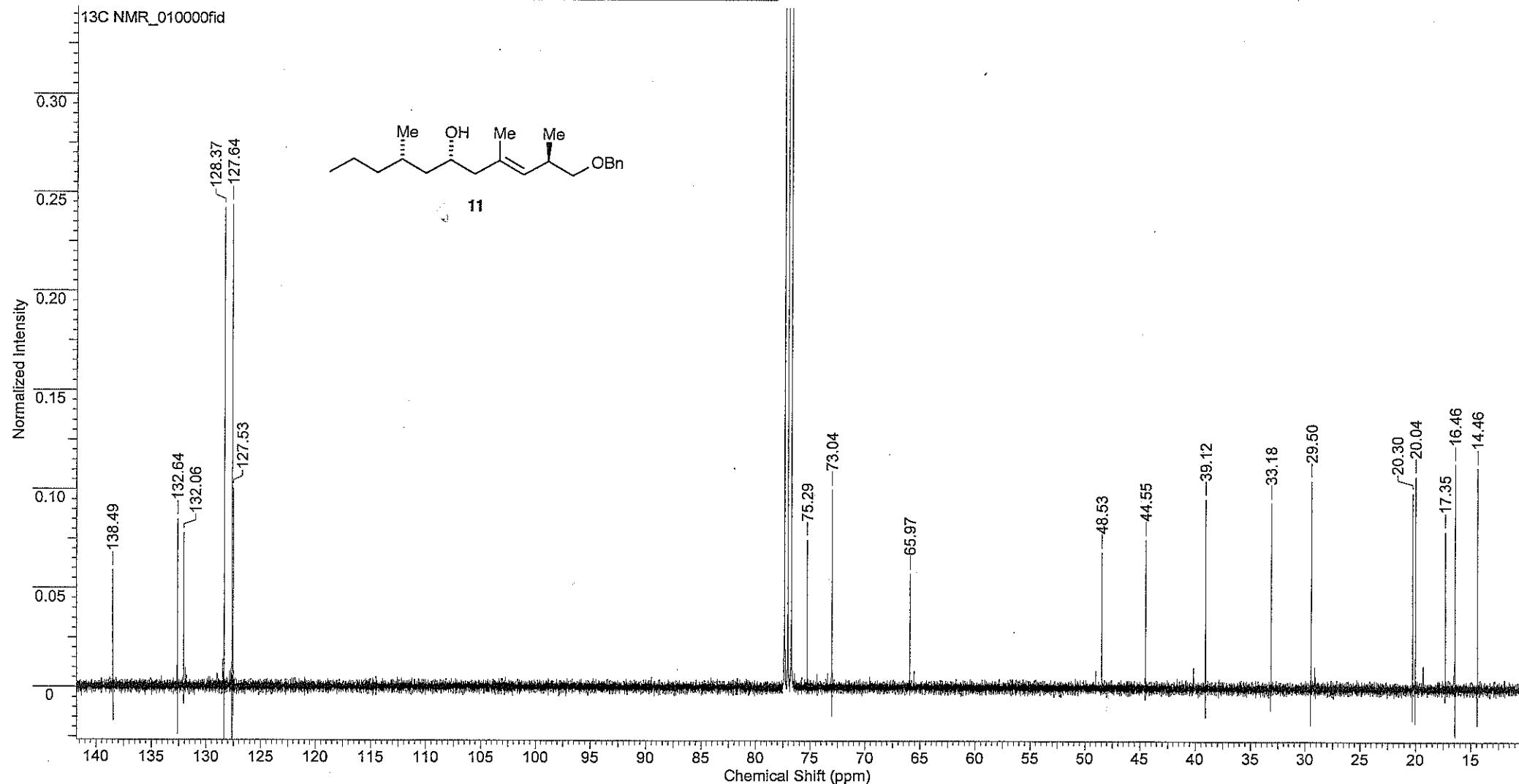
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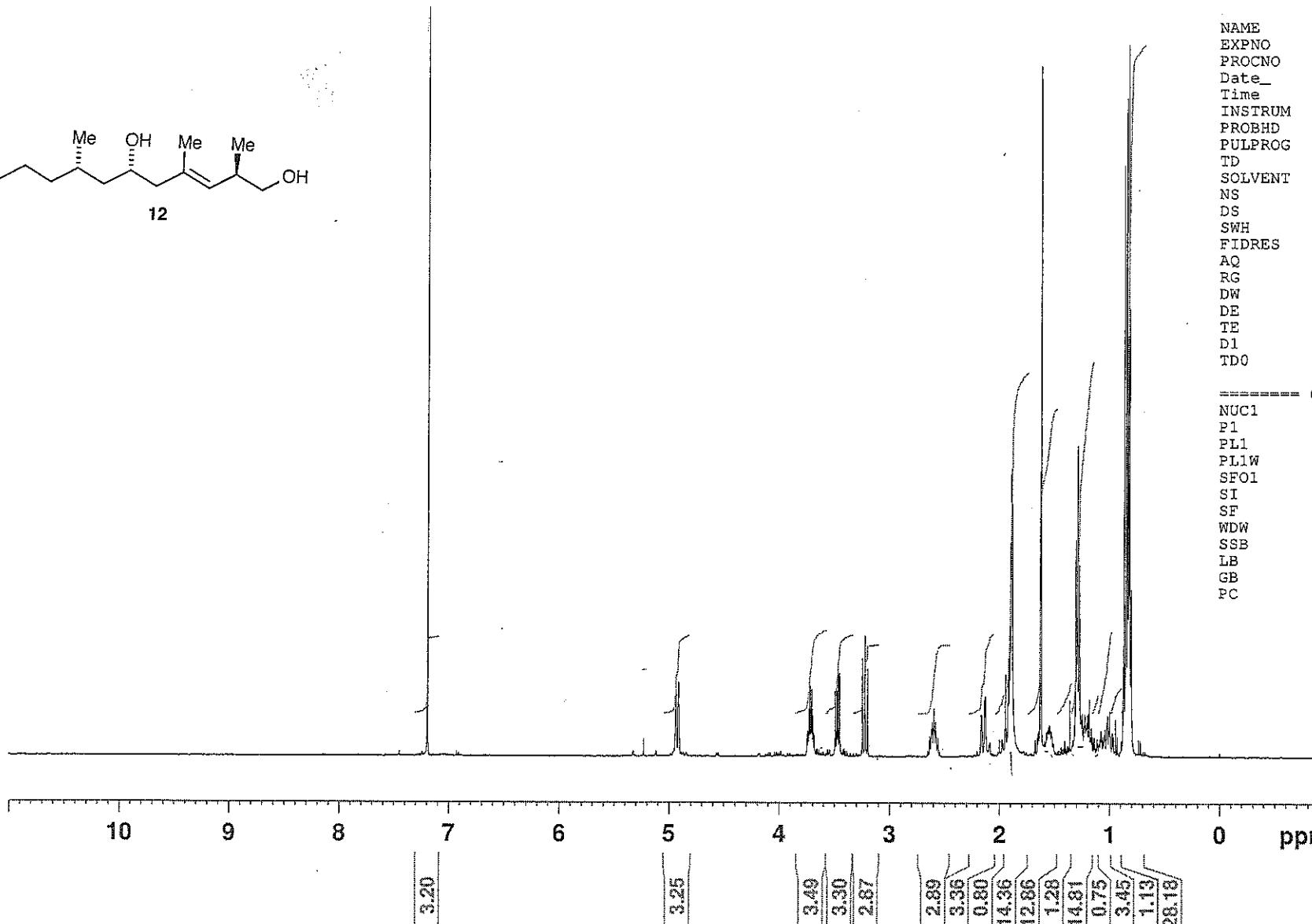
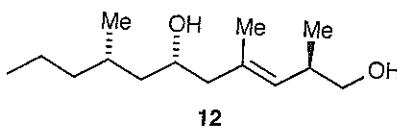
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HL089-001  
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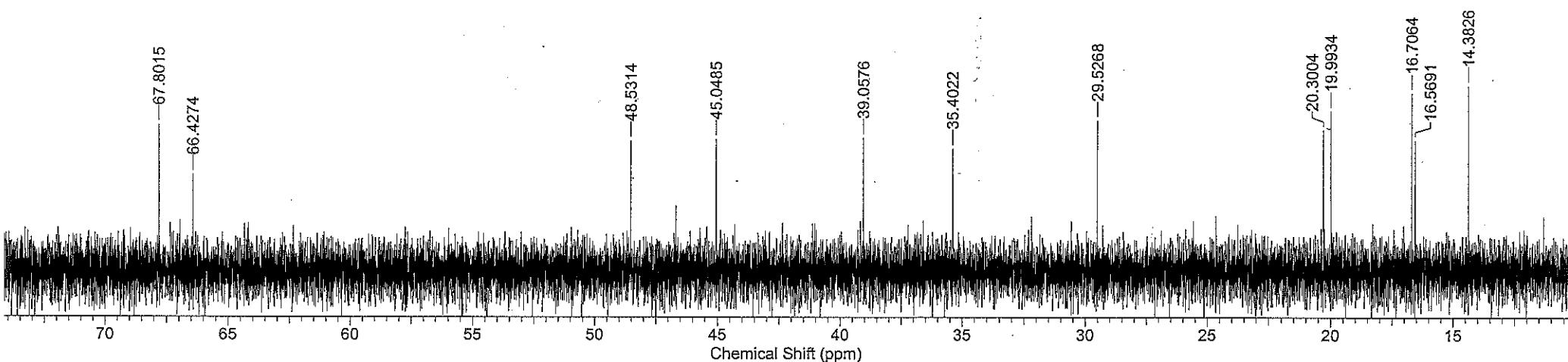
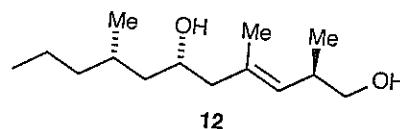


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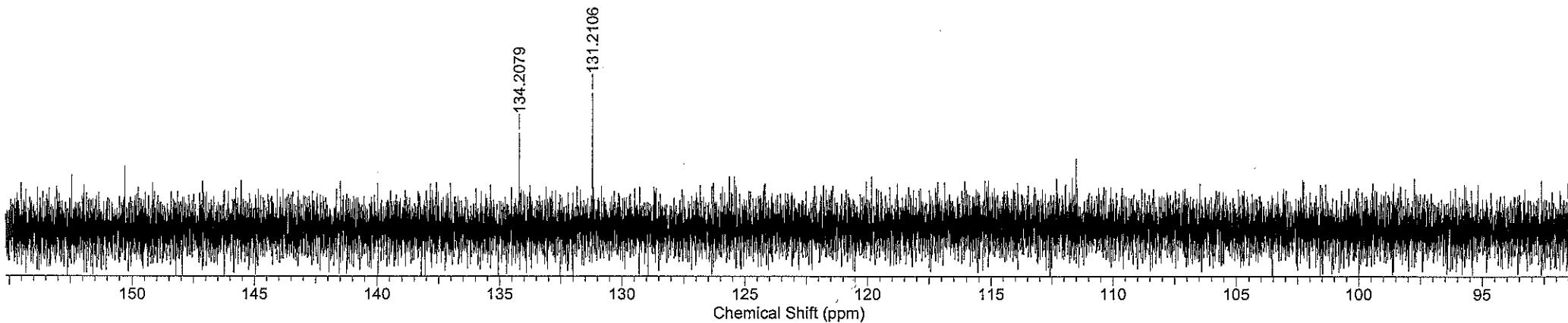
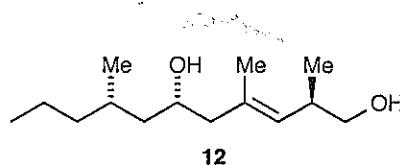
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ejt

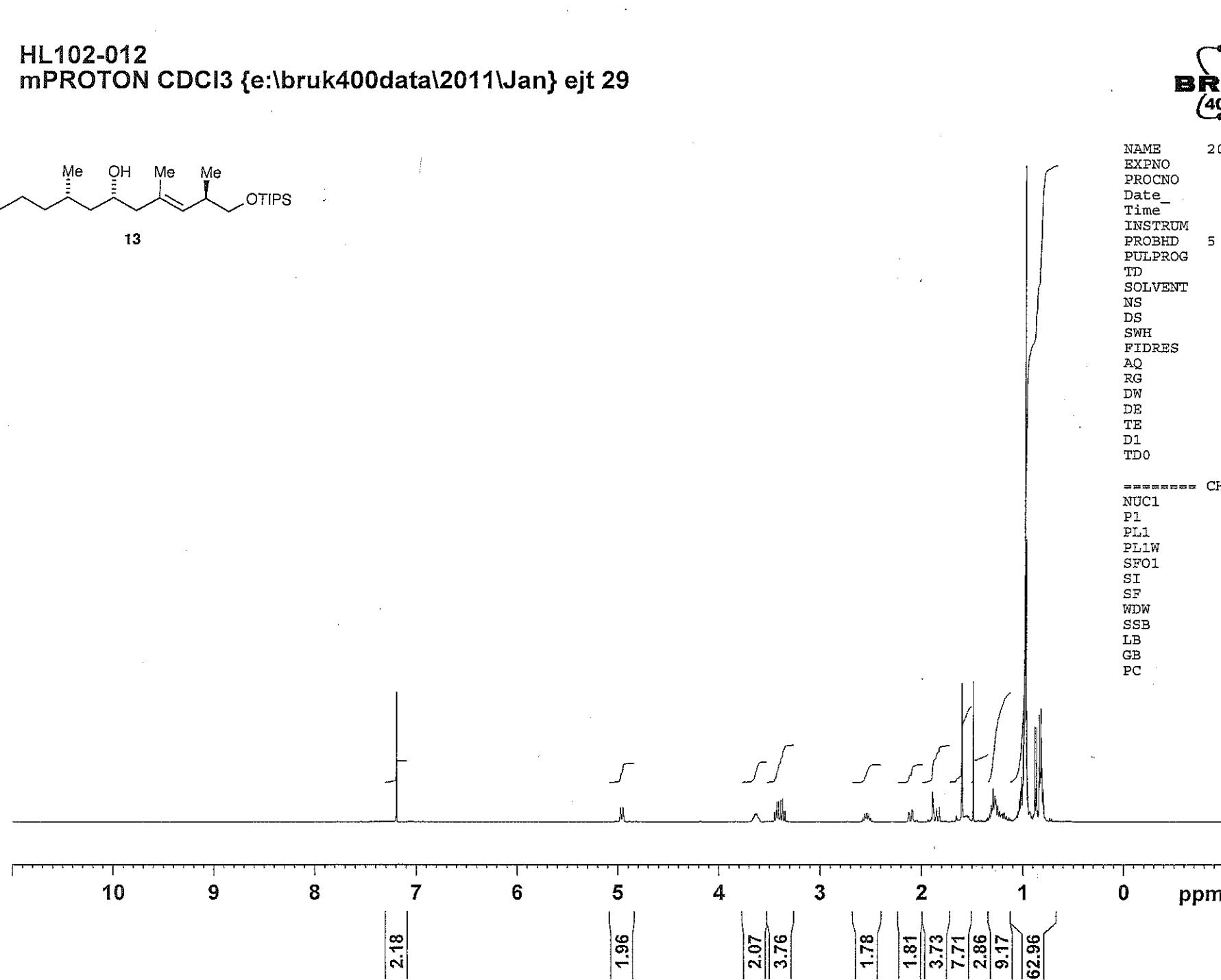
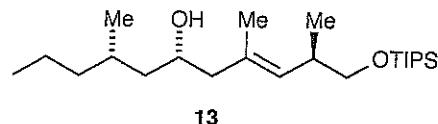


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ejt



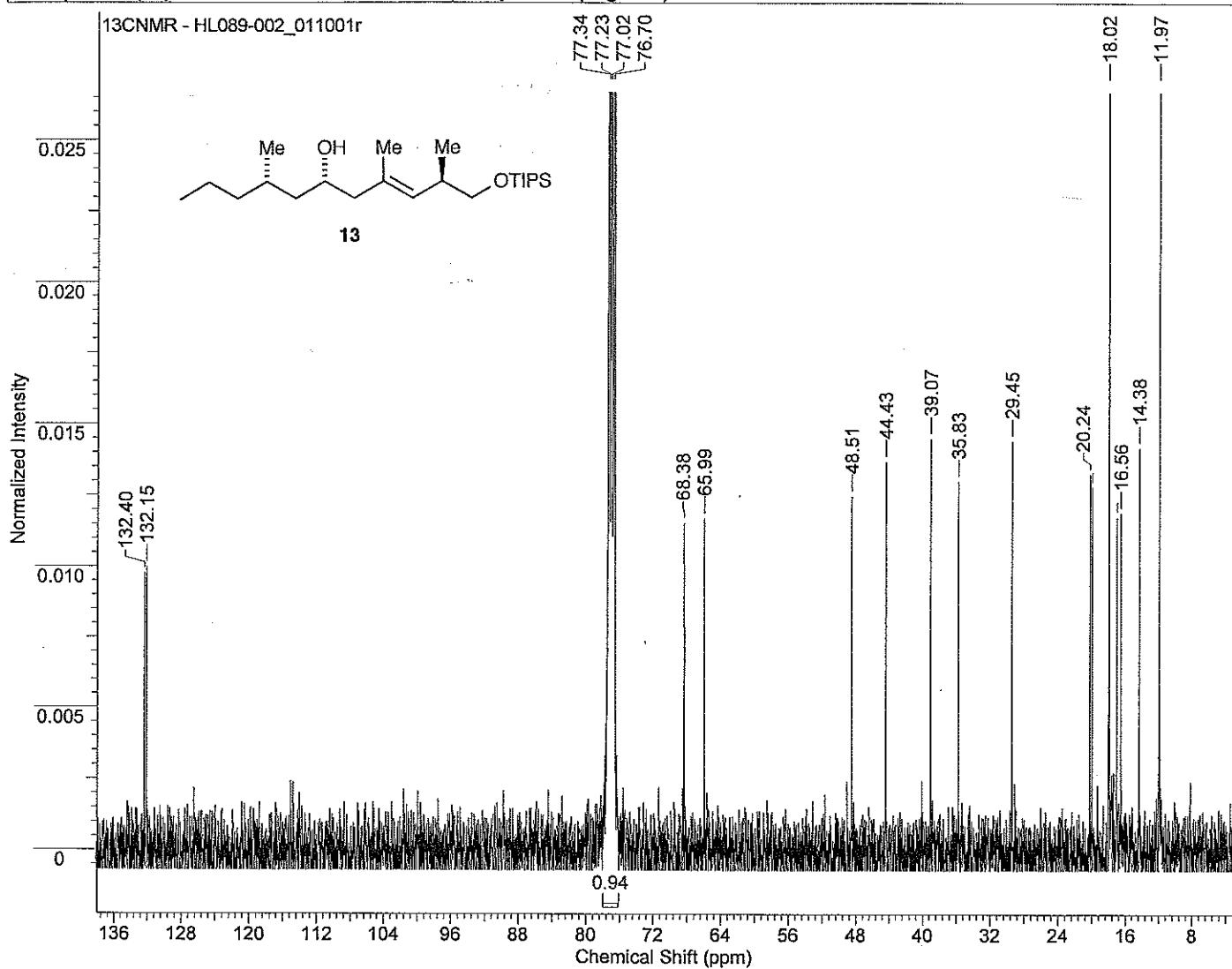
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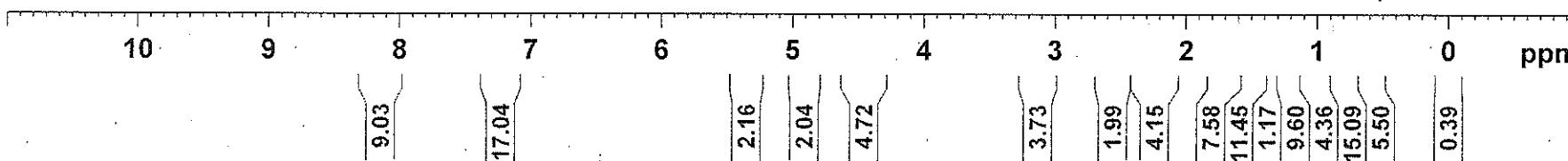
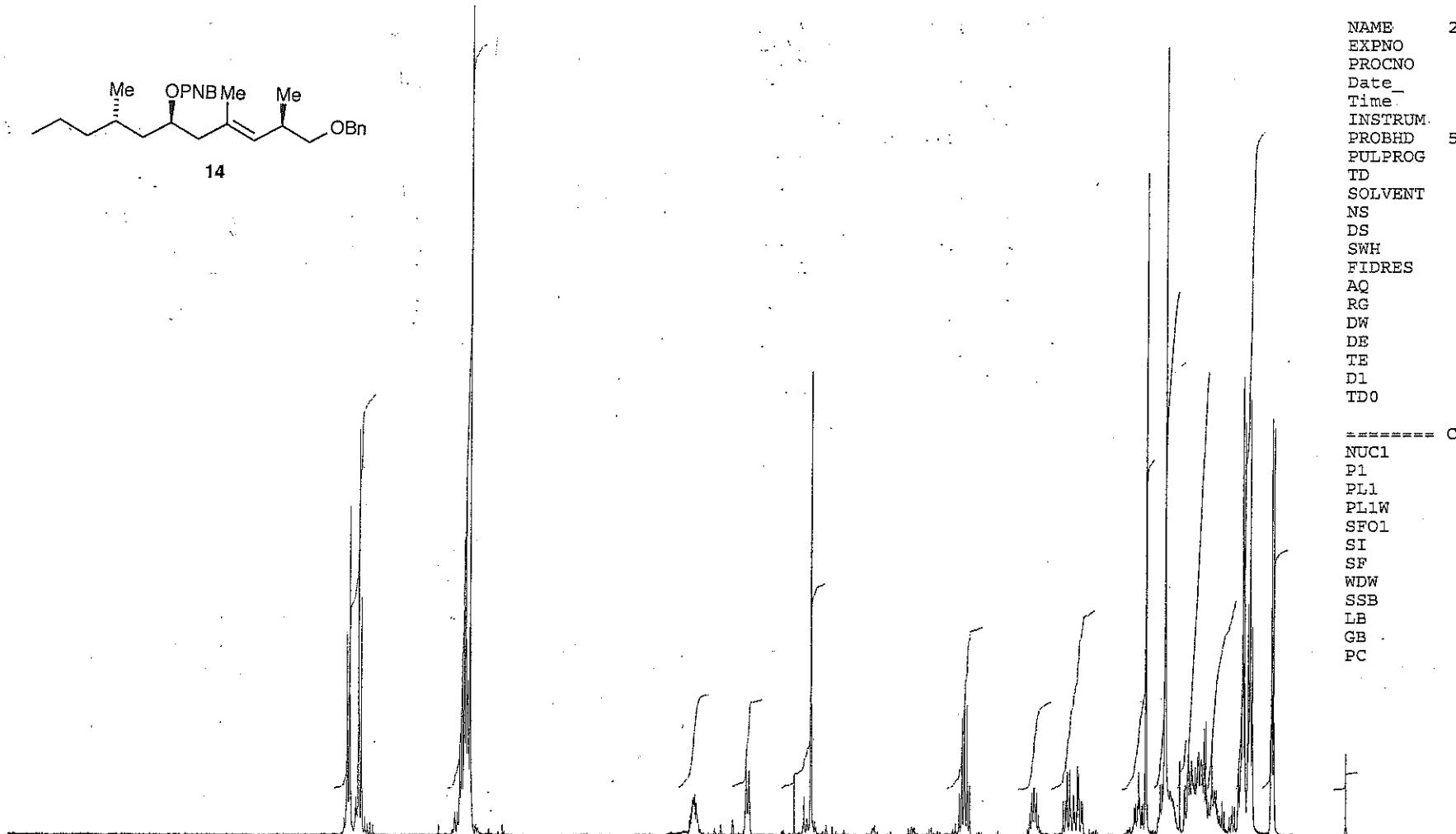
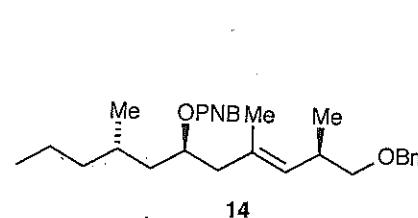
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HL048-001  
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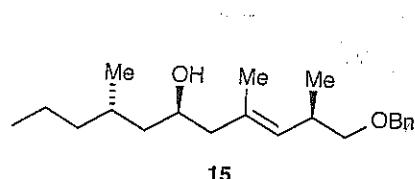


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TE 294.0 K  
D1 1.0000000 sec  
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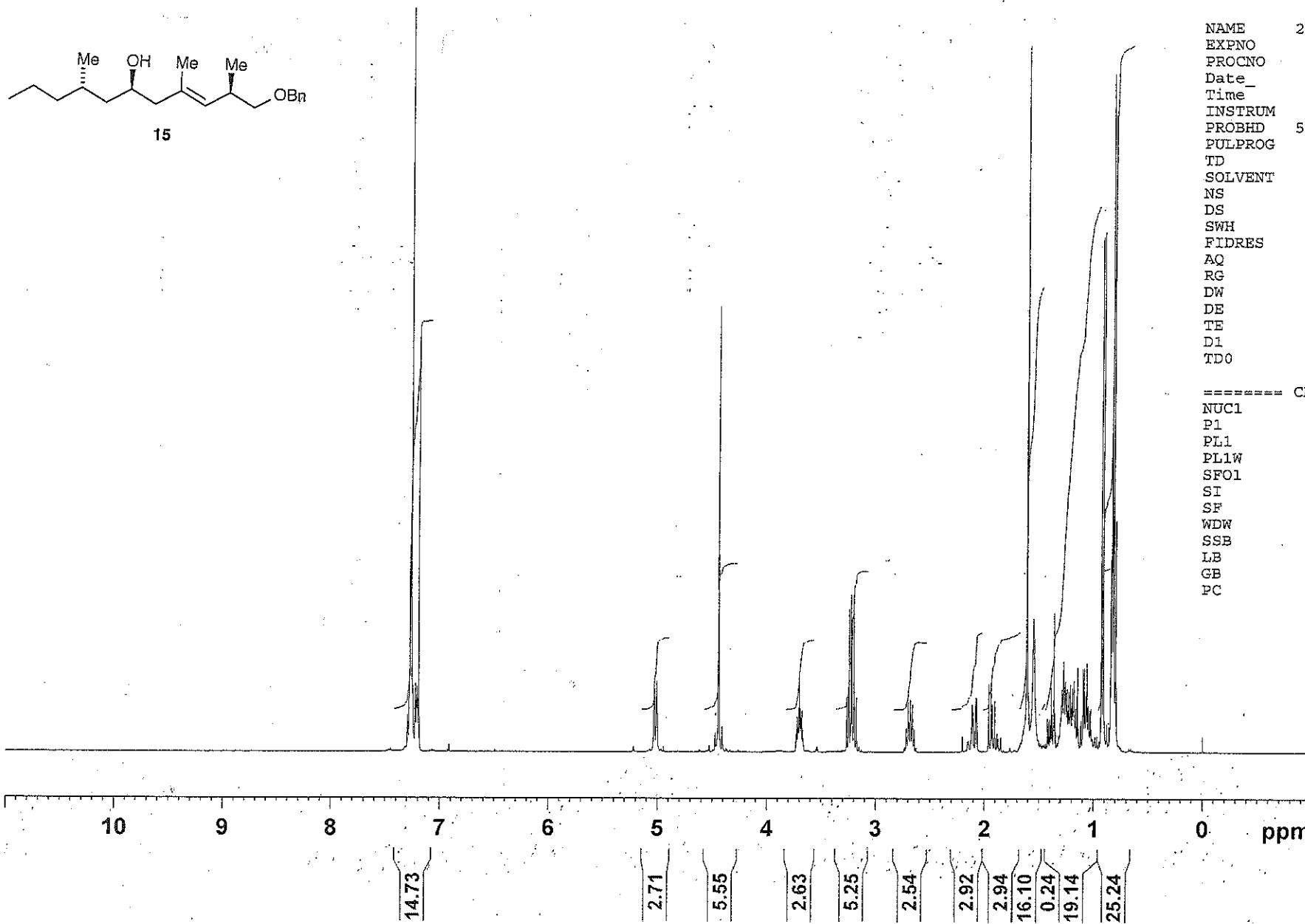
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**BRUKER**  
400 MHz



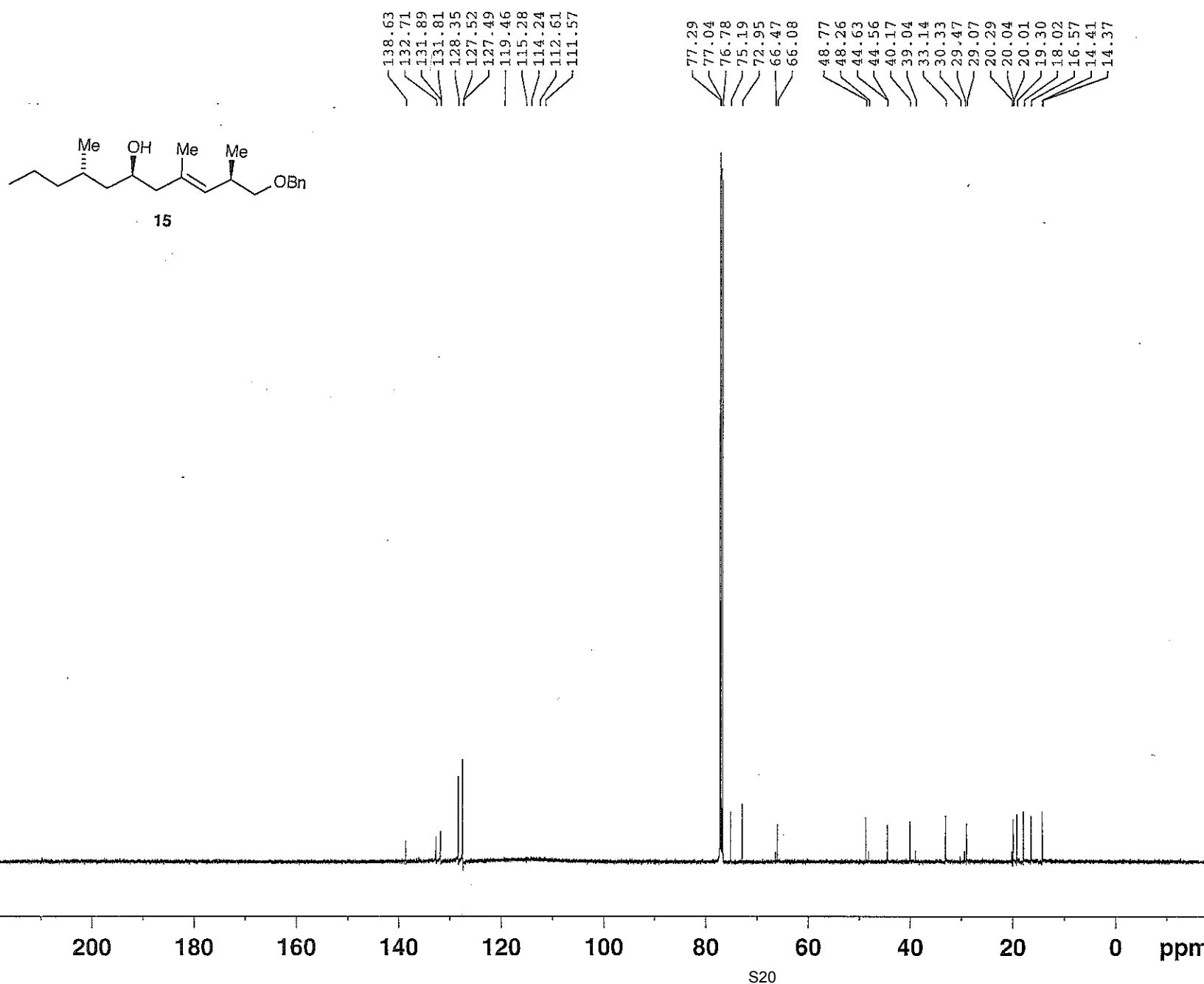
NAME 2009-10-29-ejt-1  
EXPNO 10  
PROCNO 1  
Date 20091029  
Time 16.26  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 287  
DW 60.500 usec  
DE 9.40 usec  
TE 294.2 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 ======  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
ST 32768  
SF 400.1300374 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



