Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Towards 20,20-difluorinated bryostatin: synthesis and biological evaluation of difluorinated C17,C27-fragments

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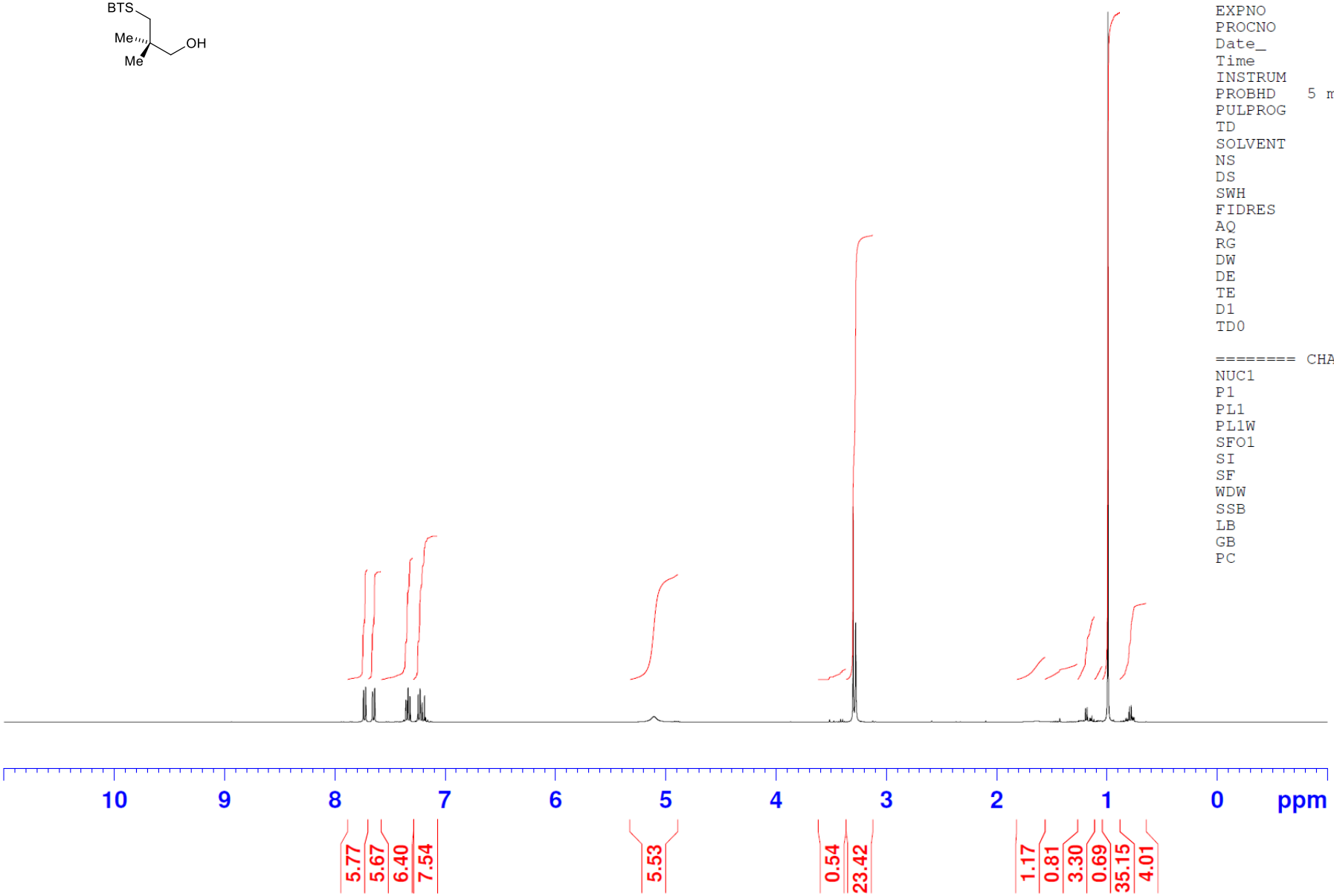
Supplementary data

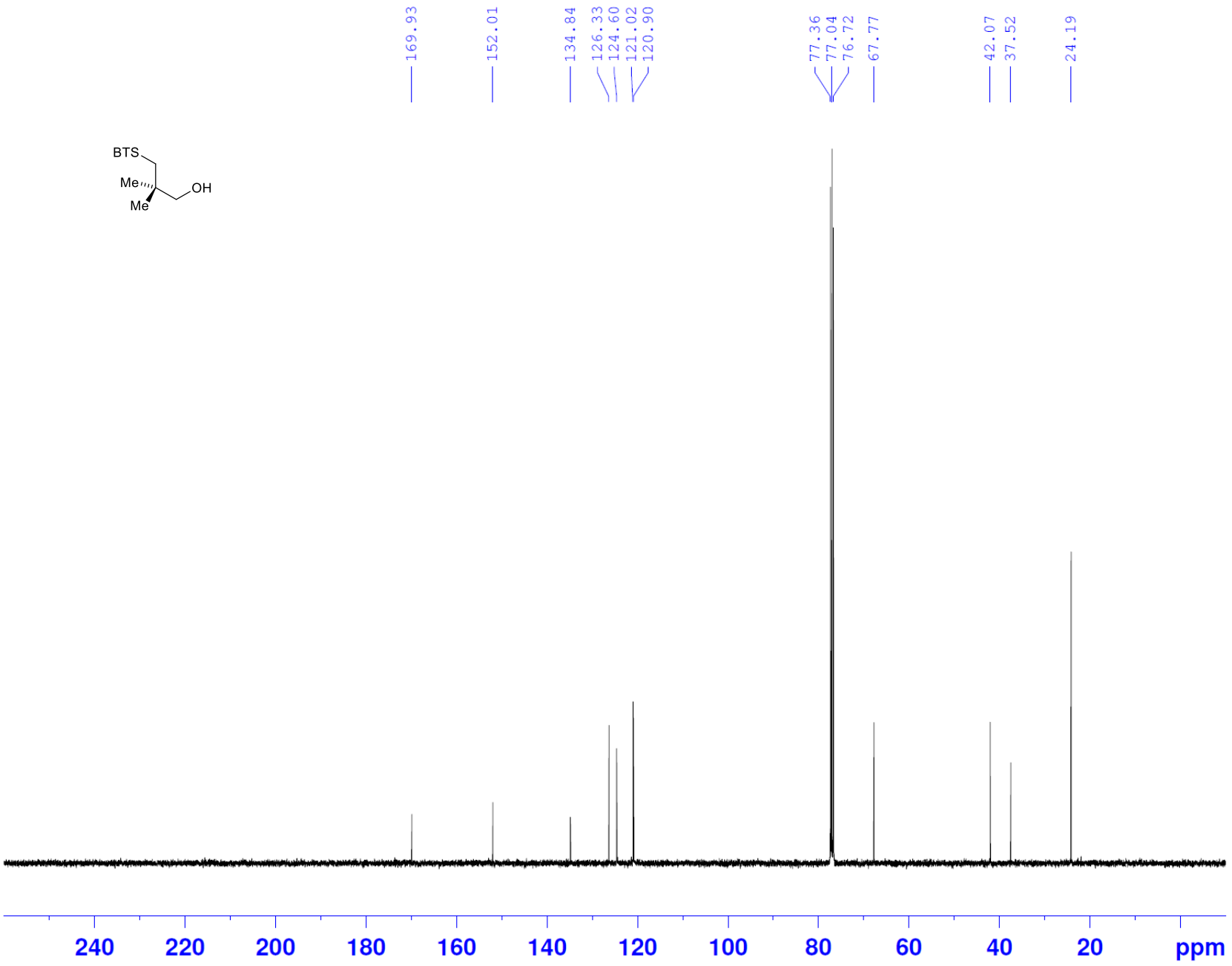
Copies of all the ^{1}H, ^{13}C and ^{19}F NMR spectra reported in this paper with expansions for some of the ^{13}C spectra to show carbon-fluorine couplings

ejt cry alcohol
mPROTON CDCl3 {e:\bruk400data\2012\Mar} ejt 38

NAME	2012-03-08-ejt-38
EXPNO	10
PROCNO	1
Date_	20120308
Time	11.47
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	203
DW	60.500 usec
DE	9.40 usec
TE	294.3 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	400.1300379 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



ejt cry alcohol
mCARBONnight CDCl3 {e:\bruk400data\2012\Mar} ejt 12



NAME	2012-03-12-ejt-12
EXPNO	10
PROCNO	1
Date_	20120312
Time	20.20
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	295.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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mPROTON CDCl3 {e:\bruk400data\2012\May} ejt 17

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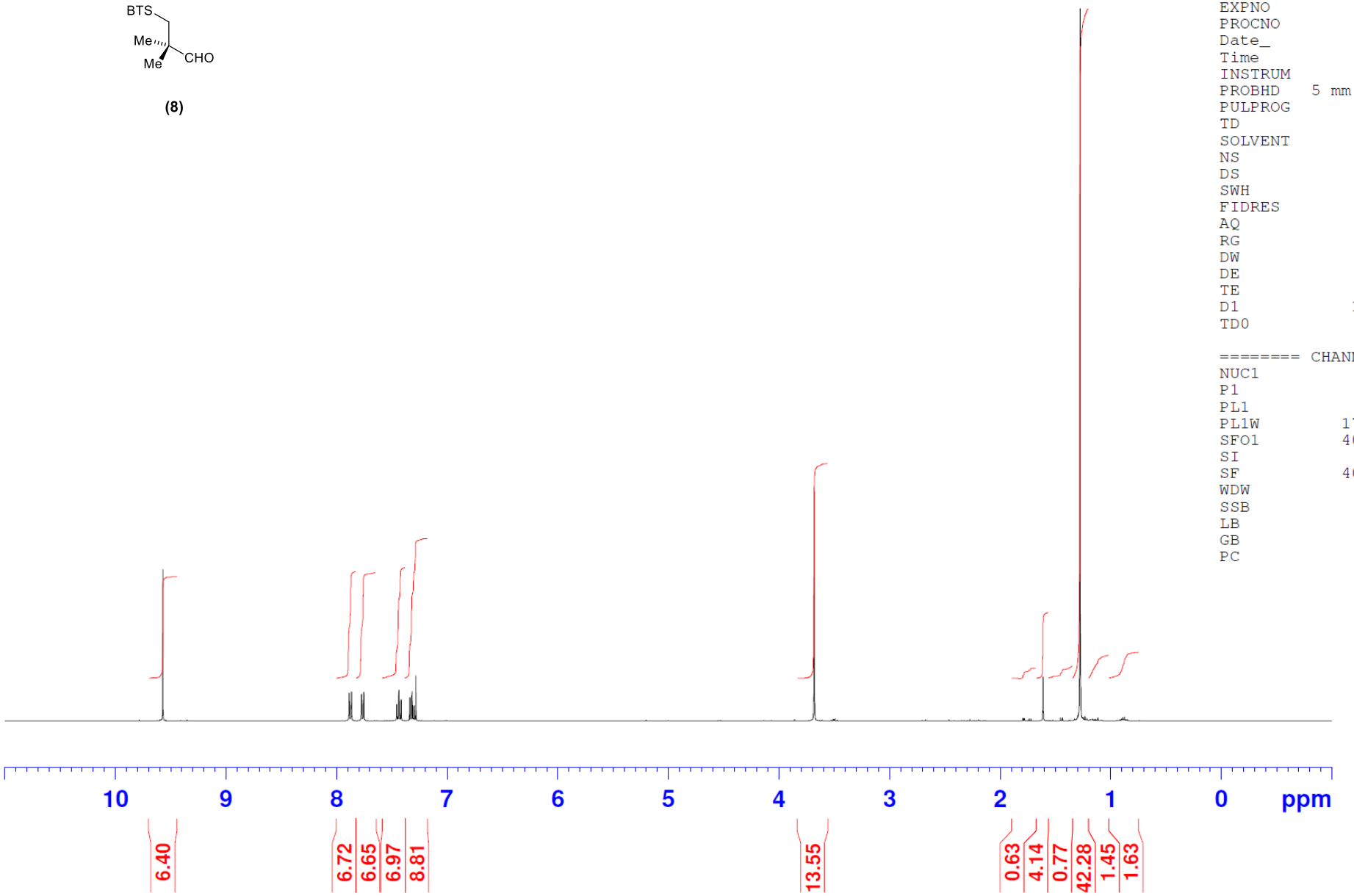
NAME	2012-05-11-ejt-17
EXPNO	10
PROCNO	1
Date_	20120511
Time	9.54
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	287
DW	60.500 usec
DE	9.40 usec
TE	293.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
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



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mCARBONnight CDCl3 {e:\bruk400data\2012\Feb} ejt 38

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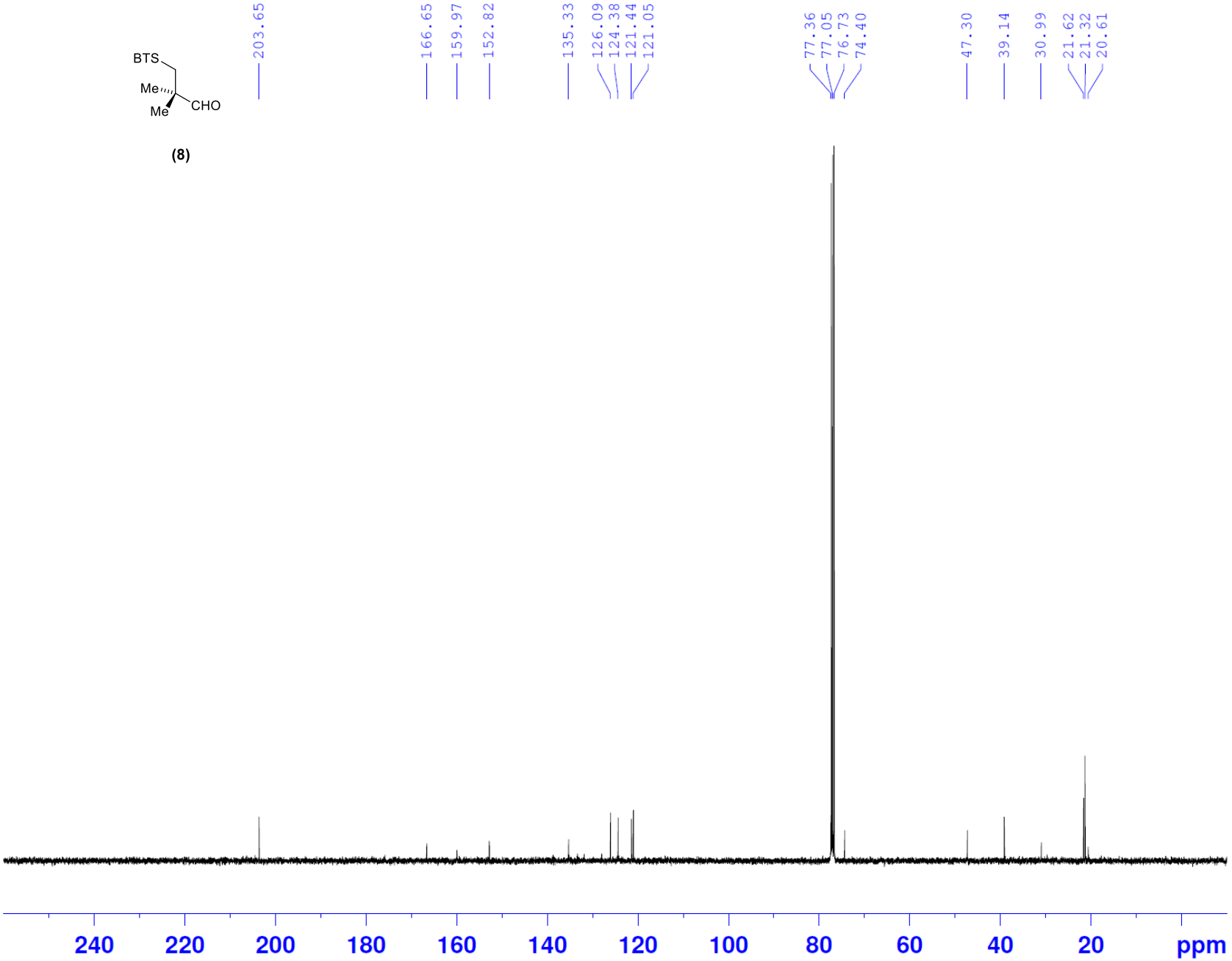

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EXPNO	10
PROCNO	1
Date_	20120208
Time	23.37
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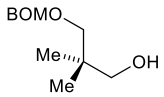
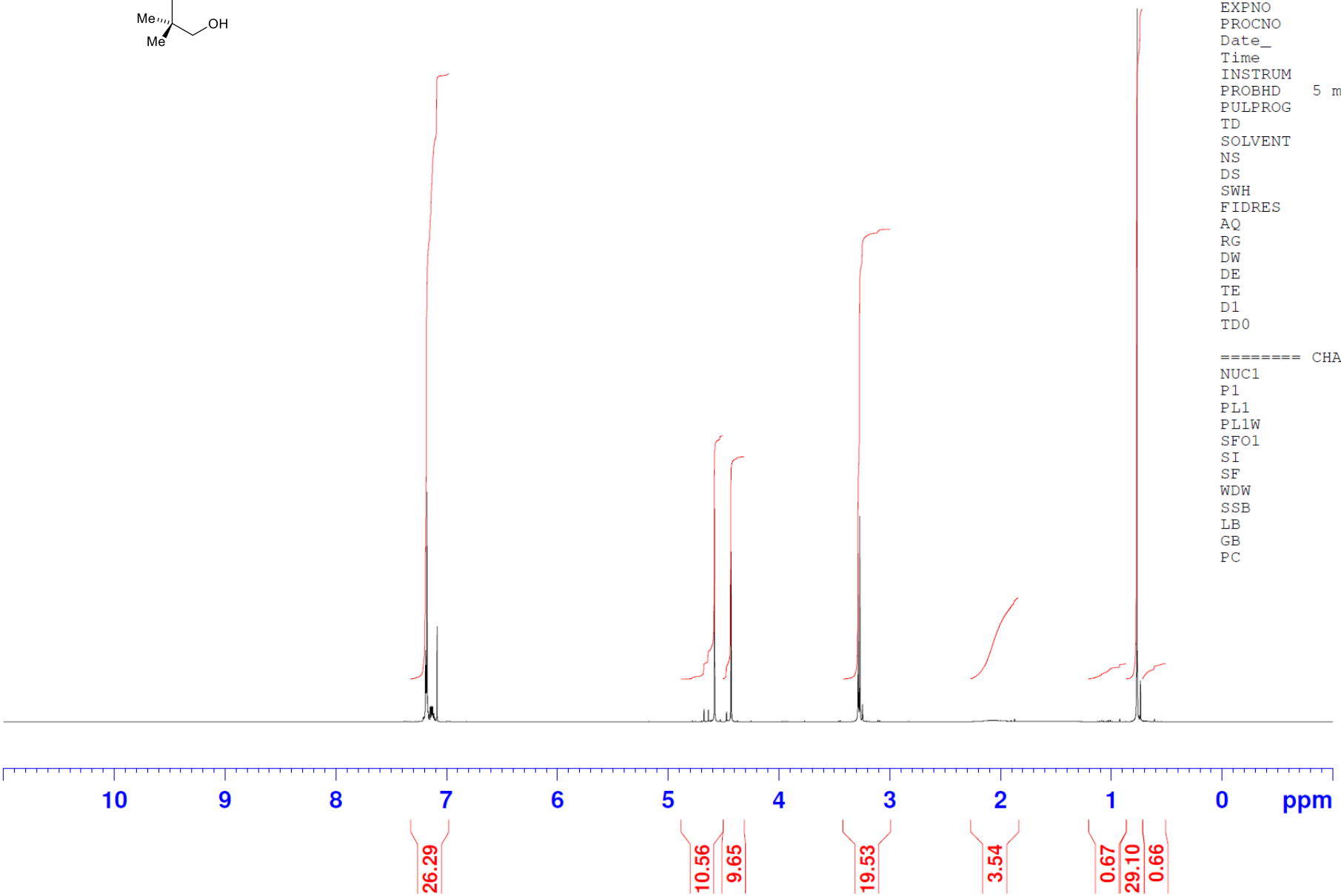
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	292.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

ejt cry bom oh
mPROTON CDCl3 {e:\bruk400data\2012\Aug} ejt 16





NAME	2012-08-07-ejt-16
EXPNO	10
PROCNO	1
Date_	20120807
Time	16.08
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	287
DW	60.500 usec
DE	9.40 usec
TE	295.2 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	400.1300790 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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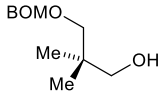
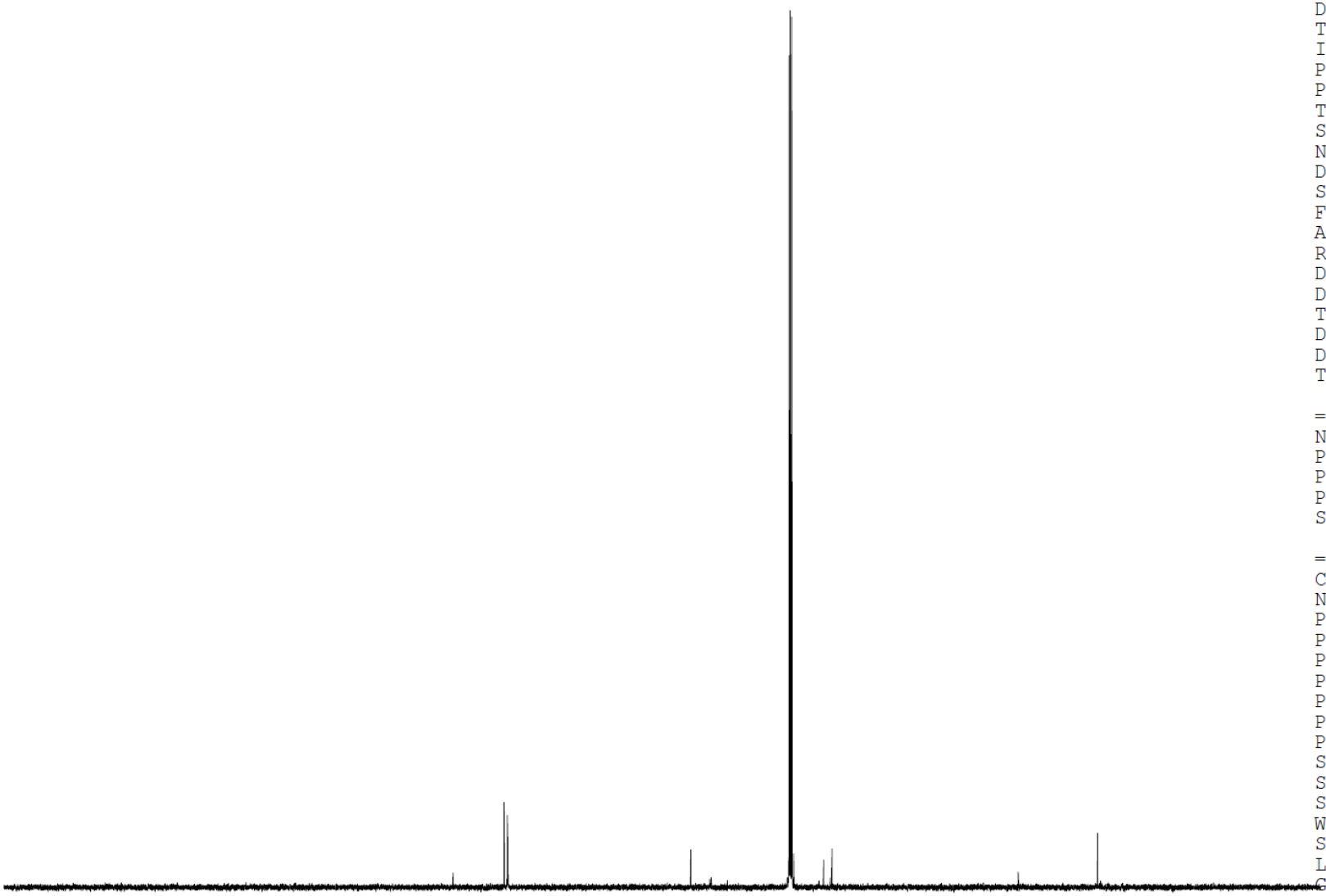
mCARBONnight CDCl3 /opt/bruk500data/2012/May ejt 2



137.63
128.51
128.48
127.92
127.88
127.84
127.78
94.93
91.55
91.28
77.61
77.29
77.04
76.79
76.48
71.09
69.90
69.57
36.09
21.82



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

NAME	2012-05-30-ejt-2
EXPNO	20
PROCNO	1
Date_	20120530
Time	18.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	512
DW	16.800 usec
DE	32.78 usec
TE	293.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.80 usec
PL1	-1.00 dB
PL1W	104.35516357 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.23 dB
PL13	120.00 dB
PL2W	25.62124252 W
PL12W	0.48484197 W
PL13W	0.00000000 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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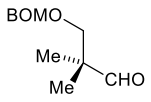
mPROTON CDCl3 {e:\bruk400data\2012\Aug} ejt 15



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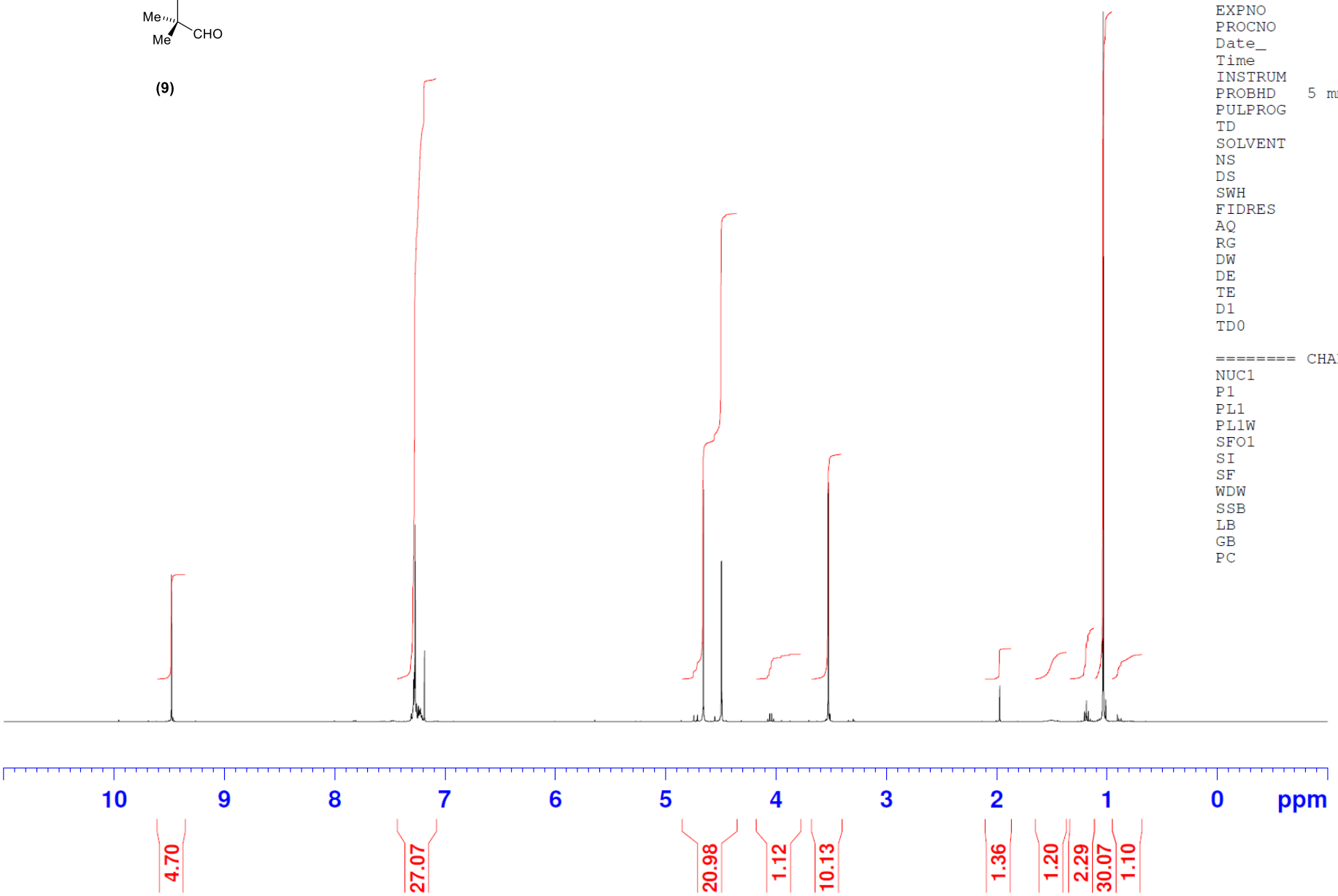

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EXPNO	10
PROCNO	1
Date_	20120808
Time	15.31
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	256
DW	60.500 usec
DE	9.40 usec
TE	295.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300387 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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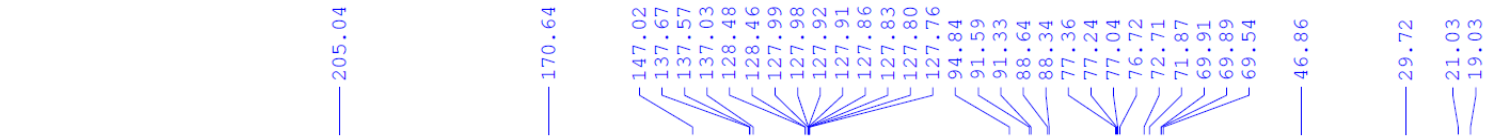
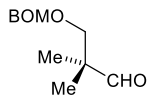
mCARBONnight CDCl3 {e:\bruk400data\2012\May} ejt 31





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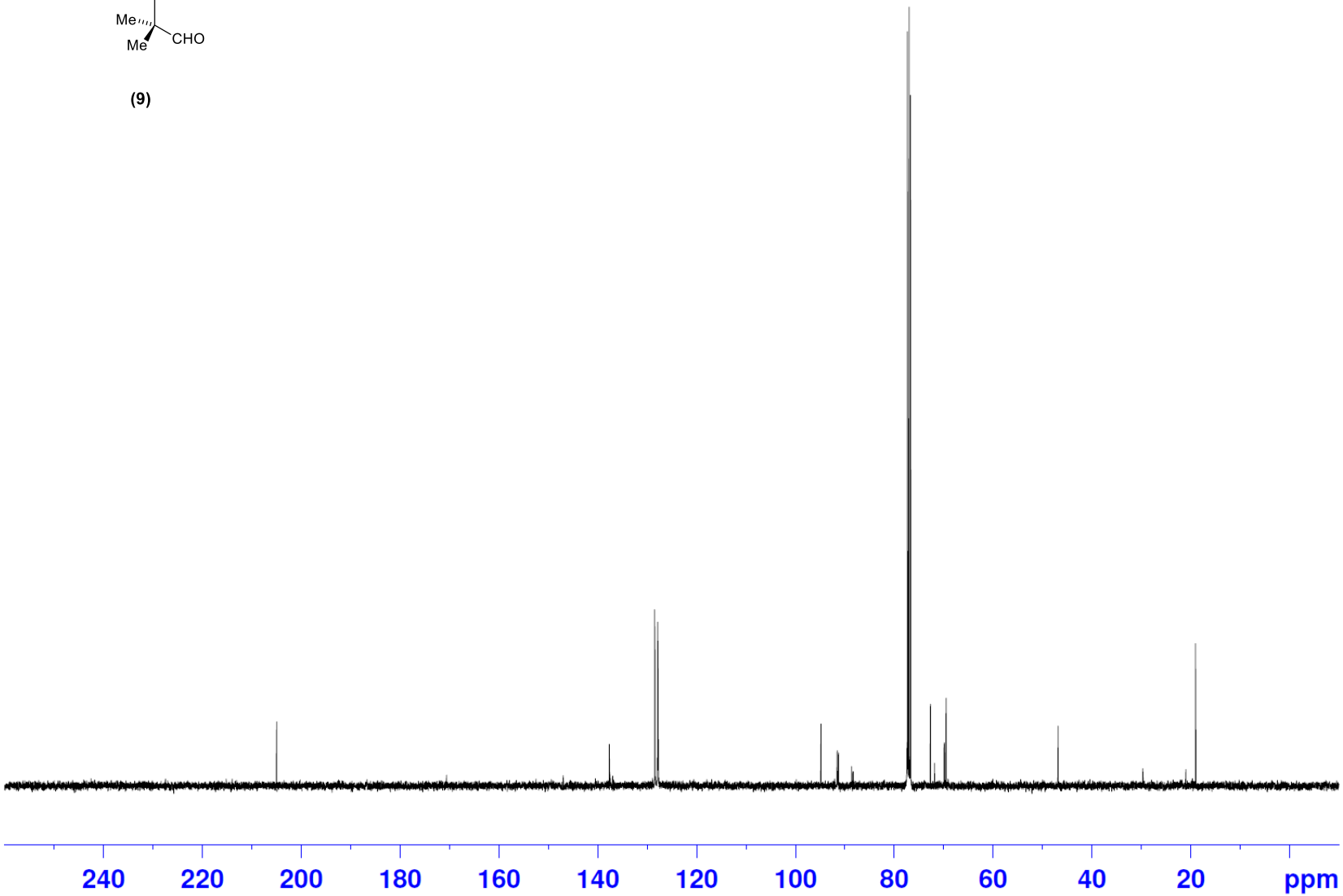
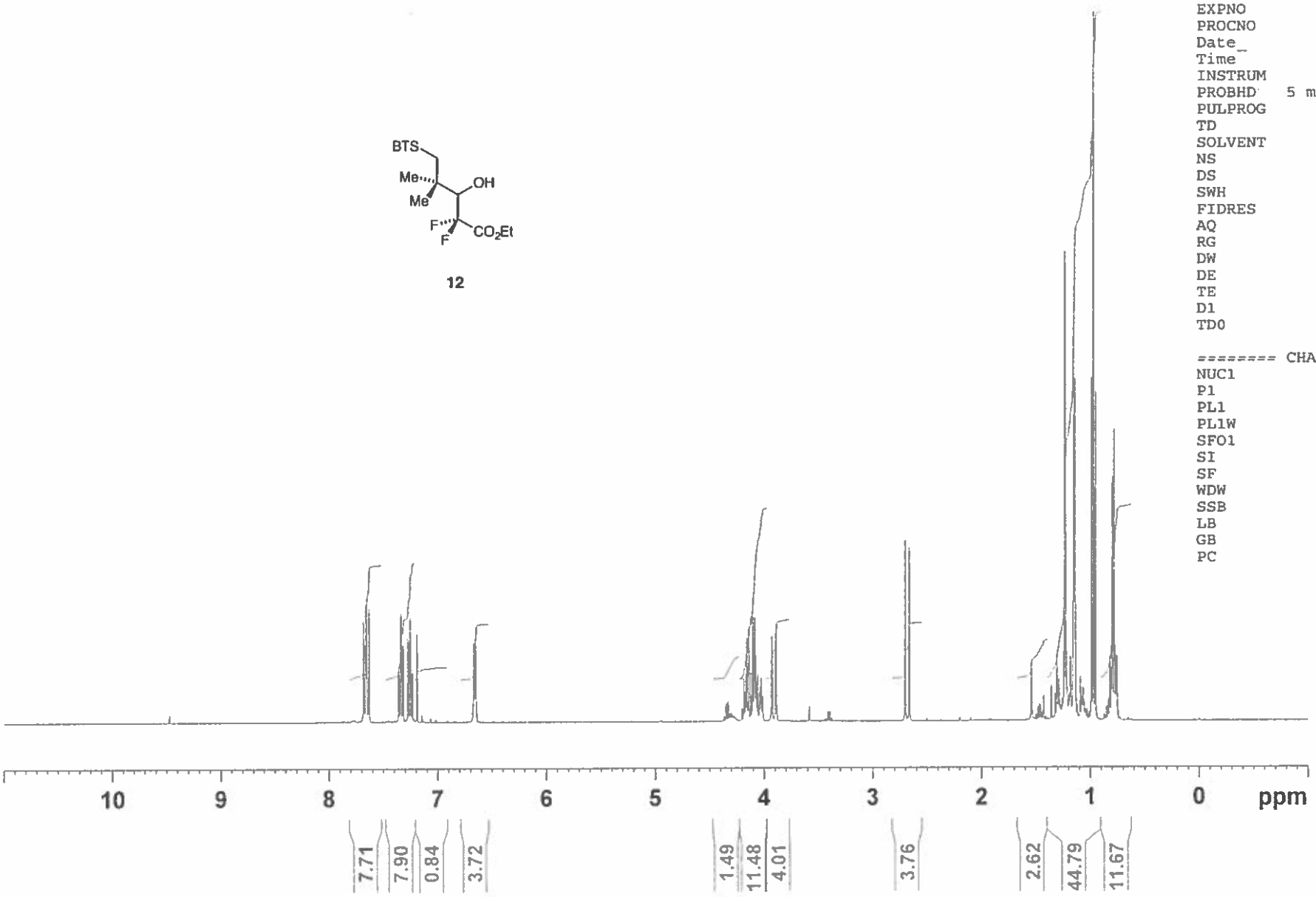


NAME	2012-05-31-ejt-31
EXPNO	11
PROCNO	1
Date_	20120601
Time	1.04
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

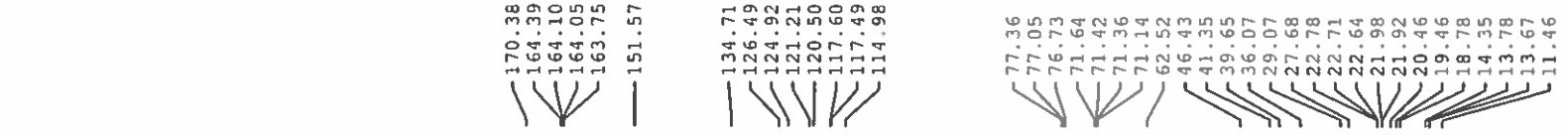
ejt cry 7-9
mPROTON CDCl3 {e:\bruk400data\2012\Feb} ejt 16

12

NAME	2012-02-06-ejt-16
EXPNO	10
PROCNO	1
Date_	20120206
Time	14.23
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	161
DW	60.500 usec
DE	9.40 usec
TE	293.7 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	400.1300376 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



ejt cry 7–9
mCARBONnight CDCl3 {e:\bruk400data\2012\Feb} ejt 16



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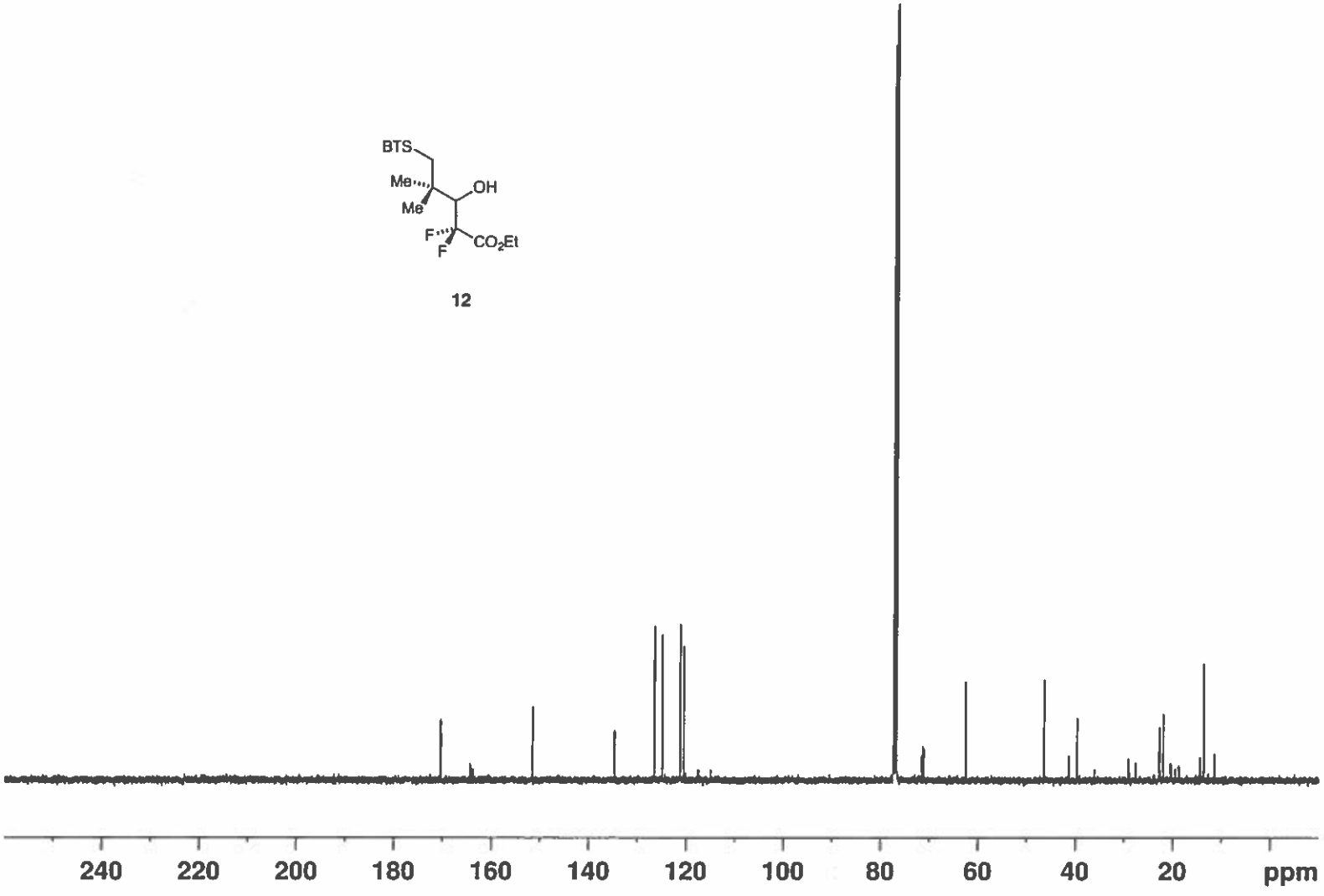

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PROCNO	1
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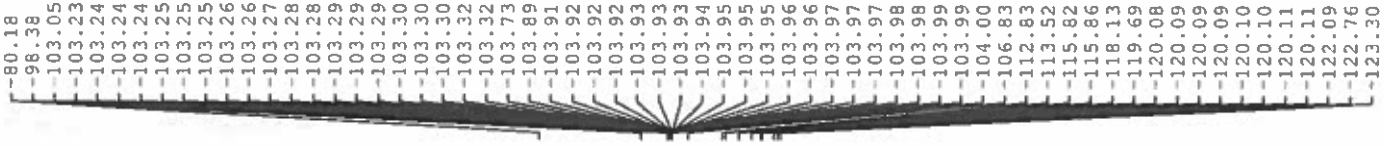
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	293.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

ejt cry 7–9
mF19CPD CDCl3 {e:\bruk400data\2012\Feb} ejt 16



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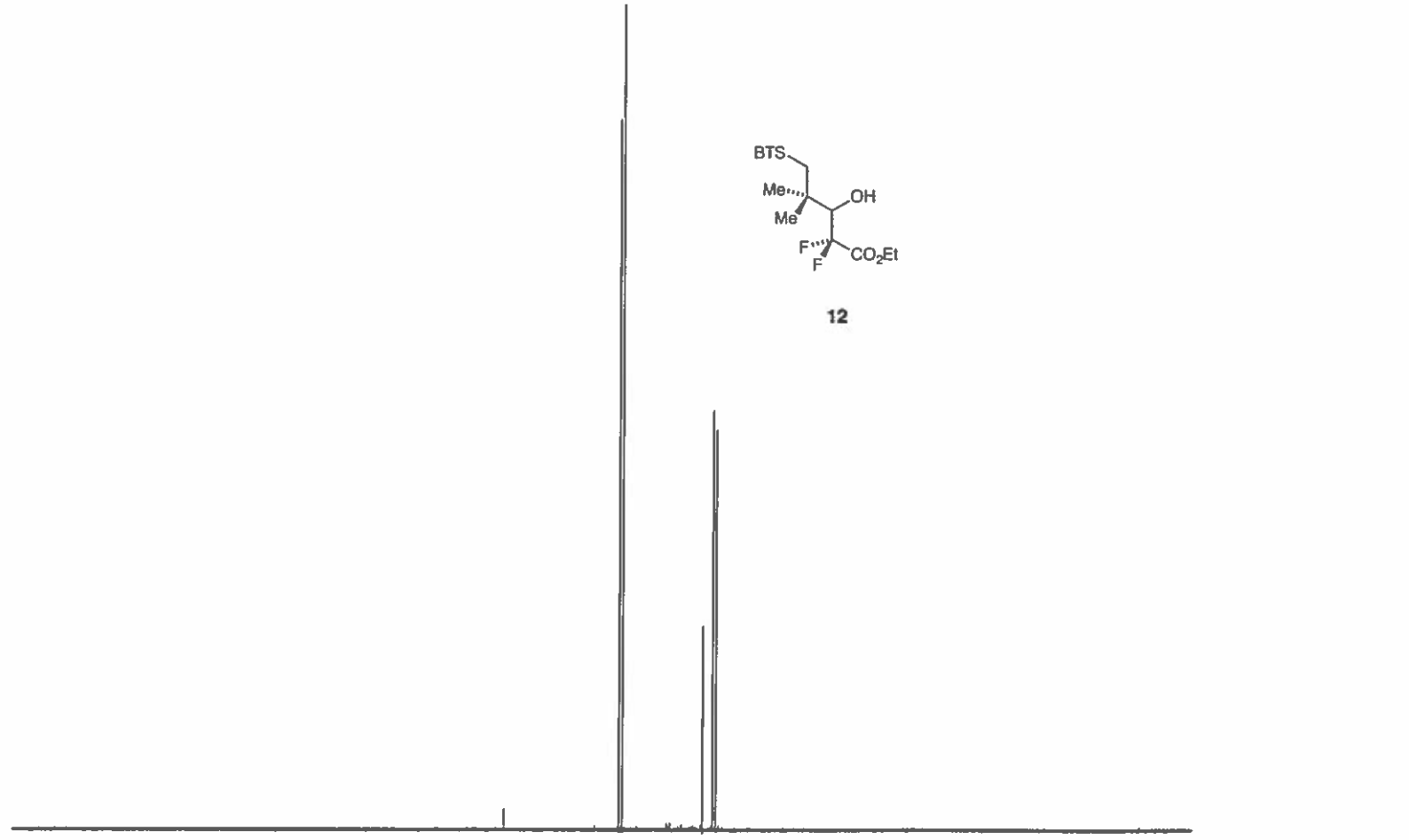

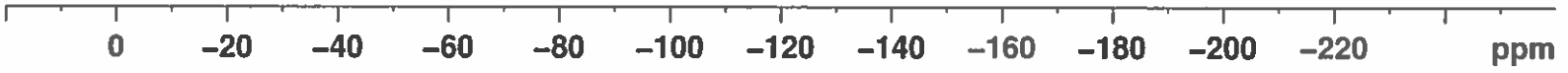

BRUKER 400 MHz

NAME	2012-02-07-ejt-16	
EXPNO	10	
PROCNO	1	
Date_	20120207	
Time	9.30	
INSTRUM	AV400	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	131072	
SOLVENT	CDCl3	
NS	32	
DS	4	
SWH	89285.711	Hz
FIDRES	0.681196	Hz
AQ	0.7340532	sec
RG	4100	
DW	5.600	usec
DE	7.51	usec
TE	292.9	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	10.70	usec
PL1	-5.00	dB
PL1W	27.00716019	W
SFO1	376.4607164	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-3.60	dB
PL12	15.31	dB
PL2W	17.83863831	W
PL12W	0.22927761	W
SFO2	400.1316005	MHz
SI	262144	
SF	376.4983660	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	2.00	

05/07/2012 12:44:14

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Date Stamp	20 Jun 2012 03:46:24						
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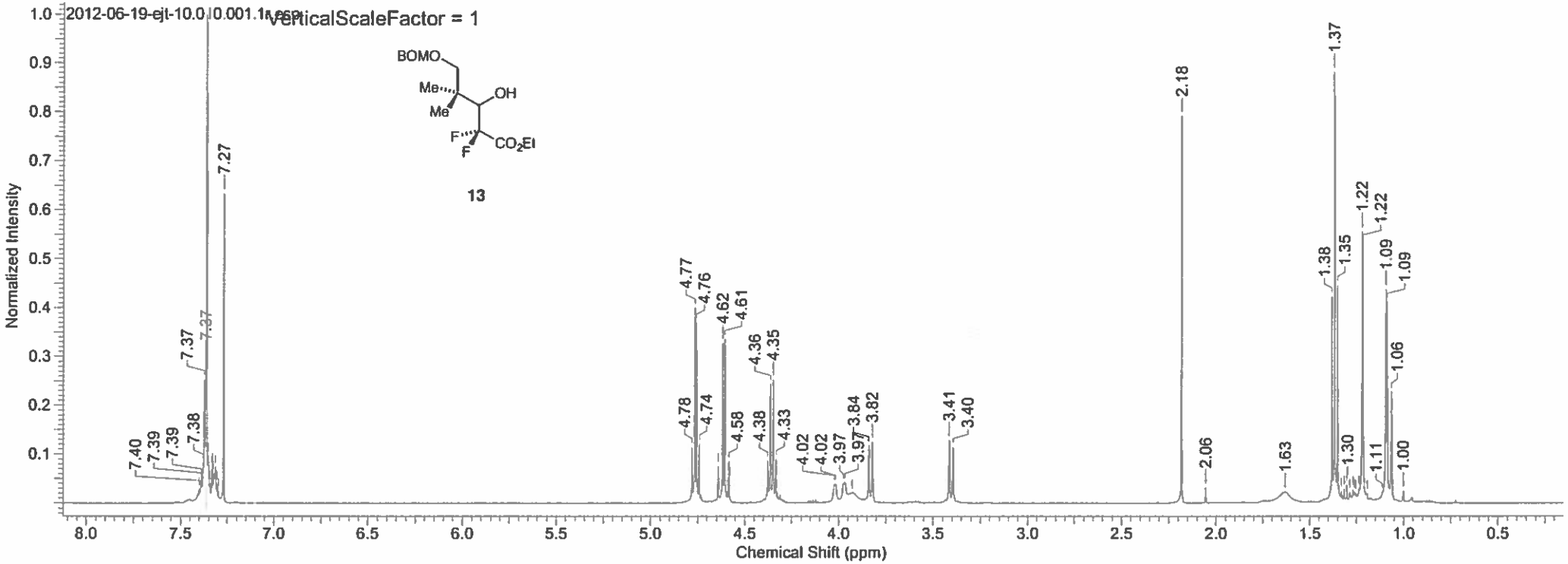
Frequency (MHz)	500.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zg30b
Receiver Gain	203.00	*SW(cyclical) (Hz)*	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3079.9768
Spectrum Type	STANDARD	*Sweep Width (Hz)*	10330.26	*Temperature (degree C)*	20.001		



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.00	501.0	0.0255	12	1.26	630.2	0.0225	23	1.37	686.0	0.0604	34	3.97	1987.4	0.0410	45	4.59	2297.3	0.0249
2	1.06	531.9	0.2281	13	1.27	634.0	0.0282	24	1.38	690.1	0.4235	35	4.02	2008.6	0.0394	46	4.61	2304.0	0.3359
3	1.07	533.7	0.0986	14	1.29	644.1	0.0230	25	1.63	815.6	0.0229	36	4.02	2012.3	0.0387	47	4.62	2309.9	0.3286
4	1.09	544.5	0.4125	15	1.30	651.0	0.0371	26	2.06	1028.1	0.0322	37	4.33	2163.7	0.0224	48	4.64	2321.6	0.0757
5	1.09	546.7	0.4379	16	1.32	658.3	0.0293	27	2.18	1091.4	0.7925	38	4.33	2167.8	0.0898	49	4.74	2372.4	0.1213
6	1.11	557.4	0.0224	17	1.33	665.2	0.0251	28	3.40	1698.0	0.1140	39	4.34	2170.6	0.0238	50	4.75	2376.1	0.0240
7	1.20	597.7	0.0200	18	1.34	672.5	0.0356	29	3.41	1707.8	0.1283	40	4.35	2175.0	0.2529	51	4.76	2379.3	0.3702
8	1.22	608.5	0.5317	19	1.35	673.4	0.0364	30	3.82	1910.8	0.1254	41	4.36	2182.3	0.2438	52	4.77	2384.0	0.4005
9	1.22	609.7	0.5571	20	1.35	675.9	0.4465	31	3.84	1920.3	0.1186	42	4.37	2186.0	0.0262	53	4.78	2391.0	0.1141
10	1.24	618.6	0.0300	21	1.36	679.4	0.0452	32	3.93	1964.7	0.0215	43	4.38	2189.2	0.0866	54	7.27	3635.9	0.6329
11	1.25	627.1	0.0214	22	1.37	683.2	0.8827	33	3.97	1983.6	0.0433	44	4.58	2292.3	0.0859	55	7.30	3650.1	0.0243

ejt cry tips
mCARBONnight CDCl3 /opt/bruk500data/2012/Jun ejt 10

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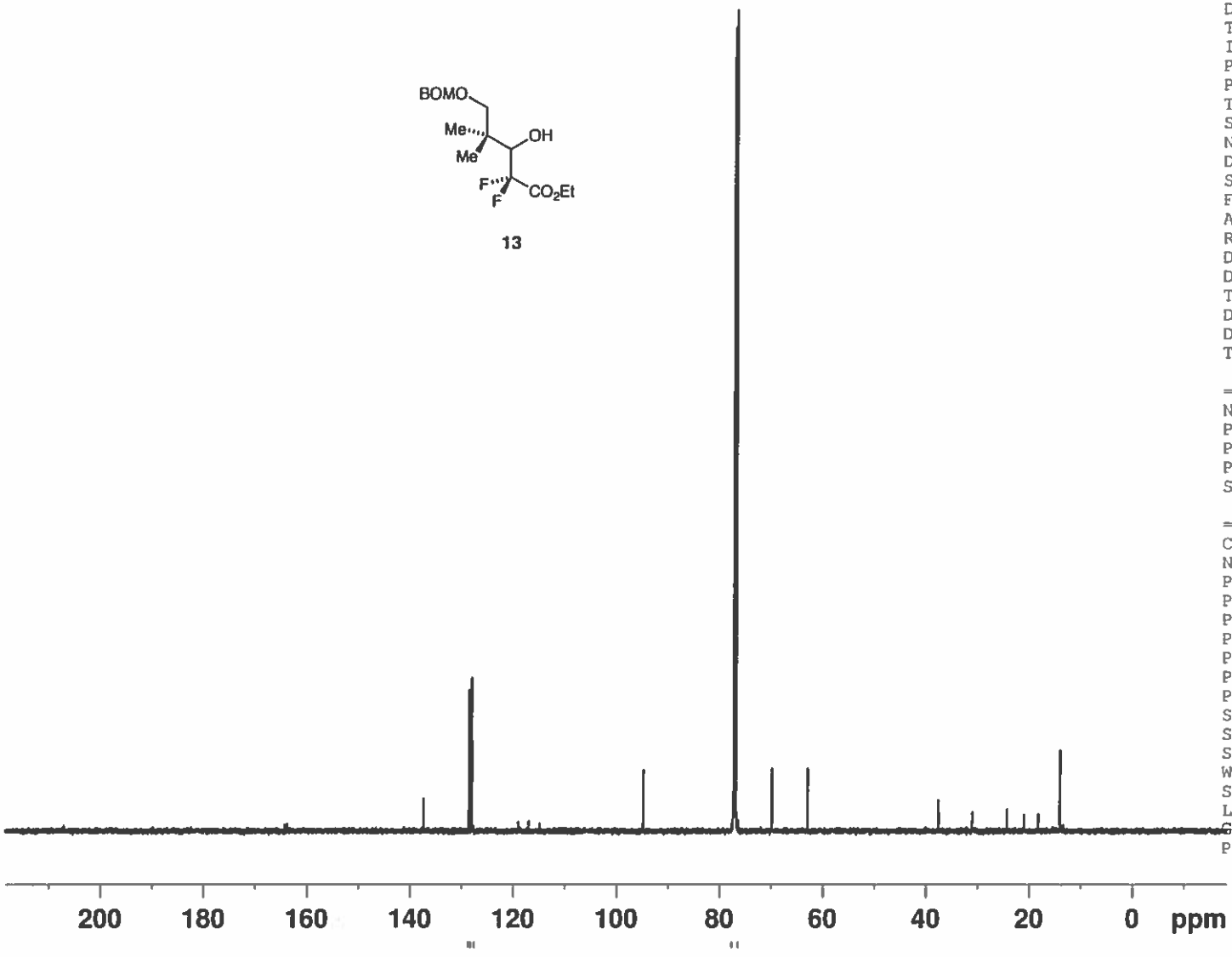
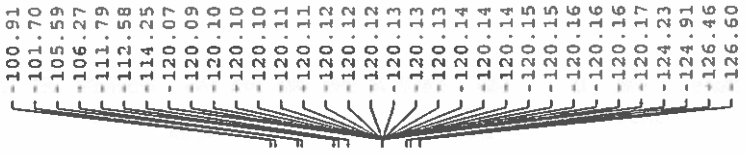
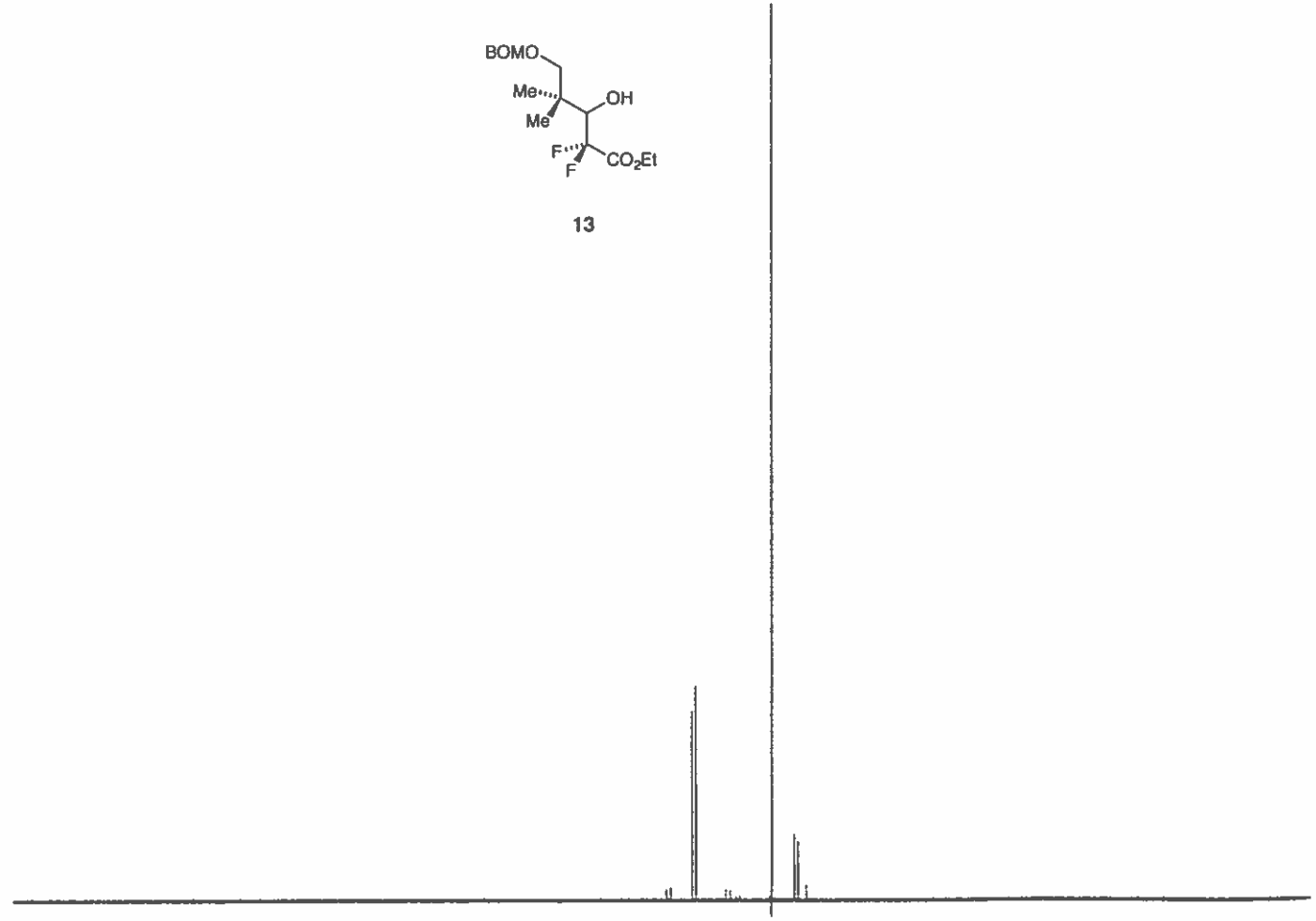


NAME	2012-06-19-ejt-10
EXPNO	11
PROCNO	1
Date_	20120620
Time	4.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	512
DW	16.800 usec
DE	32.78 usec
TE	293.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.80 usec
PL1	-1.00 dB
PL1W	104.35516357 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.23 dB
PL13	120.00 dB
PL2W	25.62124252 W
PL12W	0.48484197 W
PL13W	0.00000000 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

ejt cry zinc 2-6
mF19CPD CDCl3 {e:\bruk400data\2012\Jun} ejt 39



13



NAME	2012-06-11-ejt-39	
EXPNO	11	
PROCNO	1	
Date	20120611	
Time	12.34	
INSTRUM	AV400	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	89285.711	Hz
FIDRES	0.681196	Hz
AQ	0.7340532	sec
RG	4100	
DW	5.600	usec
DE	7.51	usec
TE	293.7	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	10.70	usec
PL1	-5.00	dB
PL1W	27.00716019	W
SFO1	376.4607164	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-3.60	dB
PL12	15.31	dB
PL2W	17.83863831	W
PL12W	0.22927761	W
SFO2	400.1316005	MHz
SI	262144	
SF	376.4983660	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	2.00	

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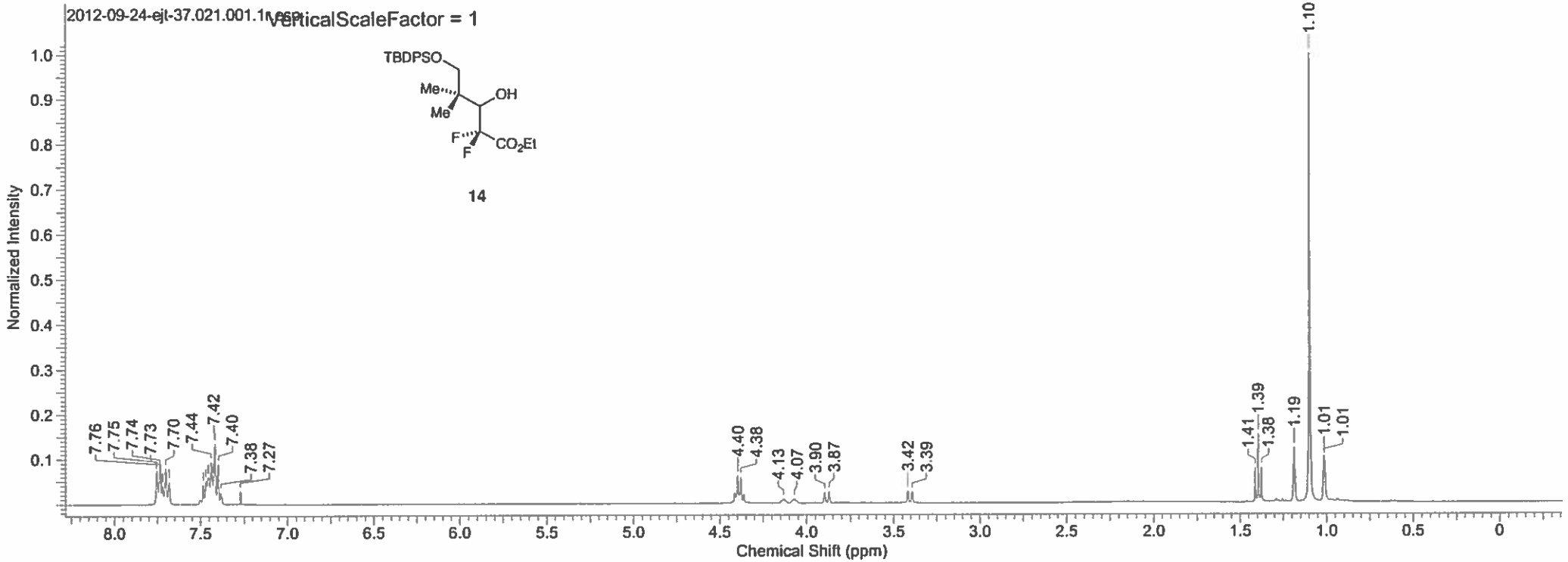
30/11/2012 13:48:52

Acquisition Time (sec)	3.9649	*Comment*	ejt cry zinc product mPROTONnight CDCl3 (e:\bruk400data\2012\Sep) ejt 37				
Date	25 Sep 2012 08:06:40			*Date Stamp*	25 Sep 2012 08:06:40		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Sep\data\ejt\nmr\2012-09-24-ejt-37\21\pdata\1\1r					*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*	90.50
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9272	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	21.100				



No.	(ppm)	(Hz)	Height
1	1.01	404.7	0.0991
2	1.01	406.0	0.1034
3	1.10	439.0	1.0000
4	1.19	474.9	0.1219
5	1.38	550.3	0.0775
6	1.39	557.3	0.1528
7	1.41	564.6	0.0761
8	3.39	1357.3	0.0242

No.	(ppm)	(Hz)	Height
9	3.42	1367.4	0.0266
10	3.87	1549.3	0.0257
11	3.90	1559.4	0.0233
12	4.07	1629.2	0.0093
13	4.13	1653.7	0.0094
14	4.38	1752.6	0.0584
15	4.40	1759.6	0.0613
16	7.27	2908.9	0.0286

No.	(ppm)	(Hz)	Height
17	7.38	2954.1	0.0268
18	7.40	2960.4	0.0893
19	7.42	2967.7	0.1354
20	7.42	2969.2	0.1038
21	7.43	2971.0	0.0623
22	7.44	2976.3	0.0944
23	7.45	2982.3	0.0596
24	7.46	2983.3	0.0587

No.	(ppm)	(Hz)	Height
25	7.46	2984.4	0.0597
26	7.47	2988.6	0.0512
27	7.49	2995.2	0.0433
28	7.68	3074.4	0.0505
29	7.70	3081.2	0.0732
30	7.70	3082.5	0.0804
31	7.72	3089.0	0.0416
32	7.72	3090.5	0.0400

No.	(ppm)	(Hz)	Height
33	7.73	3092.1	0.0258
34	7.73	3094.3	0.0699
35	7.74	3095.6	0.0802
36	7.75	3101.9	0.0759
37	7.76	3103.1	0.0708

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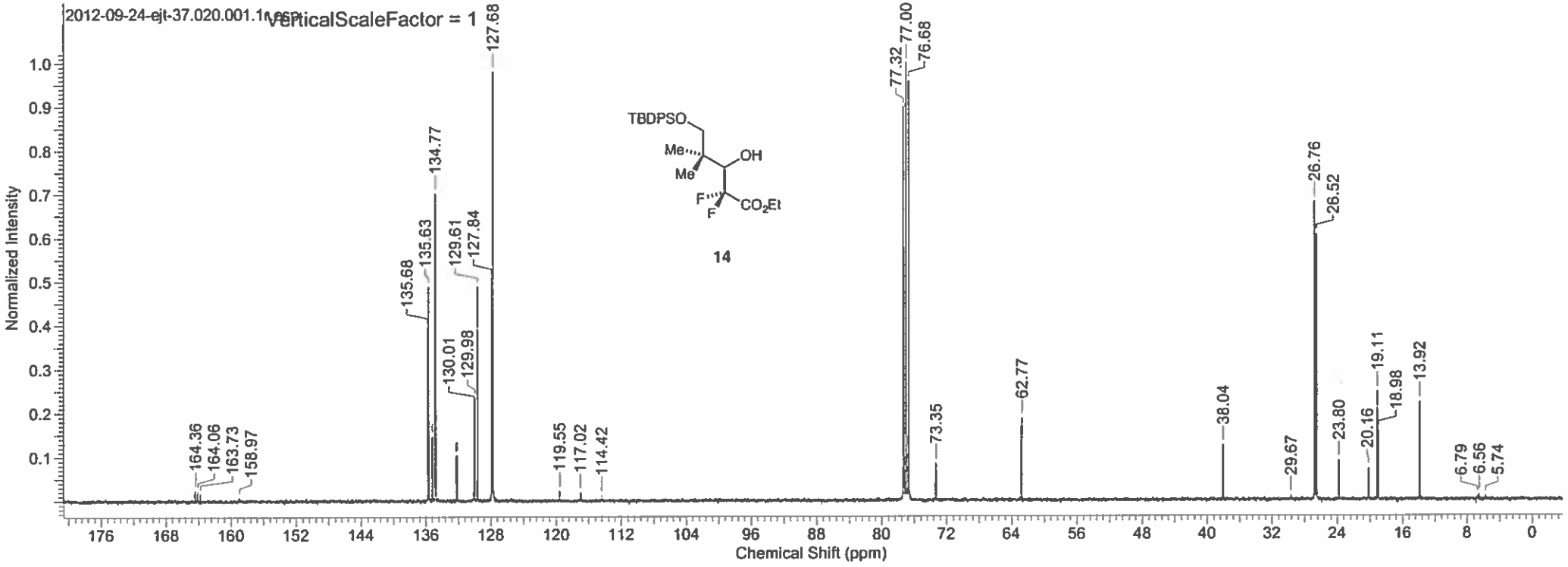
30/11/2012 13:50:44

Acquisition Time (sec)	1.0835	*Comment*	ejt cry zinc product mCARBONnight CDCl3 (e:\bruk400data\2012\Sep) ejt 37				
Date	25 Sep 2012 08:04:32	*Date Stamp*	25 Sep 2012 08:04:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Sep\data\ejt\nmr\2012-09-24-ejt-37\20\pdata\1\1r					*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	1000	*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)*	11328.5381	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30241.01	*Temperature (degree C)*	21.600				



No.	(ppm)	(Hz)	Height
1	5.74	577.1	0.0093
2	6.56	660.2	0.0119
3	6.79	683.2	0.0090
4	13.92	1400.3	0.2237
5	18.98	1909.8	0.1580
6	19.11	1922.7	0.2472
7	20.16	2027.9	0.0721
8	23.77	2391.5	0.0884
9	23.80	2394.3	0.0903

No.	(ppm)	(Hz)	Height
10	26.52	2668.4	0.6070
11	26.76	2692.4	0.6829
12	29.67	2985.0	0.0095
13	38.04	3827.6	0.1250
14	62.77	6315.7	0.1868
15	73.31	7376.2	0.0789
16	73.35	7379.9	0.0836
17	76.68	7714.9	0.9580
18	76.93	7739.8	0.0754

No.	(ppm)	(Hz)	Height
19	77.00	7747.2	1.0000
20	77.20	7767.5	0.0691
21	77.32	7779.5	0.8987
22	114.42	11511.7	0.0121
23	116.95	11766.5	0.0172
24	117.02	11773.8	0.0187
25	119.55	12028.6	0.0216
26	127.68	12846.3	0.9803
27	127.82	12860.1	0.4990

No.	(ppm)	(Hz)	Height
28	127.84	12862.0	0.5090
29	129.61	13040.1	0.4893
30	129.98	13077.9	0.2343
31	130.01	13080.7	0.2185
32	132.09	13290.2	0.1047
33	132.23	13304.0	0.1029
34	134.77	13559.7	0.7025
35	135.16	13598.4	0.1467
36	135.63	13646.4	0.4880