HL048-002

mCARBONnight CDCl<sub>3</sub> /opt/bruk500data/2009/Oct ejt 9

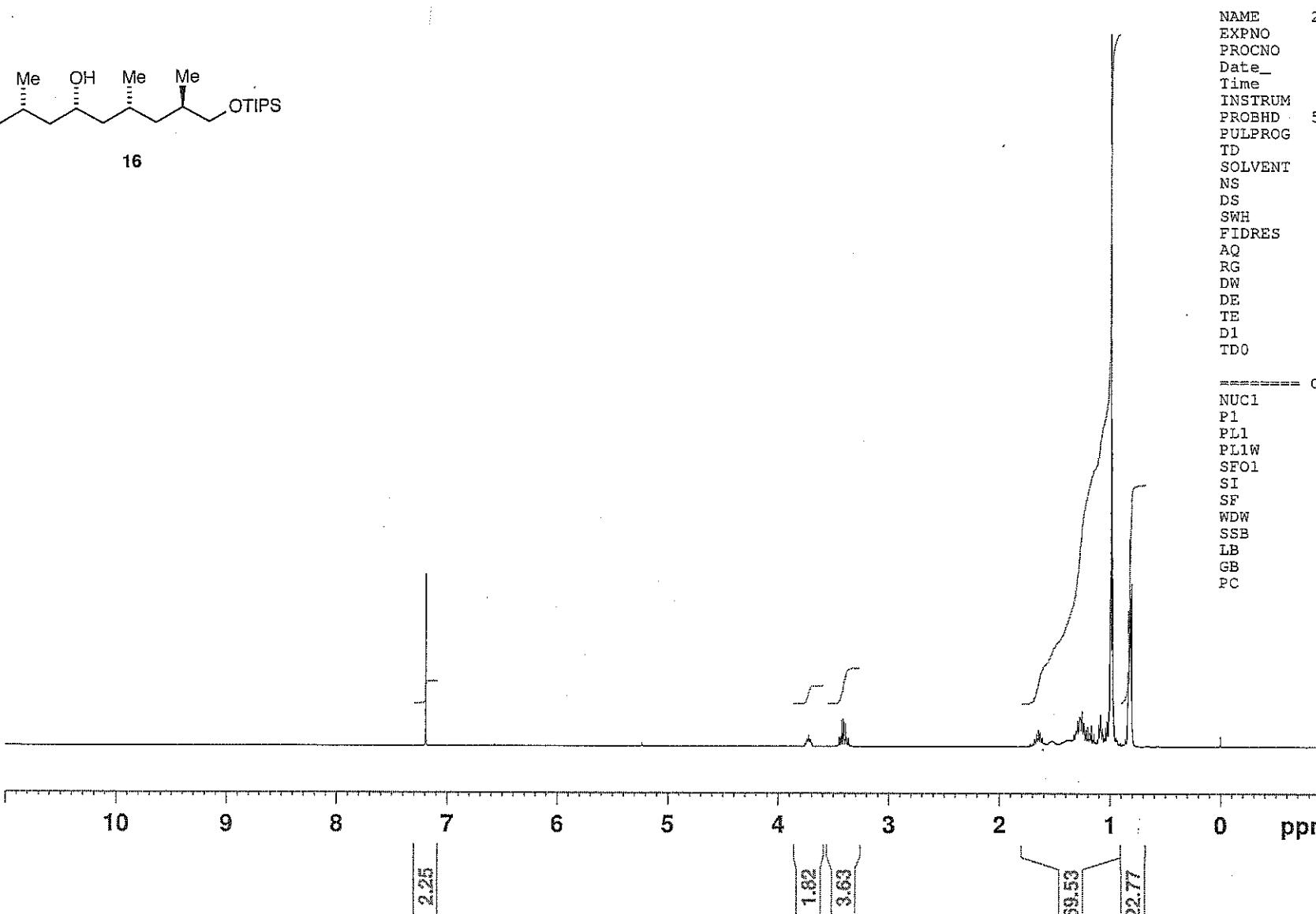
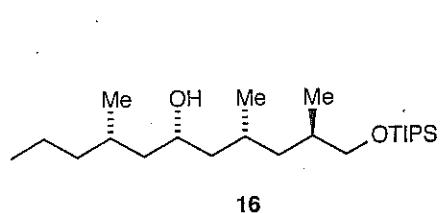


NAME 2009-10-30-ejt-9  
EXPNO 10  
PROCNO 1  
Date\_ 20091031  
Time 0.11  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 3072  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 usec  
DE 32.21 usec  
TE 293.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

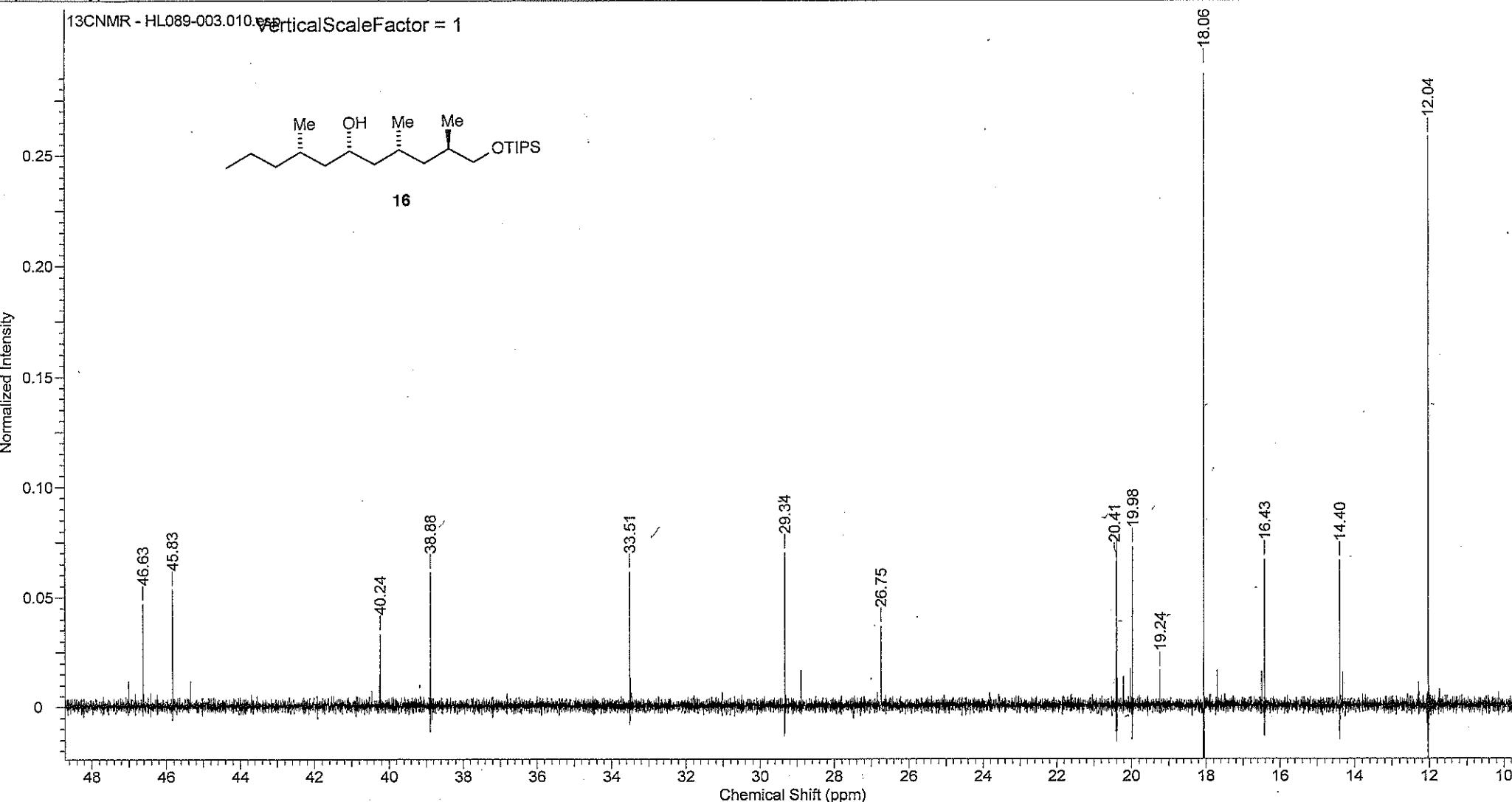
===== CHANNEL f1 =====  
NUC1 <sup>13</sup>C  
P1 11.50 usec  
PL1 -4.20 dB  
PL1W 218.02882385 W  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 <sup>1</sup>H  
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

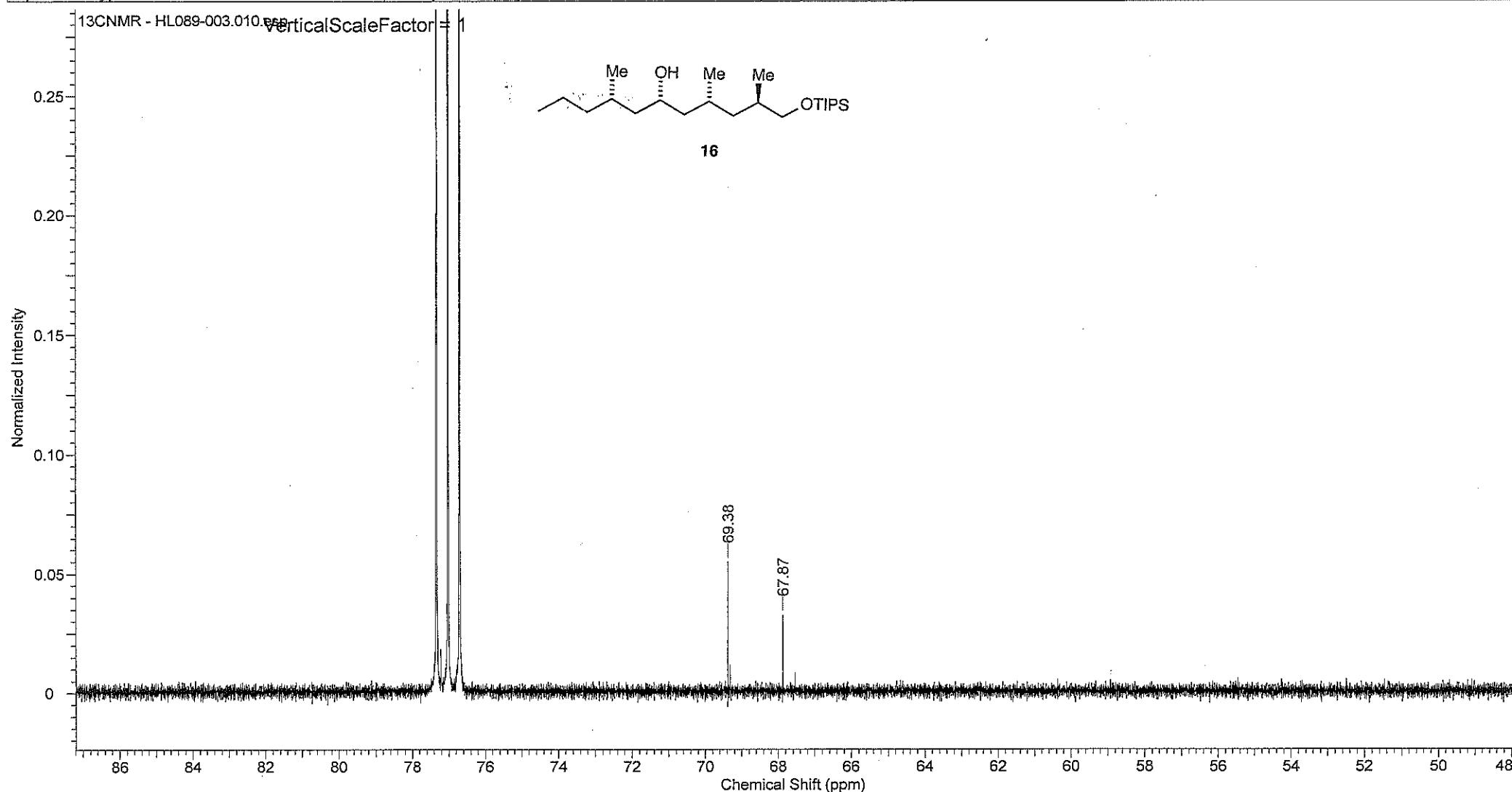
HL089-003  
mPROTON CDCl<sub>3</sub> {e:\ bruk400data\2010\Jun} ejt 12



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	<sup>13</sup> C
Origin	AV400_S	Original Points Count	32768
Points Count	262144	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	24038.37
			Temperature (degree C) 26.100



Acquisition Time (sec)	1.3631	Comment	H. Liu 0610-012 HL089-003 mCARBON CDCl <sub>3</sub> {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
Origin	AV400 S	Original Points Count	32768
Points Count	262144	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	24038.37
			Temperature (degree C) 26.100

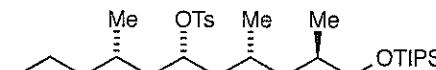


HL102-014  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2011/Jan ejt 18

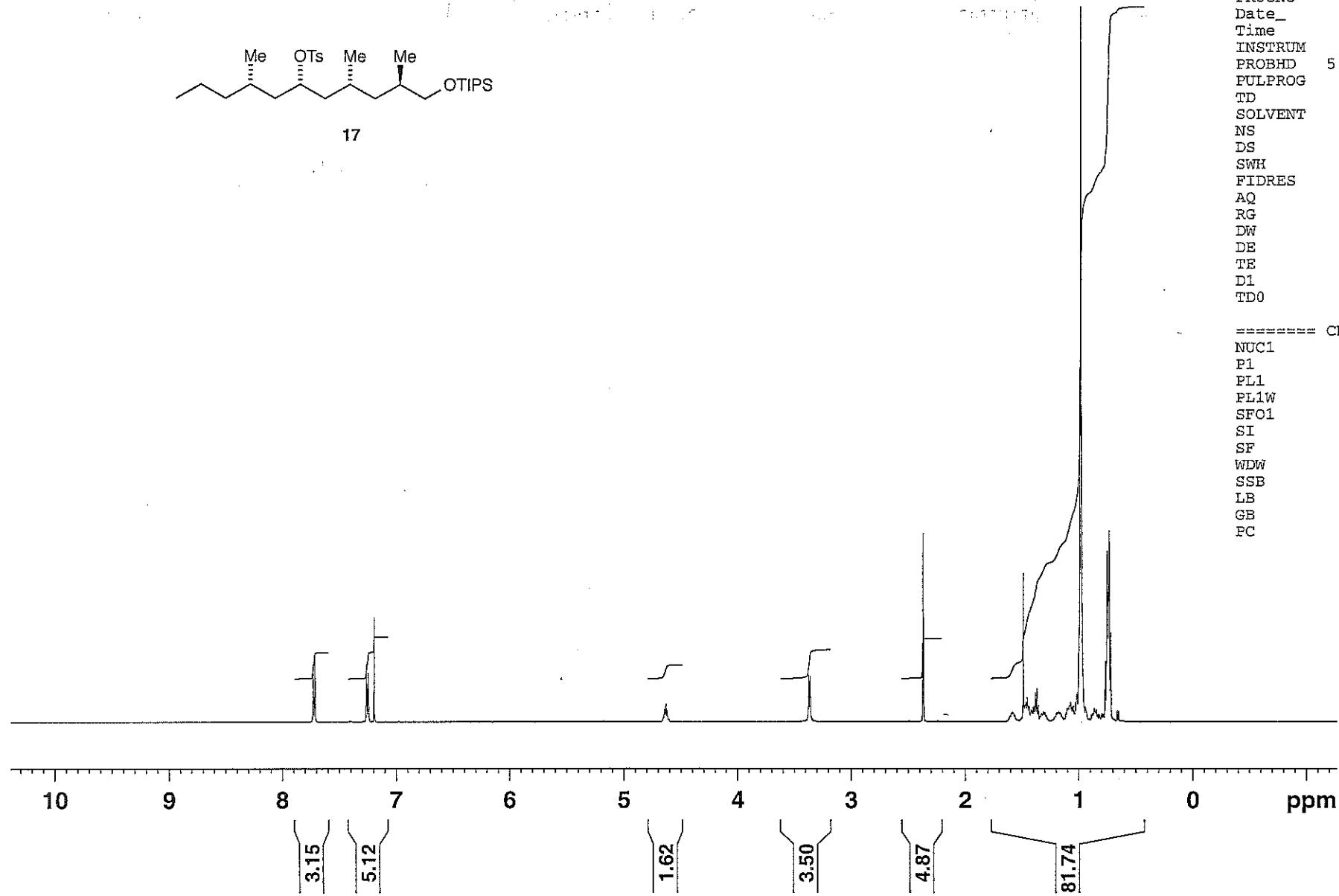


NAME 2011-01-25-ejt-18  
EXPNO 10  
PROCNO 1  
Date\_ 20110125  
Time 9.44  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 256  
DW 48.400 usec  
DE 13.38 usec  
TE 293.0 K  
D1 1.0000000 sec  
TD0 1

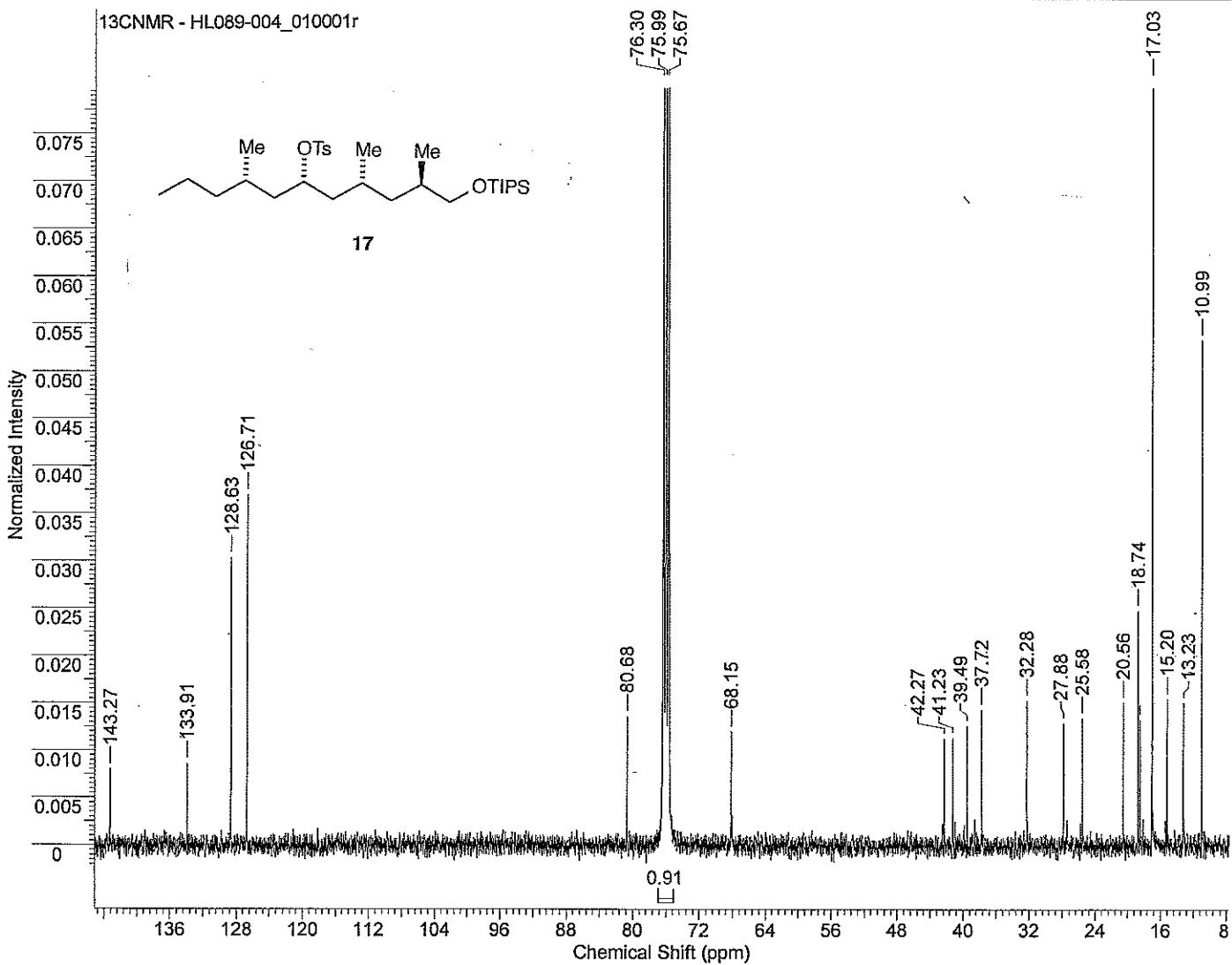
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300470 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



17



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

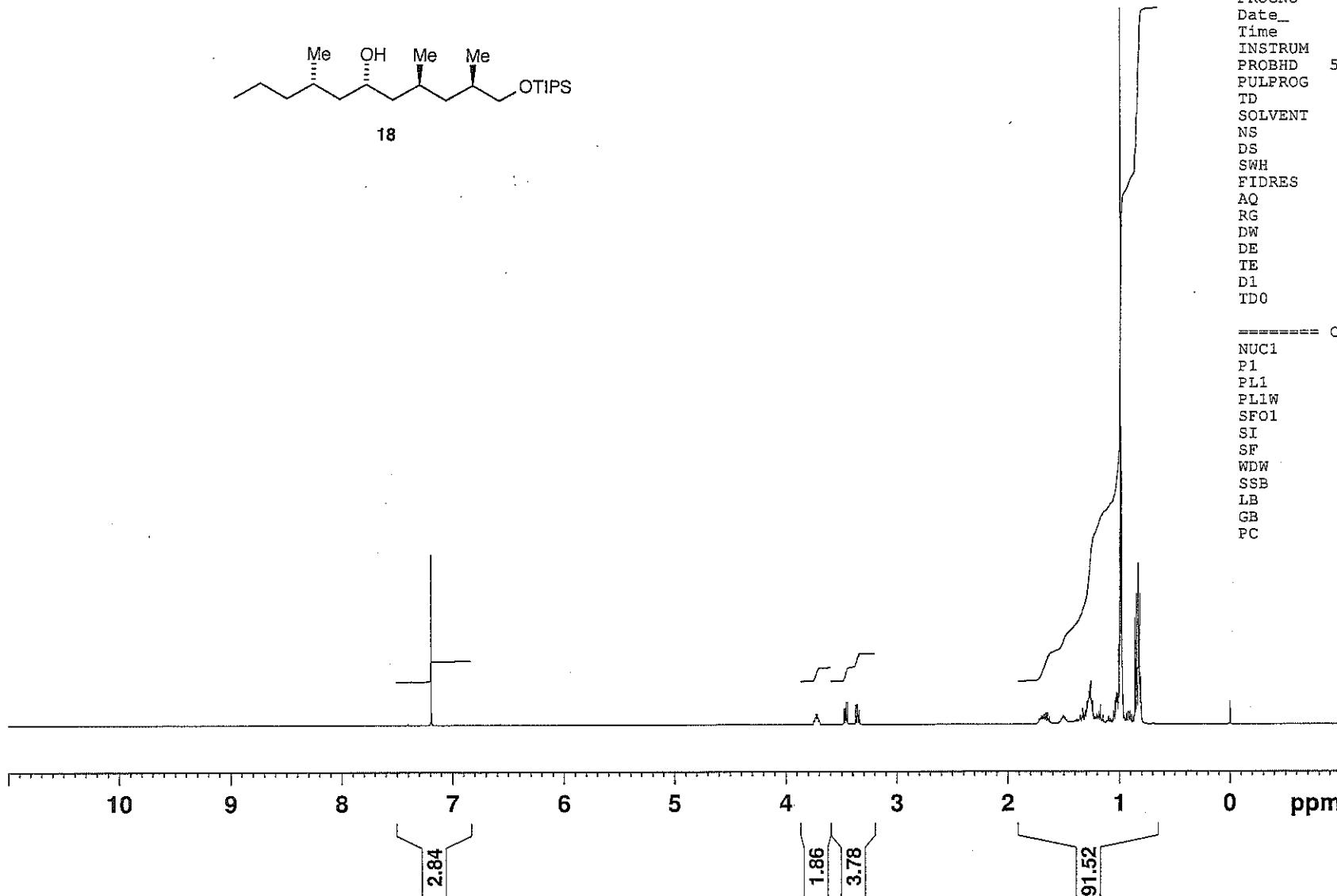


HL055-002  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2009/Dec ejt 38



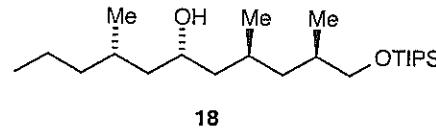
NAME 2009-12-04-ejt-38  
EXPNO 10  
PROCNO 1  
Date\_ 20091204  
Time 10.30  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 362  
DW 48.400 usec  
DE 13.38 usec  
TE 295.4 K  
D1 1.0000000 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 500.1300474 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



H liu HL055-002 . 0611-006

mCARBON CDCl<sub>3</sub> {E:\bruk400service\_data\2011\Jun} Administrator 8



NAME 2011-06-10-Administrator-8

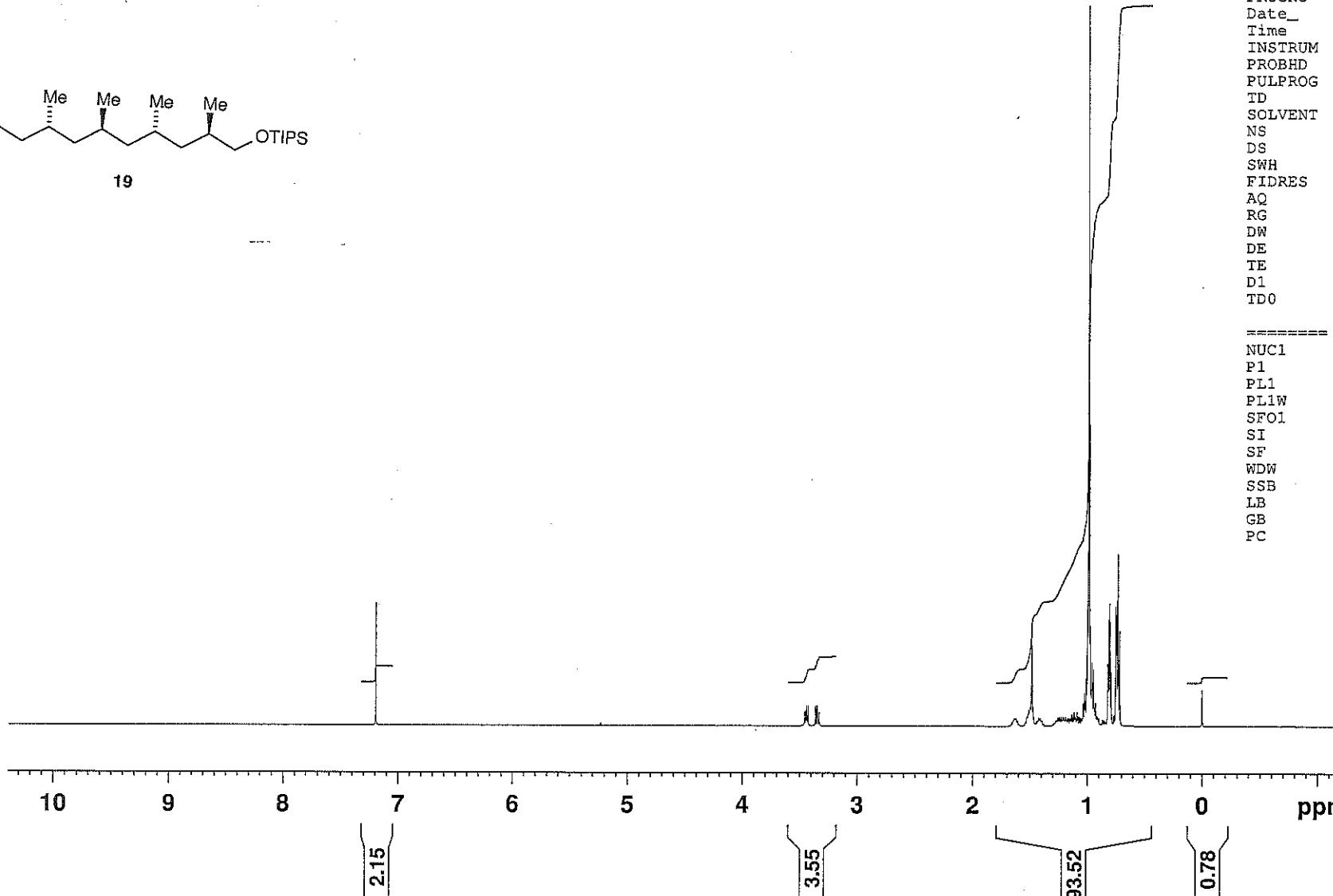
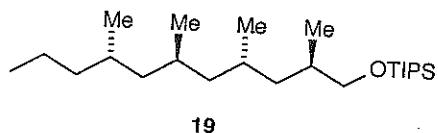
EXPNO 11  
PROCNO 1  
Date\_ 20110612  
Time\_ 21.18  
INSTRUM AV400\_S  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 10240  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 294.7 K  
D1 2.0000000 sec  
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 =====  
CPDPGR2 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

200 180 160 140 120 100 80 60 40 20 0 ppm

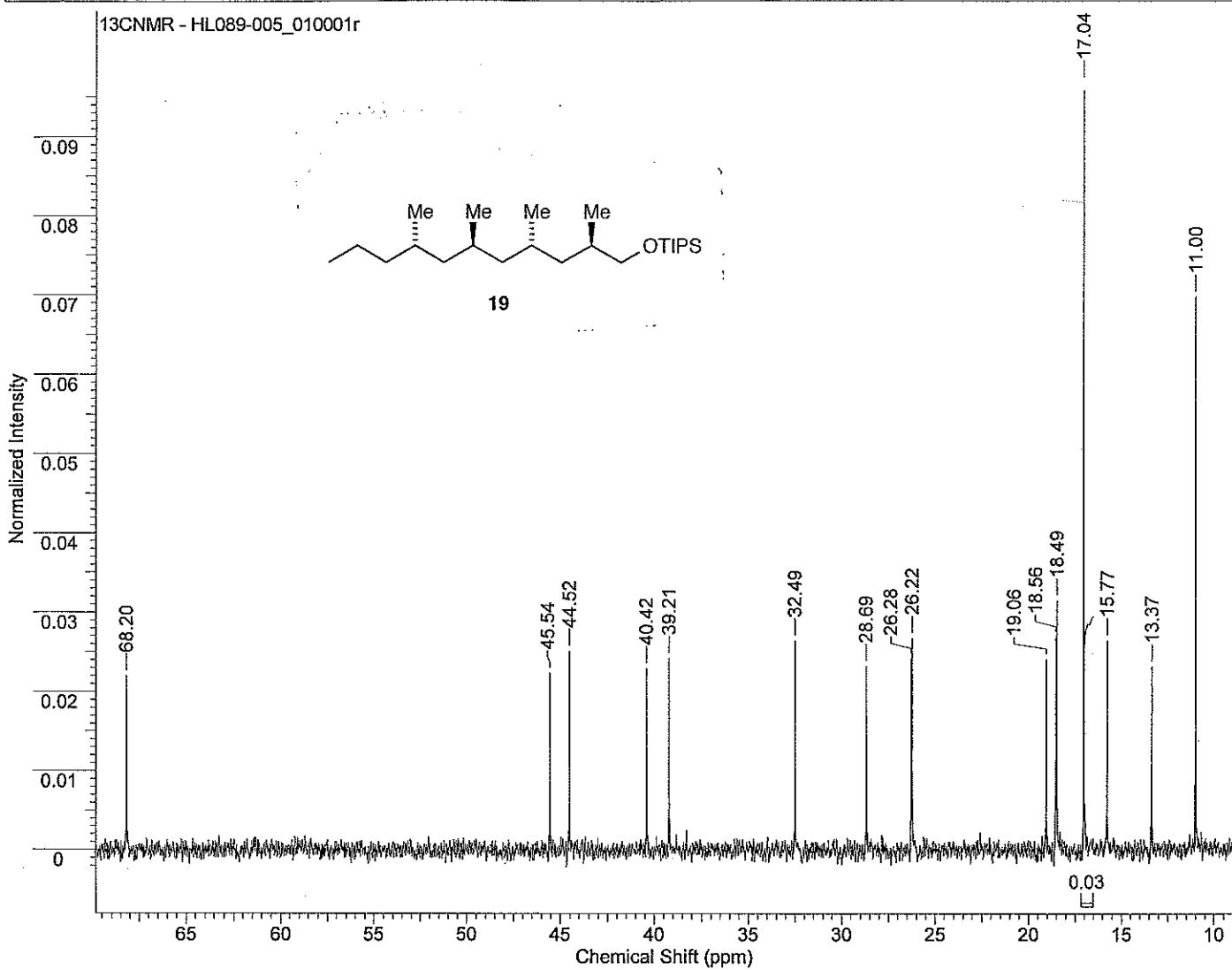
HL089-005  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2010/Jun ejt 18



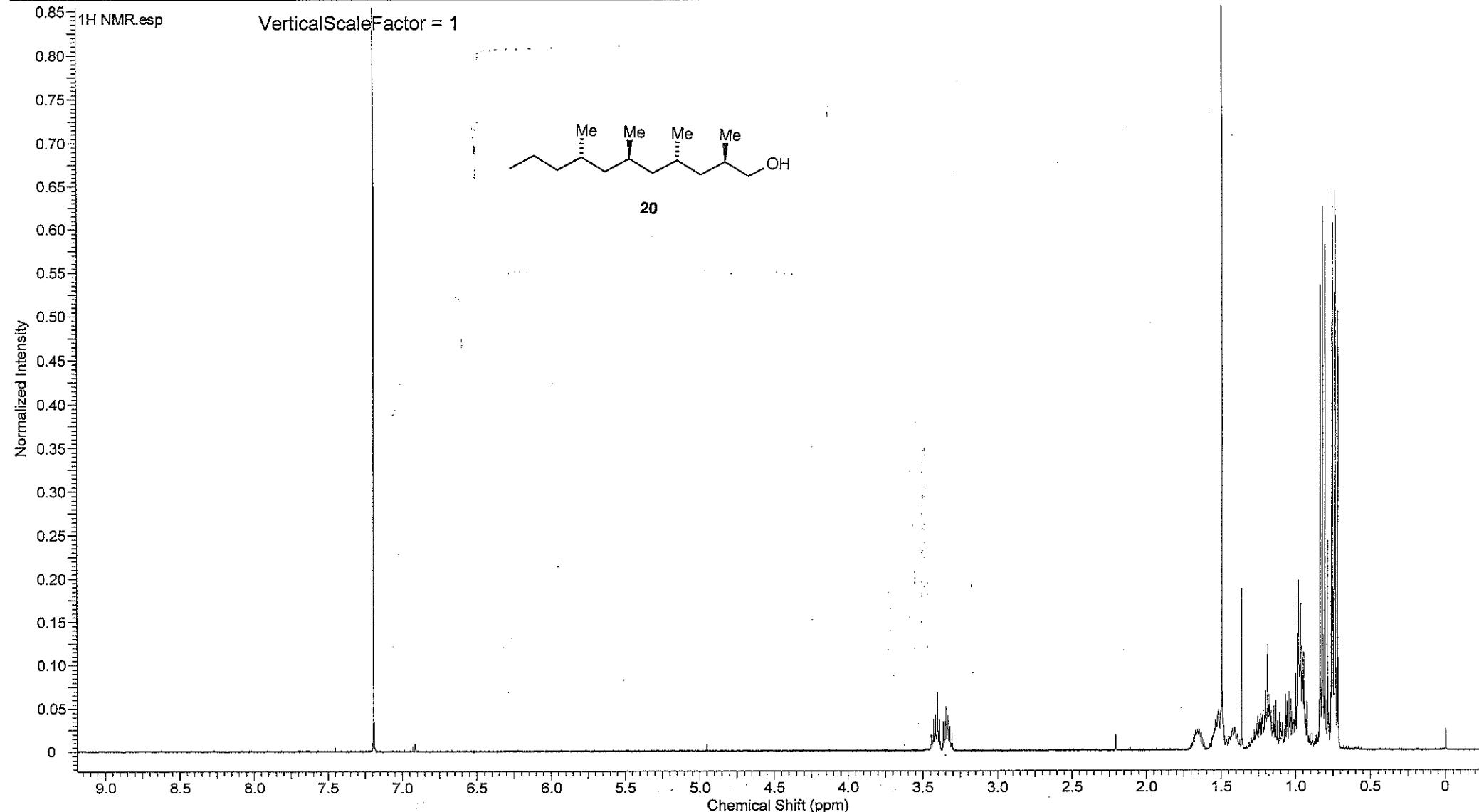
NAME 2010-06-15-ejt-18  
EXPNO 10  
PROCNO 1  
Date\_ 20100615  
Time 9.33  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 287  
DW 48.400 usec  
DE 13.38 usec  
TE 294.2 K  
D1 1.0000000 sec  
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 500.1300474 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<b>Acquisition Time (sec)</b>	1.3631
<b>Comment</b>	H. Liu 0610-022 HL089-005 mCARBON CDCl3 {E:\ bruk400service_data\2010\Jun} Administrator 22
<b>Date</b>	16 Jun 2010 07:13:04
<b>Date Stamp</b>	16 Jun 2010 07:13:04
<b>File Name</b>	E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL089 - LHS synthesis\HL089-005\13CNMR - HL089-005_010001r
<b>Frequency (MHz)</b>	100.64
<b>Nucleus</b>	13C
<b>Number of Transients</b>	11264
<b>Origin</b>	AV400_S
<b>Original Points Count</b>	32768
<b>Owner</b>	Administrator
<b>Points Count</b>	32768
<b>Pulse Sequence</b>	zgpg30
<b>Receiver Gain</b>	2050.00
<b>SW(cyclical) (Hz)</b>	24038.46
<b>Solvent</b>	CHLOROFORM-d
<b>Spectrum Offset (Hz)</b>	9960.1025
<b>Sweep Width (Hz)</b>	24037.73
<b>Temperature (degree C)</b>	24.900

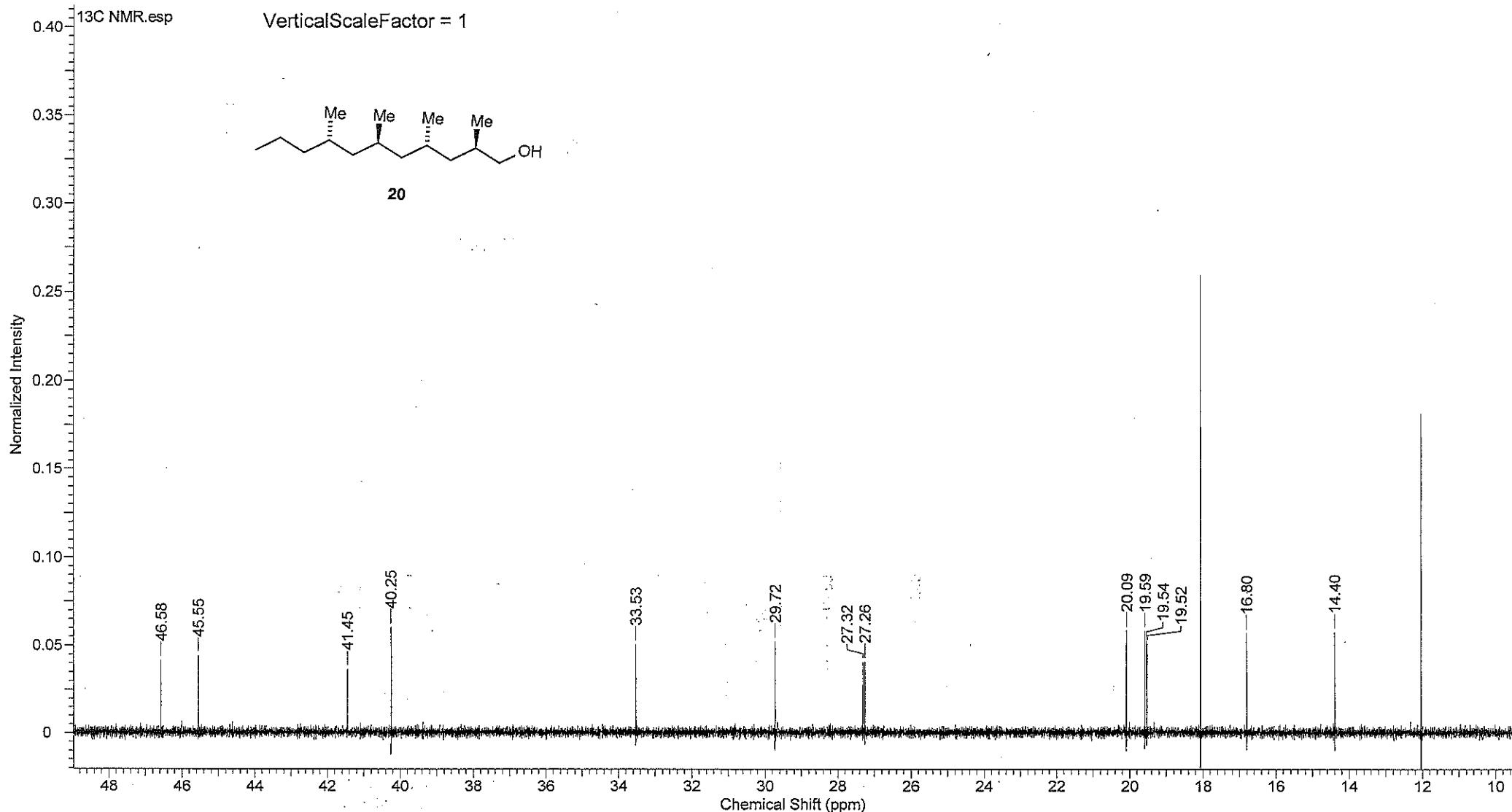


Acquisition Time (sec)	3.9649	Comment	HL102-016 mPROTON CDCl3 {e:\ bruk400\data\2011\Jan} ejt 57		Date	30 Jan 2011 20:07:28	
Date Stamp	30 Jan 2011 20:07:28	File Name	C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-016\1H NMR\fid		Origin	AV400	
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	16	Pulse Sequence	zg30b
Original Points Count	32768	Owner	Administrator	Points Count	32768	Spectrum Offset (Hz)	2434.2427
Receiver Gain	362.00	SW(cyclical) (Hz)	8264.46	Solvent	CHLOROFORM-d		
Spectrum Type	STANDARD	Sweep Width (Hz)	8264.21	Temperature (degree C)	19.100		



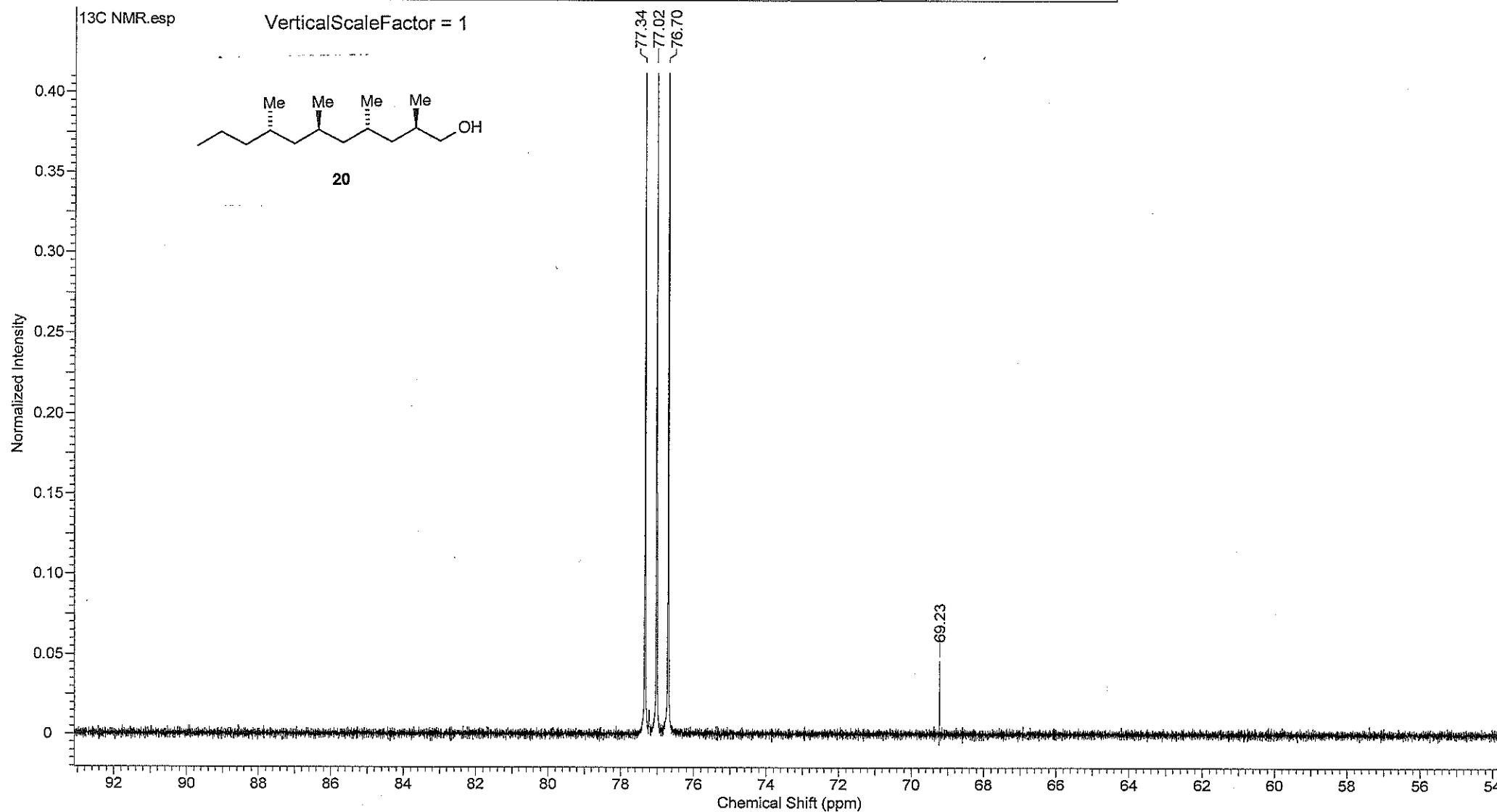
02/03/2011 17:26:38

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

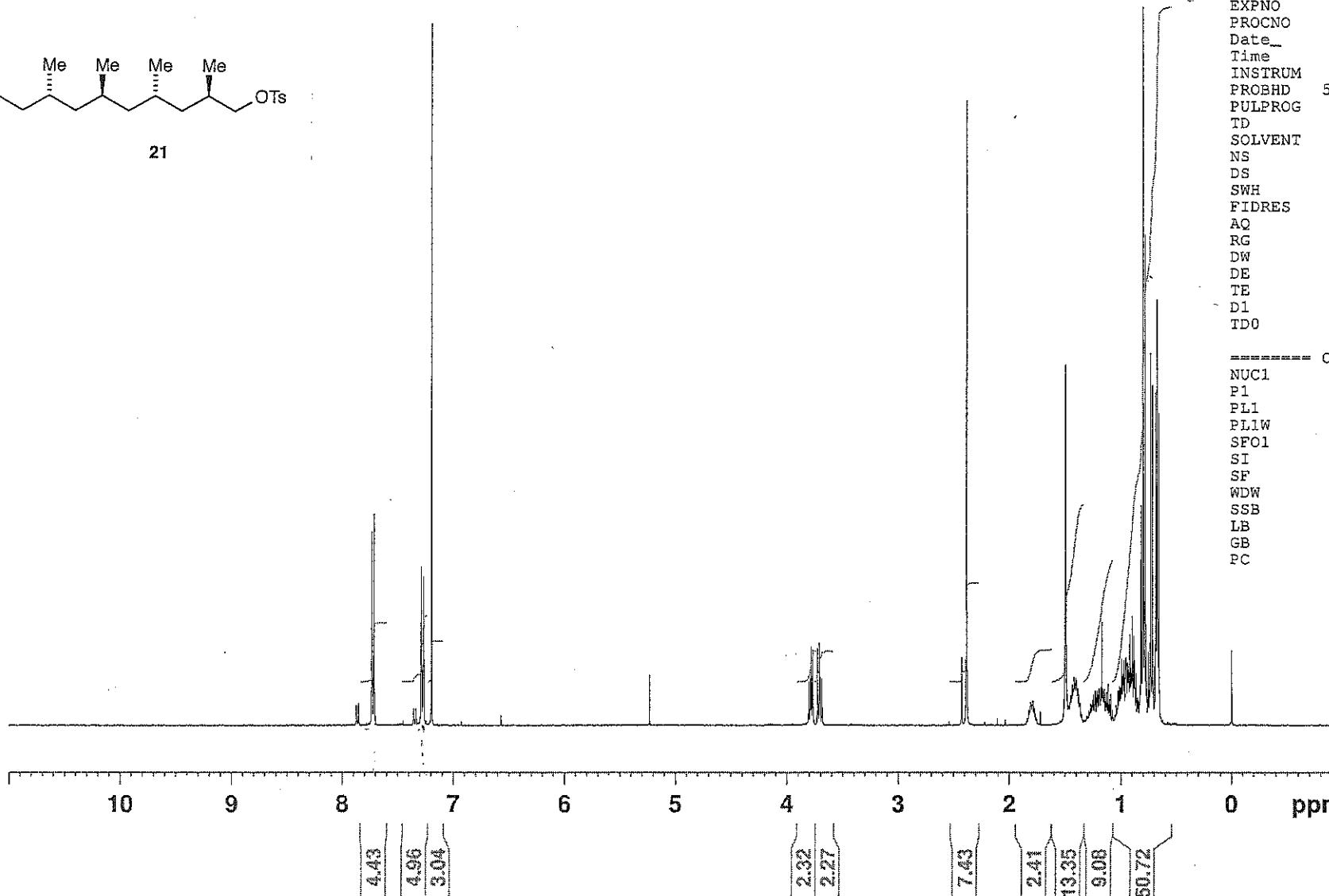
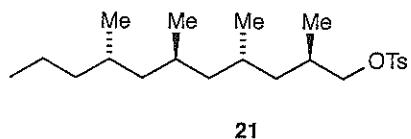


02/03/2011 17:26:46

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

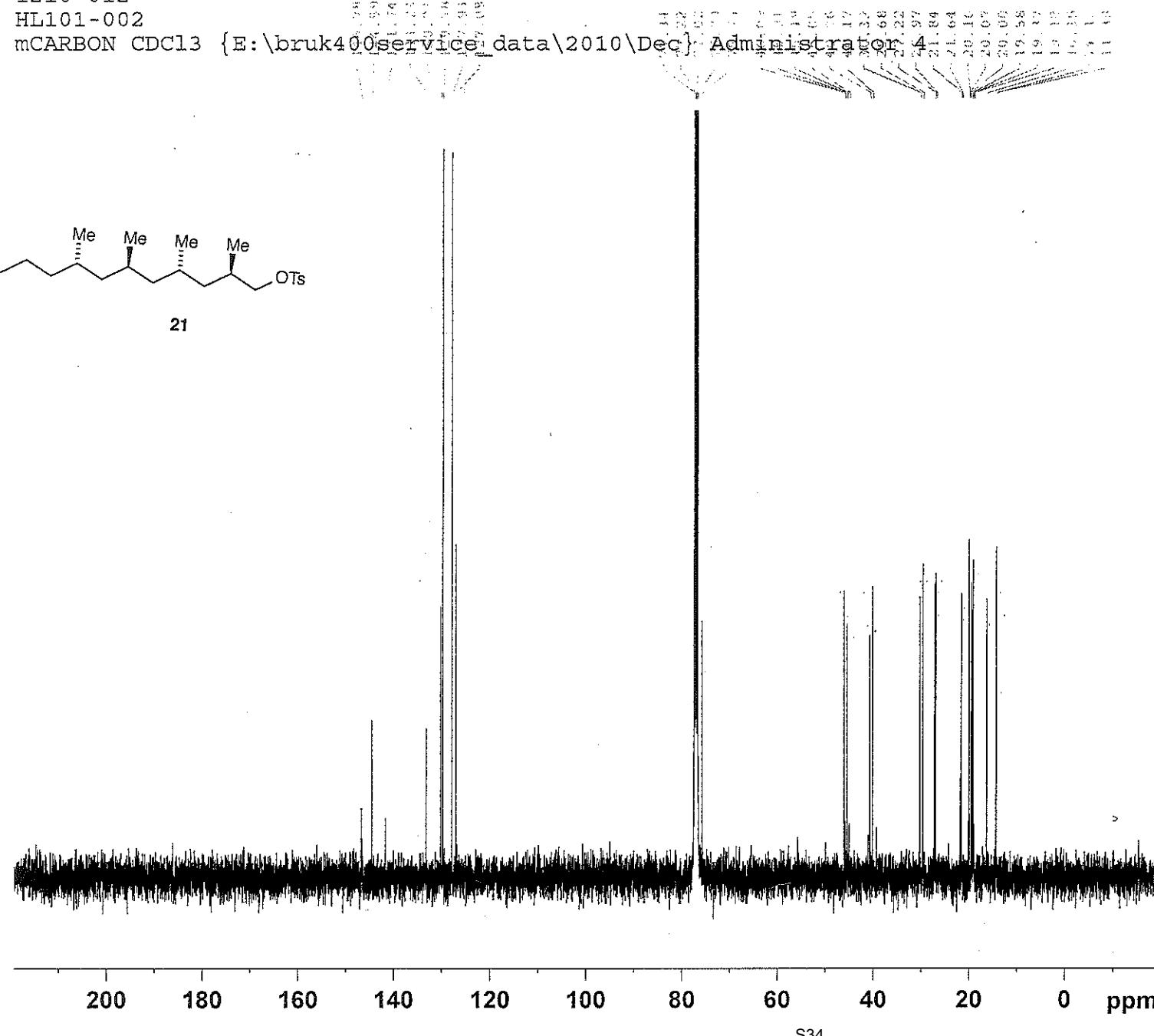
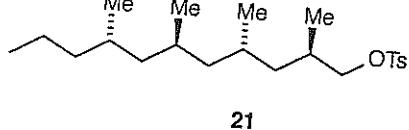


HL099-002  
mPROTON CDCl<sub>3</sub> {e:\bruk400data\2010\Nov} ejt 16



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	CDCl <sub>3</sub>
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	1.0000000 sec
TDO	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

H. Liu  
1210-012  
HL101-002  
mCARBON CDCl<sub>3</sub> {E:\bruk400service\data\2010\Dec}\Administrator



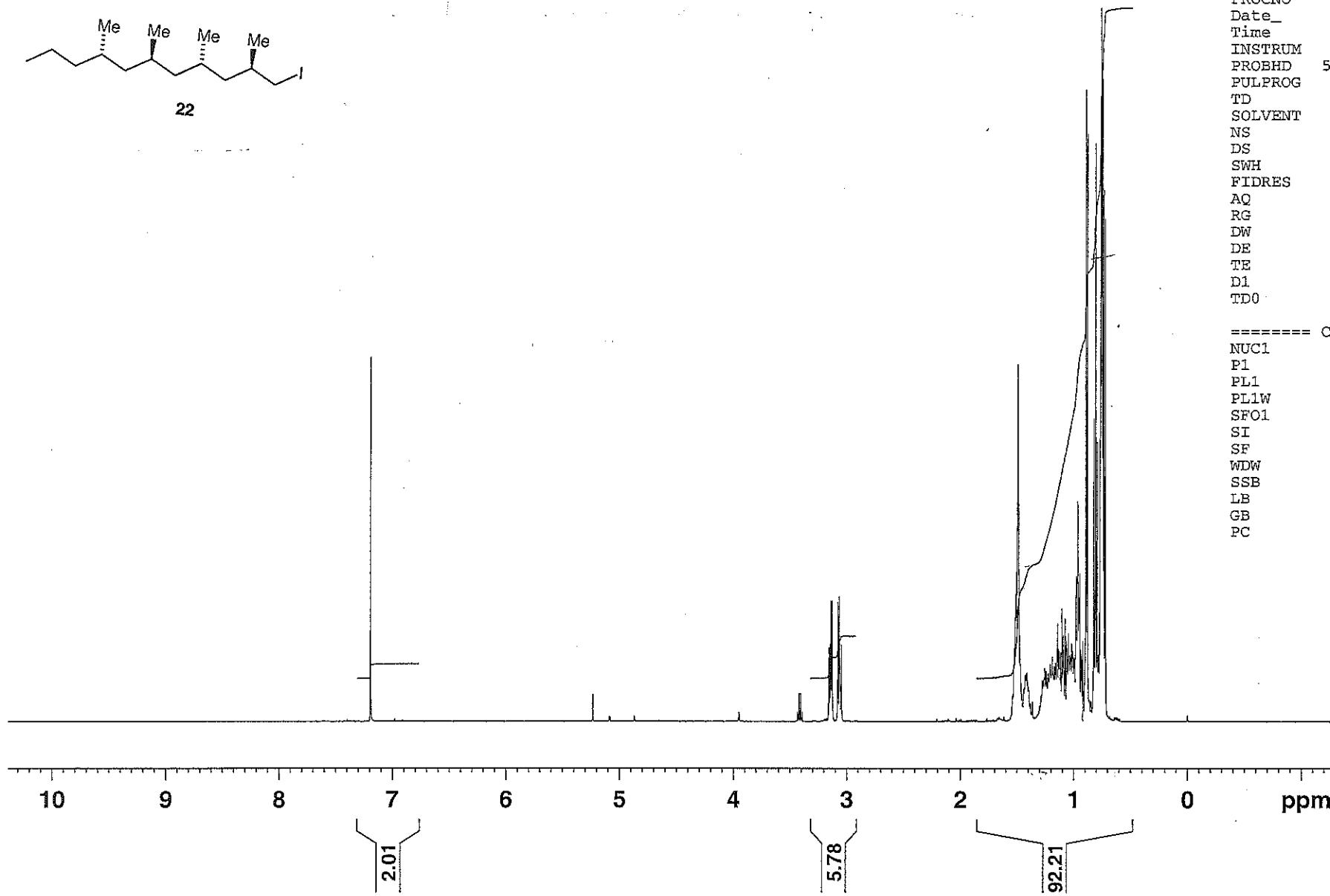
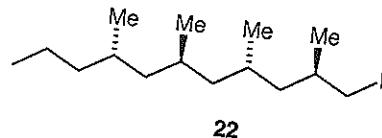
NAME 2010-12-06-Administrator-4  
EXPNO 10

PROCNO 1  
Date\_ 20101207  
Time 8.28  
INSTRUM AV400\_S  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 5000  
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 297.7 K  
D1 2.0000000 sec  
D11 0.0300000 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 =====  
CPDPG2 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

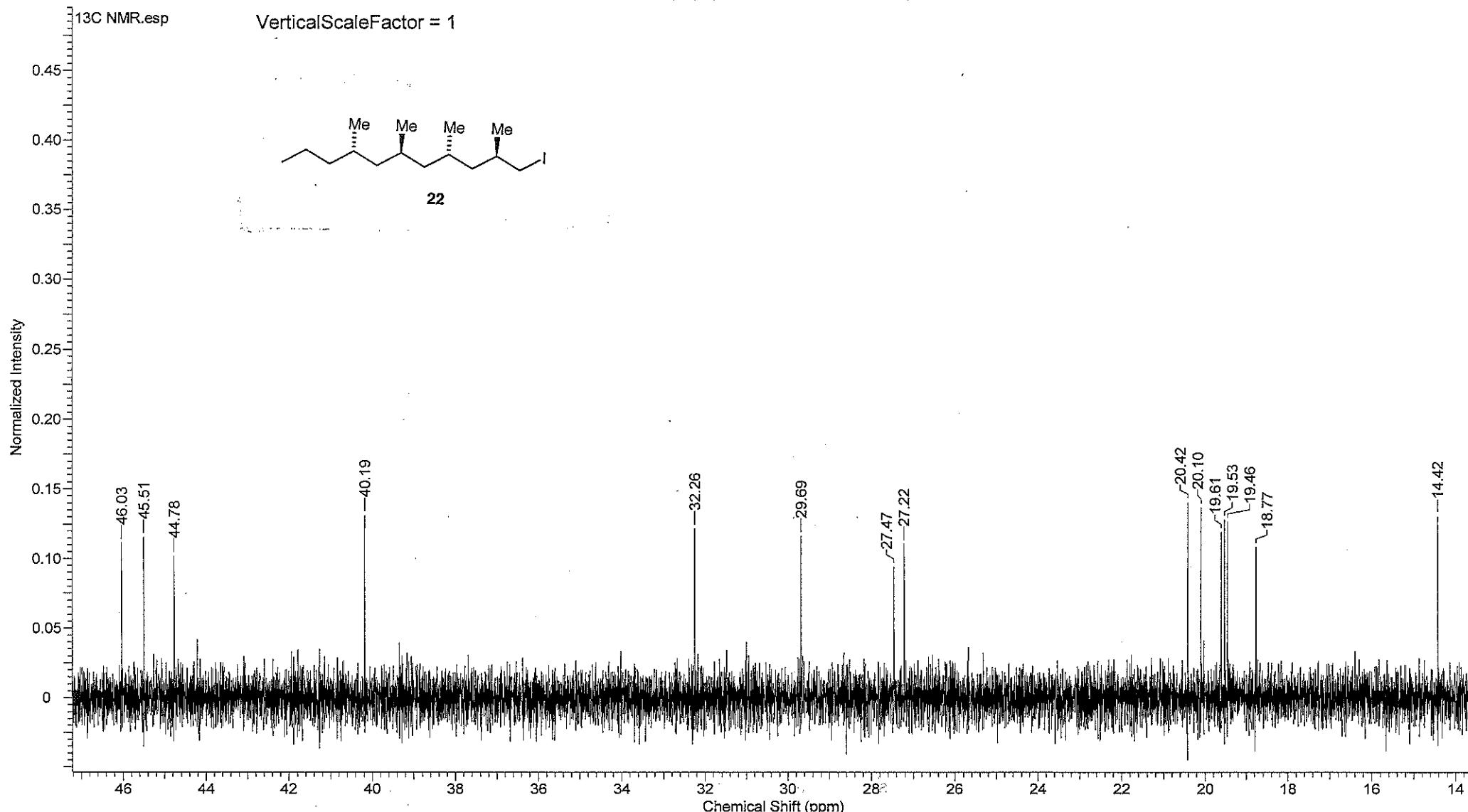
HL101-003  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2010/Dec ejt 34