No.	(ppm)	(Hz)	Height
37	135.68	13651.0	0.3960
38	158.97	15994.3	0.0089
39	163.73	16473.3	0.0166
40	164.02	16502.8	0.0220
41	164.06	16506.5	0.0221
42	164.36	16537.0	0.0238

ejty cry meli
mPROTON CDCl3 {e:\bruk400data\2012\Feb} ejt 41

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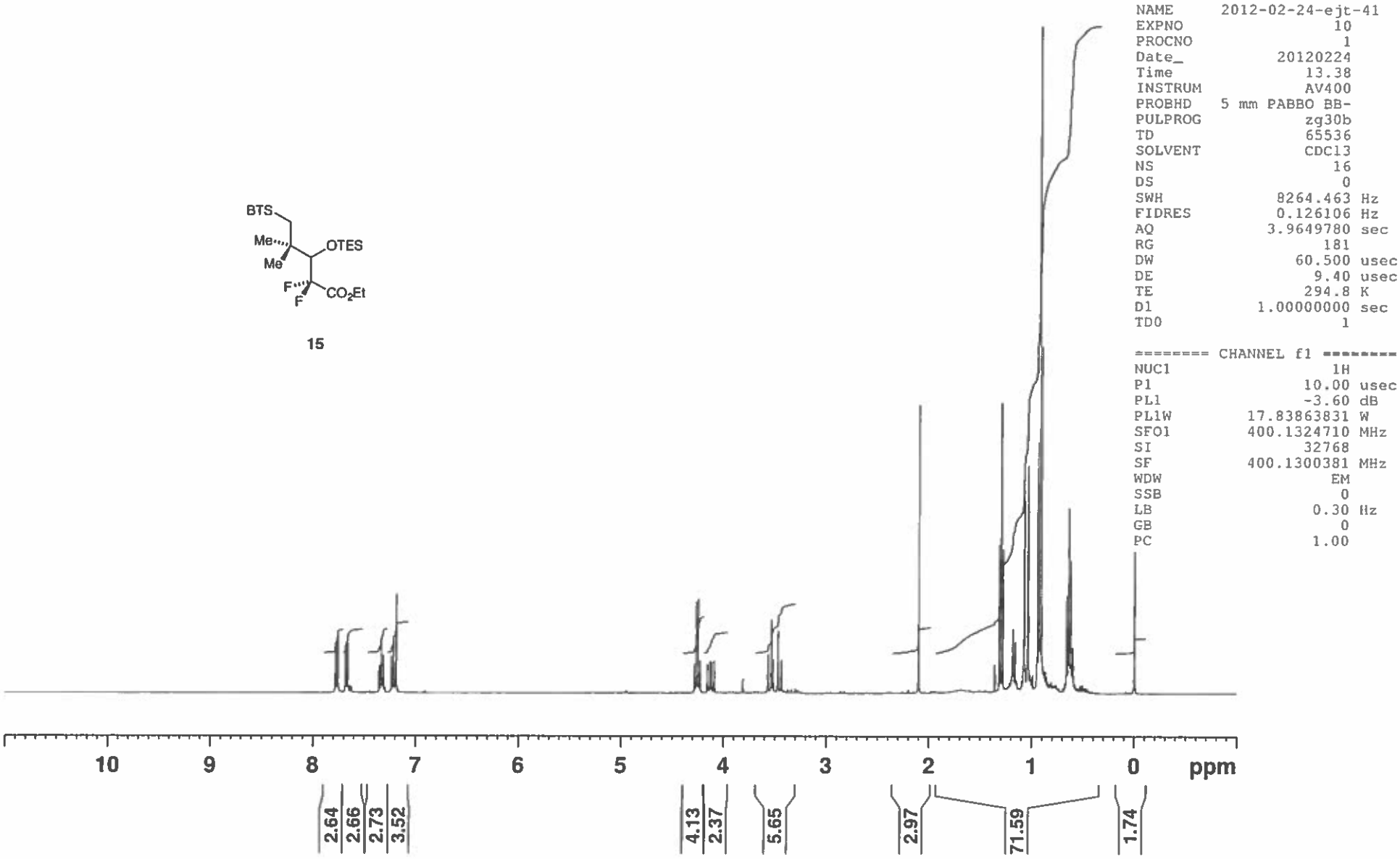

NAME	2012-02-24-ejt-41
EXPNO	10
PROCNO	1
Date_	20120224
Time	13.38
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	181
DW	60.500 usec
DE	9.40 usec
TE	294.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300381 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

ejt cry tes 3-5
mCARBONnight CDCl3 /opt/bruk500data/2012/Feb ejt 28

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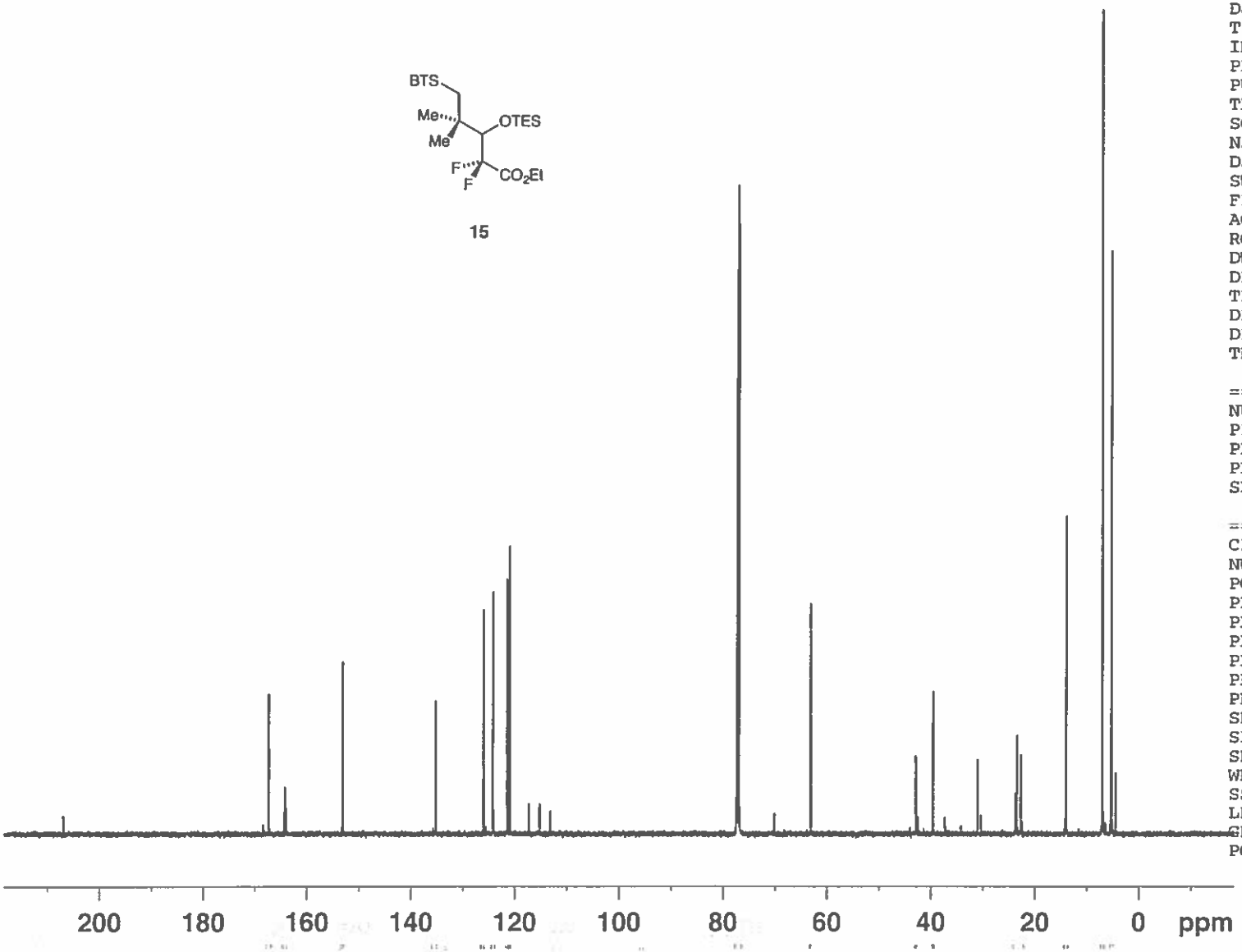
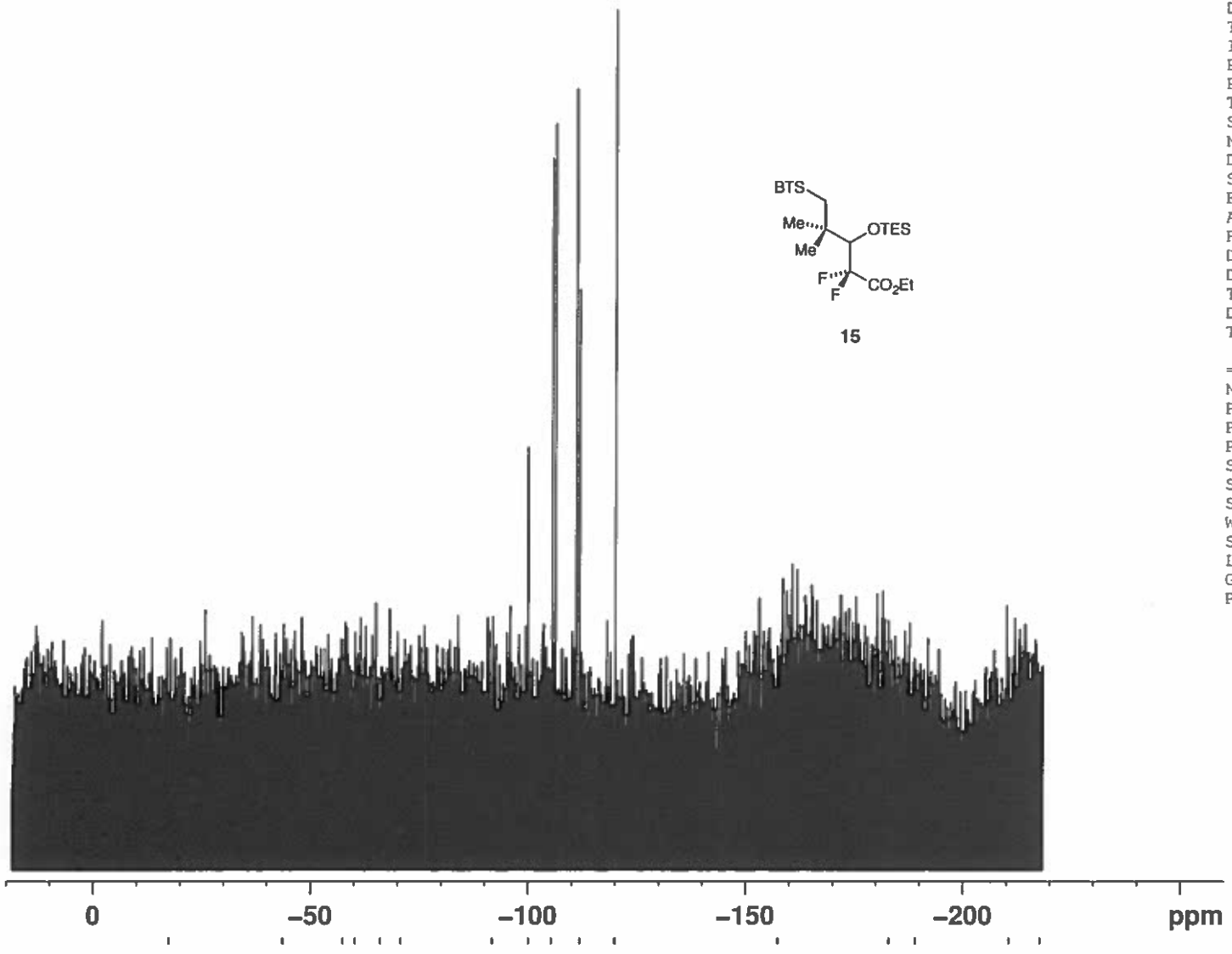


NAME	2012-02-13-ejt-28
EXPNO	12
PROCNO	1
Date_	20120214
Time	0.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	500
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	512
DW	16.800 usec
DE	32.78 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.80 usec
PL1	-1.00 dB
PL1W	104.35516357 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.23 dB
PL13	120.00 dB
PL2W	25.62124252 W
PL12W	0.48484197 W
PL13W	0.00000000 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

ejt cry tes
mF19 CDCl3 {e:\bruk400data\2012\Mar} ejt 58



15

NAME	2012-03-21-ejt-58
EXPNO	10
PROCNO	1
Date_	20120321
Time	15.43
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	11.01 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

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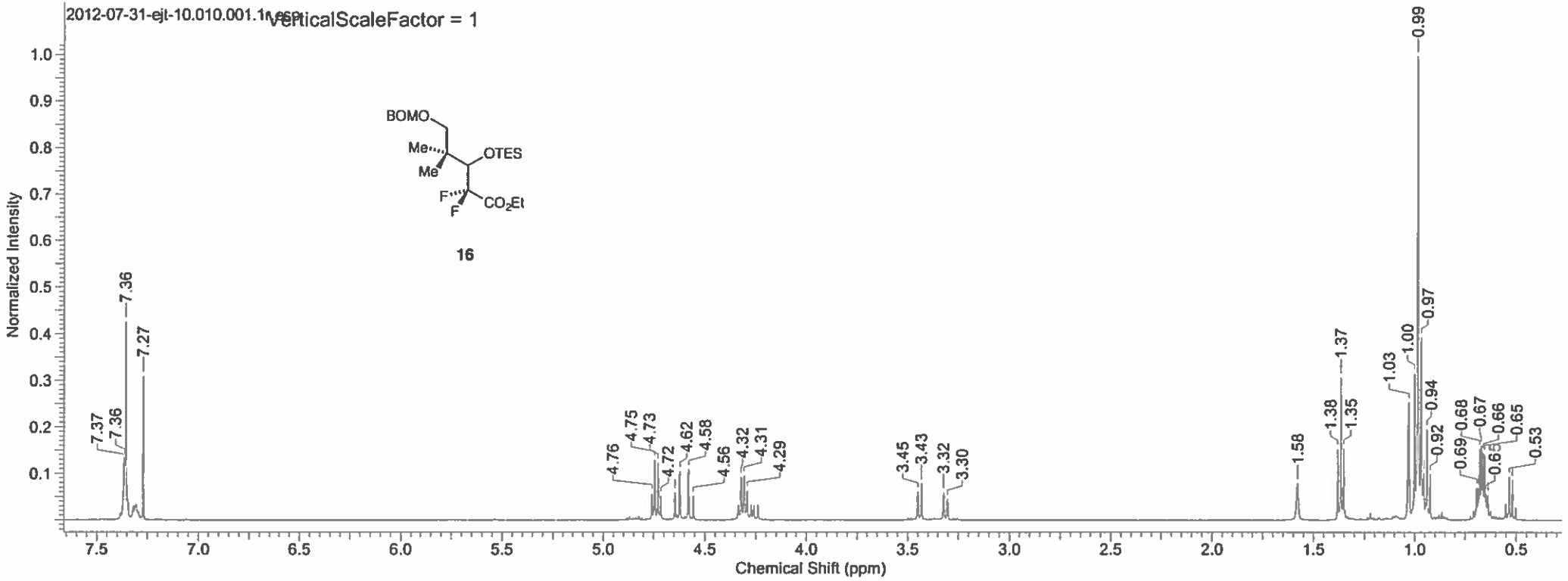
29/11/2012 16:44:47

Acquisition Time (sec)	3.1719	*Comment*	ejt cry tes prot mPROTON CDCl3 /opt/bruk500data/2012/Jul ejt 10			*Date*	31 Jul 2012 11:08:00
Date Stamp	31 Jul 2012 11:08:00	*File Name*	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500data\bruk500data\2012\Jul\data\ejt\nmr\2012-07-31-ejt-10\10\pdata\1\1r				
Frequency (MHz)	500.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zg30b
Receiver Gain	90.50	*SW(cyclical) (Hz)*	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3080.2925
Spectrum Type	STANDARD	*Sweep Width (Hz)*	10330.26	*Temperature (degree C)*	27.000		



No.	(ppm)	(Hz)	Height
1	0.52	259.2	0.0866
2	0.53	267.0	0.0938
3	0.64	319.4	0.0536
4	0.65	323.8	0.0573
5	0.65	327.6	0.1427
6	0.66	331.7	0.1452
7	0.67	335.4	0.1599
8	0.68	339.5	0.1533
9	0.69	343.6	0.0687

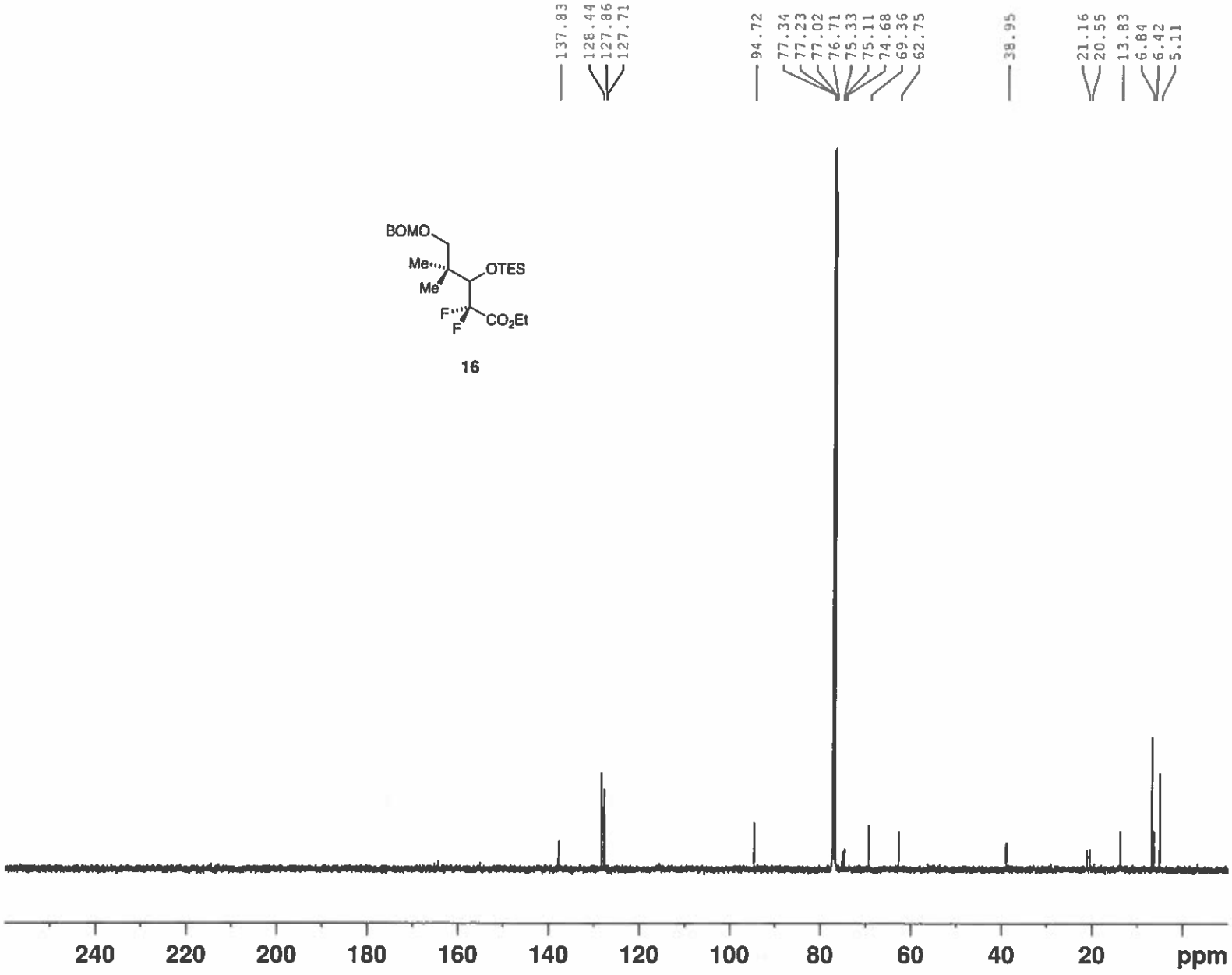
No.	(ppm)	(Hz)	Height
10	0.69	347.1	0.0698
11	0.92	461.9	0.0986
12	0.94	469.7	0.1950
13	0.96	477.6	0.1019
14	0.96	479.5	0.0617
15	0.97	484.9	0.3933
16	0.99	492.8	1.0000
17	1.00	500.6	0.3154
18	1.03	515.1	0.2534

No.	(ppm)	(Hz)	Height
19	1.35	676.2	0.1536
20	1.36	679.7	0.0425
21	1.37	683.5	0.3057
22	1.38	690.4	0.1533
23	1.58	789.4	0.0789
24	3.30	1652.3	0.0458
25	3.32	1661.4	0.0594
26	3.43	1716.3	0.0788
27	3.45	1725.4	0.0613

No.	(ppm)	(Hz)	Height
28	4.29	2146.6	0.0634
29	4.31	2153.9	0.0958
30	4.32	2161.1	0.0920
31	4.56	2278.4	0.0522
32	4.58	2290.1	0.1087
33	4.62	2311.8	0.1047
34	4.65	2323.5	0.0587
35	4.72	2358.5	0.0520
36	4.73	2365.1	0.1230

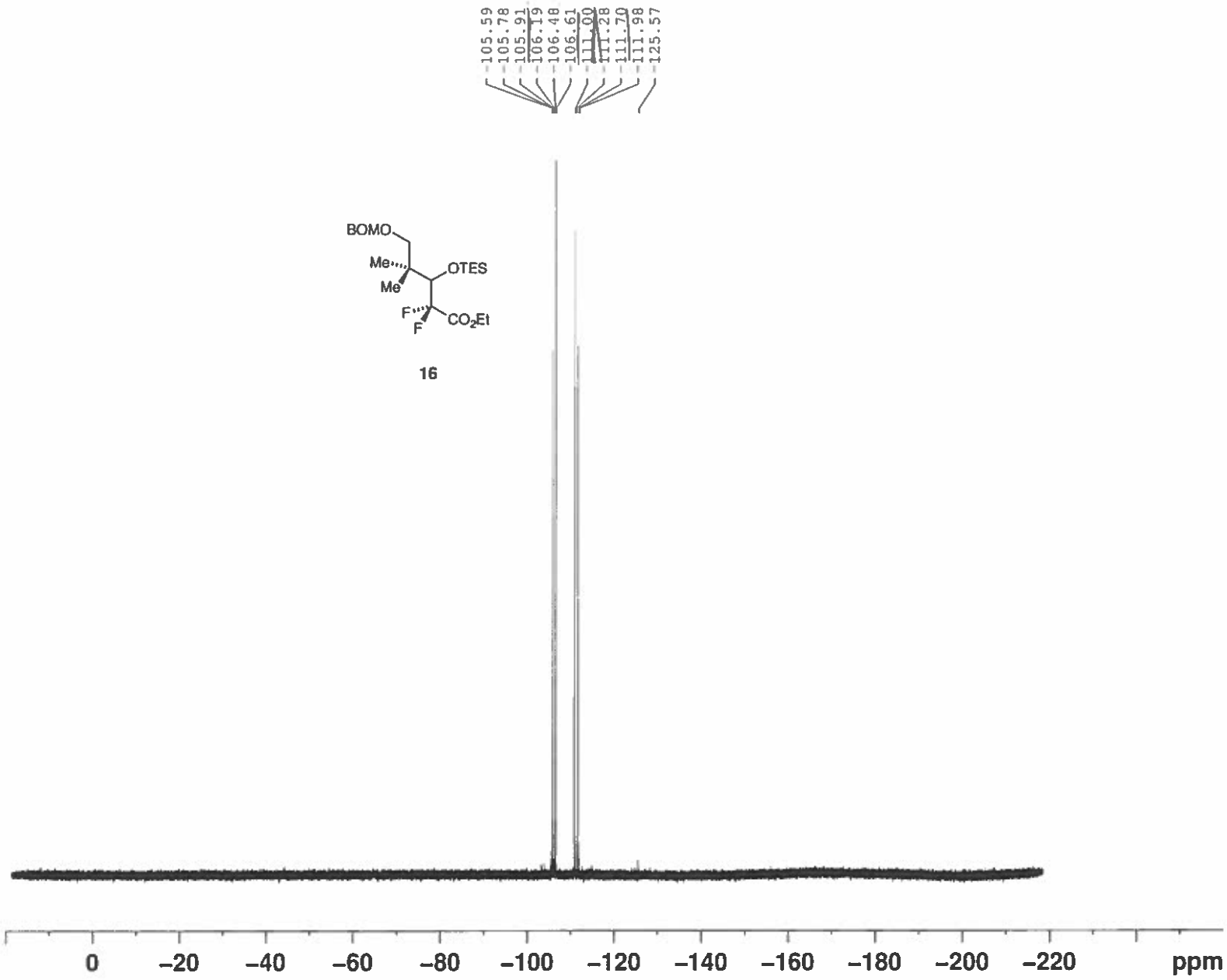
No.	(ppm)	(Hz)	Height
37	4.75	2373.3	0.1291
38	4.76	2379.9	0.0568
39	7.27	3635.9	0.3093
40	7.35	3675.0	0.0455
41	7.36	3678.8	0.4257
42	7.36	3681.7	0.1335
43	7.37	3684.5	0.1228

ejt cry tes prot
mCARBONnight CDCl3 {e:\bruk400data\2012\Jul} ejt 35



NAME	2012-07-31-ejt-35
EXPNO	11
PROCNO	1
Date_	20120801
Time	0.01
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	296.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

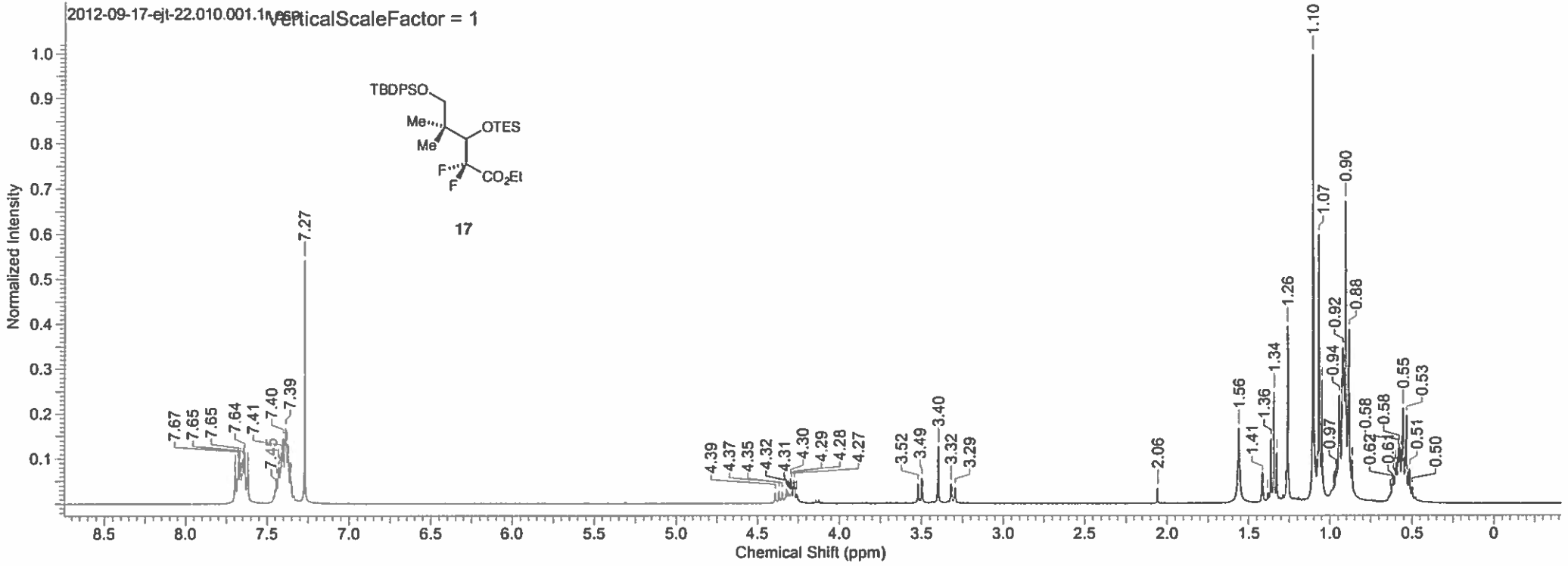
ejt cry tes prot
mF19CPD CDCl3 {e:\bruk400data\2012\Jul} ejt 35



NAME	2012-07-31-ejt-35	
EXPNO	10	
PROCNO	1	
Date_	20120731	
Time	11.44	
INSTRUM	AV400	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	89285.711	Hz
FIDRES	0.681196	Hz
AQ	0.7340532	sec
RG	4100	
DW	5.600	usec
DE	7.51	usec
TE	295.6	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	10.70	usec
PL1	-5.00	dB
PL1W	27.00716019	W
SFO1	376.4607164	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-3.60	dB
PL12	15.31	dB
PL2W	17.83863831	W
PL12W	0.22927761	W
SFO2	400.1316005	MHz
SI	262144	
SF	376.4983660	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	2.00	

30/11/2012 14:32:02

Acquisition Time (sec)	3.9649	*Comment*	ejt cry tes protection mPROTON CDCl3 (e:\bruk400data\2012\Sep) ejt 22				
Date	17 Sep 2012 15:04:48			*Date Stamp*	17 Sep 2012 15:04:48		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Sep\data\ejt\nmr\2012-09-17-ejt-22\10\pdata\1\1r					*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*	287.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.6750	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	22.200				



No.	(ppm)	(Hz)	Height
1	0.50	198.9	0.0365
2	0.51	205.2	0.0761
3	0.53	213.1	0.1953
4	0.54	217.3	0.0733
5	0.55	220.9	0.2121
6	0.56	225.2	0.1204
7	0.58	230.2	0.1316
8	0.58	233.0	0.1224
9	0.59	236.0	0.0720
10	0.60	238.3	0.0895
11	0.60	240.5	0.0780

No.	(ppm)	(Hz)	Height
12	0.61	244.1	0.0597
13	0.61	245.8	0.0438
14	0.62	247.9	0.0422
15	0.63	251.6	0.0247
16	0.86	345.7	0.0959
17	0.88	353.0	0.3885
18	0.90	360.9	0.6733
19	0.91	362.4	0.5130
20	0.92	366.7	0.3024
21	0.92	368.7	0.3475
22	0.93	370.4	0.2798

No.	(ppm)	(Hz)	Height
23	0.94	377.0	0.2404
24	0.95	378.3	0.2398
25	0.96	383.8	0.0689
26	0.97	386.3	0.0770
27	0.97	389.4	0.0415
28	0.98	391.6	0.0350
29	1.05	419.6	0.2737
30	1.07	426.7	0.5991
31	1.08	432.5	0.0672
32	1.09	434.5	0.0747
33	1.10	440.8	1.0000

No.	(ppm)	(Hz)	Height
34	1.26	503.4	0.3944
35	1.27	508.1	0.0415
36	1.33	530.6	0.1129
37	1.34	537.7	0.2470
38	1.36	544.7	0.1441
39	1.38	552.0	0.0236
40	1.41	564.4	0.0379
41	1.41	565.9	0.0633
42	1.42	567.4	0.0394
43	1.56	624.4	0.1664
44	2.06	822.9	0.0340

No.	(ppm)	(Hz)	Height
45	3.29	1318.0	0.0350
46	3.32	1327.8	0.0429
47	3.40	1359.1	0.1272
48	3.49	1398.5	0.0558
49	3.52	1408.3	0.0440
50	4.26	1704.4	0.0213
51	4.27	1709.4	0.0484
52	4.28	1711.7	0.0527
53	4.29	1716.5	0.0498
54	4.30	1718.8	0.0555
55	4.31	1723.6	0.0223

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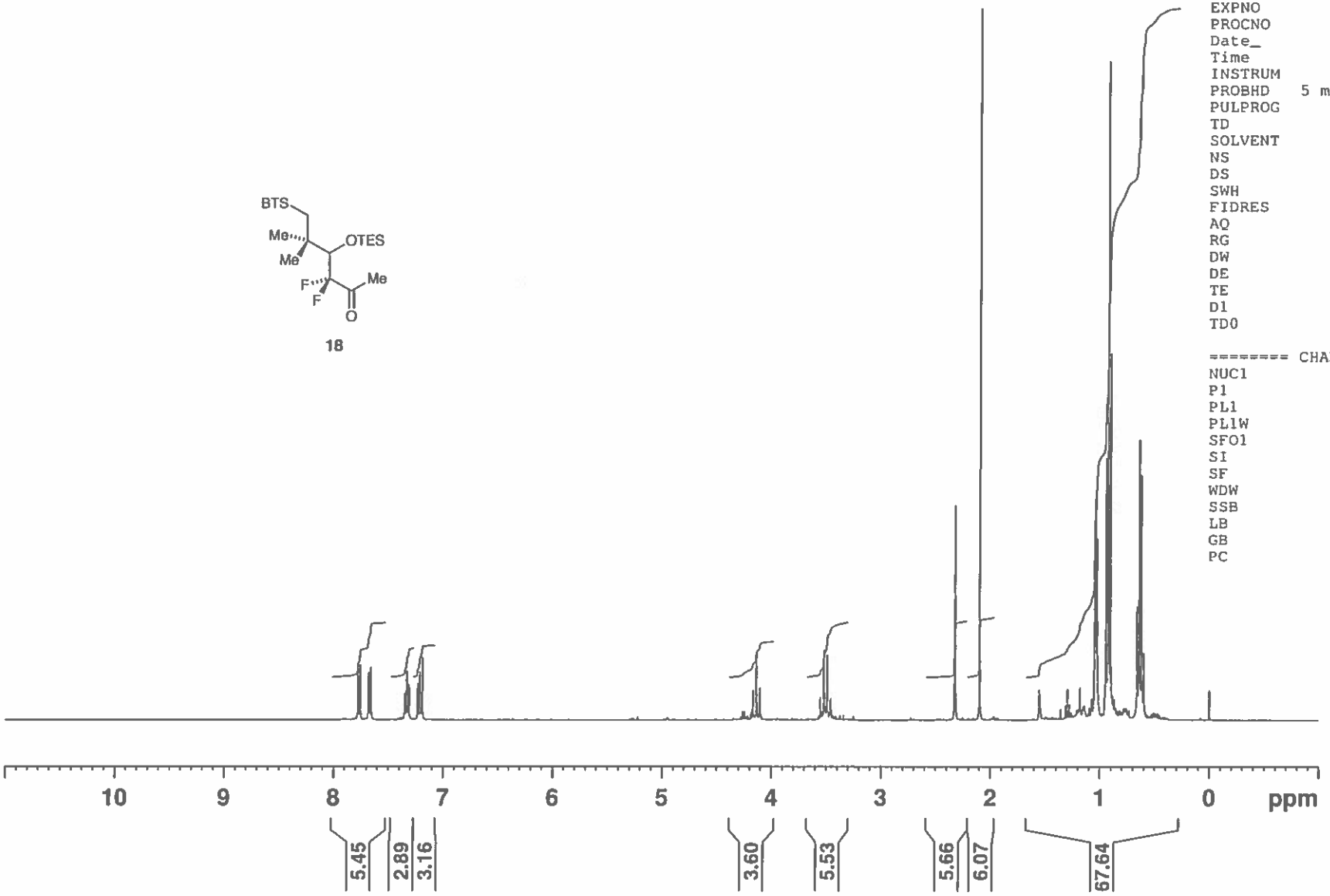
mPROTON CDCl3 {e:\bruk400data\2012\Mar} ejt 38

18

NAME	2012-03-01-ejt-38
EXPNO	10
PROCNO	1
Date_	20120301
Time	14.22
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	144
DW	60.500 usec
DE	9.40 usec
TE	295.0 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	400.1300383 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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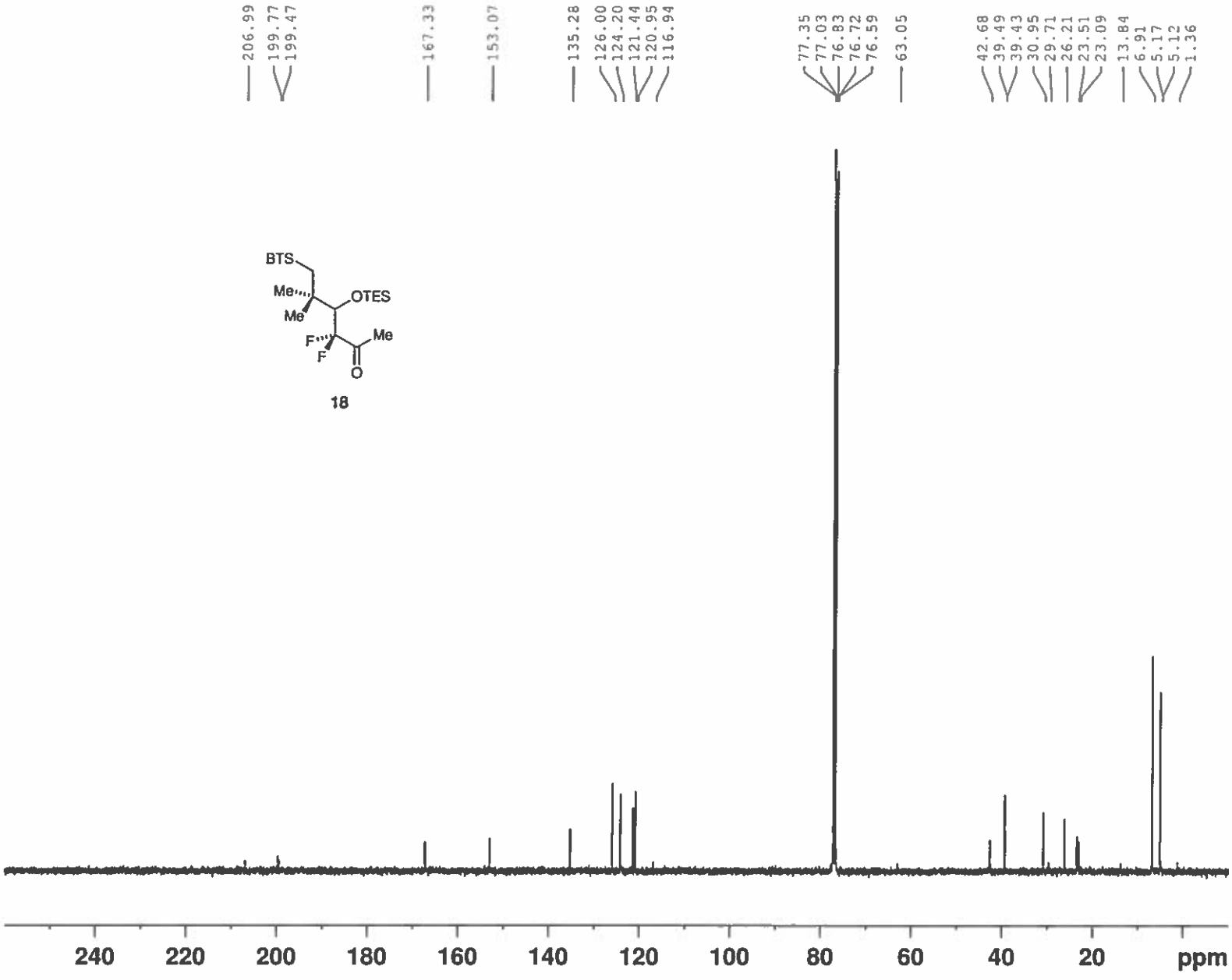
mCARBONnight CDCl3 {e:\bruk400data\2012\Mar} ejt 38



NAME	2012-03-01-ejt-38
EXPNO	11
PROCNO	1
Date_	20120302
Time	6.17
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	295.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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mF19CPD CDCl3 {e:\bruk400data\2012\Mar} ejt 38

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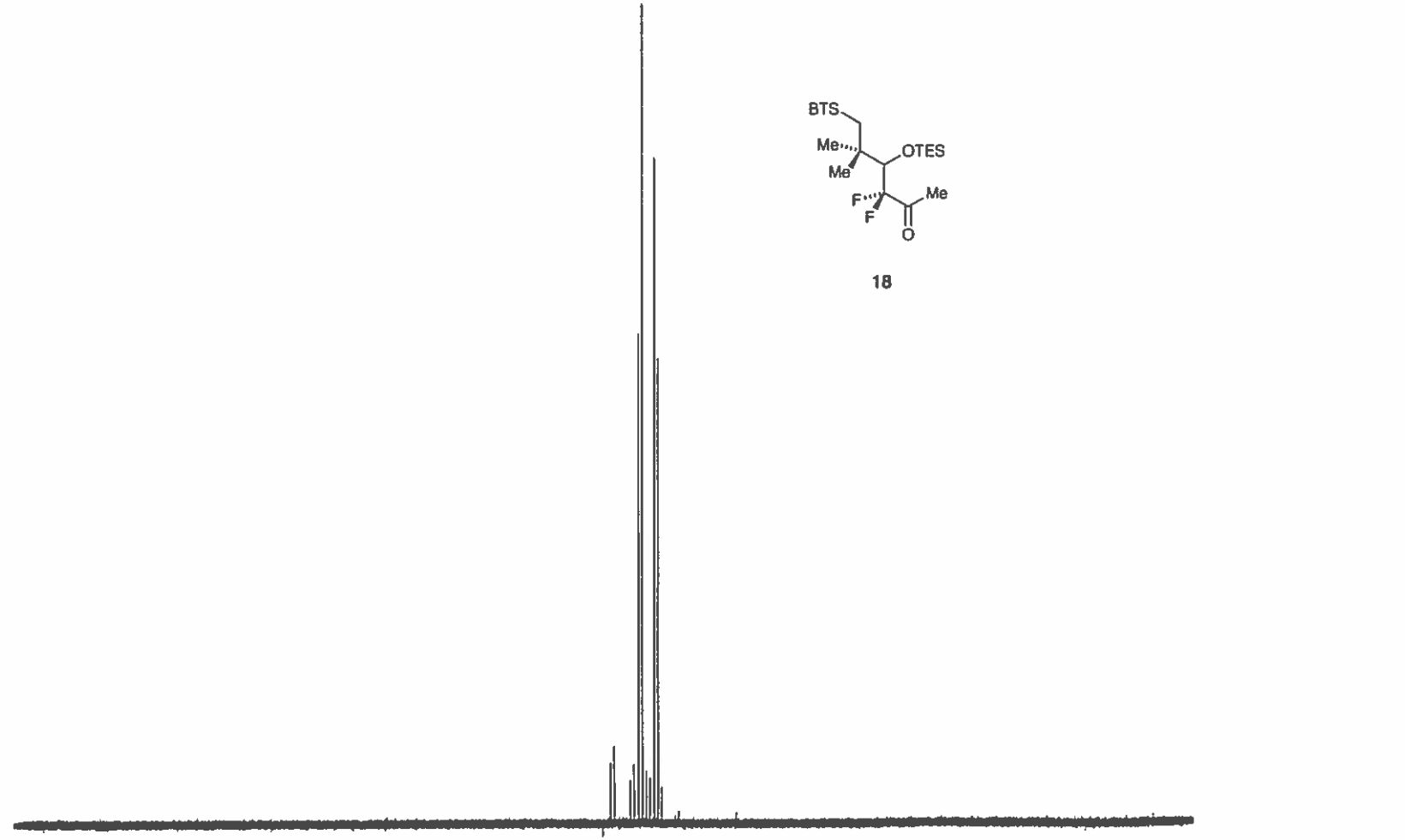

NAME	2012-03-01-ejt-38
EXPNO	12
PROCNO	1
Date_	20120301
Time	14.23
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgig
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	7.51 usec
TE	295.1 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
SFO2	400.1316005 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

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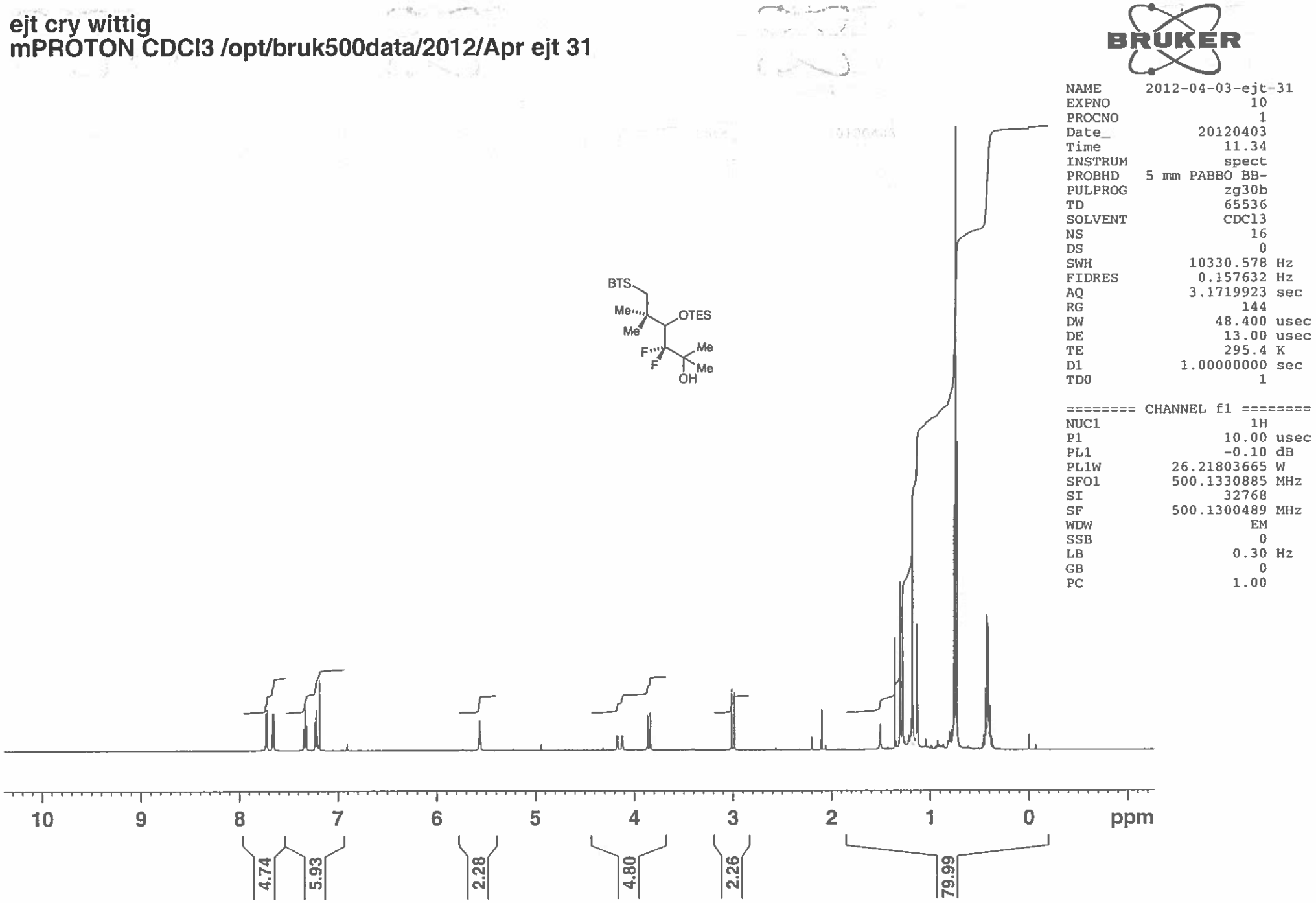
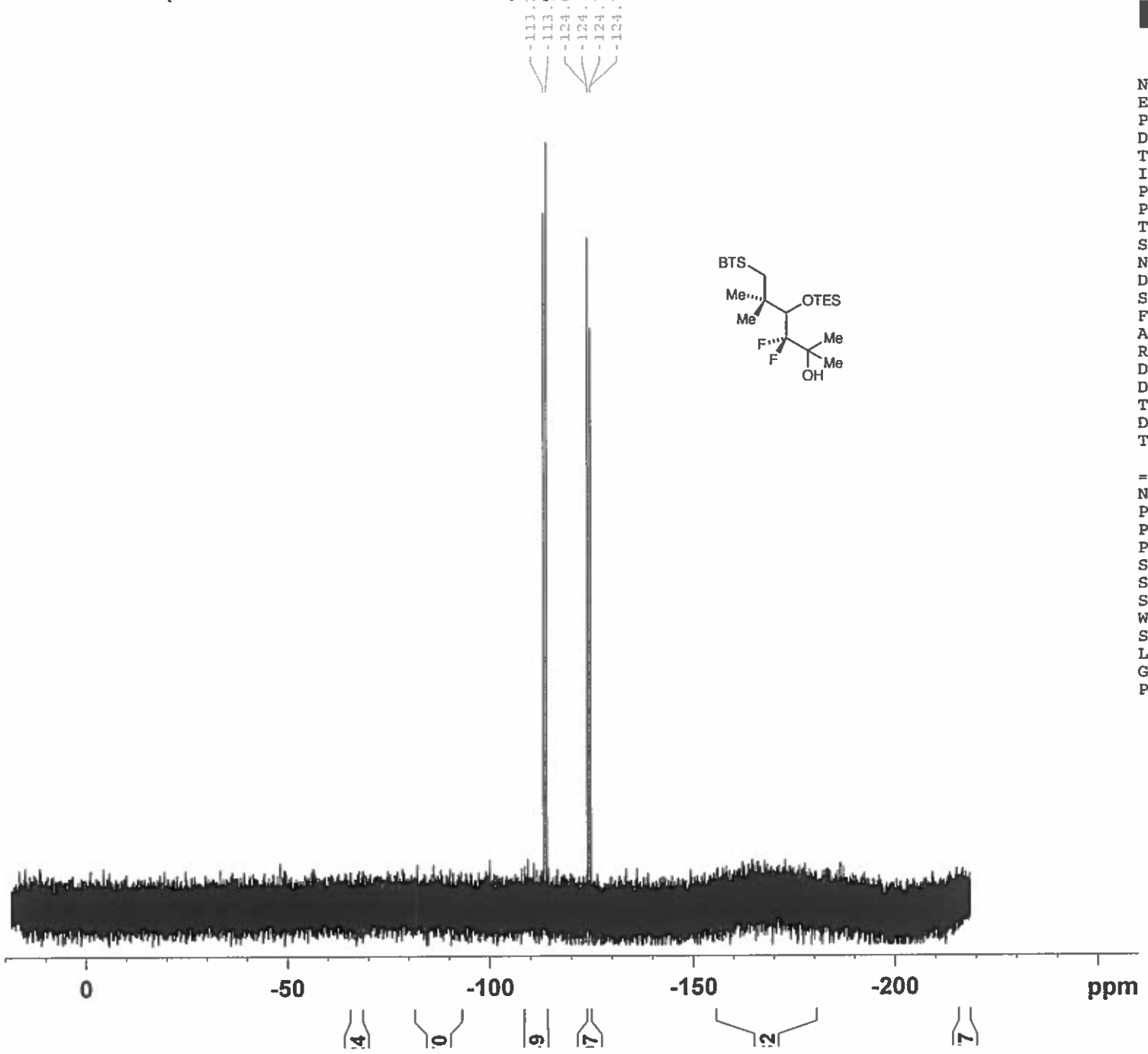
mPROTON CDCl3 /opt/bruk500data/2012/Apr ejt 31



ejt cry mesylate r2
mF19 CDCl3 {e:\bruk400data\2012\Mar} ejt 60

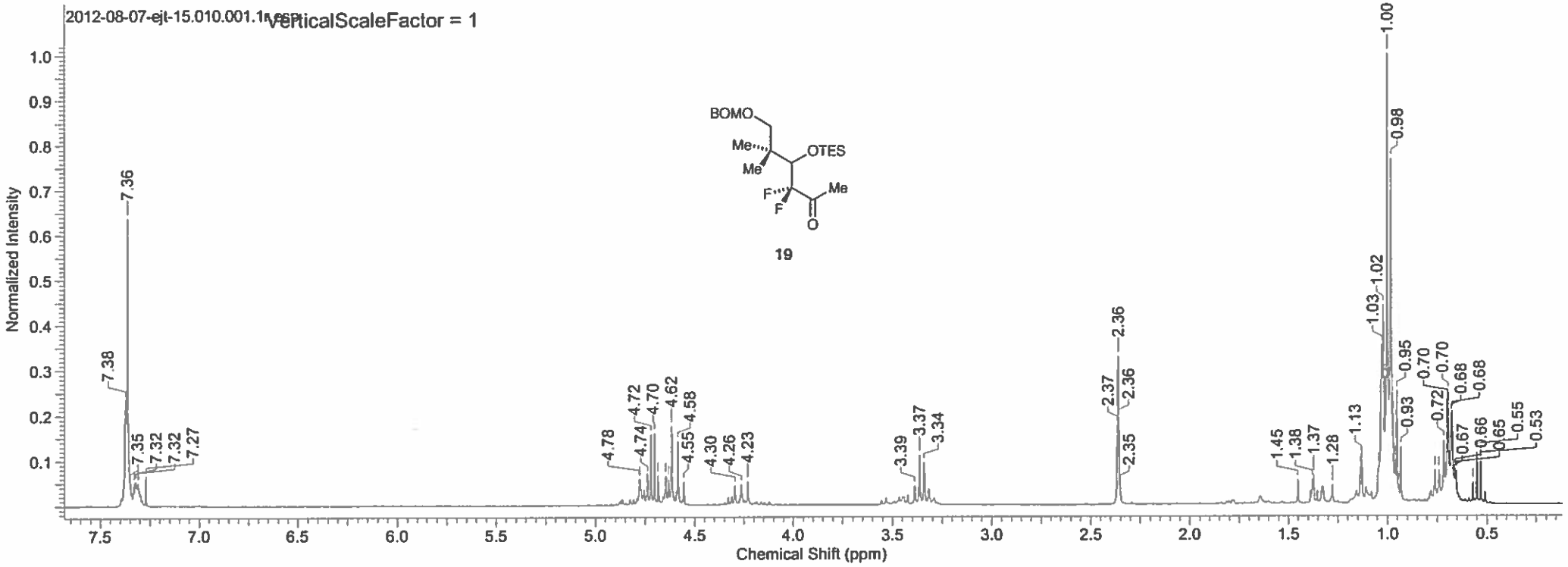


BRUKER 400 MHz

NAME	2012-03-30-ejt-60
EXPNO	10
PROCNO	1
Date_	20120330
Time	17.57
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	11.01 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

29/11/2012 17:03:06

Acquisition Time (sec)	3.9649	*Comment*	ejt cry meli mPROTON CDCl3 {e:\bruk400data\2012\Aug} ejt 15			*Date*	07 Aug 2012 16:04:32
Date Stamp	07 Aug 2012 16:04:32						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Aug\data\ejt\nmr\2012-08-07-ejt-15\10\pdata\1\1r					*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*	57.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9272	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	22.200				

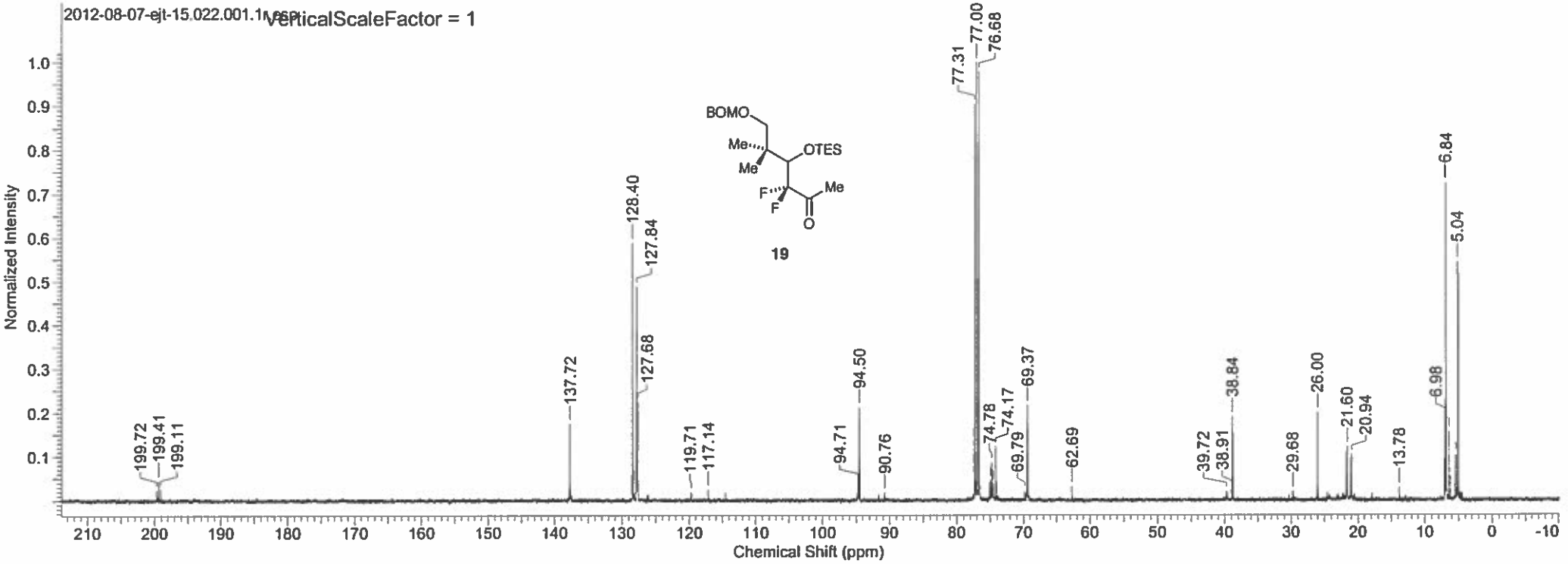


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.53	212.0	0.0952	12	0.71	282.9	0.0629	23	1.00	400.7	1.0000	34	1.45	581.3	0.0545	45	4.55	1822.4	0.0519
2	0.55	220.1	0.1146	13	0.72	287.2	0.1403	24	1.01	404.7	0.2829	35	2.35	941.7	0.0446	46	4.58	1834.0	0.1428
3	0.57	228.2	0.0492	14	0.74	296.8	0.0743	25	1.02	408.8	0.4415	36	2.36	943.5	0.1913	47	4.62	1846.9	0.1761
4	0.65	262.0	0.0748	15	0.76	304.9	0.0762	26	1.03	410.5	0.2809	37	2.36	945.2	0.3289	48	4.63	1853.2	0.0599
5	0.66	264.3	0.0802	16	0.93	373.5	0.1267	27	1.03	412.1	0.3534	38	2.37	946.7	0.1756	49	4.65	1858.7	0.0647
6	0.67	266.8	0.0663	17	0.94	377.2	0.0432	28	1.04	417.9	0.0848	39	3.34	1337.2	0.0945	50	4.69	1874.6	0.0660
7	0.68	270.3	0.2067	18	0.95	381.3	0.2509	29	1.13	451.9	0.0942	40	3.37	1346.5	0.1099	51	4.70	1881.2	0.1598
8	0.68	272.1	0.2004	19	0.96	385.1	0.0987	30	1.13	453.4	0.1088	41	3.39	1355.8	0.0427	52	4.72	1888.5	0.1570
9	0.69	275.1	0.0892	20	0.97	389.4	0.1997	31	1.28	511.2	0.0430	42	4.23	1692.8	0.0518	53	4.74	1895.1	0.0676
10	0.70	278.6	0.2478	21	0.98	392.9	0.7667	32	1.37	549.0	0.0650	43	4.26	1706.1	0.0454	54	4.74	1896.8	0.0426
11	0.70	279.6	0.2340	22	0.99	396.9	0.2736	33	1.38	552.0	0.0558	44	4.30	1719.0	0.0431	55	4.78	1910.7	0.0575

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

30/11/2012 10:40:20

Acquisition Time (sec)	1.0835	*Comment*	ejt cry meli mCARBONnight CDCl3 {e:\bruk400data\2012\Aug} ejt 15			*Date*	08 Aug 2012 01:51:12
Date Stamp	08 Aug 2012 01:51:12						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Aug\data\ejt\nmr\2012-08-07-ejt-15\22\pdata\1\1r					*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	1000	*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)*	11330.3838	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30241.01	*Temperature (degree C)*	23.100				



No.	(ppm)	(Hz)	Height
1	5.04	506.9	0.5443
2	5.40	542.9	0.1020
3	5.47	550.3	0.0425
4	6.26	629.7	0.0241
5	6.38	641.7	0.1556
6	6.74	678.6	0.0747
7	6.77	681.4	0.1883
8	6.80	684.1	0.1352
9	6.84	687.8	0.7244
10	6.98	702.6	0.1890

No.	(ppm)	(Hz)	Height
11	13.78	1386.5	0.0286
12	20.94	2107.3	0.1033
13	21.12	2124.8	0.0187
14	21.60	2172.8	0.1212
15	26.00	2615.8	0.1999
16	29.68	2985.9	0.0199
17	38.84	3907.9	0.1899
18	38.91	3915.3	0.0243
19	39.72	3996.5	0.0196
20	62.69	6307.4	0.0302

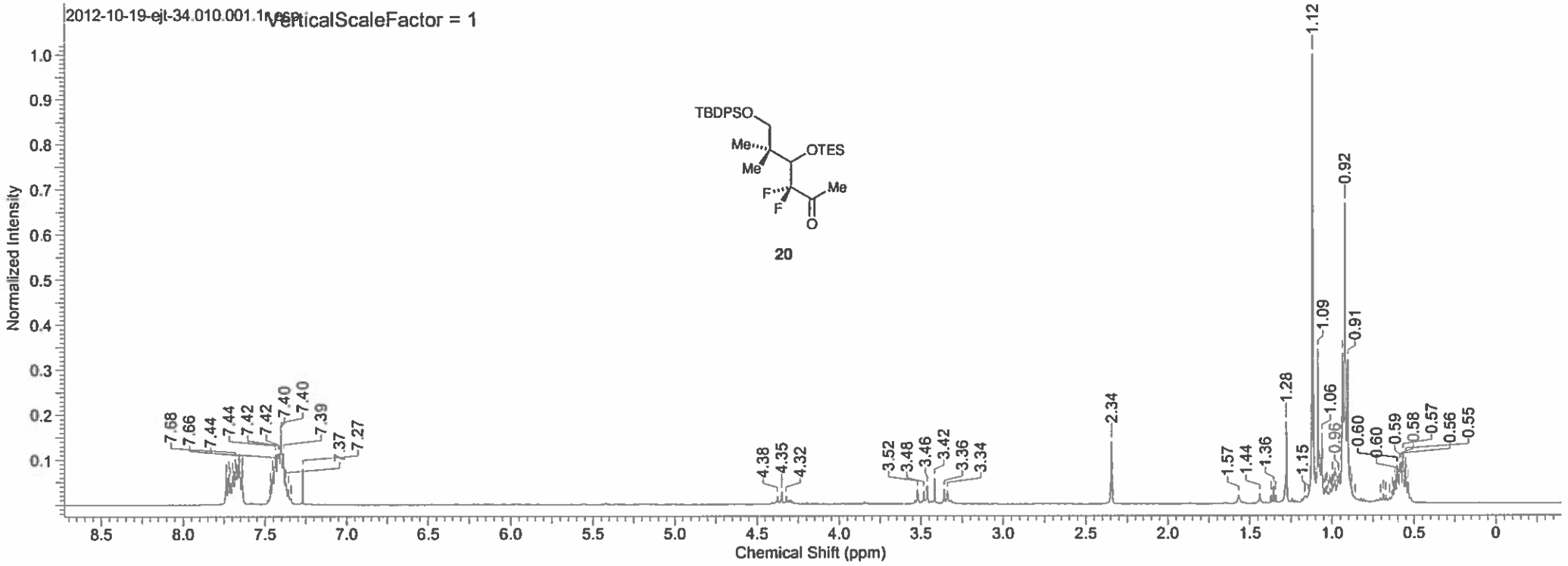
No.	(ppm)	(Hz)	Height
21	69.31	6973.8	0.0433
22	69.37	6979.3	0.2156
23	69.45	6987.6	0.0507
24	69.79	7021.8	0.0204
25	74.17	7462.0	0.1225
26	74.54	7499.8	0.0398
27	74.63	7509.1	0.0360
28	74.78	7523.8	0.0857
29	75.02	7547.8	0.0449
30	76.68	7714.9	0.9789

No.	(ppm)	(Hz)	Height
31	77.00	7747.2	1.0000
32	77.31	7778.6	0.9035
33	90.76	9131.5	0.0177
34	94.50	9508.1	0.2119
35	94.68	9525.6	0.0300
36	94.71	9529.3	0.0407
37	117.14	11785.8	0.0240
38	119.71	12044.3	0.0187
39	127.68	12846.3	0.2237
40	127.82	12860.1	0.2858

No.	(ppm)	(Hz)	Height
41	127.84	12862.0	0.4885
42	127.93	12871.2	0.0317
43	128.40	12918.3	0.5878
44	137.72	13856.9	0.1744
45	137.80	13864.2	0.0260
46	199.11	20033.0	0.0260
47	199.41	20063.4	0.0447
48	199.72	20093.9	0.0240

29/11/2012 13:22:34

Acquisition Time (sec)	3.1719	*Comment*	ejt cry meli 3 mPROTON CDCl3 /opt/bruk500data/2012/Oct ejt 34			*Date*	19 Oct 2012 11:33:36
Date Stamp	19 Oct 2012 11:33:36						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500data\bruk500data\2012\Oct\data\ejt\nmr\2012-10-19-ejt-34\10\pdata\1\1r						
Frequency (MHz)	500.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zg30b
Receiver Gain	50.80	*SW(cyclical) (Hz)*	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3080.2925
Spectrum Type	STANDARD	*Sweep Width (Hz)*	10330.26	*Temperature (degree C)*	27.000		



No.	(ppm)	(Hz)	Height
1	0.54	267.7	0.0431
2	0.54	268.9	0.0464
3	0.55	276.8	0.1038
4	0.56	282.5	0.0932
5	0.57	284.7	0.1130
6	0.58	290.4	0.0931
7	0.59	294.5	0.0897
8	0.60	298.6	0.0594
9	0.60	302.3	0.0853
10	0.61	306.4	0.0326
11	0.62	309.9	0.0520

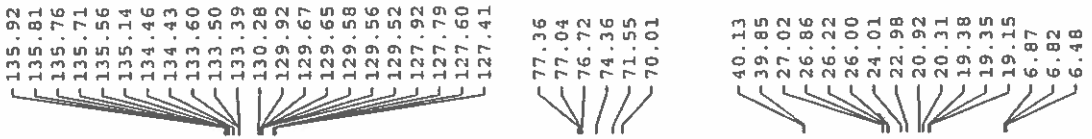
No.	(ppm)	(Hz)	Height
12	0.63	314.0	0.0186
13	0.63	317.2	0.0284
14	0.65	325.0	0.0140
15	0.67	336.7	0.0190
16	0.69	344.9	0.0219
17	0.71	352.8	0.0133
18	0.86	430.3	0.0132
19	0.88	441.1	0.0372
20	0.89	446.1	0.0547
21	0.91	453.4	0.3225
22	0.92	461.2	0.6680

No.	(ppm)	(Hz)	Height
23	0.94	469.1	0.3353
24	0.96	478.9	0.0683
25	0.96	481.4	0.0615
26	0.97	486.8	0.0406
27	0.98	491.5	0.0507
28	0.99	494.7	0.0414
29	1.00	499.4	0.0647
30	1.01	504.7	0.0289
31	1.01	506.3	0.0330
32	1.01	507.3	0.0349
33	1.02	511.4	0.0228

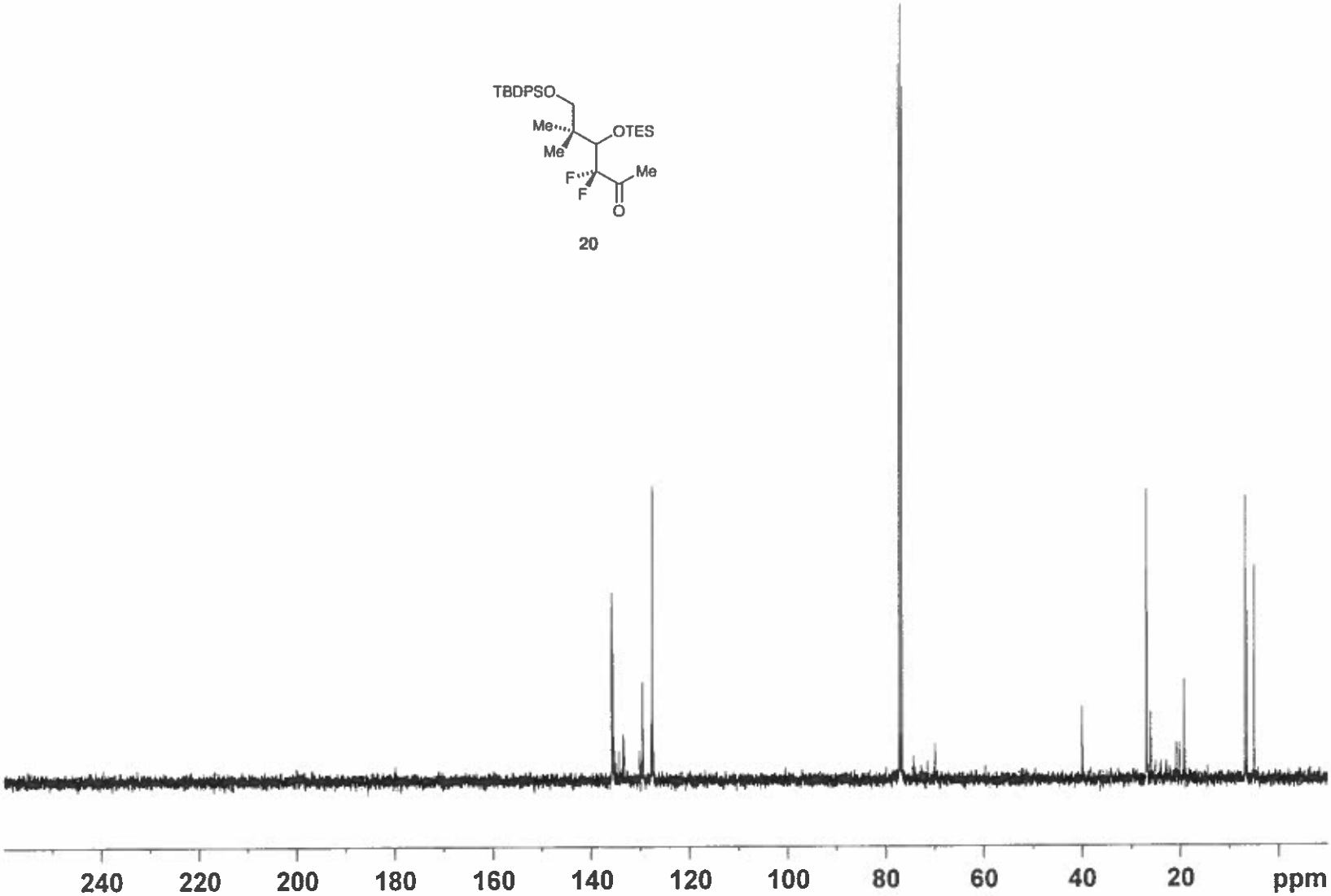
No.	(ppm)	(Hz)	Height
34	1.03	517.0	0.0402
35	1.04	518.6	0.0352
36	1.04	522.4	0.0359
37	1.06	531.2	0.1567
38	1.07	534.1	0.0731
39	1.07	536.9	0.0888
40	1.08	537.8	0.0738
41	1.09	542.9	0.3437
42	1.10	551.7	0.0526
43	1.12	559.9	1.0000
44	1.15	572.8	0.0205