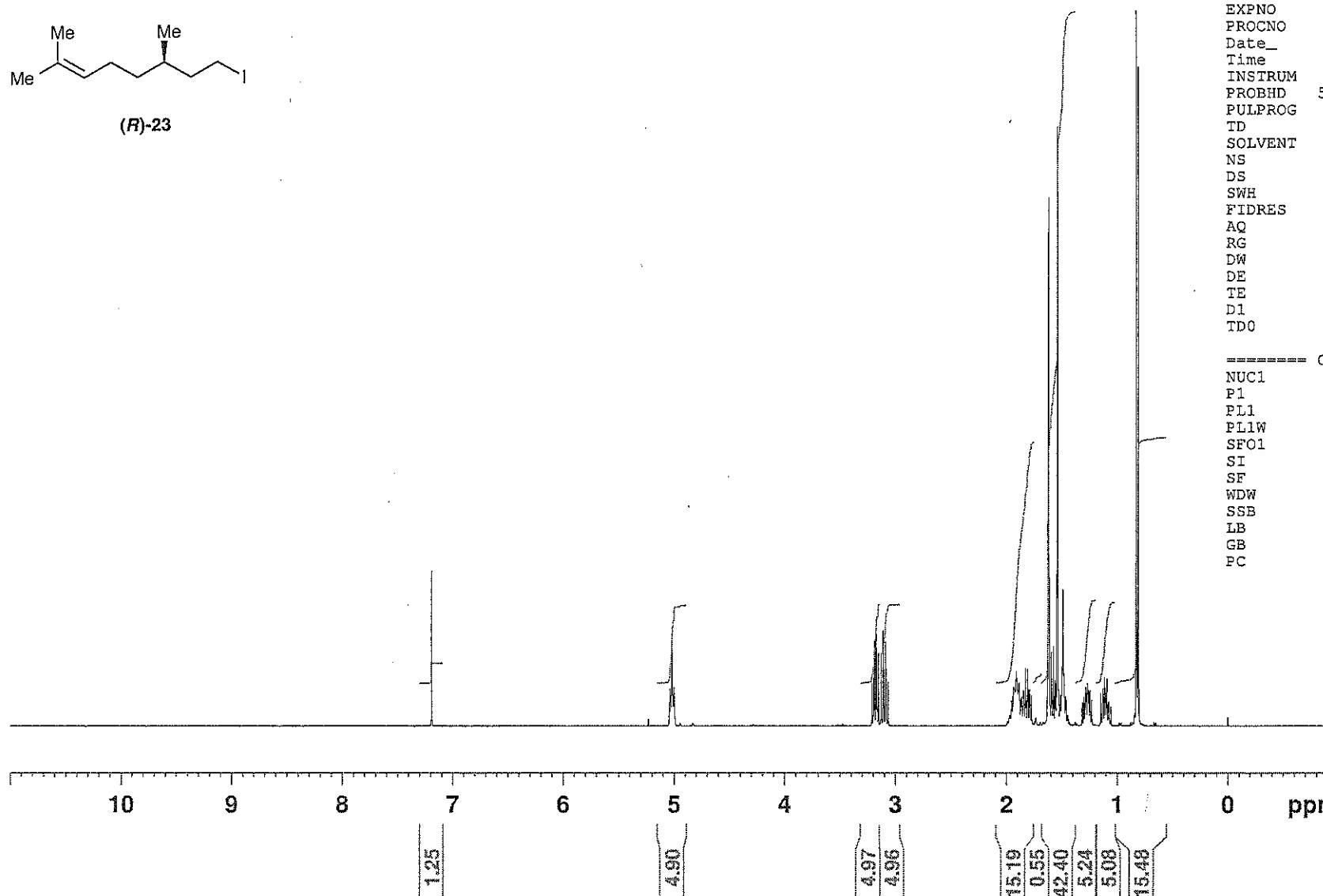
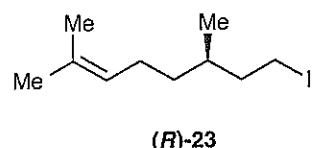
NAME 2010-12-07-ejt-34  
EXPNO 10  
PROCNO 1  
Date\_ 20101207  
Time 9.28  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 287  
DW 48.400 usec  
DE 13.38 usec  
TE 292.6 K  
D1 1.0000000 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 500.1300469 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<i>Acquisition Time (sec)</i>	1.1010	<i>Comment</i>	HL101-003 mCARBON CDCl <sub>3</sub> /opt/bruk500data/2010/Dec ejt 34	<i>Date</i>	07 Dec 2010 09:42:24
<i>Date Stamp</i>	07 Dec 2010 09:42:24	<i>File Name</i>	C:\Users\Leo\Desktop\Experiments Folder\Experiment 101-150\HL102 - Project Intermediate Characterization\HL102-018\13C NMR\fid		
<i>Frequency (MHz)</i>	125.76	<i>Nucleus</i>	<sup>13</sup> C	<i>Number of Transients</i>	256
<i>Original Points Count</i>	32768	<i>Owner</i>	vnmr1	<i>Points Count</i>	262144
<i>Receiver Gain</i>	512.00	<i>SW(cyclical) (Hz)</i>	29761.90	<i>Solvent</i>	CHLOROFORM-d
<i>Spectrum Type</i>	STANDARD	<i>Sweep Width (Hz)</i>	29761.79	<i>Temperature (degree C)</i>	19.803



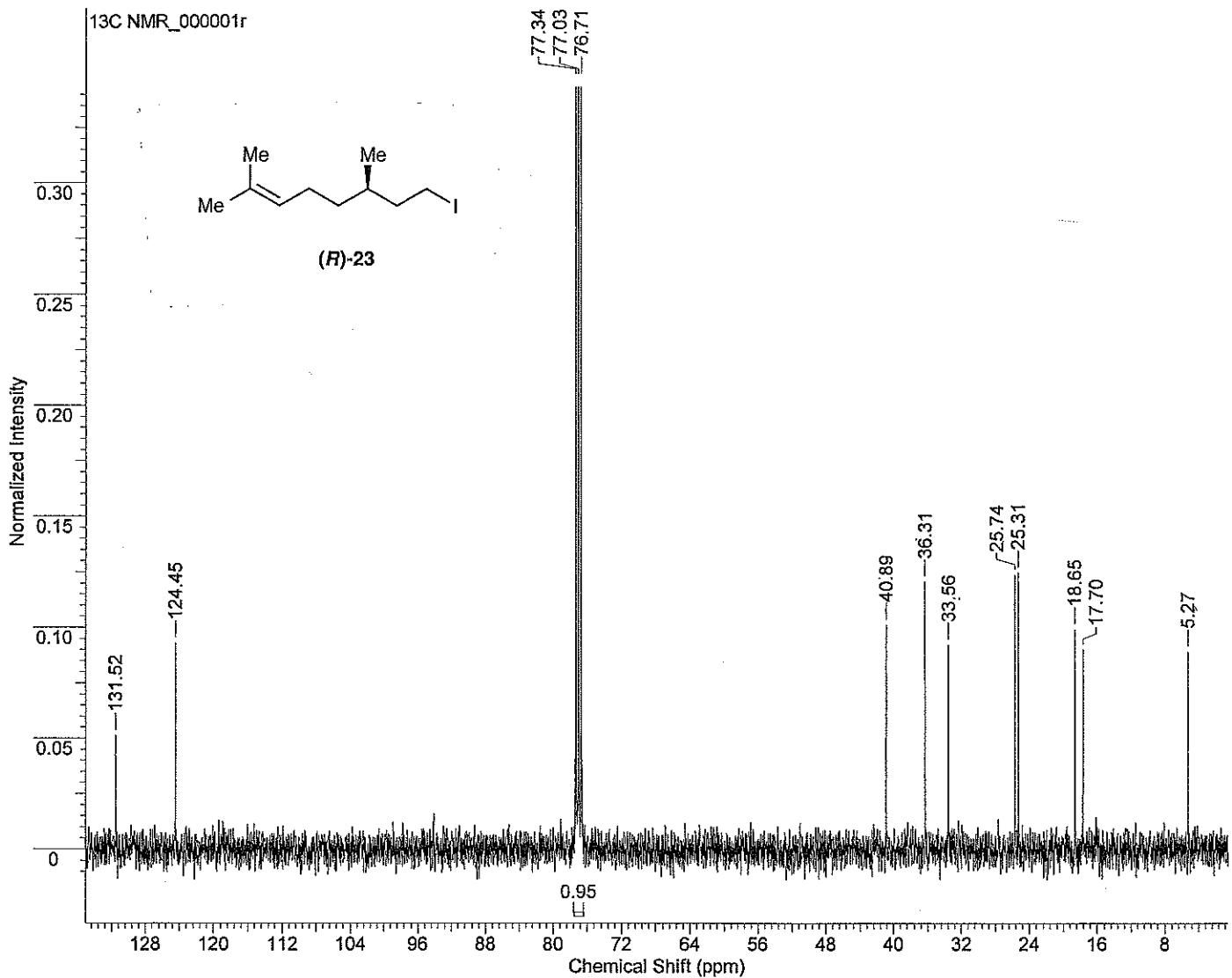
HL092-002  
mPROTON CDCl<sub>3</sub> {e:\bruk400data\2010\Aug} ejt 40



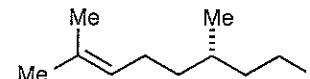
NAME 2010-08-12-ejt-40  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20100812  
 Time 15.16  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 256  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 293.9 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PLL -3.60 dB  
 PLLW 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

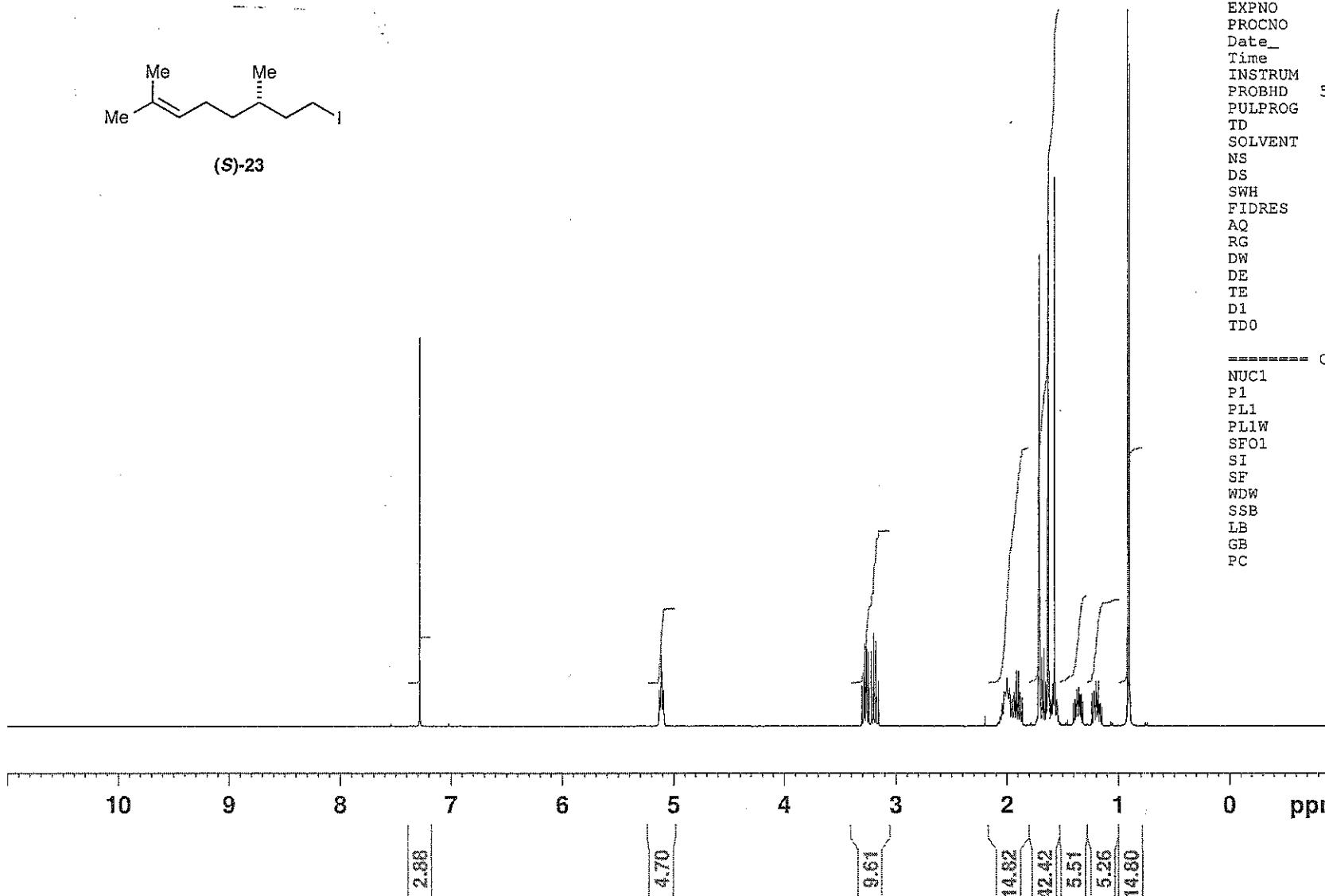
<b>Acquisition Time (sec)</b>	1.0835	<b>Comment</b>	HL092-002 mCARBON CDCl3 {e:\bruk400\data\2010\Aug} ejt 40
<b>Date</b>	12 Aug 2010 14:30:24	<b>Date Stamp</b>	12 Aug 2010 14:30:24
<b>File Name</b>	E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL092 - (R)-citronellol iodonation\HL092-002\13C NMR_000001r		
<b>Frequency (MHz)</b>	100.61	<b>Nucleus</b>	13C
<b>Number of Transients</b>	256	<b>Origin</b>	AV400
<b>Original Points Count</b>	32768	<b>Owner</b>	Administrator
<b>Points Count</b>	32768	<b>Pulse Sequence</b>	zgpg30
<b>Receiver Gain</b>	512.00	<b>SW(cyclical) (Hz)</b>	30241.94
<b>Solvent</b>	CHLOROFORM-d	<b>Spectrum Offset (Hz)</b>	11335.2197
<b>Sweep Width (Hz)</b>	30241.01	<b>Temperature (degree C)</b>	21.500



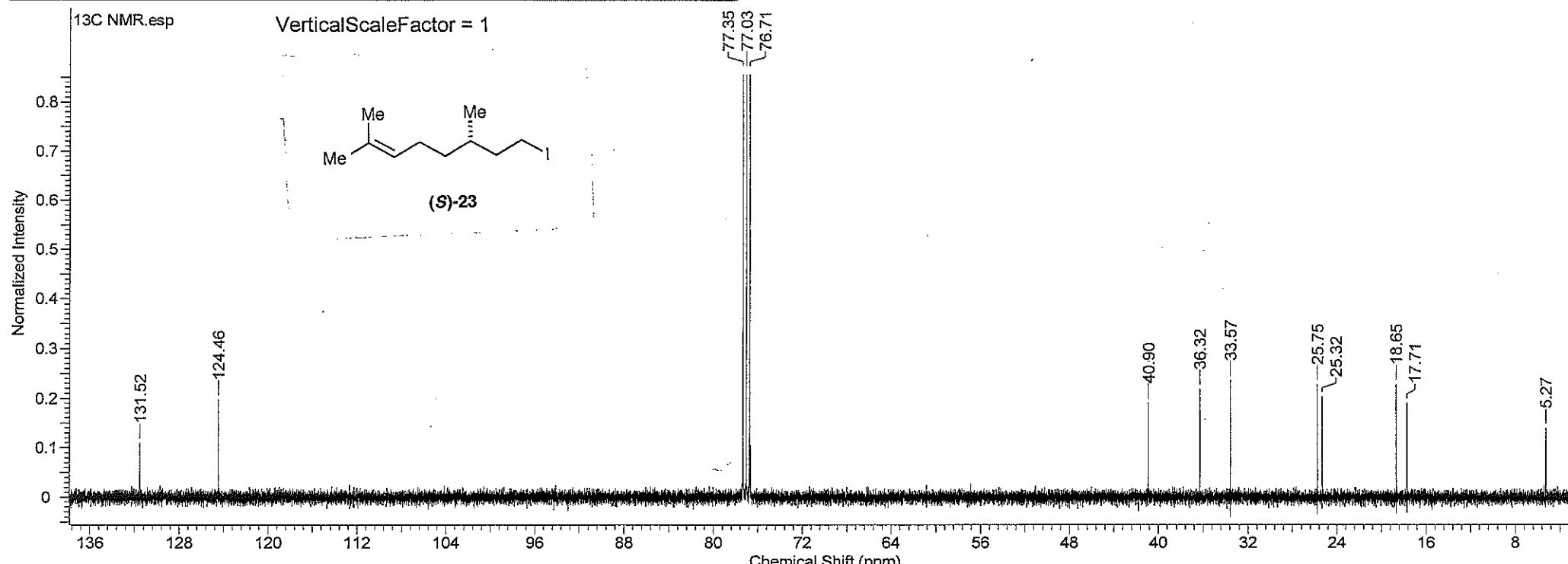
HL102-029  
mPROTON CDCl<sub>3</sub> {e:\bruk400data\2011\Feb} ejt 8



(S)-23

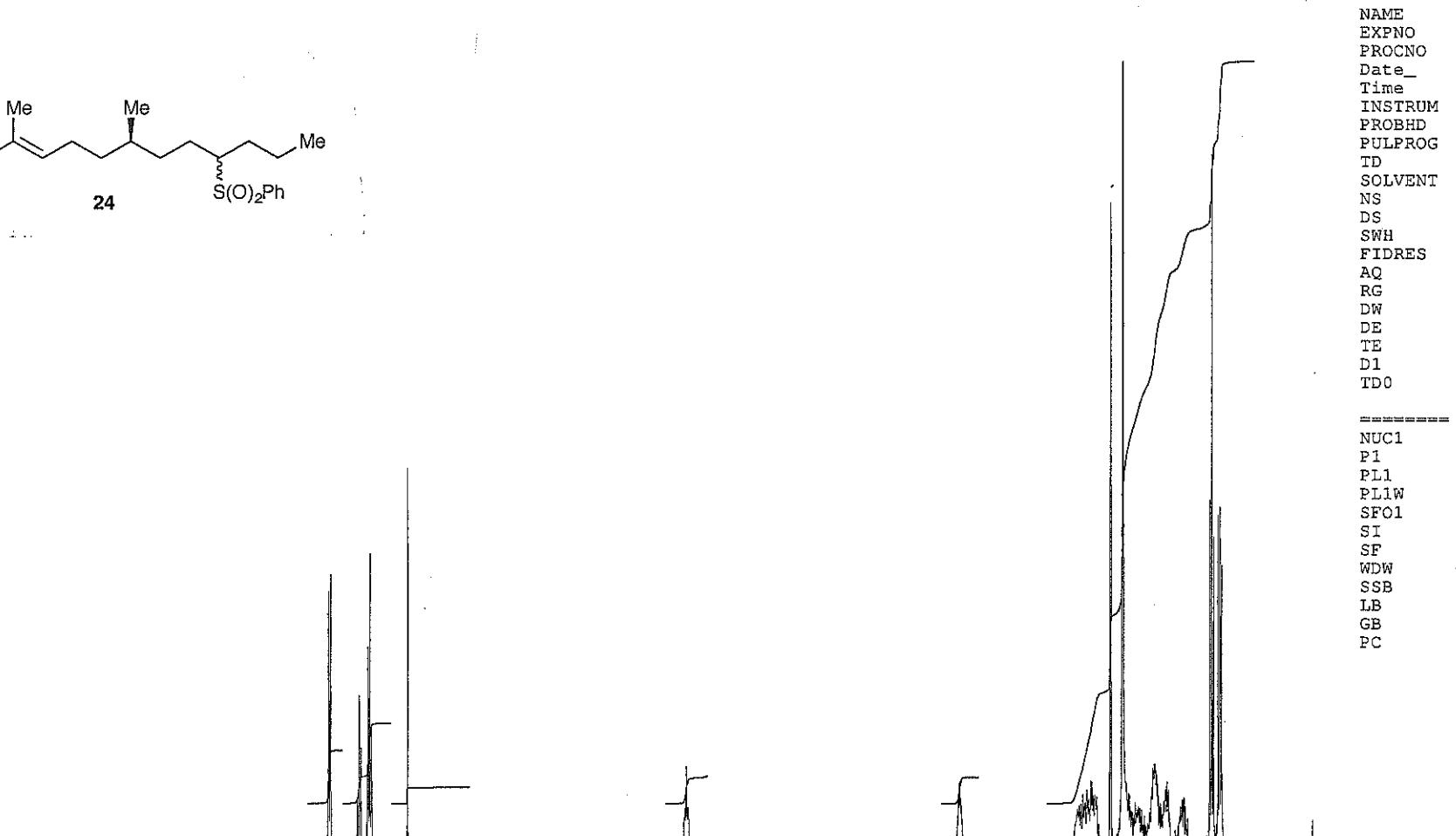
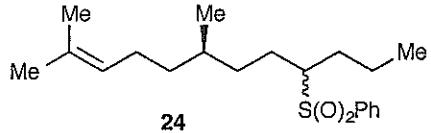


Acquisition Time (sec)	1.0835	Comment	HL092-002 mCARBON CDCl3 {e:\ bruk400data\2010\Aug} eit 40	Date	12 Aug 2010 15:30:24
Date Stamp	12 Aug 2010 15:30:24				
File Name	C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL092 - (R)-citronellol iodonation\HL092-002\13C NMR\fid		Frequency (MHz)	100.61	
Nucleus	13C	Number of Transients	256	Origin	AV400
Owner	Administrator	Points Count	1048576	Original Points Count	32768
SW(cyclical) (Hz)	30241.94	Solvent	CHLOROFORM-d	Pulse Sequence	zgpg30
Sweep Width (Hz)	30241.91	Temperature (degree C)	21.500	Spectrum Offset (Hz)	11335.2197
				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

HL093-001  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2010/Sep ejt 14

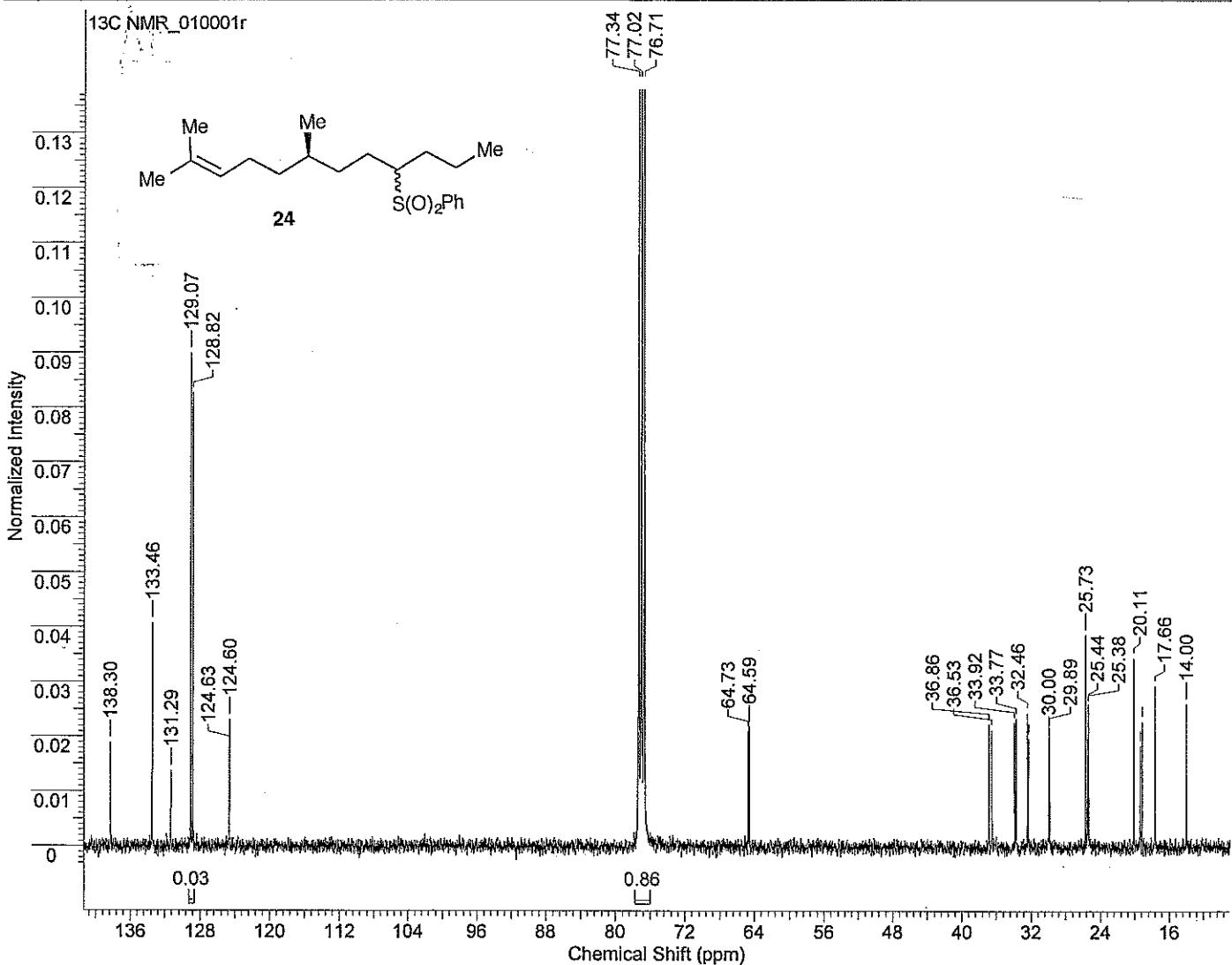


NAME 2010-09-20-ejt-14  
EXPNO 10  
PROCNO 1  
Date\_ 20100920  
Time 12.12  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 322  
DW 48.400 usec  
DE 13.38 usec  
TE 294.2 K  
D1 1.0000000 sec  
TDO 1

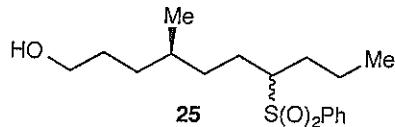
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300471 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

10 9 8 7 6 5 4 3 2 1 0 ppm  
5.61 8.50 1.72  
2.88  
2.78  
78.50

<b>Acquisition Time (sec)</b>	1.3631
<b>Comment</b>	Leo 0910-040 HL093-001 mCARBON CDCl <sub>3</sub> {E:\ bruk400service_data\2010\Sep} Administrator 56
<b>Date</b>	20 Sep 2010 10:57:04
<b>Date Stamp</b>	20 Sep 2010 10:57:04
<b>File Name</b>	E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL093 - Sulfone alkylation\HL093-001\13C NMR_010001r
<b>Frequency (MHz)</b>	100.64
<b>Nucleus</b>	<sup>13</sup> C
<b>Number of Transients</b>	10240
<b>Origin</b>	AV400_S
<b>Original Points Count</b>	32768
<b>Owner</b>	Administrator
<b>Points Count</b>	32768
<b>Pulse Sequence</b>	zgpg30
<b>Receiver Gain</b>	2050.00
<b>SW(cyclical) (Hz)</b>	24038.46
<b>Solvent</b>	CHLOROFORM-d
<b>Spectrum Offset (Hz)</b>	10063.3350
<b>Sweep Width (Hz)</b>	24037.73
<b>Temperature (degree C)</b>	23.600



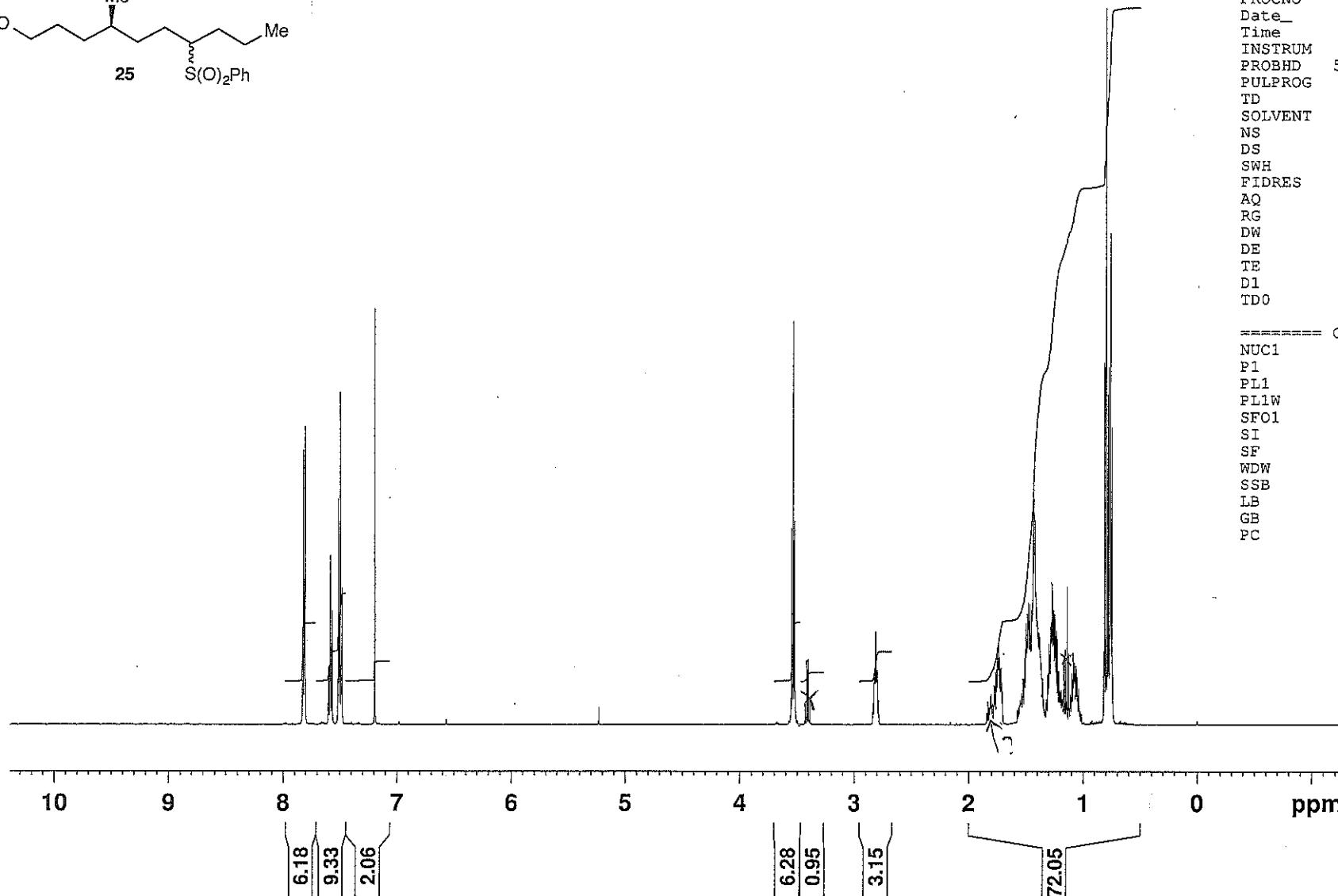
HL093-002  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2010/Sep ejt 15