No.	(ppm)	(Hz)	Height
45	1.16	581.4	0.0182
46	1.17	584.8	0.0152
47	1.28	639.0	0.1818
48	1.34	671.2	0.0200
49	1.36	678.5	0.0397
50	1.37	685.7	0.0202
51	1.44	719.8	0.0216
52	1.57	784.1	0.0186
53	2.34	1172.8	0.1382
54	3.34	1670.6	0.0283
55	3.36	1680.4	0.0327

ejt cry meli
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} ejt 20



20



NAME	2012-09-28-ejt-20
EXPNO	13
PROCNO	1
Date_	20120929
Time	10.56
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	295.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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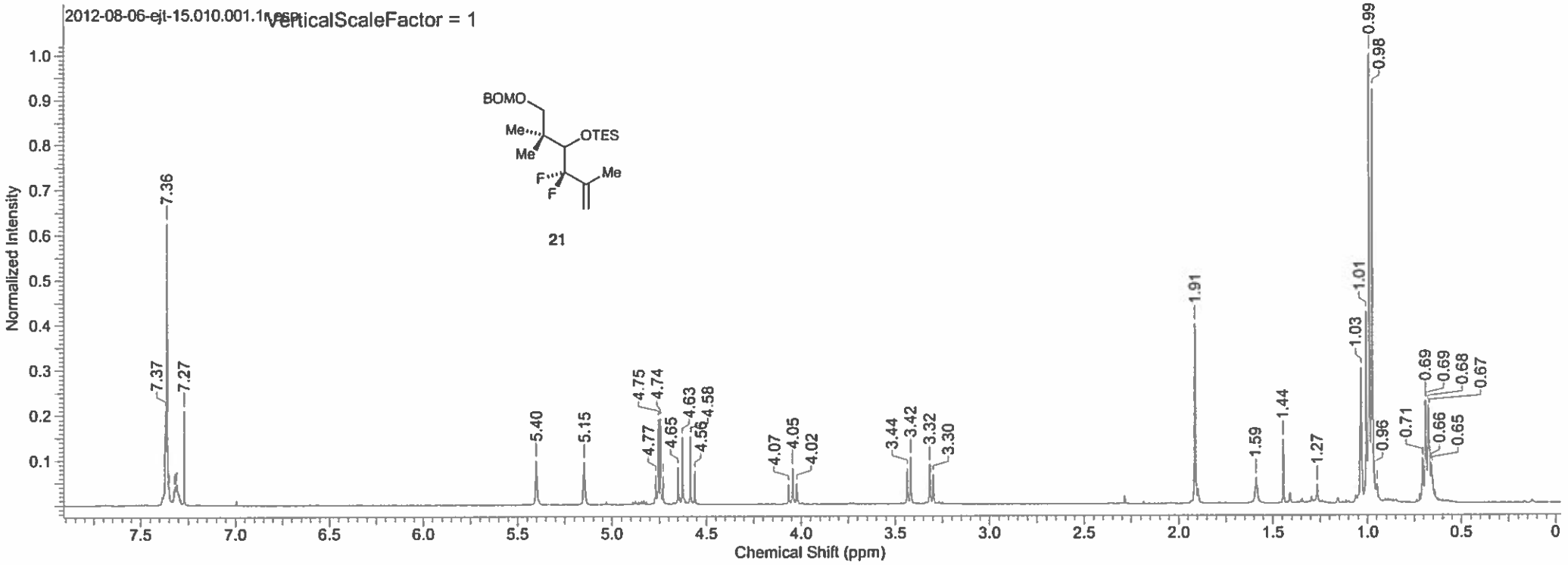
30/11/2012 11:35:13

Acquisition Time (sec)	3.1719	*Comment*	ejt cry wittig mPROTON CDCl3 /opt/bruk500data/2012/Aug ejt 15			*Date*	06 Aug 2012 11:08:00
Date Stamp	06 Aug 2012 11:08:00						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500data\bruk500data\2012\Aug\data\ejt\nmr\2012-08-06-ejt-15\10\pdata\1\1r						
Frequency (MHz)	500.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zg30b
Receiver Gain	90.50	*SW(cyclical) (Hz)*	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3080.2925
Spectrum Type	STANDARD	*Sweep Width (Hz)*	10330.26	*Temperature (degree C)*	19.310		



No.	(ppm)	(Hz)	Height
1	0.65	327.6	0.0833
2	0.66	330.7	0.0898
3	0.67	335.8	0.2117
4	0.68	338.6	0.2200
5	0.69	344.0	0.2262
6	0.69	346.2	0.2280
7	0.70	352.2	0.0968
8	0.71	354.0	0.1020
9	0.95	474.8	0.0435

No.	(ppm)	(Hz)	Height
10	0.96	481.7	0.0726
11	0.98	487.7	0.9220
12	0.99	495.3	1.0000
13	1.01	503.5	0.4271
14	1.03	517.4	0.3013
15	1.27	632.7	0.0427
16	1.44	722.6	0.1420
17	1.59	794.5	0.0578
18	1.91	956.8	0.3996

No.	(ppm)	(Hz)	Height
19	3.30	1649.5	0.0662
20	3.32	1658.6	0.0885
21	3.42	1709.4	0.1050
22	3.44	1718.5	0.0793
23	4.02	2012.3	0.0466
24	4.05	2023.1	0.0813
25	4.07	2033.8	0.0442
26	4.56	2281.3	0.0744
27	4.58	2292.9	0.1522

No.	(ppm)	(Hz)	Height
28	4.63	2314.0	0.1497
29	4.65	2325.7	0.0829
30	4.73	2365.7	0.0640
31	4.74	2372.4	0.1916
32	4.75	2377.7	0.1894
33	4.77	2384.3	0.0667
34	5.15	2575.1	0.0948
35	5.40	2701.8	0.0979
36	7.27	3635.9	0.2110

No.	(ppm)	(Hz)	Height
37	7.31	3654.5	0.0471
38	7.31	3657.7	0.0381
39	7.32	3659.6	0.0439
40	7.32	3663.1	0.0375
41	7.35	3676.0	0.0414
42	7.36	3681.0	0.6262
43	7.37	3684.5	0.2032
44	7.37	3686.1	0.2121

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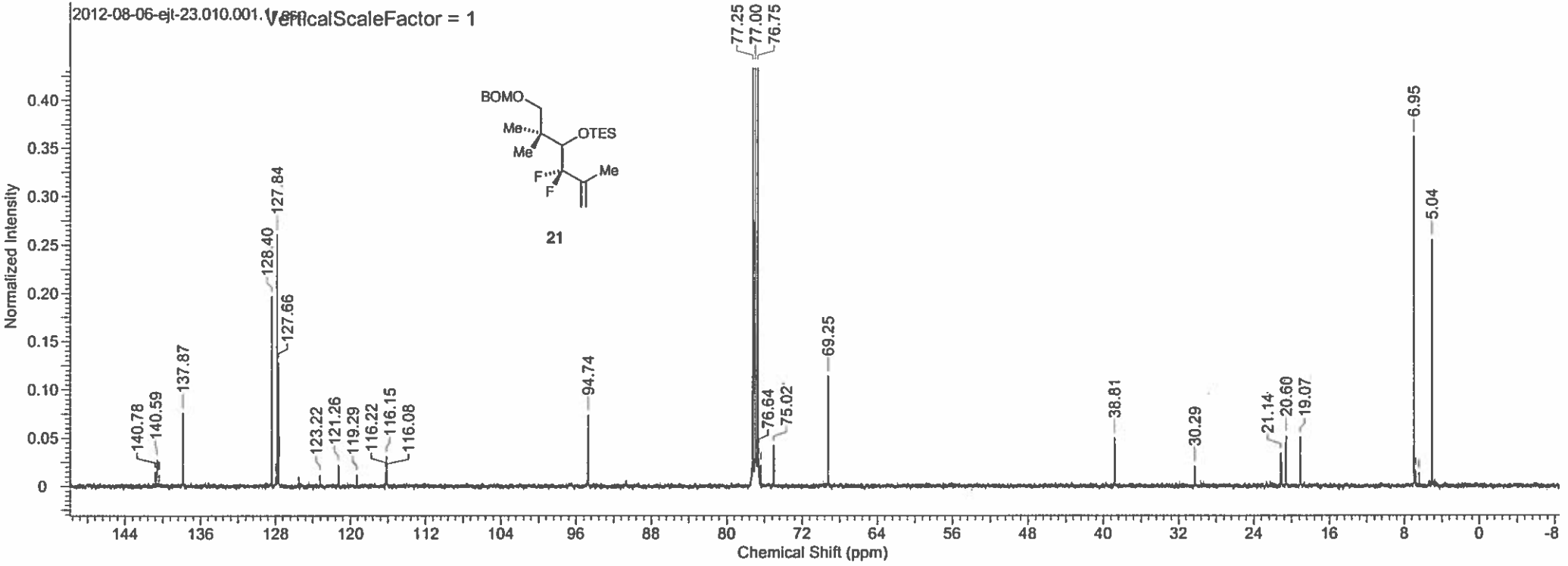
30/11/2012 11:46:40

Acquisition Time (sec)	1.1010	*Comment*	ejt cry wittig mCARBONnight CDCl3 /opt/bruk500data/2012/Aug ejt 23			*Date*	06 Aug 2012 14:26:24
Date Stamp	06 Aug 2012 14:26:24						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500data\bruk500data\2012\Aug\data\ejt\nmr\2012-08-06-ejt-23\10\pdata\1\1r						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	1000	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12570.2578
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	19.803		



No.	(ppm)	(Hz)	Height
1	5.04	633.4	0.2561
2	6.41	806.0	0.0136
3	6.76	849.6	0.0164
4	6.95	874.1	0.3625
5	19.05	2395.5	0.0298
6	19.07	2398.2	0.0512
7	20.60	2590.7	0.0517

No.	(ppm)	(Hz)	Height
8	21.14	2657.9	0.0346
9	30.29	3808.7	0.0208
10	38.81	4880.5	0.0501
11	69.25	8708.8	0.1144
12	75.02	9434.5	0.0423
13	76.41	9609.8	0.0225
14	76.64	9637.9	0.0394

No.	(ppm)	(Hz)	Height
15	76.75	9651.6	0.9667
16	76.86	9666.1	0.0343
17	77.00	9683.3	1.0000
18	77.25	9715.1	0.9716
19	94.74	11914.0	0.0742
20	116.08	14598.0	0.0146
21	116.15	14607.0	0.0313

No.	(ppm)	(Hz)	Height
22	116.22	14616.1	0.0151
23	119.29	15002.1	0.0117
24	121.26	15249.2	0.0223
25	123.22	15496.2	0.0117
26	127.66	16054.8	0.1289
27	127.74	16064.8	0.0119
28	127.84	16076.6	0.2612

No.	(ppm)	(Hz)	Height
29	127.99	16095.7	0.0101
30	128.40	16147.4	0.1971
31	137.87	17338.2	0.0763
32	140.40	17657.0	0.0125
33	140.59	17680.6	0.0279
34	140.78	17704.2	0.0156

ejt cry wittig
mF19 CDCl3 {e:\bruk400data\2012\Aug} ejt 14

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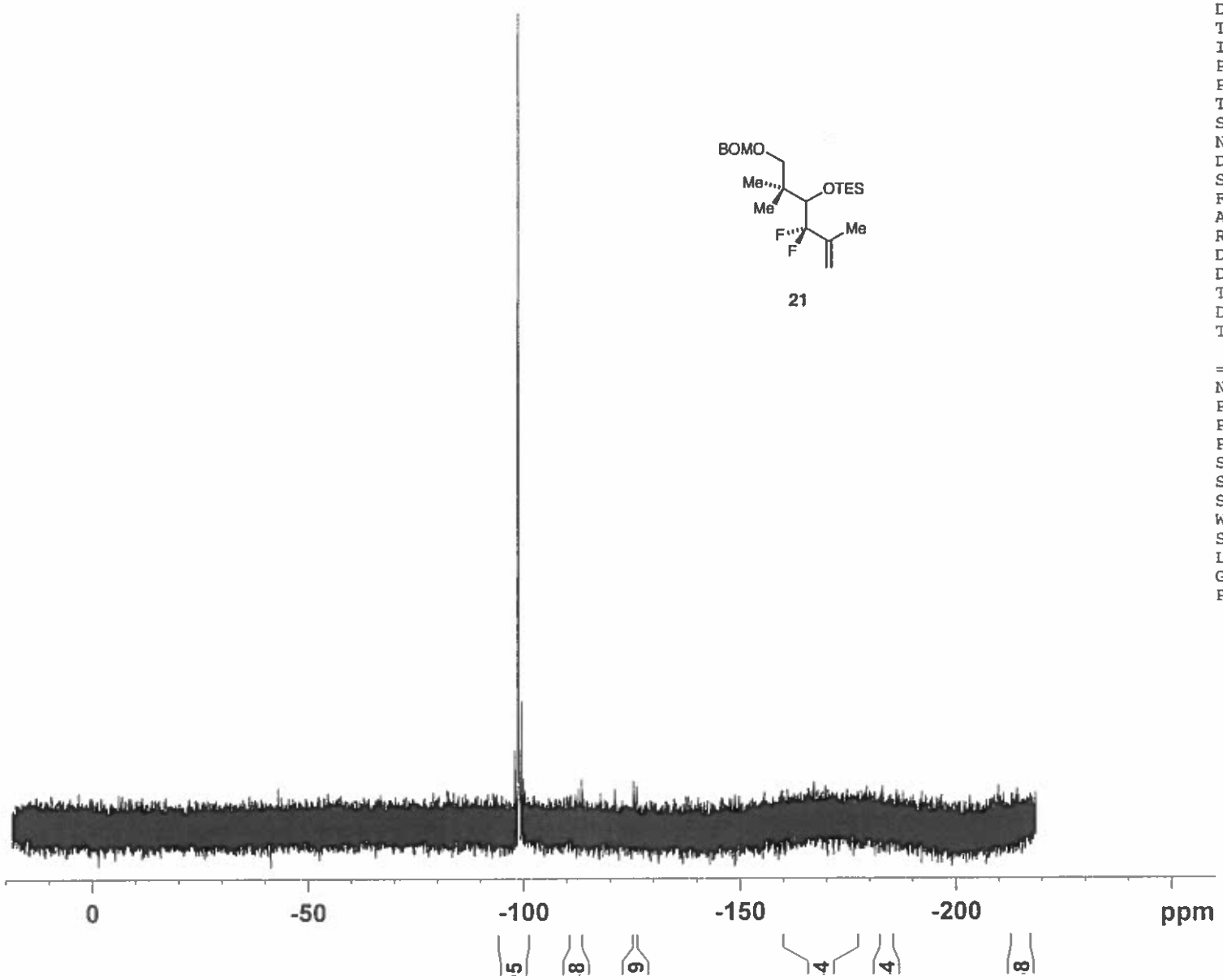

NAME	2012-08-07-ejt-14
EXPNO	10
PROCNO	1
Date_	20120807
Time	15.57
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	11.01 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

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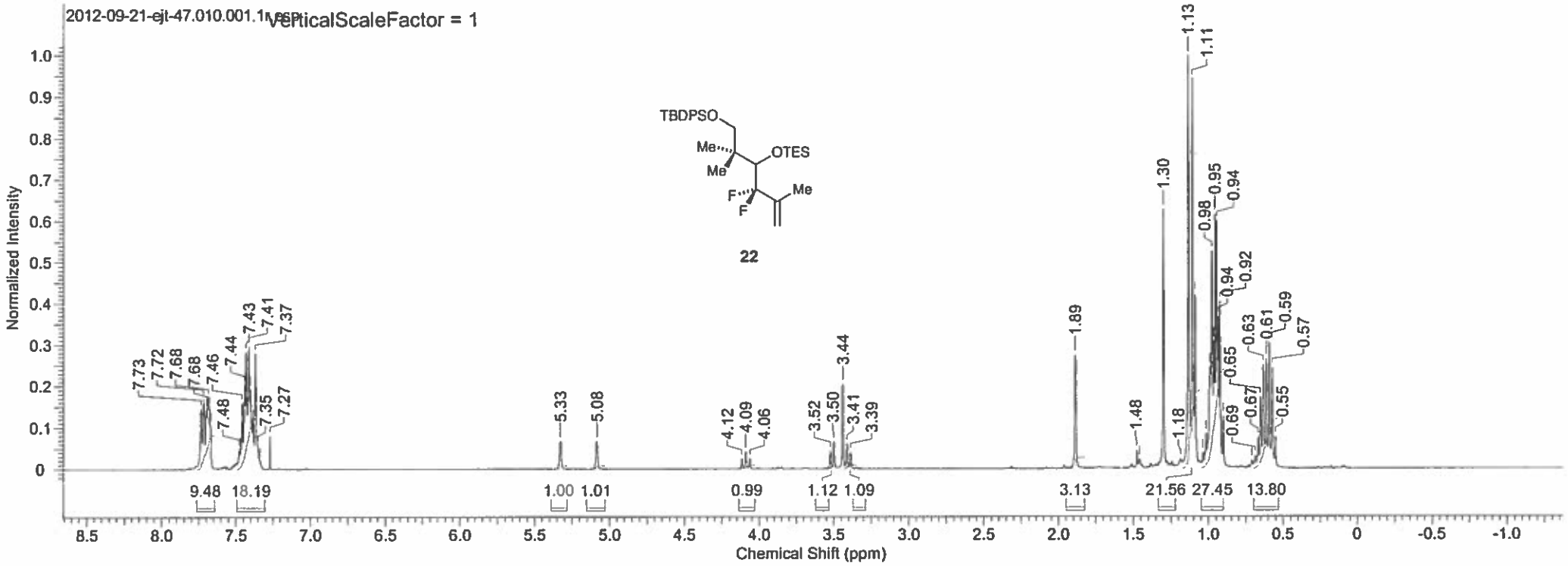
23/11/2012 15:30:05

Acquisition Time (sec)	3.9649	*Comment*	ejt cry wittig mPROTONnight CDCl3 (e:\bruk400data\2012\Sep) ejt 47			*Date*	23 Sep 2012 05:48:00
Date Stamp	23 Sep 2012 05:48:00						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Sep\data\ejt\nmr\2012-09-21-ejt-47\10\pdata\1\1r					*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*	40.30
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9272	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	21.200				



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	5311 .. 0.69	3.7977647	1.79901200e+8	13.79776478
2	3997 .. 1.04	27.4501934	3.57907424e+8	27.45019341
3	0554 .. 1.17	21.5567245	2.81065856e+8	21.55672455
4	3255 .. 1.94	3.12946820	4.08033520e+7	3.12946820
5	3494 .. 3.43	1.09304404	1.42515790e+7	1.09304404
6	4723 .. 3.56	1.11904001	1.45905260e+7	1.11904001

No.	(ppm)	Value	Absolute Value	Non-Negative Value
7	0295 .. 4.130	0.98917204	1.28972510e+7	0.98917204
8	0290 .. 5.151	1.01108396	1.31829480e+7	1.01108396
9	2830 .. 5.381	1.00019169	1.30409290e+7	1.00019169
10	8067 .. 7.491	8.18846893	2.37149088e+8	18.18846893
11	6426 .. 7.769	9.48153591	1.23624344e+8	9.48153591

No.	(ppm)	(Hz)	Height
1	0.55	220.6	0.0768
2	0.57	228.4	0.2431
3	0.59	236.5	0.3054

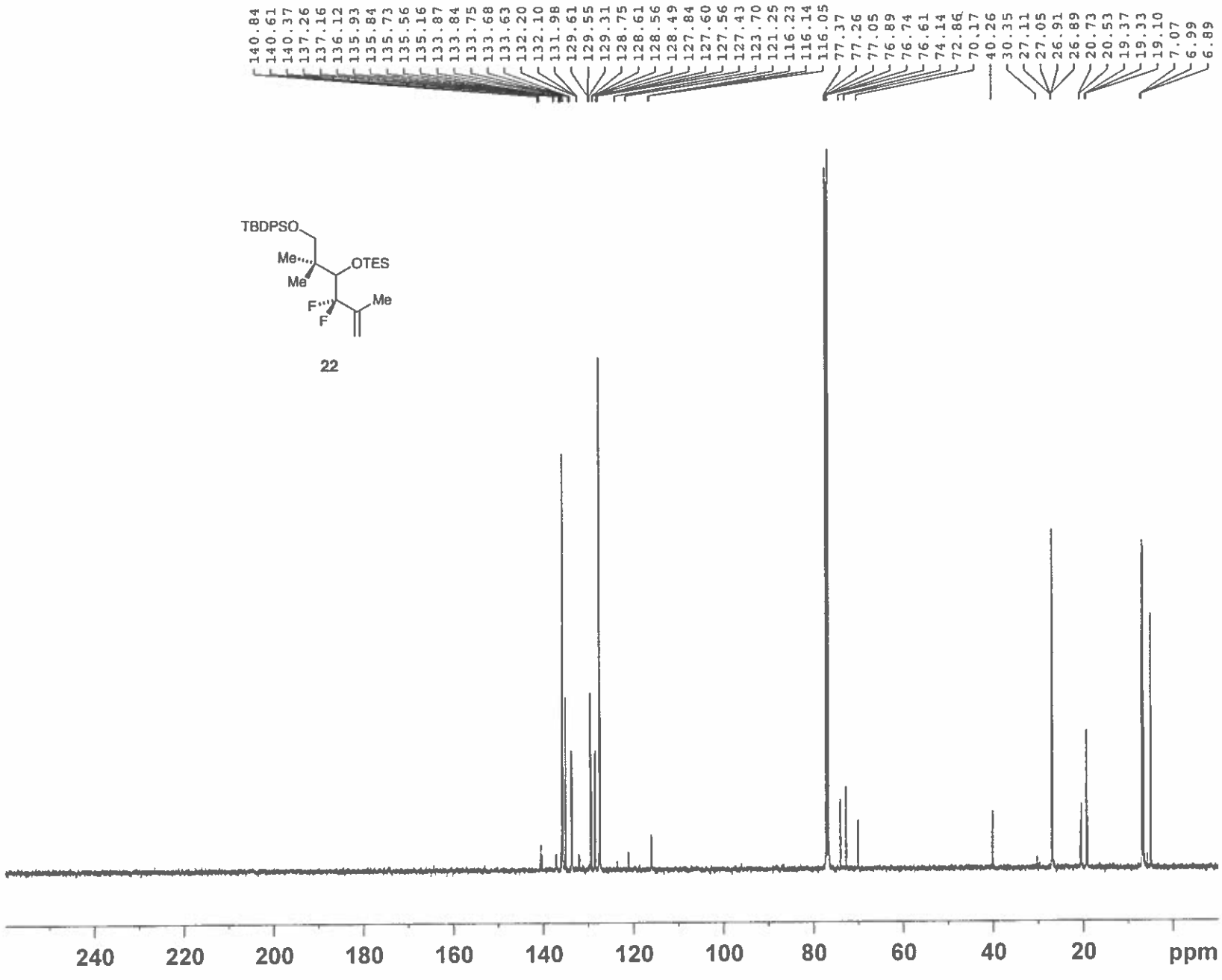
No.	(ppm)	(Hz)	Height
4	0.61	244.6	0.2646
5	0.63	252.7	0.2509
6	0.65	259.7	0.1726

No.	(ppm)	(Hz)	Height
7	0.67	267.0	0.0752
8	0.69	274.6	0.0313
9	0.71	283.7	0.0202

No.	(ppm)	(Hz)	Height
10	0.90	360.9	0.1269
11	0.92	369.7	0.4047
12	0.94	374.2	0.3671

No.	(ppm)	(Hz)	Height
13	0.94	377.8	0.6009
14	0.95	382.0	0.6156
15	0.96	385.8	0.3093

ejt cry wittig
mCARBONnight CDCl3 {e:\bruk400data\2012\Sep} ejt 47

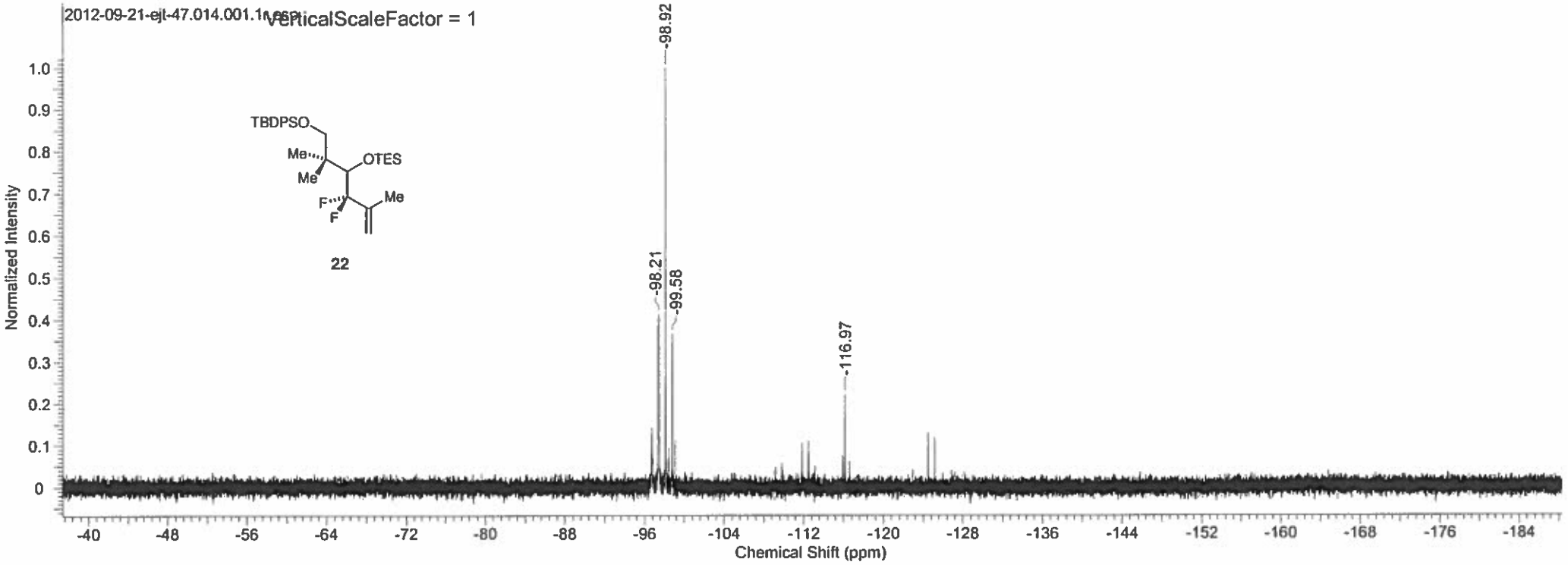


BRUKER 400 MHz

NAME	2012-09-21-ejt-47
EXPNO	11
PROCNO	1
Date_	20120923
Time	6.40
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	294.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

24/09/2012 09:56:17

Acquisition Time (sec)	0.7340	***Comment***	ejt cry wittig mF19CPD CDCl3 (e:\bruk400data\2012\Sep) ejt 47			***Date***	21 Sep 2012 17:08:32
Date Stamp	21 Sep 2012 17:08:32						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Sep\data\ejt\nmr\2012-09-21-ejt-47\14\pdata\1\1r					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Origin***	AV400	***Original Points Count***	65536
Owner	Administrator	***Points Count***	262144	***Pulse Sequence***	zgig	***Receiver Gain***	4100.00
SW(cyclical) (Hz)	89285.71	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	-37649.5977	***Spectrum Type***	STANDARD
Sweep Width (Hz)	89285.37	***Temperature (degree C)***	21.300				



No.	(ppm)	(Hz)	Height
1	-116.97	-44039.7	0.2203
2	-99.58	-37493.1	0.3652
3	-98.92	-37241.4	1.0000
4	-98.21	-36974.7	0.4116

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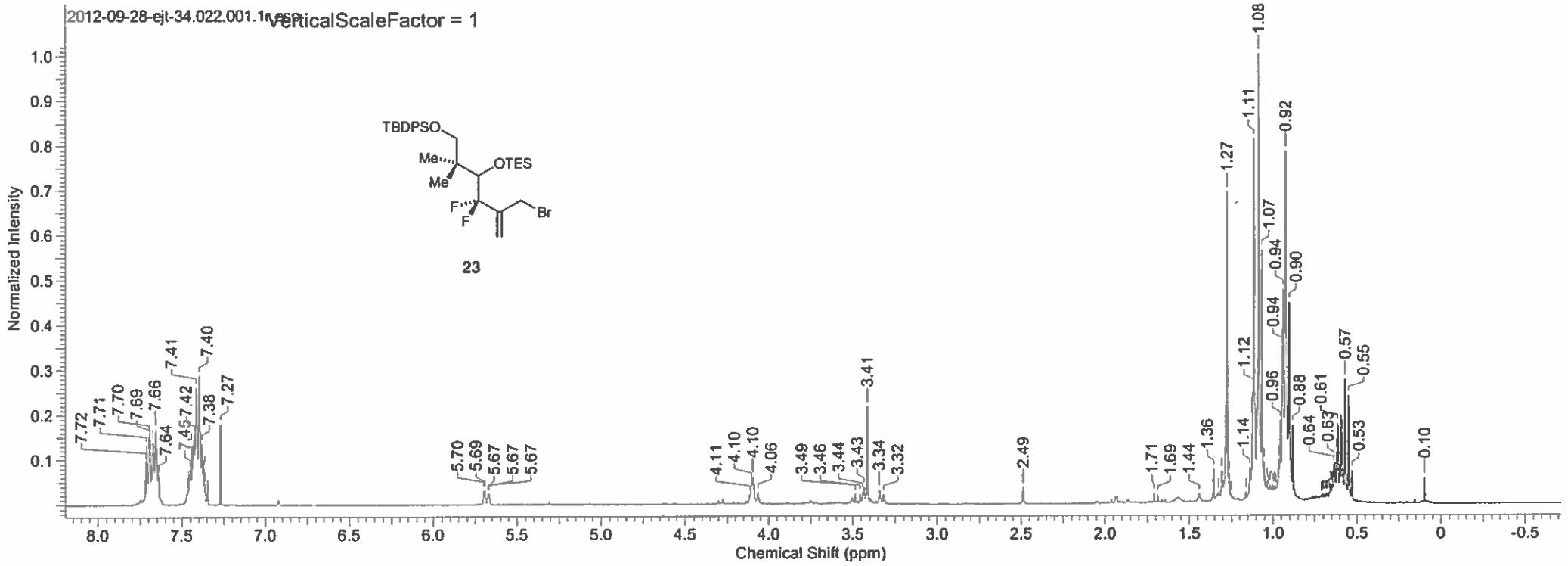
30/11/2012 16:12:31

Acquisition Time (sec)	3.9649	*Comment*	ejt cry bromination mPROTONnight CDCl3 (e:\bruk400data\2012\Sep) ejt 34				
Date	29 Sep 2012 06:41:20			*Date Stamp*	29 Sep 2012 06:41:20		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Sep\data\ejt\nmr\2012-09-28-ejt-34\22\pdata\1\1r					*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*	90.50
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9272	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	21.900				



No.	(ppm)	(Hz)	Height
1	0.10	39.3	0.0569
2	0.53	211.5	0.0728
3	0.55	219.6	0.2398
4	0.57	227.4	0.2773
5	0.58	232.0	0.0477
6	0.59	235.8	0.1562
7	0.59	236.8	0.1676
8	0.60	240.0	0.0879
9	0.61	244.8	0.1781
10	0.62	247.9	0.1145
11	0.63	252.7	0.0927

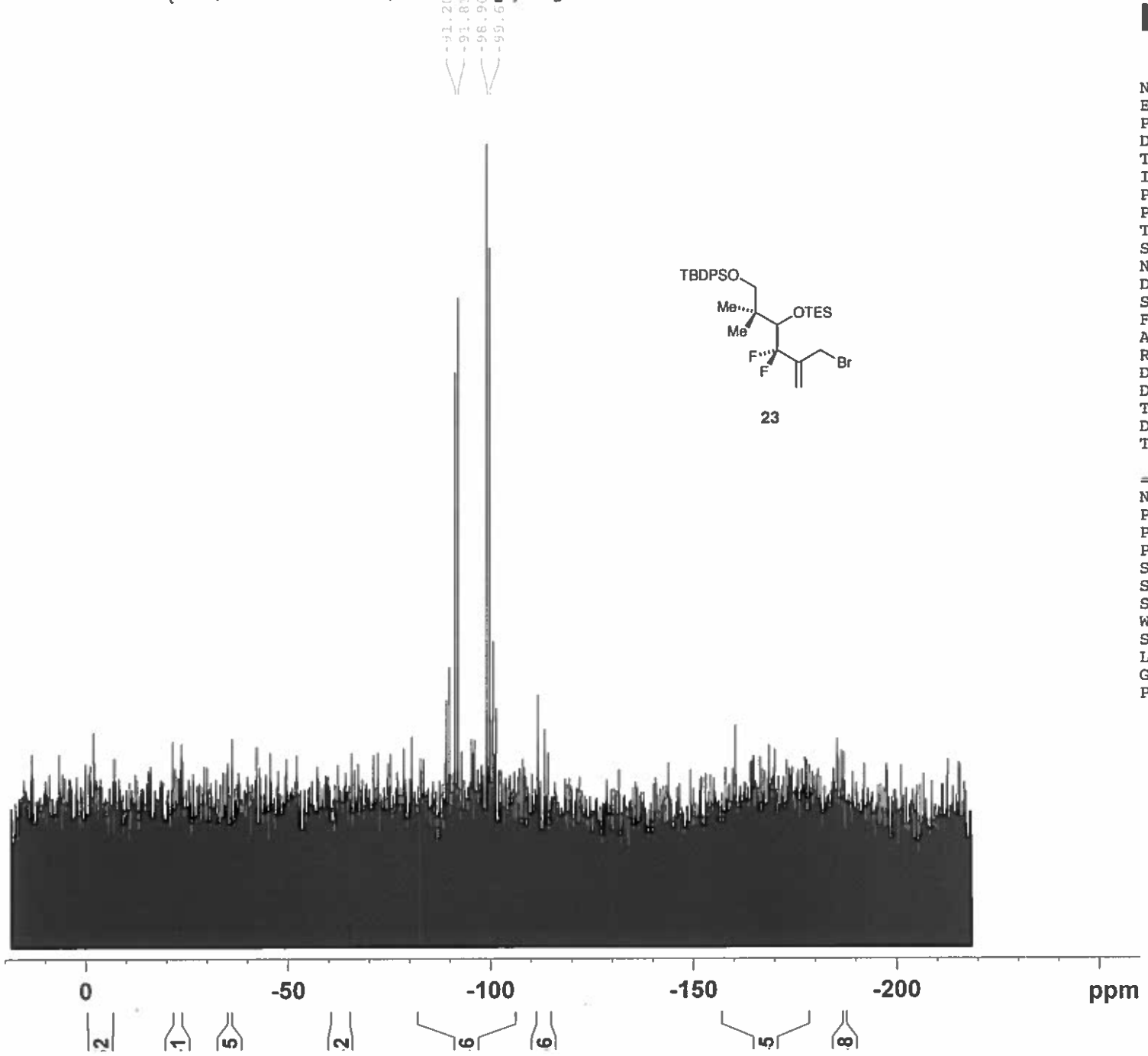
No.	(ppm)	(Hz)	Height
12	0.64	255.4	0.0854
13	0.65	258.7	0.0423
14	0.66	262.7	0.0431
15	0.67	266.3	0.0256
16	0.67	270.1	0.0215
17	0.68	273.3	0.0229
18	0.69	277.4	0.0206
19	0.70	281.4	0.0220
20	0.71	284.9	0.0185
21	0.88	352.3	0.1744
22	0.90	360.9	0.4475

No.	(ppm)	(Hz)	Height
23	0.92	369.2	0.7846
24	0.94	374.7	0.4768
25	0.94	377.2	0.3485
26	0.96	382.8	0.1848
27	0.96	386.1	0.0974
28	0.98	391.6	0.0344
29	0.99	394.1	0.0378
30	0.99	396.4	0.0415
31	1.00	398.7	0.0372
32	1.01	402.2	0.0435
33	1.02	407.3	0.0412

No.	(ppm)	(Hz)	Height
34	1.02	410.0	0.0333
35	1.04	414.6	0.0491
36	1.05	421.1	0.0929
37	1.07	426.4	0.5648
38	1.07	430.0	0.1603
39	1.08	433.5	1.0000
40	1.09	436.8	0.2914
41	1.11	444.8	0.8124
42	1.12	447.9	0.2577
43	1.14	455.2	0.0789
44	1.16	465.0	0.0262

No.	(ppm)	(Hz)	Height
45	1.25	500.8	0.0197
46	1.26	505.6	0.0664
47	1.27	510.2	0.6938
48	1.31	522.3	0.0724
49	1.33	530.8	0.0254
50	1.36	542.4	0.0765
51	1.44	577.0	0.0218
52	1.69	675.4	0.0202
53	1.71	683.2	0.0231
54	2.49	995.7	0.0366
55	3.32	1328.1	0.0218

ejt cry bromination
mF19 CDCl3 {e:\bruk400data\2012\Sep} ejt 34



23

NAME	2012-09-28-ejt-34
EXPNO	20
PROCNO	1
Date_	20120928
Time	13.29
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	11.01 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

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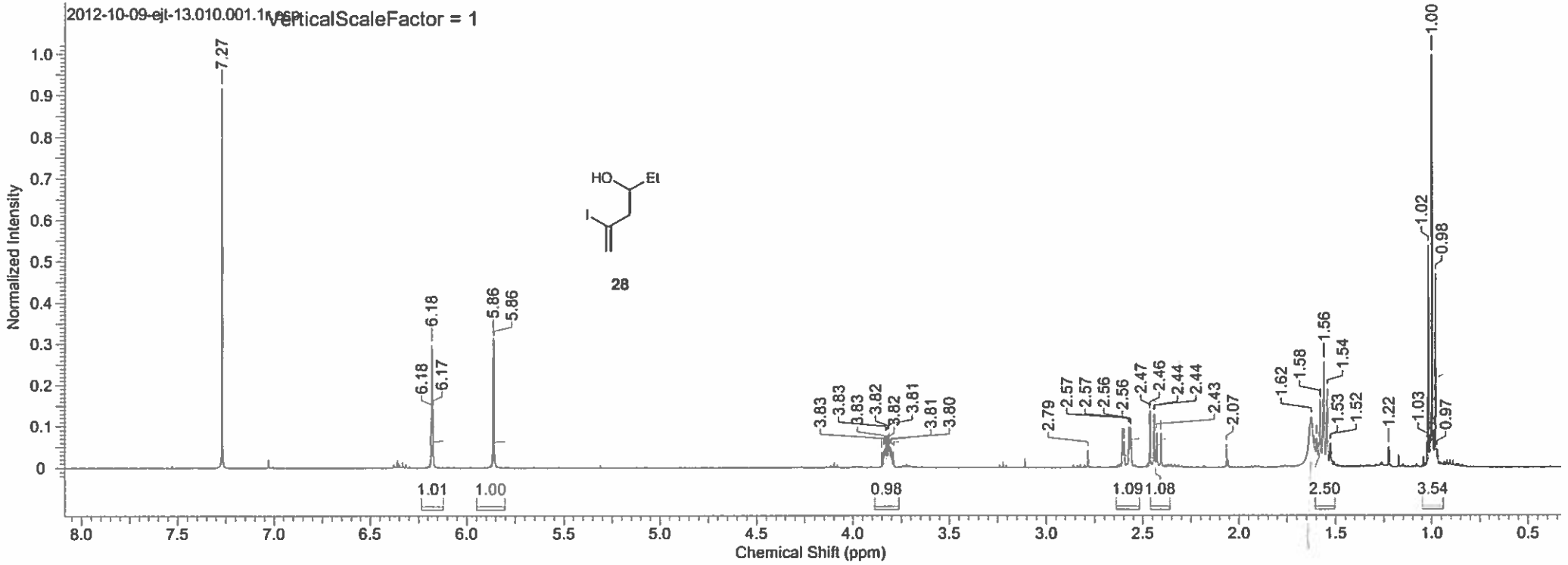
20/11/2012 17:35:28

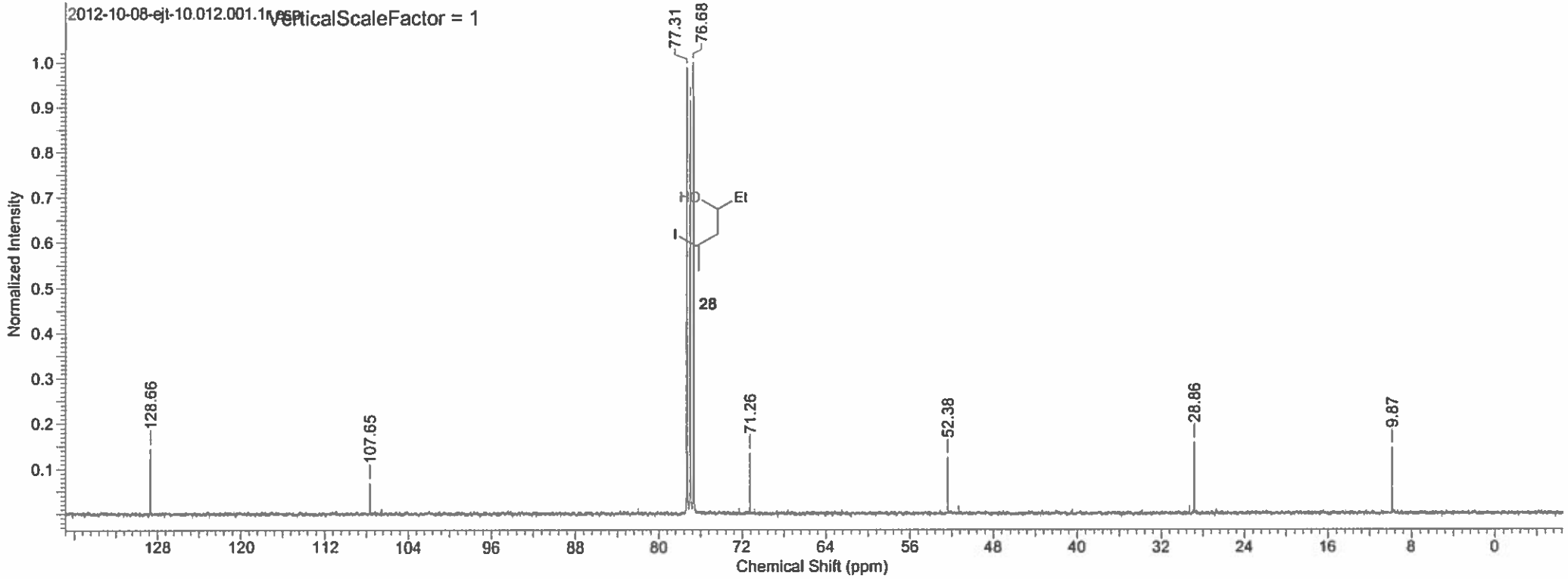
Acquisition Time (sec)	3.9649	*Comment*	ejt cry vinyl iodide mPROTON CDCl3 (e:\bruk400data\2012\Oct) ejt 13			*Date*	09 Oct 2012 12:46:08
Date Stamp	09 Oct 2012 12:46:08						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Oct\data\ejt\nmr\2012-10-09-ejt-13\10\pdata\1\1r					*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*	322.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9272	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	21.300				



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	9398 .. 1.04	3.54017091	1.01245312e+8	3.54017091
2	5041 .. 1.602	2.49626207	7.13905760e+7	2.49626207
3	3854 .. 2.48	1.07680511	3.07955380e+7	1.07680511
4	5185 .. 2.63	1.09013748	3.11768320e+7	1.09013748
5	7612 .. 3.88	0.97696531	2.79402220e+7	0.97696531
6	8027 .. 5.94	1.00033140	2.86084700e+7	1.00033140
7	1198 .. 6.23	1.00761056	2.88166460e+7	1.00761056

20/11/2012 17:36:58

Acquisition Time (sec)	1.0835	*Comment*	ejt cry iodide 10 mCARBONnight CDCl3 {e:\bruk400data\2012\Oct} ejt 10			*Date*	08 Oct 2012 19:35:44
Date Stamp	08 Oct 2012 19:35:44	*File Name*	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2012\Oct\data\ejt\nmr\2012-10-08-ejt-10\12\pdata\1\1r				
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	800	*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)*	11332.2295
Spectrum Type	STANDARD	*Sweep Width (Hz)*	30241.01	*Temperature (degree C)*	22.900		

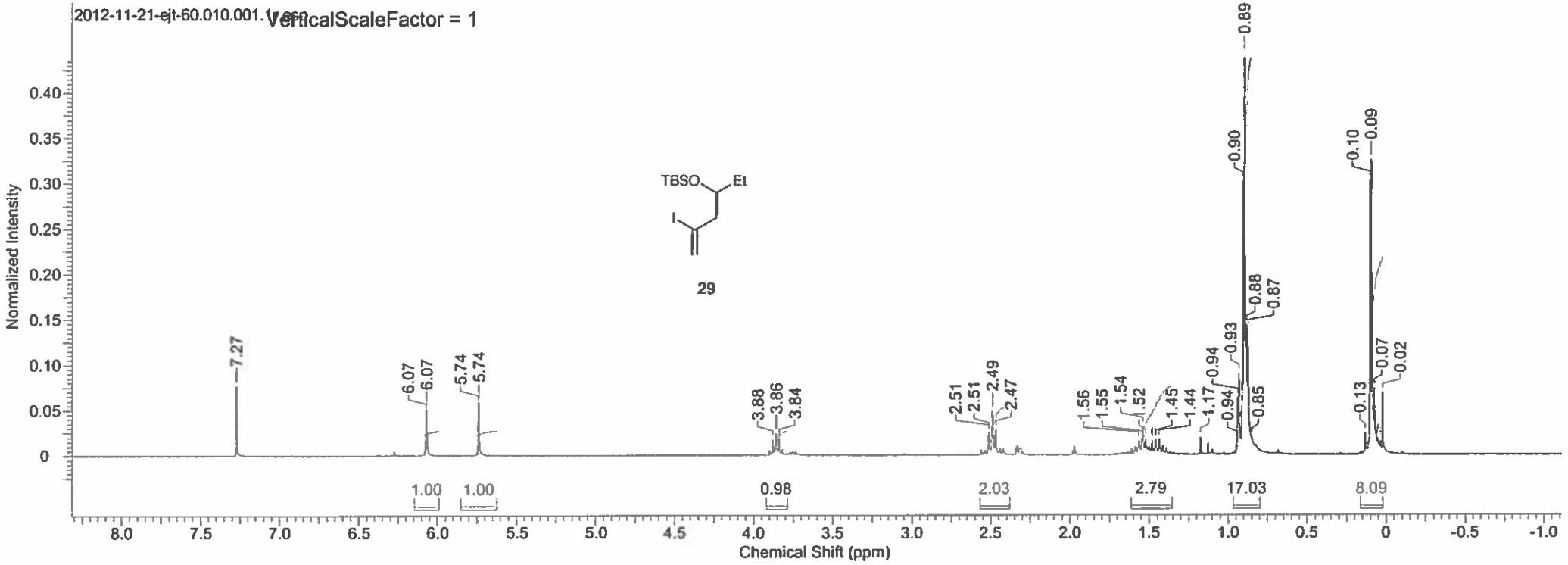


No.	(ppm)	(Hz)	Height
1	9.87	993.3	0.1460
2	28.86	2903.7	0.1572
3	52.38	5270.1	0.1243
4	71.26	7169.4	0.1335
5	76.68	7714.9	1.0000
6	77.00	7747.2	0.9152
7	77.31	7778.6	0.9874
8	107.65	10830.6	0.0683
9	128.66	12945.0	0.1445

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

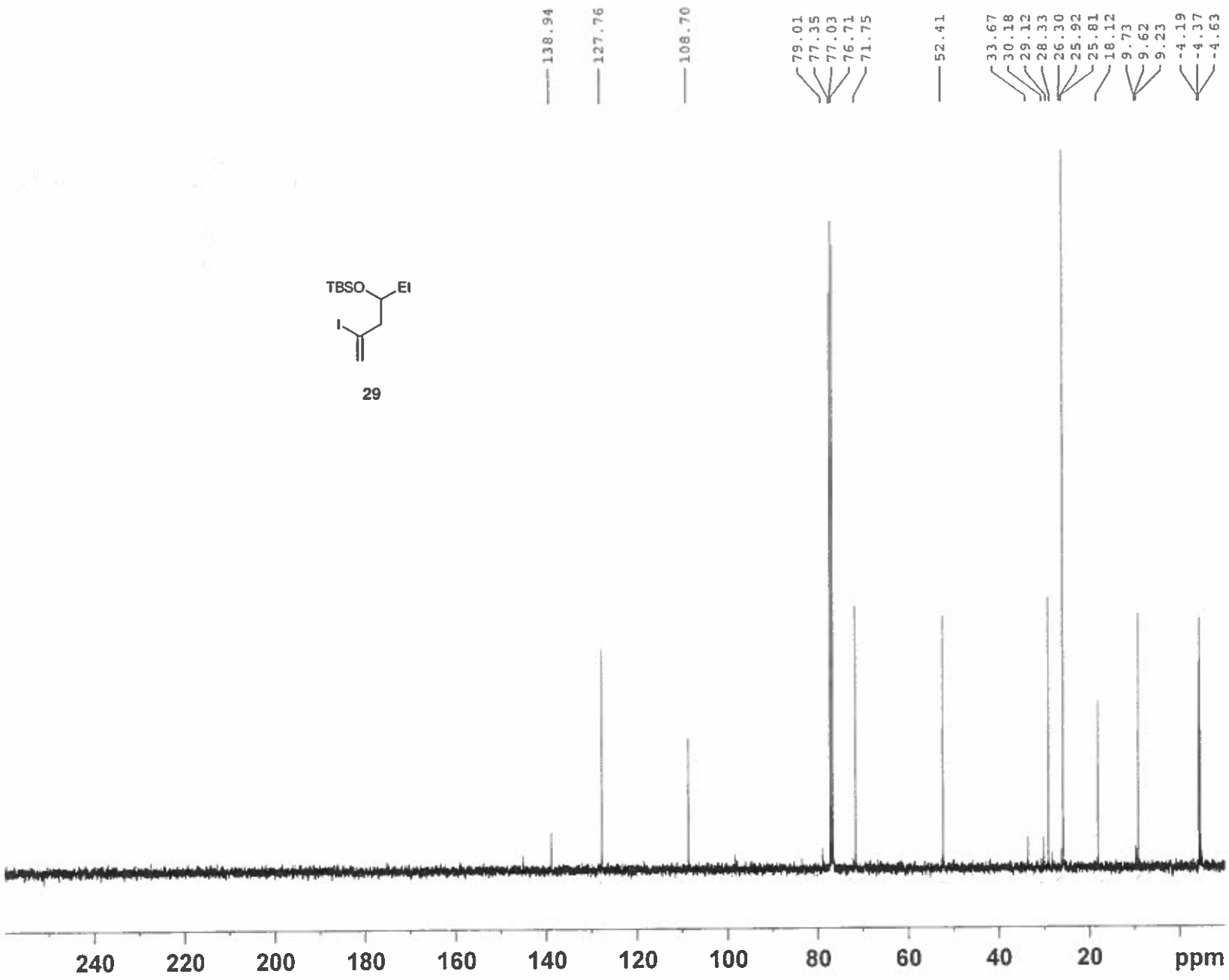
21/11/2012 11:54:23

Acquisition Time (sec)	5.3084	*Comment*	ejt cry vinyl mPROTON CDCl3 {E:\bruk300data\2012\Nov} ejt 60			*Date*	21 Nov 2012 10:22:56
Date Stamp	21 Nov 2012 10:22:56						
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk300data\2012\Nov\data\ejt\nmr\2012-11-21-ejt-60\10\pdata\1\1r					*Frequency (MHz)*	299.95
Nucleus	1H	*Number of Transients*	16	*Origin*	DPX300	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	456.10
SW(cyclical) (Hz)	6172.84	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	1848.6169	*Spectrum Type*	STANDARD
Sweep Width (Hz)	6172.65	*Temperature (degree C)*	27.000				



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	0223 .. 0.16	8.08682060	4.68993120e+8	8.08682060
2	7955 .. 0.96	7.02706337	9.87480256e+8	17.02706337
3	3579 .. 1.61	2.78549266	1.61543936e+8	2.78549266
4	3810 .. 2.56	2.03447366	1.17988776e+8	2.03447366
5	7869 .. 3.91	0.98051947	5.68649760e+7	0.98051947
6	6223 .. 5.84	0.99646074	5.77894880e+7	0.99646074
7	9894 .. 6.14	0.99959248	5.79711120e+7	0.99959248

EJT-PRM46 TBS vinyl iodide data
mCARBONnight CDCl3 {e:\bruk400data\2012\Nov} ejt 58

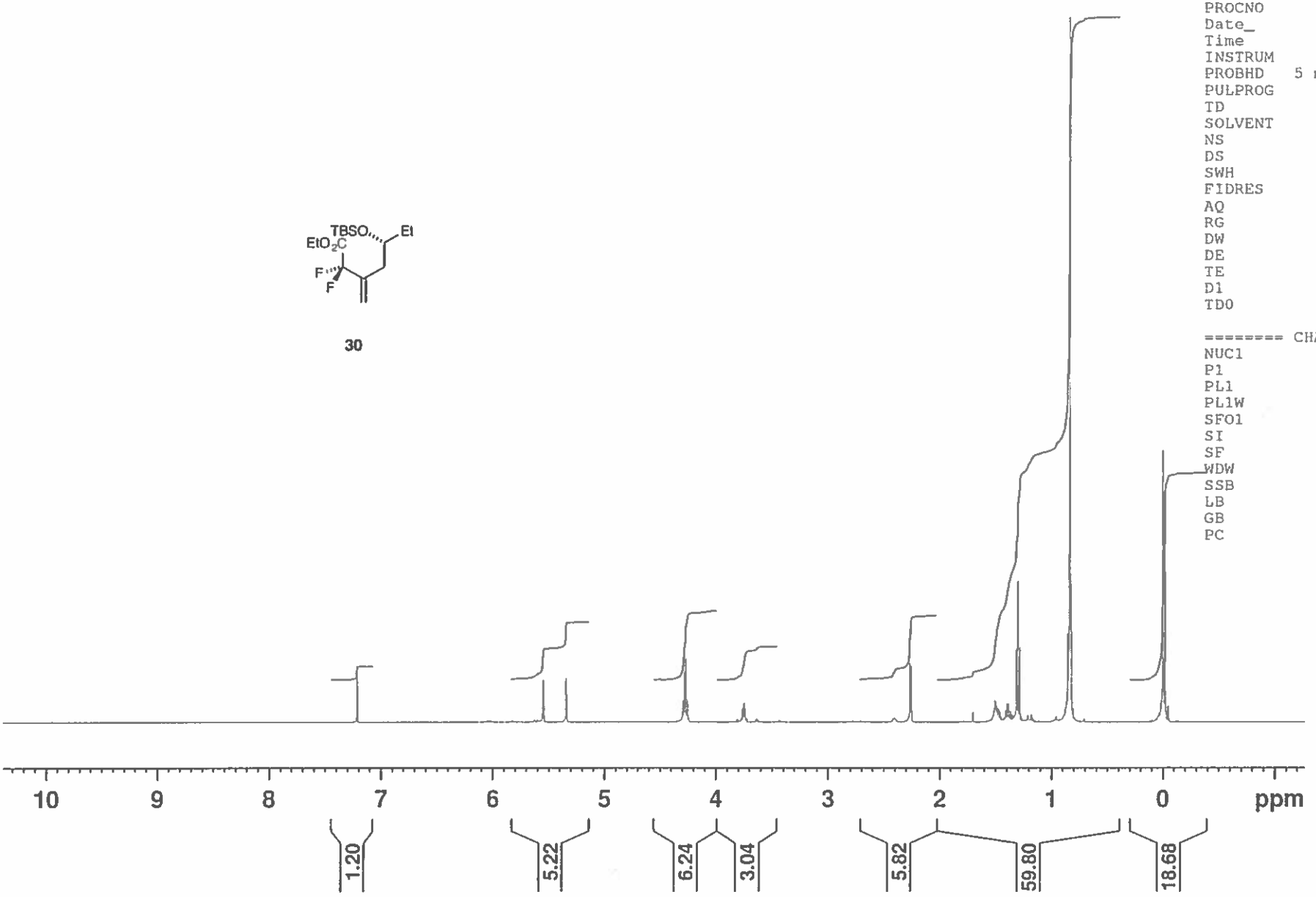


NAME	2012-11-28-ejt-58
EXPNO	10
PROCNO	1
Date_	20121129
Time	20.00
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	30241.936 Hz
FIDRES	0.461455 Hz
AQ	1.0835786 sec
RG	512
DW	16.533 usec
DE	7.83 usec
TE	293.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
PL1W	34.91522217 W
SFO1	100.6241042 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

EJT-PRM48c f4-5 8mg full data
mPROTONnight CDCl3 /opt/bruk500data/2013/Jan ejt 31

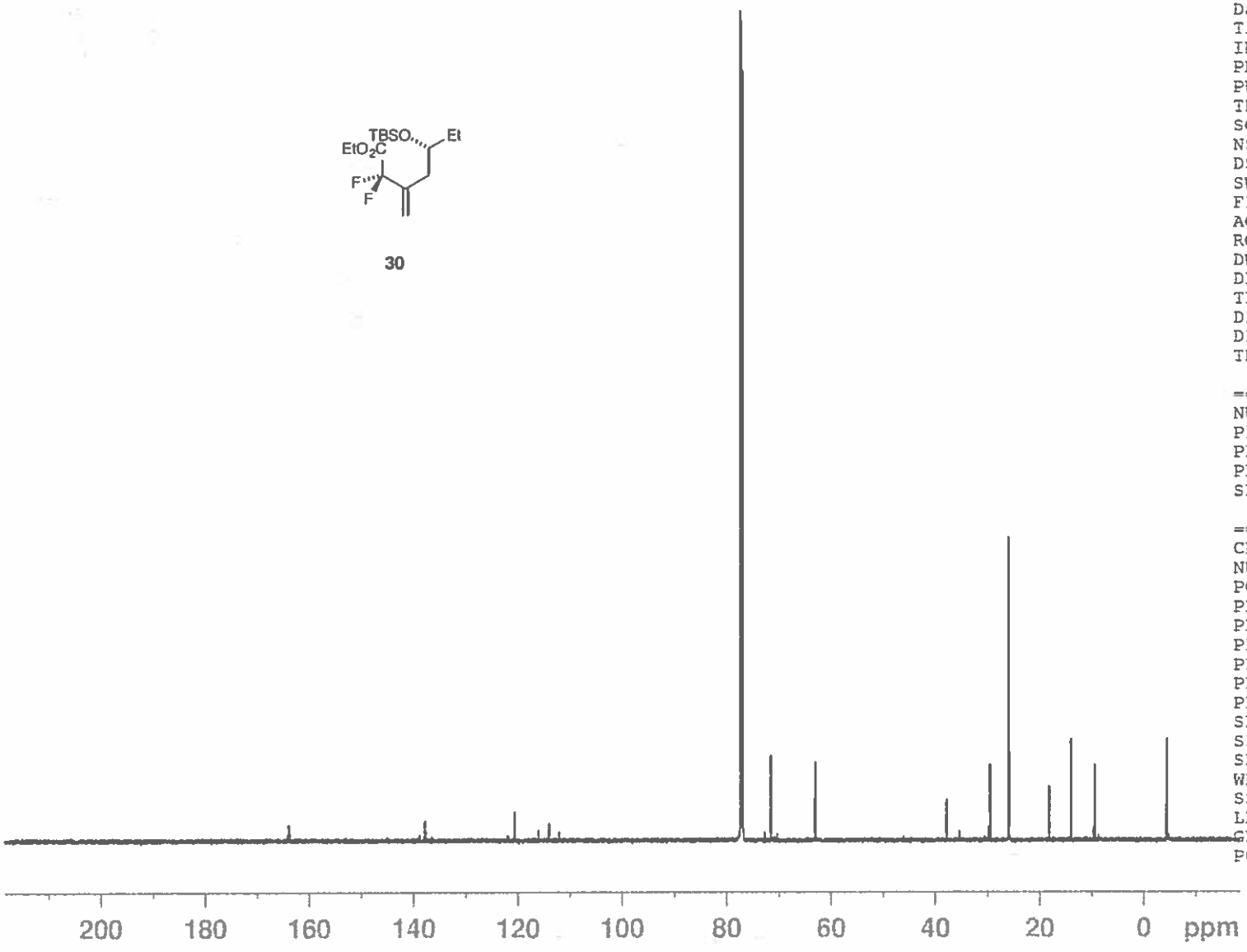
30

NAME	2013-01-10-ejt-31
EXPNO	11
PROCNO	1
Date_	20130110
Time	21.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	90.5
DW	48.400 usec
DE	13.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300359 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



EJT-PRM48c f4-5 8mg full data
mCARBONnight CDCl3 /opt/bruk500data/2013/Jan ejt 31

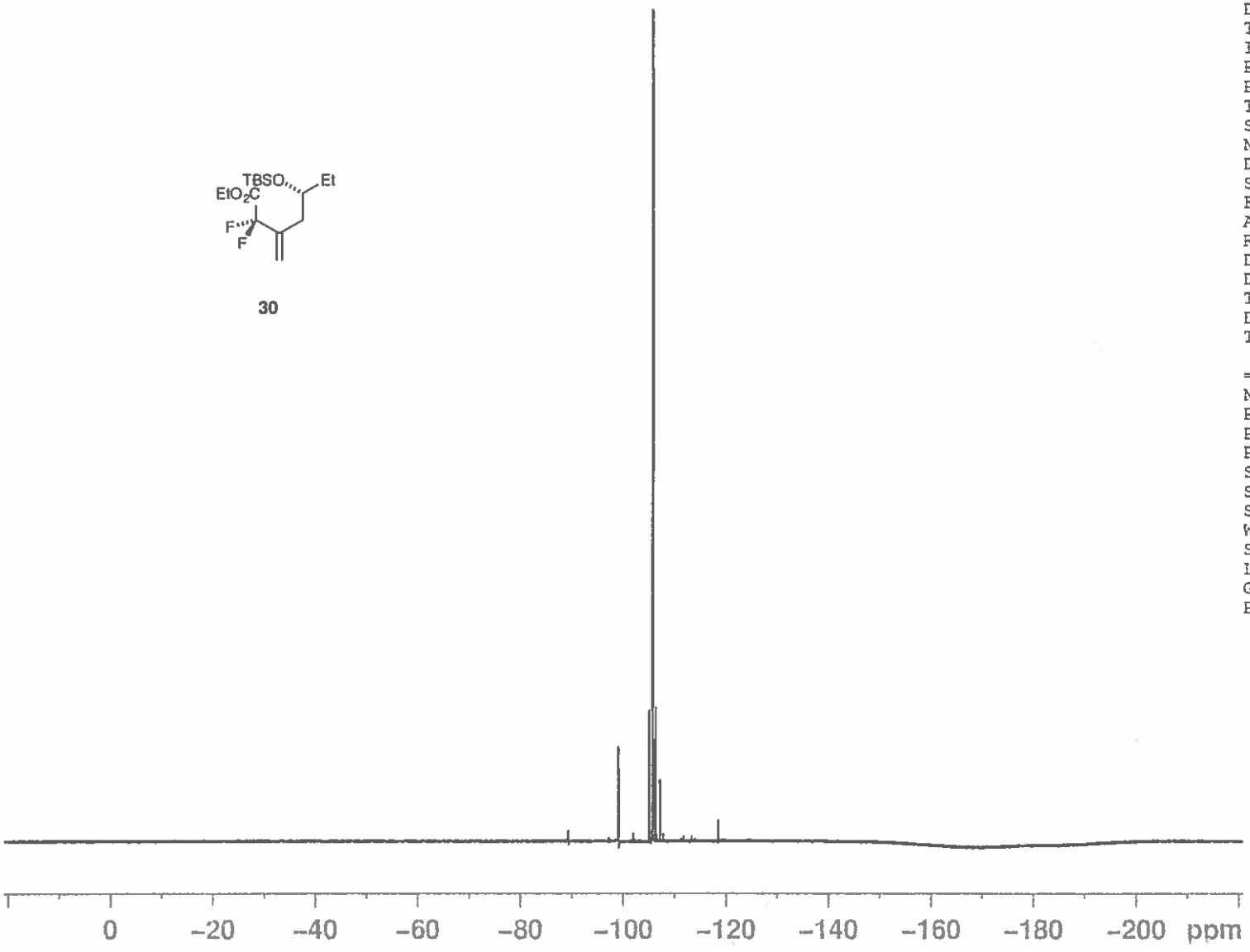
30



NAME	2013-01-10-ejt-31
EXPNO	10
PROCNO	1
Date_	20130110
Time	21.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2000
DS	2
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	512
DW	16.800 usec
DE	32.78 usec
TE	293.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	13C
P1	8.80 usec
PL1	-1.00 dB
PL1W	104.35516357 W
SFO1	125.7703643 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.23 dB
PL13	120.00 dB
PL2W	25.62124252 W
PL12W	0.48484197 W
PL13W	0.00000000 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

EJT-PRM48c f4-5 8mg
m19F CDCl3 /opt/bruk500data/2013/Jan ejt 29

30

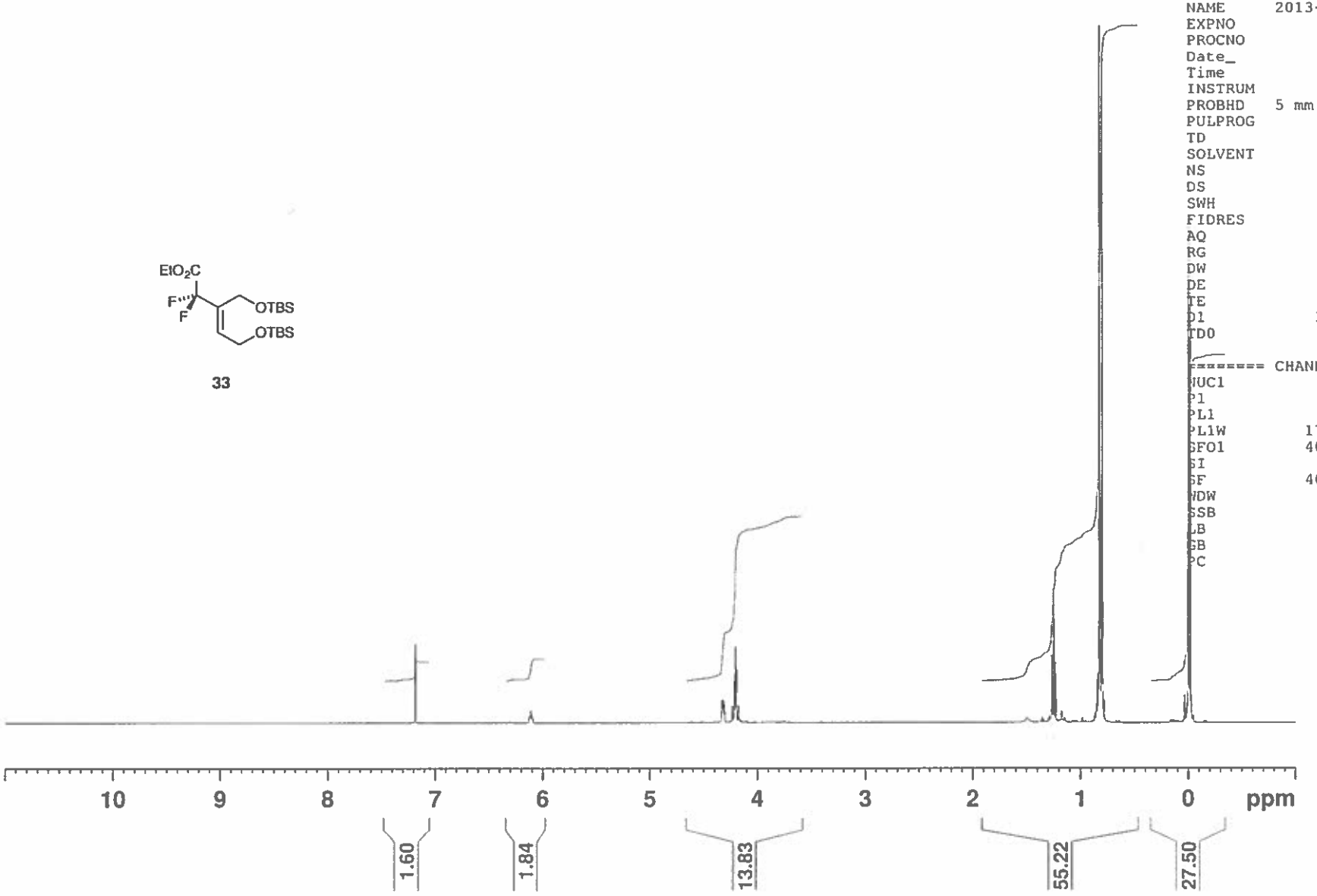


NAME	2013-01-10-ejt-29
EXPNO	12
PROCNO	1
Date_	20130110
Time	17.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	113636.367 Hz
FIDRES	0.866977 Hz
AQ	0.5767668 sec
RG	203
DW	4.400 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	17.50 usec
PL1	-2.90 dB
PL1W	48.97788239 W
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

EJT–PRM65 Product data
mPROTONnight CDCl3 {e:\bruk400data\2013\May} ejt 40

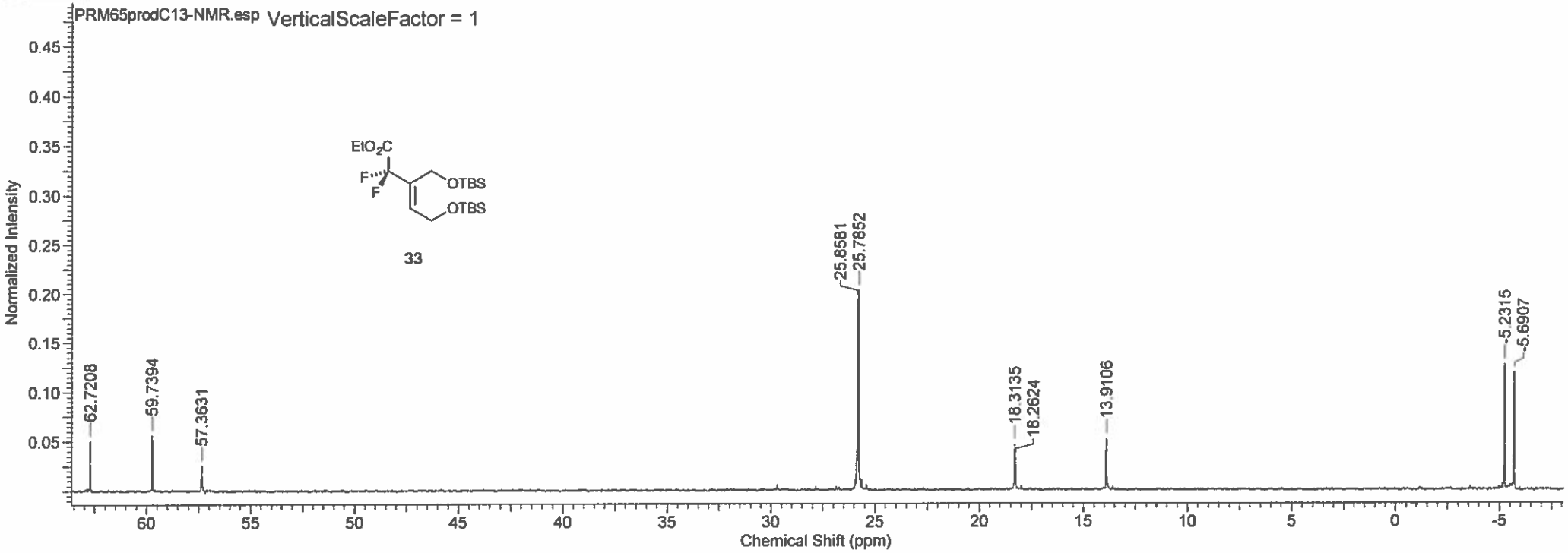
33

NAME	2013-05-02-ejt-40
EXPNO	11
PROCNO	1
Date_	20130503
Time	2.19
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	203
DW	60.500 usec
DE	9.40 usec
TE	300.0 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	400.1300401 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



12/06/2013 18:27:58

Acquisition Time (sec)	1.3631	***Comment***	P. Mears EJT-PRM 65 Prod data 0513-008 mCARBON CDCl3 {E:\bruk400service_data\2013\May} Administrator 24		
Date	10 May 2013 09:34:08	***Date Stamp***	10 May 2013 09:34:08		
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400SERVICE_DATA\2013\MAY\DATA\ADMINISTRATOR\NMR\2013-05-09-ADMINISTRATOR-24\12\PDATA\1\1R				
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
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.100



No.	(ppm)	(Hz)	Height
1	-5.69	-572.7	0.1186
2	-5.23	-526.5	0.1268
3	13.91	1399.9	0.0515