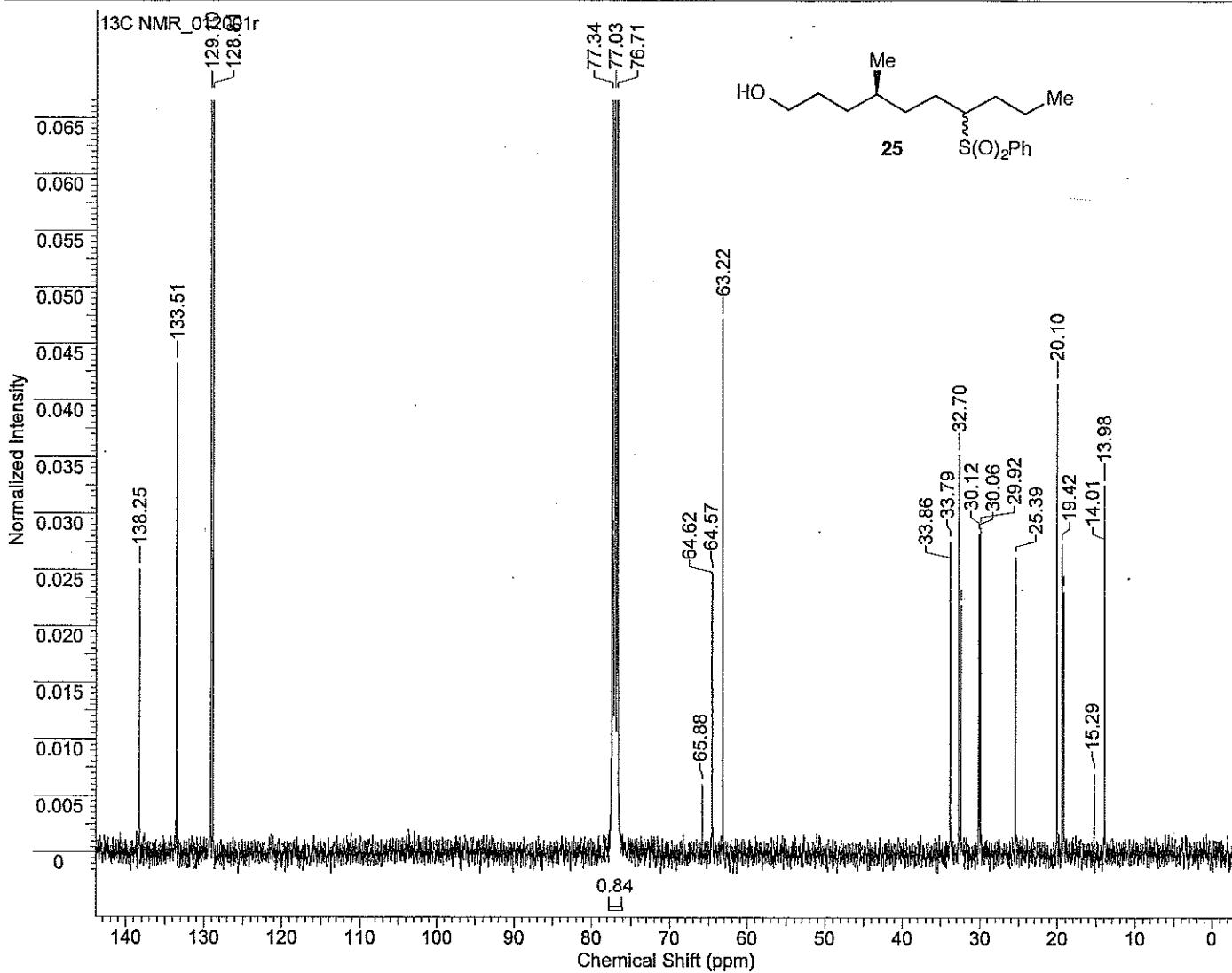
NAME 2010-09-20-ejt-15  
EXPNO 10  
PROCNO 1  
Date 20100920  
Time 12.16  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 322  
DW 48.400 usec  
DE 13.38 usec  
TE 294.3 K  
D1 1.00000000 sec  
TDO 1

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

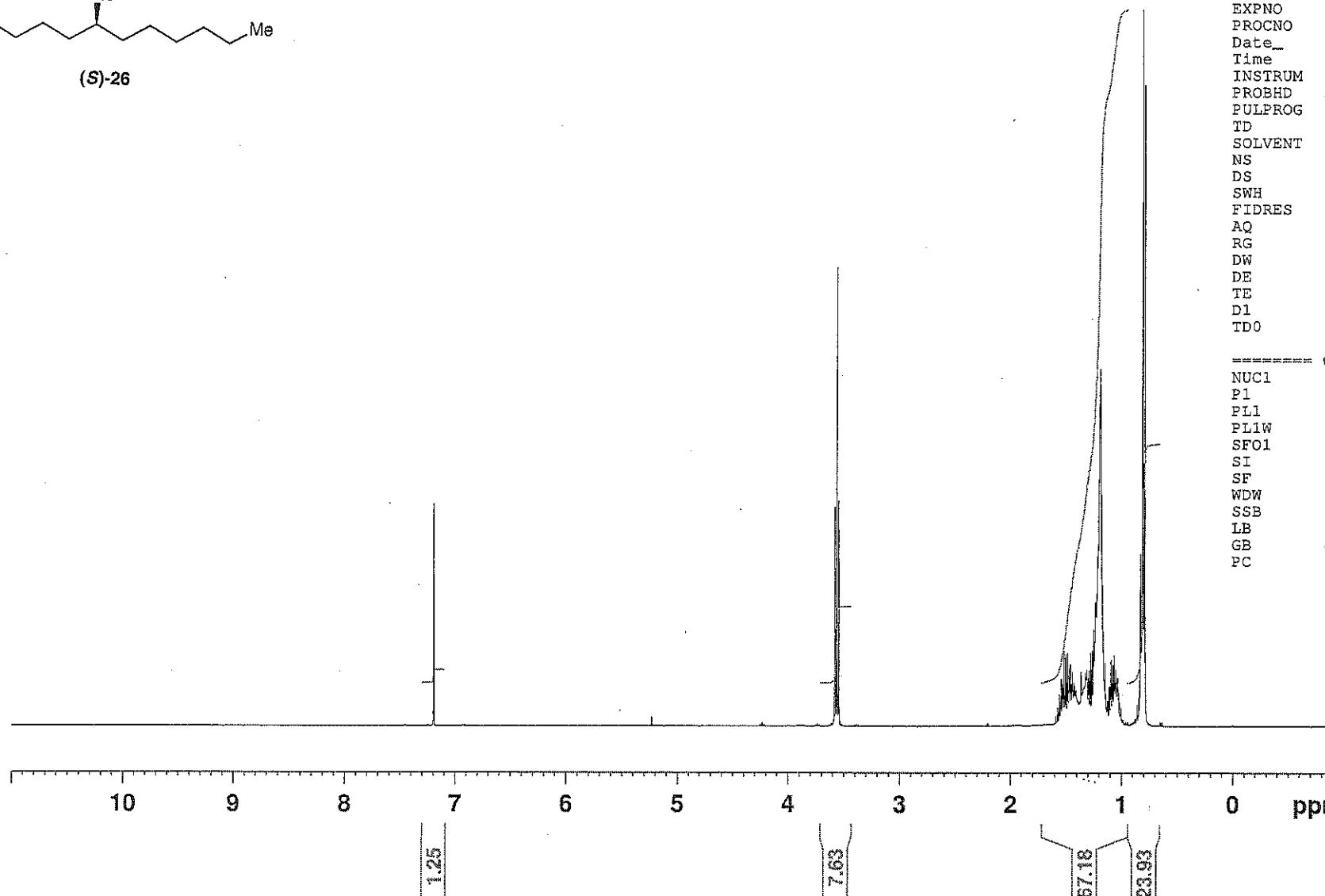
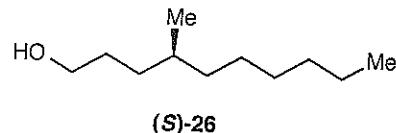
NUC1	1H
P1	8.20 usec
PL1	3.25 dB
PL1W	12.12272263 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300463 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



<b>Acquisition Time (sec)</b>	1.3631
<b>Comment</b>	Leo 0910-043 HI093-002 mCARBON CDCl <sub>3</sub> (E:\ bruk400service_data\2010\Sep) Administrator 8
<b>Date</b>	22 Sep 2010 14:17:36
<b>Date Stamp</b>	22 Sep 2010 14:17:36
<b>File Name</b>	E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL093 - Sulfone alkylation\HL093-002\13C NMR_012001r
<b>Frequency (MHz)</b>	100.64
<b>Number of Transients</b>	12000
<b>Original Points Count</b>	32768
<b>Points Count</b>	32768
<b>Receiver Gain</b>	2050.00
<b>Solvent</b>	CHLOROFORM-d
<b>Sweep Width (Hz)</b>	24037.73
<b>Nucleus</b>	13C
<b>Origin</b>	AV400_S
<b>Owner</b>	Administrator
<b>Pulse Sequence</b>	zgpg30
<b>SW(cyclical) (Hz)</b>	24038.46
<b>Spectrum Offset (Hz)</b>	10063.3350
<b>Temperature (degree C)</b>	23.600

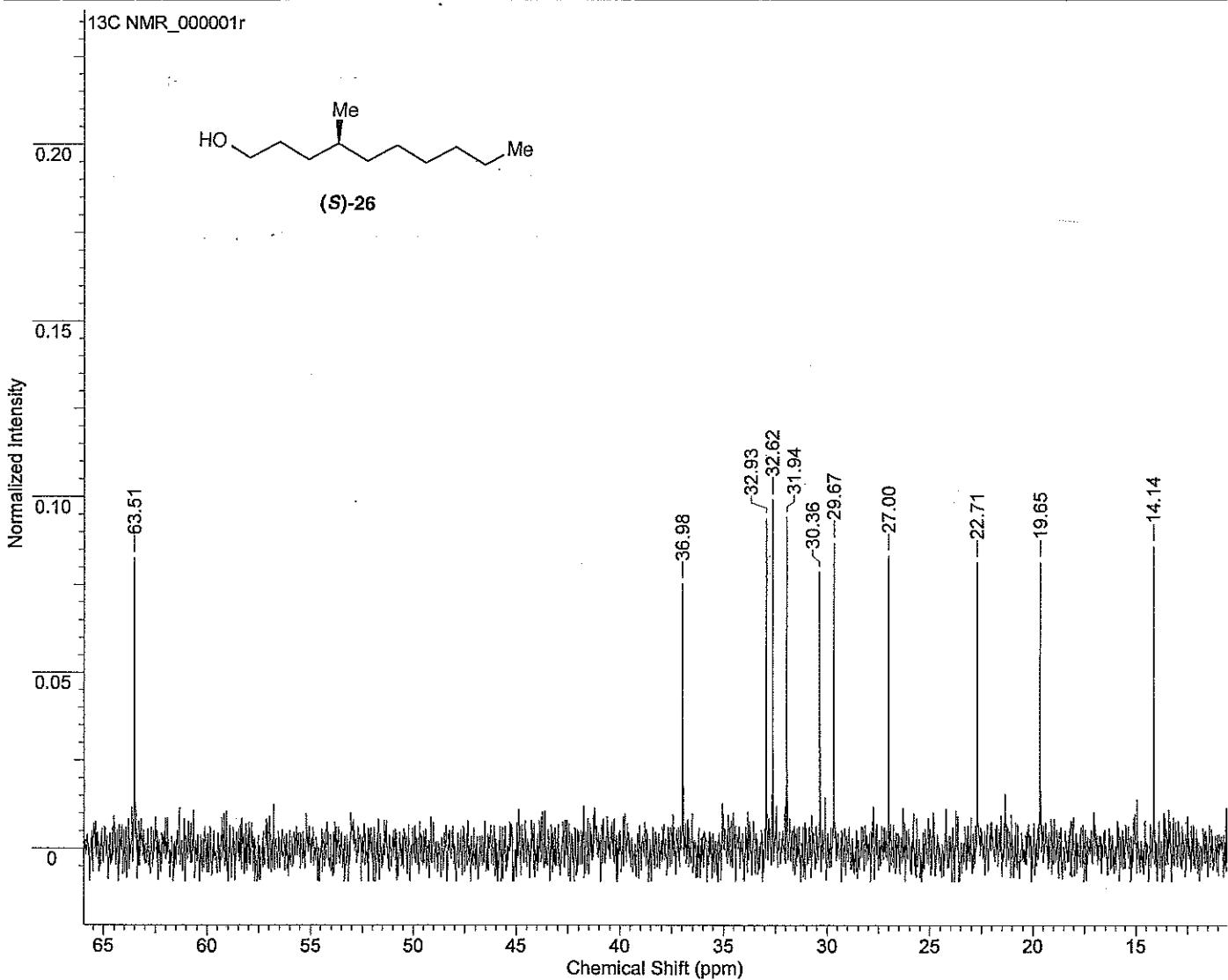


HL094-001  
mPROTON CDCl<sub>3</sub> {e:\ bruk400data\2010\Sep} ejt 54



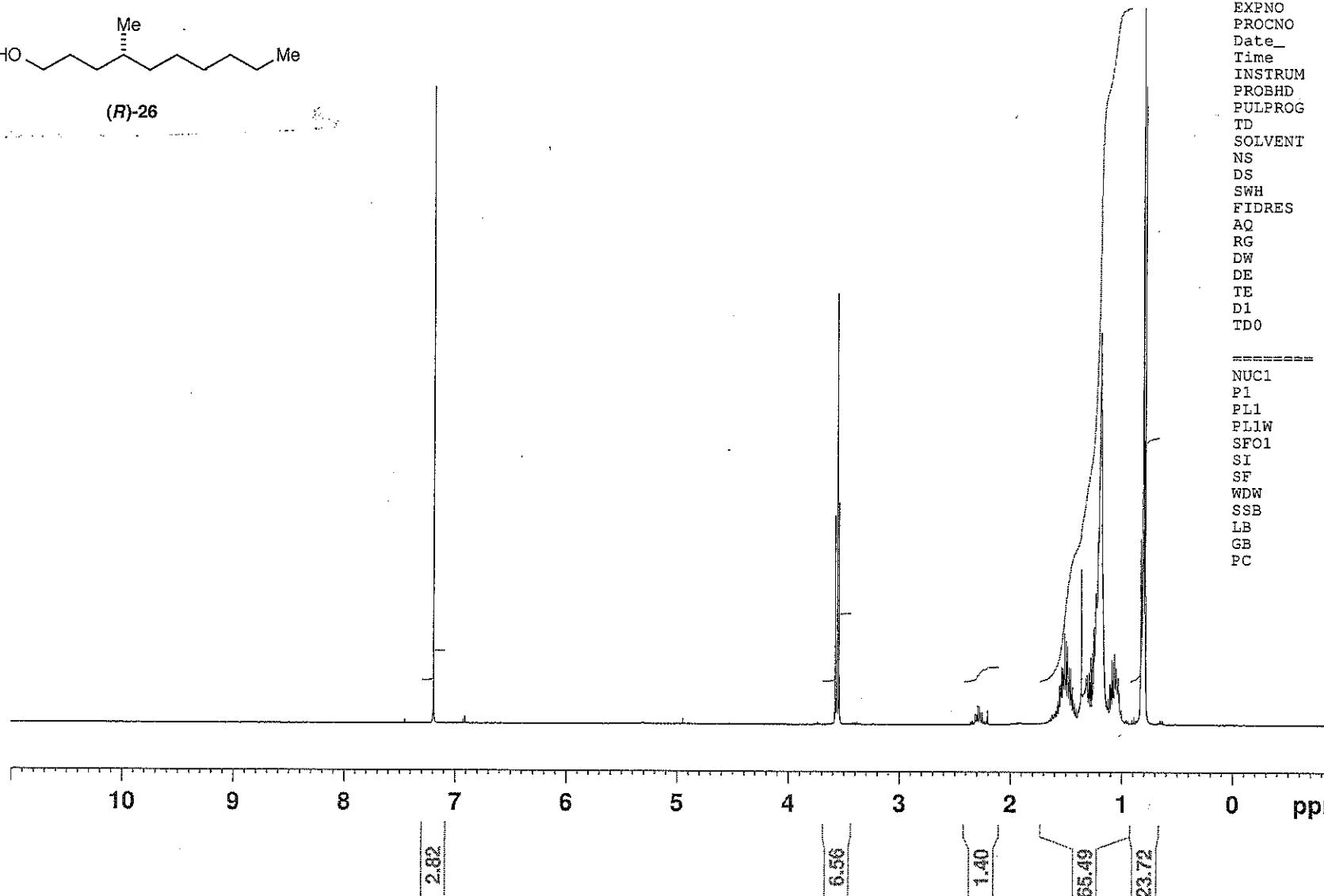
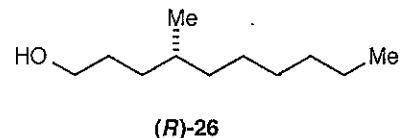
NAME	2010-09-23-ejt-54
EXPNO	10
PROCNO	1
Date_	20100923
Time	17.25
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl <sub>3</sub>
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	256
DW	60.500 usec
DE	9.40 usec
TE	293.6 K
D1	1.00000000 sec
TDO	1
===== CHANNEL f1 =====	
NUC1	1H
P1	10.00 usec
P1L	-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

<b>Acquisition Time (sec)</b>	1.0835	<b>Comment</b>	HL094-001 mCARBON CDCl3 {e:\ bruk400\data\2010\Sep} ejt 50
<b>Date</b>	23 Sep 2010 13:05:04	<b>Date Stamp</b>	23 Sep 2010 13:05:04
<b>File Name</b>	E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL094 - Dithiane formation\HL094-001\13C NMR_000001r		
<b>Frequency (MHz)</b>	100.61	<b>Nucleus</b>	13C
<b>Number of Transients</b>	256	<b>Origin</b>	AV400
<b>Original Points Count</b>	32768	<b>Owner</b>	Administrator
<b>Points Count</b>	32768	<b>Pulse Sequence</b>	zgpg30
<b>Receiver Gain</b>	512.00	<b>SW(cyclical) (Hz)</b>	30241.94
<b>Solvent</b>	CHLOROFORM-d	<b>Spectrum Offset (Hz)</b>	11335.2197
<b>Sweep Width (Hz)</b>	30241.01	<b>Temperature (degree C)</b>	21.300



HL102-032  
mPROTON CDCl<sub>3</sub> {e:\bruk400data\2011\Feb} ejt 45

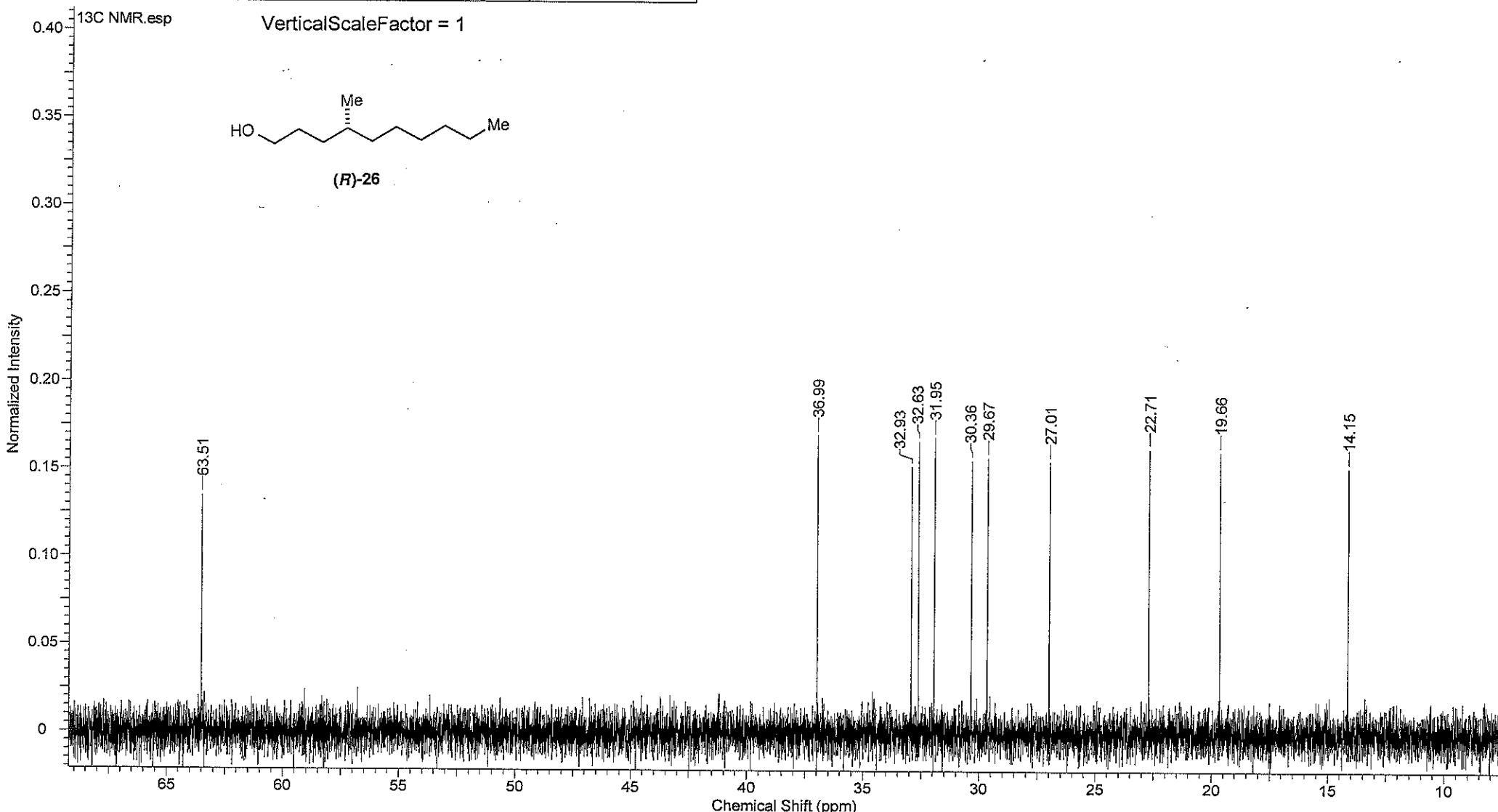
**BRUKER**  
400 MHz



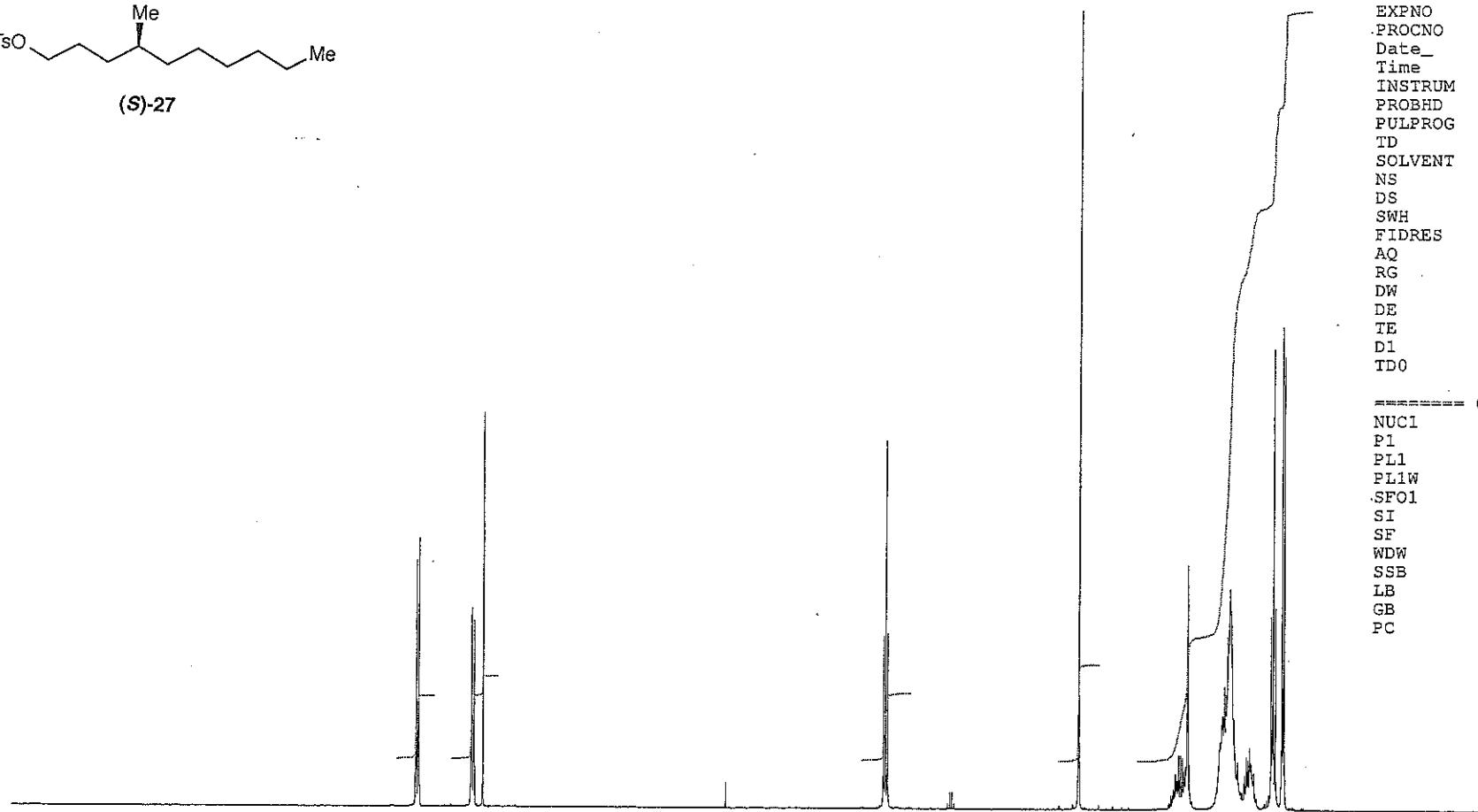
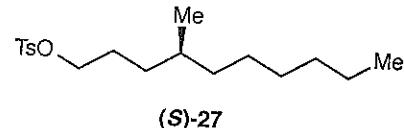
NAME 2011-02-25-ejt-45  
EXPNO 10  
PROCNO 1  
Date 20110225  
Time 10.32  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 406  
DW 60.500 usec  
DE 9.40 usec  
TE 293.4 K  
D1 1.00000000 sec  
TDO 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SF01 400.1324710 MHz  
SI 32768  
SF 400.1300366 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3/15/2011 10:04:19 AM

Acquisition Time (sec)	1.0835	Comment	HL094-001 mCARBON CDCl3 {e:\ bruk400data\2010\Sep} ejt 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 CDCl<sub>3</sub> {e:\ bruk400data\2010\Nov} ejt 12



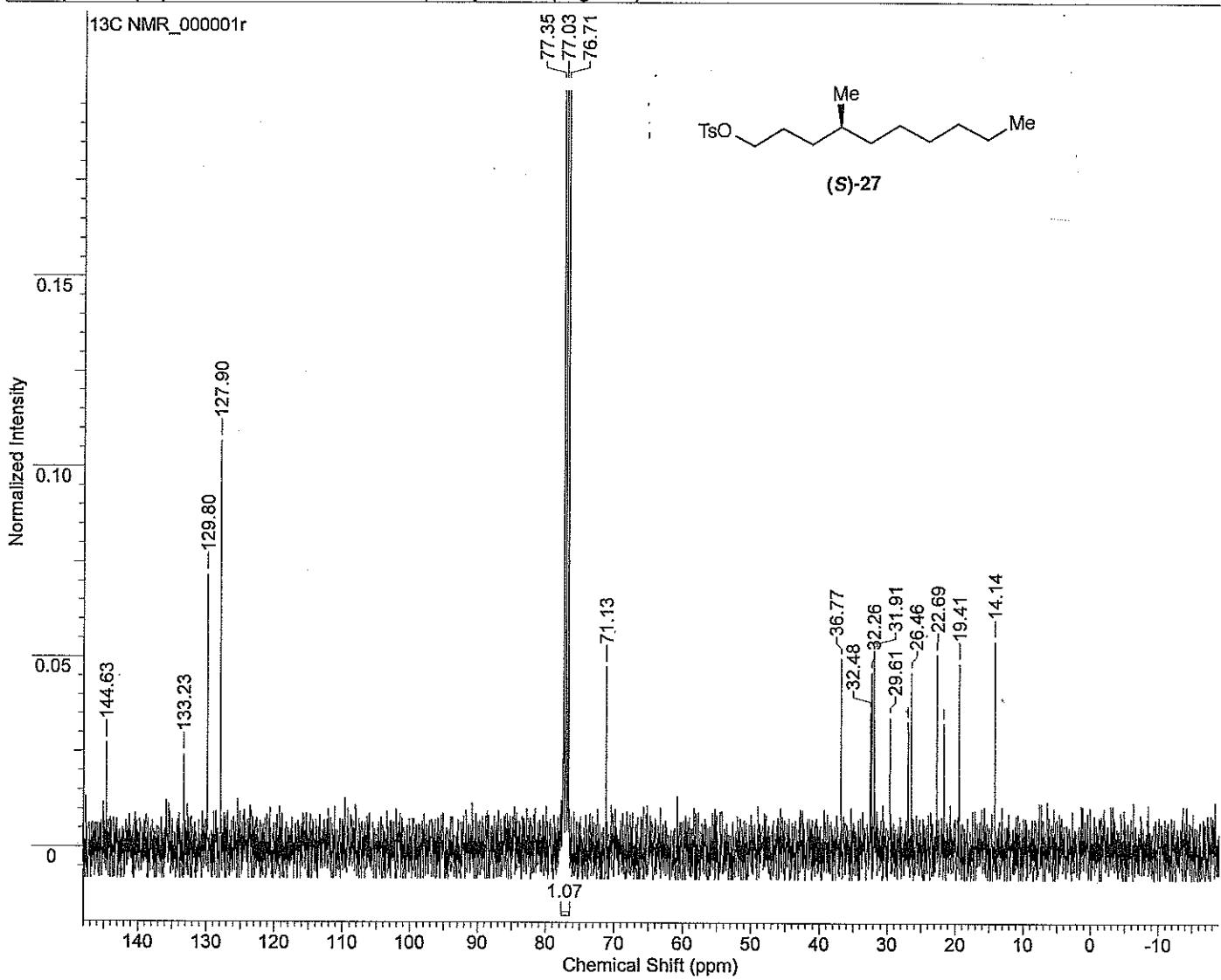
NAME 2010-11-16-ejt-12  
 EXPNO 10  
 PROCNO 1  
 Date 20101117  
 Time 4.53  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 406  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 292.9 K  
 D1 1.00000000 sec  
 TDO 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