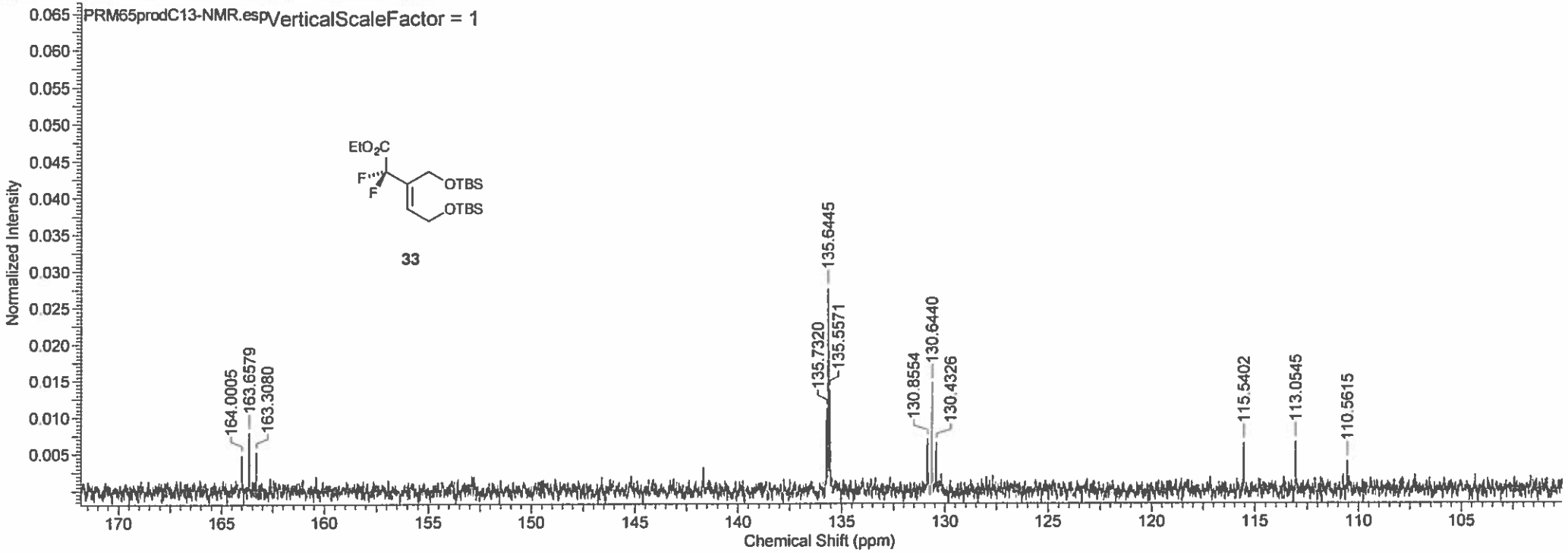
No.	(ppm)	(Hz)	Height
4	18.26	1837.9	0.0326
5	18.31	1843.0	0.0457
6	25.79	2595.0	0.2026

No.	(ppm)	(Hz)	Height
7	25.82	2598.6	0.0350
8	25.86	2602.3	0.1934
9	57.36	5772.9	0.0262

No.	(ppm)	(Hz)	Height
10	59.74	6012.1	0.0566
11	62.72	6312.1	0.0509

12/06/2013 18:28:32

Acquisition Time (sec)	1.3631	***Comment***	P. Mears EJT-PRM 65 Prod data 0513-008 mCARBON CDCl3 {E:\bruk400service_data\2013\May} Administrator 24		
Date	10 May 2013 09:34:08	***Date Stamp***	10 May 2013 09:34:08		
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400SERVICE_DATA\2013\MAY\DATA\ADMINISTRATOR\NMR\2013-05-09-ADMINISTRATOR-24\12\PDATA\1\1R				
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
Spectrum Type	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	25.100



No.	(ppm)	(Hz)	Height
1	-5.69	-572.7	0.1186
2	-5.23	-526.5	0.1268
3	13.91	1399.9	0.0515
4	18.26	1837.9	0.0326
5	18.31	1843.0	0.0457

No.	(ppm)	(Hz)	Height
6	25.79	2595.0	0.2026
7	25.82	2598.6	0.0350
8	25.86	2602.3	0.1934
9	57.36	5772.9	0.0262
10	59.74	6012.1	0.0566

No.	(ppm)	(Hz)	Height
11	62.72	6312.1	0.0509
12	110.56	11126.7	0.0039
13	113.05	11377.6	0.0066
14	115.54	11627.7	0.0063
15	130.43	13126.5	0.0064

No.	(ppm)	(Hz)	Height
16	130.64	13147.7	0.0146
17	130.86	13169.0	0.0069
18	135.56	13642.2	0.0137
19	135.64	13651.0	0.0274
20	135.73	13659.8	0.0111

No.	(ppm)	(Hz)	Height
21	163.31	16435.0	0.0053
22	163.66	16470.2	0.0079
23	164.00	16504.7	0.0049

EJT-PRM65 l/s prod 10mg
mF19 CDCl3 {e:\bruk400data\2013\Feb} ejt 31

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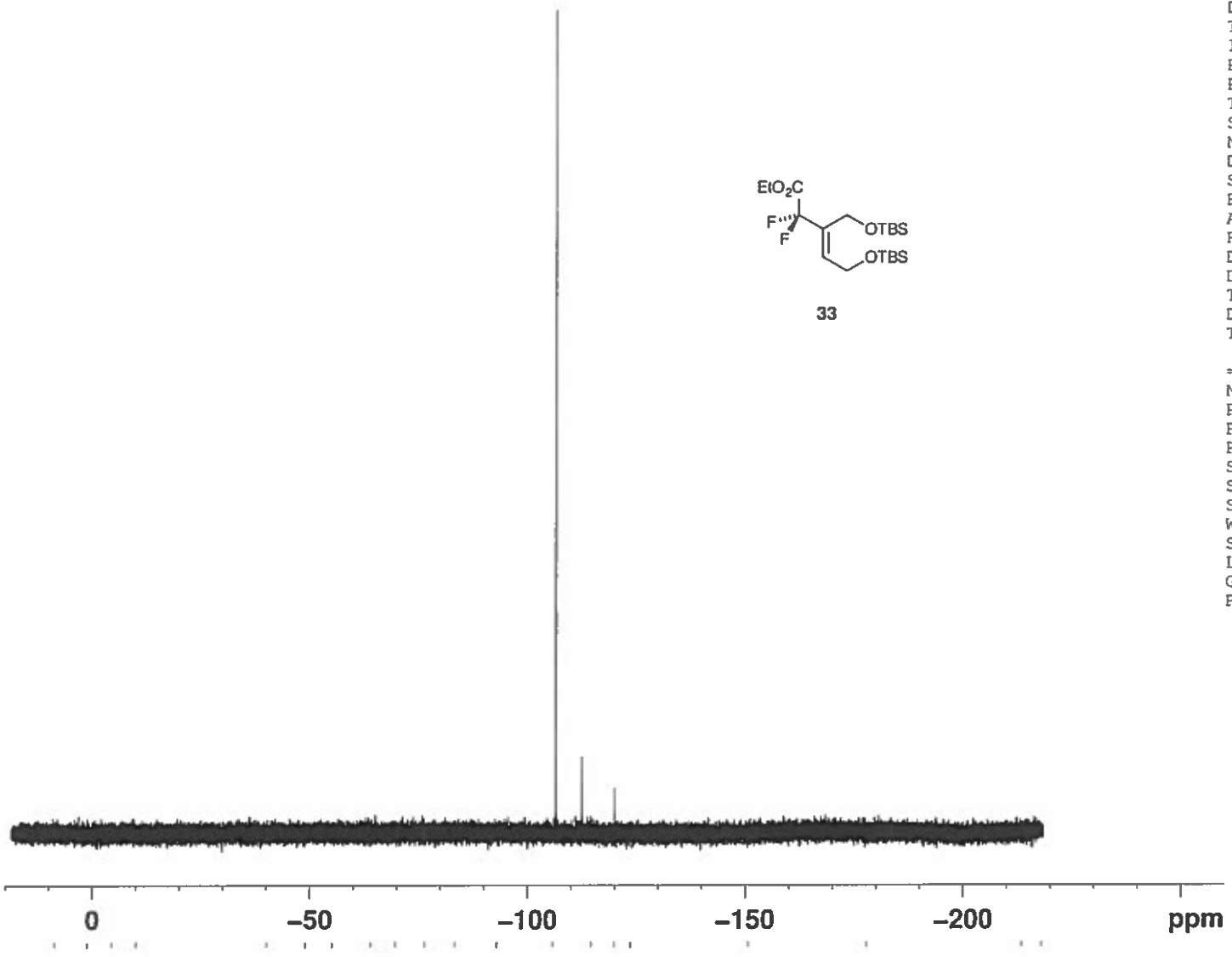
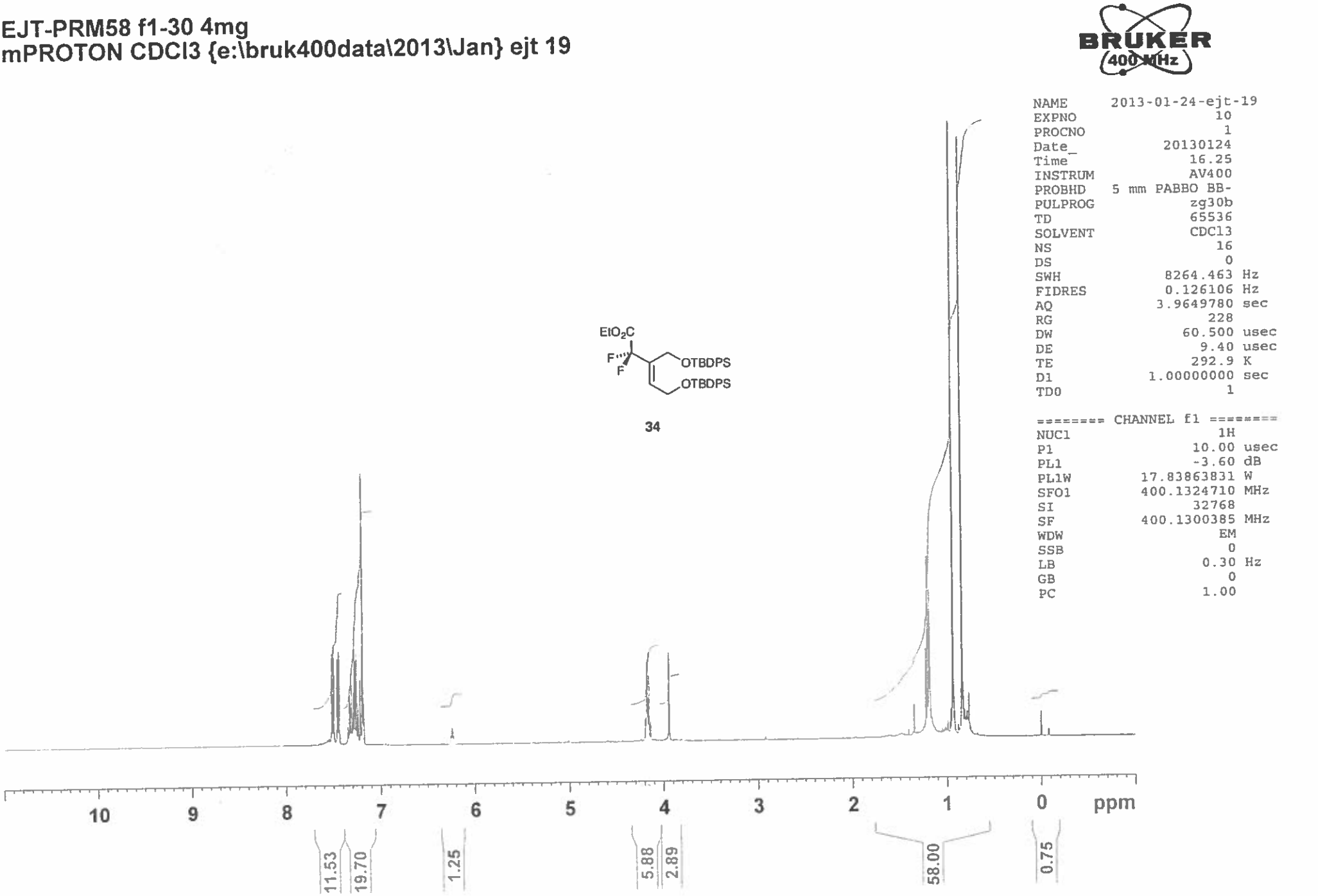
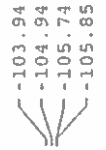


NAME	2013-02-14-ejt-31
EXPNO	12
PROCNO	1
Date_	20130214
Time	12.58
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	11.01 usec
TE	292.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

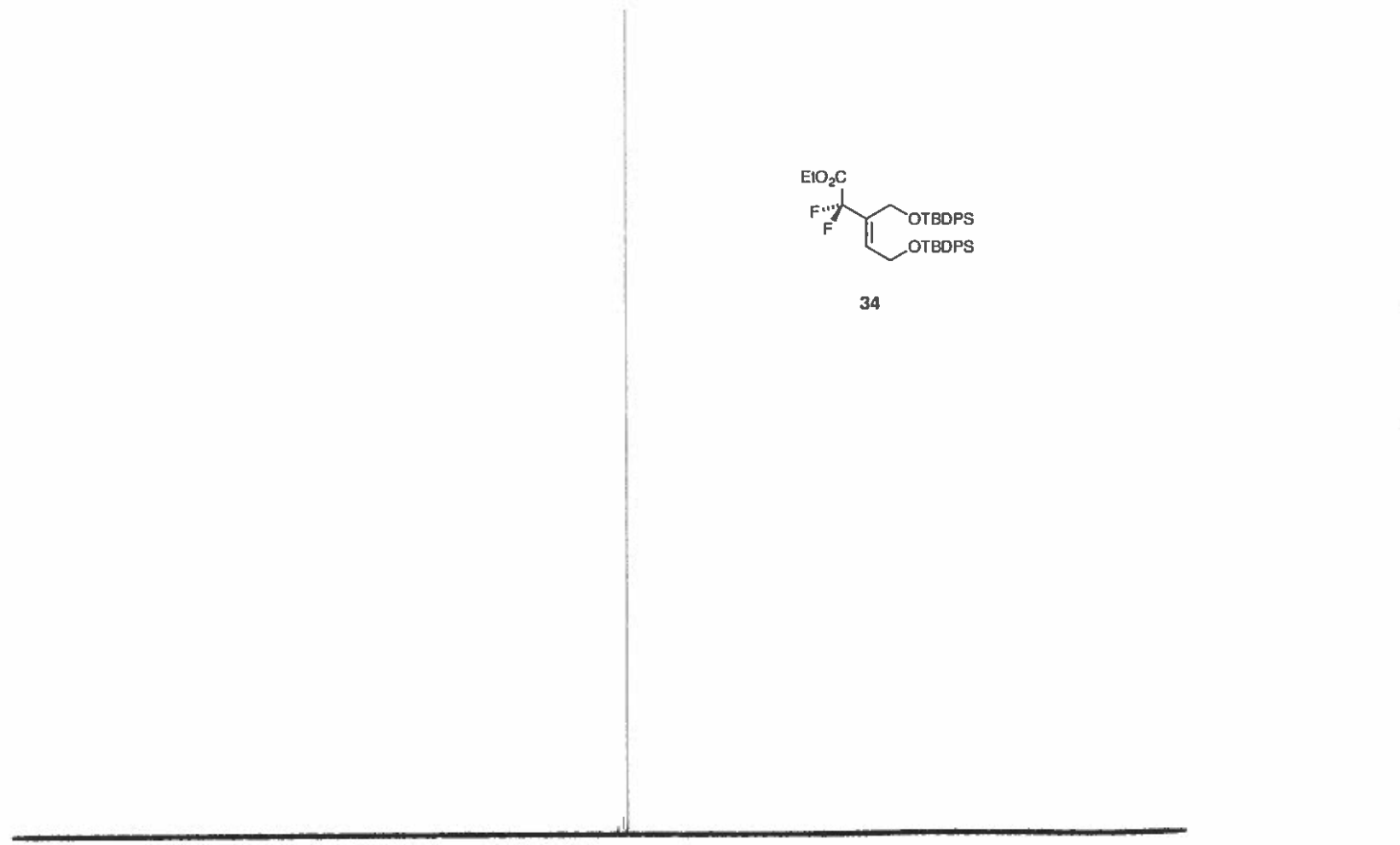
EJT-PRM58 f1-30 4mg
mPROTON CDCl3 {e:\bruk400data\2013\Jan} ejt 19



EJT-PRM58 f1-30 4mg
mF19CPD CDCl3 {e:\bruk400data\2013\Jan} ejt 19

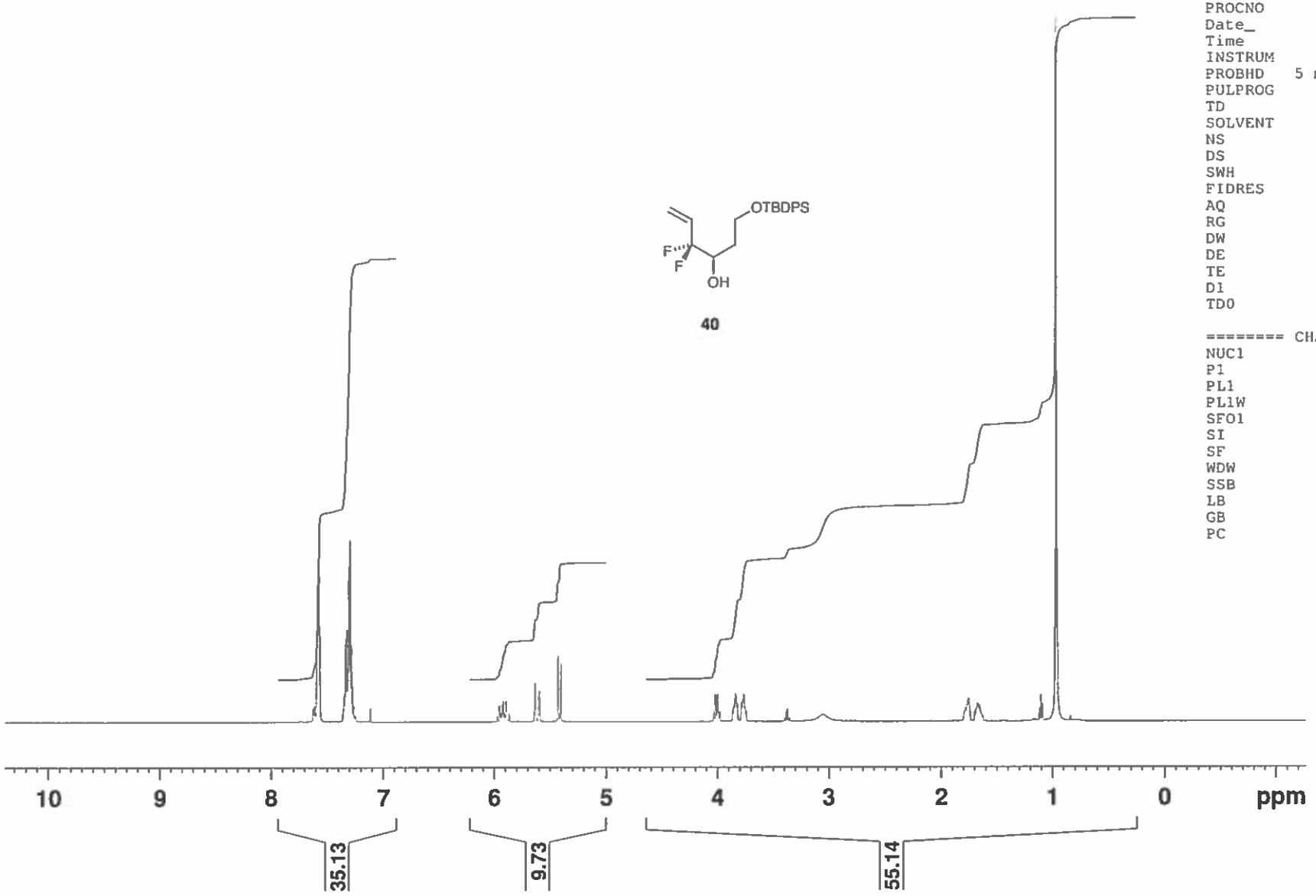


34



NAME	2013-01-24-ejt-19
EXPNO	12
PROCNO	1
Date_	20130124
Time	16.28
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgig
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	7.51 usec
TE	293.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
SFO2	400.1316005 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

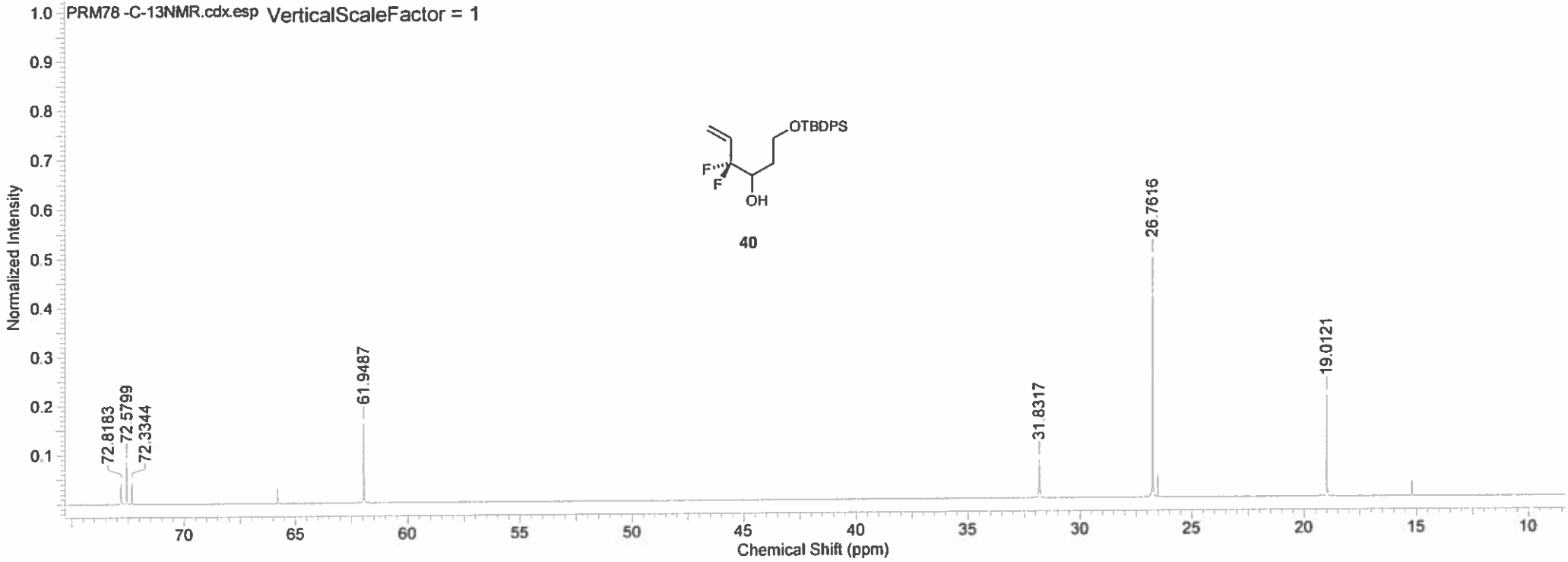
EJT–PRM78 Prod data
mPROTONnight CDCl3 /opt/oldbruk500data.11vii11/2013/May ejt 23



NAME	2013-05-06-ejt-23
EXPNO	14
PROCNO	1
Date_	20130506
Time	23.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	18
DW	48.400 usec
DE	13.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300840 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

23/05/2014 17:17:55

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM78 Prod data mCARBONnight CDCl3 /opt/oldbruk500data 11vii11/2013/May ejt 23				
Date	06 May 2013 22:20:00	*Date Stamp*	06 May 2013 22:20:00				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\MAY\DATA\EJT\NMR\2013-05-06-EJT-23\10\PDATA\1\1R						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	3000	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12562.9922
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	25.128		

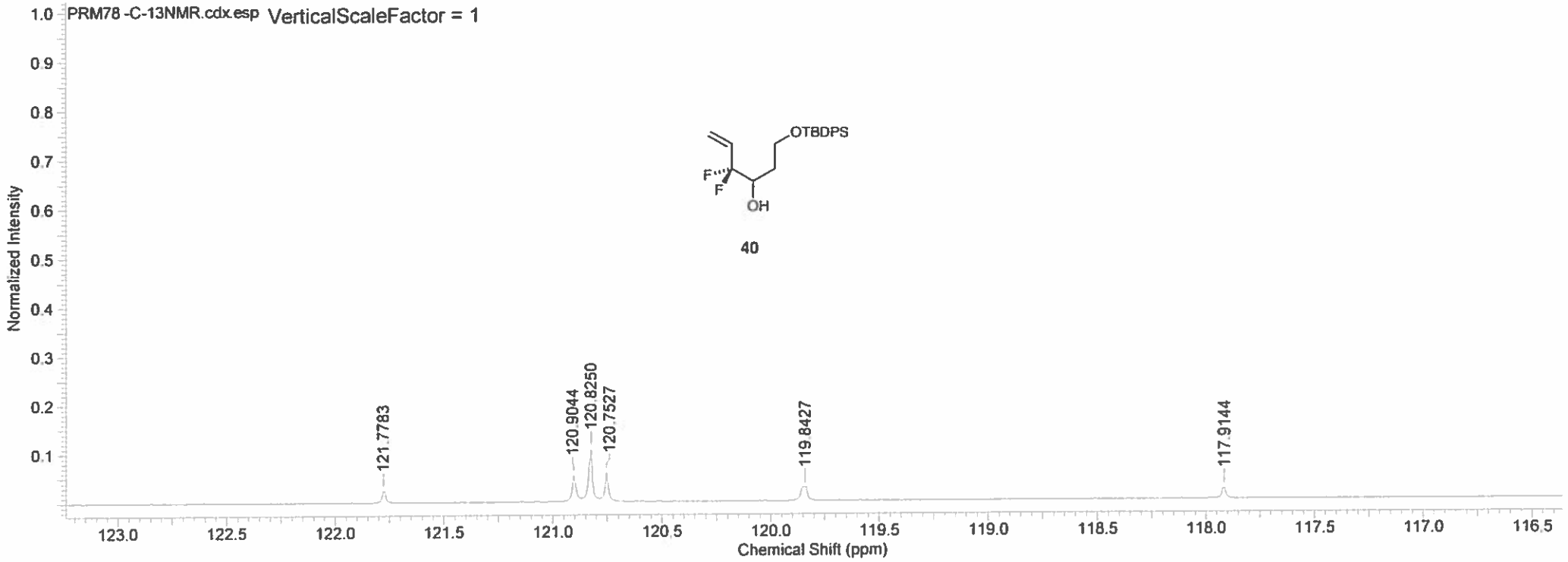


No.	(ppm)	(Hz)	Height
1	19.01	2390.9	0.2061
2	26.76	3365.5	0.4888
3	31.83	4003.1	0.0785
4	61.95	7790.5	0.1612
5	72.33	9096.6	0.0455
6	72.58	9127.5	0.0859
7	72.82	9157.5	0.0440

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

23/05/2014 17:23:24

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM78 Prod data mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2013/May ejt 23				
Date	06 May 2013 22:20:00	*Date Stamp*	06 May 2013 22:20:00				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\MAY\DATA\EJT\NMR\2013-05-06-EJT-23\10\PDATA\1\1R						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	3000	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12562.9922
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	25.128		



40

No.	(ppm)	(Hz)	Height
1	19.01	2390.9	0.2061
2	26.76	3365.5	0.4888
3	31.83	4003.1	0.0785
4	61.95	7790.5	0.1612
5	72.33	9096.6	0.0455

No.	(ppm)	(Hz)	Height
6	72.58	9127.5	0.0859
7	72.82	9157.5	0.0440
8	117.91	14828.6	0.0221
9	119.84	15071.2	0.0281
10	120.75	15185.6	0.0599

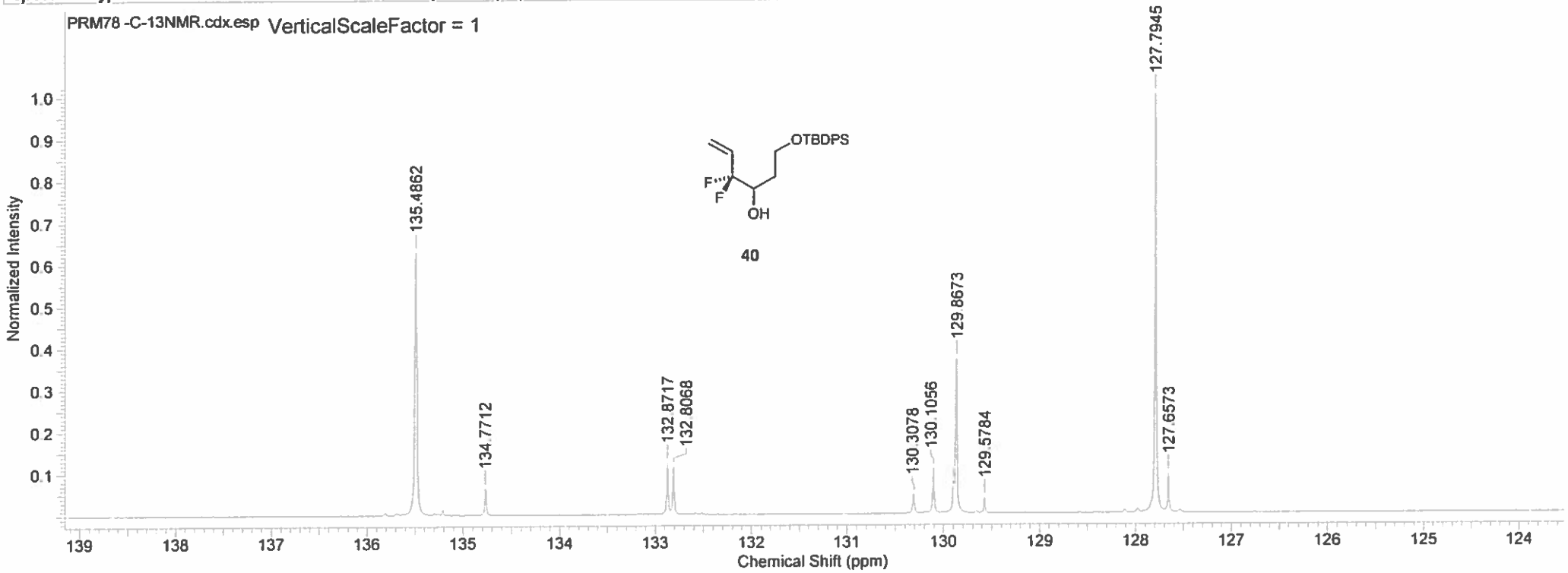
No.	(ppm)	(Hz)	Height
11	120.82	15194.7	0.1070
12	120.90	15204.7	0.0546
13	121.78	15314.6	0.0234
14	127.66	16053.9	0.0923
15	127.79	16071.2	1.0000

No.	(ppm)	(Hz)	Height
16	129.58	16295.5	0.0367
17	129.87	16331.8	0.3682
18	129.90	16335.5	0.0755
19	130.11	16361.8	0.1076
20	130.31	16387.2	0.0446

No.	(ppm)	(Hz)	Height
21	132.81	16701.5	0.1135
22	132.87	16709.7	0.1225
23	134.77	16948.5	0.0635
24	135.49	17038.4	0.6292

23/05/2014 17:53:06

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM78 Prod data mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2013/May ejt 23				
Date	06 May 2013 22:20:00	*Date Stamp*	06 May 2013 22:20:00				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\MAY\DATA\EJT\NMR\2013-05-06-EJT-23\10\PDATA\1\1R						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	3000	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12562.9922
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	25.128		



No.	(ppm)	(Hz)	Height
1	19.01	2390.9	0.2061
2	26.76	3365.5	0.4888
3	31.83	4003.1	0.0785
4	61.95	7790.5	0.1612
5	72.33	9096.6	0.0455

No.	(ppm)	(Hz)	Height
6	72.58	9127.5	0.0859
7	72.82	9157.5	0.0440
8	117.91	14828.6	0.0221
9	119.84	15071.2	0.0281
10	120.75	15185.6	0.0599

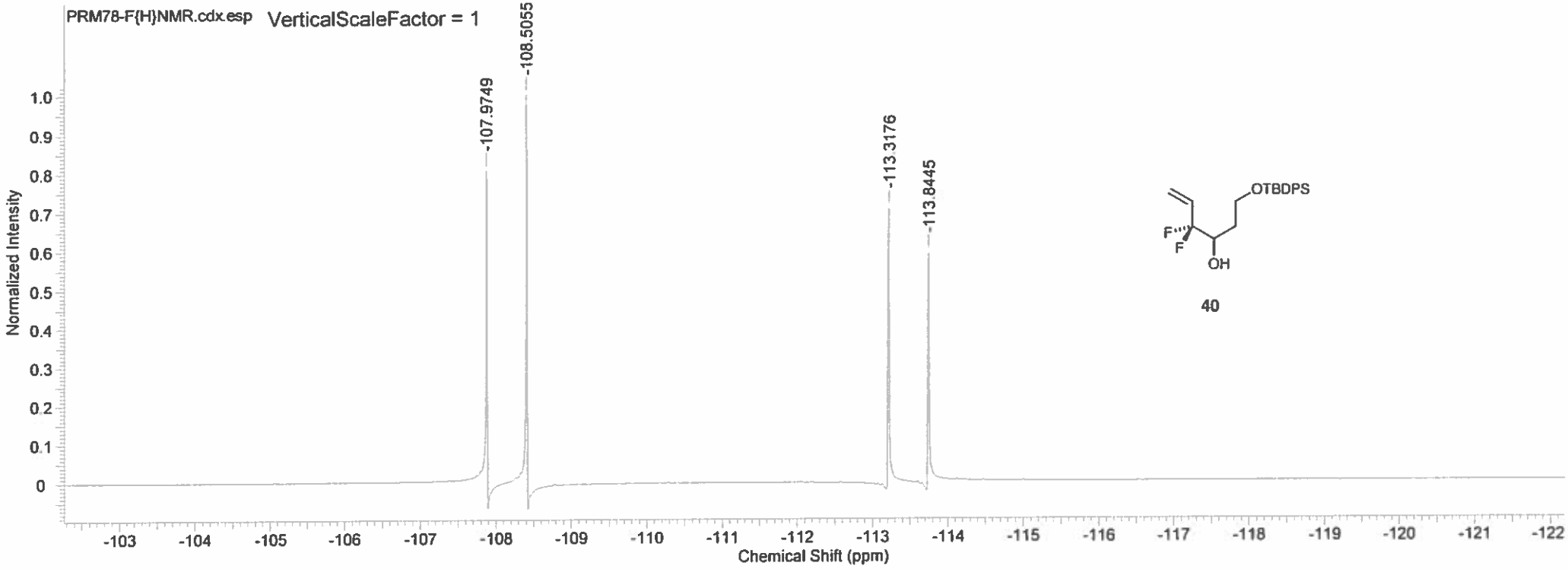
No.	(ppm)	(Hz)	Height
11	120.82	15194.7	0.1070
12	120.90	15204.7	0.0546
13	121.78	15314.6	0.0234
14	127.66	16053.9	0.0923
15	127.79	16071.2	1.0000

No.	(ppm)	(Hz)	Height
16	129.58	16295.5	0.0367
17	129.87	16331.8	0.3682
18	129.90	16335.5	0.0755
19	130.11	16361.8	0.1076
20	130.31	16387.2	0.0446

No.	(ppm)	(Hz)	Height
21	132.81	16701.5	0.1135
22	132.87	16709.7	0.1225
23	134.77	16948.5	0.0635
24	135.49	17038.4	0.6292

23/05/2014 18:08:10

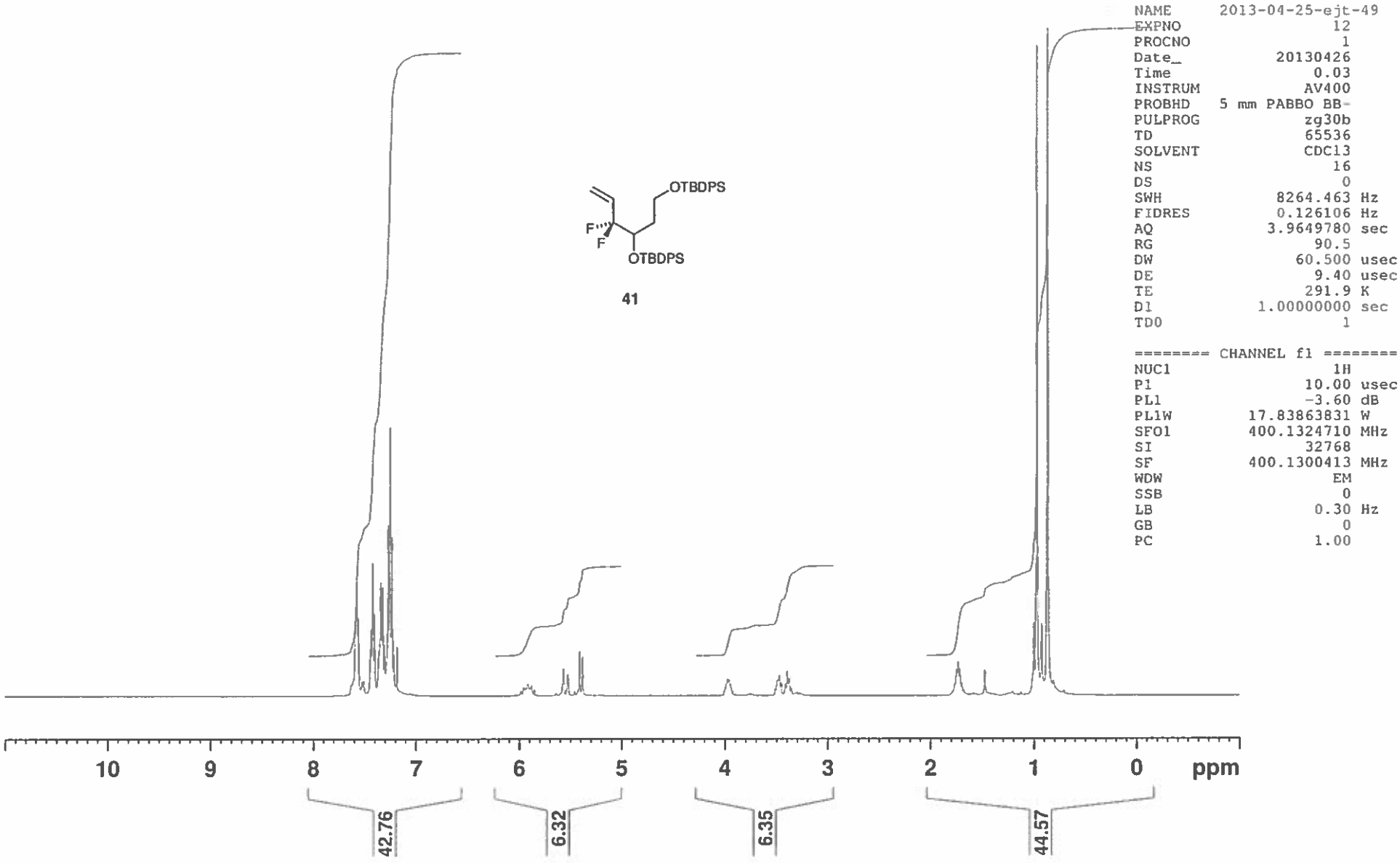
Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM78 Prod data m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2013/May ejt 23				
Date	06 May 2013 22:24:16	*Date Stamp*	06 May 2013 22:24:16				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\MAY\DATA\EJT\NMR\2013-05-06-EJT-23\12\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn
Receiver Gain	287.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	27.000		



40

No.	(ppm)	(Hz)	Height
1	-113.84	-53574.4	0.5903
2	-113.32	-53326.4	0.7057
3	-108.51	-51061.9	1.0000
4	-107.97	-50812.2	0.8064

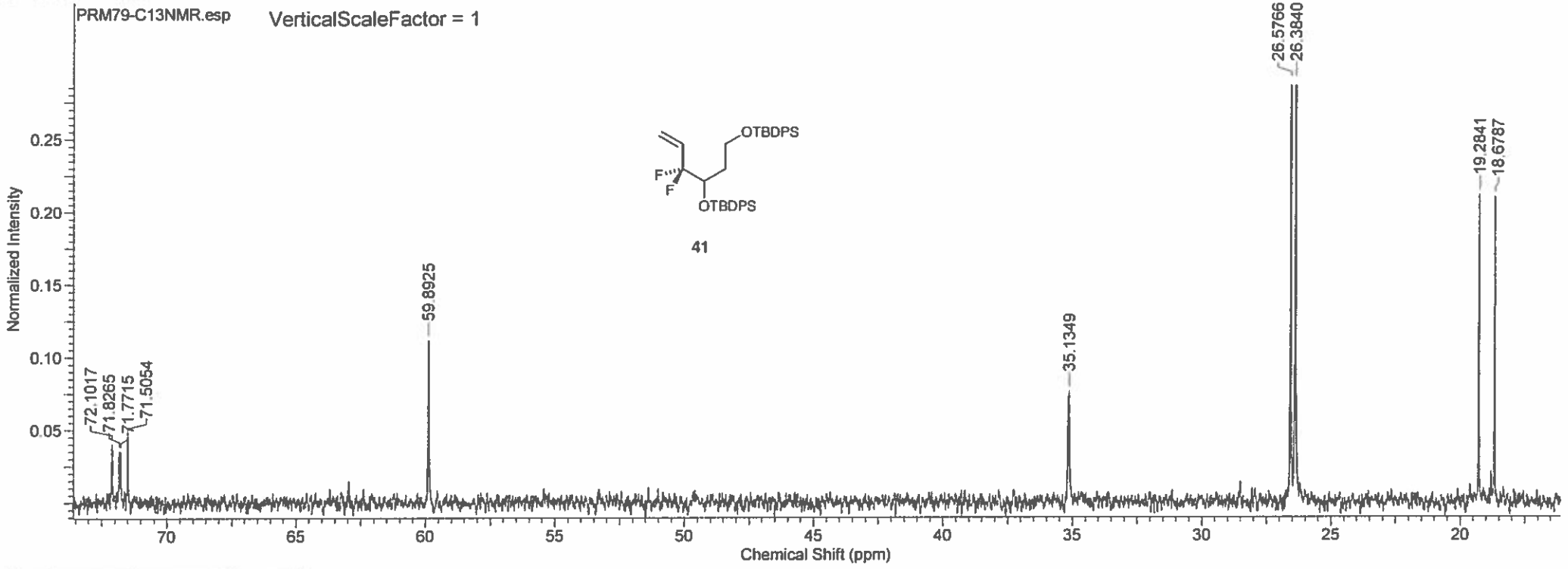
EJT–PRM77/79 Prod data
mPROTONnight CDCl3 {e:\bruk400data\2013\Apr} ejt 49



NAME	2013-04-25-ejt-49
EXPNO	12
PROCNO	1
Date_	20130426
Time	0.03
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	90.5
DW	60.500 usec
DE	9.40 usec
TE	291.9 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	400.1300413 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

12/06/2013 11:53:18

Acquisition Time (sec)	1.0835	***Comment***	EJT-PRM77/79 Prod data mCARBONnight CDCl3 {e:\bruk400data\2013\Apr} ejt 49				
Date	25 Apr 2013 23:47:28	***Date Stamp***	25 Apr 2013 23:47:28				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2013\APR\DATA\EJT\NMR\2013-04-25-EJT-49\10\PDATA\1\1R						
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	600	***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)***	11297.1592
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30241.01	***Temperature (degree C)***	19.400		

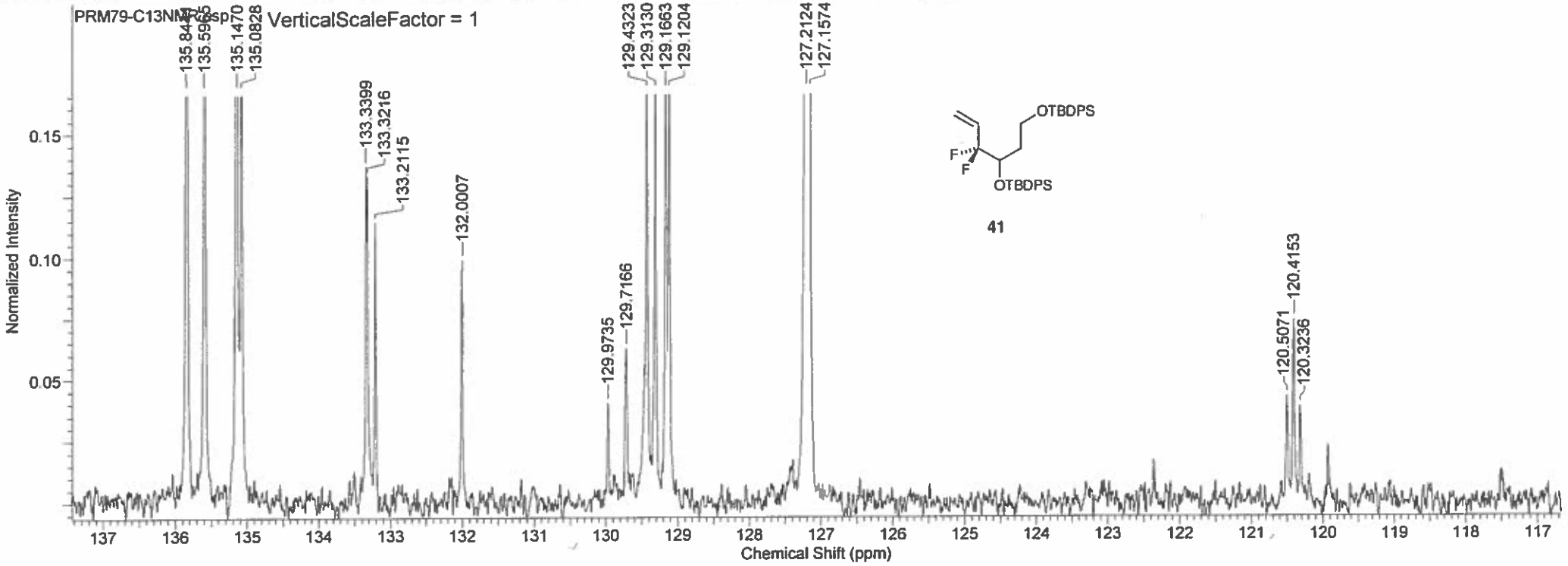


No.	(ppm)	(Hz)	Height
1	18.68	1879.3	0.2102
2	19.28	1940.2	0.2114
3	26.38	2654.6	0.5291
4	26.58	2673.9	0.5033
5	35.13	3535.0	0.0761
6	59.89	6026.0	0.1114
7	71.51	7194.4	0.0453
8	71.77	7221.1	0.0348
9	71.83	7226.7	0.0355
10	72.10	7254.3	0.0405

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

12/06/2013 11:53:48

Acquisition Time (sec)	1.0835	*Comment*	EJT-PRM77/79 Prod data mCARBONnight CDCl3 {e:\bruk400data\2013\Apr} ejt 49				
Date	25 Apr 2013 23:47:28	*Date Stamp*	25 Apr 2013 23:47:28				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2013\APR\DATA\EJT\NMR\2013-04-25-EJT-49\10\PDATA\1\1R						
Frequency (MHz)	100.61	*Nucleus*	13C	*Number of Transients*	600	*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)*	11297.1592
Spectrum Type	STANDARD	*Sweep Width (Hz)*	30241.01	*Temperature (degree C)*	19.400		



41

No.	(ppm)	(Hz)	Height
1	18.68	1879.3	0.2102
2	19.28	1940.2	0.2114
3	26.38	2654.6	0.5291
4	26.58	2673.9	0.5033
5	35.13	3535.0	0.0761
6	59.89	6026.0	0.1114

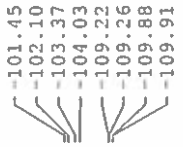
No.	(ppm)	(Hz)	Height
7	71.51	7194.4	0.0453
8	71.77	7221.1	0.0348
9	71.83	7226.7	0.0355
10	72.10	7254.3	0.0405
11	120.32	12106.1	0.0384
12	120.42	12115.3	0.0735

No.	(ppm)	(Hz)	Height
13	120.51	12124.5	0.0424
14	127.16	12793.7	0.4051
15	127.21	12799.2	0.7568
16	129.12	12991.2	0.1982
17	129.17	12995.8	0.2313
18	129.31	13010.5	0.1777

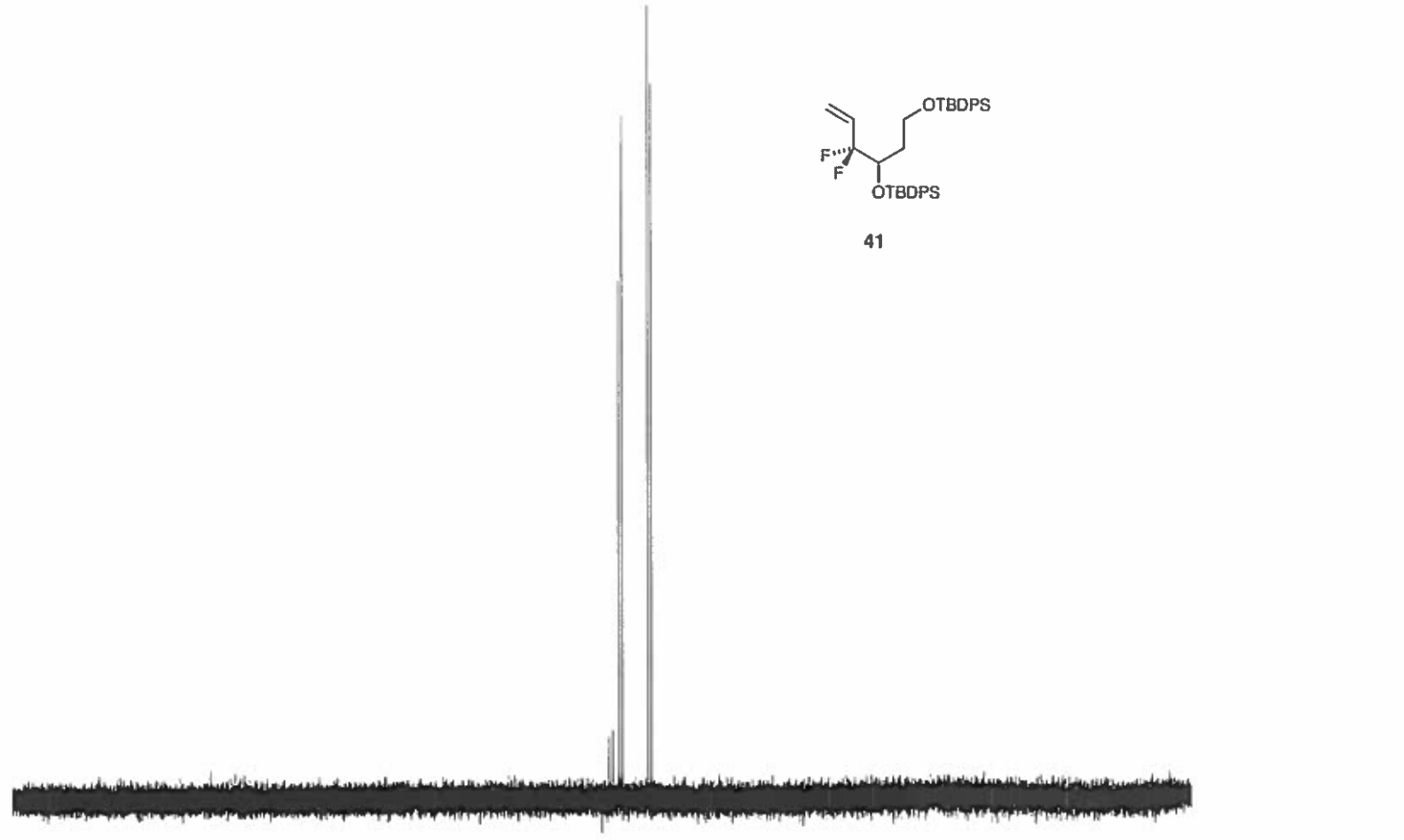
No.	(ppm)	(Hz)	Height
19	129.43	13022.5	0.1720
20	129.72	13051.2	0.0625
21	129.97	13077.0	0.0402
22	132.00	13281.0	0.0988
23	133.21	13402.8	0.1141
24	133.32	13413.9	0.1326

No.	(ppm)	(Hz)	Height
25	133.34	13415.7	0.1369
26	135.08	13591.1	0.4275
27	135.15	13597.5	0.4308
28	135.60	13642.7	0.3973
29	135.84	13667.7	0.3377

EJT-PRM77 f5-11 86mg
mF19CPD CDCl3 {e:\bruk400data\2013\Apr} ejt 56



41

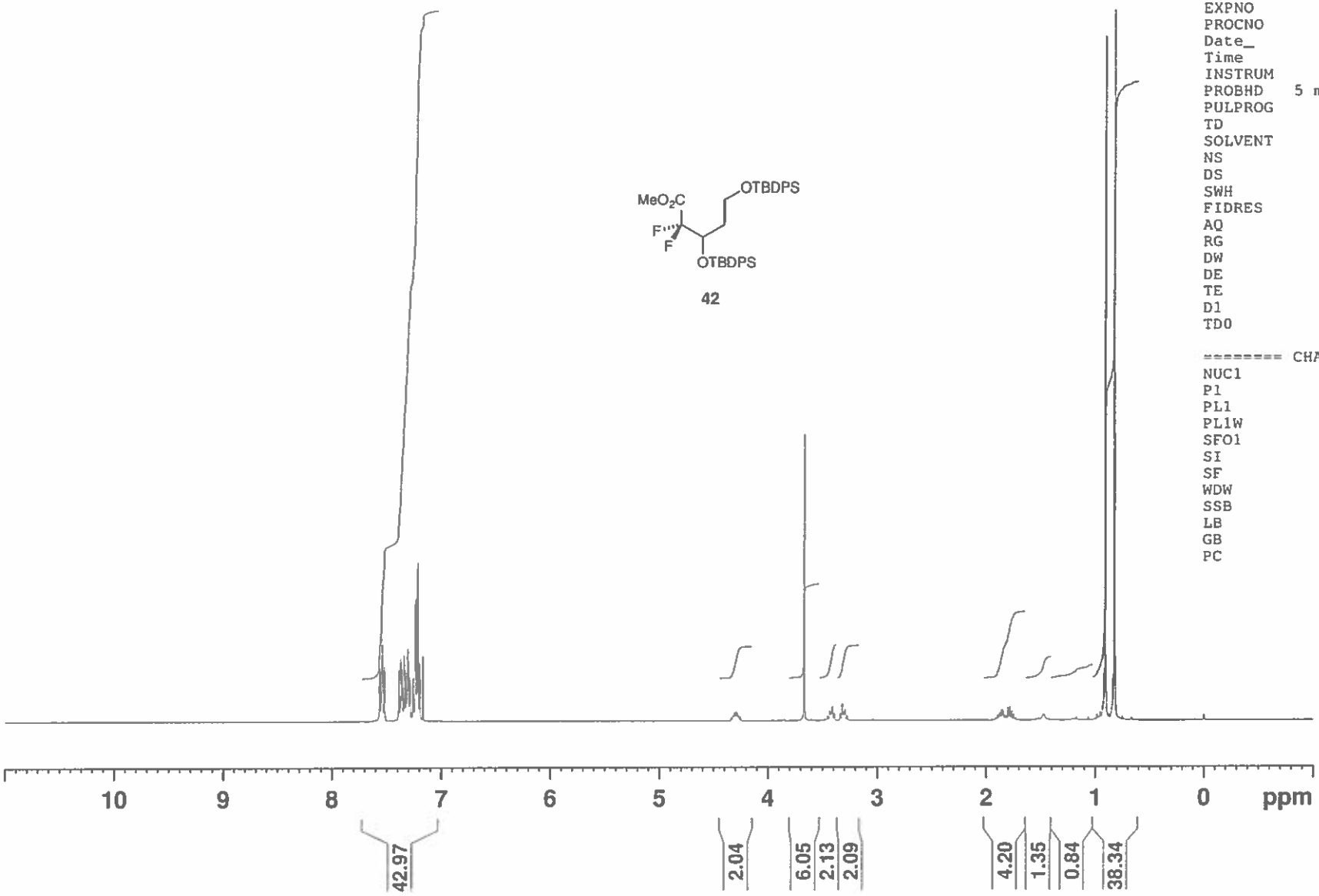


NAME	2013-04-24-ejt-56	
EXPNO	11	
PROCNO	1	
Date_	20130424	
Time	18.18	
INSTRUM	AV400	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	89285.711	Hz
FIDRES	0.681196	Hz
AQ	0.7340532	sec
RG	4100	
DW	5.600	usec
DE	7.51	usec
TE	293.3	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	10.70	usec
PL1	-5.00	dB
PL1W	27.00716019	W
SFO1	376.4607164	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-3.60	dB
PL12	15.31	dB
PL2W	17.83863831	W
PL12W	0.22927761	W
SFO2	400.1316005	MHz
SI	262144	
SF	376.4983660	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	2.00	

EJT–PRM89 f10–24 20mg
mPROTON CDCl3 {e:\bruk400data\2013\May} ejt 11

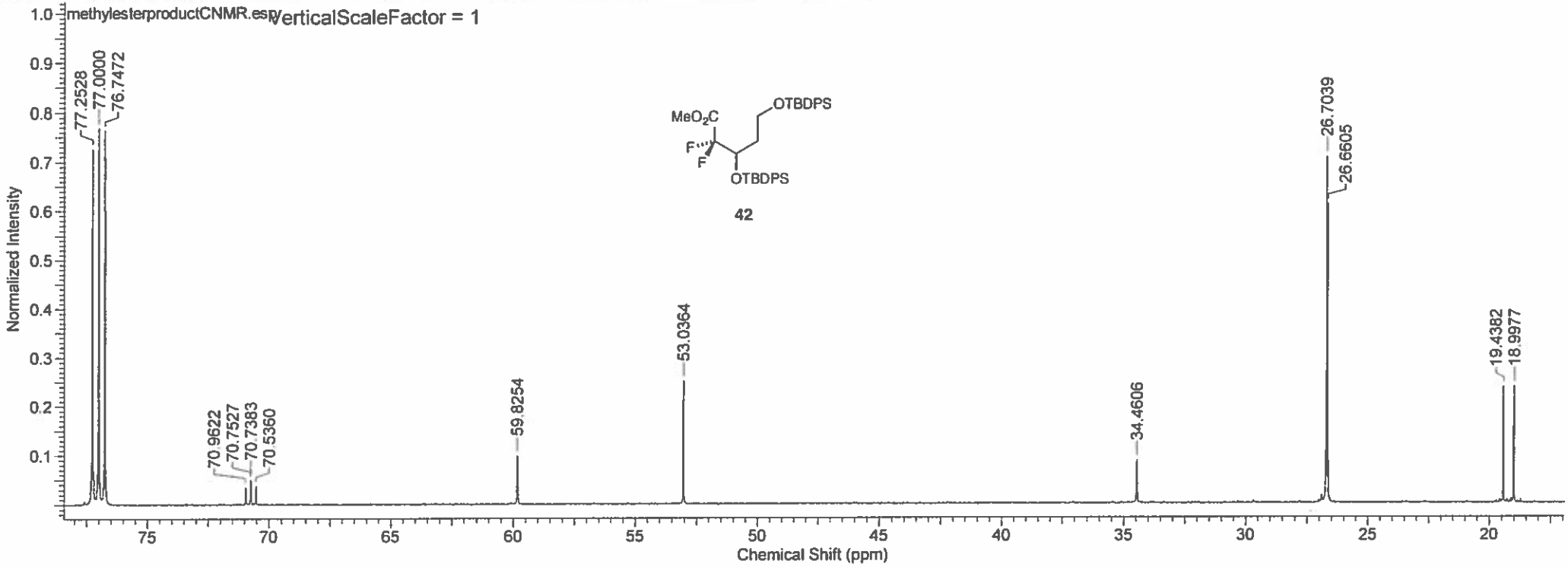
42

NAME	2013-05-29-ejt-11
EXPNO	10
PROCNO	1
Date_	20130529
Time	12.38
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	144
DW	60.500 usec
DE	9.40 usec
TE	294.4 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	400.1300464 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



12/06/2013 11:05:49

Acquisition Time (sec)	1.1010	***Comment***	EJT-PRM80 methyl ester mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2013/Jun ejt 26				
Date	07 Jun 2013 03:50:40	***Date Stamp***	07 Jun 2013 03:50:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\JUN\DATA\EJT\NMR\2013-06-06-EJT-26\11\PDATA\1\1R						
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	3072	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12569.3496
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.128		



No.	(ppm)	(Hz)	Height
1	19.00	2389.1	0.2368
2	19.44	2444.5	0.2365
3	26.66	3352.8	0.6122

No.	(ppm)	(Hz)	Height
4	26.70	3358.2	0.7079
5	34.46	4333.7	0.0876
6	53.04	6669.7	0.2506

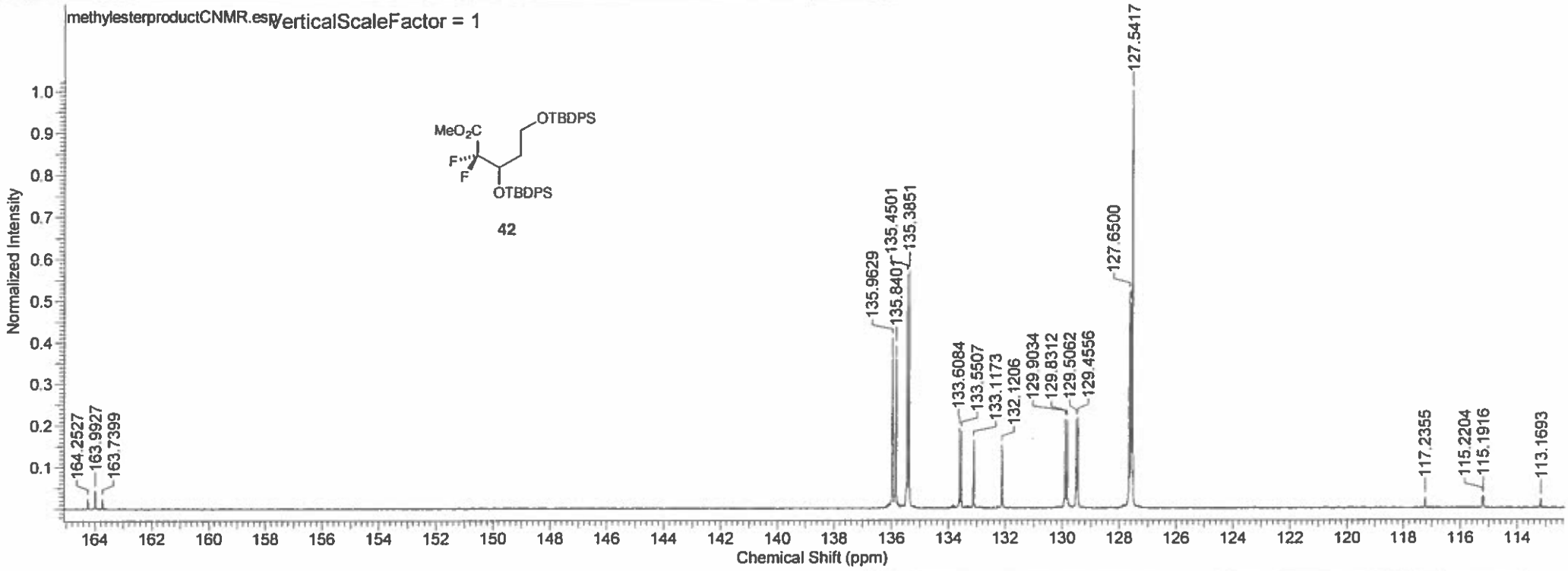
No.	(ppm)	(Hz)	Height
7	59.83	7523.5	0.0992
8	70.54	8870.5	0.0373
9	70.74	8895.9	0.0510

No.	(ppm)	(Hz)	Height
10	70.75	8897.7	0.0487
11	70.96	8924.0	0.0351
12	76.75	9651.6	0.7640

No.	(ppm)	(Hz)	Height
13	77.00	9683.3	0.7680
14	77.25	9715.1	0.7269

12/06/2013 11:06:19

Acquisition Time (sec)	1.1010	***Comment***	EJT-PRM80 methyl ester mCARBONnight CDCl3 /opt/otdbruk500data.11vii11/2013/Jun ejt 26				
Date	07 Jun 2013 03:50:40	***Date Stamp***	07 Jun 2013 03:50:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\JUN\DATA\EJT\NMR\2013-06-06-EJT-26\11\PDATA\1\1R						
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	3072	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12569.3496
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.128		



No.	(ppm)	(Hz)	Height
1	19.00	2389.1	0.2368
2	19.44	2444.5	0.2365
3	26.66	3352.8	0.6122
4	26.70	3358.2	0.7079
5	34.46	4333.7	0.0876
6	53.04	6669.7	0.2506
7	59.83	7523.5	0.0992
8	70.54	8870.5	0.0373

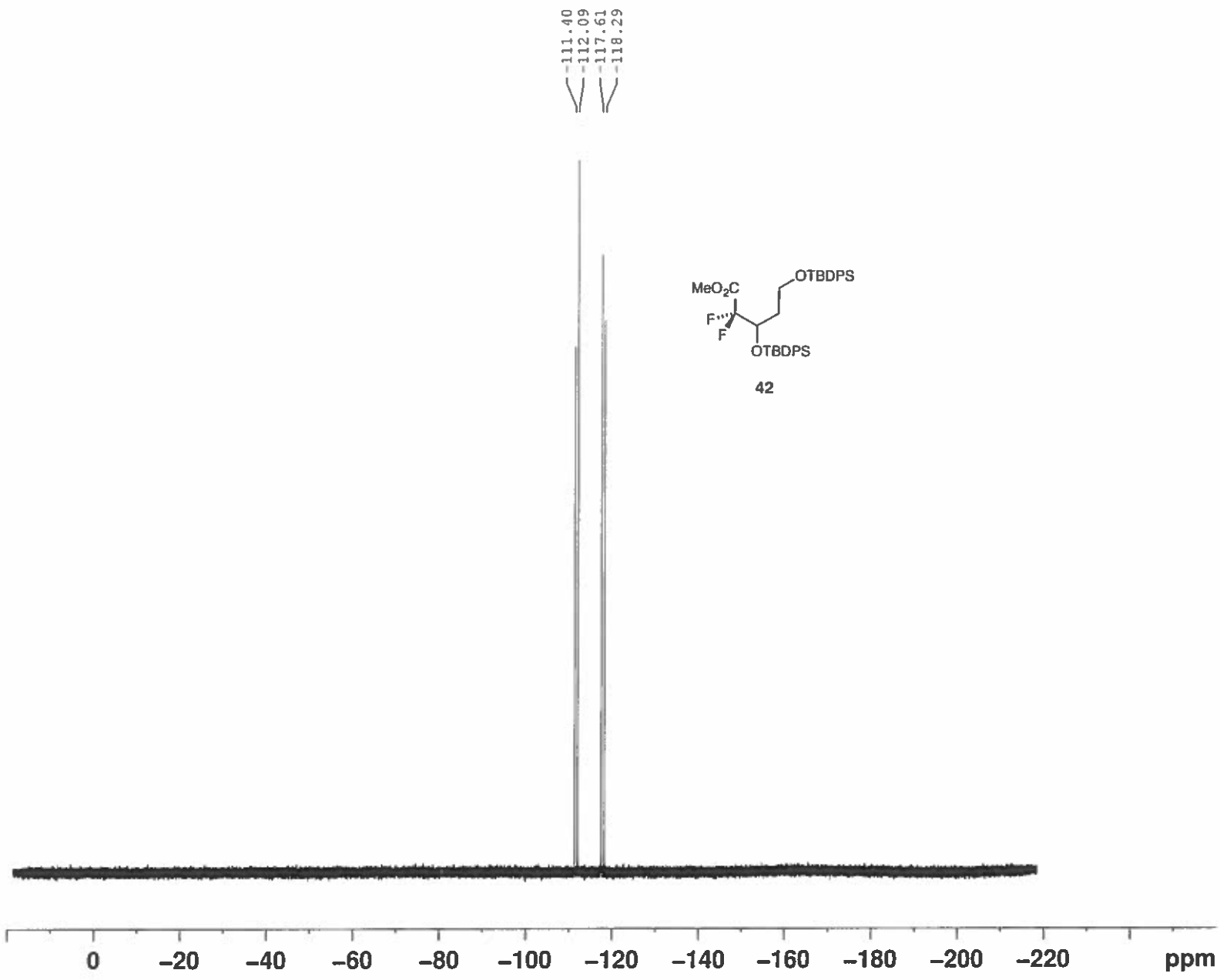
No.	(ppm)	(Hz)	Height
9	70.74	8895.9	0.0510
10	70.75	8897.7	0.0487
11	70.96	8924.0	0.0351
12	76.75	9651.6	0.7640
13	77.00	9683.3	0.7680
14	77.25	9715.1	0.7269
15	113.17	14231.9	0.0225
16	115.19	14486.2	0.0292

No.	(ppm)	(Hz)	Height
17	115.22	14489.9	0.0265
18	117.24	14743.3	0.0254
19	127.54	16039.4	1.0000
20	127.59	16045.7	0.4926
21	127.65	16053.0	0.5199
22	129.46	16280.1	0.2176
23	129.51	16286.4	0.2148
24	129.83	16327.3	0.2114

No.	(ppm)	(Hz)	Height
25	129.90	16336.4	0.2136
26	132.12	16615.2	0.1516
27	133.12	16740.5	0.1625
28	133.55	16795.0	0.1850
29	133.61	16802.3	0.1924
30	135.39	17025.7	0.5682
31	135.45	17033.9	0.5619
32	135.84	17083.0	0.3899

No.	(ppm)	(Hz)	Height
33	135.96	17098.4	0.4091
34	163.74	20591.6	0.0256
35	163.99	20623.4	0.0439
36	164.25	20656.1	0.0261

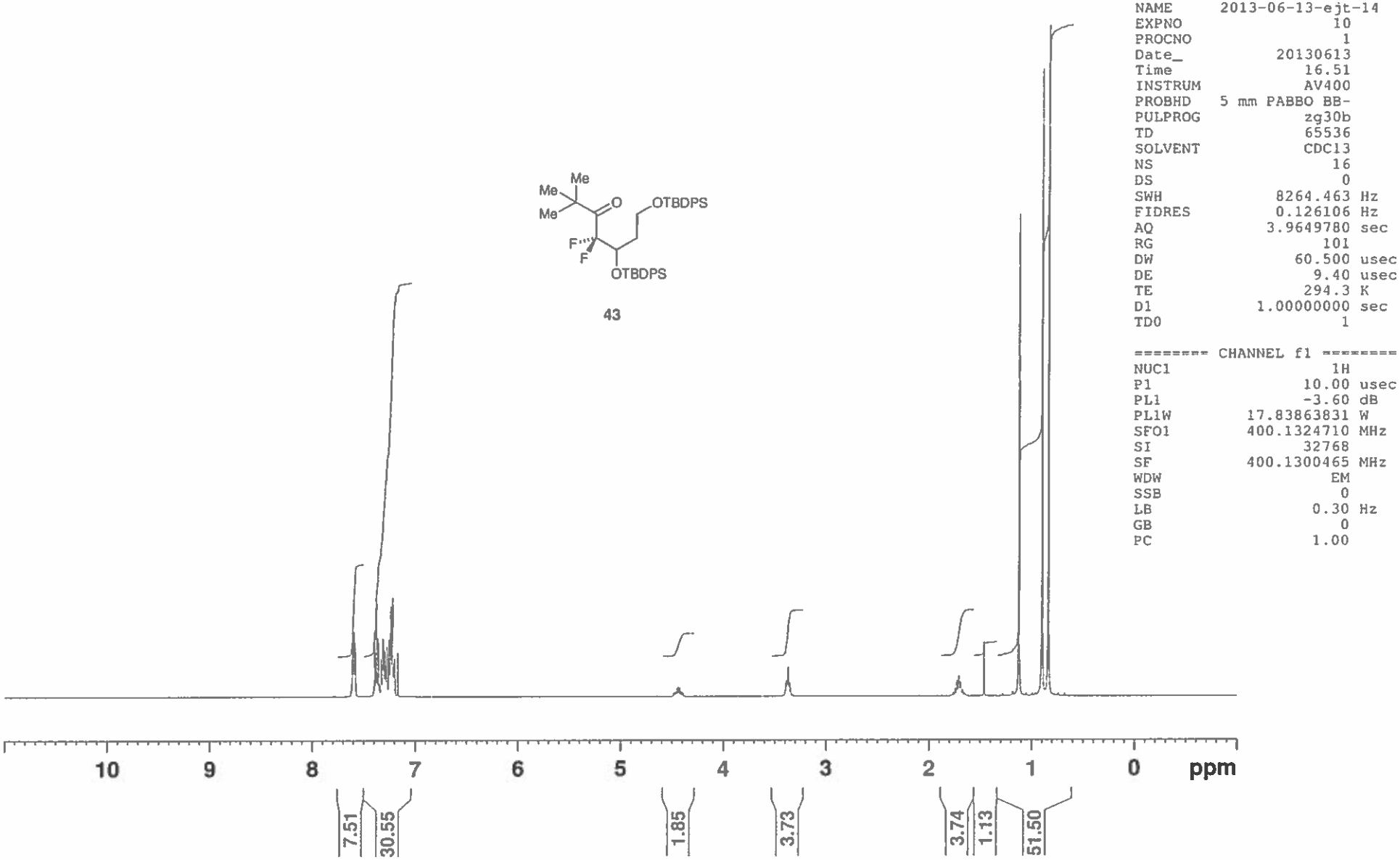
EJT-PRM89 f10-24 20mg
mF19CPD CDCl3 {e:\bruk400data\2013\May} ejt 11