5.87 7.81 6.34 9.14 70.85

Acquisition Time (sec)	1.0835	Comment	HL098-001 mCARBONnight CDCl3 {e:\ bruk400\data\2010\Nov} eit 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

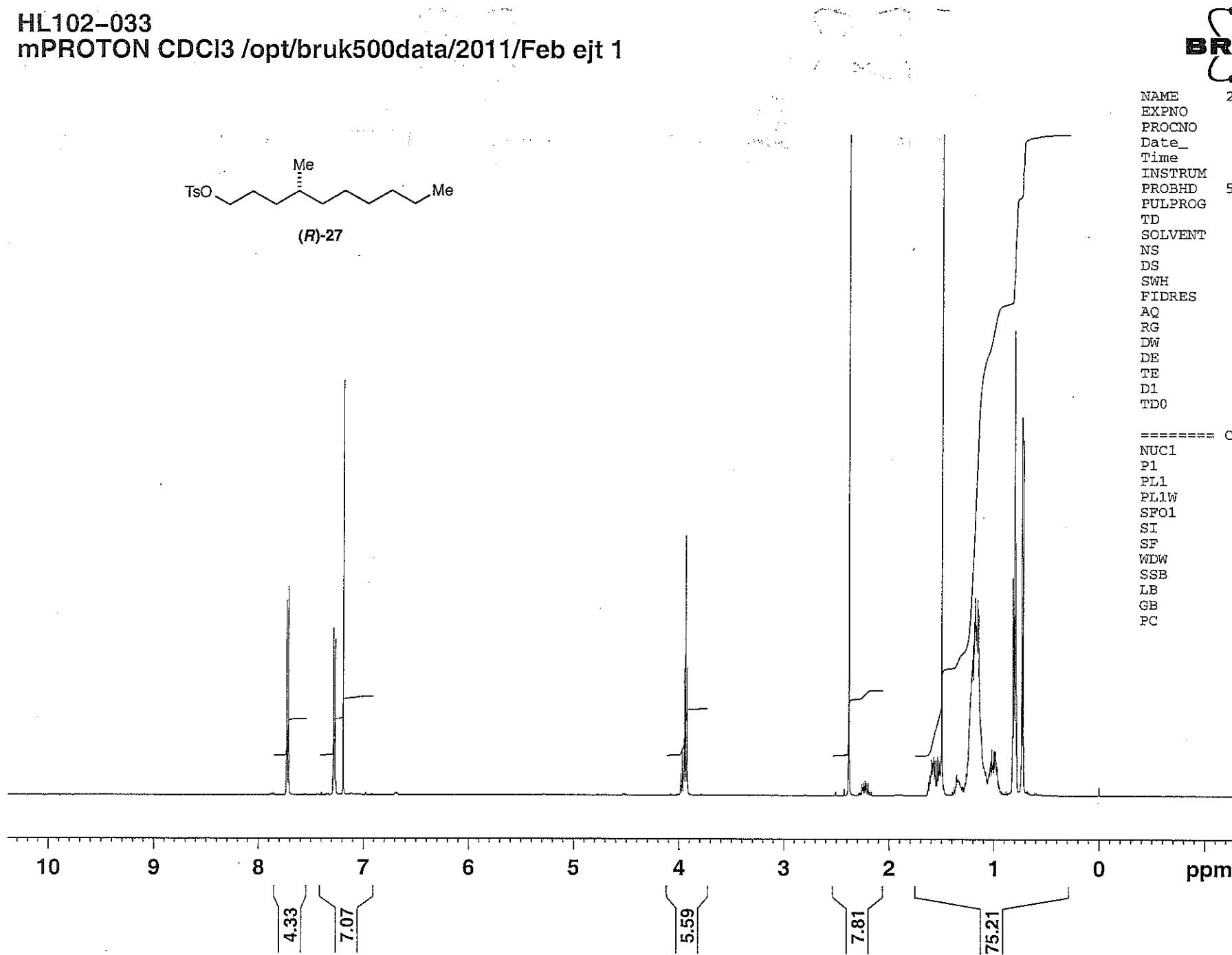


HL102-033  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2011/Feb ejt 1

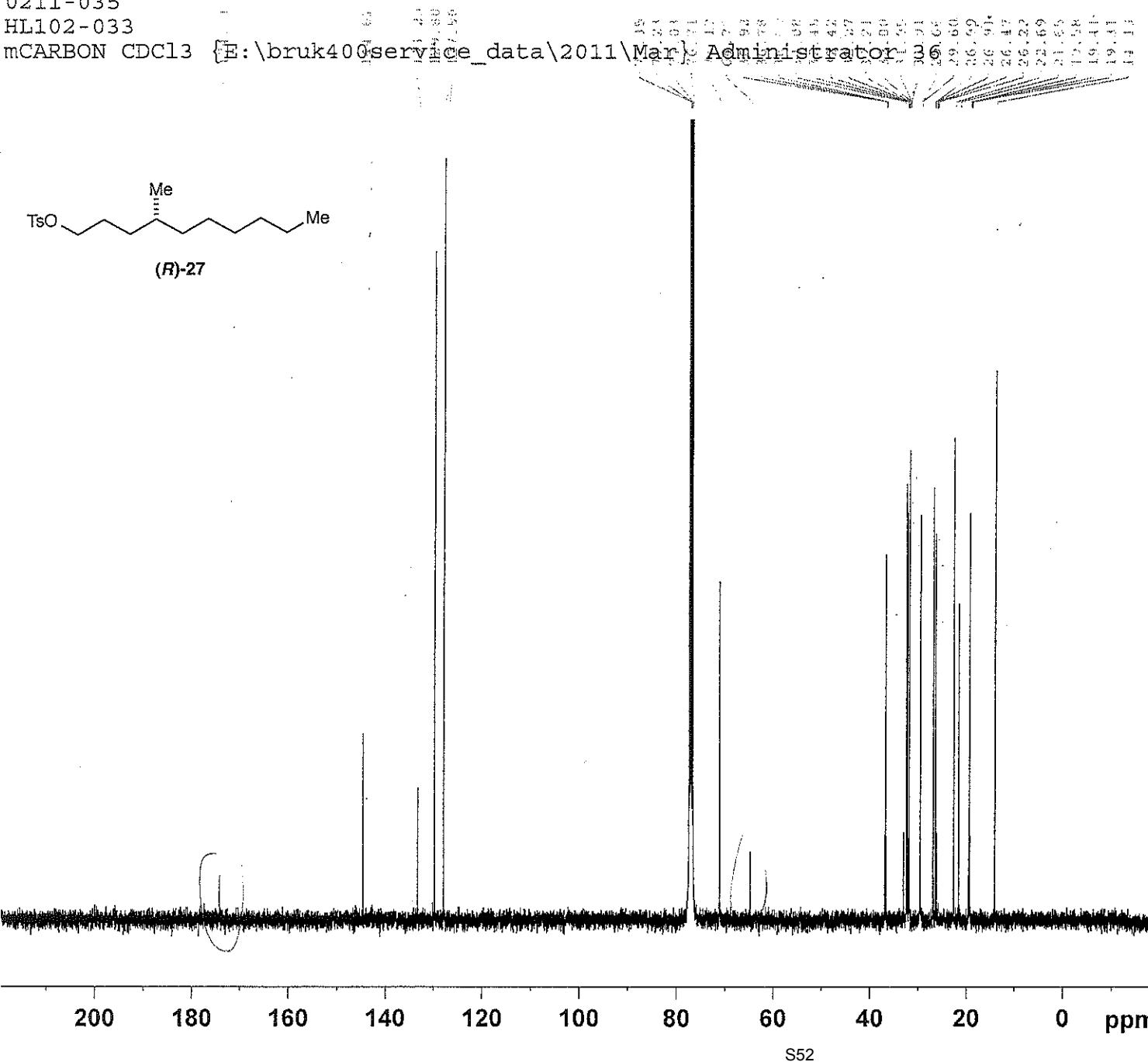


NAME 2011-02-28-ejt-1  
EXPNO 10  
PROCNO 1  
Date\_ 20110228  
Time 11.15  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 322  
DW 48.400 usec  
DE 13.38 usec  
TE 290.6 K  
D1 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 CDCl<sub>3</sub> [E:\bruk40\service\_data\2011\Mar] Administrator 36



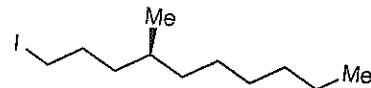
NAME 2011-03-07-Administrator-36

EXPNO 10  
PROCNO 1  
Date 20110307  
Time 15.37  
INSTRUM AV400\_S  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

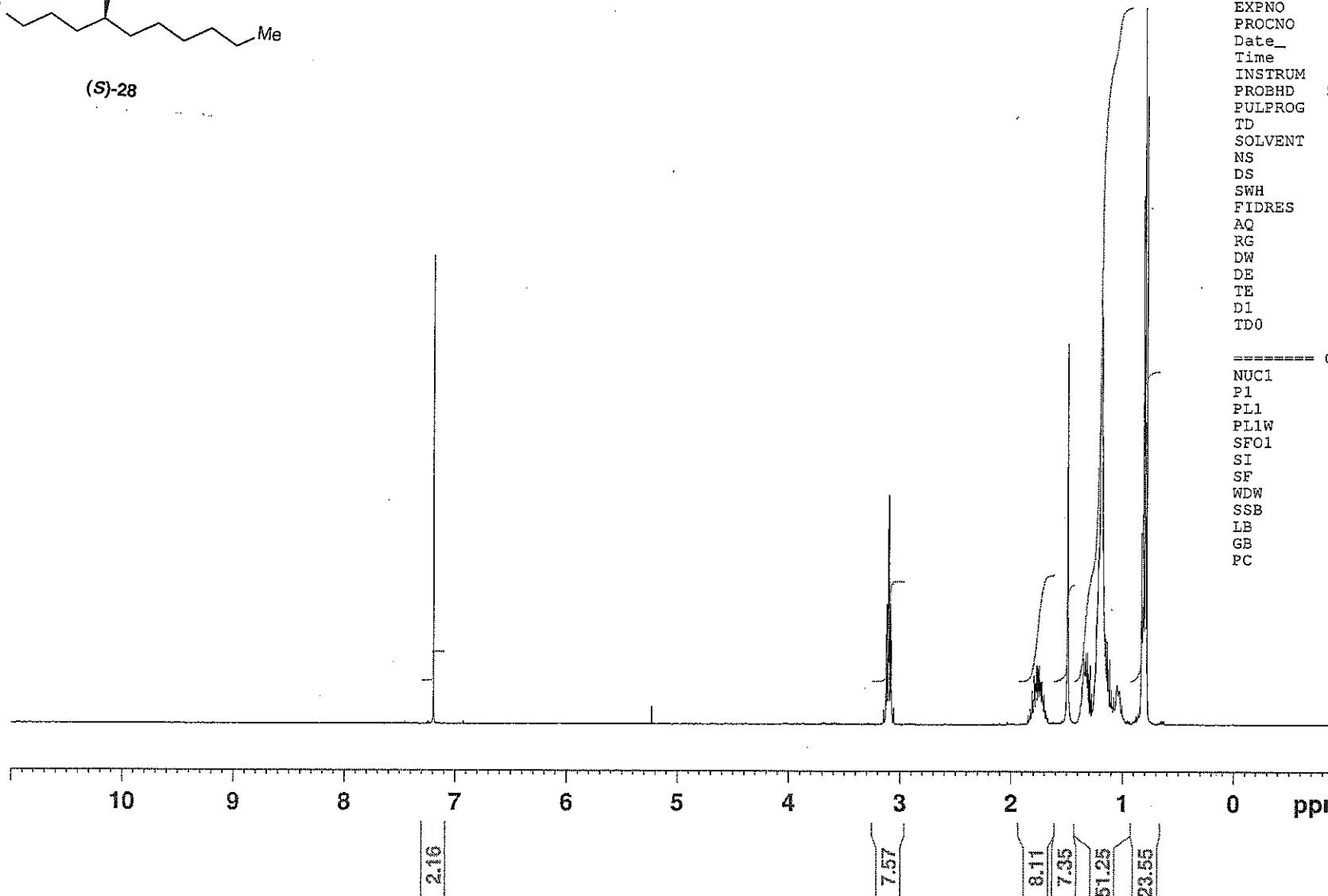
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 33.91046524 W  
SFO1 100.6479773 MHz

===== CHANNEL f2 =====  
CPDPGR2 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 CDCl<sub>3</sub> {e:\bruk400data\2010\Sep} ejt 10



(S)-28



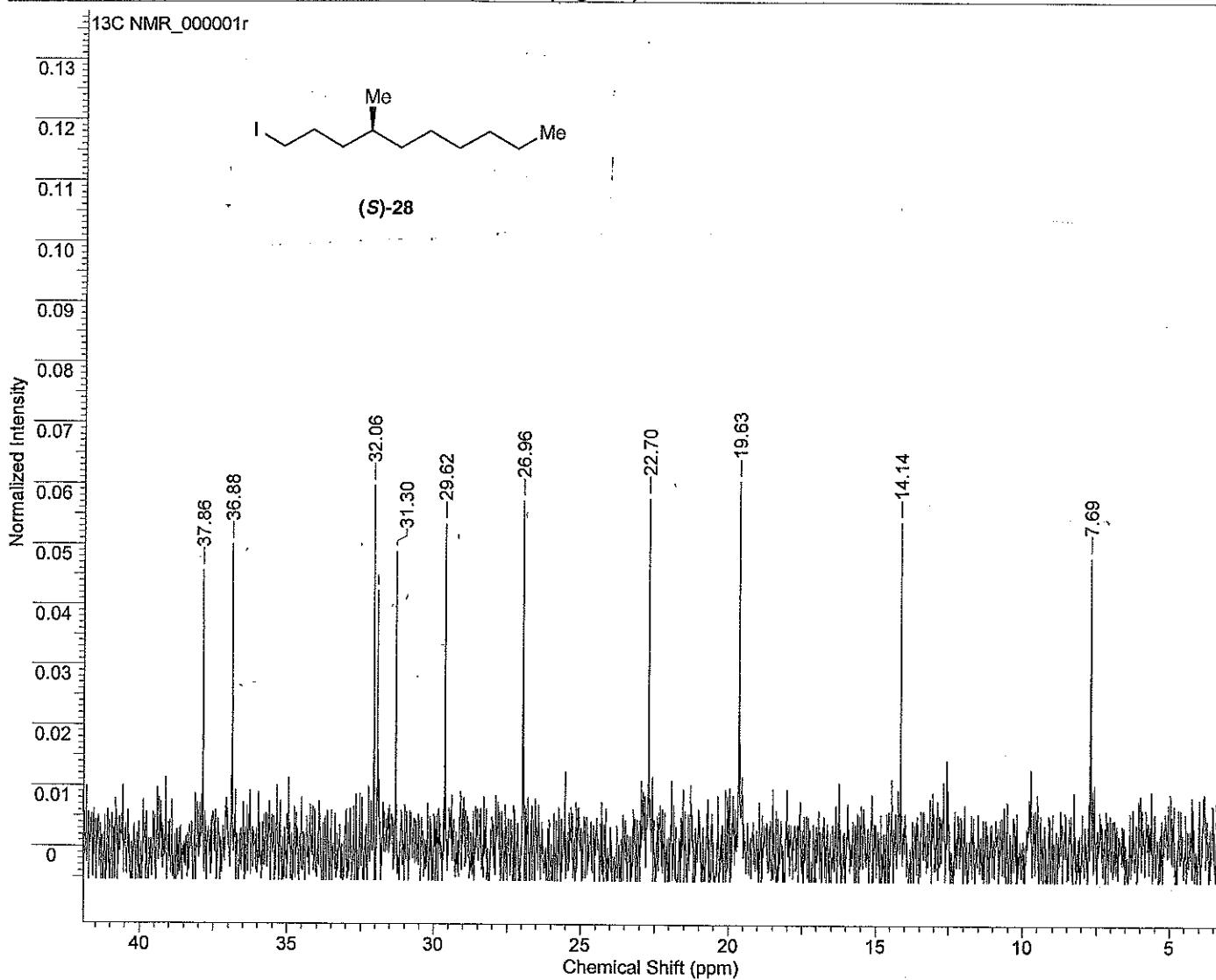
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NAME      2010-09-27-ejt-10
EXPNO        10
PROCNO       1
Date_   20100927
Time     10.29
INSTRUM   AV400
PROBHD   5 mm PABBO BB-
PULPROG  zg30b
TD        65536
SOLVENT    CDC13
NS         16
DS          0
SWH       8264.463 Hz
FIDRES    0.126106 Hz
AQ        3.9649780 sec
RG          322
DW        60.500 usec
DE        9.40  usec
TE        293.9 K
D1      1.00000000 sec
TDO         1