42

NAME	2013-05-29-ejt-11	
EXPNO	11	
PROCNO	1	
Date_	20130529	
Time	12.39	
INSTRUM	AV400	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	89285.711	Hz
FIDRES	0.681196	Hz
AQ	0.7340532	sec
RG	4100	
DW	5.600	usec
DE	7.51	usec
TE	294.6	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	10.70	usec
PL1	-5.00	dB
PL1W	27.00716019	W
SFO1	376.4607164	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-3.60	dB
PL12	15.31	dB
PL2W	17.83863831	W
PL12W	0.22927761	W
SFO2	400.1316005	MHz
SI	262144	
SF	376.4983660	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	2.00	

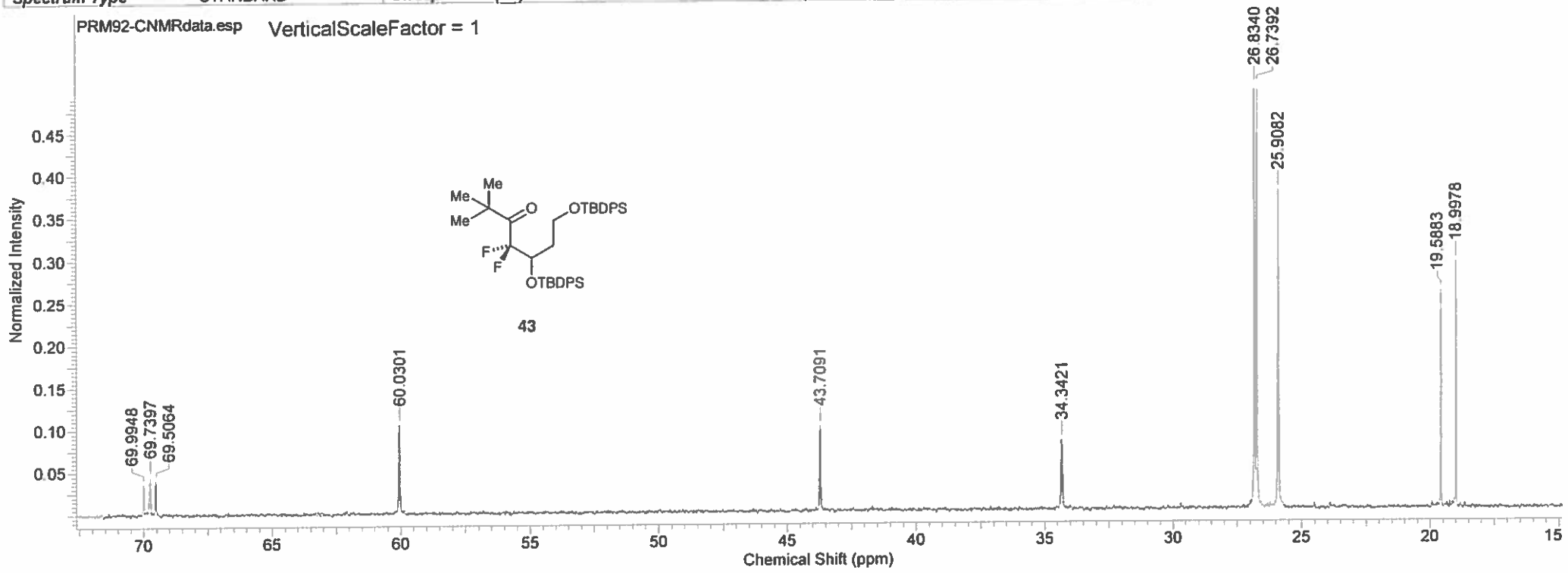
EJT-PRM92 prod fracs 40mg
mPROTON CDCl3 {e:\bruk400data\2013\Jun} ejt 14



NAME	2013-06-13-ejt-14
EXPNO	10
PROCNO	1
Date_	20130613
Time	16.51
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	101
DW	60.500 usec
DE	9.40 usec
TE	294.3 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	400.1300465 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

16/08/2013 13:28:26

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM92 prod data mCARBON_A CDCl3 {E:\bruk400service_data\2013\Aug} ejt 12				
Date	16 Aug 2013 13:01:04	*Date Stamp*	16 Aug 2013 13:01:04				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400SERVICE_DATA\2013\AUG\DATA\EJT\NMR\2013-08-16-EJT-12\10\PDATA\1\1R						
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	256	*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)*	10052.9766
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	25.100		



No.	(ppm)	(Hz)	Height
1	19.00	1911.9	0.2909
2	19.59	1971.3	0.2561
3	25.91	2607.3	0.3759
4	26.74	2691.0	0.6812
5	26.83	2700.5	0.7331
6	34.34	3456.1	0.0819
7	43.71	4398.8	0.1006

No.	(ppm)	(Hz)	Height
8	60.03	6041.3	0.1051
9	69.51	6995.0	0.0402
10	69.74	7018.5	0.0451
11	69.99	7044.1	0.0362
12	115.58	11632.0	0.0139
13	118.16	11891.0	0.0151
14	120.77	12154.4	0.0177

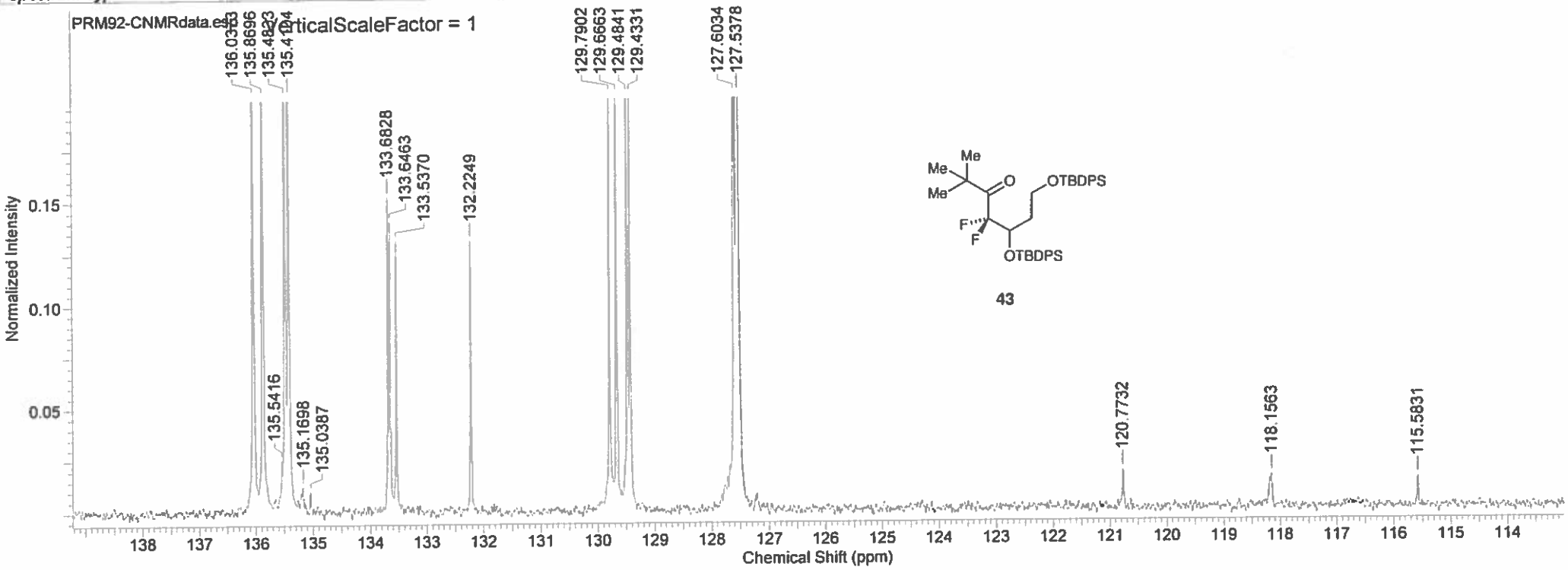
No.	(ppm)	(Hz)	Height
15	127.54	12835.1	1.0000
16	127.60	12841.7	0.4956
17	129.43	13025.9	0.2381
18	129.48	13031.0	0.2207
19	129.67	13049.3	0.2017
20	129.79	13061.8	0.2198
21	132.22	13306.8	0.1308

No.	(ppm)	(Hz)	Height
22	133.54	13438.9	0.1312
23	133.65	13449.9	0.1402
24	133.68	13453.6	0.1522
25	135.04	13590.0	0.0101
26	135.17	13603.2	0.0124
27	135.41	13627.4	0.5391
28	135.48	13634.8	0.4682

No.	(ppm)	(Hz)	Height
29	135.54	13640.6	0.0254
30	135.87	13673.6	0.4506
31	136.04	13690.5	0.3669
32	204.29	20559.2	0.0217
33	204.57	20587.0	0.0263
34	204.84	20614.2	0.0223

16/08/2013 13:27:53

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM92 prod data mCARBON_A CDCl3 (E:\bruk400service_data\2013\Aug) ejt 12				
Date	16 Aug 2013 13:01:04	*Date Stamp*	16 Aug 2013 13:01:04				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400SERVICE_DATA\2013\AUG\DATA\EJT\NMR\2013-08-16-EJT-12\10\PDATA\1\1R						
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	256	*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)*	10052.9766
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	25.100		



43

No.	(ppm)	(Hz)	Height
1	115.58	11632.0	0.0139
2	118.16	11891.0	0.0151
3	120.77	12154.4	0.0177
4	127.54	12835.1	1.0000
5	127.60	12841.7	0.4956

No.	(ppm)	(Hz)	Height
6	129.43	13025.9	0.2381
7	129.48	13031.0	0.2207
8	129.67	13049.3	0.2017
9	129.79	13061.8	0.2198
10	132.22	13306.8	0.1308

No.	(ppm)	(Hz)	Height
11	133.54	13438.9	0.1312
12	133.65	13449.9	0.1402
13	133.68	13453.6	0.1522
14	135.04	13590.0	0.0101
15	135.17	13603.2	0.0124

No.	(ppm)	(Hz)	Height
16	135.41	13627.4	0.5391
17	135.48	13634.8	0.4682
18	135.54	13640.6	0.0254
19	135.87	13673.6	0.4506
20	136.04	13690.5	0.3669

No.	(ppm)	(Hz)	Height
21	204.29	20559.2	0.0217
22	204.57	20587.0	0.0263
23	204.84	20614.2	0.0223

16/08/2013 13:27:10

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM92 prod data mCARBON_A CDCl3 (E:\bruk400service_data\2013\Aug) ejt 12				
Date	16 Aug 2013 13:01:04	*Date Stamp*	16 Aug 2013 13:01:04				
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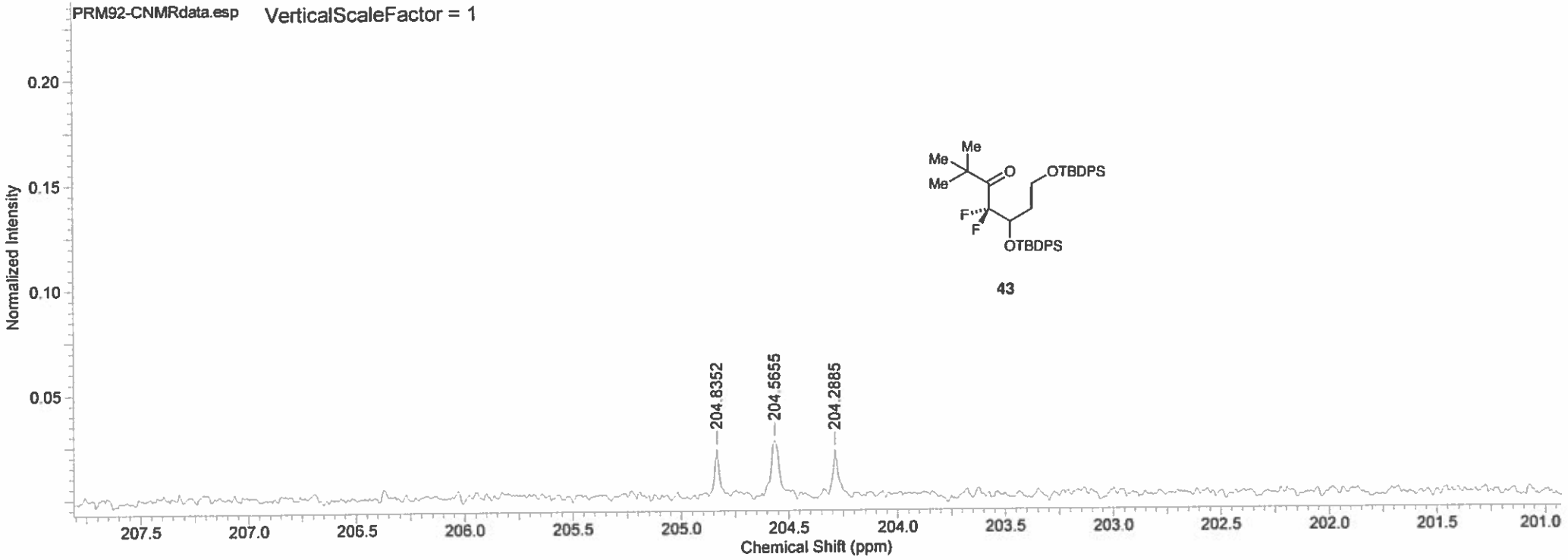
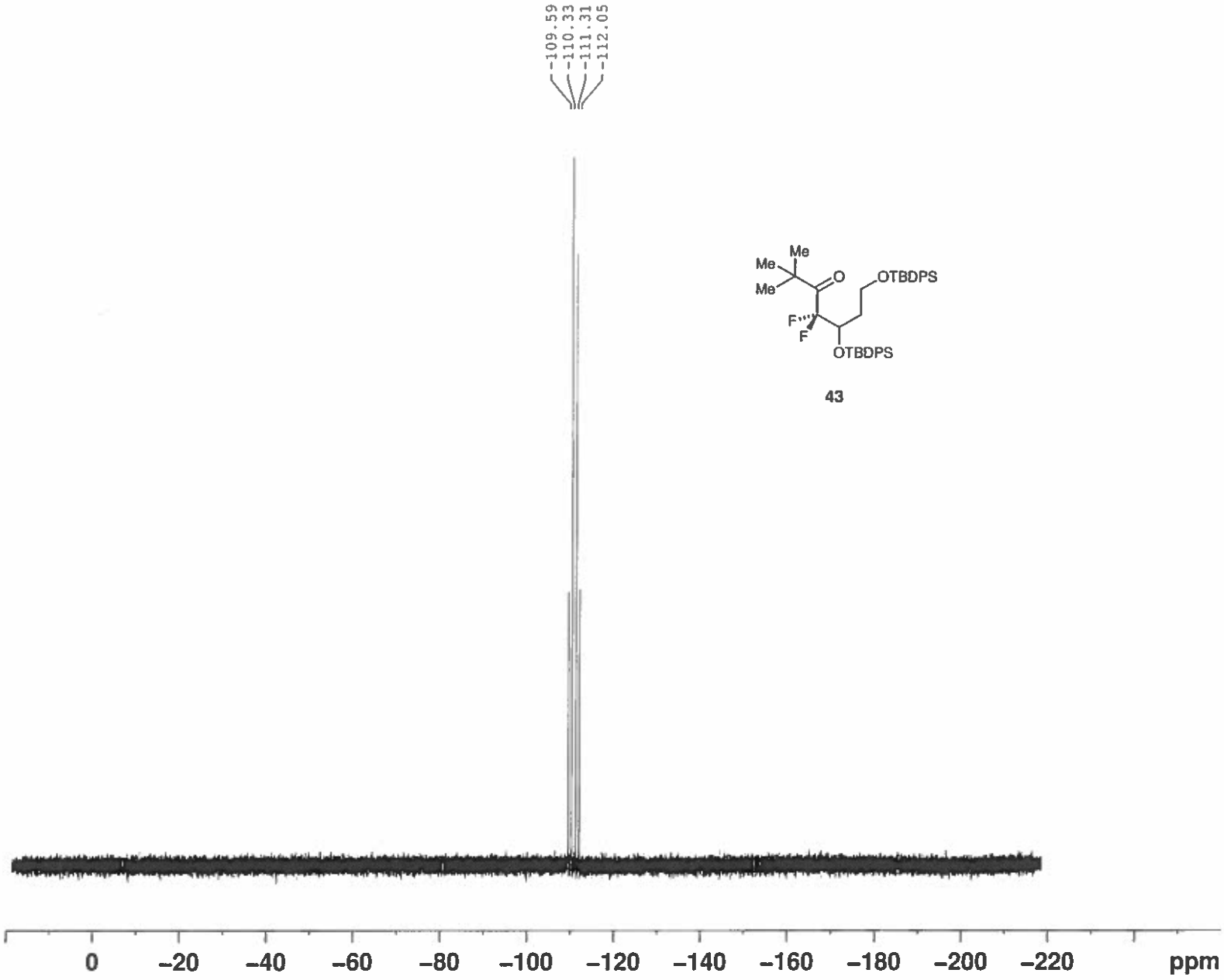
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	256	*Origin*	AV400_S
Original Points Count	32768	*Owner*	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	2050.00	*SW(cyclical) (Hz)*	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10052.9766
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	25.100		



43

No.	(ppm)	(Hz)	Height
1	204.29	20559.2	0.0217
2	204.57	20587.0	0.0263
3	204.84	20614.2	0.0223

EJT–PRM92 prod fracs 40mg
mF19CPD CDCl3 {e:\bruk400data\2013\Jun} ejt 14

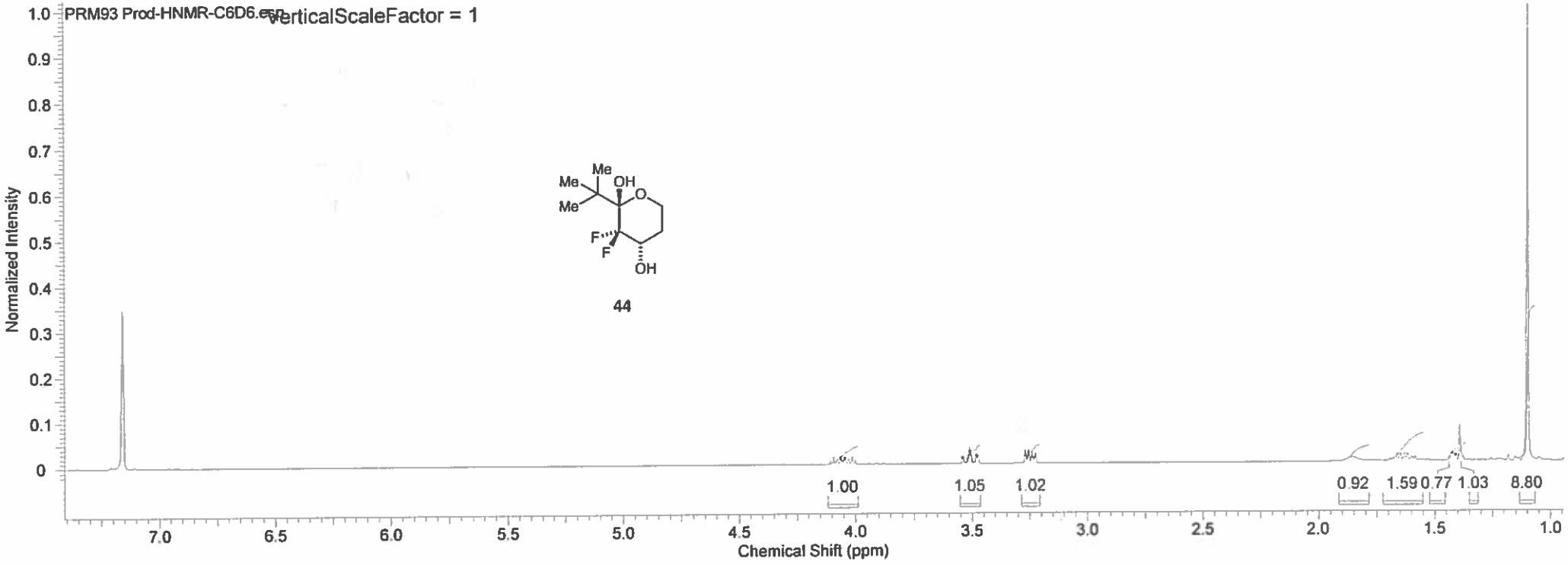


43

NAME	2013-06-13-ejt-14
EXPNO	11
PROCNO	1
Date_	20130613
Time	16.53
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgig
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	7.51 usec
TE	294.5 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	15.31 dB
PL2W	17.83863831 W
PL12W	0.22927761 W
SFO2	400.1316005 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

17/09/2013 11:11:49

Acquisition Time (sec)	3.9846	*Comment*	EJT-PRM93 Product data C-13 mPROTON C6D6 {E:\bruk400service_data\2013\Sep} Administrator 4				
Date	16 Sep 2013 13:05:20	*Date Stamp*	16 Sep 2013 13:05:20				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-16-Administrator-4\10\fid						
Frequency (MHz)	400.23	*Nucleus*	1H	*Number of Transients*	16	*Origin*	AV400_S
Original Points Count	32768	*Owner*	Administrator	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	181.00	*SW(cyclical) (Hz)*	8223.68	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	2424.5730
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8223.43	*Temperature (degree C)*	21.000		



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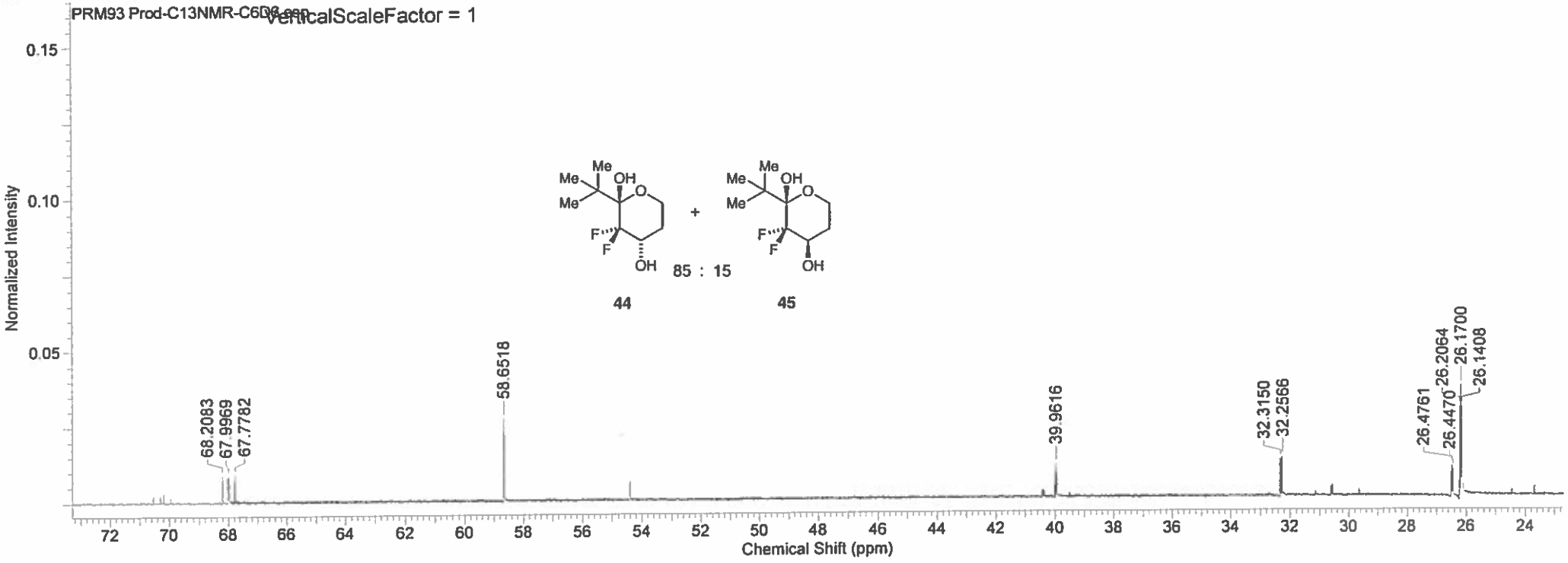
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	0663 .. 1.138	.79730225	3.25690757e+10	8.79730225
2	3673 .. 1.401	.02738047	3.80353306e+9	1.02738047
3	4051 .. 1.470	.77102357	2.85445734e+9	0.77102357
4	5520 .. 1.721	.59436548	5.90260582e+9	1.59436548
5	7838 .. 1.910	.91760439	3.39712384e+9	0.91760439
6	2054 .. 3.281	.02023995	3.77709773e+9	1.02023995
7	4649 .. 3.551	.04753137	3.87813530e+9	1.04753137
8	9897 .. 4.110	.99798036	3.69468902e+9	0.99798036

17/09/2013 19:18:31

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM93 Product data C-13 mCARBON C6D6 (E:\bruk400service_data\2013\Sep) Administrator 4				
Date	16 Sep 2013 13:56:32	*Date Stamp*	16 Sep 2013 13:56:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-16-Administrator-4\13\fid						
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*	BENZENE-d6	*Spectrum Offset (Hz)*	10119.6650
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	21.000		



No.	(ppm)	(Hz)	Height
1	26.14	2630.8	0.0291
2	26.17	2633.7	0.0362
3	26.21	2637.4	0.0290

No.	(ppm)	(Hz)	Height
4	26.45	2661.6	0.0085
5	26.48	2664.5	0.0096
6	32.26	3246.2	0.0127

No.	(ppm)	(Hz)	Height
7	32.31	3252.1	0.0121
8	39.96	4021.7	0.0109
9	58.65	5902.6	0.0272

No.	(ppm)	(Hz)	Height
10	67.78	6821.1	0.0091
11	68.00	6843.1	0.0086
12	68.21	6864.3	0.0088

17/09/2013 19:19:15

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM93 Product data C-13 mCARBON C6D6 {E:\bruk400service_data\2013\Sep} Administrator 4				
Date	16 Sep 2013 13:56:32	*Date Stamp*	16 Sep 2013 13:56:32				
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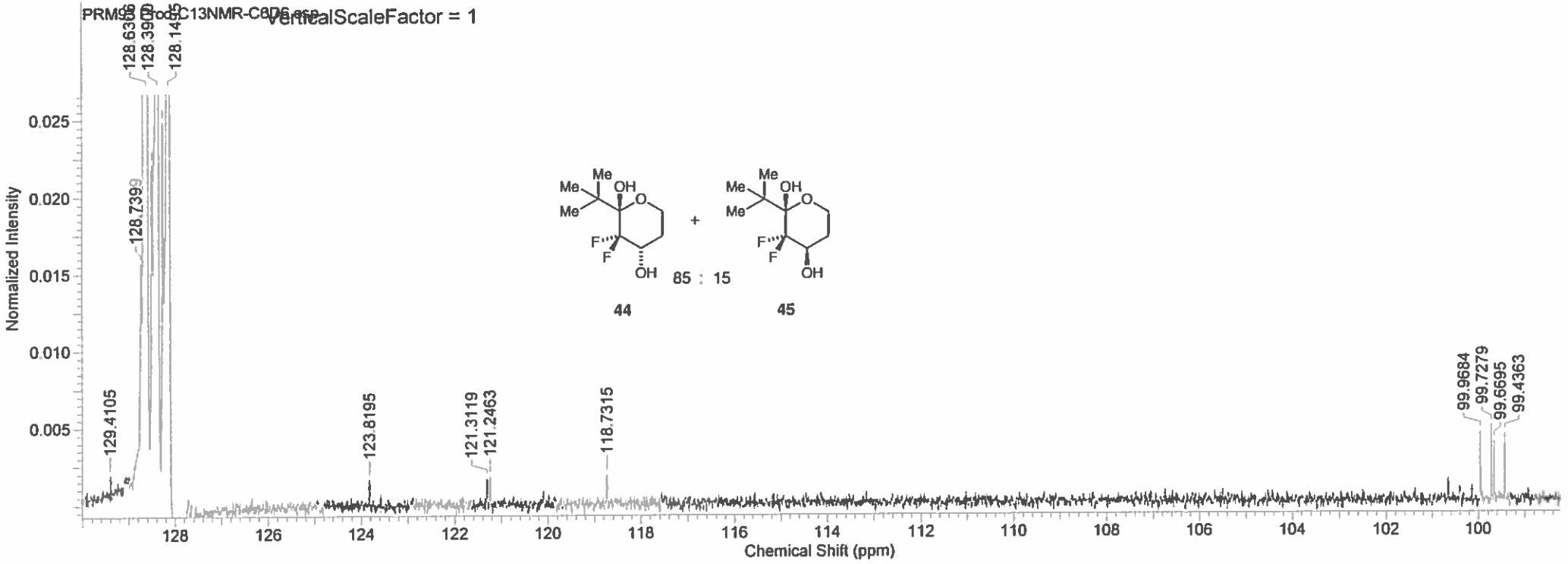
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	12000	*Origin*	AV400_S
Original Points Count	32768	*Owner*	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	2050.00	*SW(cyclical) (Hz)*	24038.46	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	10119.6650
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	21.000		



44 45

No.	(ppm)	(Hz)	Height
1	26.14	2630.8	0.0291
2	26.17	2633.7	0.0362
3	26.21	2637.4	0.0290
4	26.45	2661.6	0.0085
5	26.48	2664.5	0.0096
6	32.26	3246.2	0.0127

No.	(ppm)	(Hz)	Height
7	32.31	3252.1	0.0121
8	39.96	4021.7	0.0109
9	58.65	5902.6	0.0272
10	67.78	6821.1	0.0091
11	68.00	6843.1	0.0086
12	68.21	6864.3	0.0088

No.	(ppm)	(Hz)	Height
13	99.44	10007.1	0.0043
14	99.67	10030.5	0.0039
15	99.73	10036.4	0.0049
16	99.97	10060.6	0.0045
17	118.73	11948.9	0.0019
18	121.25	12202.0	0.0018

No.	(ppm)	(Hz)	Height
19	121.31	12208.6	0.0017
20	123.82	12460.9	0.0016
21	128.15	12896.7	0.9836
22	128.27	12909.2	0.0249
23	128.39	12920.9	1.0000
24	128.51	12932.6	0.0222

No.	(ppm)	(Hz)	Height
25	128.63	12945.1	0.9943
26	128.74	12956.1	0.0157
27	129.41	13023.6	0.0020

EJT-PRM93 Prod crystals CD2Cl2
m19F CD2Cl2 /opt/oldbruk500data.11vii11/2013/Sep ejt 23

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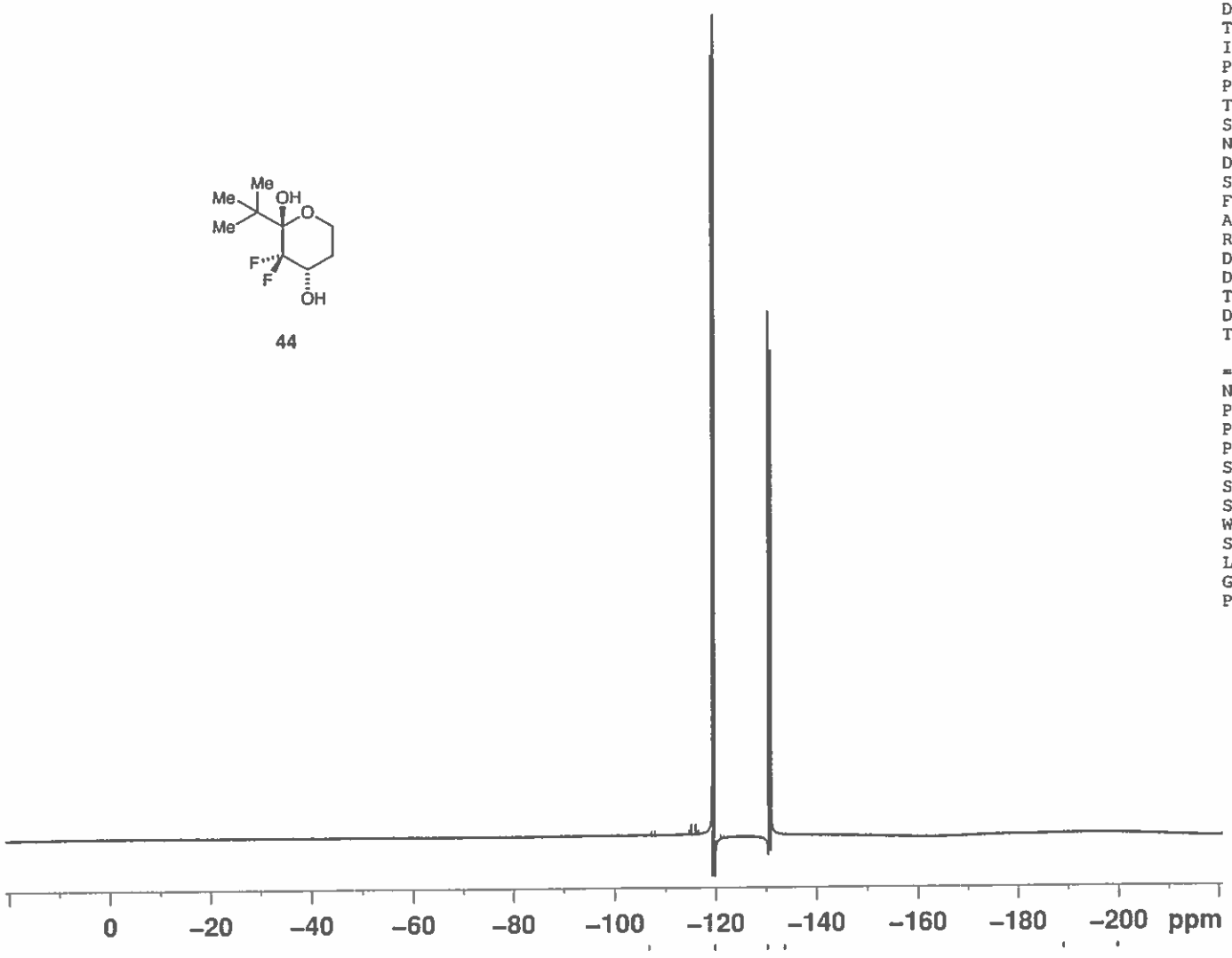
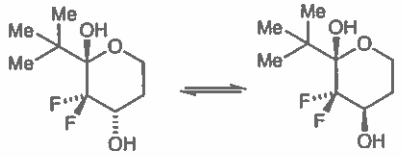


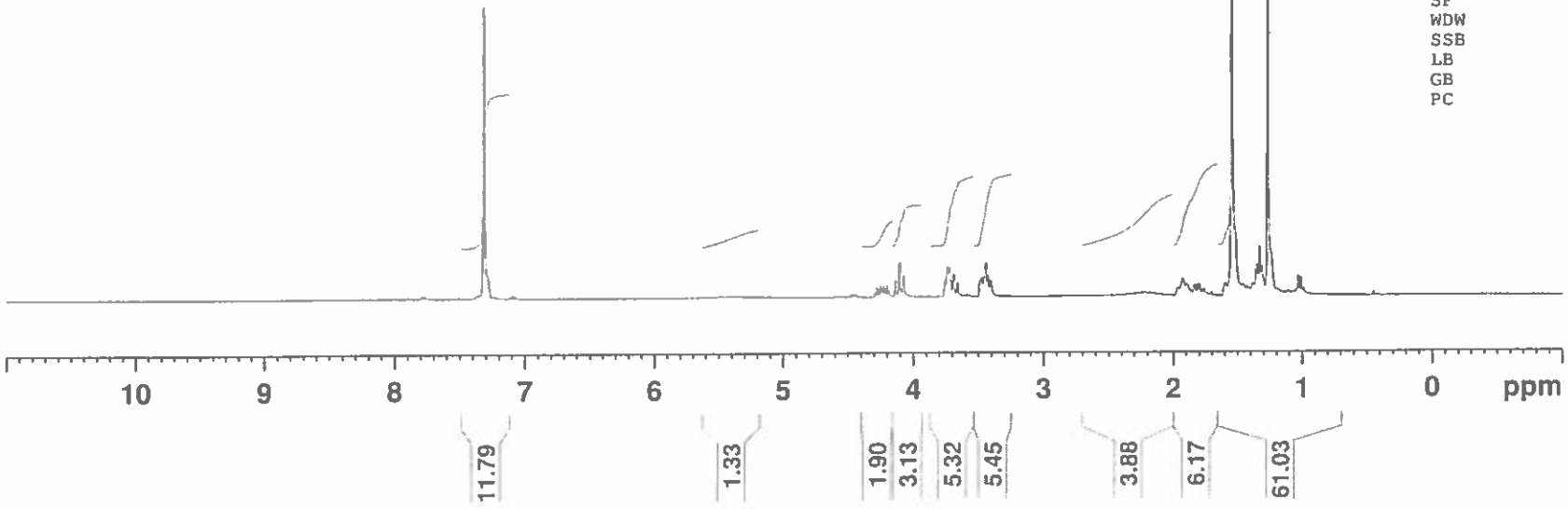
NAME	2013-09-10-ejt-23	
EXPNO	11	
PROCNO	1	
Date_	20130910	
Time	14.54	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgflqn	
TD	131072	
SOLVENT	CD2Cl2	
NS	16	
DS	4	
SWH	113636.367	Hz
FIDRES	0.866977	Hz
AQ	0.5767668	sec
RG	28.5	
DW	4.400	usec
DE	6.50	usec
TE	300.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	17.50	usec
PL1	-2.90	dB
PL1W	48.97788239	W
SFO1	470.5453180	MHz
SI	65536	
SF	470.5923770	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

EJT-PRM93 Prod crystals in C6D6 2*o/n
mPROTON C6D6 {e:\bruk400data\2013\Sep} ejt 17



44 45

NAME	2013-09-12-ejt-17
EXPNO	10
PROCNO	1
Date_	20130912
Time	10.13
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	C6D6
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	114
DW	60.500 usec
DE	8.45 usec
TE	293.3 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	1H
P1	14.50 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



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Date	12 Sep 2013 06:00:48	*Date Stamp*	12 Sep 2013 06:00:48				
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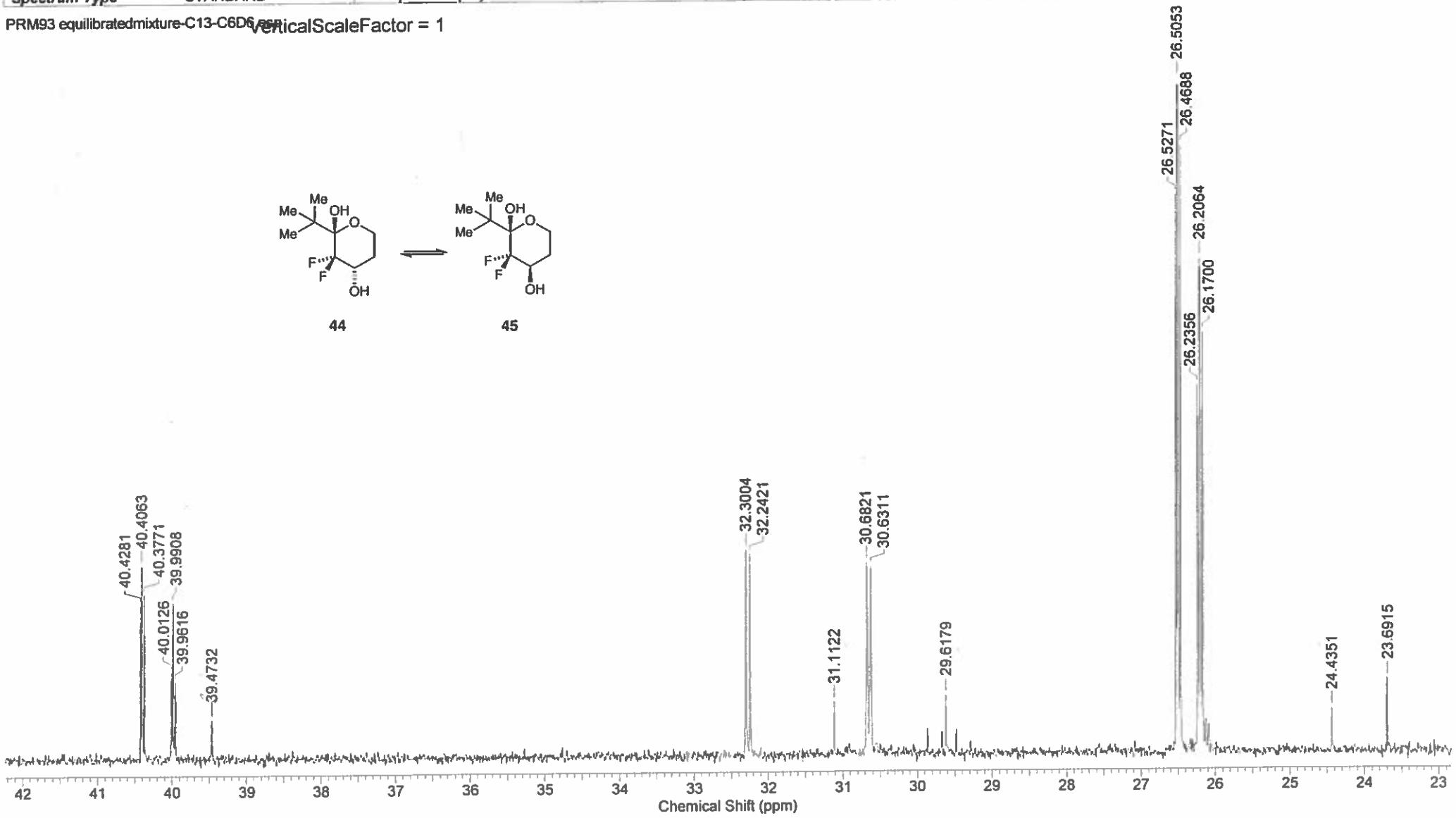
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	12000	*Origin*	AV400_S
Original Points Count	32768	*Owner*	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	2050.00	*SW(cyclical) (Hz)*	24038.46	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	10119.6650
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	18.900		

PRM93 equilibratedmixture-C13-C6D6.esp verticalScaleFactor = 1

44 45



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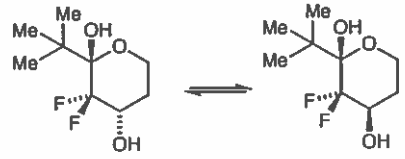
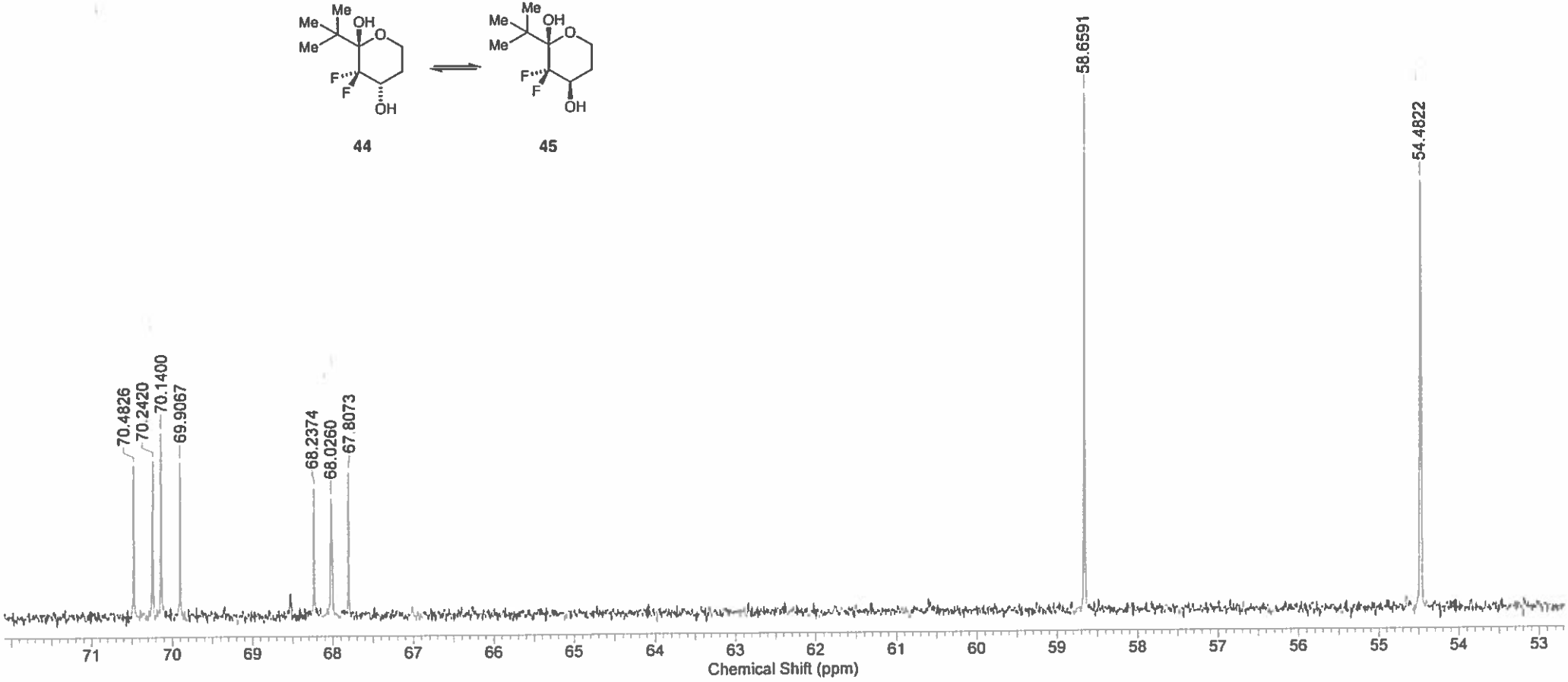
Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM93 Prod crystals mCARBON C6D6 {E:\bruk400service_data\2013\Sep} Administrator 10				
Date	12 Sep 2013 06:00:48	*Date Stamp*	12 Sep 2013 06:00:48				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-11-Administrator-10\10\fid						
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*	BENZENE-d6	*Spectrum Offset (Hz)*	10119.6650
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	18.900		

PRM93 equilibratedmixture-C13-C6D6.esp VerticalScaleFactor = 1



44

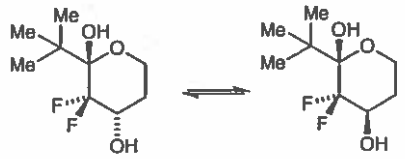
45



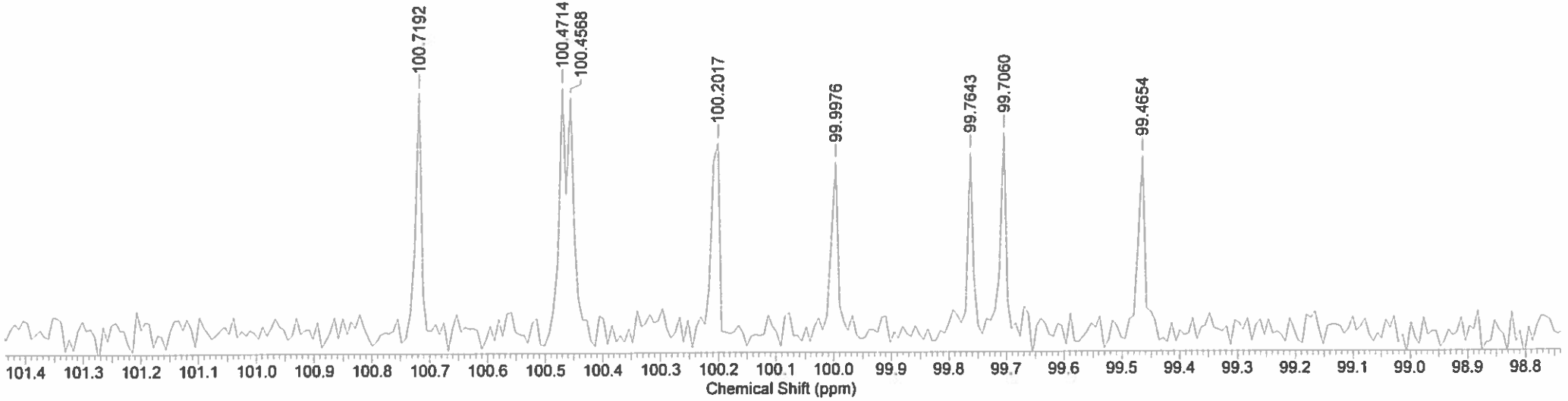
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM93 Prod crystals mCARBON C6D6 (E:\bruk400service_data\2013\Sep) Administrator 10				
Date	12 Sep 2013 06:00:48	*Date Stamp*	12 Sep 2013 06:00:48				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-11-Administrator-10\10\fid						
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*	BENZENE-d6	*Spectrum Offset (Hz)*	10119.6650
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	18.900		

PRM93 equilibratedmixture-C13-C6D6.esp



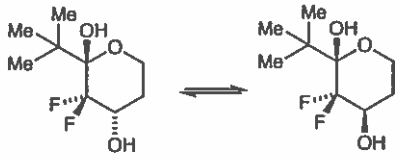
44 45



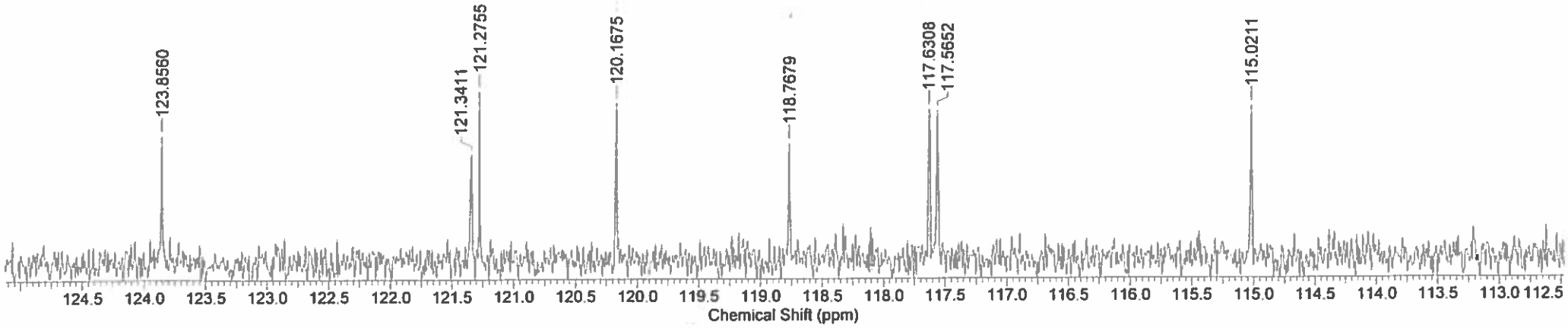
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM93 Prod crystals mCARBON C6D6 (E:\bruk400service_data\2013\Sep) Administrator 10				
Date	12 Sep 2013 06:00:48	*Date Stamp*	12 Sep 2013 06:00:48				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-11-Administrator-10\10\fid						
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*	BENZENE-d6	*Spectrum Offset (Hz)*	10119.6650
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	18.900		

PRM93 equilibratedmixture-C13-C6D6.esp

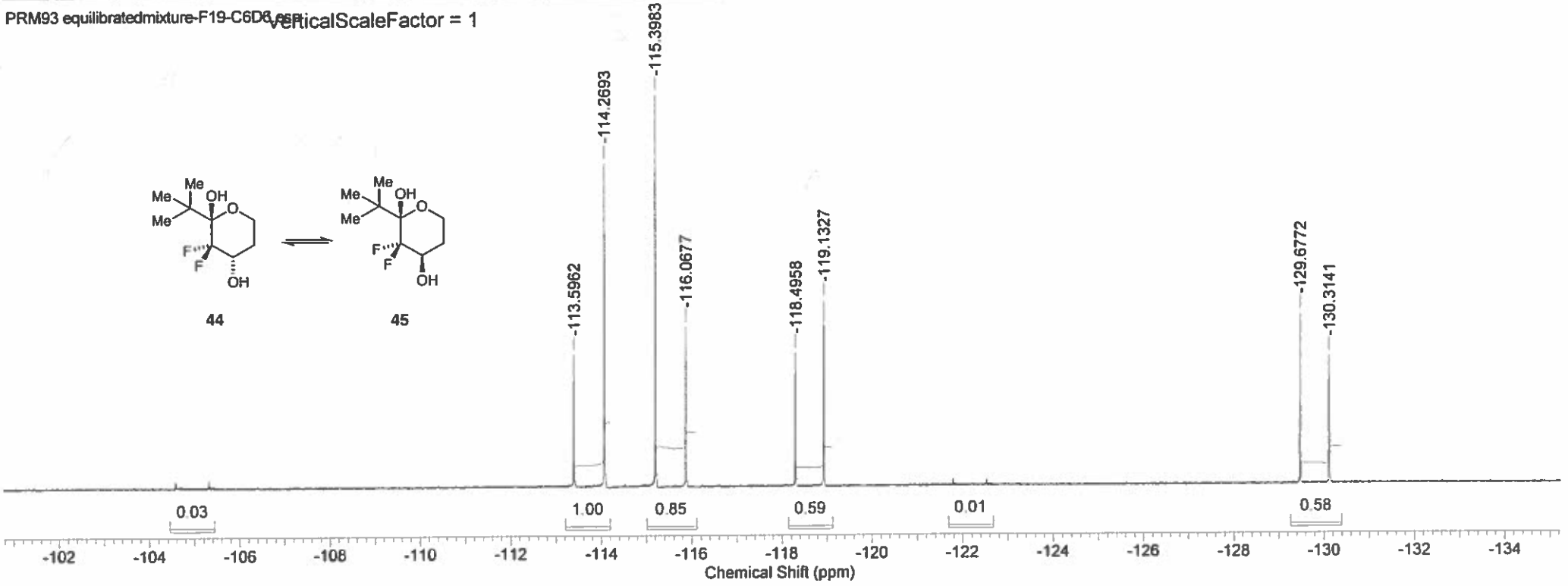


44 45



Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM93 Prod crystals in C6D6 2*o/n mF19CPD C6D6 {e:\bruk400data\2013\Sep} ejt 17				
Date	12 Sep 2013 10:14:40	*Date Stamp*	12 Sep 2013 10:14:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2013\Sep\data\ejt\nmr\2013-09-12-ejt-17\11\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	Administrator	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	4100.00
SW(cyclical) (Hz)	89285.71	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	20.500				

PRM93 equilibratedmixture-F19-C6D6.esp VerticalScaleFactor = 1

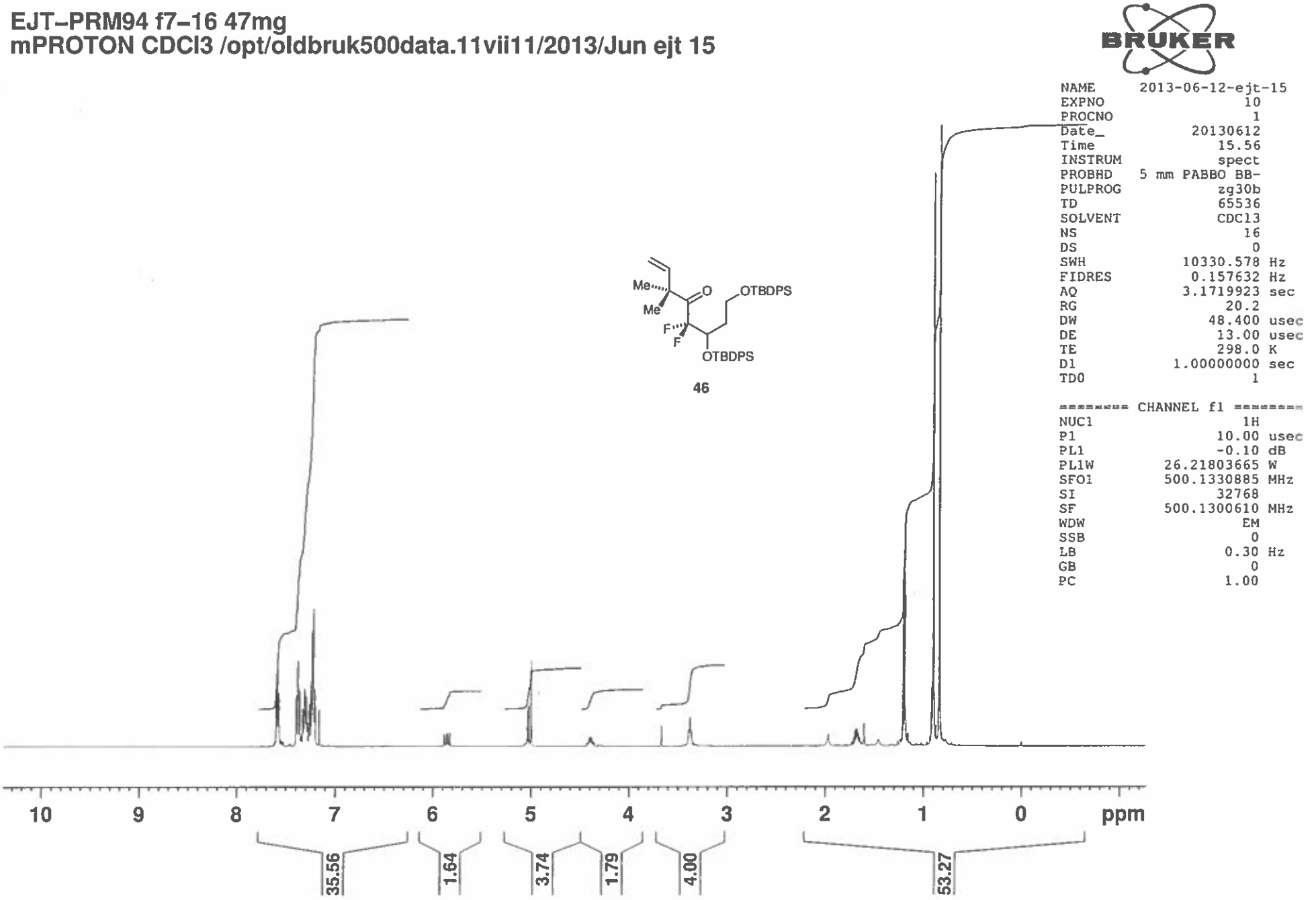


44

45

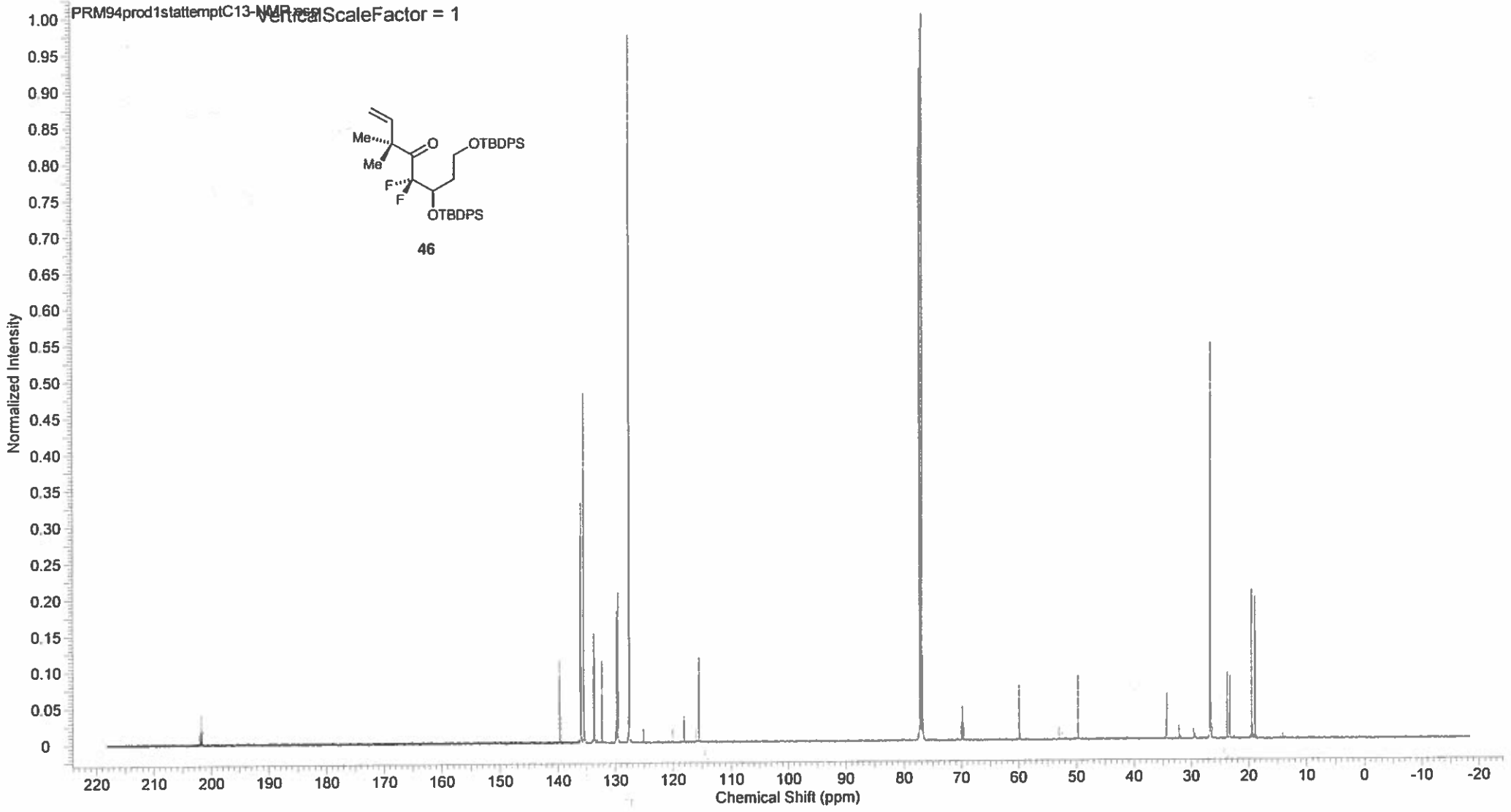
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	5932 .. -129	0.57895821	1.36767340e+7	0.57895821
2	3756 .. -121	0.00921777	2.17751453e+5	0.00921777
3	3266 .. -118	0.59456044	1.40453060e+7	0.59456044
4	3128 .. -115	0.84520292	1.99662340e+7	0.84520292
5	3975 .. -113	1.00384212	2.37137700e+7	1.00384212
6	5377 .. -104	0.02603587	6.15045438e+5	0.02603587

EJT–PRM94 f7–16 47mg
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2013/Jun ejt 15



26/07/2013 11:08:37

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM94 Prod data mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2013/Jun ejt 15				
Date	13 Jun 2013 04:54:40	*Date Stamp*	13 Jun 2013 04:54:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\JUN\DATA\EJT\NMR\2013-06-12-EJT-15\20\PDATA\1\1R						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	3072	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.1670
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	25.029		



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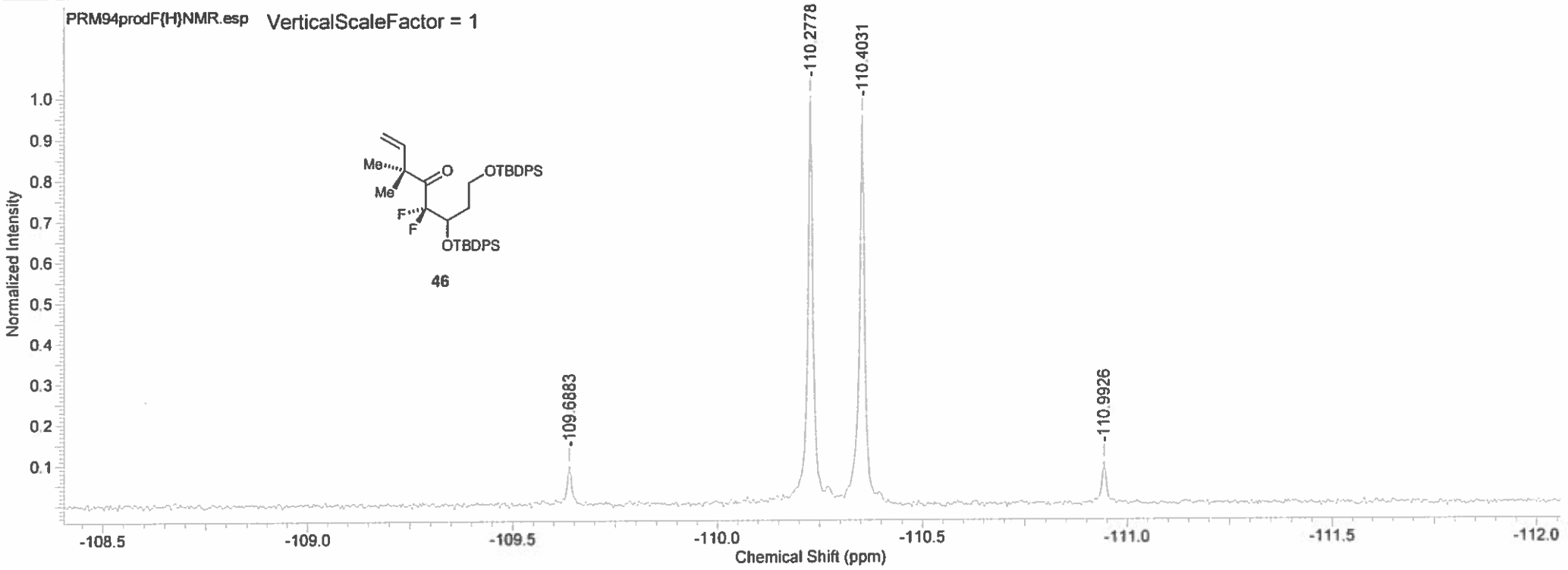
29/05/2014 15:09:13

Acquisition Time (sec)	0.5767	*Comment*	ETJ-PRM94 prod fracs 354mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2013/Aug ejt 1				
Date	24 Aug 2013 18:04:00	*Date Stamp*	24 Aug 2013 18:04:00				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500data\bruk500data\2013\Aug\data\ejt\nmr\2013-08-24-ejt-1\12\fid					*Frequency (MHz)*	470.59
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn	*Receiver Gain*	32.00
SW(cyclical) (Hz)	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	113634.63	*Temperature (degree C)*	27.000				

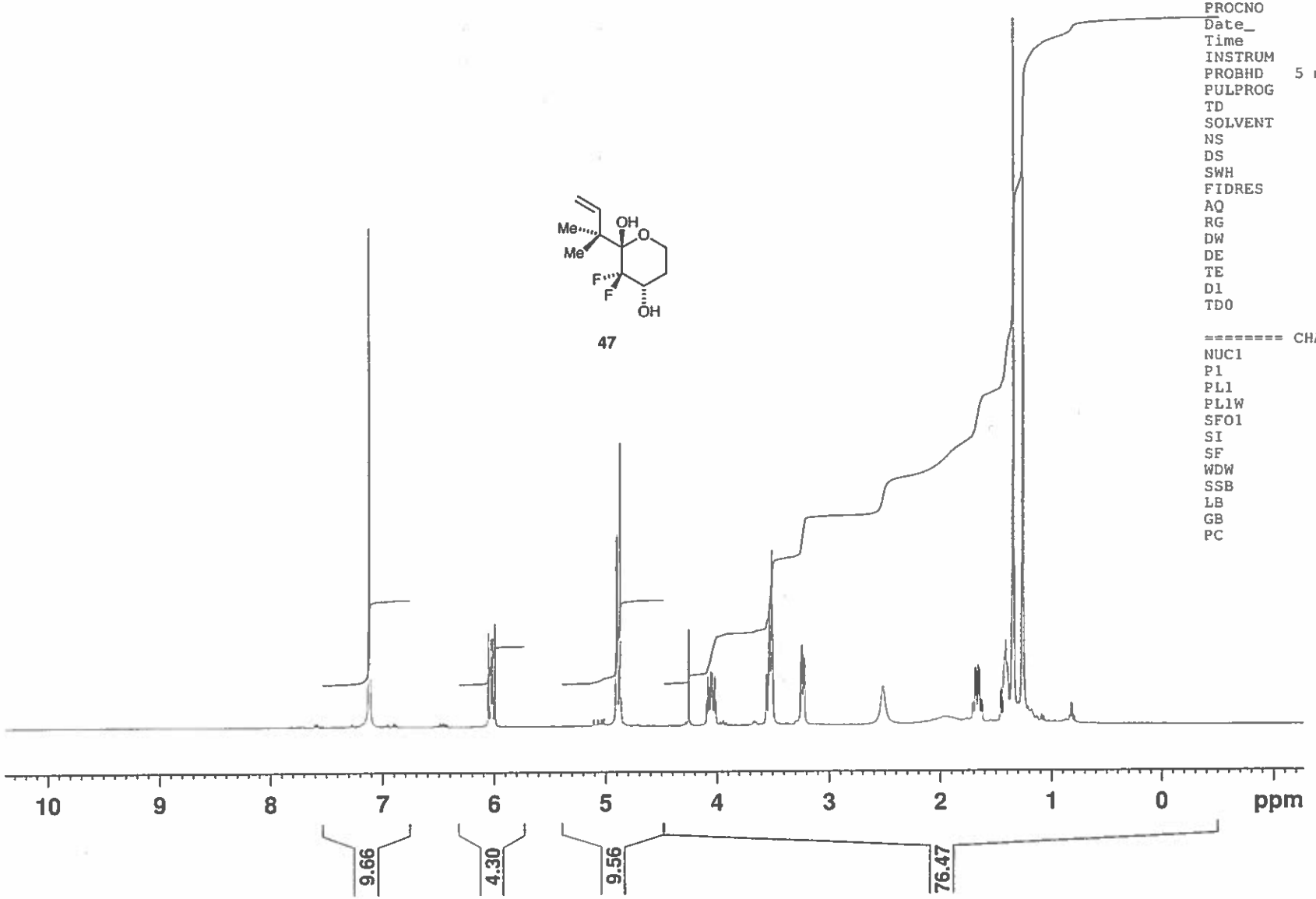


46

No.	(ppm)	(Hz)	Height
1	-110.99	-52232.3	0.1008
2	-110.40	-51954.8	0.9523
3	-110.28	-51895.9	1.0000
4	-109.69	-51618.5	0.0963

EJT-PRM95 Product data
mPROTON C6D6 /opt/oldbruk500data.11vii11/2013/Sep ejt 11

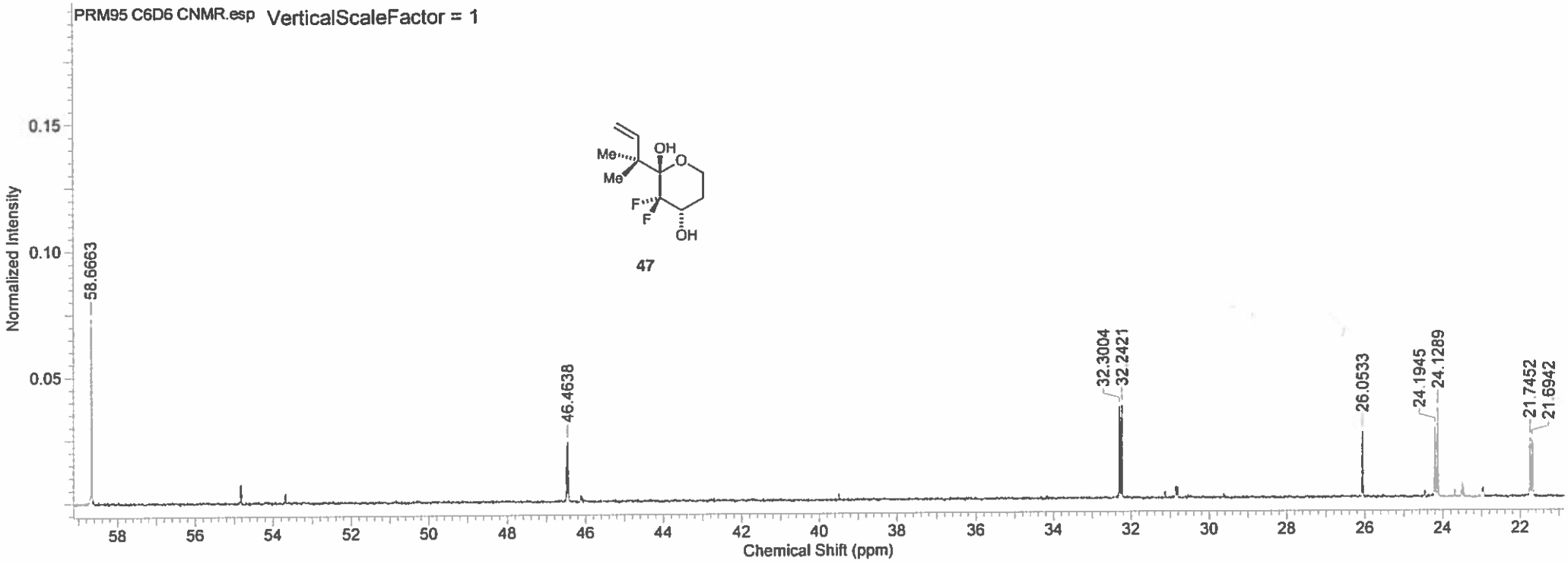
47



NAME	2013-09-20-ejt-11
EXPNO	10
PROCNO	1
Date_	20130920
Time	10.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	C6D6
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	22.6
DW	48.400 usec
DE	13.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300778 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

23/09/2013 18:37:19

Acquisition Time (sec)	1.3631	*Comment*	P Mears 0913-081 ejt-prm95 prod xtals mCARBON C6D6 {E:\bruk400service_data\2013\Sep} Administrator 13				
Date	20 Sep 2013 10:46:40	*Date Stamp*	20 Sep 2013 10:46:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-20-Administrator-13\11\fid						
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	6144	*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*	BENZENE-d6	*Spectrum Offset (Hz)*	10120.3975
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	21.700		

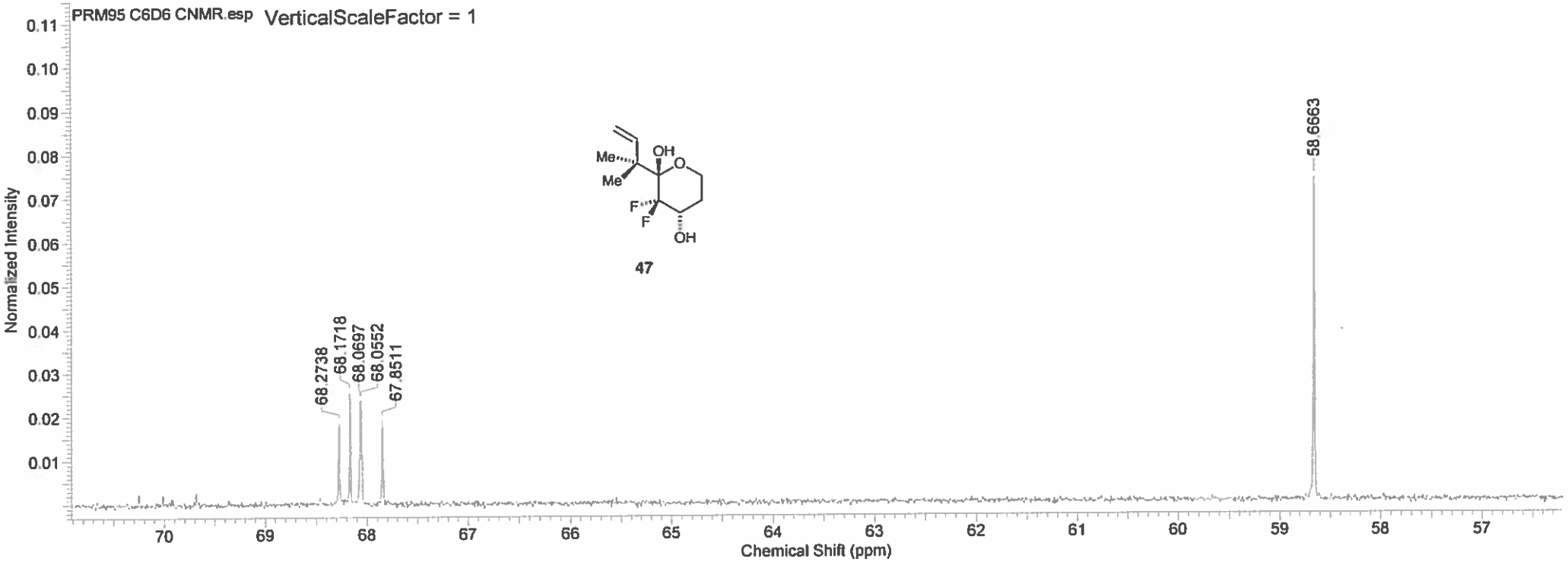


47

No.	(ppm)	(Hz)	Height
1	21.69	2183.3	0.0226
2	21.75	2188.4	0.0232
3	24.13	2428.3	0.0351
4	24.19	2434.9	0.0275
5	26.05	2622.0	0.0258
6	32.24	3244.8	0.0365
7	32.30	3250.6	0.0363
8	46.46	4676.0	0.0235
9	58.67	5904.1	0.0736

23/09/2013 18:40:51

Acquisition Time (sec)	1.3631	*Comment*	P Mears 0913-081 ejt-prm95 prod xtals mCARBON C6D6 {E:\bruk400service_data\2013\Sep} Administrator 13				
Date	20 Sep 2013 10:46:40	*Date Stamp*	20 Sep 2013 10:46:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-20-Administrator-13\11\fid						
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	6144	*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*	BENZENE-d6	*Spectrum Offset (Hz)*	10120.3975
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	21.700		



47

No.	(ppm)	(Hz)	Height
1	21.69	2183.3	0.0226
2	21.75	2188.4	0.0232
3	24.13	2428.3	0.0351

No.	(ppm)	(Hz)	Height
4	24.19	2434.9	0.0275
5	26.05	2622.0	0.0258
6	32.24	3244.8	0.0365

No.	(ppm)	(Hz)	Height
7	32.30	3250.6	0.0363
8	46.46	4676.0	0.0235
9	58.67	5904.1	0.0736

No.	(ppm)	(Hz)	Height
10	67.85	6828.4	0.0191
11	68.06	6848.9	0.0237
12	68.07	6850.4	0.0235

No.	(ppm)	(Hz)	Height
13	68.17	6860.7	0.0255
14	68.27	6870.9	0.0183

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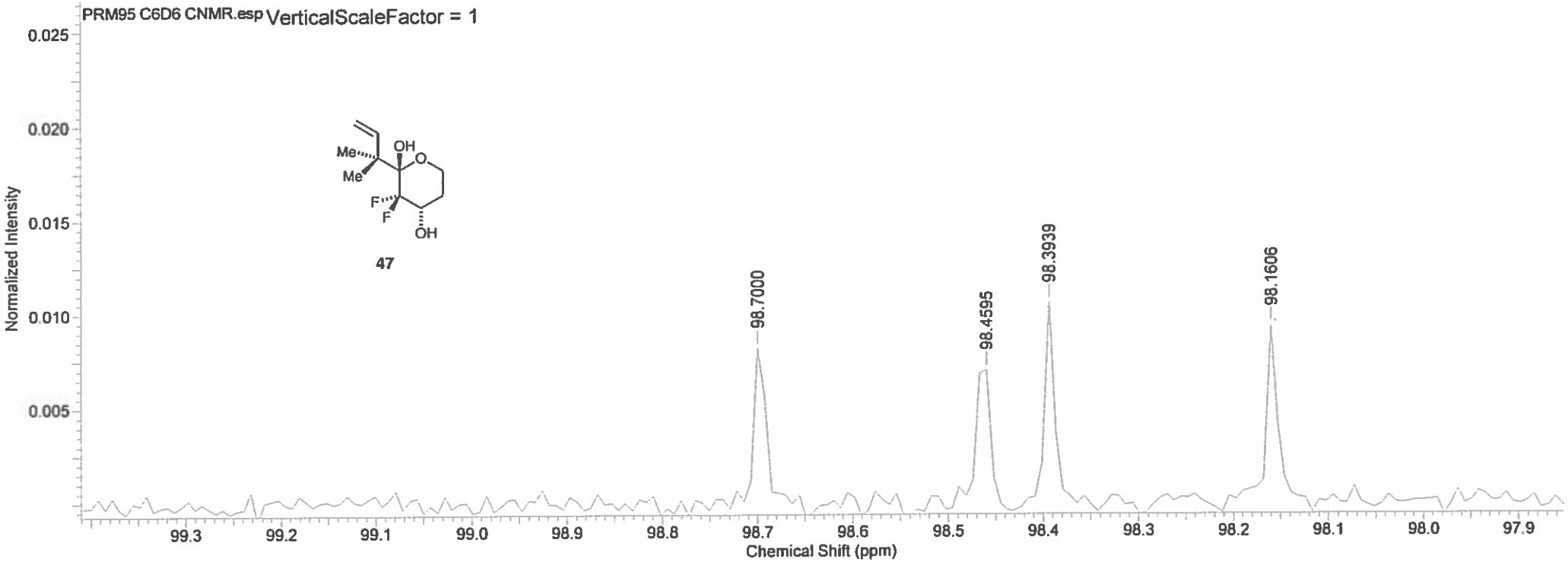
23/09/2013 18:43:57

Acquisition Time (sec)	1.3631	*Comment*	P Mears 0913-081 ejt-prm95 prod xtals mCARBON C6D6 {E:\bruk400service_data\2013\Sep} Administrator 13				
Date	20 Sep 2013 10:46:40	*Date Stamp*	20 Sep 2013 10:46:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-20-Administrator-13\11\fid						
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	6144	*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*	BENZENE-d6	*Spectrum Offset (Hz)*	10120.3975
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	21.700		



No.	(ppm)	(Hz)	Height
1	21.69	2183.3	0.0226
2	21.75	2188.4	0.0232
3	24.13	2428.3	0.0351
4	24.19	2434.9	0.0275

No.	(ppm)	(Hz)	Height
5	26.05	2622.0	0.0258
6	32.24	3244.8	0.0365
7	32.30	3250.6	0.0363
8	46.46	4676.0	0.0235

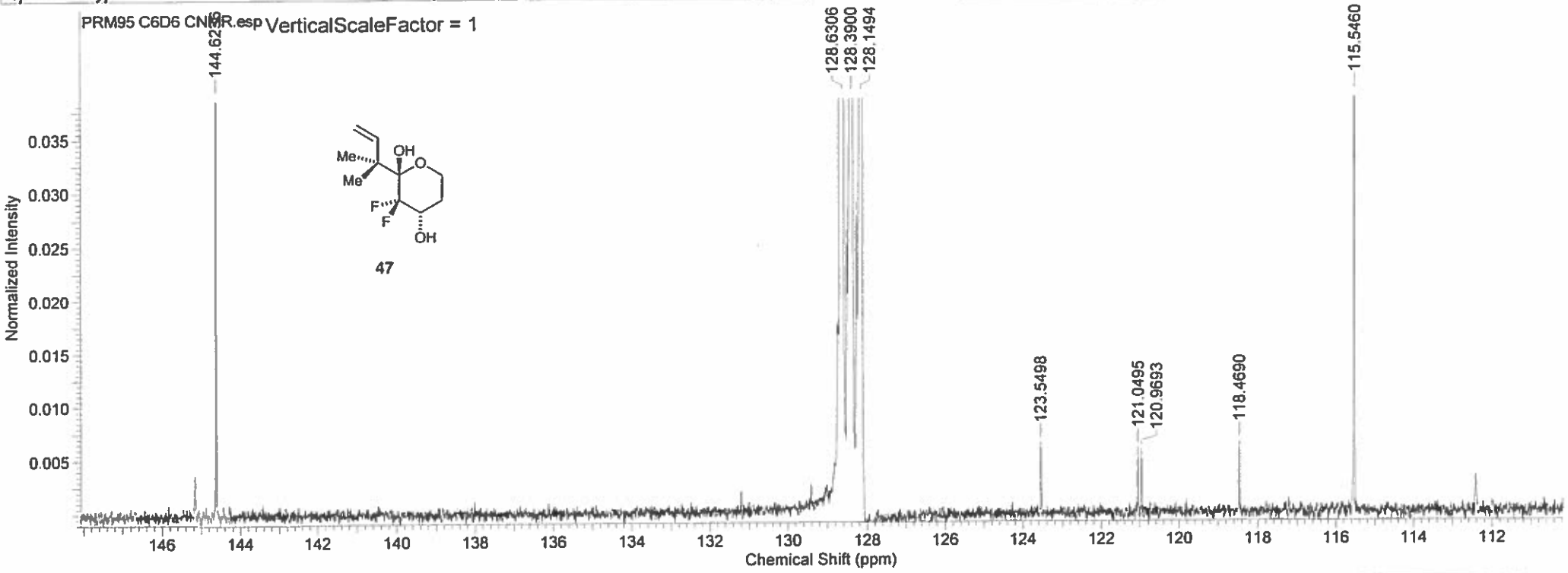
No.	(ppm)	(Hz)	Height
9	58.67	5904.1	0.0736
10	67.85	6828.4	0.0191
11	68.06	6848.9	0.0237
12	68.07	6850.4	0.0235

No.	(ppm)	(Hz)	Height
13	68.17	6860.7	0.0255
14	68.27	6870.9	0.0183
15	98.16	9878.7	0.0092
16	98.39	9902.2	0.0105

No.	(ppm)	(Hz)	Height
17	98.46	9908.8	0.0069
18	98.70	9933.0	0.0081

23/09/2013 18:46:37

Acquisition Time (sec)	1.3631	*Comment*	P Mears 0913-081 ejt-prm95 prod xtals mCARBON C6D6 (E:\bruk400service_data\2013\Sep) Administrator 13				
Date	20 Sep 2013 10:46:40	*Date Stamp*	20 Sep 2013 10:46:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400service_data\2013\Sep\data\Administrator\nmr\2013-09-20-Administrator-13\11\fid						
Frequency (MHz)	100.64	*Nucleus*	13C	*Number of Transients*	6144	*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*	BENZENE-d6	*Spectrum Offset (Hz)*	10120.3975
Spectrum Type	STANDARD	*Sweep Width (Hz)*	24037.73	*Temperature (degree C)*	21.700		



No.	(ppm)	(Hz)	Height
1	21.69	2183.3	0.0226
2	21.75	2188.4	0.0232
3	24.13	2428.3	0.0351
4	24.19	2434.9	0.0275
5	26.05	2622.0	0.0258
6	32.24	3244.8	0.0365

No.	(ppm)	(Hz)	Height
7	32.30	3250.6	0.0363
8	46.46	4676.0	0.0235
9	58.67	5904.1	0.0736
10	67.85	6828.4	0.0191
11	68.06	6848.9	0.0237
12	68.07	6850.4	0.0235

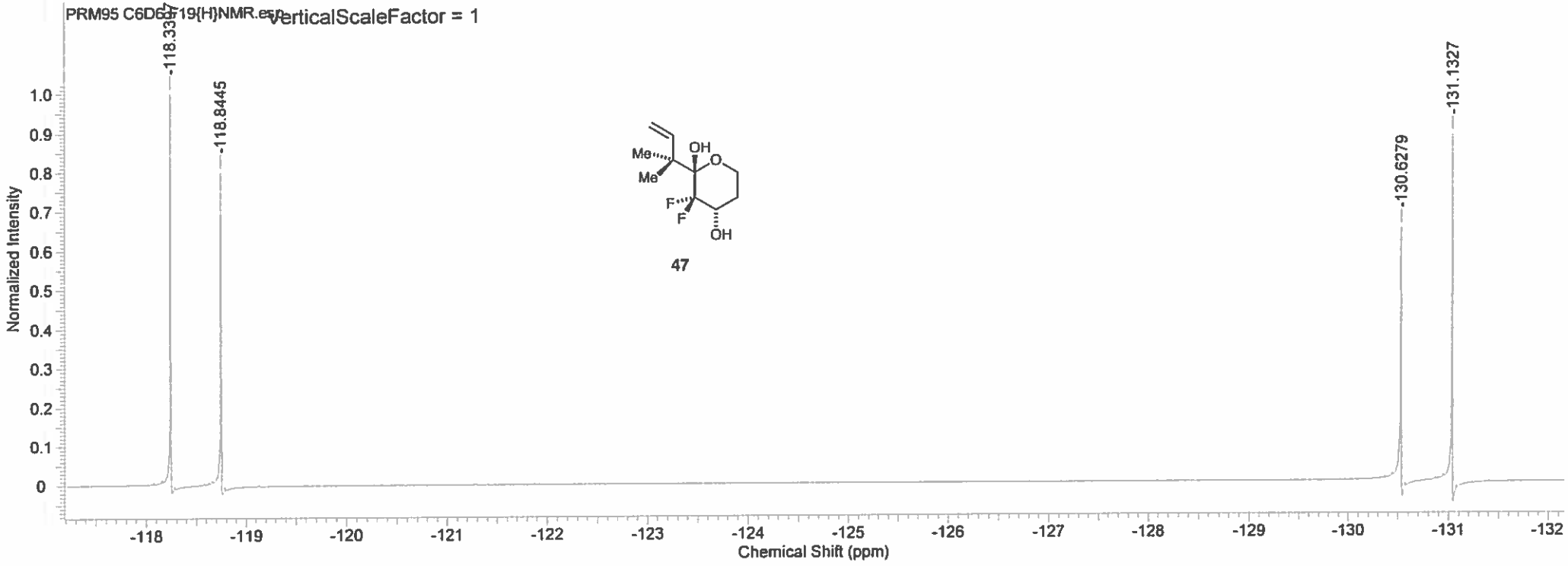
No.	(ppm)	(Hz)	Height
13	68.17	6860.7	0.0255
14	68.27	6870.9	0.0183
15	98.16	9878.7	0.0092
16	98.39	9902.2	0.0105
17	98.46	9908.8	0.0069
18	98.70	9933.0	0.0081

No.	(ppm)	(Hz)	Height
19	115.55	11628.3	0.0593
20	118.47	11922.5	0.0063
21	120.97	12174.1	0.0056
22	121.05	12182.2	0.0058
23	123.55	12433.8	0.0063
24	128.15	12896.7	0.9879

No.	(ppm)	(Hz)	Height
25	128.27	12909.2	0.0277
26	128.39	12920.9	1.0000
27	128.51	12932.6	0.0251
28	128.63	12945.1	0.9899
29	144.62	14554.6	0.0523

20/09/2013 11:40:52

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM95 Product data m19FCPD C6D6 /opt/oldbruk500data.11vii11/2013/Sep ejt 11				
Date	20 Sep 2013 10:40:16	*Date Stamp*	20 Sep 2013 10:40:16				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2013\SEP\DATA\EJT\NMR\2013-09-20-EJT-11\12\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn
Receiver Gain	32.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	27.000		



No.	(ppm)	(Hz)	Height
1	-131.13	-61710.1	0.8834
2	-130.63	-61472.5	0.6455
3	-118.84	-55927.3	0.7986
4	-118.34	-55689.8	1.0000

EJT–PRM95 prod crystals over weekend equilibrated
mPROTON C6D6 {e:\bruk400data\2013\Sep} ejt 37

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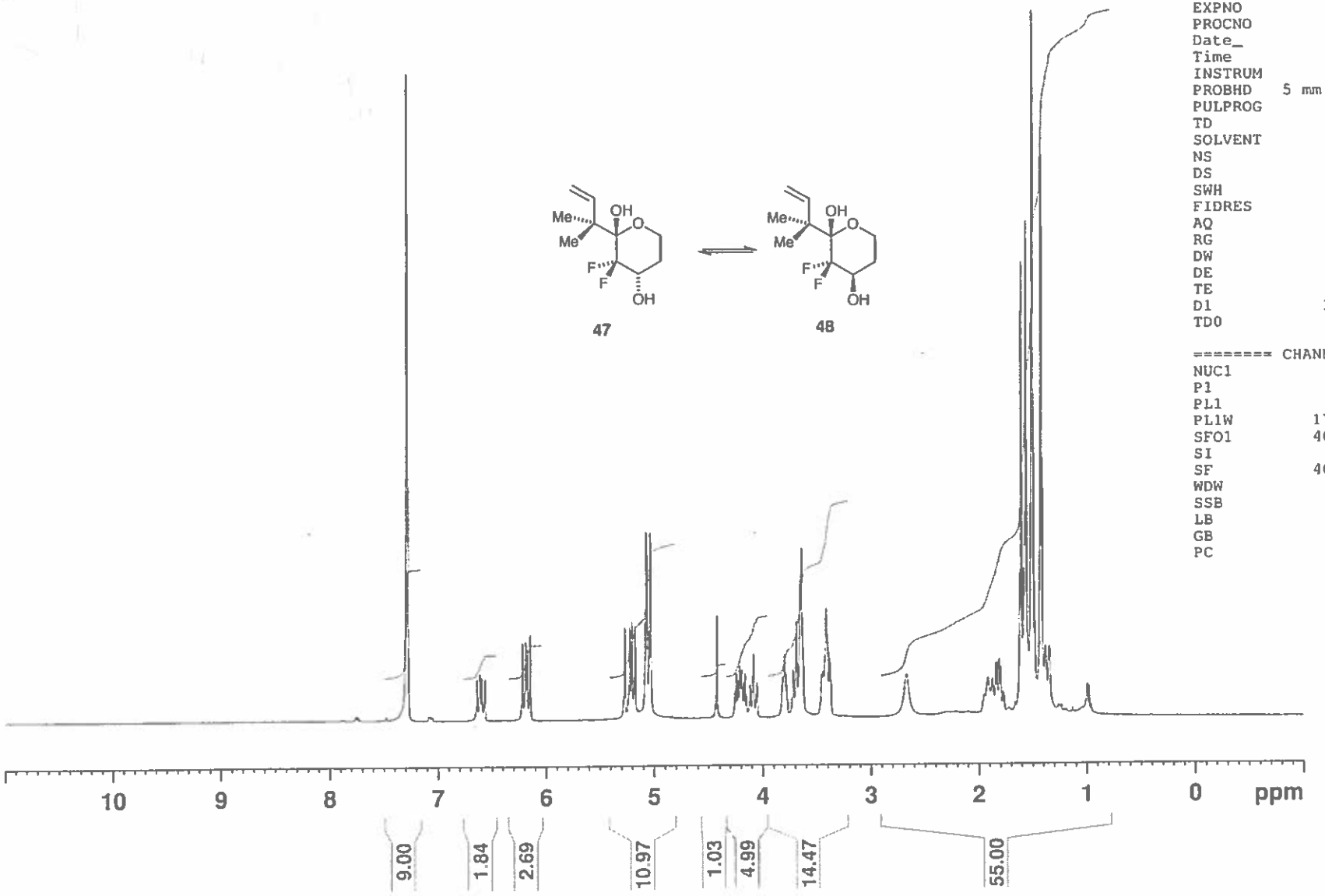
NAME	2013-09-23-ejt-37
EXPNO	10
PROCNO	1
Date_	20130923
Time	11.40
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	C6D6
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	101
DW	60.500 usec
DE	8.45 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 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



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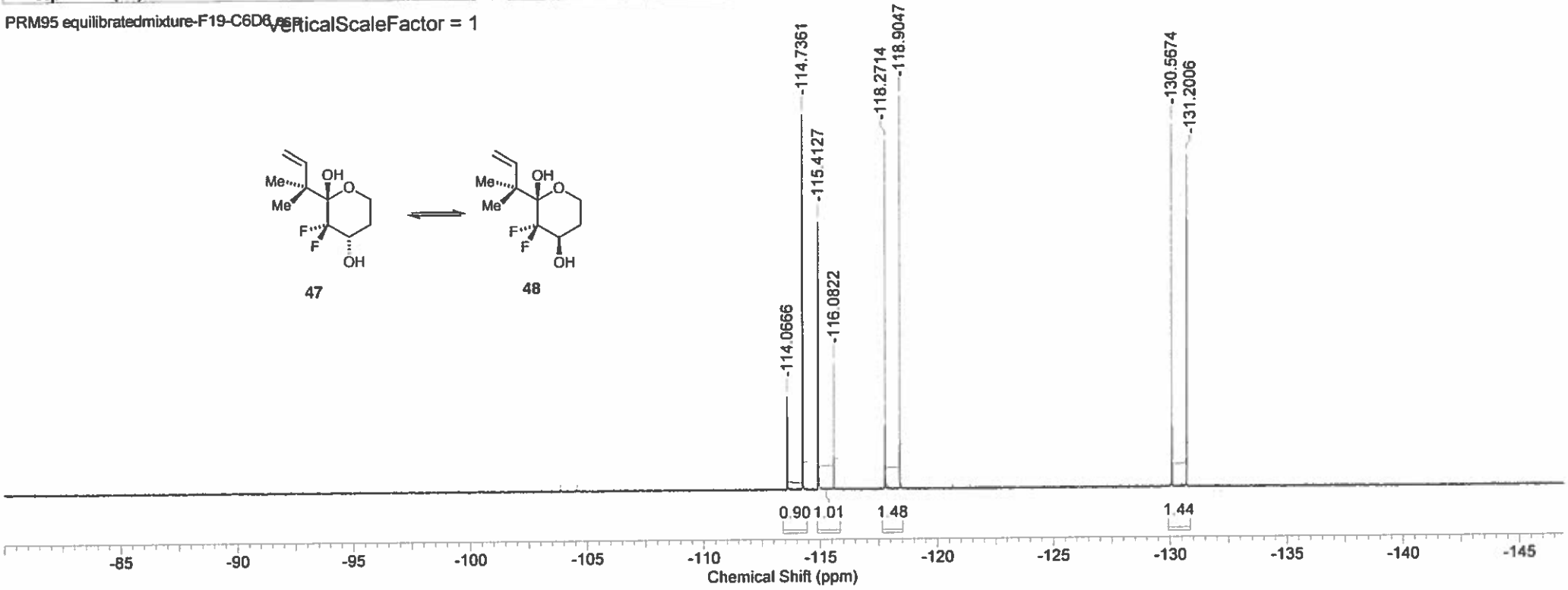
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM95 prod crystals over weekend equilibrated mF19CPD C6D6 (e:\bruk400data\2013\Sep) ejt 37				
Date	23 Sep 2013 11:42:08	*Date Stamp*	23 Sep 2013 11:42:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400data\2013\Sep\data\ejt\nmr\2013-09-23-ejt-37\11\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	Administrator	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	4100.00
SW(cyclical) (Hz)	89285.71	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	22.300				

PRM95 equilibratedmixture-F19-C6D6.esp VerticalScaleFactor = 1

47

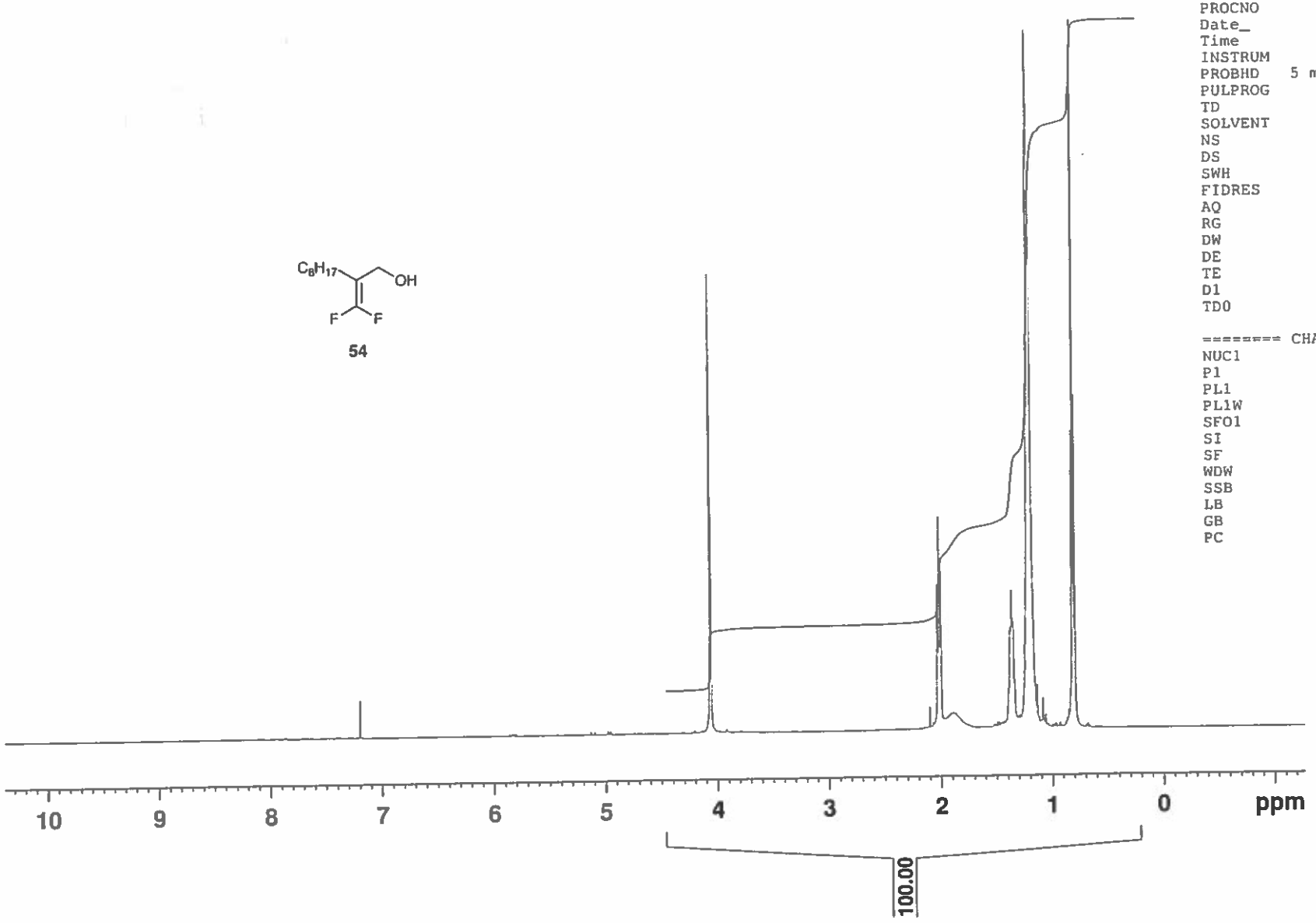
48



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	3493 .. -130	1.44295704	2.36217000e+7	1.44295704
2	0336 .. -116	1.48149800	2.42526280e+7	1.48149800
3	2540 .. -115	1.00809872	1.65029200e+7	1.00809872
4	9284 .. -113	0.89820582	1.47039360e+7	0.89820582

EJT–PRM115 product data allylic alcohol
mPROTONnight CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 3

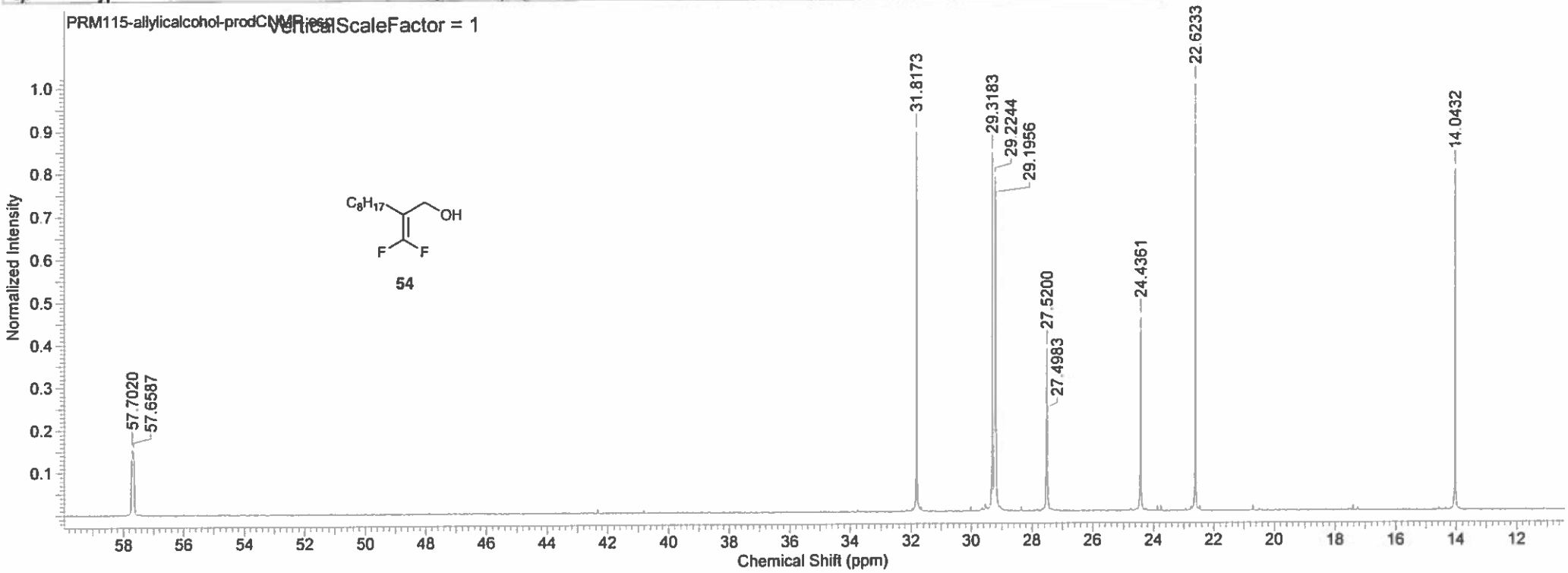
54



NAME	2014-01-12-ejt-3	
EXPNO	11	
PROCNO	1	
Date_	20140112	
Time	17.54	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30b	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	0	
SWH	10330.578	Hz
FIDRES	0.157632	Hz
AQ	3.1719923	sec
RG	16	
DW	48.400	usec
DE	13.00	usec
TE	300.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-0.10	dB
PL1W	26.21803665	W
SFO1	500.1330885	MHz
SI	32768	
SF	500.1300437	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

15/01/2014 15:51:49

Acquisition Time (sec)	1.1010	***Comment***	EJT-PRM115 product data allylic alcohol mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 3				
Date	12 Jan 2014 17:50:56	***Date Stamp***	12 Jan 2014 17:50:56				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\JAN\DATA\EJT\NMR\2014-01-12-EJT-3\10\PDATA\1\1R						
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	3072	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12571.1670
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	20.099		



No.	(ppm)	(Hz)	Height
1	14.04	1766.0	0.7988
2	22.62	2845.1	1.0000
3	24.44	3073.0	0.4542

No.	(ppm)	(Hz)	Height
4	27.50	3458.1	0.2238
5	27.52	3460.9	0.3816
6	29.20	3671.6	0.7282

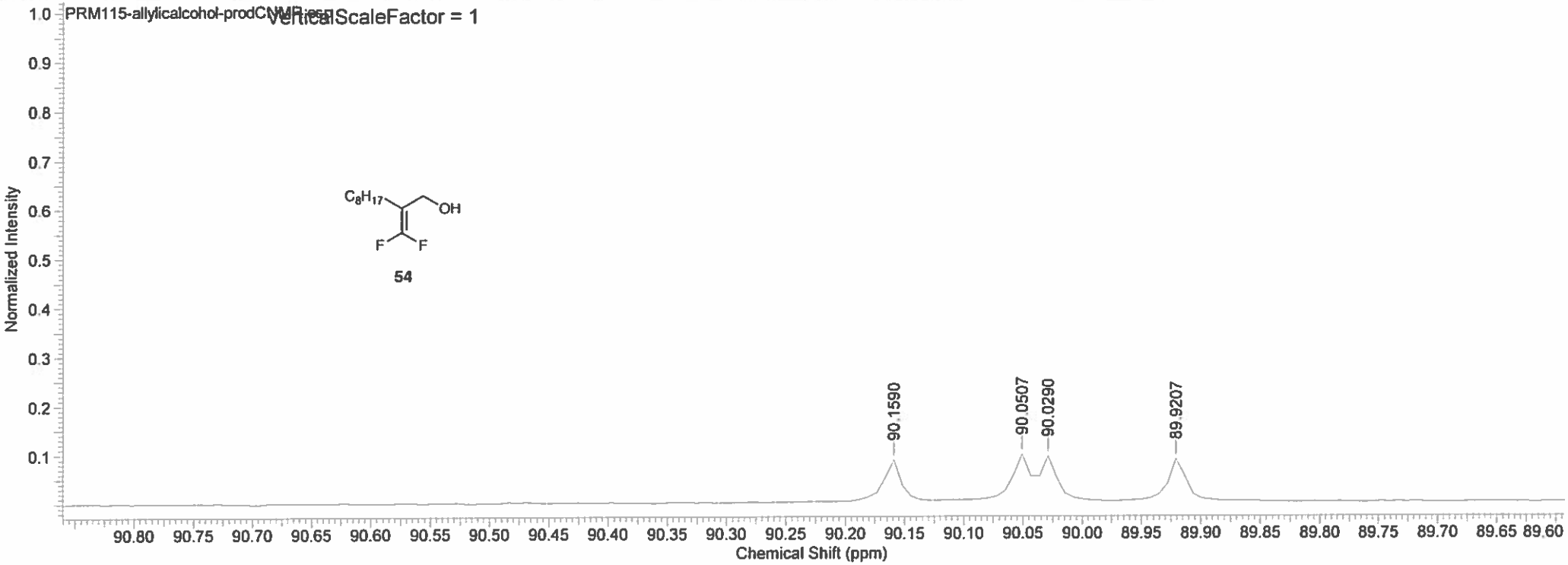
No.	(ppm)	(Hz)	Height
7	29.22	3675.2	0.7842
8	29.32	3687.0	0.8407
9	31.82	4001.3	0.8907

No.	(ppm)	(Hz)	Height
10	57.66	7251.0	0.1504
11	57.70	7256.5	0.1568

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

15/01/2014 15:52:04

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM115 product data allylic alcohol mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 3				
Date	12 Jan 2014 17:50:56	*Date Stamp*	12 Jan 2014 17:50:56				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\JAN\DATA\EJT\NMR\2014-01-12-EJT-3\10\PDATA\1\1R						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	3072	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.1670
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	20.099		



No.	(ppm)	(Hz)	Height
1	14.04	1766.0	0.7988
2	22.62	2845.1	1.0000
3	24.44	3073.0	0.4542

No.	(ppm)	(Hz)	Height
4	27.50	3458.1	0.2238
5	27.52	3460.9	0.3816
6	29.20	3671.6	0.7282

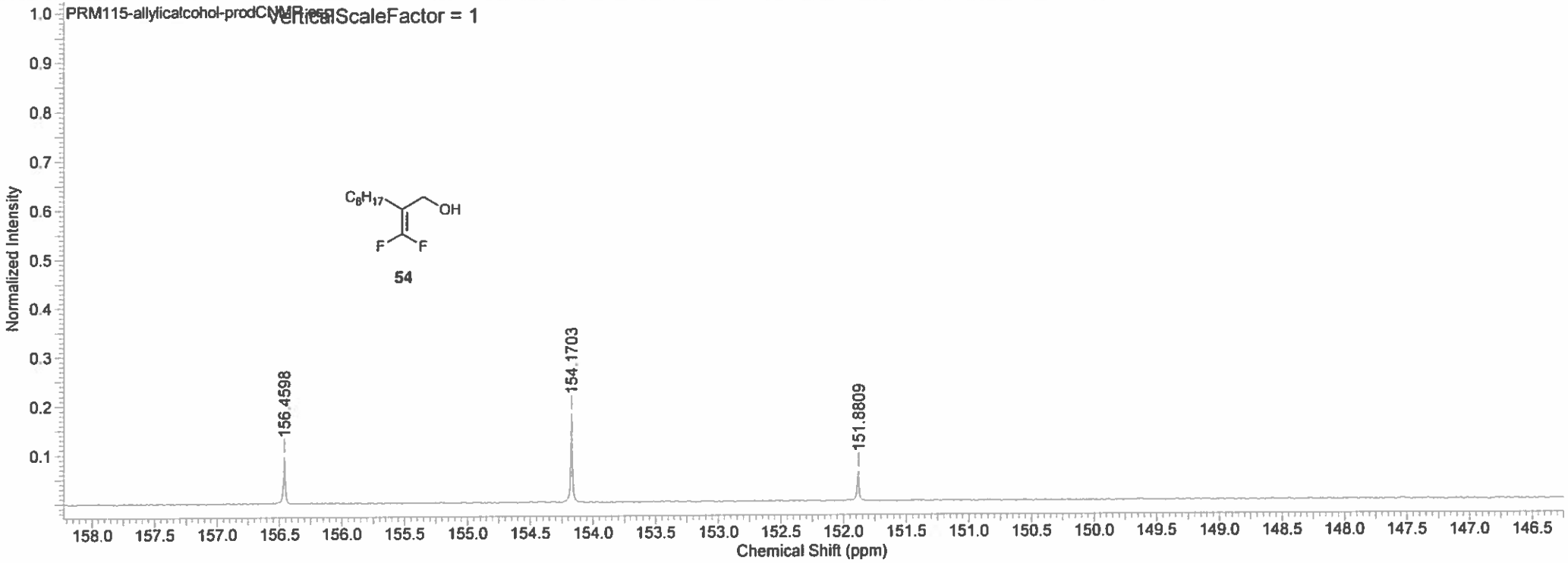
No.	(ppm)	(Hz)	Height
7	29.22	3675.2	0.7842
8	29.32	3687.0	0.8407
9	31.82	4001.3	0.8907

No.	(ppm)	(Hz)	Height
10	57.66	7251.0	0.1504
11	57.70	7256.5	0.1568
12	89.92	11308.2	0.0872

No.	(ppm)	(Hz)	Height
13	90.03	11321.9	0.0938
14	90.05	11324.6	0.0980
15	90.16	11338.2	0.0866

15/01/2014 15:52:22

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM115 product data allylic alcohol mCARBONnight CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 3				
Date	12 Jan 2014 17:50:56	*Date Stamp*	12 Jan 2014 17:50:56				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\JAN\DATA\EJT\NMR\2014-01-12-EJT-3\10\PDATA\1\1R						
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	3072	*Origin*	spect
Original Points Count	32768	*Owner*	vnmr1	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	512.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.1670
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	20.099		



54

No.	(ppm)	(Hz)	Height
1	14.04	1766.0	0.7988
2	22.62	2845.1	1.0000
3	24.44	3073.0	0.4542
4	27.50	3458.1	0.2238

No.	(ppm)	(Hz)	Height
5	27.52	3460.9	0.3816
6	29.20	3671.6	0.7282
7	29.22	3675.2	0.7842
8	29.32	3687.0	0.8407

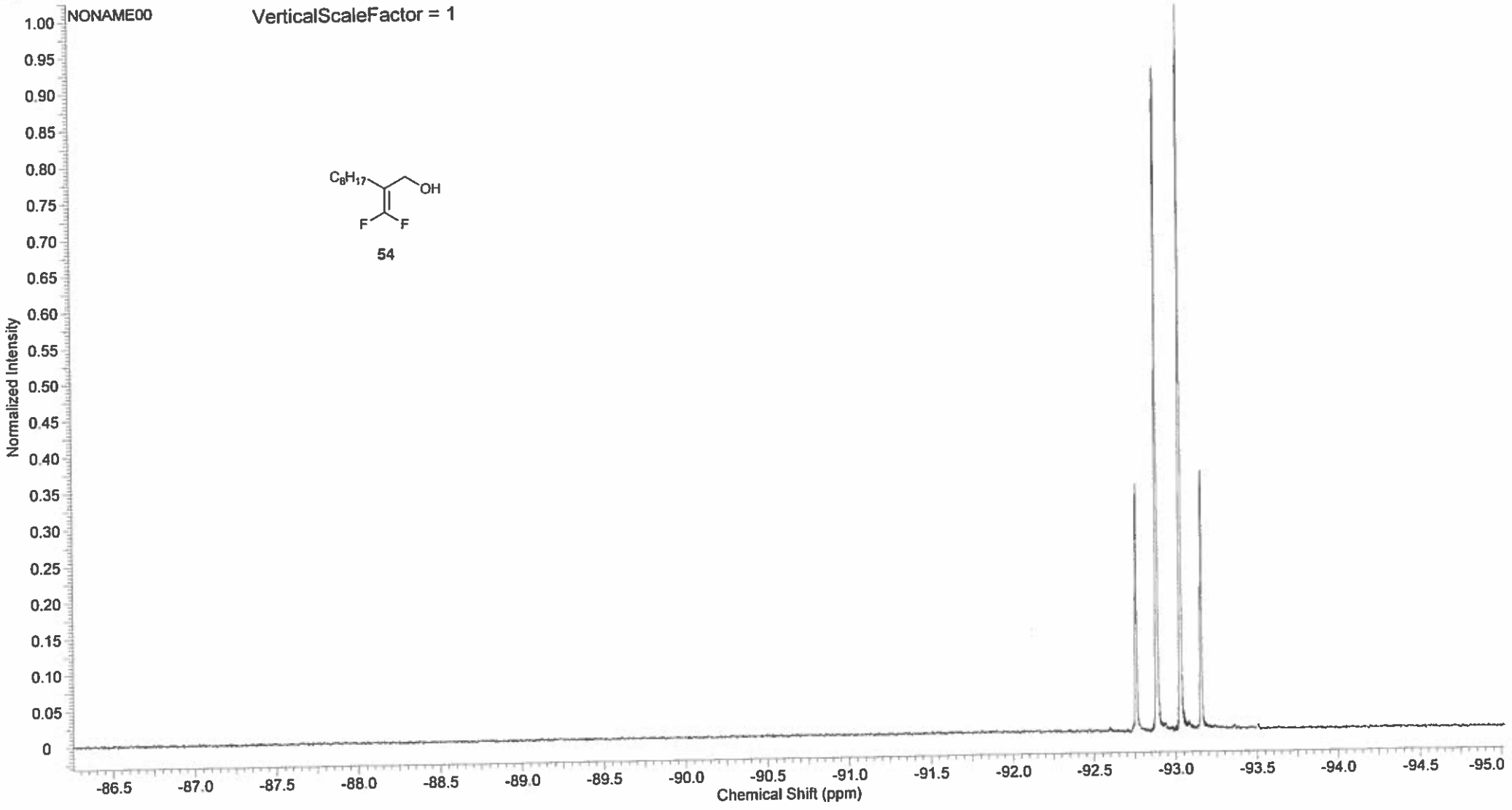
No.	(ppm)	(Hz)	Height
9	31.82	4001.3	0.8907
10	57.66	7251.0	0.1504
11	57.70	7256.5	0.1568
12	89.92	11308.2	0.0872

No.	(ppm)	(Hz)	Height
13	90.03	11321.9	0.0938
14	90.05	11324.6	0.0980
15	90.16	11338.2	0.0866
16	151.88	19100.2	0.0602

No.	(ppm)	(Hz)	Height
17	154.17	19388.1	0.1808
18	156.46	19676.0	0.0960

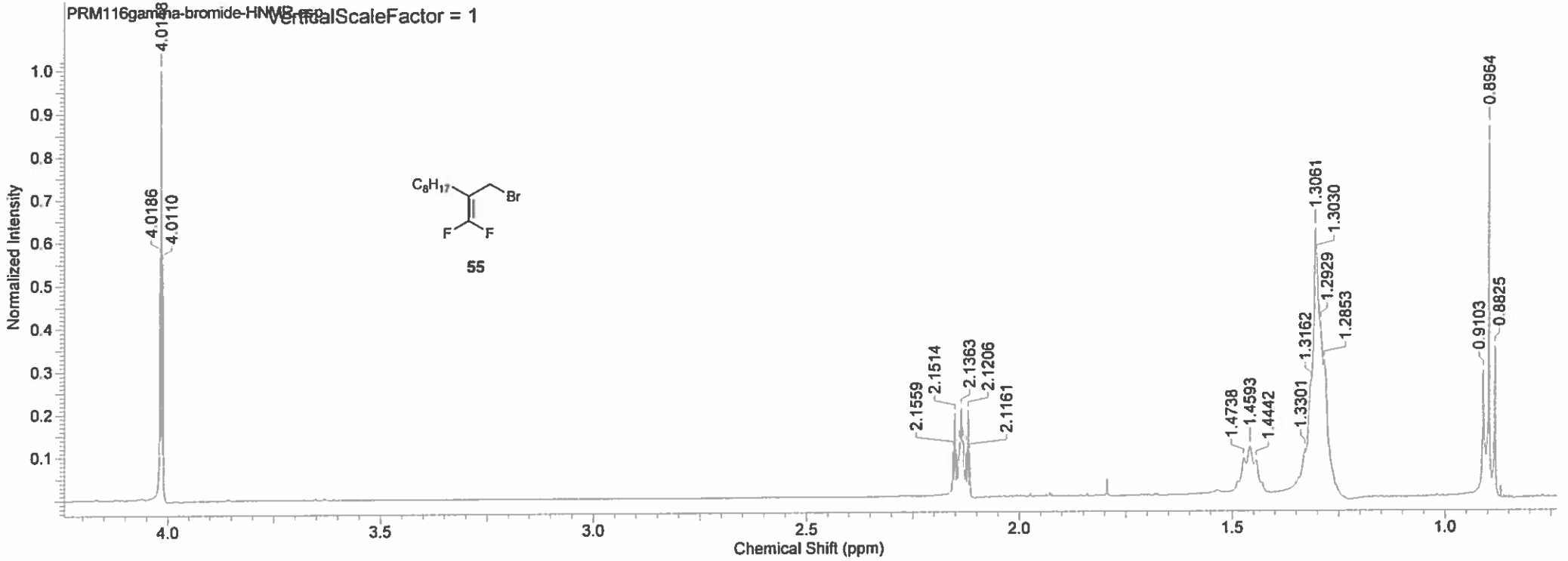
19/12/2013 12:59:59

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM115E prod fracs 94mg mF19CPD CDCl3 (e:\bruk400data\2013\Dec) ejt 9				
Date	18 Dec 2013 12:50:08	*Date Stamp*	18 Dec 2013 12:50:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2013\DEC\DATA\EJT\NMR\2013-12-18-EJT-9\11\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	20.700		



20/01/2014 16:07:15

Acquisition Time (sec)	3.1719	*Comment*	EJT-PRM116 gamma-bromide data mPROTONnight CDCl3 (F:\bruk500_b_data\2014\Jan) ejt 15				
Date	13 Jan 2014 16:08:32	*Date Stamp*	13 Jan 2014 16:08:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500bdata\2014\Jan\data\ejt\nmr\2014-01-13-ejt-15\10\fid					*Frequency (MHz)*	500.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	20.20
SW(cyclical) (Hz)	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3079.6614	*Spectrum Type*	STANDARD
Sweep Width (Hz)	10330.26	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	0.88	441.4	0.3473
2	0.90	448.3	0.8616
3	0.91	455.2	0.2924
4	1.29	642.8	0.3156
5	1.29	646.6	0.4054

No.	(ppm)	(Hz)	Height
6	1.30	651.7	0.5638
7	1.31	653.2	0.6235
8	1.32	658.3	0.2676
9	1.33	665.2	0.1092
10	1.44	722.3	0.0831

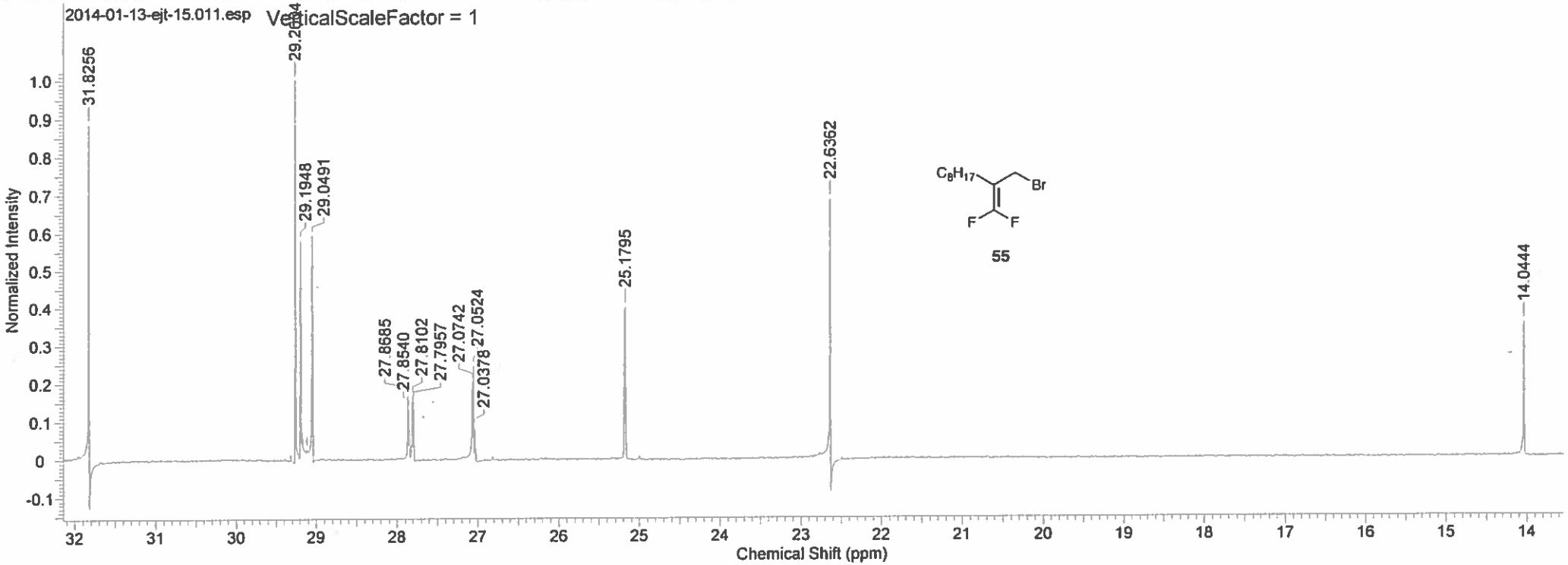
No.	(ppm)	(Hz)	Height
11	1.46	729.8	0.1155
12	1.47	737.1	0.0883
13	2.12	1058.3	0.1030
14	2.12	1060.6	0.2010
15	2.12	1062.8	0.1131

No.	(ppm)	(Hz)	Height
16	2.13	1066.2	0.1312
17	2.13	1067.2	0.1312
18	2.14	1068.4	0.2079
19	2.14	1070.6	0.1279
20	2.15	1073.8	0.1106

No.	(ppm)	(Hz)	Height
21	2.15	1076.0	0.1937
22	2.16	1078.2	0.1086
23	4.01	2006.0	0.5535
24	4.01	2007.9	1.0000
25	4.02	2009.8	0.5684

15/01/2014 10:25:12

Acquisition Time (sec)	1.0912	*Comment*	EJT-PRM116 gamma-bromide data mCARBONnight CDCl3 (F:\bruk500_b_data\2014\Jan) ejt 15				
Date	13 Jan 2014 20:50:08	*Date Stamp*	13 Jan 2014 20:50:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500bdata\2014\Jan\data\ejt\nmr\2014-01-13-ejt-15\11\fid					*Frequency (MHz)*	125.76
Nucleus	13C	*Number of Transients*	3096	*Origin*	spect	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	4597.60
SW(cyclical) (Hz)	30030.03	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12574.2715	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	14.04	1766.2	0.3511
2	22.64	2846.7	0.6830
3	25.18	3166.5	0.4006
4	27.04	3400.2	0.0841
5	27.05	3402.0	0.2455

No.	(ppm)	(Hz)	Height
6	27.07	3404.8	0.2039
7	27.80	3495.5	0.1549
8	27.81	3497.4	0.1686
9	27.85	3502.9	0.1310
10	27.87	3504.7	0.1670

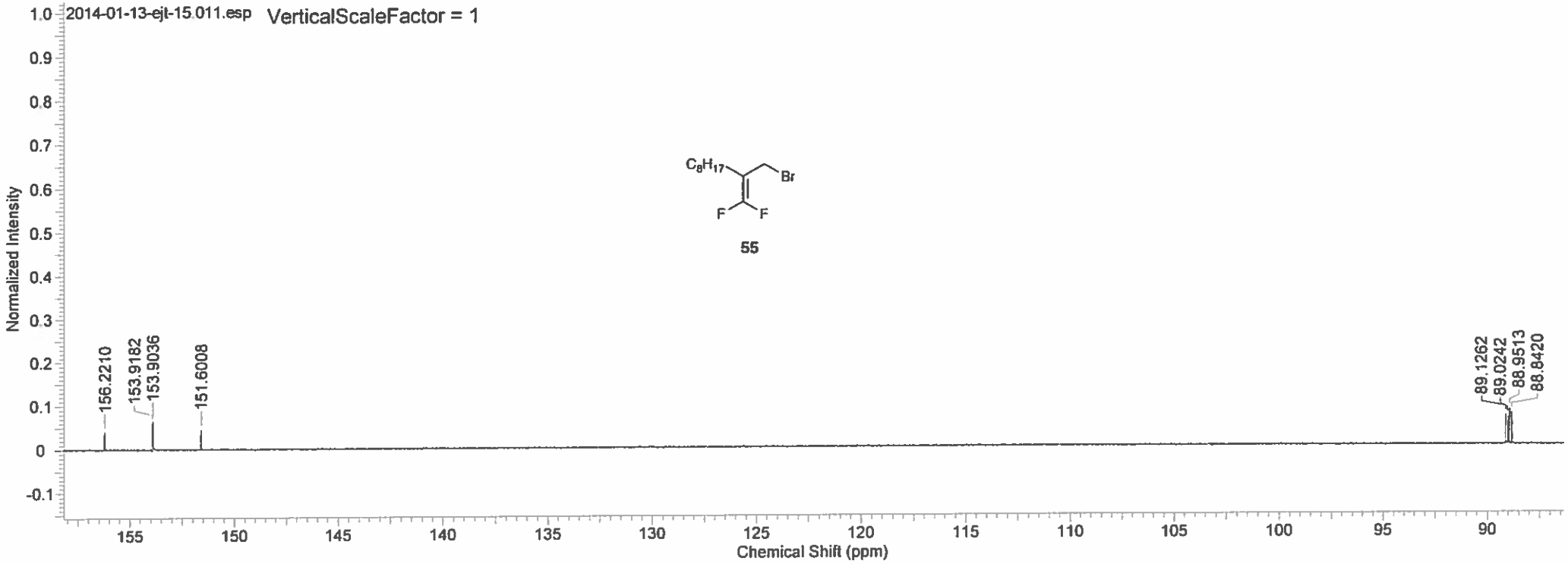
No.	(ppm)	(Hz)	Height
11	29.05	3653.1	0.5937
12	29.11	3661.4	0.0268
13	29.19	3671.5	0.5800
14	29.26	3679.7	1.0000
15	31.83	4002.3	0.8875

No.	(ppm)	(Hz)	Height
16	88.84	11172.6	0.0722
17	88.95	11186.3	0.0809
18	89.02	11195.5	0.0630
19	89.13	11208.3	0.0664
20	151.60	19065.0	0.0455

No.	(ppm)	(Hz)	Height
21	153.90	19354.6	0.0672
22	153.92	19356.4	0.0605
23	156.22	19646.0	0.0411

15/01/2014 10:24:55

Acquisition Time (sec)	1.0912	*Comment*	EJT-PRM116 gamma-bromide data mCARBONnight CDCl3 {F:\bruk500_b_data\2014\Jan} ejt 15				
Date	13 Jan 2014 20:50:08	*Date Stamp*	13 Jan 2014 20:50:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500bdata\2014\Jan\data\ejt\nmr\2014-01-13-ejt-15\11\fid					*Frequency (MHz)*	125.76
Nucleus	13C	*Number of Transients*	3096	*Origin*	spect	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	4597.60
SW(cyclical) (Hz)	30030.03	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12574.2715	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				



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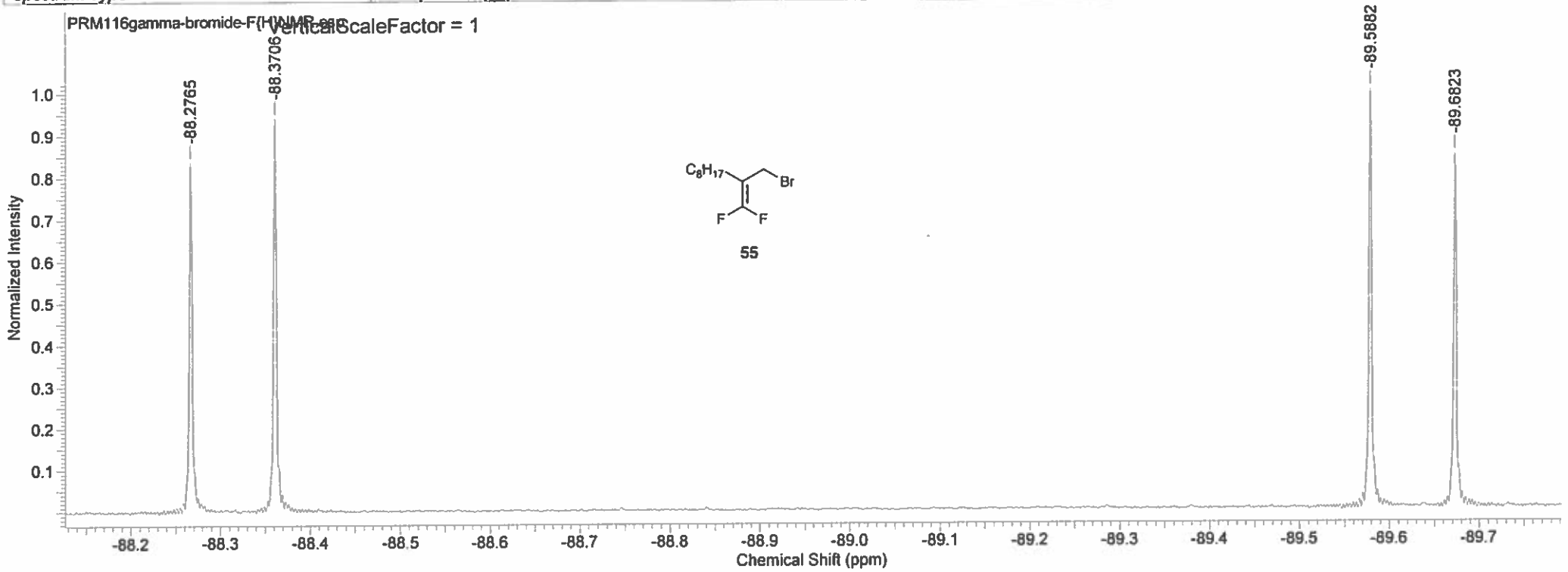
No.	(ppm)	(Hz)	Height
1	88.84	11172.6	0.0722
2	88.95	11186.3	0.0809
3	89.02	11195.5	0.0630
4	89.13	11208.3	0.0664
5	151.60	19065.0	0.0455
6	153.90	19354.6	0.0672
7	153.92	19356.4	0.0605
8	156.22	19646.0	0.0411

20/01/2014 15:51:13

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM116 f3+4 117mg mF19CPD CDCl3 (e:\bruk400data\2014\Jan) ejt 42				
Date	13 Jan 2014 12:33:04	*Date Stamp*	13 Jan 2014 12:33:04				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\JAN\DATA\EJT\NMR\2014-01-13-EJT-42\11\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	20.800		

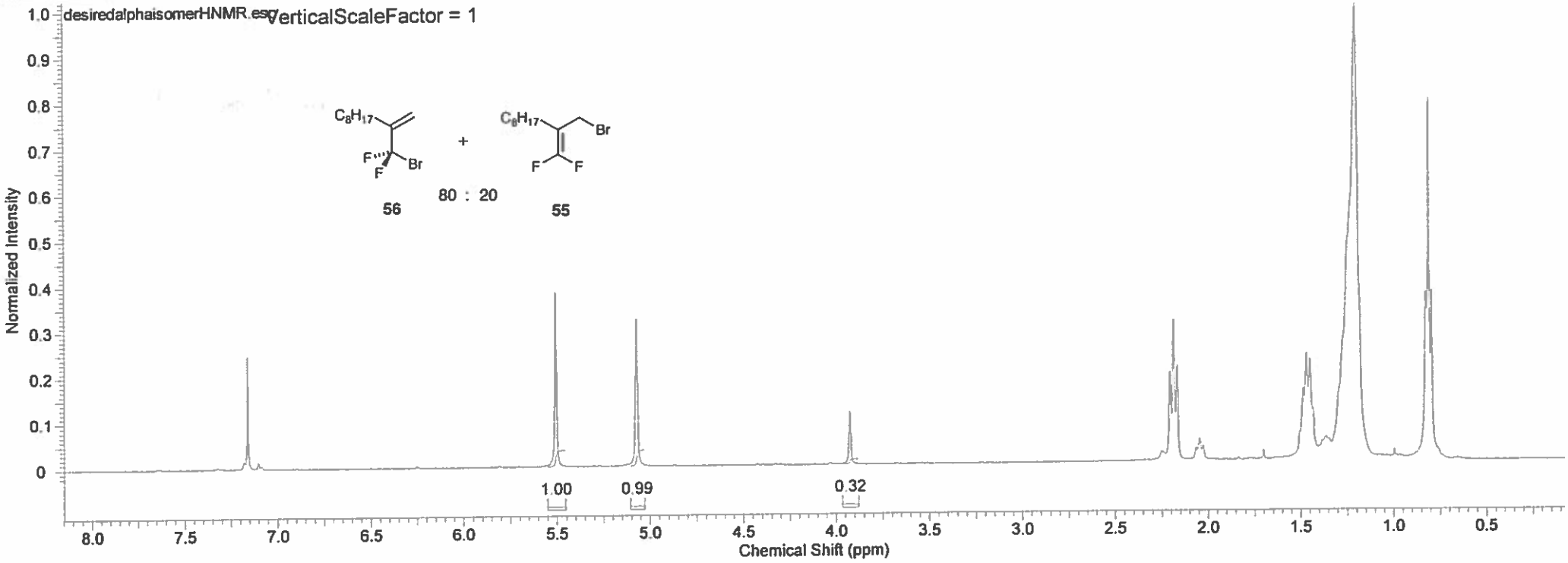


55

No.	(ppm)	(Hz)	Height
1	-89.68	-33765.3	0.8449
2	-89.59	-33729.8	1.0000
3	-88.37	-33271.4	0.9398
4	-88.28	-33236.0	0.8364

13/01/2014 13:10:24

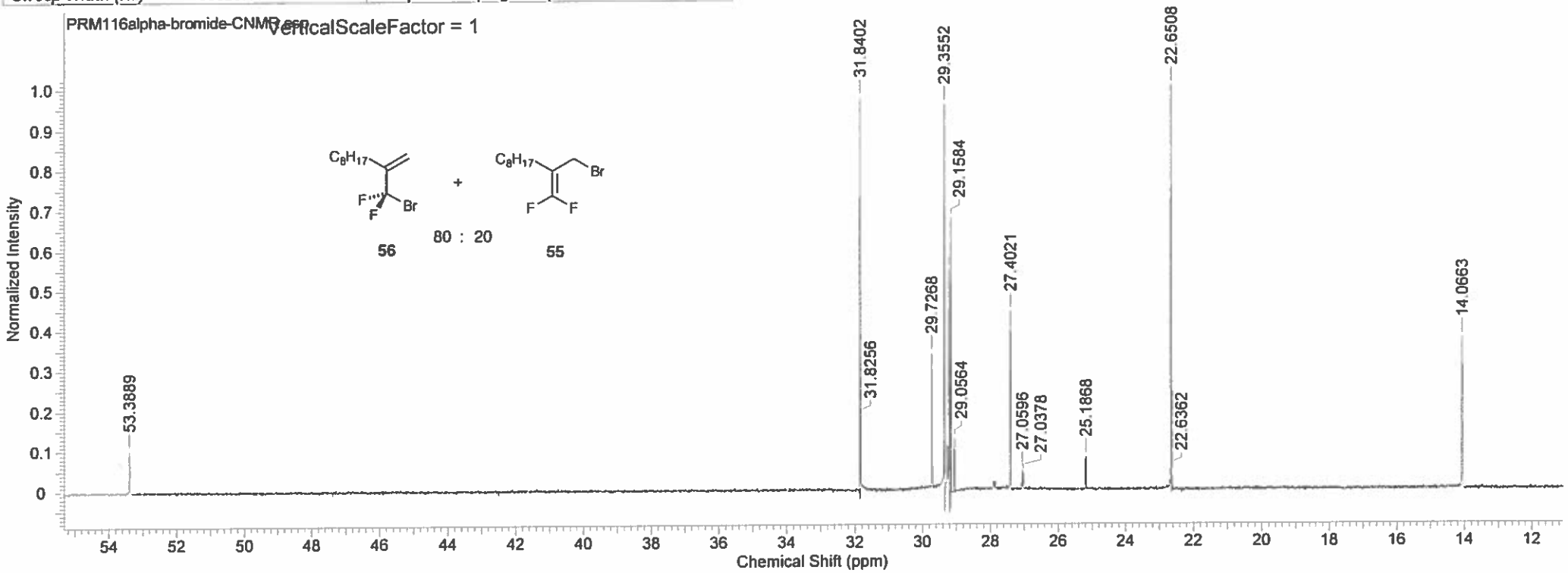
Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM120 reflux o/n tol-d8 mPROTON CDCl3 {e:\bruk400data\2014\Jan} ejt 28				
Date	10 Jan 2014 10:46:24	*Date Stamp*	10 Jan 2014 10:46:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\JAN\DATA\EJT\NMR\2014-01-10-EJT-28\10\PDATA\1\1R						
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	128.00	*SW(cyclical) (Hz)*	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2421.3662
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8264.21	*Temperature (degree C)*	20.400		



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	3791 .. 3.960	0.31848073	6.23530000e+6	0.31848073
2	5303 .. 5.100	0.99194330	1.94205280e+7	0.99194330
3	4545 .. 5.550	0.99989295	1.95761680e+7	0.99989295

15/01/2014 12:18:01

Acquisition Time (sec)	1.0912	*Comment*	EJT-PRM116l alpha-bromide data mCARBONnight CDCl3 {F:\bruk500_b_data\2014\Jan} ejt 16				
Date	14 Jan 2014 01:48:48	*Date Stamp*	14 Jan 2014 01:48:48				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500bdata\2014\Jan\data\ejt\nmr\2014-01-13-ejt-16\11\fid					*Frequency (MHz)*	125.76
Nucleus	13C	*Number of Transients*	3096	*Origin*	spect	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	4096.00
SW(cyclical) (Hz)	30030.03	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12574.2715	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	14.07	1768.9	0.3709
2	22.64	2846.7	0.0414
3	22.65	2848.5	1.0000
4	25.19	3167.4	0.0763
5	27.04	3400.2	0.0358

No.	(ppm)	(Hz)	Height
6	27.06	3403.0	0.0437
7	27.40	3446.0	0.4405
8	29.06	3654.1	0.1222
9	29.16	3666.9	0.6740
10	29.21	3673.3	0.5448

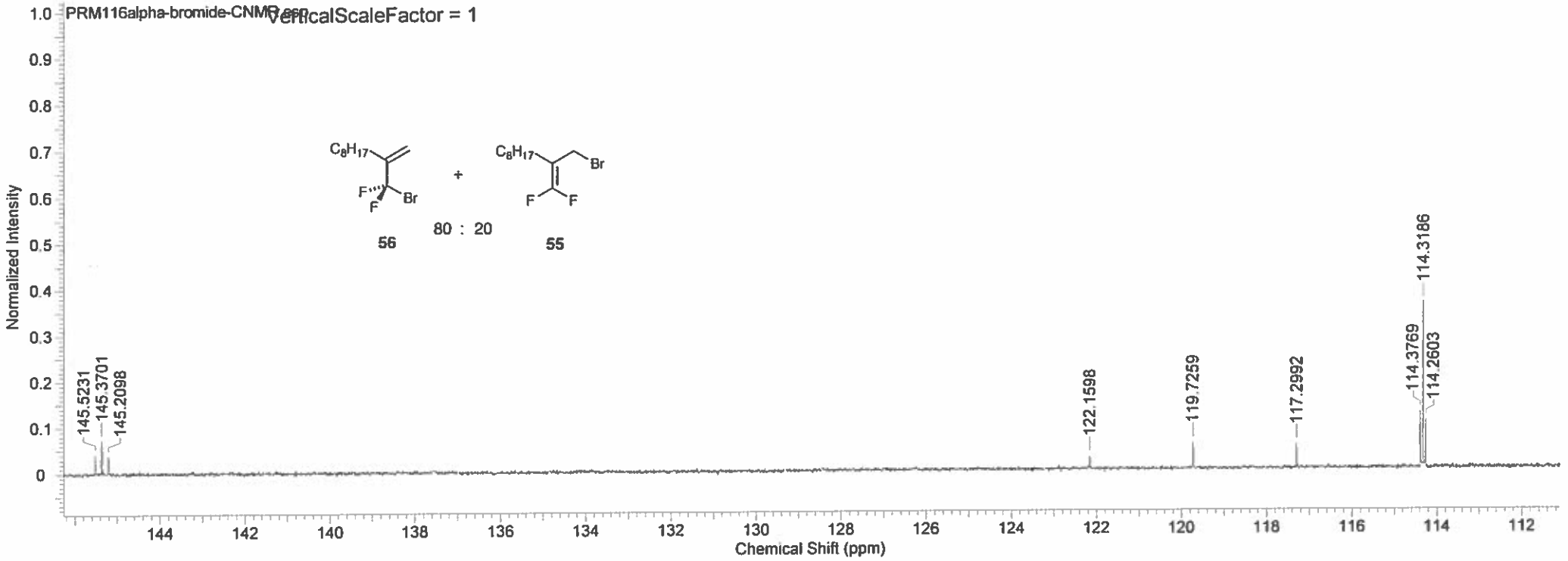
No.	(ppm)	(Hz)	Height
11	29.27	3680.6	0.1341
12	29.36	3691.6	0.9545
13	29.73	3738.4	0.3351
14	31.83	4002.3	0.1738
15	31.84	4004.1	0.9721