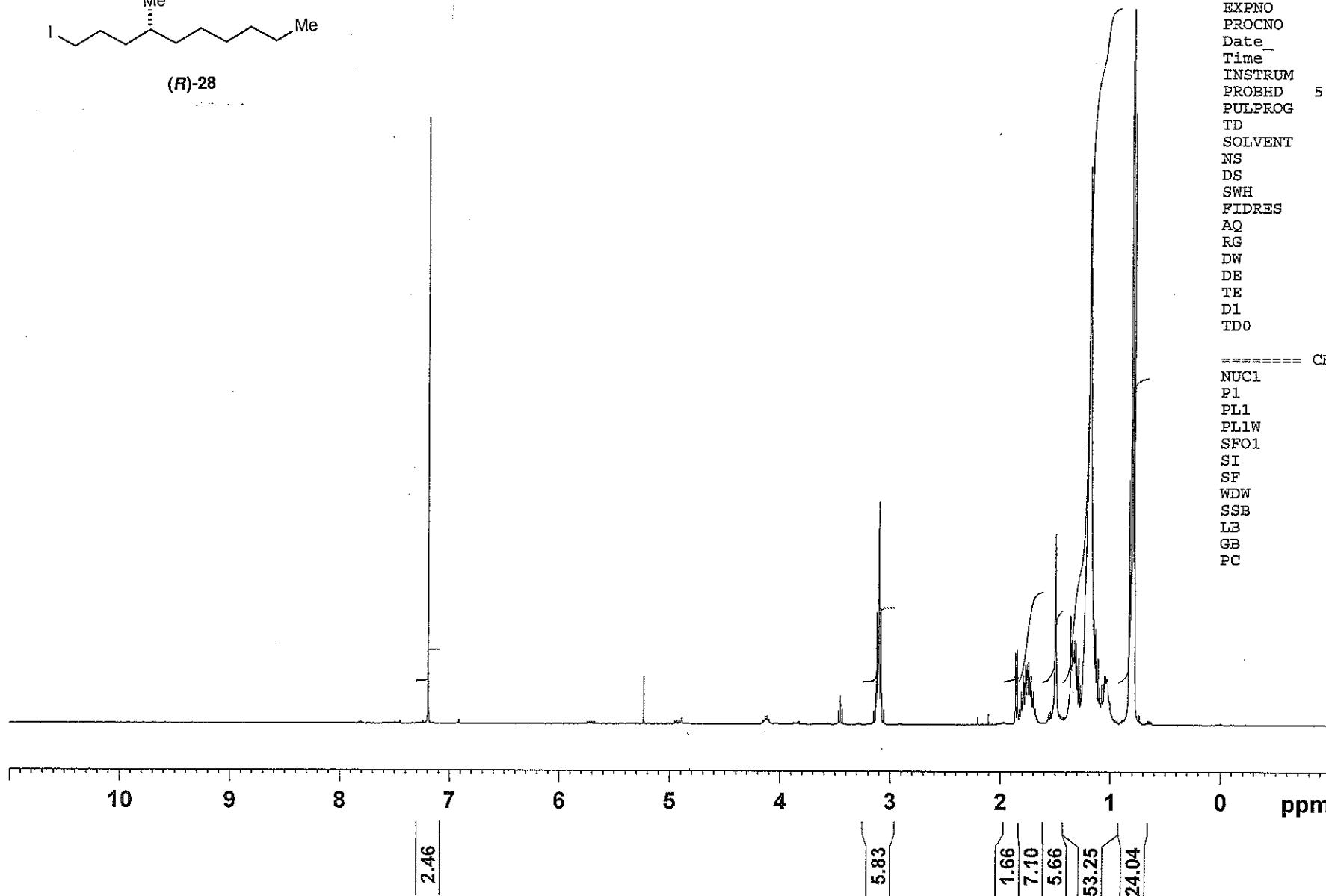
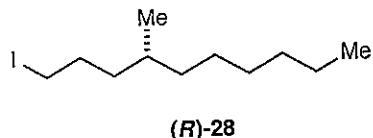
===== CHANNEL f1 =====
NUC1        1H
P1        10.00 usec
PL1       -3.50 dB
PL1W    17.83863831 W
SFO1    400.1324710 MHz
SI        32768
SF      400.1300368 MHz
WDW         EM
SSB          0
LB        0.30 Hz
GB          0
PC        1.00

```

Acquisition Time (sec)	1.0835	Comment	HL094-002 mCARBON CDCl <sub>3</sub> {e:\ bruk400\data\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	<sup>13</sup> C
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



HL100-007  
mPROTON CDCl<sub>3</sub> {e:\bruk400data\2010\Dec} ejt 22

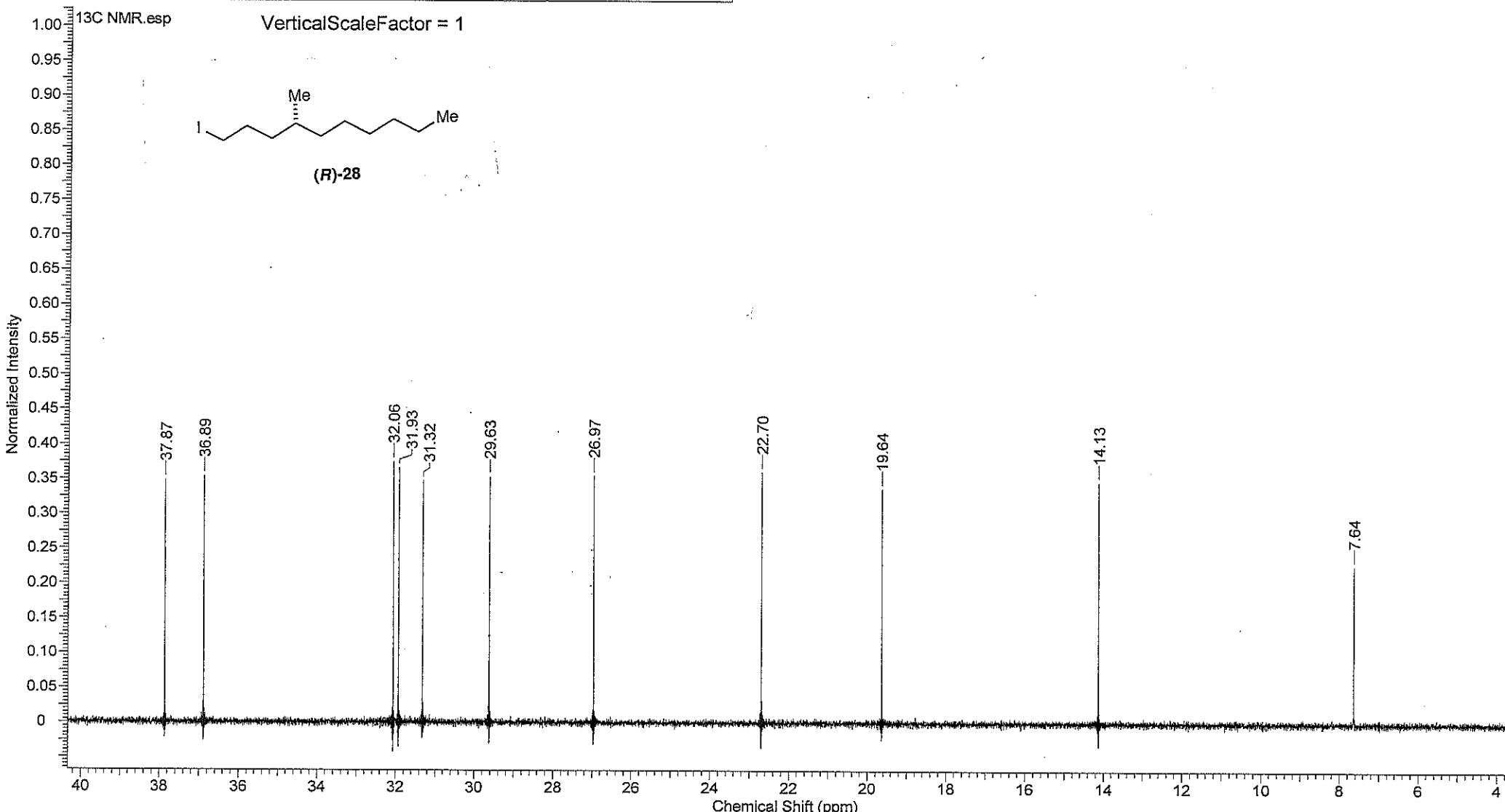


NAME 2010-12-03-ejt-22  
EXPNO 20  
PROCNO 1  
Date 20101203  
Time 14.50  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 322  
DW 60.500 usec  
DE 9.40 usec  
TE 290.5 K  
D1 1.0000000 sec  
TDO 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

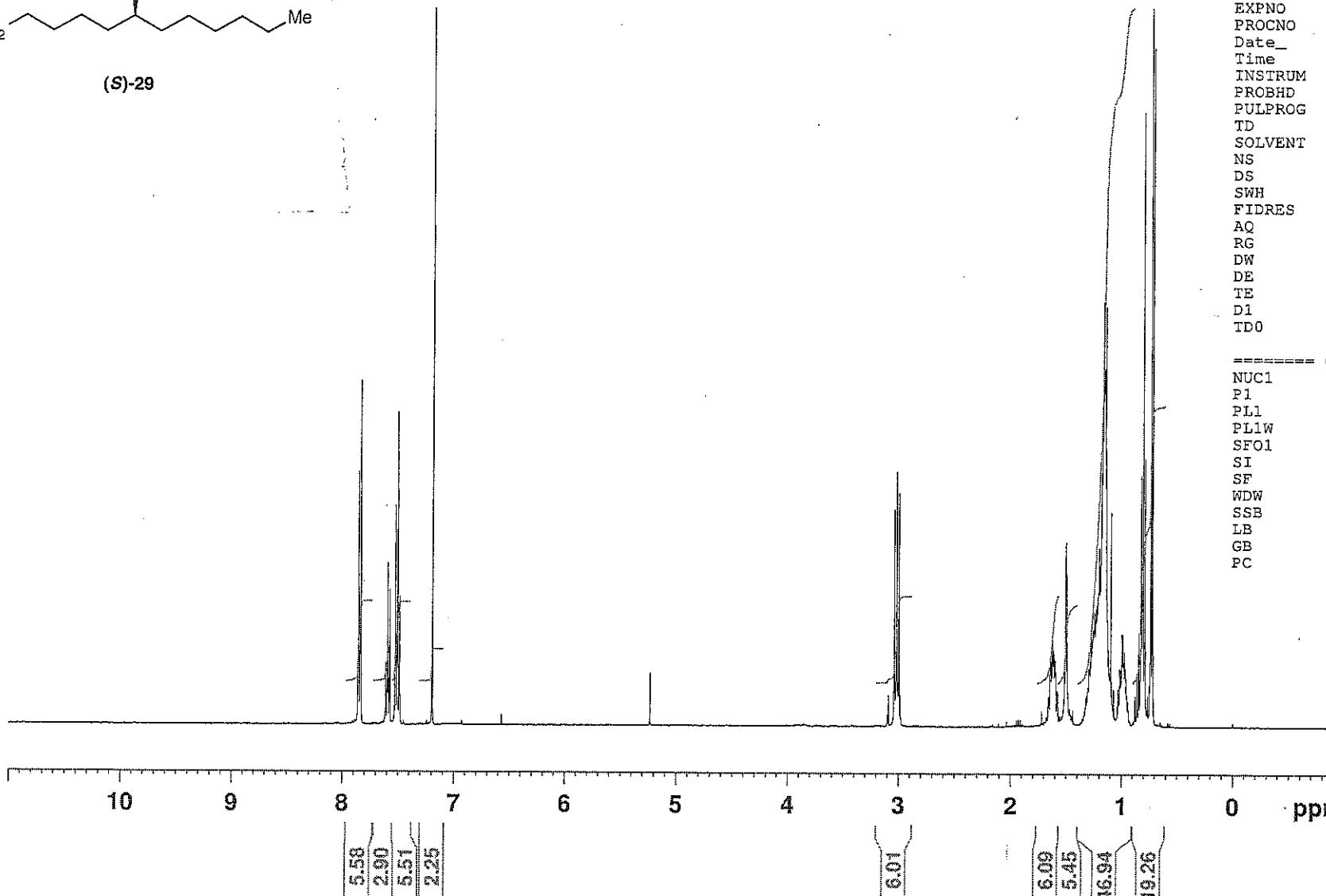
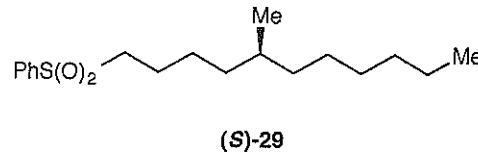
3/15/2011 10:07:46 AM

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 CDCl<sub>3</sub> {e:\bruk400data\2010\Nov} ejt 7

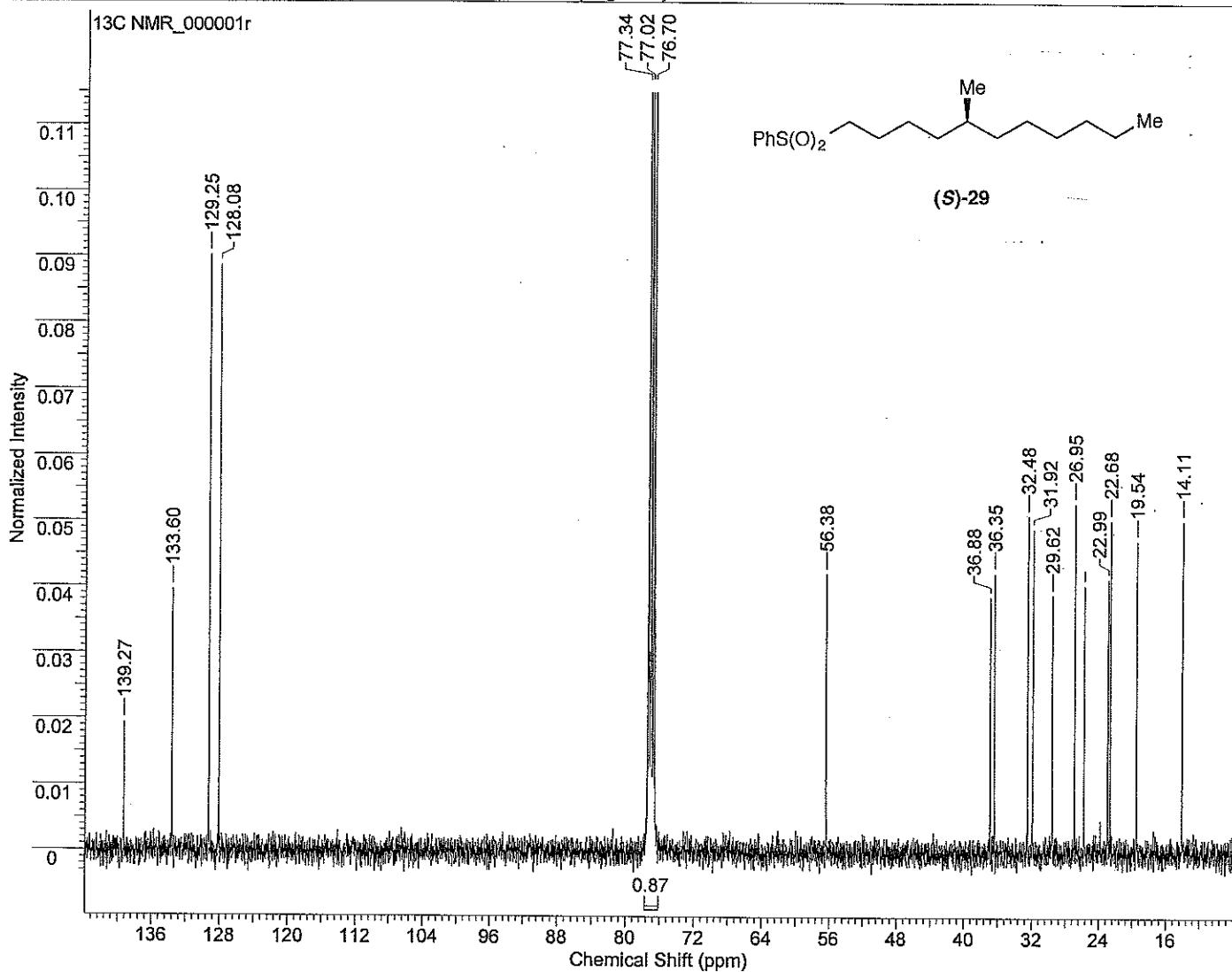
**BRUKER**  
400 MHz



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 CDCl<sub>3</sub>  
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 1.0000000 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

<b>Acquisition Time (sec)</b>	1.3631		
<b>Comment</b>	Leo 1110-055 HL098-003 mCARBON CDCl <sub>3</sub> {E:\bruk400service\data\2010\Nov\Administrator.18}		
<b>Date</b>	19 Nov 2010 08:36:16	<b>Date Stamp</b>	19 Nov 2010 08:36:16
<b>File Name</b>	E:\Postgraduate Database\Experiment Database\Experiment 51-100\HL098 - RHS sulfone synthesis\HL098-003\13C NMR_000001r		
<b>Frequency (MHz)</b>	100.64	<b>Nucleus</b>	<sup>13</sup> C
<b>Number of Transients</b>	4096	<b>Origin</b>	AV400_S
<b>Original Points Count</b>	32768	<b>Owner</b>	Administrator
<b>Points Count</b>	32768	<b>Pulse Sequence</b>	zgpg30
<b>Receiver Gain</b>	2050.00	<b>SW(cyclical) (Hz)</b>	24038.46
<b>Solvent</b>	CHLOROFORM-d	<b>Spectrum Offset (Hz)</b>	10063.3350
<b>Sweep Width (Hz)</b>	24037.73	<b>Temperature (degree C)</b>	25.100

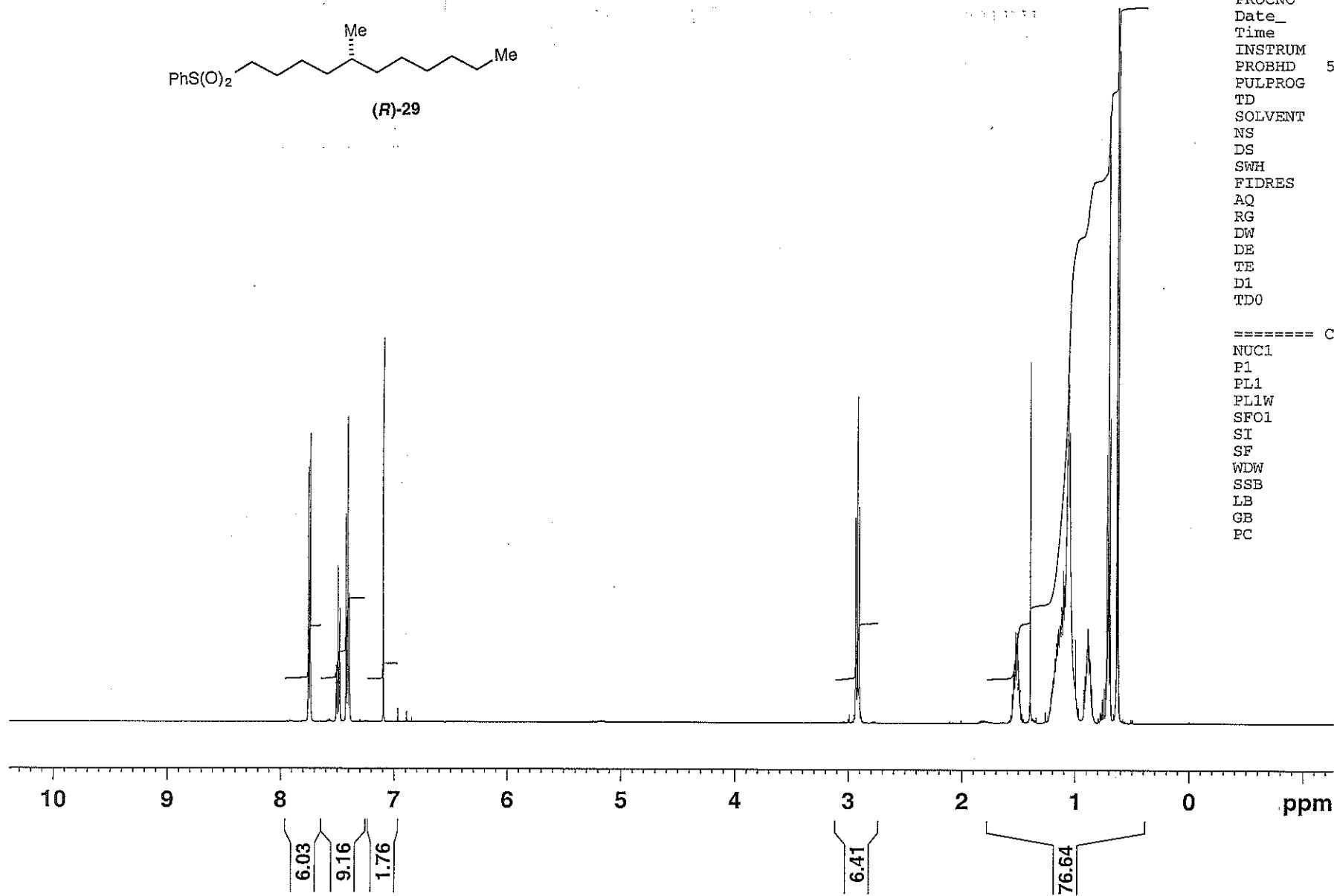


HL102-035  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2011/Jan ejt 1



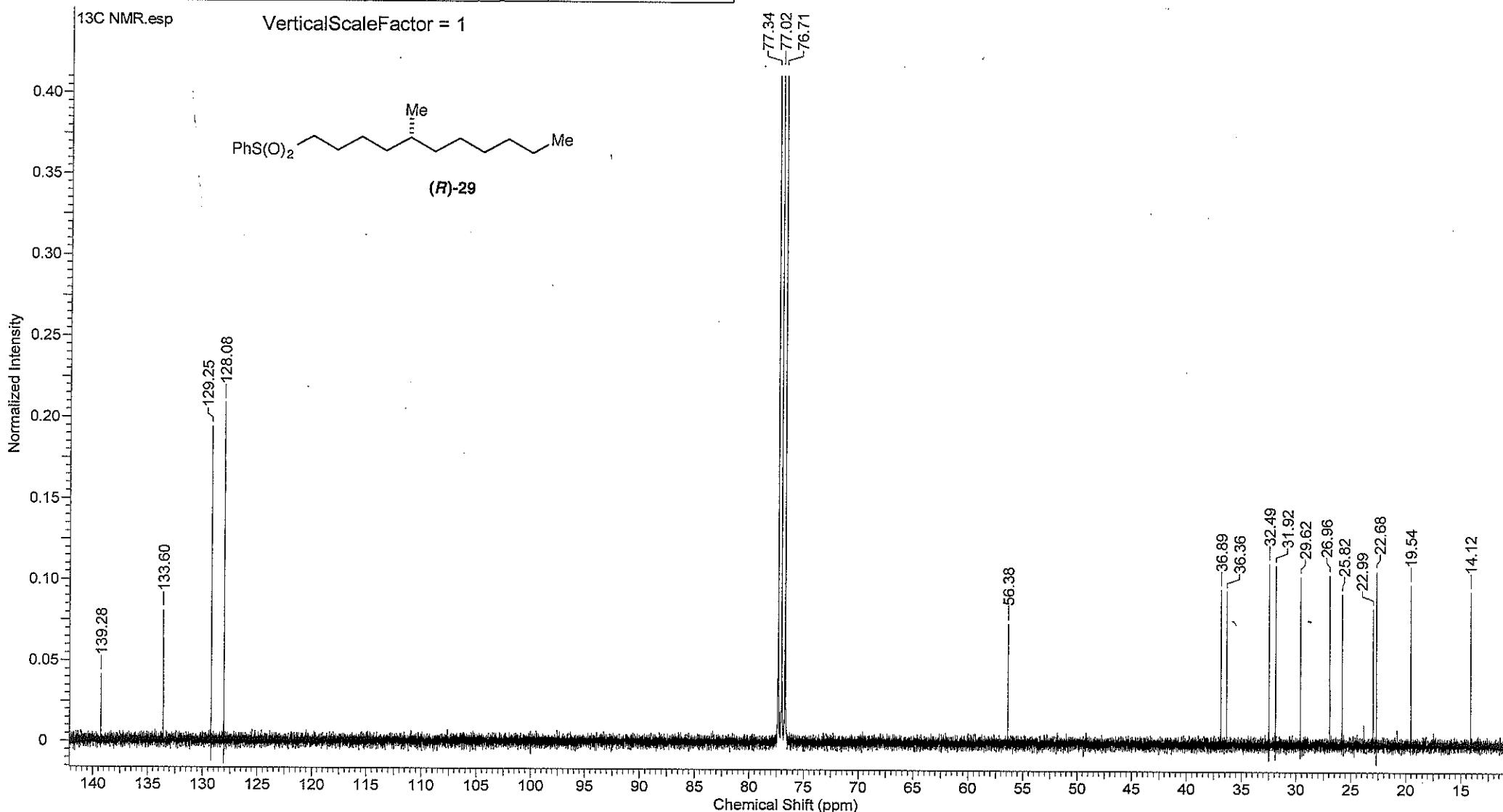
NAME 2011-01-31-ejt-1  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20110131  
 Time 10.49  
 INSTRUM spect  
 PROBHD 5 mm TXI 1H/D-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1719923 sec  
 RG 228  
 DW 48.400 usec  
 DE 13.38 usec  
 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

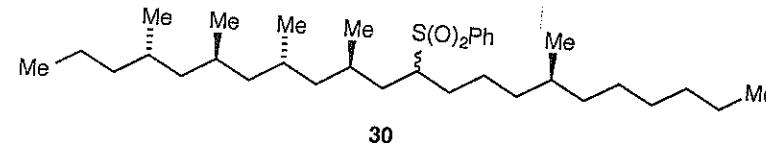


3/15/2011 10:09:13 AM

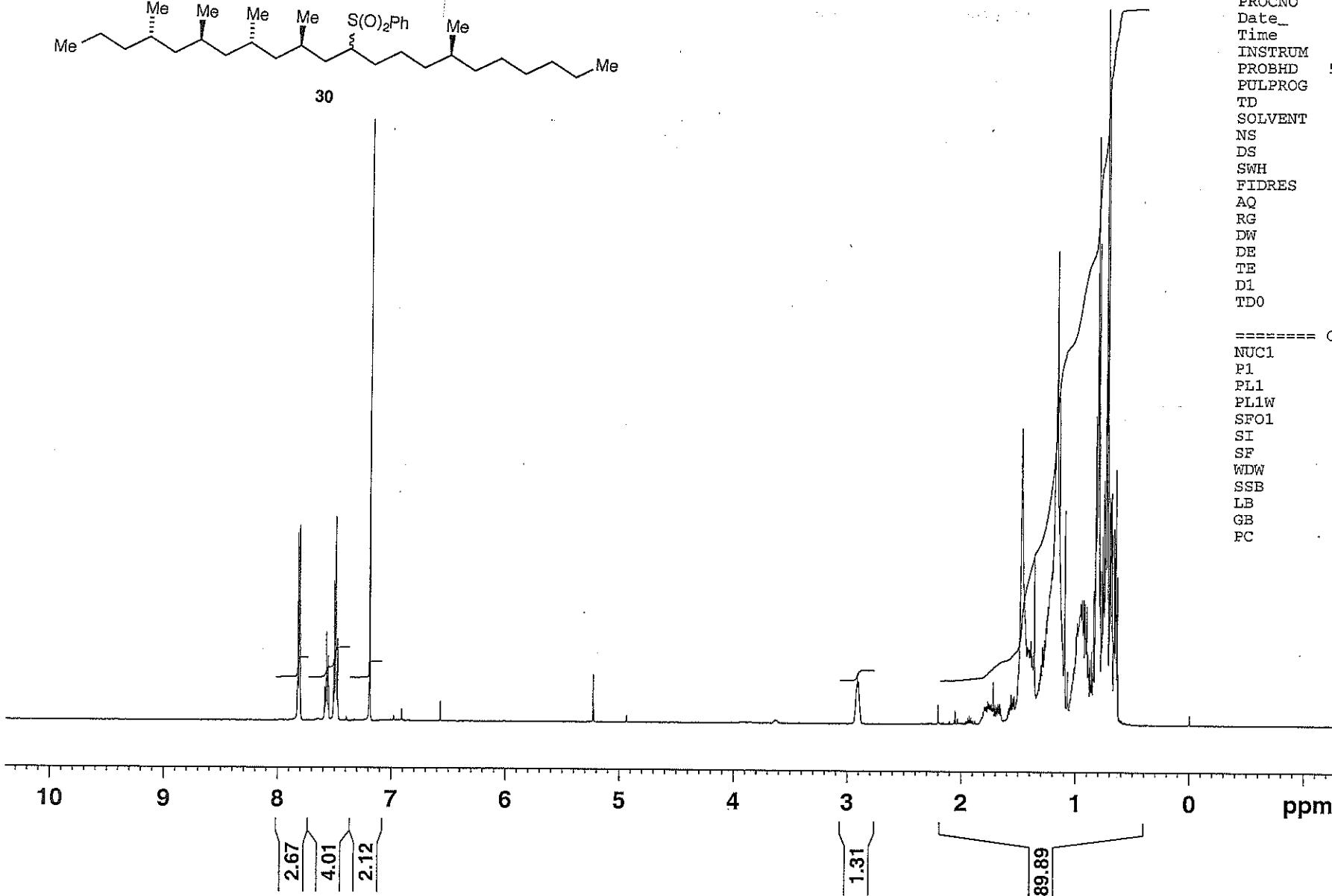
<b>Acquisition Time (sec)</b>	1.3631	<b>Comment</b>	Leo 1110-055 HL098-003 mCARBON CDCl3 {E:\ bruk400service_data\2010\Nov} Administrator 18		
<b>Date</b>	19 Nov 2010 08:36:16	<b>Date Stamp</b>	19 Nov 2010 08:36:16		
<b>File Name</b>	C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL098 - RHS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



HL099-004  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2010/Nov ejt 12



30

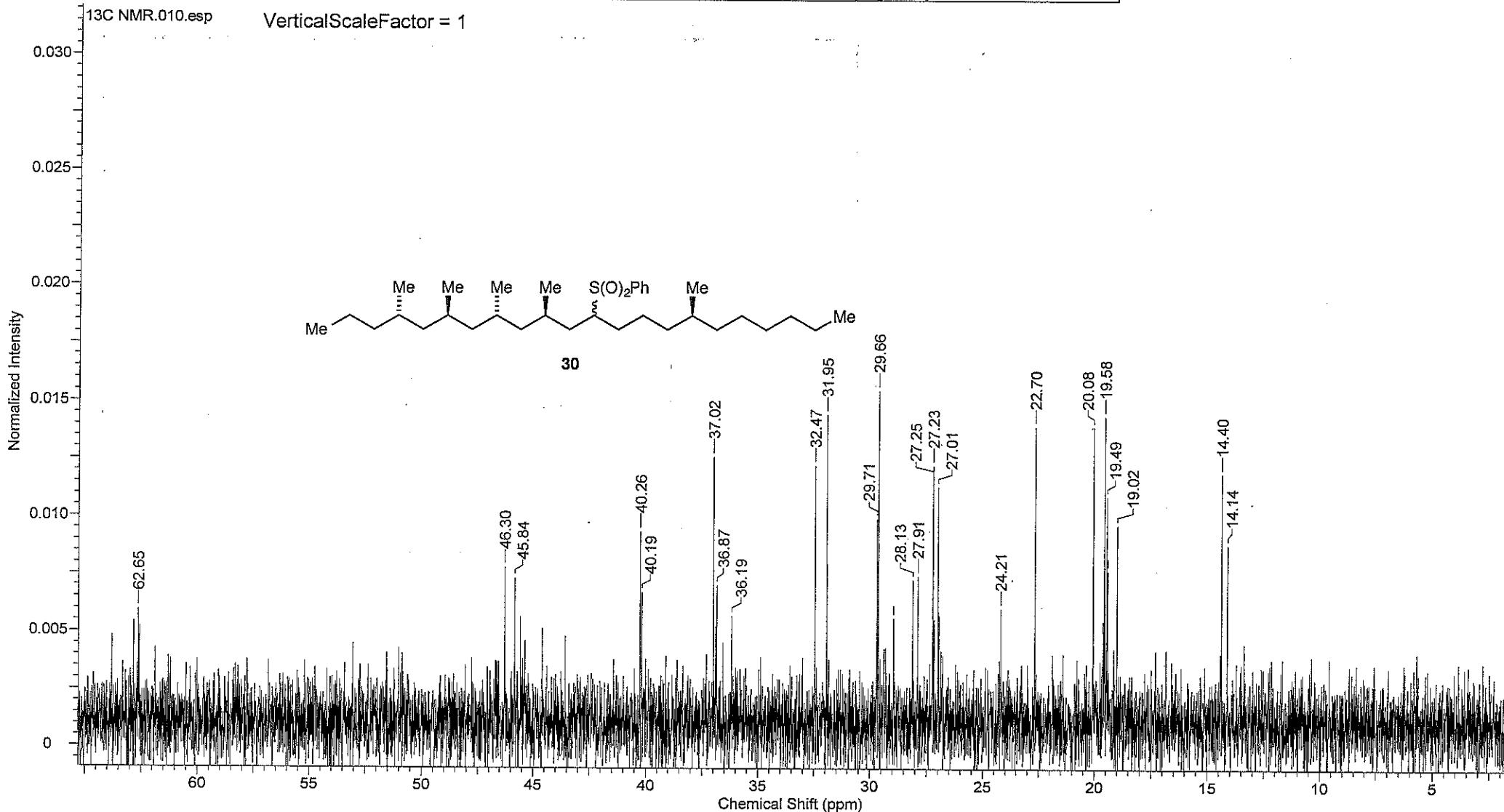


NAME 2010-11-22-ejt-12  
EXPNO 10  
PROCNO 1  
Date\_ 20101122  
Time 12.10  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 322  
DW 48.400 usec  
DE 13.38 usec  
TE 298.1 K  
D1 1.0000000 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 500.1300479 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

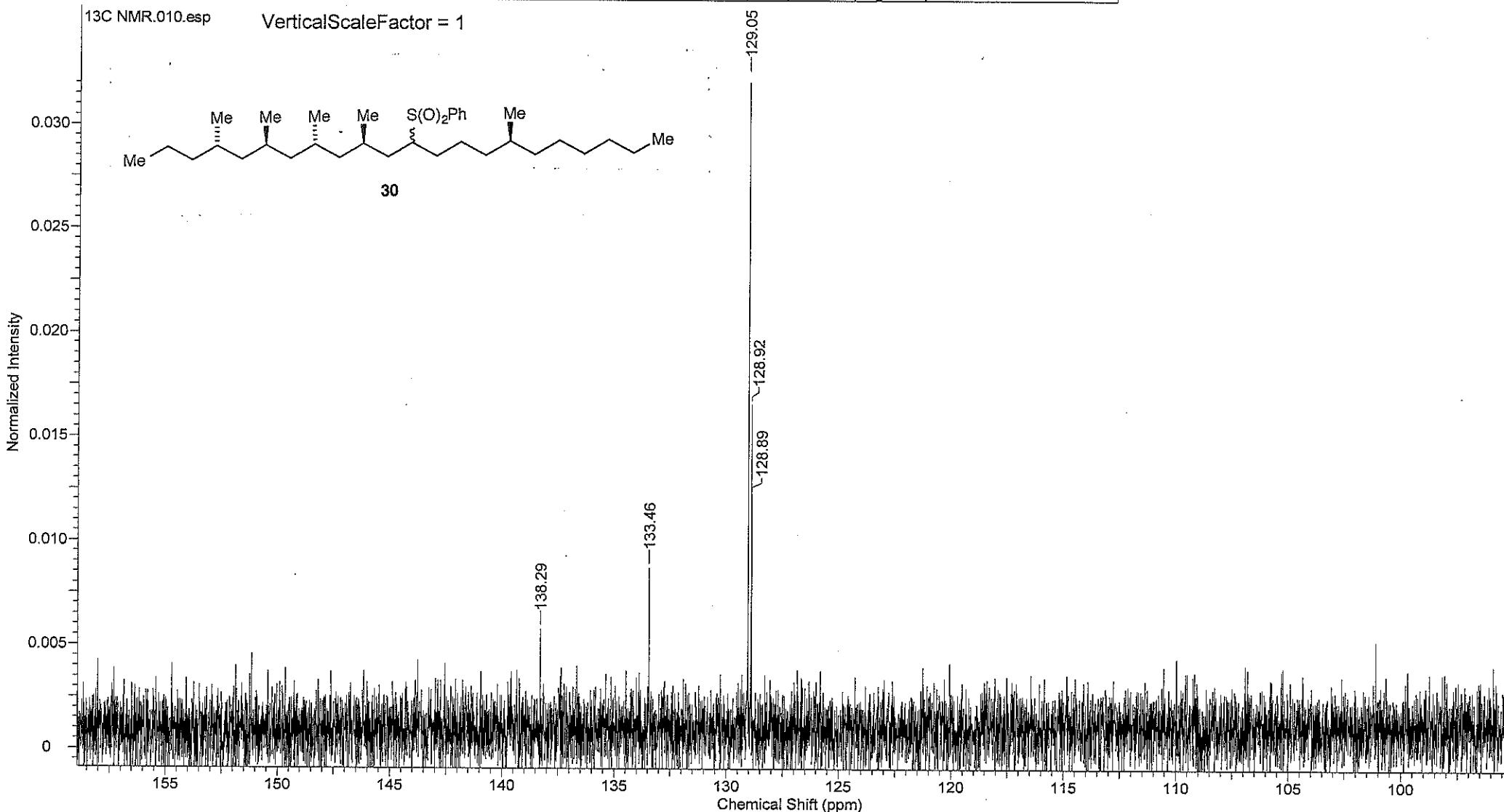
3/8/2011 11:33:58 AM

Acquisition Time (sec)	1.3631	Comment	Leo 1110-062 HL099-004 mCARBON CDCl <sub>3</sub> {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



3/8/2011 11:34:05 AM

Acquisition Time (sec)	1.3631	Comment	Leo 1110-062 HL099-004 mCARBON CDCl <sub>3</sub> {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