No.	(ppm)	(Hz)	Height
16	53.39	6714.1	0.1016
17	114.26	14369.1	0.1056
18	114.32	14376.5	0.3611
19	114.38	14383.8	0.1226
20	117.30	14751.3	0.0533

No.	(ppm)	(Hz)	Height
21	119.73	15056.5	0.0576
22	122.16	15362.6	0.0286
23	145.21	18261.3	0.0397
24	145.37	18281.4	0.0736
25	145.52	18300.7	0.0430

15/01/2014 12:16:32

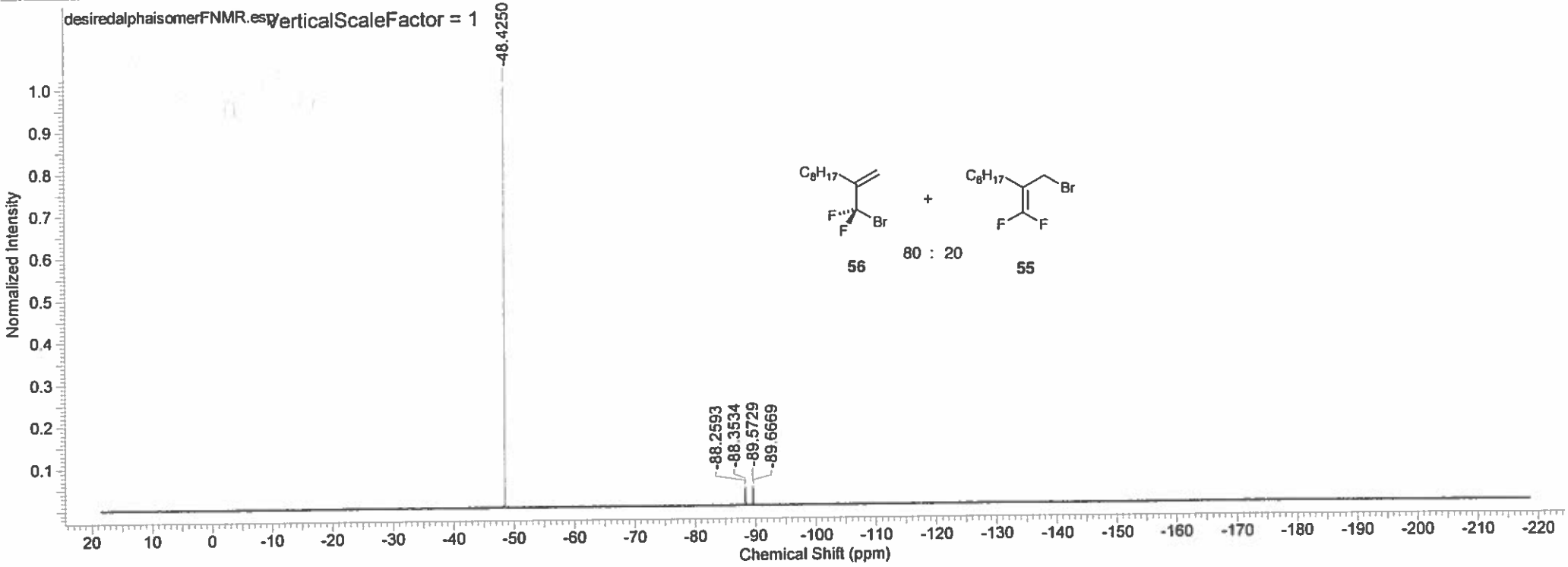
Acquisition Time (sec)	1.0912	*Comment*	EJT-PRM116I alpha-bromide data mCARBONnight CDCl3 {F:\bruk500_b_data\2014\Jan} ejt 16				
Date	14 Jan 2014 01:48:48	*Date Stamp*	14 Jan 2014 01:48:48				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500bdata\2014\Jan\data\ejt\nmr\2014-01-13-ejt-16\11\fid					*Frequency (MHz)*	125.76
Nucleus	13C	*Number of Transients*	3096	*Origin*	spect	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	4096.00
SW(cyclical) (Hz)	30030.03	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12574.2715	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	114.26	14369.1	0.1056
2	114.32	14376.5	0.3611
3	114.38	14383.8	0.1226
4	117.30	14751.3	0.0533
5	119.73	15056.5	0.0576
6	122.16	15362.6	0.0286
7	145.21	18261.3	0.0397
8	145.37	18281.4	0.0736
9	145.52	18300.7	0.0430

13/01/2014 13:10:16

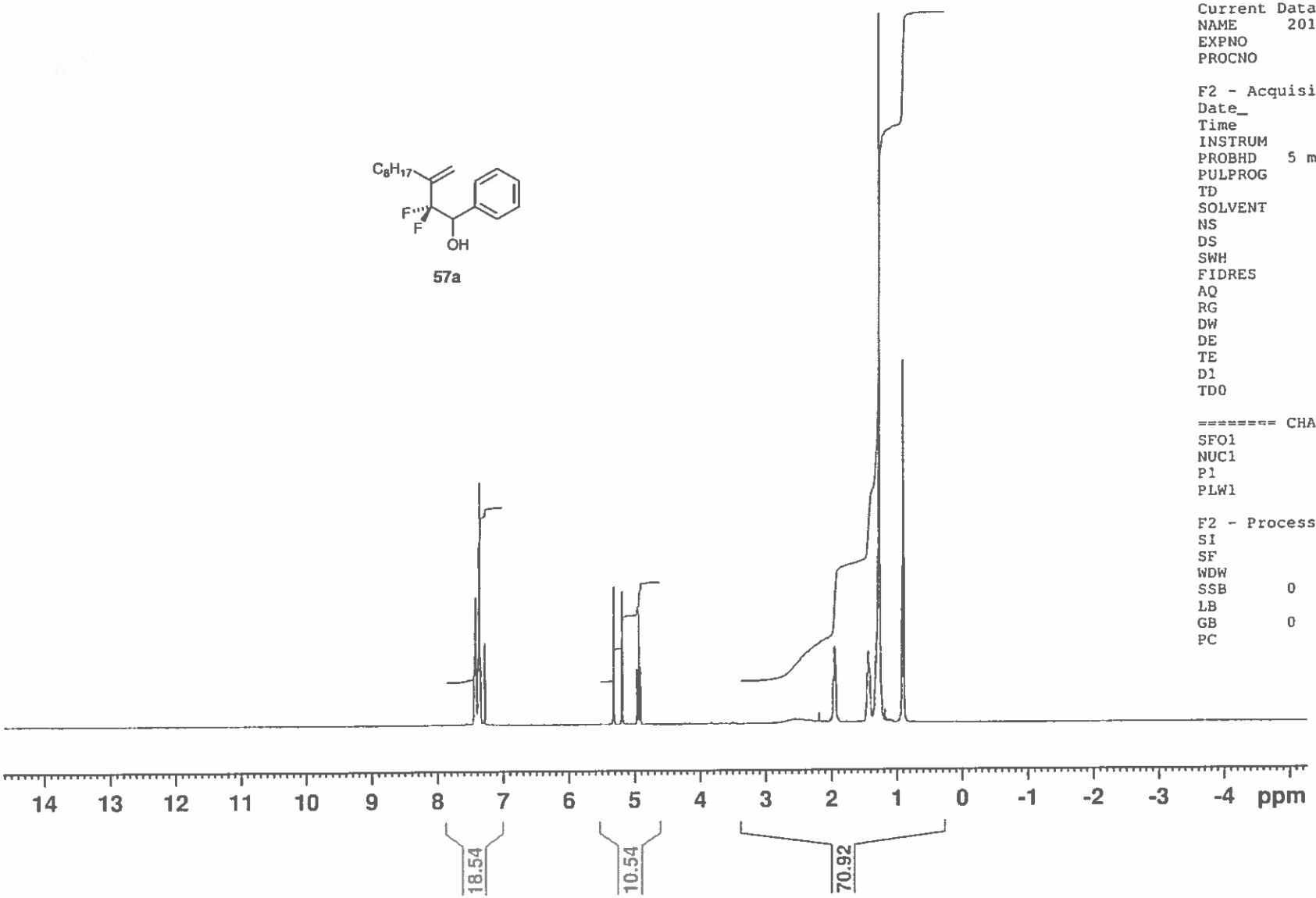
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM120 reflux o/n tol-d8 mF19CPD CDCl3 (e:\bruk400data\2014\Jan) ejt 28				
Date	10 Jan 2014 10:48:32	*Date Stamp*	10 Jan 2014 10:48:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\JAN\DATA\EJT\NMR\2014-01-10-EJT-28\11\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	20.700		



No.	(ppm)	(Hz)	Height
1	-89.67	-33759.5	0.0402
2	-89.57	-33724.0	0.0467
3	-88.35	-33264.9	0.0441
4	-88.26	-33229.5	0.0391
5	-48.43	-18231.9	1.0000

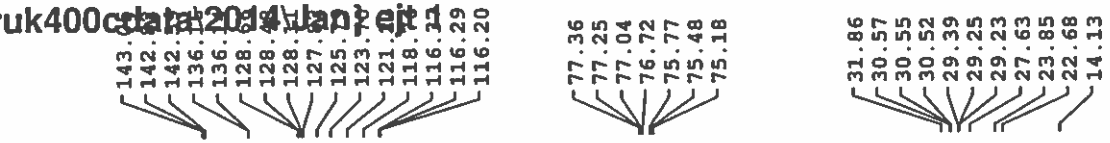
EJT-PRM123A prod data
mPROTON_A_night CDCl3 {e:\bruk400cdata\2014\Jan} ejt 1

57a

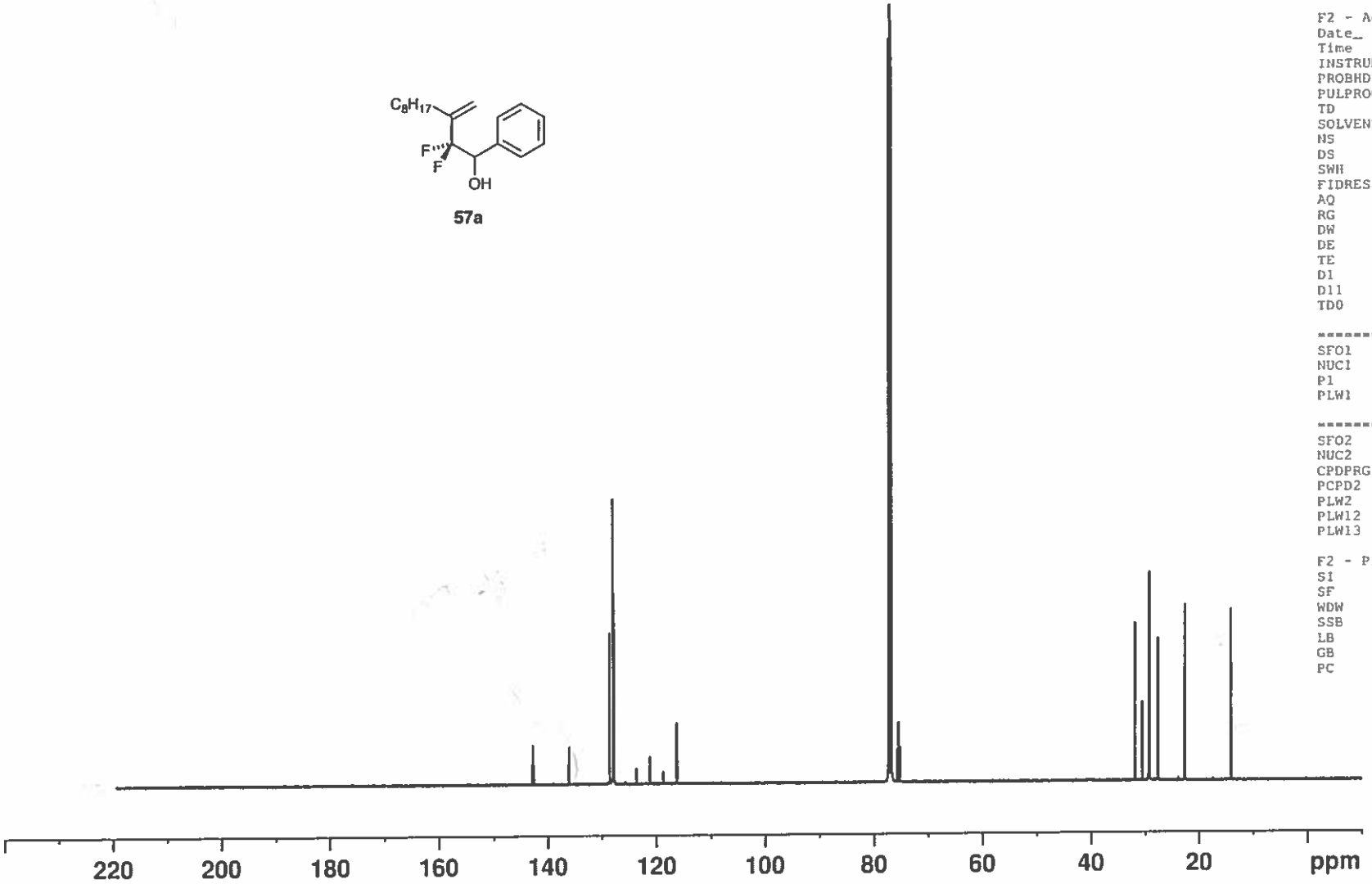



```
Current Data Parameters
NAME      2014-01-27-ejt-1
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140127
Time                  22.55
INSTRUM               spect
PROBHD   5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                     80.6
DW                   60.800 usec
DE                   10.00 usec
TE                   295.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          400.0718803 MHz
NUC1                     1H
P1                    12.00 usec
PLW1           7.40000010 W

F2 - Processing parameters
SI                    32768
SF            400.0700000 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

EJT-PRM123A prod data
mCARBON_B CDCl3 {e:\bruk400data\2014\jan\ejt-1



57a



BRUKER 400 MHz

Current Data Parameters
NAME 2014-01-27-ejt-1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140127
Time 22.53
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 41.77 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

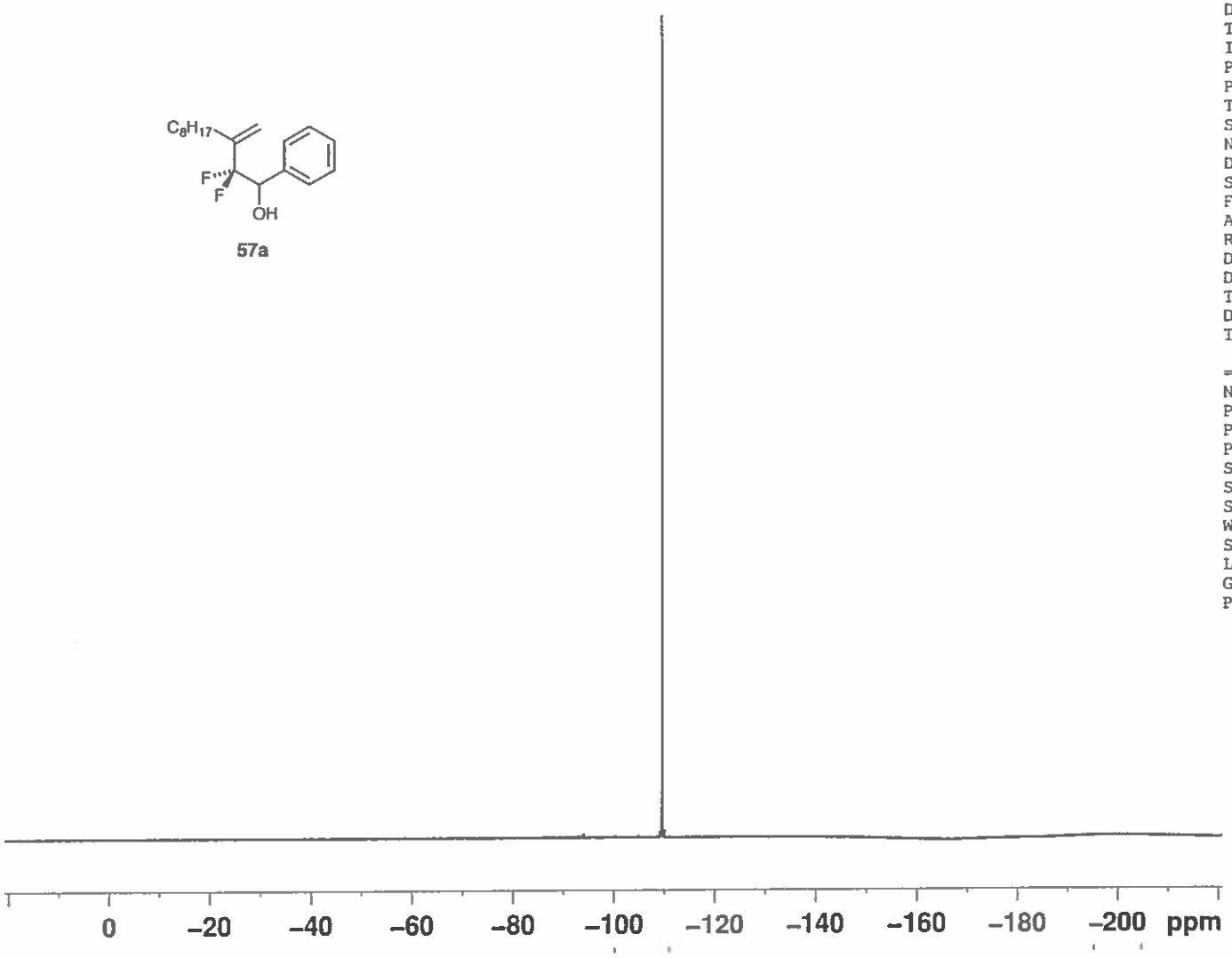
======== CHANNEL f1 ========
SFO1 100.6077384 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976820 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

EJT-PRM123A f25-43 29mg
m19F CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 34

57a

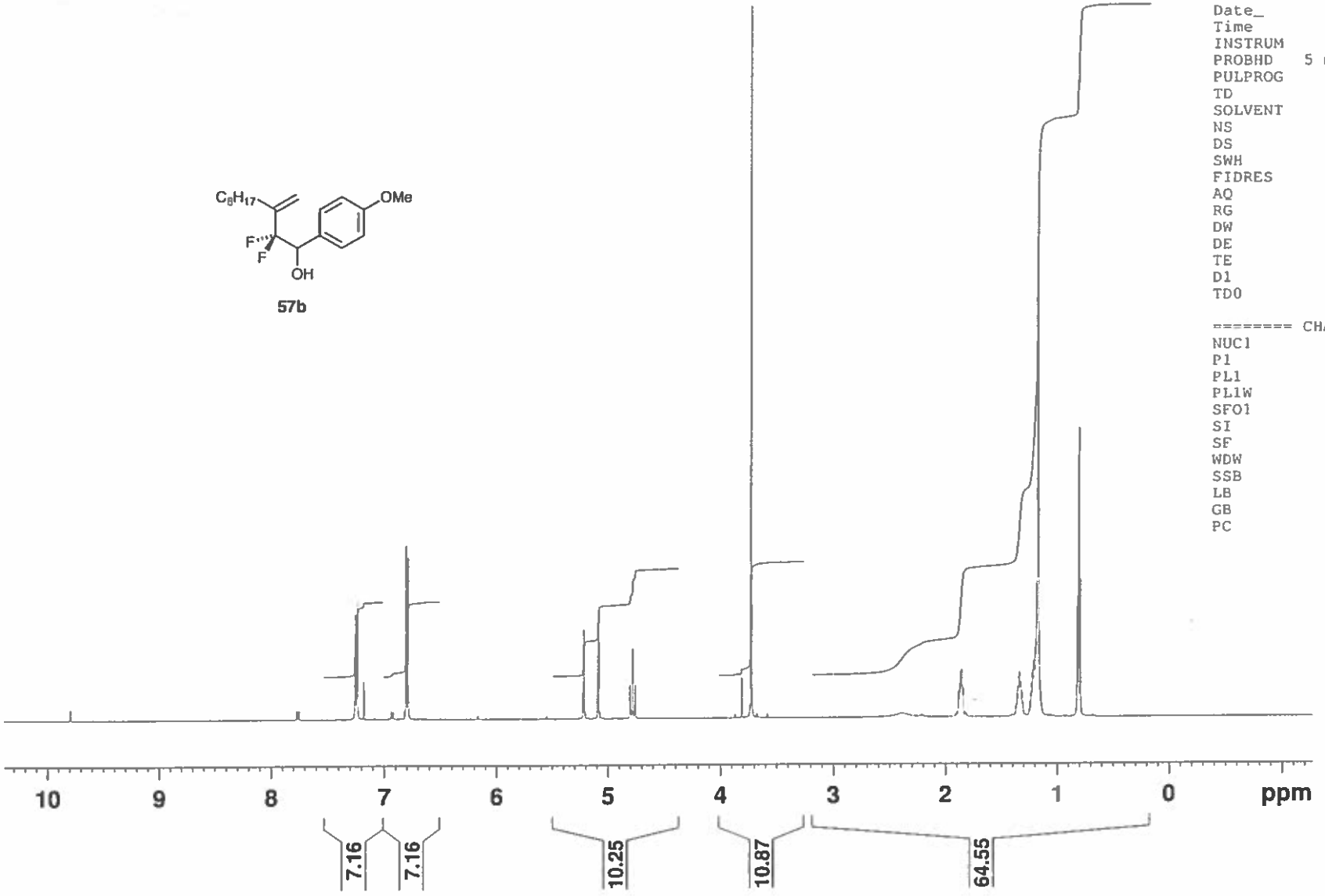


NAME	2014-01-27-ejt-34
EXPNO	11
PROCNO	1
Date_	20140127
Time	14.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	113636.367 Hz
FIDRES	0.866977 Hz
AQ	0.5767668 sec
RG	203
DW	4.400 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	12.38 usec
PL1	-0.10 dB
PL1W	25.70395851 W
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

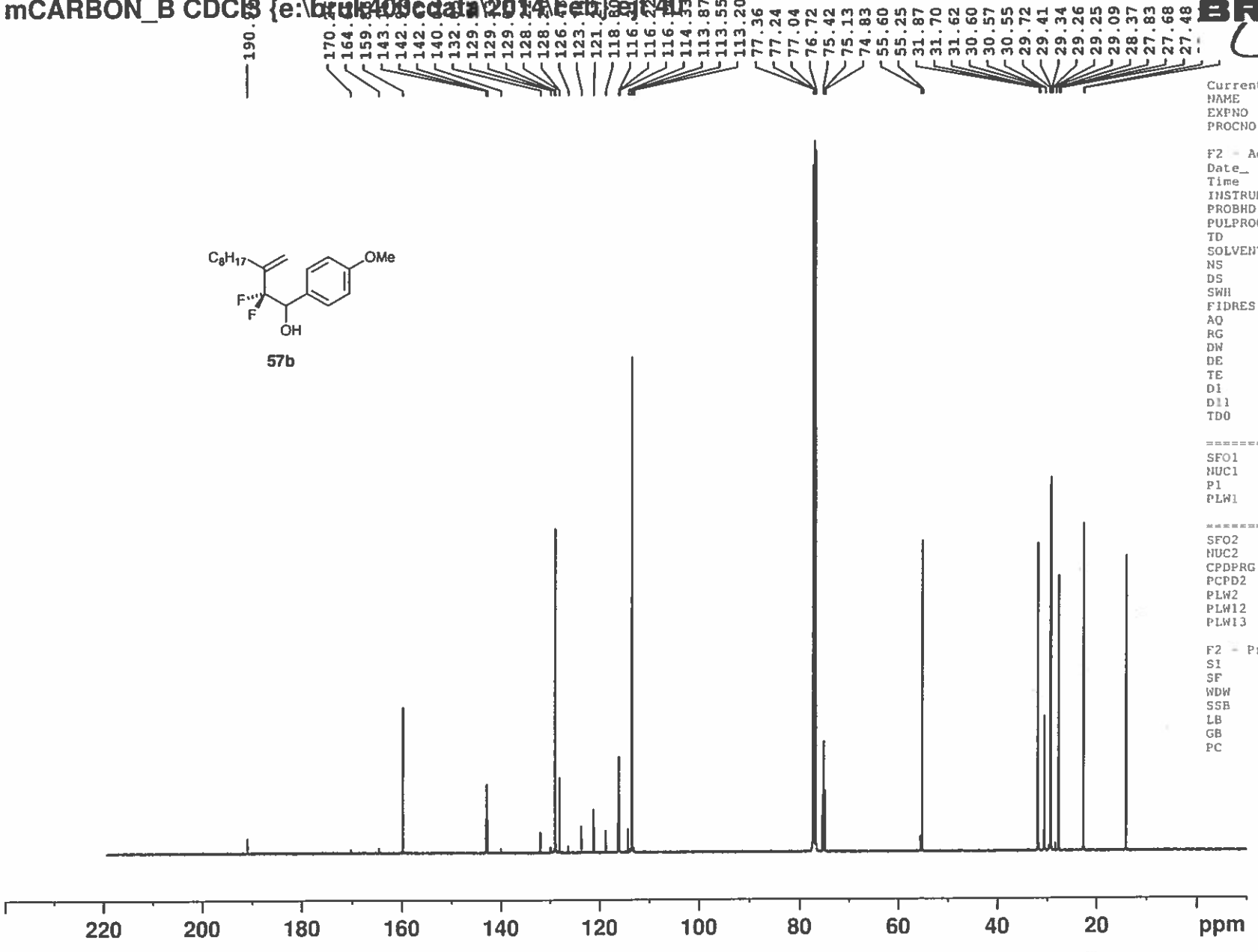
EJT–PRM123B prod data
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 25

57b

NAME	2014-02-10-ejt-25
EXPNO	10
PROCNO	1
Date_	20140210
Time	17.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	20.2
DW	48.400 usec
DE	13.00 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300522 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



EJT-PRM123B prod data
mCARBON_B CDCl3 {e:\bruk400cdata\2014\Feb\ejt-40



Current Data Parameters
NAME 2014-02-10-ejt-40
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140211
Time 21.30
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 41.77 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

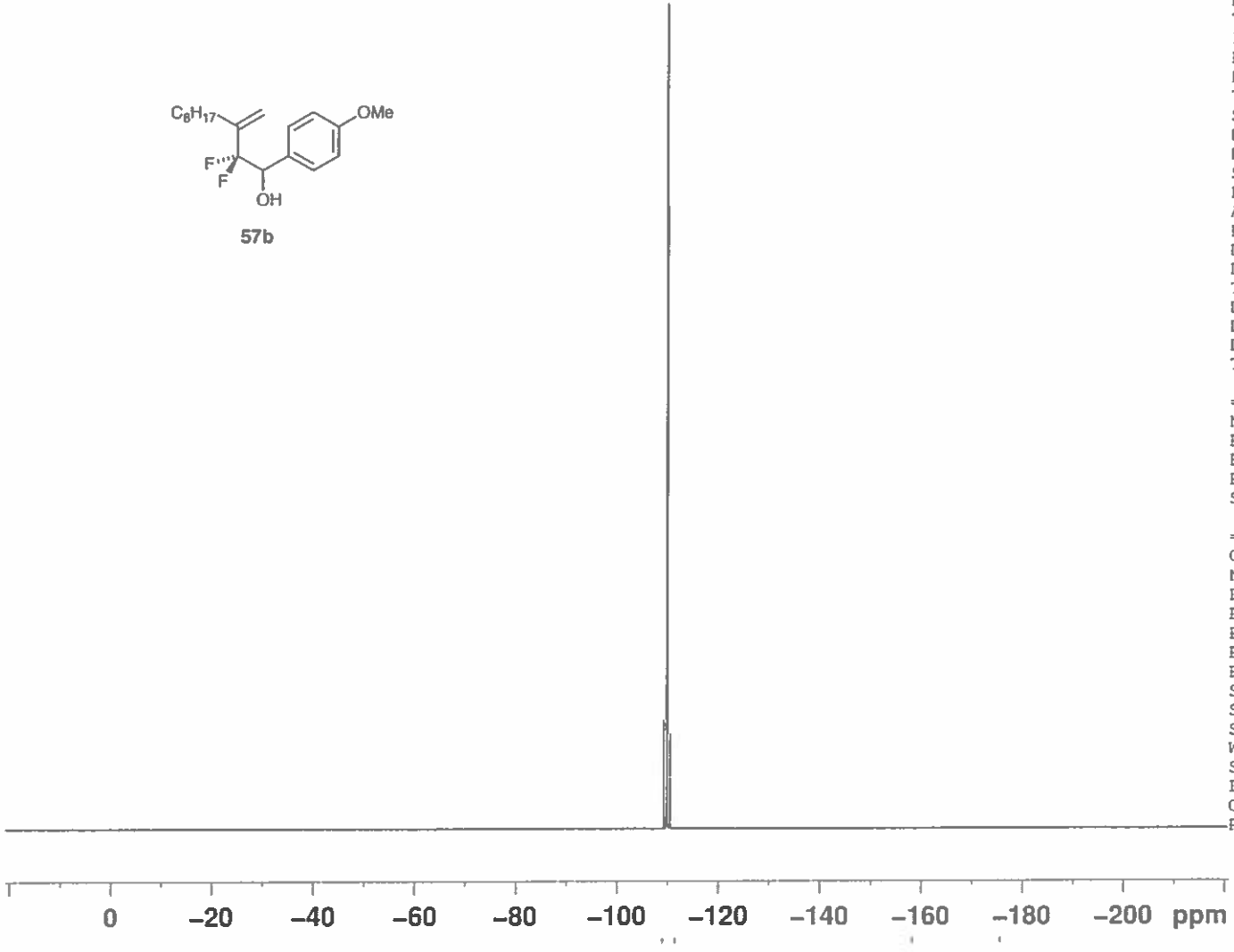
======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

EJT-PRM123B prod data
m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 25

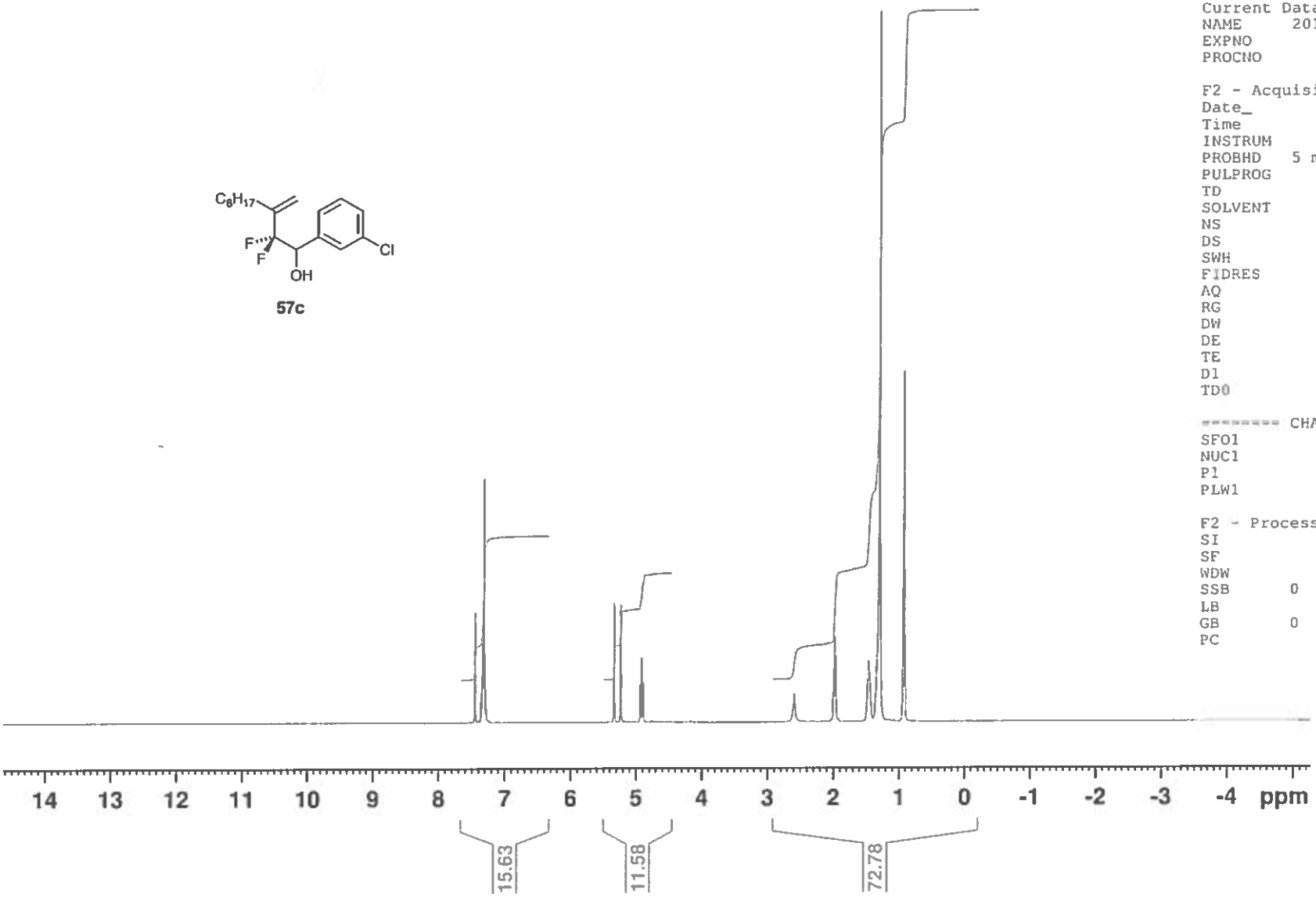
57b



NAME	2014-02-10-ejt-25	
EXPNO	12	
PROCNO	1	
Date_	20140210	
Time	17.50	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgfhigqn	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	113636.367	Hz
FIDRES	0.866977	Hz
AQ	0.5767668	sec
RG	32	
DW	4.400	usec
DE	6.50	usec
TE	294.3	K
D1	1.00000000	sec
D11	0.03000000	sec
D12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	12.38	usec
PL1	-0.10	dB
PL1W	25.70395851	W
SFO1	470.5453180	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.00	dB
PL12	17.23	dB
PL2W	25.62124252	W
PL12W	0.48484197	W
SFO2	500.1320005	MHz
SI	65536	
SF	470.5923770	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

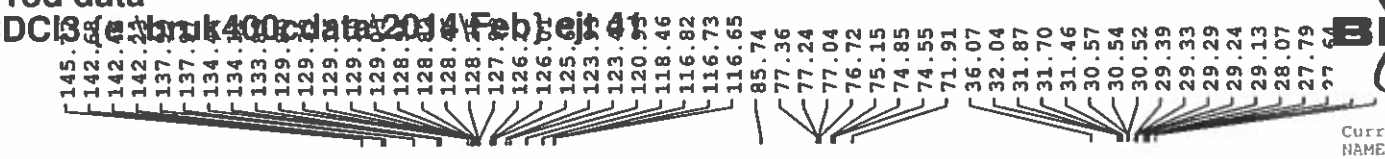
EJT-PRM123C Prod data
mPROTON_A_night CDCl3 {e:\bruk400cdata\2014\Feb} ejt 41

57c




```
Current Data Parameters
NAME      2014-02-10-ejt-41
EXPNO                    21
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140211
Time                  23.18
INSTRUM               spect
PROBHD   5 mm CPPBBO BB
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                      36
DW                  60.800 usec
DE                  10.00 usec
TE                  298.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.0718803 MHz
NUC1                    1H
P1                  12.00 usec
PLW1            7.40000010 W

F2 - Processing parameters
SI                   32768
SF              400.0700000 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

EJT-PRM123C Prod data
mCARBON_B CDCl3 {c:\bruk400\data\2014\Feb} ejt 41



57c

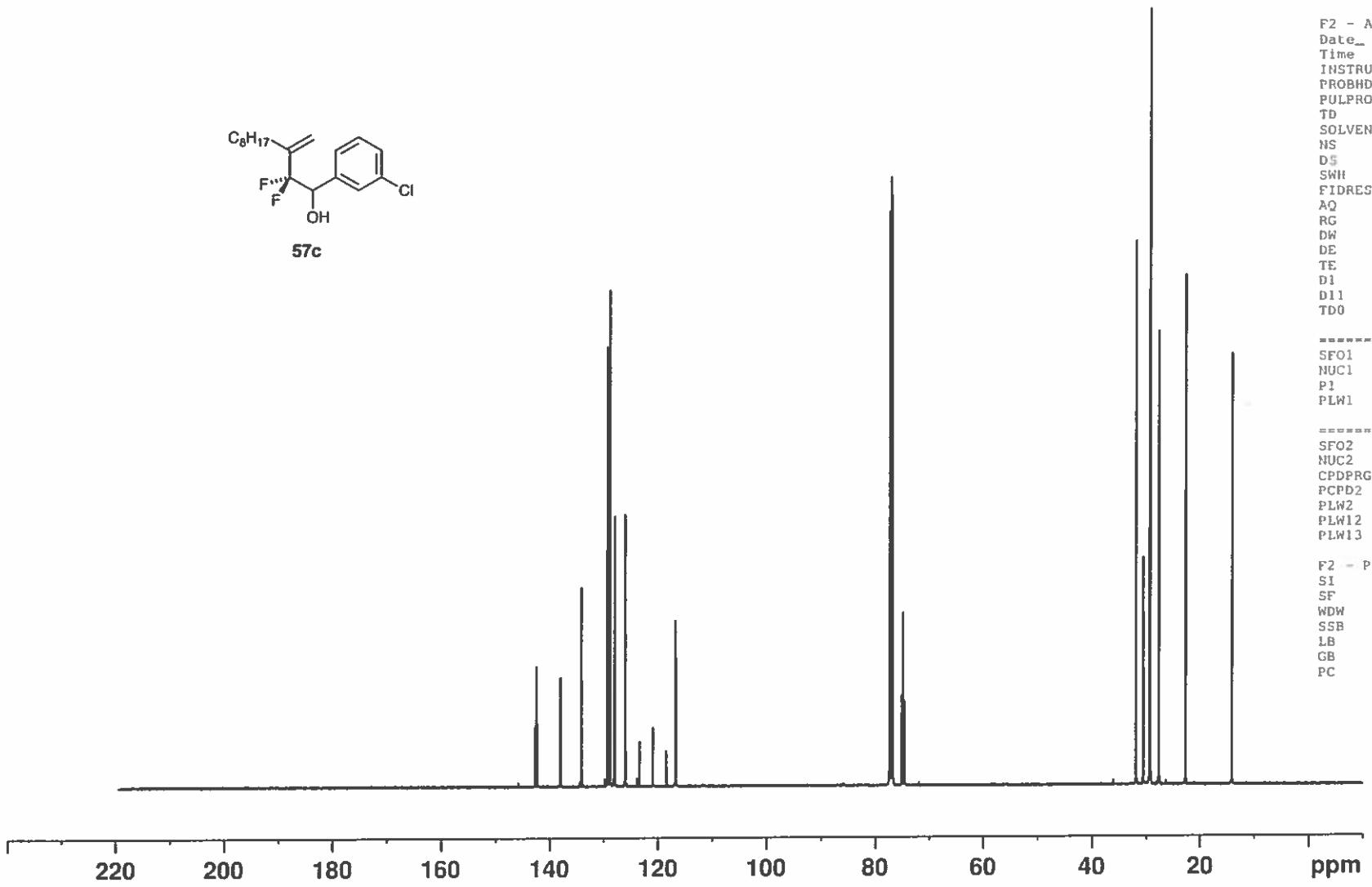
Current Data Parameters
NAME 2014-02-10-ejt-41
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140211
Time 23.16
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 71.8
DW 20.800 usec
DE 41.77 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

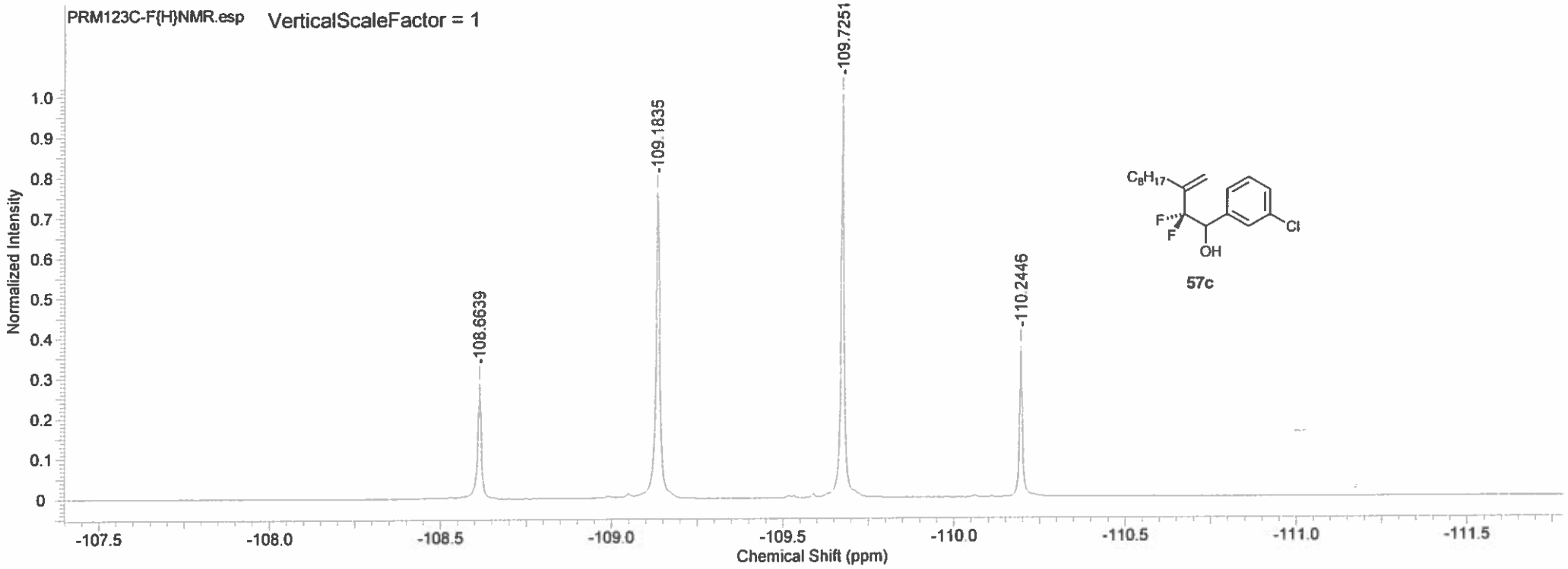
======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



18/02/2014 16:44:47

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM123C prod m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 10				
Date	11 Feb 2014 09:33:52	*Date Stamp*	11 Feb 2014 09:33:52				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\FEB\DATA\EJT\NMR\2014-02-11-EJT-10\12\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn
Receiver Gain	32.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	21.184		

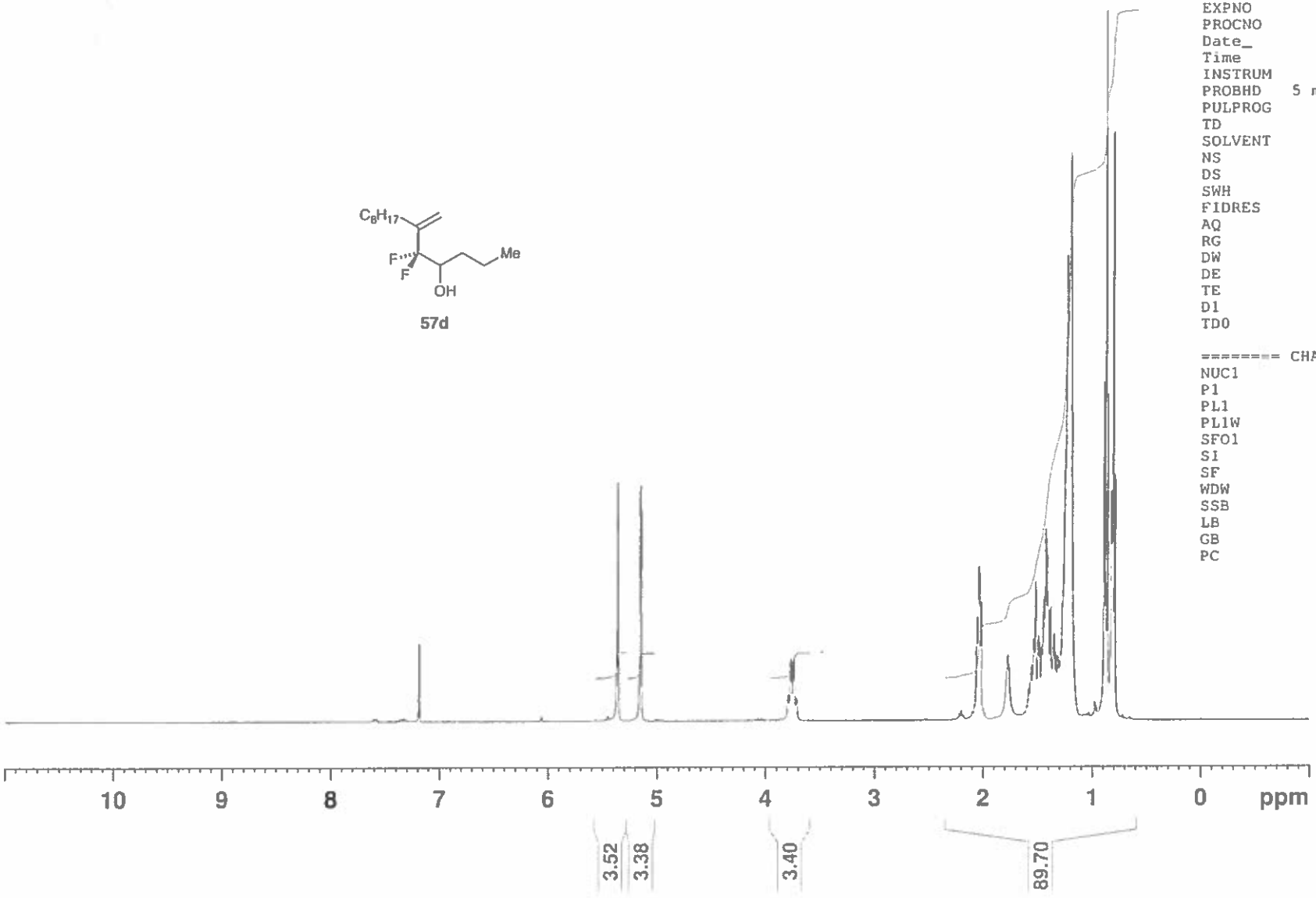


No.	(ppm)	(Hz)	Height
1	-110.24	-51880.3	0.3719
2	-109.73	-51635.8	1.0000
3	-109.18	-51380.9	0.7599
4	-108.66	-51136.4	0.2865

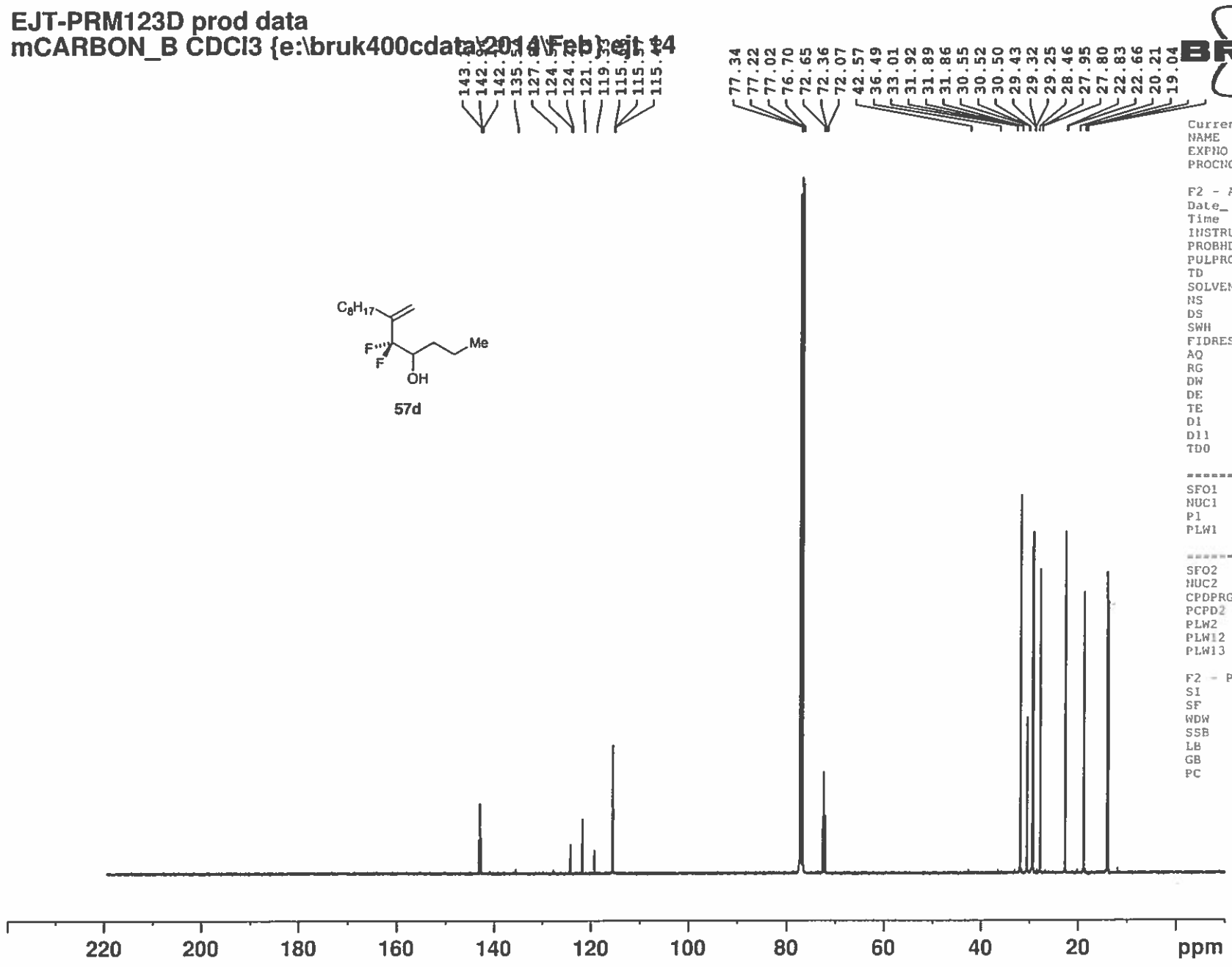
EJT–PRM123D prod f12–26 48mg
mPROTON CDCl3 {e:\bruk400data\2014\Feb} ejt 27

57d

NAME	2014-02-14-ejt-27
EXPNO	10
PROCNO	1
Date_	20140214
Time	15.25
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	90.5
DW	60.500 usec
DE	8.45 usec
TE	294.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300369 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



EJT-PRM123D prod data
mCARBON_B CDCl3 {e:\bruk400cdata\2014\Feb}ejt 14



Current Data Parameters
NAME 2014-02-14-ejt-14
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140215
Time 4.54
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 71.8
DW 20.800 usec
DE 41.77 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

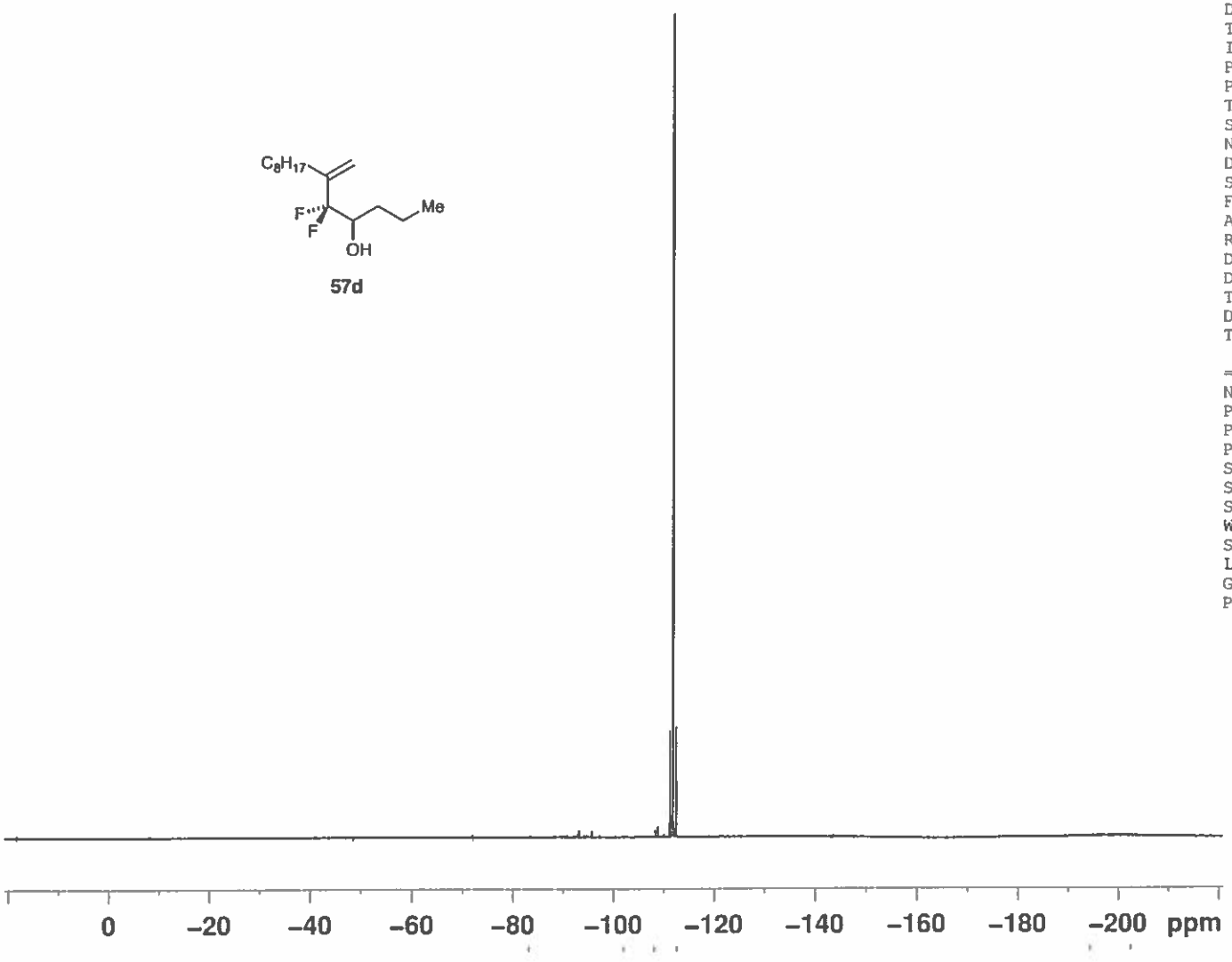
======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

EJT-PRM123D crude 60mg
m19F CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 3

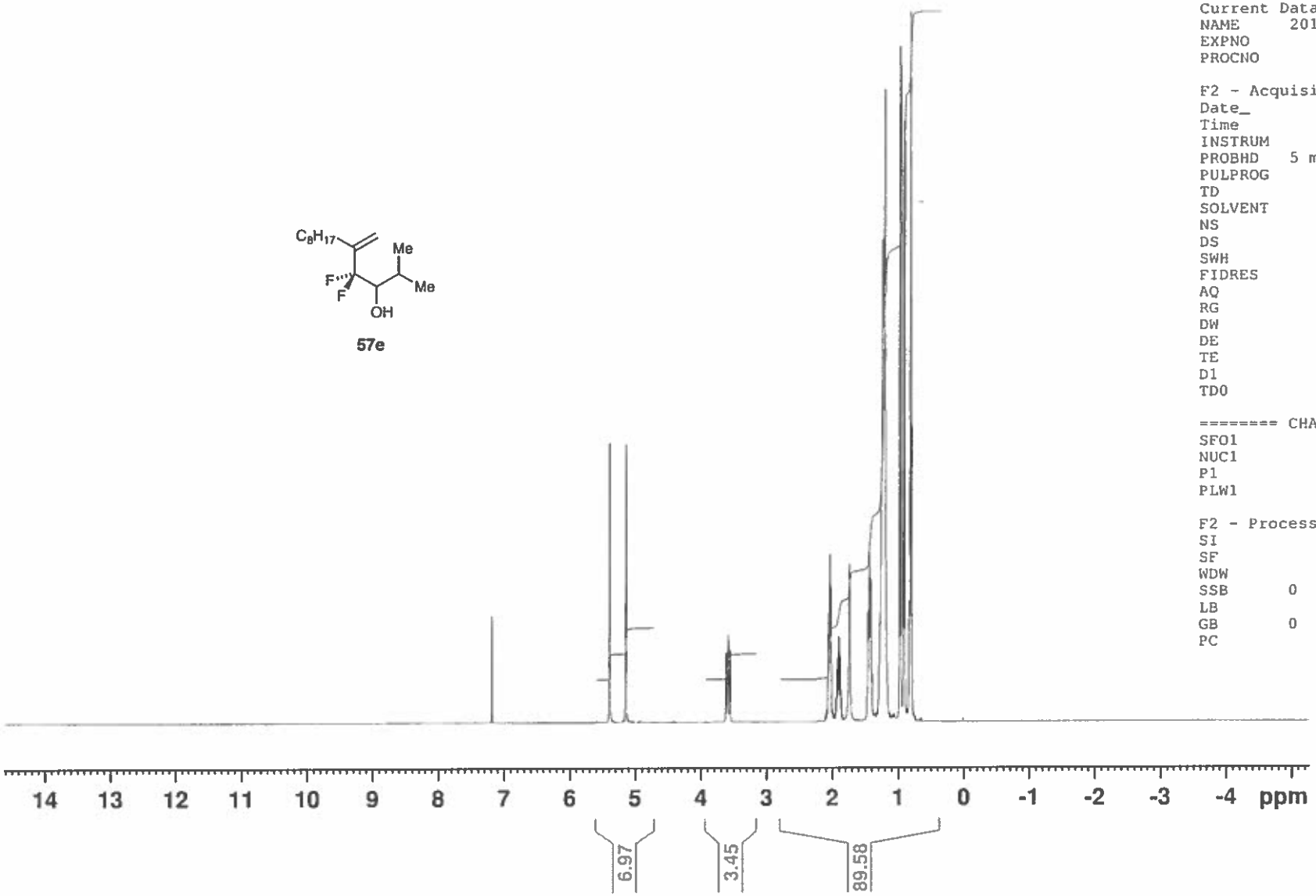
57d



NAME	2014-02-14-ejt-3
EXPNO	11
PROCNO	1
Date_	20140214
Time	11.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	113636.367 Hz
FIDRES	0.866977 Hz
AQ	0.5767668 sec
RG	203
DW	4.400 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	12.38 usec
PL1	-0.10 dB
PL1W	25.70395851 W
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

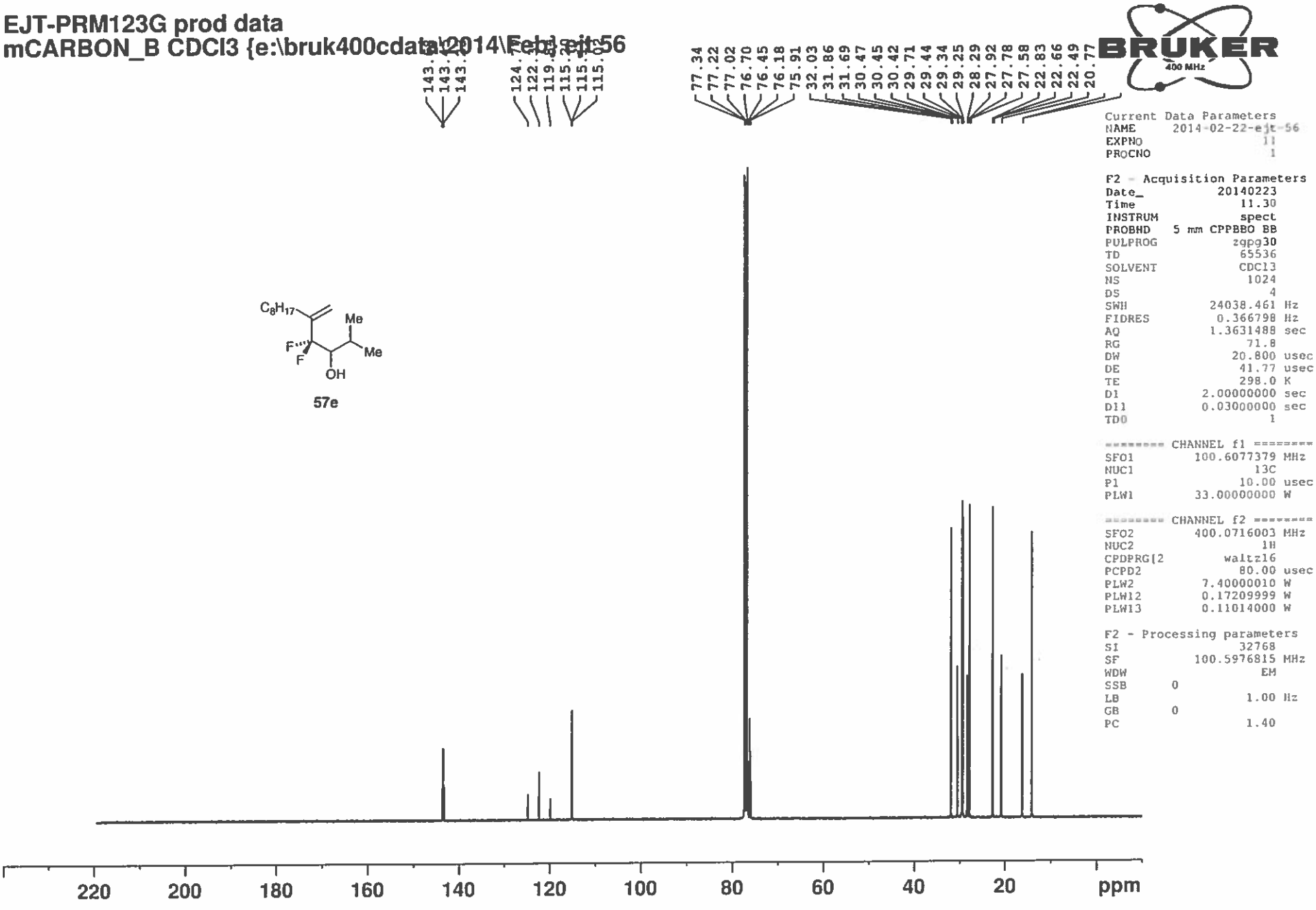
EJT-PRM123G prod data
mPROTON_A_night CDCl3 {e:\bruk400cdata\2014\Feb} ejt 56