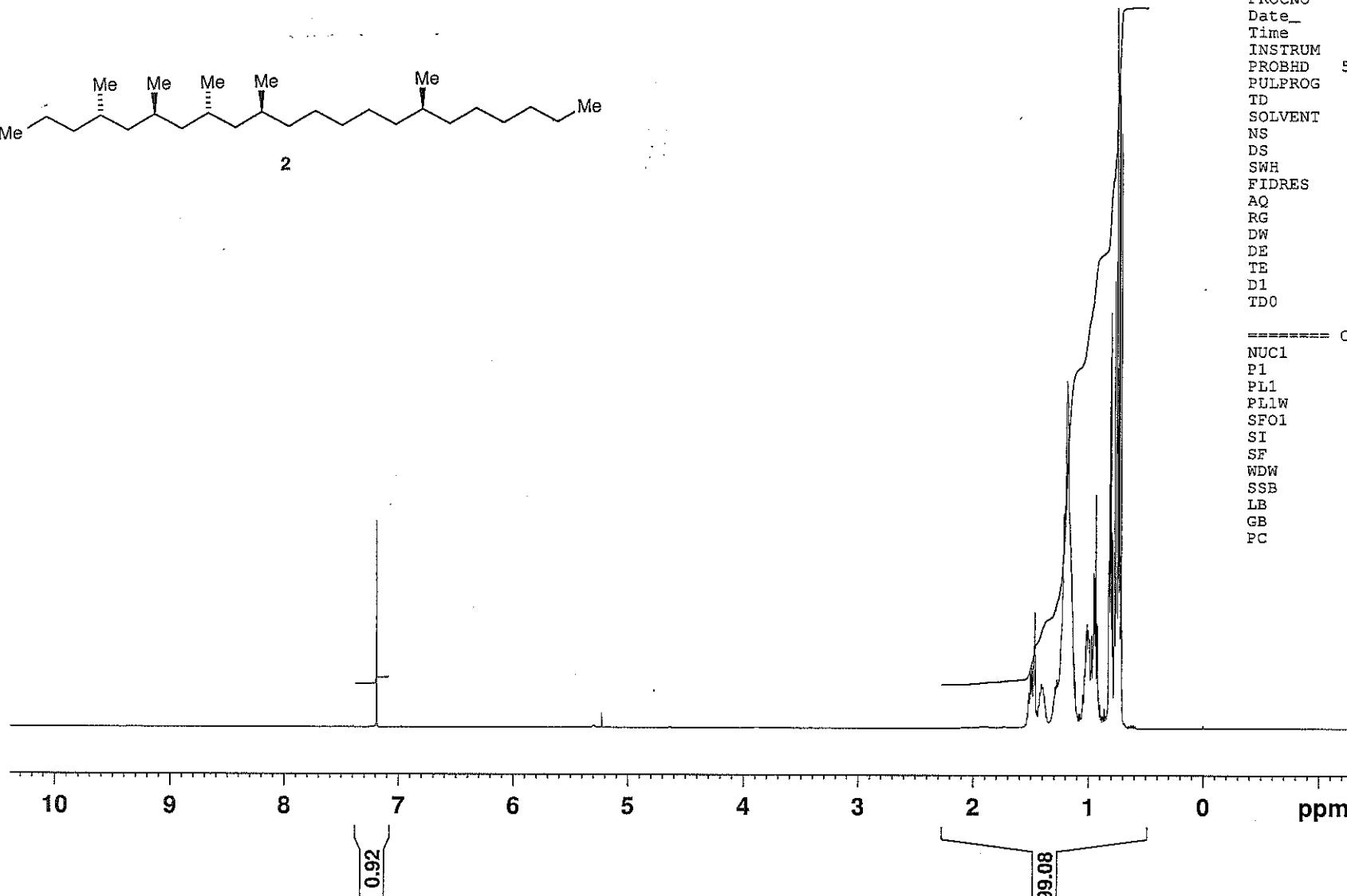
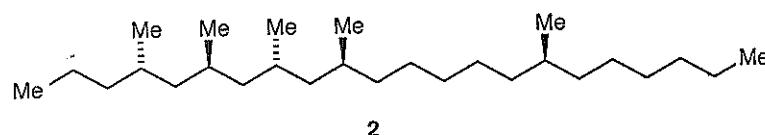


HL099-005  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2010/Nov ejt 39

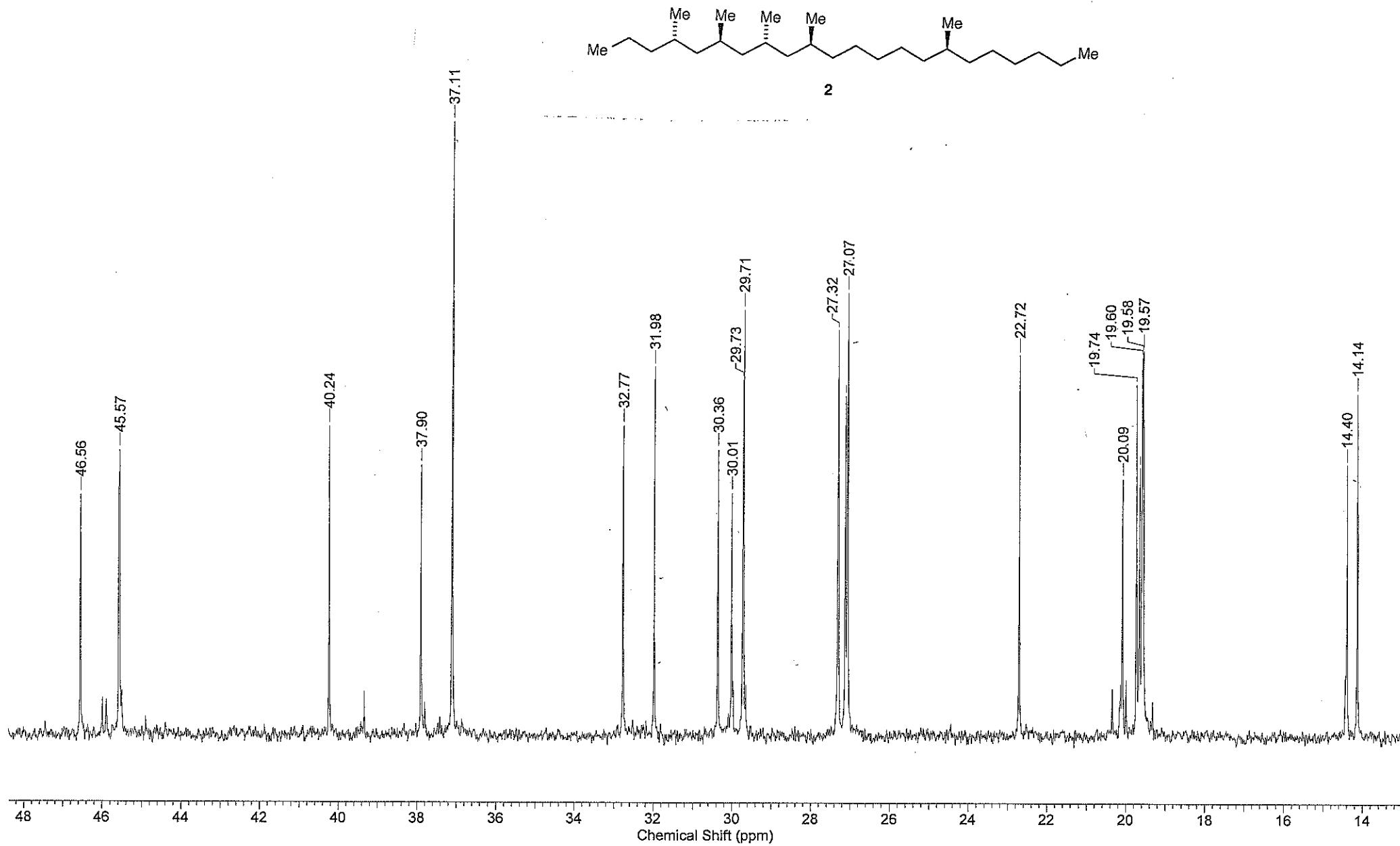


NAME 2010-11-23-ejt-39  
EXPNO 10  
PROCNO 1  
Date\_ 20101124  
Time 2.43  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 144  
DW 48.400 usec  
DE 13.38 usec  
TE 298.1 K  
D1 1.0000000 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 500.1300486 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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

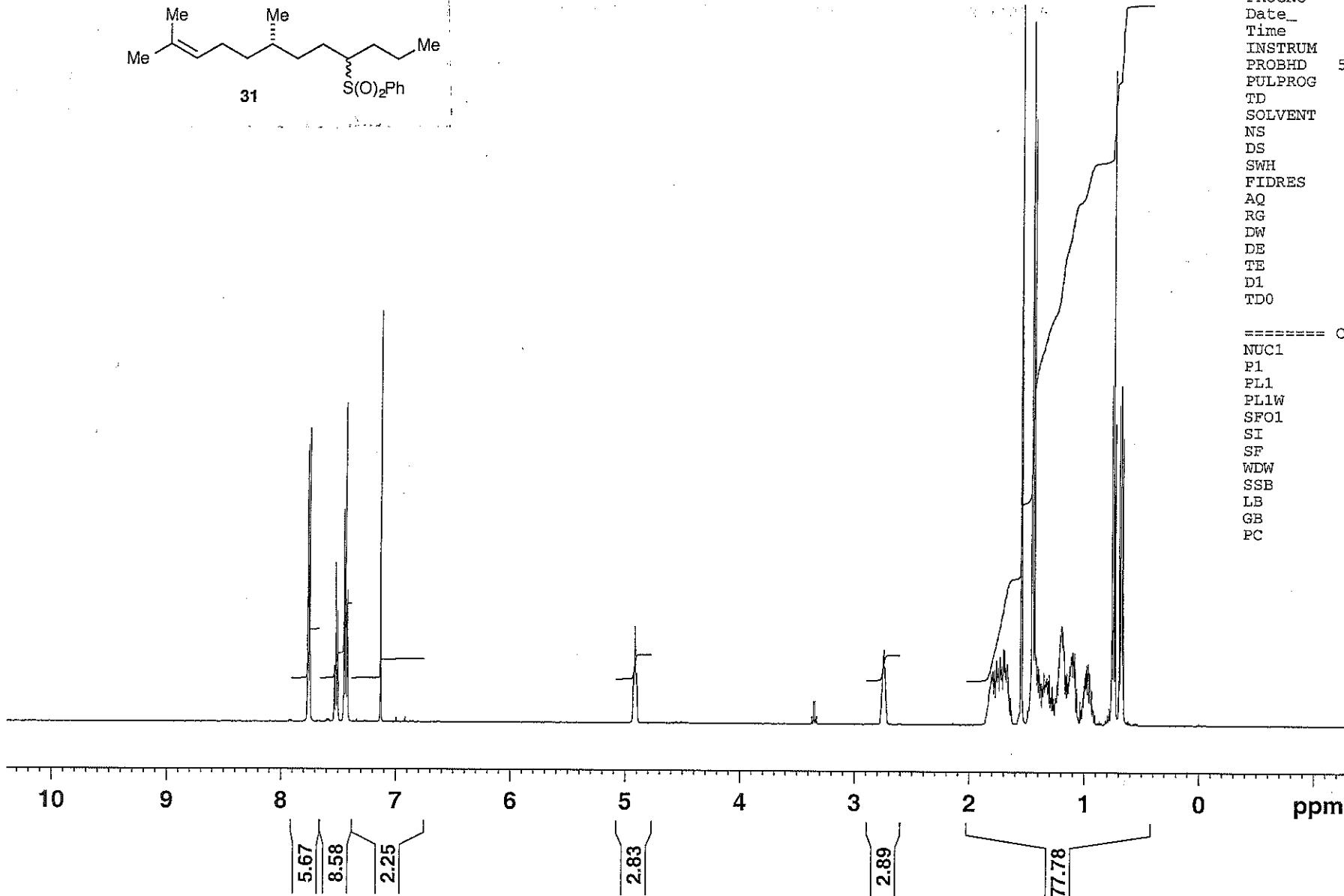


HL102-030  
mPROTON CDCl<sub>3</sub> /opt/bruk500data/2011/Feb ejt 8

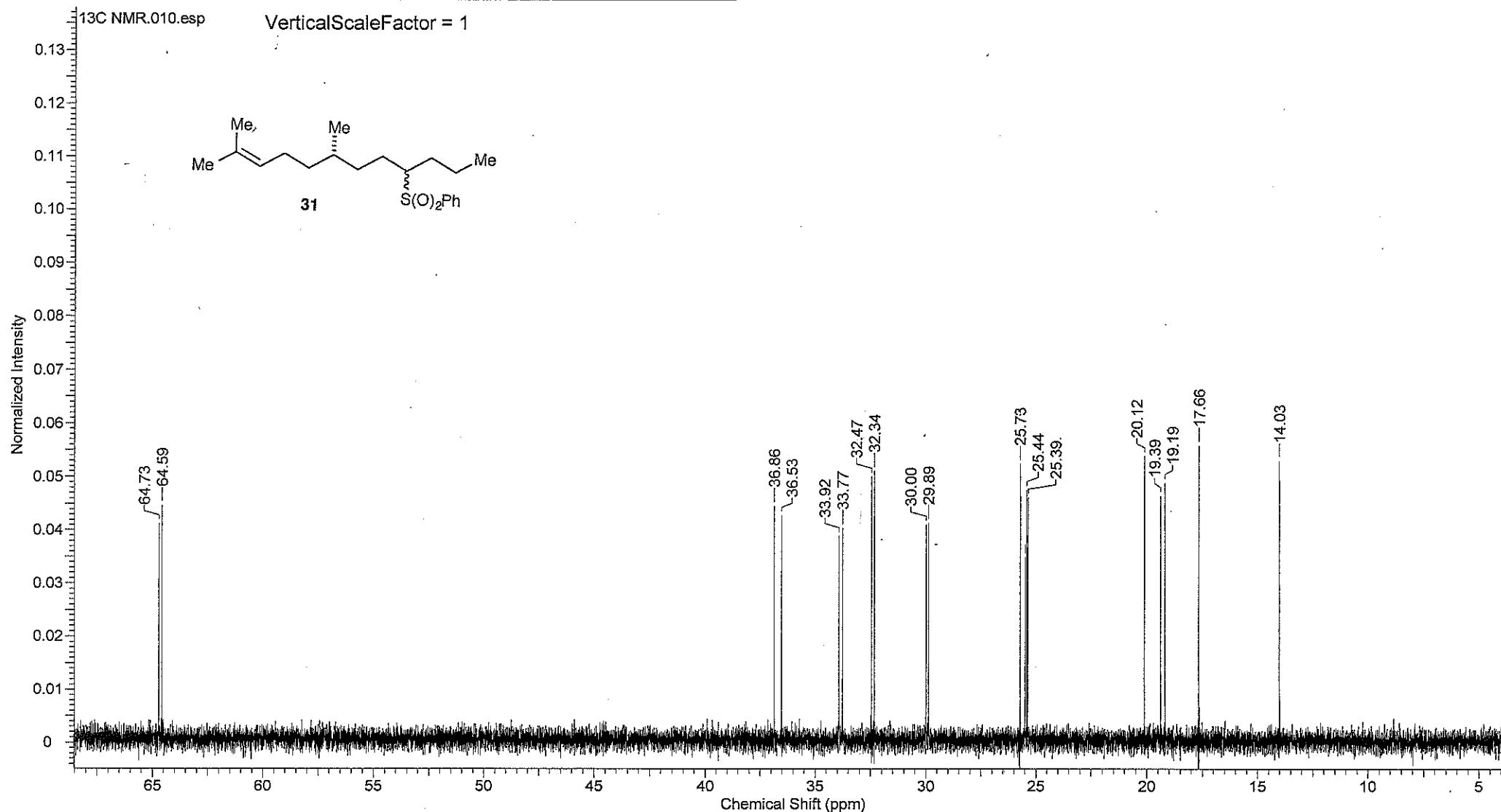


NAME 2011-02-15-ejt-8  
EXPNO 10  
PROCNO 1  
Date\_ 20110215  
Time 16.17  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 287  
DW 48.400 usec  
DE 13.38 usec  
TE 293.2 K  
D1 1.00000000 sec  
TD0 1

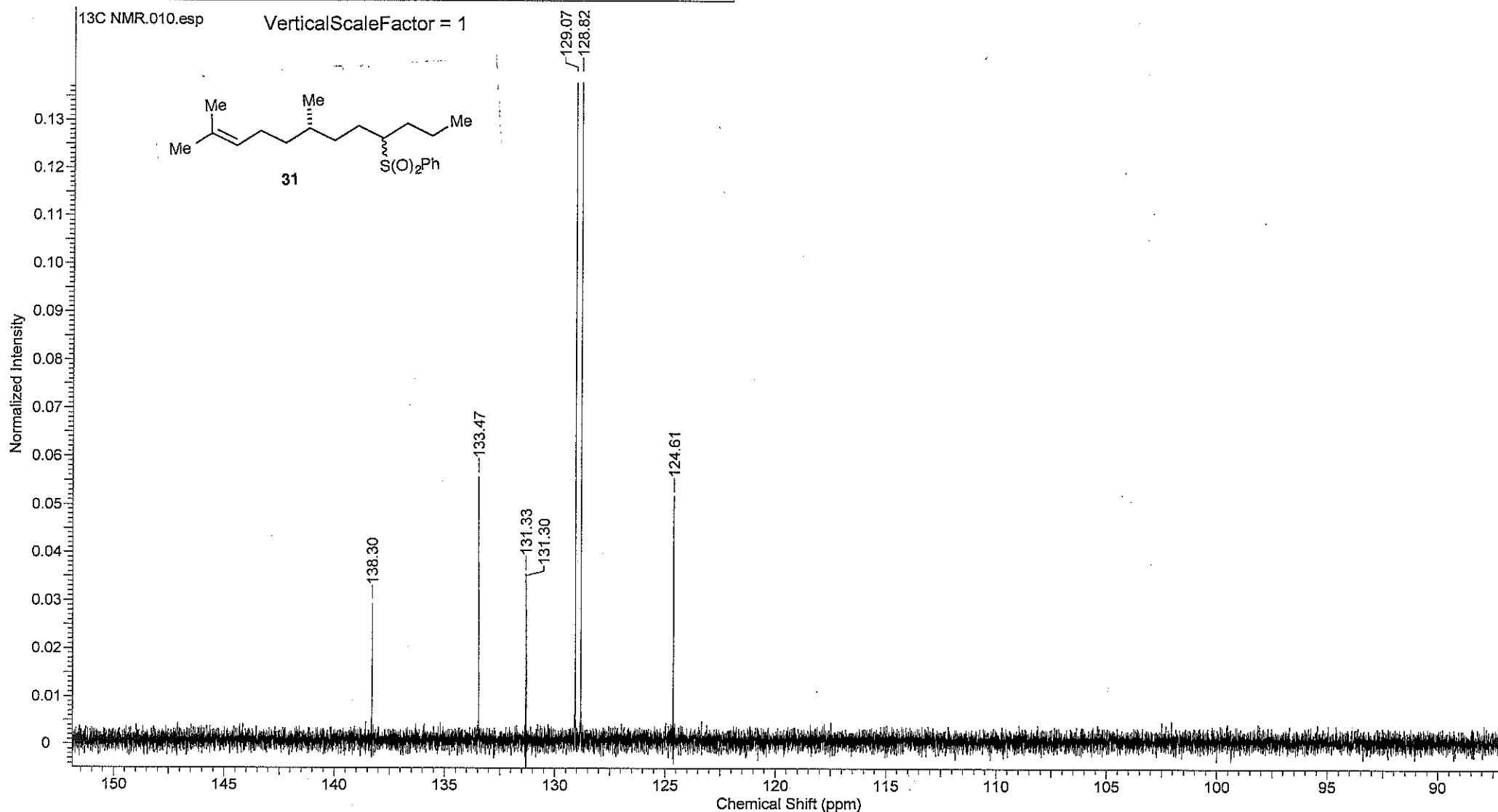
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300773 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Acquisition Time (sec)	1.3631	Comment	Leo 0910-040 HL093-001 mCARBON 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\f1d			Frequency (MHz)	100.64
Nucleus	13C	Number of Transients	10240	Origin	AV400_S
Owner	Administrator	Points Count	1048576	Pulse Sequence	zpgpg30
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



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



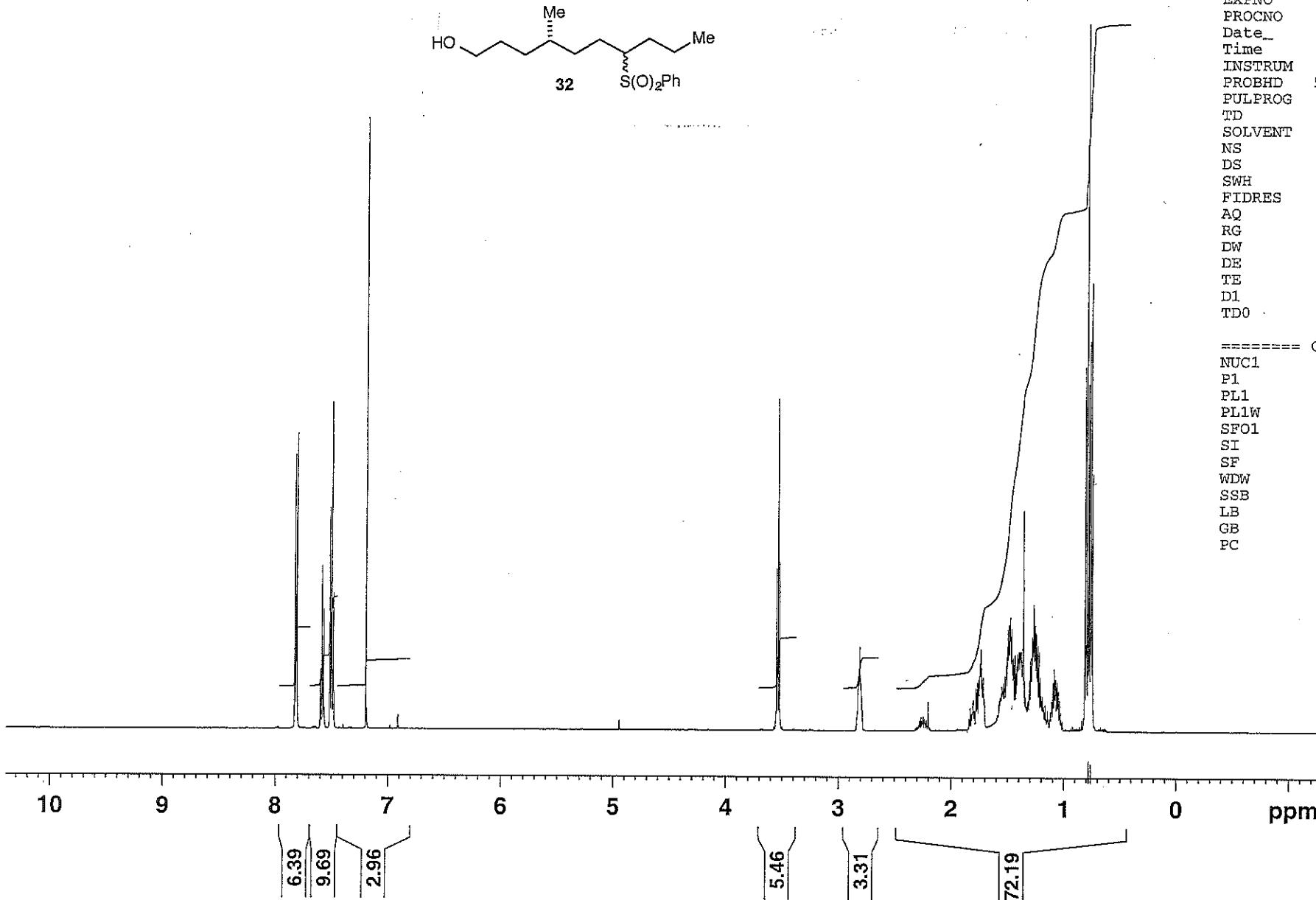
HL102-031

mPROTON CDCl<sub>3</sub> /opt/bruk500data/2011/Feb ejt 5

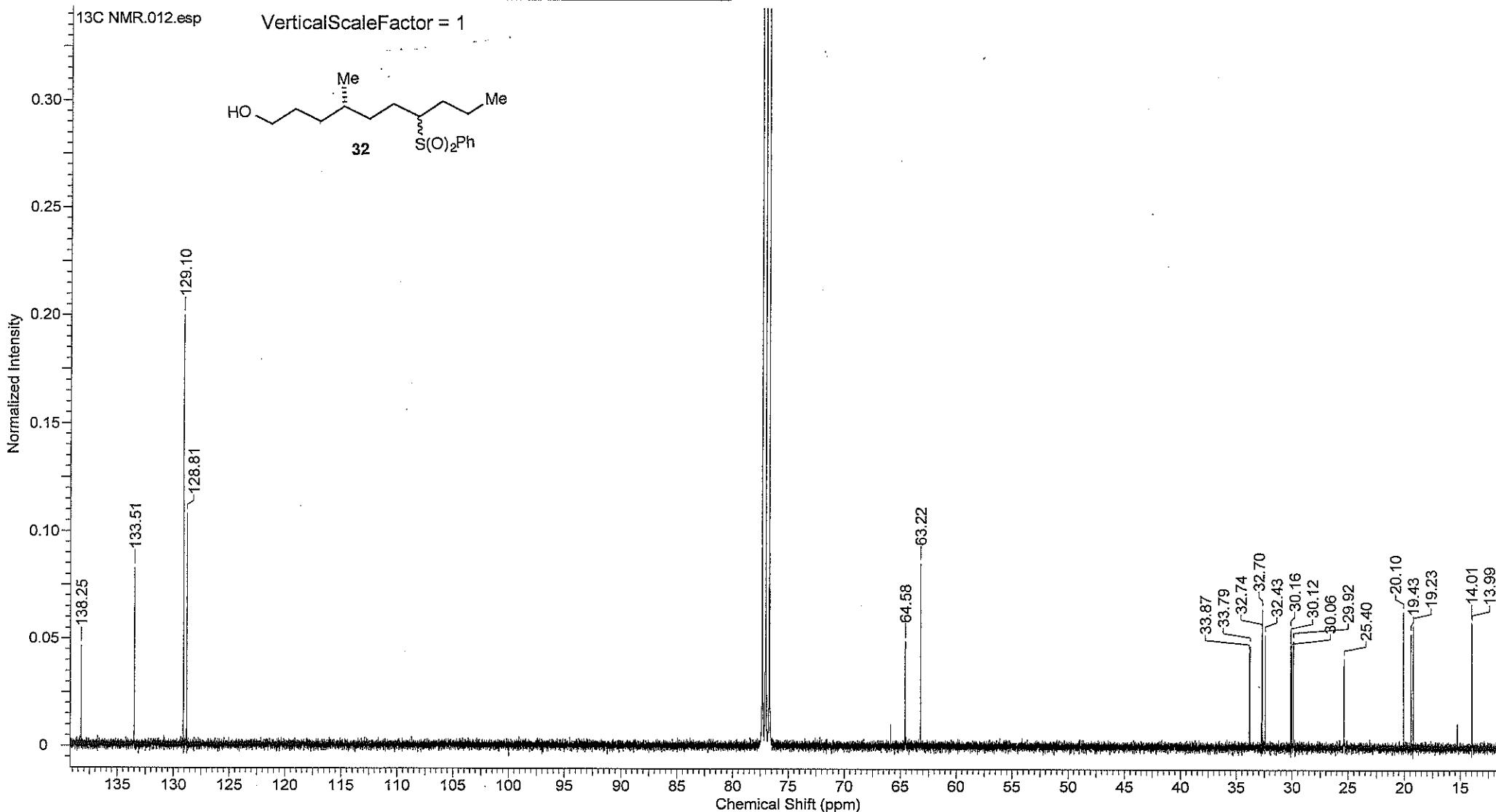


NAME 2011-02-23-ejt-5  
EXPNO 10  
PROCNO 1  
Date\_ 20110223  
Time 9.31  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 322  
DW 48.400 usec  
DE 13.38 usec  
TE 294.7 K  
D1 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

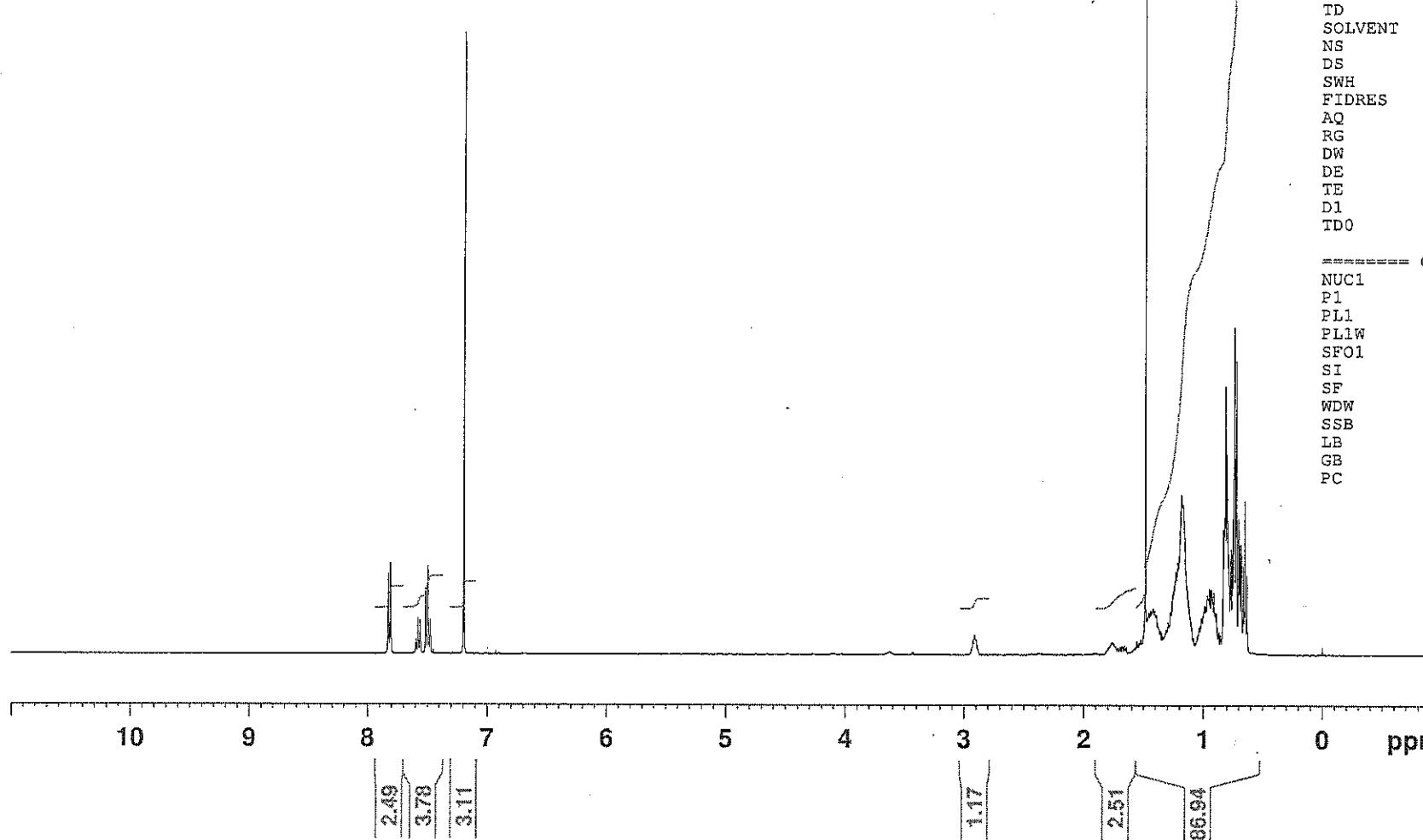
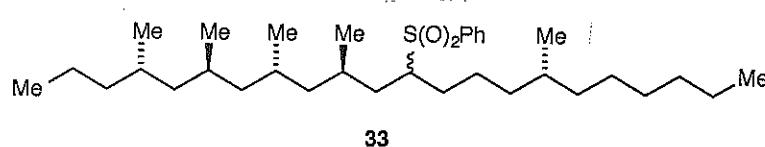


Acquisition Time (sec)	1.3631	Comment	Leo 0910-043 HL093-002 mCARBON CDCl3 {E:\bruk400service_data\2010\Sep} Administrator 8		
Date	22 Sep 2010 15:17:36	Date Stamp	22 Sep 2010 15:17:36		
File Name	C:\Users\Leo\Desktop\Experiments Folder\Experiment 51-100\HL093 - Sulfone alkylation\HL093-002\13C NMR\12\fid			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 CDCl<sub>3</sub> {e:\bruk400data\2011\Feb} ejt 60

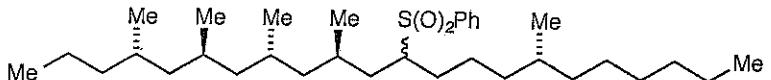
**BRUKER**  
400MHz



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 CDC13  
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 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.50 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

H. Liu  
0211-003  
HL102-036  
mCARBON CDCl<sub>3</sub> {E:\bruk400service\data\2011\Feb\Administrator-18}



33



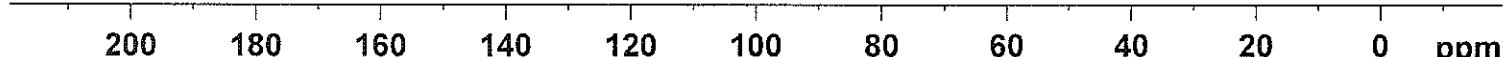
2011-02-03-Administrator-18

NAME 10  
EXPNO 1  
PROCNO 1  
Date\_ 20110203  
Time 14.50  
INSTRUM AV400\_S  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
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  
TB 298.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

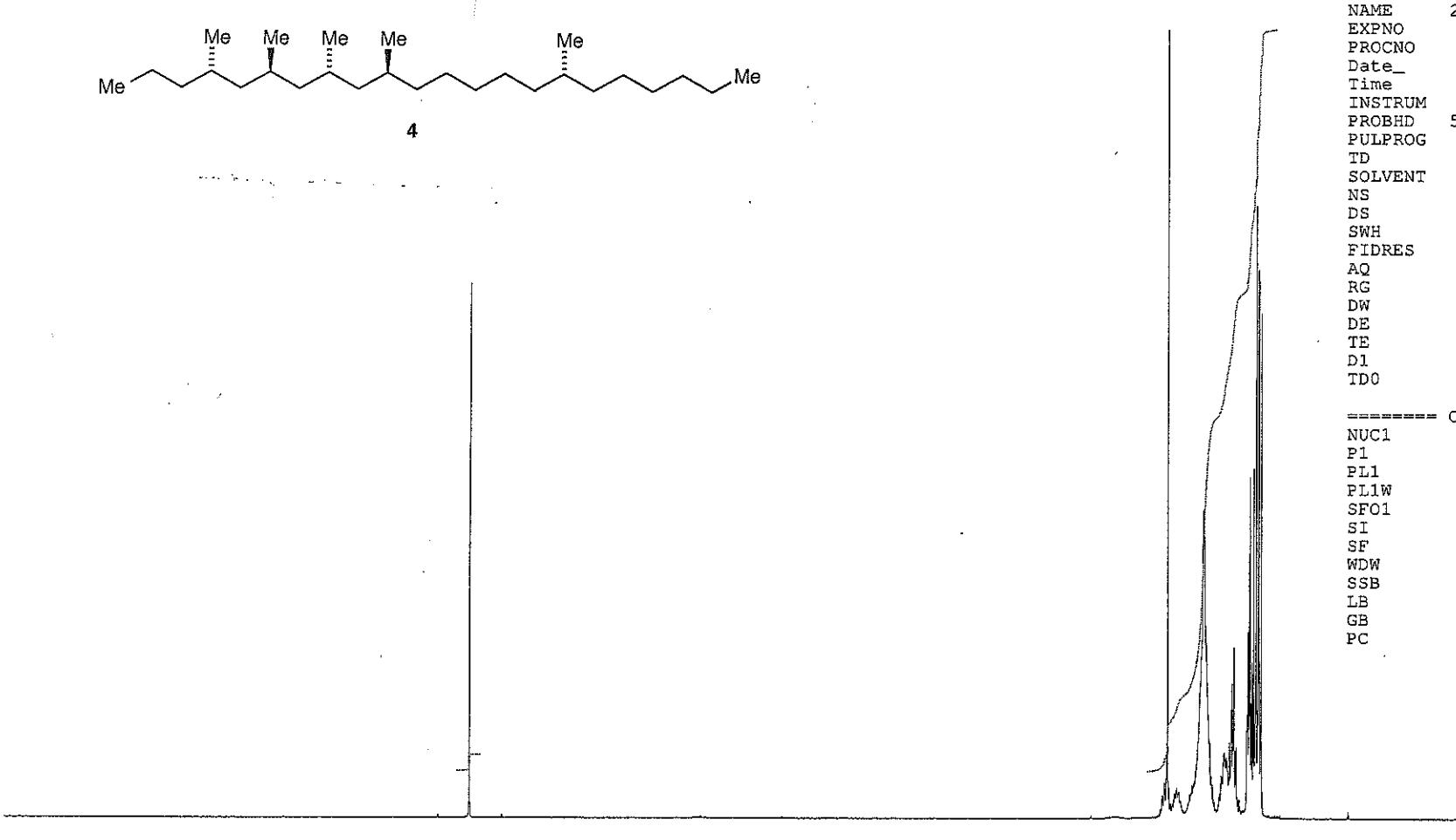
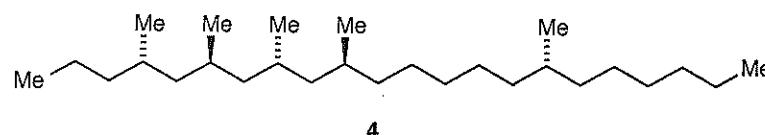
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 33.91046524 W  
SFO1 100.6479773 MHz

===== 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

$\delta$  C (125MHz, CDCl<sub>3</sub>) 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, 133.88, 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 1.0000000 sec  
TDO 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 CDCl <sub>3</sub> {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
Origin	AV400 S	Original Points Count	32768
Points Count	131072	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Sweep Width (Hz)	24038.28	Temperature (degree C)	22.500