57e



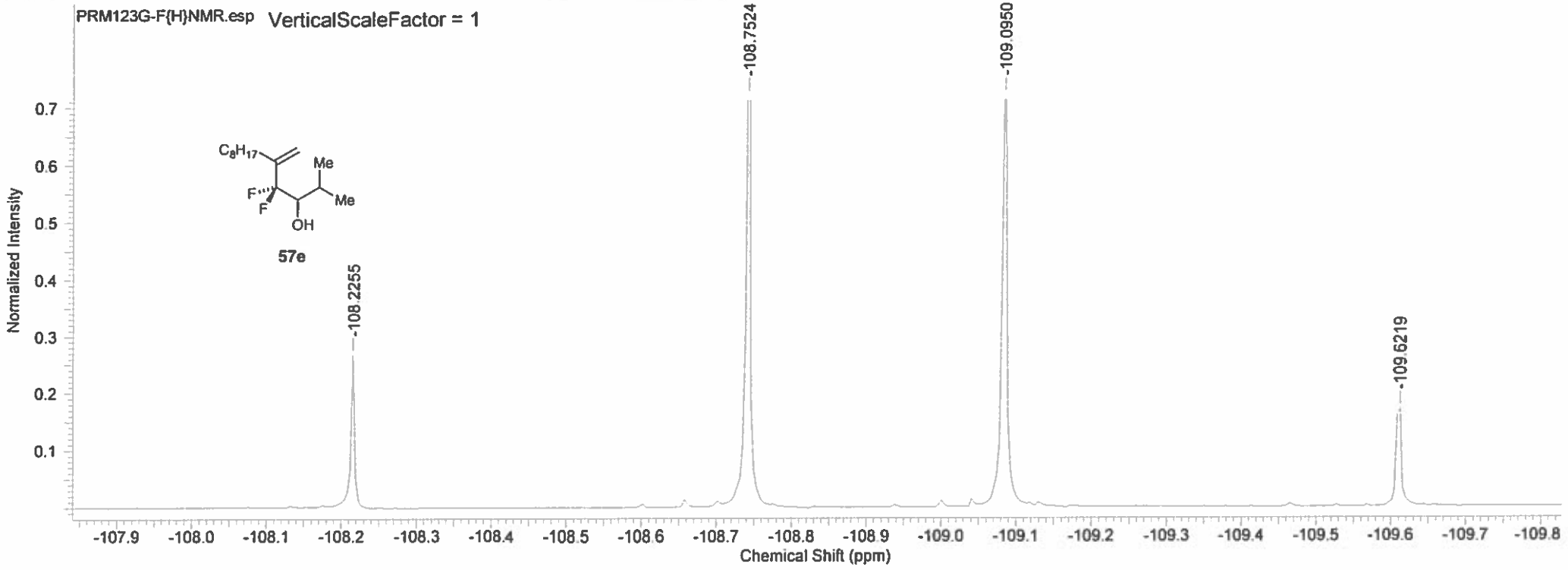

```
Current Data Parameters
NAME      2014-02-22-ejt-56
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140223
Time                 10.30
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                    45.2
DW                  60.800 usec
DE                  10.00 usec
TE                  298.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.0718803 MHz
NUC1                    1H
P1                   12.00 usec
PLW1           7.40000010 W

F2 - Processing parameters
SI                   32768
SF            400.0700371 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

EJT-PRM123G prod data
mCARBON_B CDCl3 {e:\bruk400cdata\2014\Feb\ejt-56



24/02/2014 15:06:46

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM123G prod m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Feb ejt 56				
Date	23 Feb 2014 18:54:56	*Date Stamp*	23 Feb 2014 18:54:56				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500data\bruk500data\2014\Feb\data\ejt\nmr\2014-02-23-ejt-56\12\fid					*Frequency (MHz)*	470.59
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn	*Receiver Gain*	32.00
SW(cyclical) (Hz)	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	113634.63	*Temperature (degree C)*	27.000				

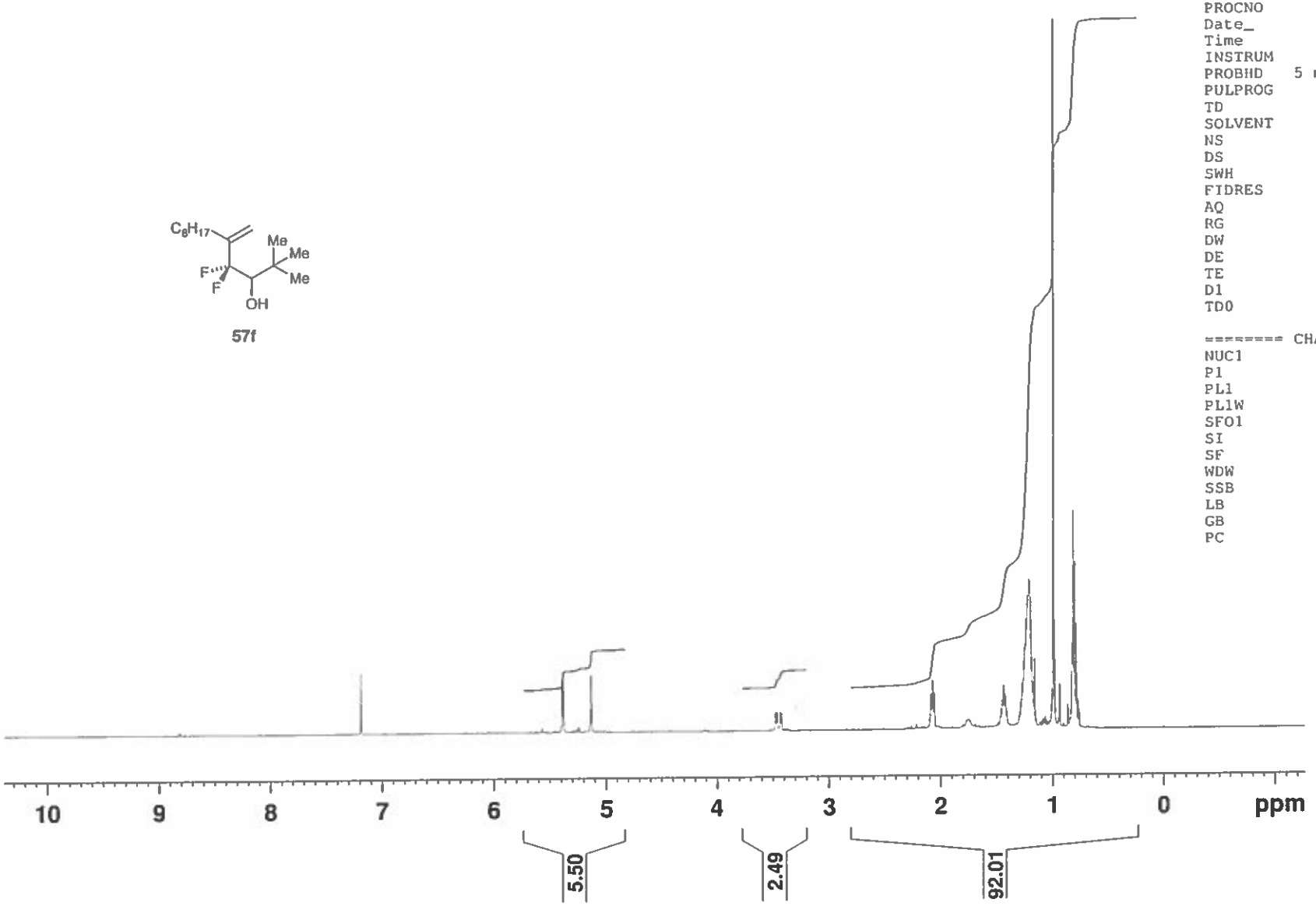


No.	(ppm)	(Hz)	Height
1	-109.62	-51587.2	0.1688
2	-109.10	-51339.3	0.8761
3	-108.75	-51178.0	1.0000
4	-108.23	-50930.1	0.2675

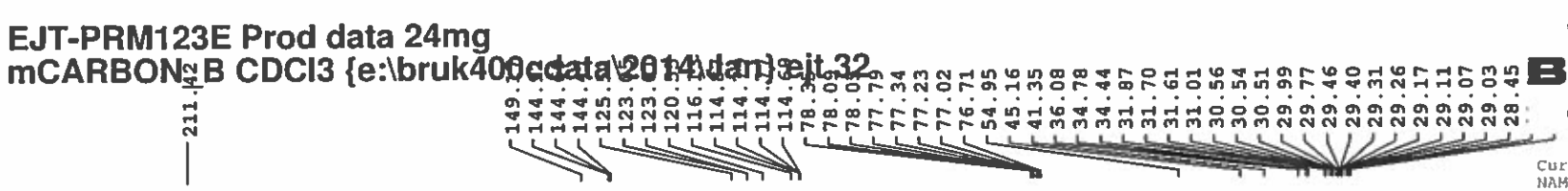
EJT–PRM123E f8–15 24mg
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 29

57f

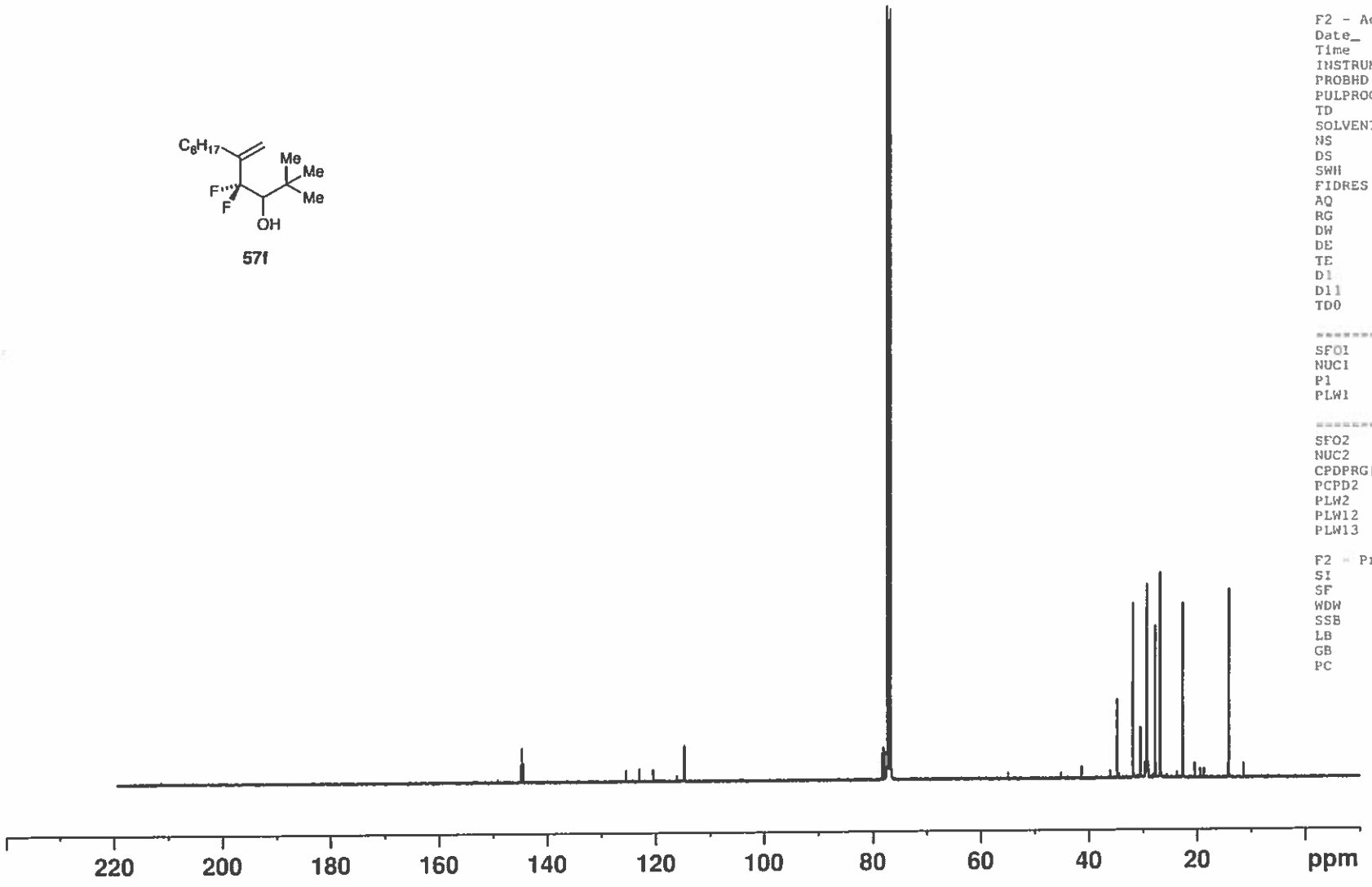
NAME	2014-01-28-ejt-29
EXPNO	10
PROCNO	1
Date_	20140128
Time	16.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	25.4
DW	48.400 usec
DE	13.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300482 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



EJT-PRM123E Prod data 24mg
mCARBON_B CDCl3 {e:\bruk400\data\2014\dan}ejt 32



571



BRUKER 400 MHz

Current Data Parameters
NAME 2014-01-28-ejt-32
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140129
Time 19.09
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 71.8
DW 20.800 usec
DE 41.77 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

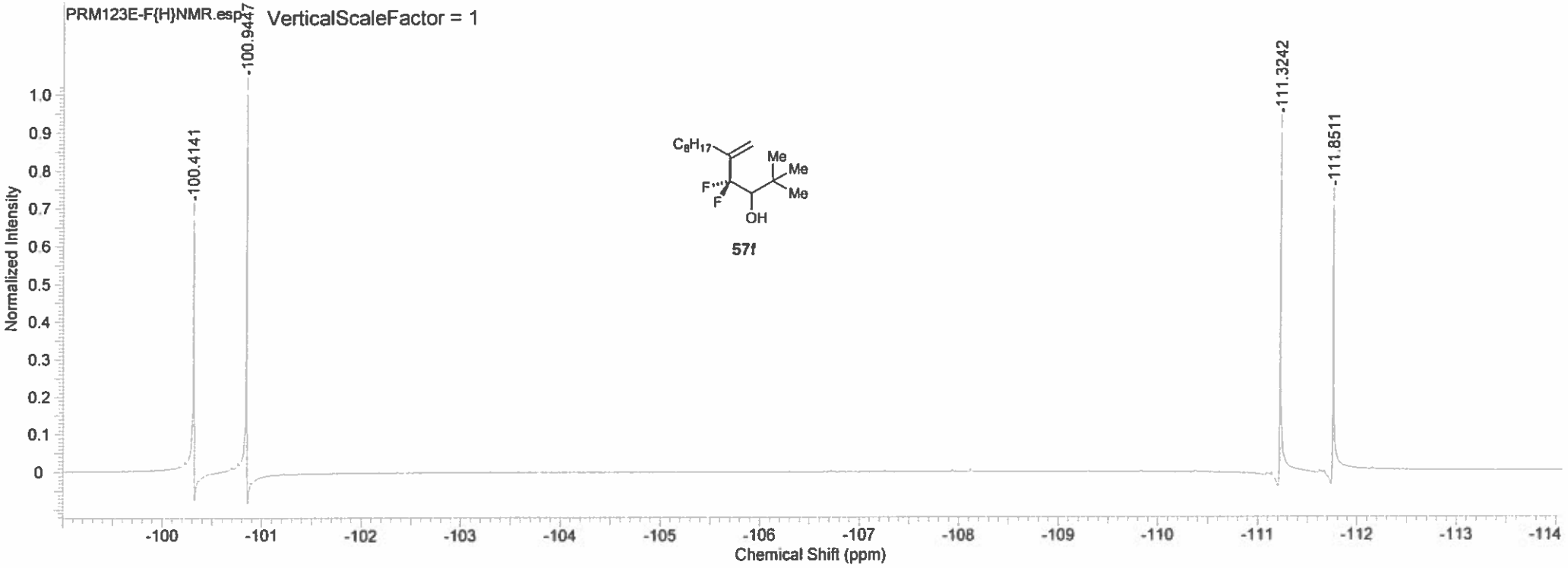
======== CHANNEL f1 ========
SFO1 100.6077384 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976820 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

30/01/2014 11:37:52

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM123E f8-15 24mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Jan ejt 29				
Date	28 Jan 2014 16:19:12	*Date Stamp*	28 Jan 2014 16:19:12				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\JAN\DATA\EJT\NMR\2014-01-28-EJT-29\12\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn
Receiver Gain	32.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	27.000		

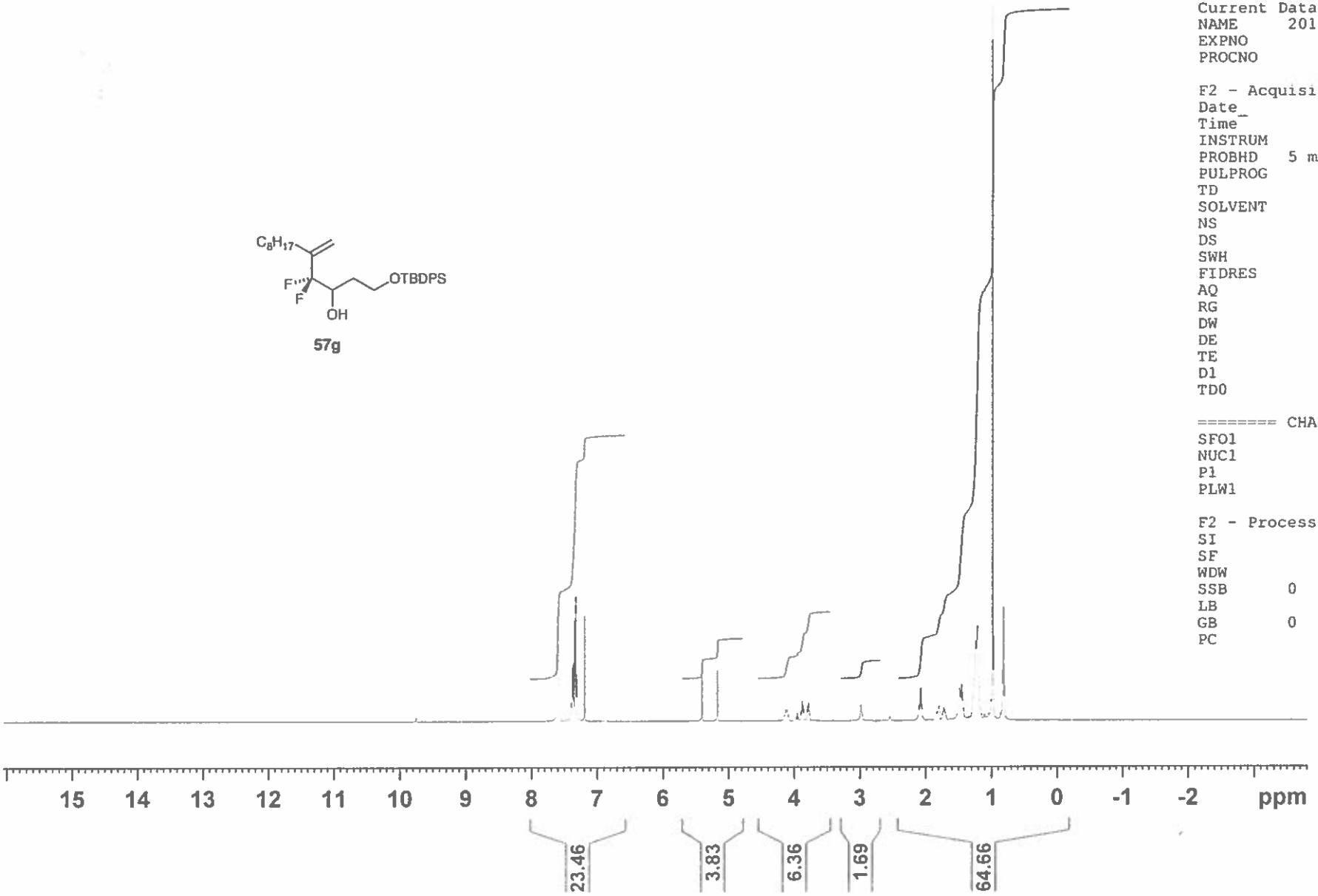


57*f*

No.	(ppm)	(Hz)	Height
1	-111.85	-52636.3	0.7016
2	-111.32	-52388.3	0.8938
3	-100.94	-47503.8	1.0000
4	-100.41	-47254.1	0.6694

P. Mears
EJT-PRM 120 prod F31-41
0214-029
mPROTON CDCl3 {E:\bruk500cdata\2014\Feb} staff 29

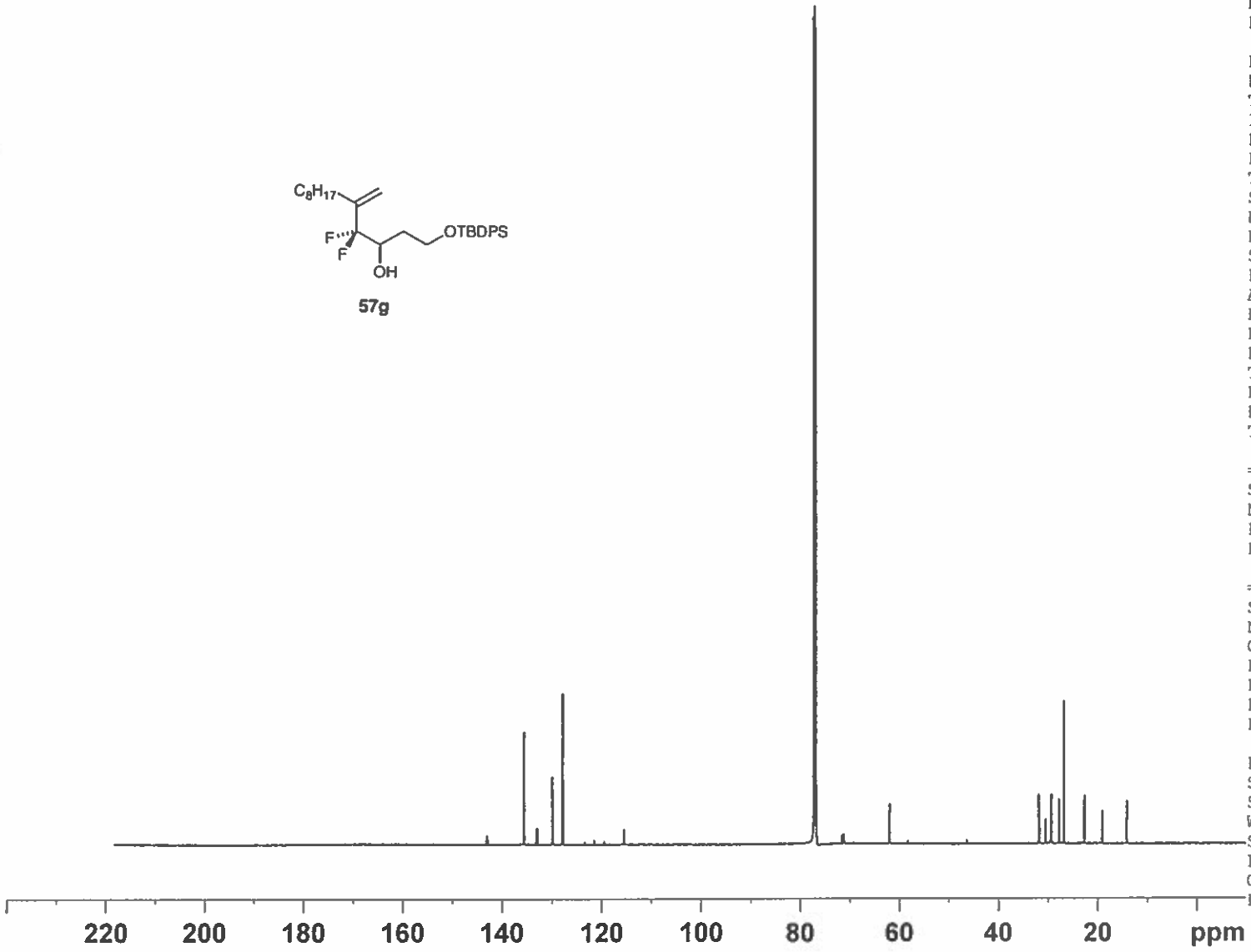
57g




```
Current Data Parameters
NAME      2014-02-18-staff-29
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140218
Time                  15.28
INSTRUM               spect
PROBHD    5 mm CPPBBO BB
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                      47.9
DW                   50.000 usec
DE                   13.87 usec
TE                   298.2 K
D1               1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1          500.1930889 MHz
NUC1                    1H
P1                   13.00 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                      65536
SF            500.1900500 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

mCARBON CDCl3 {E:\bruk500cdata\2014\Feb} staff 29

57g



Current Data Parameters
NAME 2014-02-18-staff-29
EXPNO 11
PROCNO 1

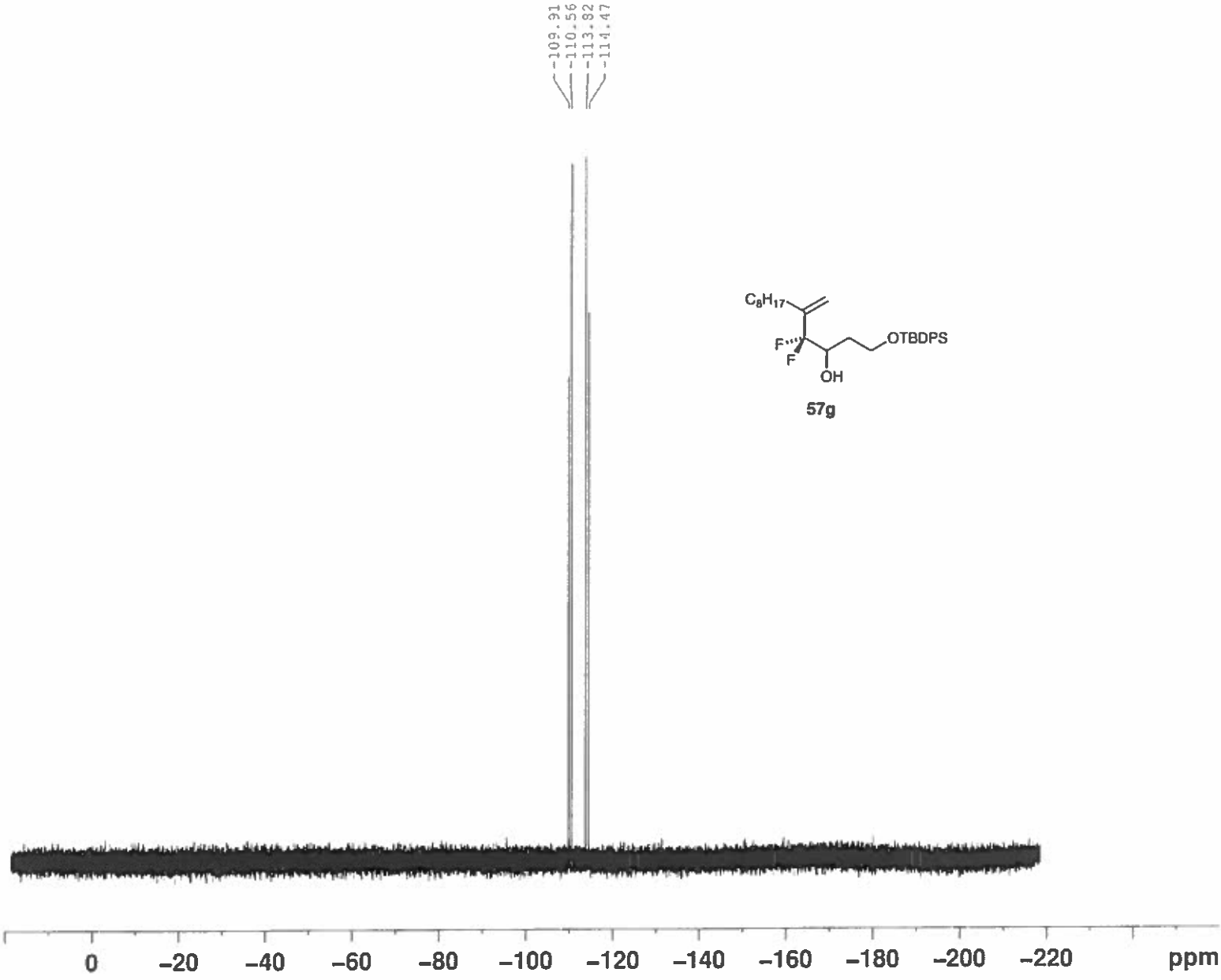
F2 - Acquisition Parameters
Date_ 20140218
Time 17.17
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 184.4
DW 16.800 usec
DE 102.82 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7854504 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.59999847 W

======== CHANNEL f2 ========
SFO2 500.1920008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.28622001 W
PLW13 0.18318000 W

F2 - Processing parameters
SI 32768
SF 125.7728760 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

EJT-PRM120 f95-113 24mg
mF19CPD CDCl3 {e:\bruk400data\2014\Feb} ejt 1



57g

NAME	2014-02-13-ejt-1
EXPNO	11
PROCNO	1
Date_	20140213
Time	13.50
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zgig
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	4100
DW	5.600 usec
DE	7.51 usec
TE	294.3 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	10.70 usec
PL1	-5.00 dB
PL1W	27.00716019 W
SFO1	376.4607164 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-3.60 dB
PL12	12.14 dB
PL2W	17.83863831 W
PL12W	0.47573122 W
SFO2	400.1316005 MHz
SI	262144
SF	376.4983660 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

EJT-PRM145 f5-13 113mg
mPROTON_A_night CDCl3 {e:\bruk400cdata\2014\Mar} ejt 11

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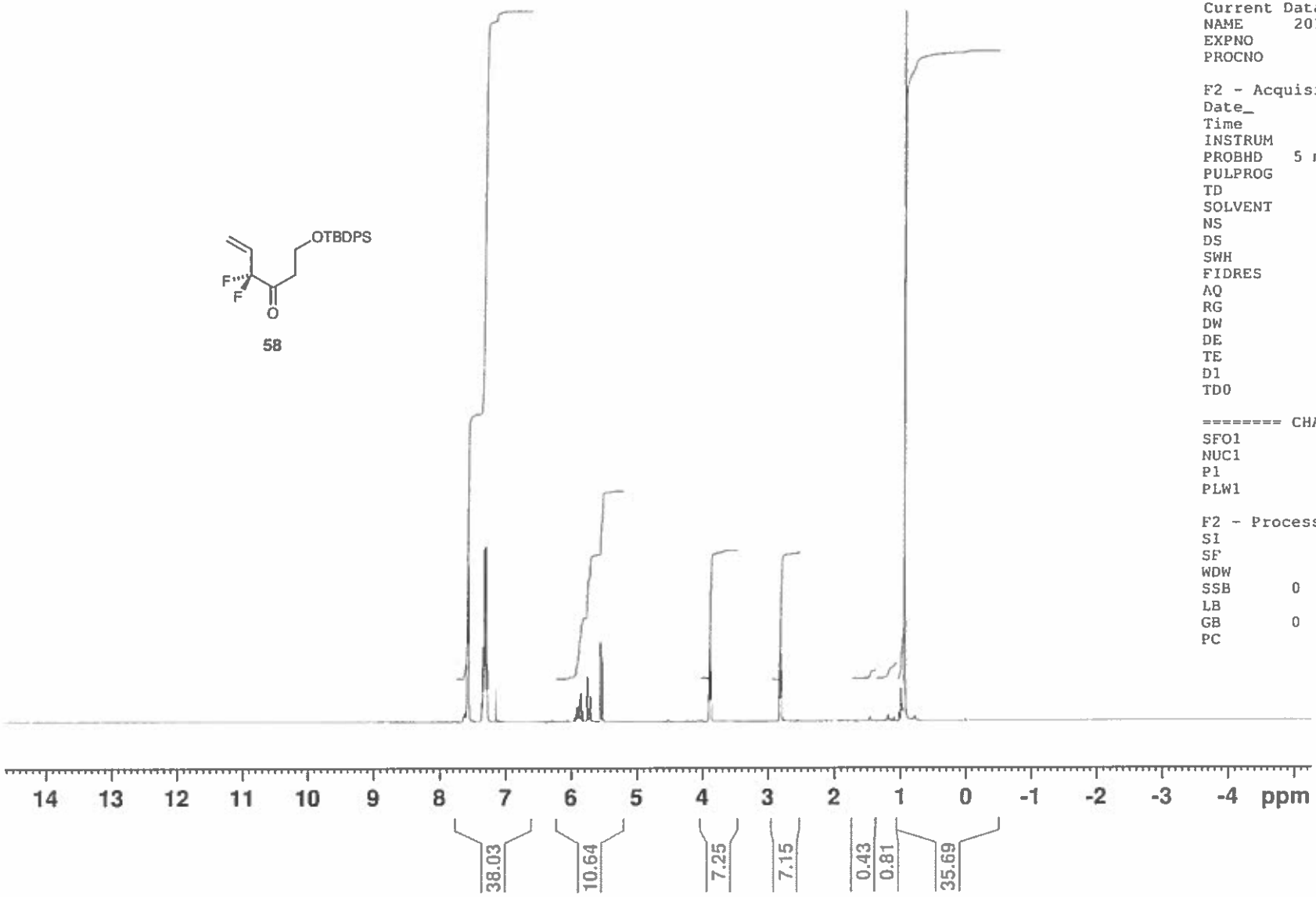
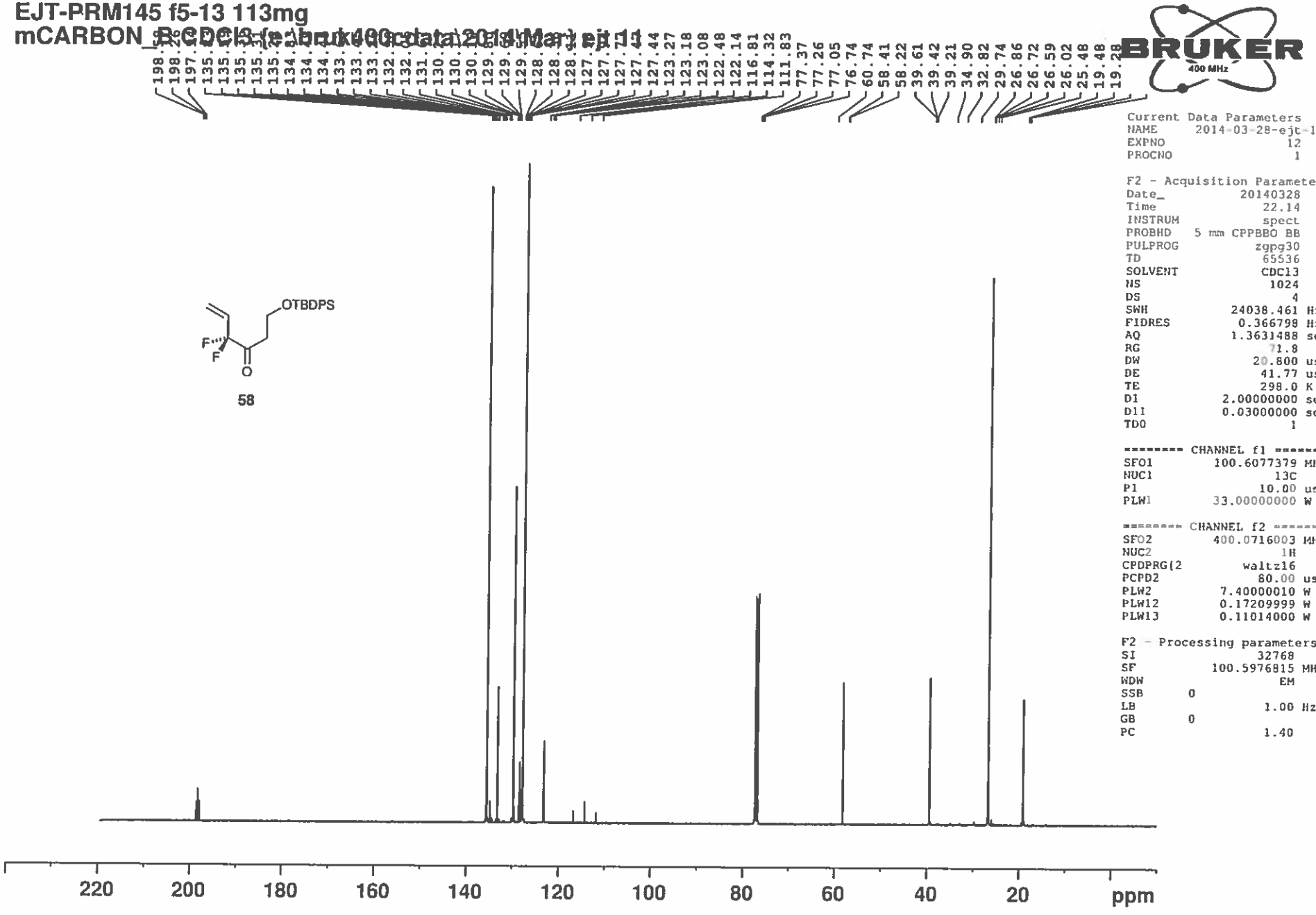



```
Current Data Parameters
NAME      2014-03-28-ejt-11
EXPNO                   13
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140328
Time                 22.16
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                    40.3
DW                  60.800 usec
DE                  10.00 usec
TE                  298.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.0718803 MHz
NUC1                   1H
P1                  12.00 usec
PLW1          7.40000010 W

F2 - Processing parameters
SI                  32768
SF           400.0700535 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

EJT-PRM145 f5-13 113mg

mCARBON_B:CDCl3-(e:\bruk400\data\2014\Mar) ejt 11



BRUKER 400 MHz

Current Data Parameters

NAME	2014-03-28-ejt-11
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20140328
Time	22.14
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631488 sec
RG	71.8
DW	20.800 usec
DE	41.77 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

SFO1	100.6077379 MHz
NUC1	13C
P1	10.00 usec
PLW1	33.00000000 W

======== CHANNEL f2 ========

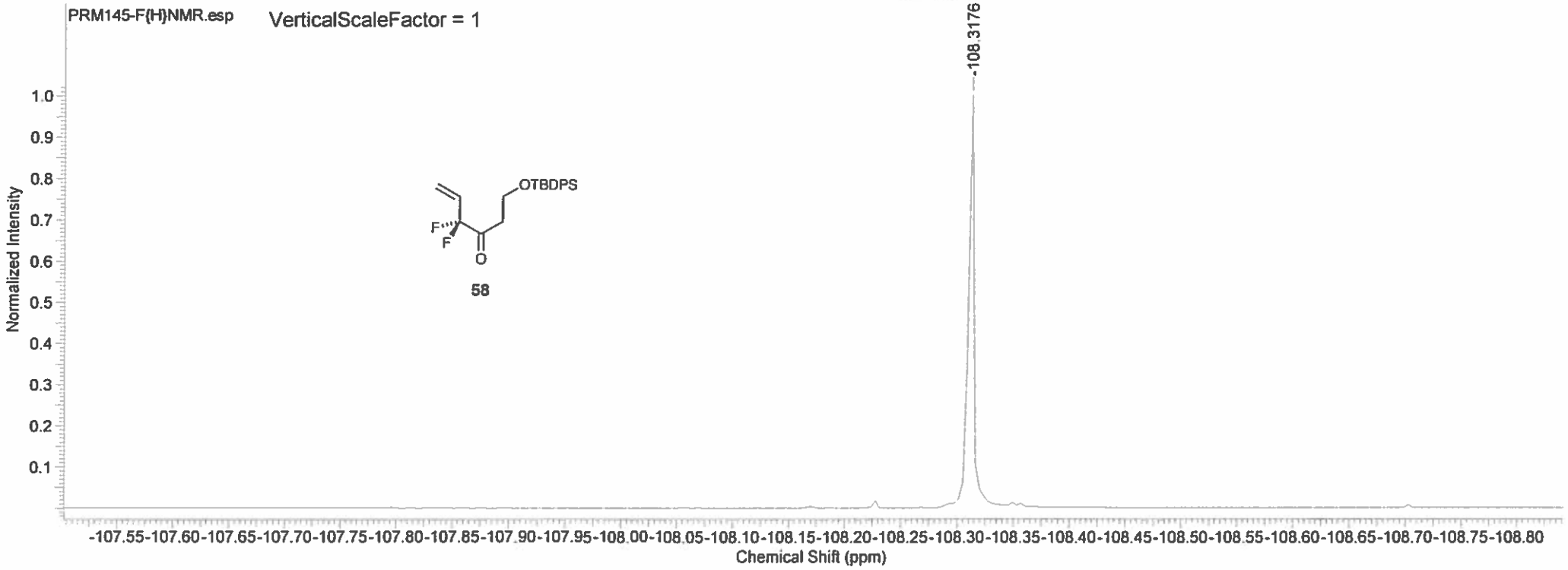
SFO2	400.0716003 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	7.40000010 W
PLW12	0.17209999 W
PLW13	0.11014000 W

F2 - Processing parameters

SI	32768
SF	100.5976815 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

07/04/2014 13:54:05

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM145 f3-7 40mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 5				
Date	26 Mar 2014 14:26:08	*Date Stamp*	26 Mar 2014 14:26:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\MAR\DATA\EJT\NMR\2014-03-26-EJT-5\12\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgflhigqn
Receiver Gain	575.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	27.000		



No.	(ppm)	(Hz)	Height
1	-108.32	-50973.4	1.0000

EJT-PRM146 phosphoranylidene f14-24 20mg
mPROTON_A CDCl3 {e:\bruk400cdata\2014\Apr} ejt 42

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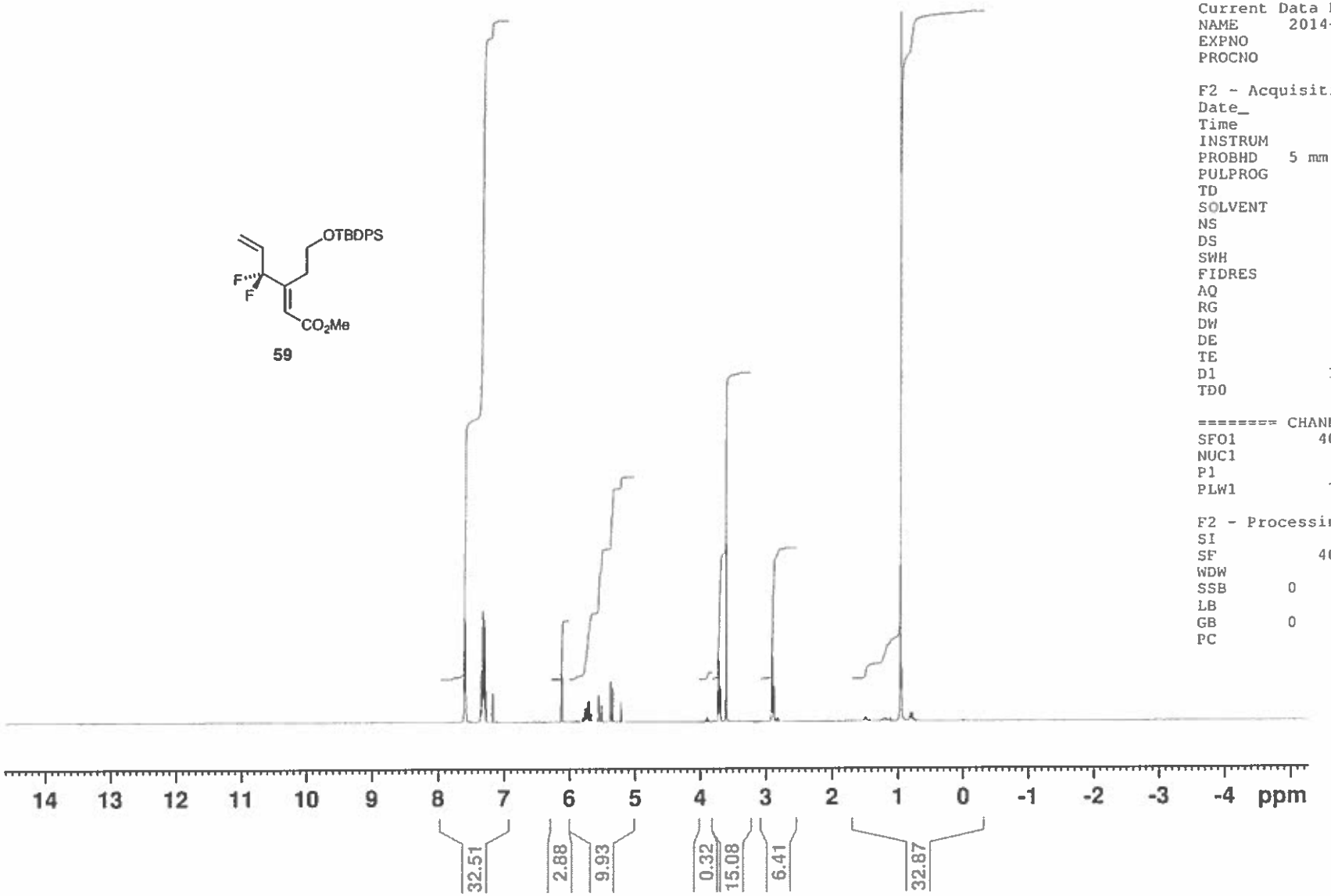
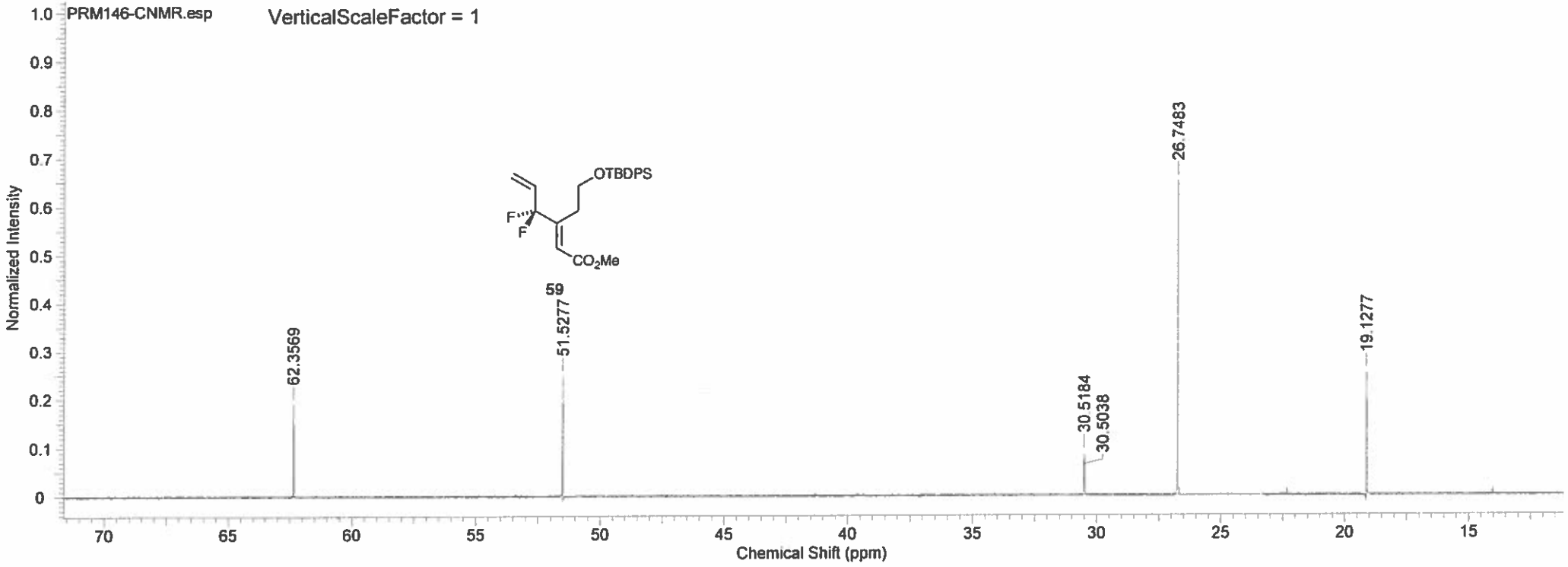



```
Current Data Parameters
NAME      2014-04-01-ejt-42
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140401
Time                  12.26
INSTRUM               spect
PROBHD    5 mm CPPBBO BB
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     90.5
DW                  62.400 usec
DE                  10.00 usec
TE                  298.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.0719003 MHz
NUC1                   1H
P1                  12.00 usec
PLW1           7.40000010 W

F2 - Processing parameters
SI                   65536
SF             400.0700435 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

07/04/2014 15:31:32

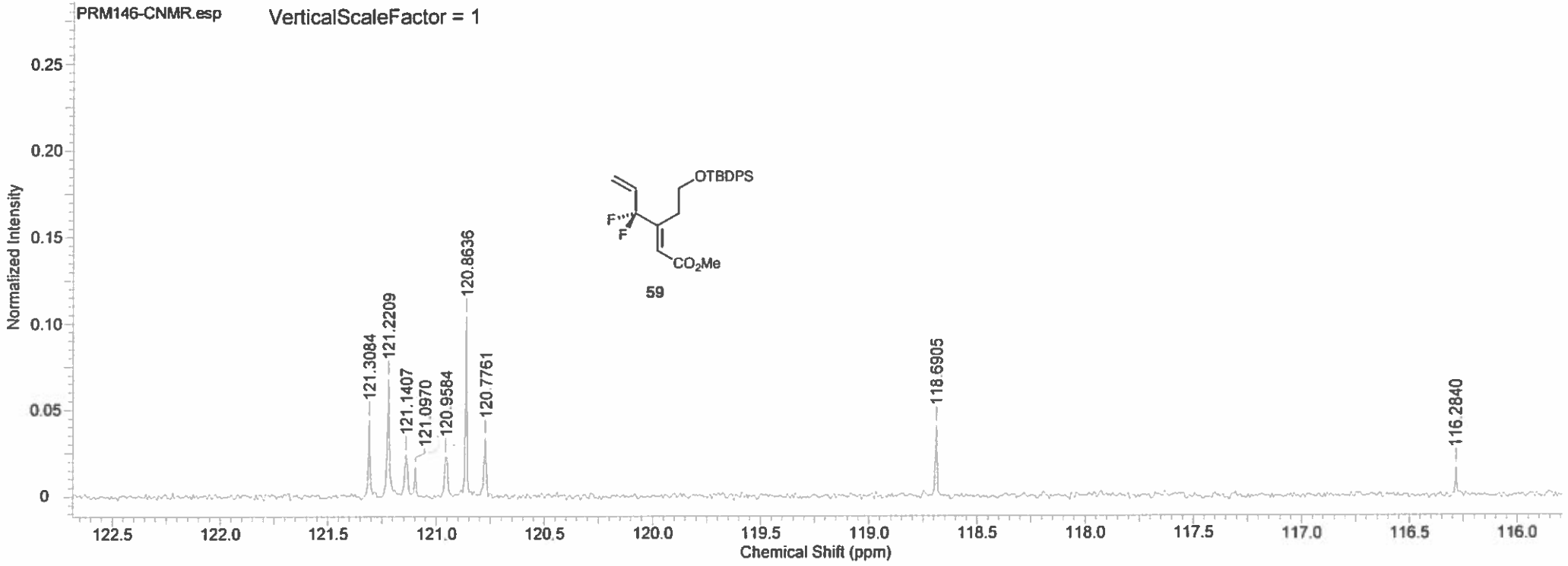
Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM146 prod alkene mCARBON_B CDCl3 {e:\bruk400cdata\2014\Apr} ejt 24				
Date	03 Apr 2014 19:05:52			*Date Stamp*	03 Apr 2014 19:05:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2014\Apr\data\ejt\nmr\2014-04-03-ejt-24\10\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10052.8125	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	19.13	1924.2	0.2521
2	26.75	2690.8	0.6509
3	30.50	3068.6	0.0458
4	30.52	3070.1	0.0862
5	30.53	3071.5	0.0407
6	51.53	5183.6	0.2488
7	62.36	6273.0	0.1910

07/04/2014 15:34:44

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM146 prod alkene mCARBON_B CDCl3 (e:\bruk400cdata\2014\Apr) ejt 24				
Date	03 Apr 2014 19:05:52			*Date Stamp*	03 Apr 2014 19:05:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2014\Apr\data\ejt\nmr\2014-04-03-ejt-24\10\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10052.8125	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	19.13	1924.2	0.2521
2	26.75	2690.8	0.6509
3	30.50	3068.6	0.0458
4	30.52	3070.1	0.0862

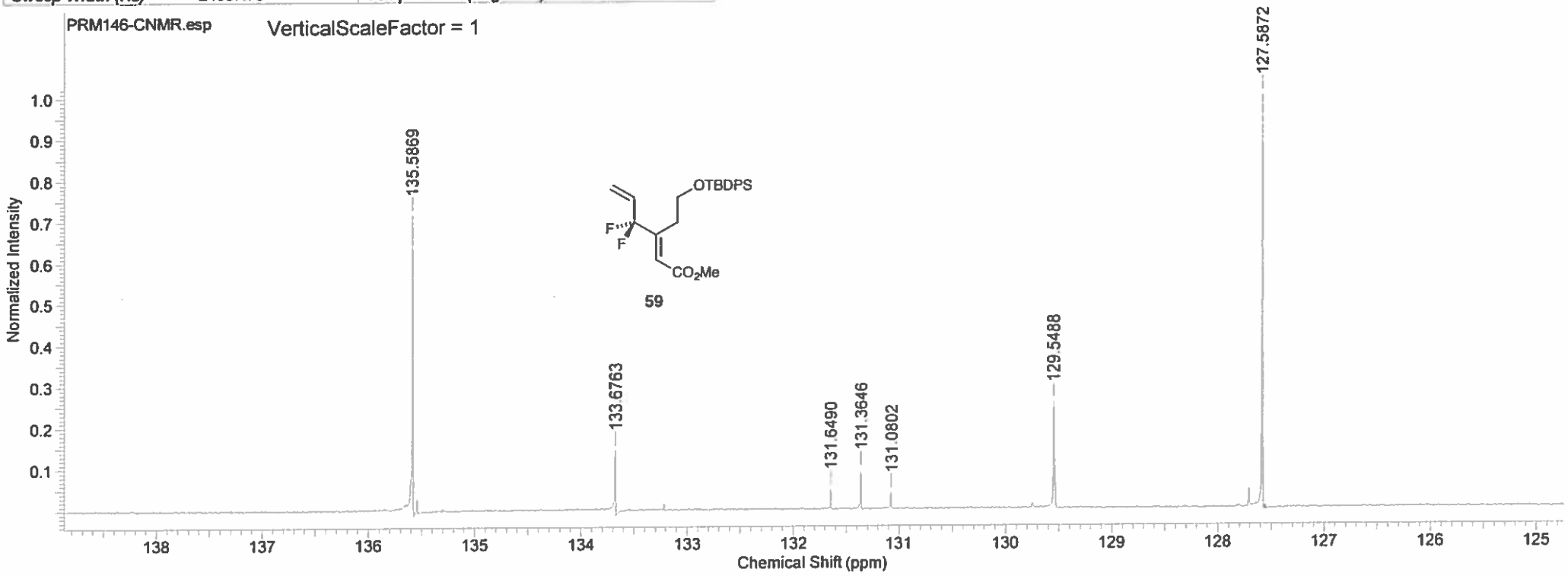
No.	(ppm)	(Hz)	Height
5	30.53	3071.5	0.0407
6	51.53	5183.6	0.2488
7	62.36	6273.0	0.1910
8	116.28	11697.9	0.0158

No.	(ppm)	(Hz)	Height
9	118.69	11940.0	0.0403
10	120.78	12149.8	0.0338
11	120.86	12158.6	0.1039
12	120.96	12168.1	0.0228

No.	(ppm)	(Hz)	Height
13	121.10	12182.1	0.0171
14	121.14	12186.5	0.0241
15	121.22	12194.5	0.0676
16	121.31	12203.3	0.0440

07/04/2014 15:41:55

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM146 prod alkene mCARBON_B CDCl3 {e:\bruk400cdata\2014\Apr} ejt 24				
Date	03 Apr 2014 19:05:52			*Date Stamp*	03 Apr 2014 19.05:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2014\Apr\data\ejt\nmr\2014-04-03-ejt-24\10\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10052.8125	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	19.13	1924.2	0.2521
2	26.75	2690.8	0.6509
3	30.50	3068.6	0.0458
4	30.52	3070.1	0.0862
5	30.53	3071.5	0.0407

No.	(ppm)	(Hz)	Height
6	51.53	5183.6	0.2488
7	62.36	6273.0	0.1910
8	116.28	11697.9	0.0158
9	118.69	11940.0	0.0403
10	120.78	12149.8	0.0338

No.	(ppm)	(Hz)	Height
11	120.86	12158.6	0.1039
12	120.96	12168.1	0.0228
13	121.10	12182.1	0.0171
14	121.14	12186.5	0.0241
15	121.22	12194.5	0.0676

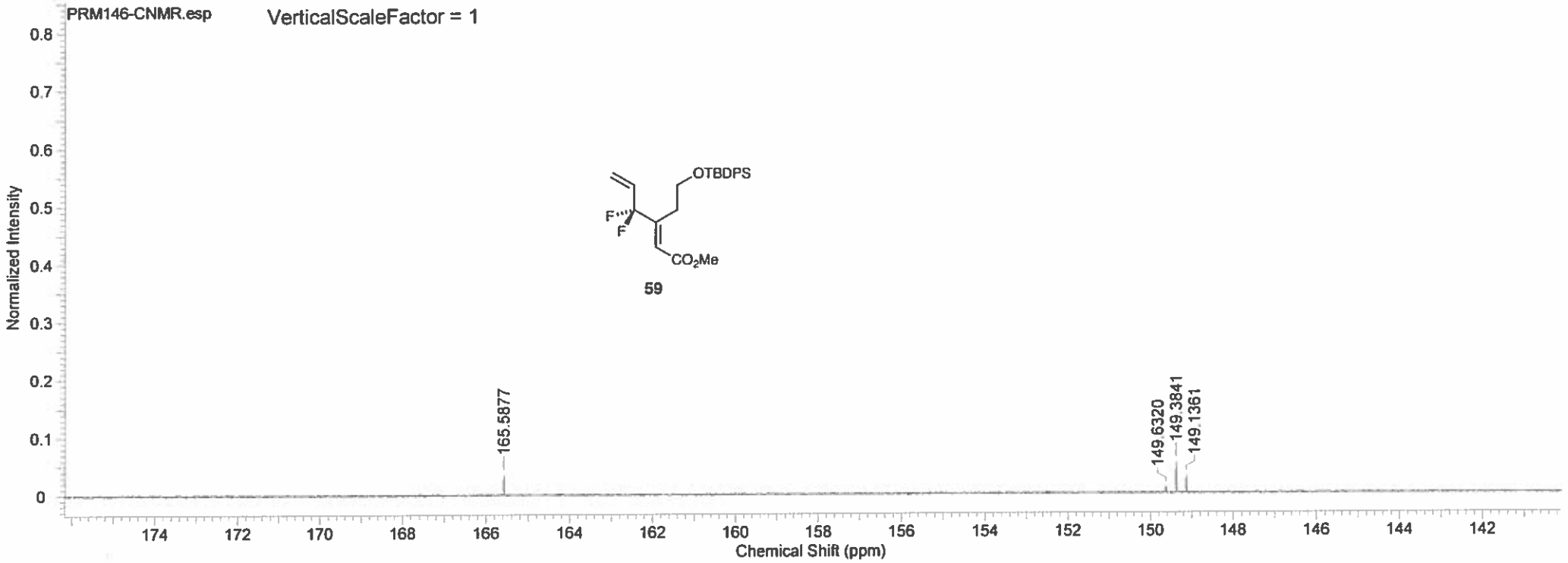
No.	(ppm)	(Hz)	Height
16	121.31	12203.3	0.0440
17	127.59	12835.0	1.0000
18	129.55	13032.3	0.2574
19	131.08	13186.4	0.0393
20	131.36	13215.0	0.0929

No.	(ppm)	(Hz)	Height
21	131.65	13243.6	0.0470
22	133.68	13447.5	0.1445
23	135.59	13639.7	0.7165

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

07/04/2014 15:45:55

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM146 prod alkene mCARBON_B CDCl3 {e:\bruk400cdata\2014\Apr} ejt 24				
Date	03 Apr 2014 19:05:52			*Date Stamp*	03 Apr 2014 19:05:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2014\Apr\data\ejt\nmr\2014-04-03-ejt-24\10\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10052.8125	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	19.13	1924.2	0.2521
2	26.75	2690.8	0.6509
3	30.50	3068.6	0.0458
4	30.52	3070.1	0.0862
5	30.53	3071.5	0.0407
6	51.53	5183.6	0.2488

No.	(ppm)	(Hz)	Height
7	62.36	6273.0	0.1910
8	116.28	11697.9	0.0158
9	118.69	11940.0	0.0403
10	120.78	12149.8	0.0338
11	120.86	12158.6	0.1039
12	120.96	12168.1	0.0228

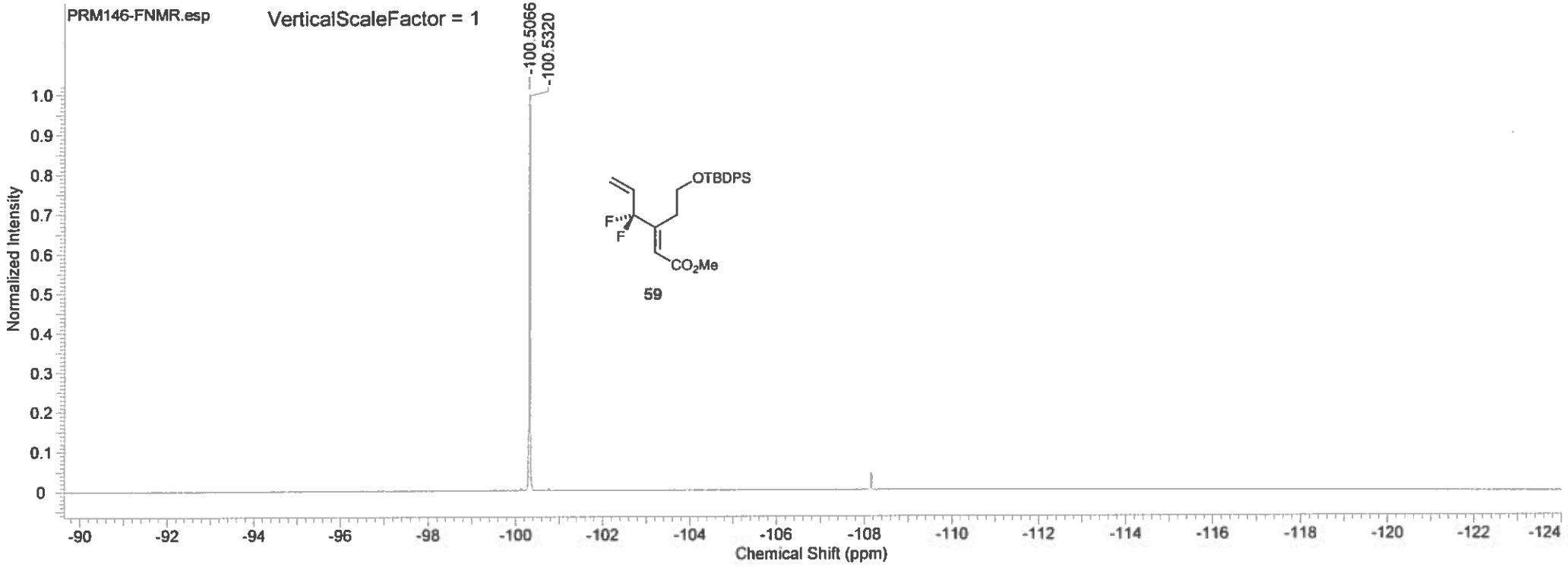
No.	(ppm)	(Hz)	Height
13	121.10	12182.1	0.0171
14	121.14	12186.5	0.0241
15	121.22	12194.5	0.0676
16	121.31	12203.3	0.0440
17	127.59	12835.0	1.0000
18	129.55	13032.3	0.2574

No.	(ppm)	(Hz)	Height
19	131.08	13186.4	0.0393
20	131.36	13215.0	0.0929
21	131.65	13243.6	0.0470
22	133.68	13447.5	0.1445
23	135.59	13639.7	0.7165
24	149.14	15002.7	0.0301

No.	(ppm)	(Hz)	Height
25	149.38	15027.7	0.0526
26	149.63	15052.6	0.0103
27	165.59	16657.7	0.0357

07/04/2014 16:11:28

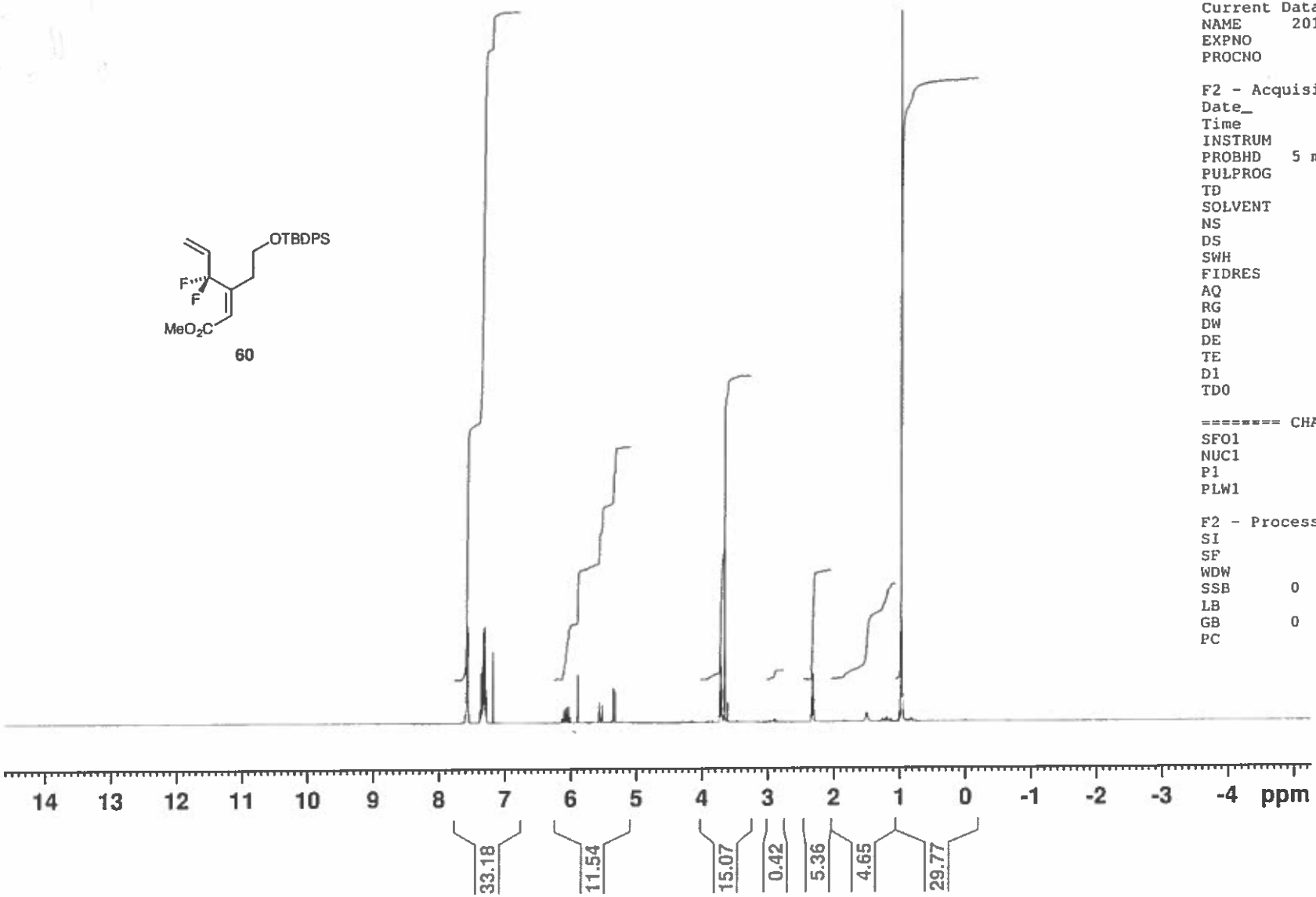
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM146 phosphoranylidene f14-24 20mg mF19_cryo CDCl3 (e:\bruk400cdata\2014\Apr) ejt 42				
Date	01 Apr 2014 12:29:04	*Date Stamp*	01 Apr 2014 12:29:04				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2014\Apr\data\ejt\nmr\2014-04-01-ejt-42\11\fid					*Frequency (MHz)*	376.44
Nucleus	19F	*Number of Transients*	4	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zg	*Receiver Gain*	16.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37644.8594	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	25.000				



No.	(ppm)	(Hz)	Height
1	-100.53	-37844.4	0.9733
2	-100.51	-37834.9	1.0000

EJT-PRM146 isomer data
mPROTON_A_night CDCl3 {e:\bruk400cdata\2014\Apr} ejt 18

60

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Current Data Parameters
NAME      2014-04-29-ejt-18
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140430
Time                   3.52
INSTRUM               spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                       114
DW                    60.800 usec
DE                    10.00 usec
TE                    298.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            400.0718803 MHz
NUC1                      1H
P1                    12.00 usec
PLW1           7.40000010 W

F2 - Processing parameters
SI                        32768
SF              400.0700399 MHz
WDW                       EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
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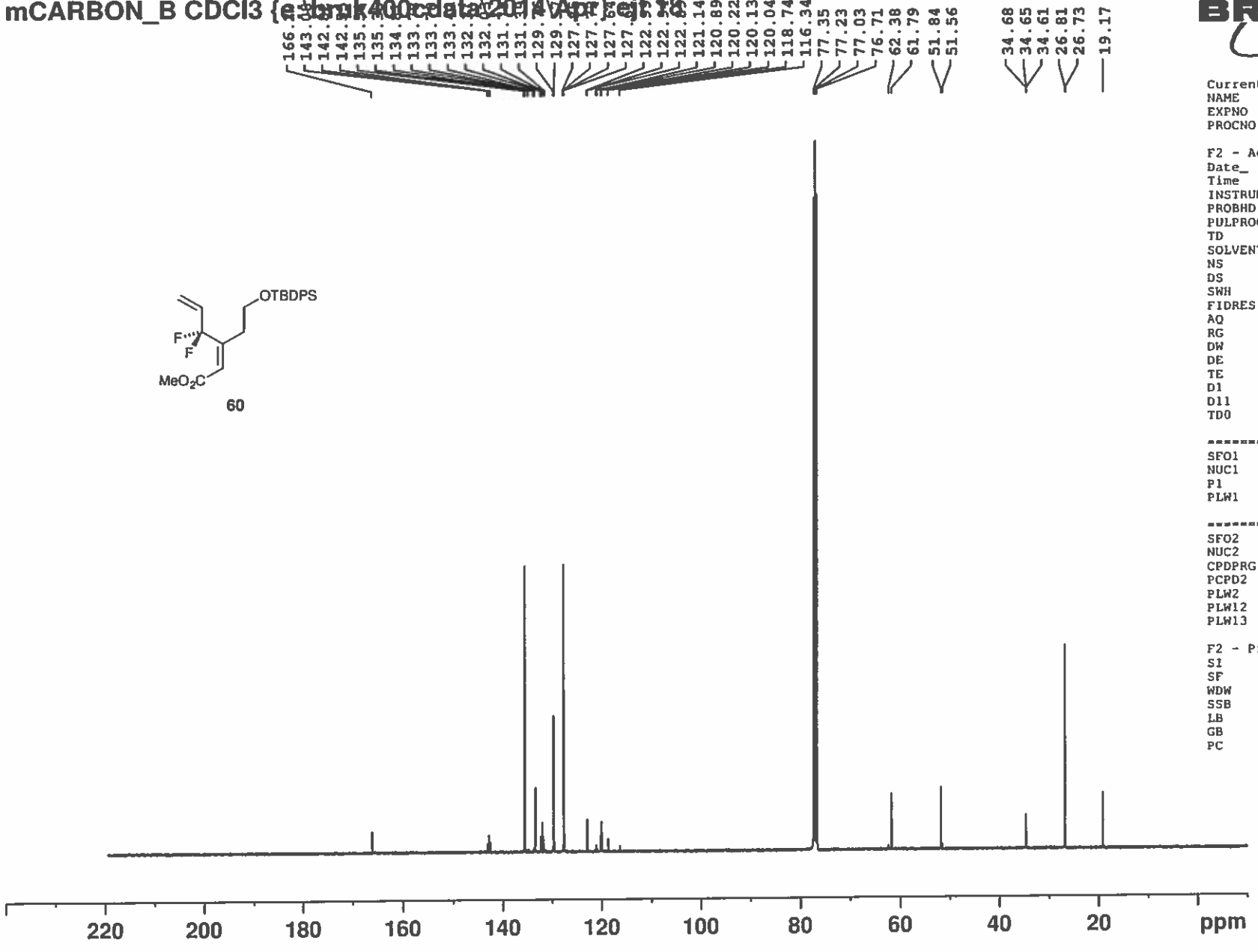
EJT-PRM146 isomer data
mCARBON_B CDCl3 {e:\bruk400c\data\2014_Apr\ejt-18



BRUKER 400 MHz

Current Data Parameters
NAME 2014-04-29-ejt-18
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140430
Time 3.49
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 41.77 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

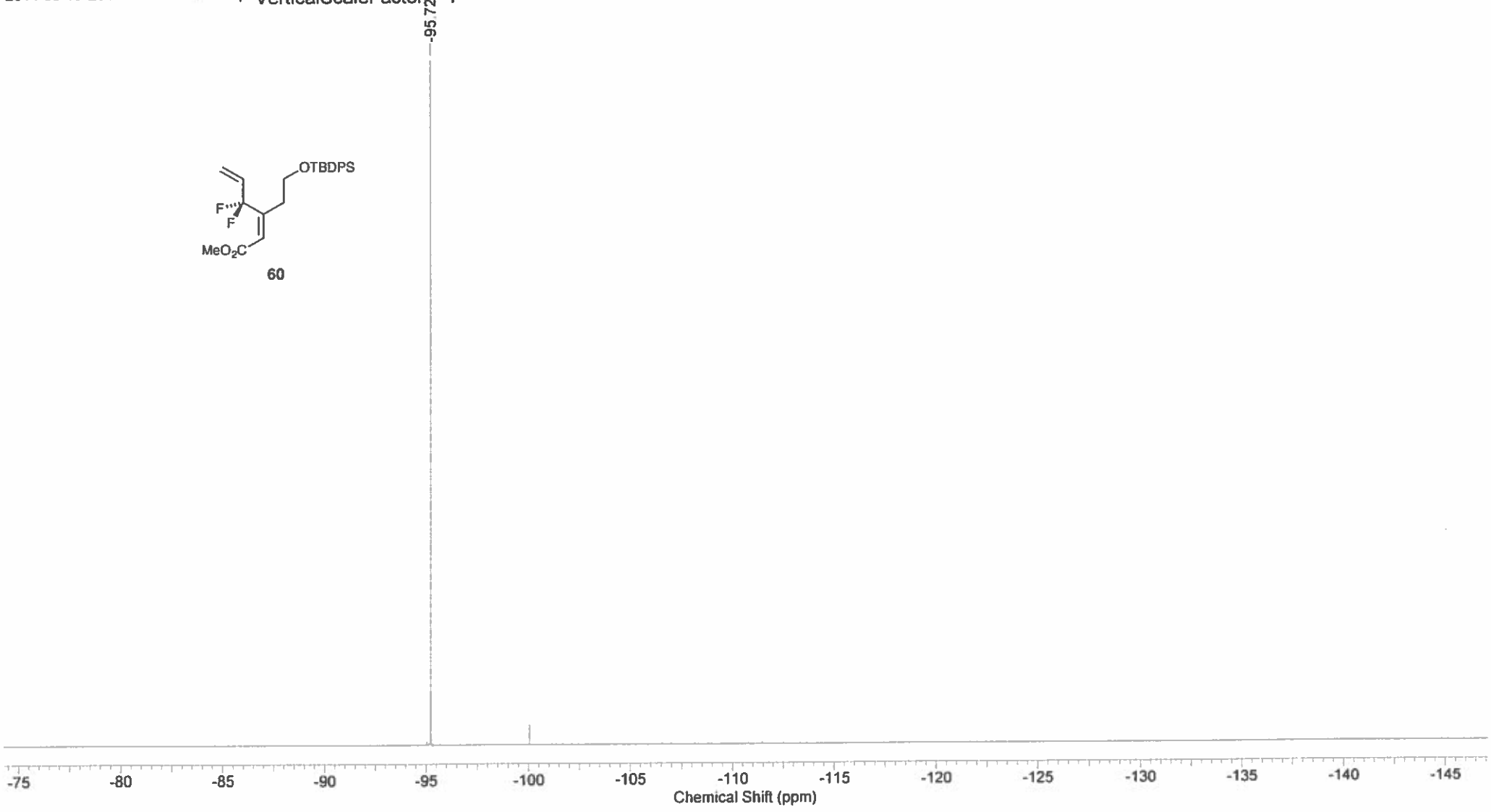
======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM146 f44-48 40mg mF19CPD CDCl3 {e:\bruk400data\2014\May} ejt 23				
Date	19 May 2014 19:08:00	*Date Stamp*	19 May 2014 19:08:00				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\MAY\DATA\EJT\NMR\2014-05-19-EJT-23\22\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	22.600		

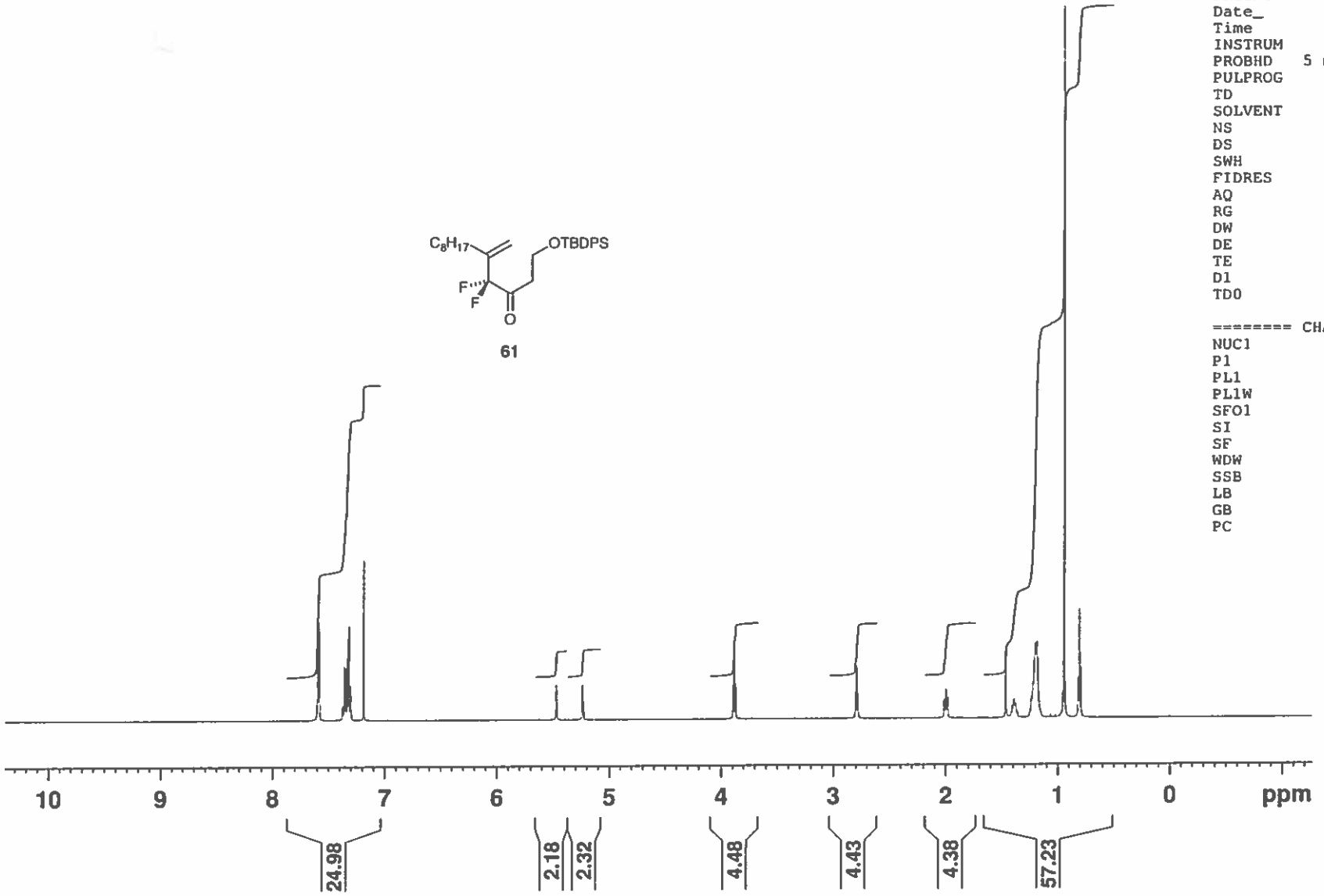
2014-05-19-EJT-23.022.001.1R.esp VerticalScaleFactor[3] 1

60



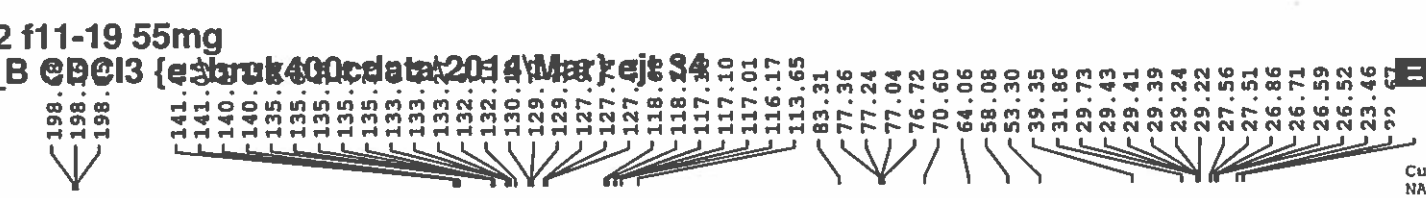
EJT–PRM132 f5–10 7mg
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 28

61

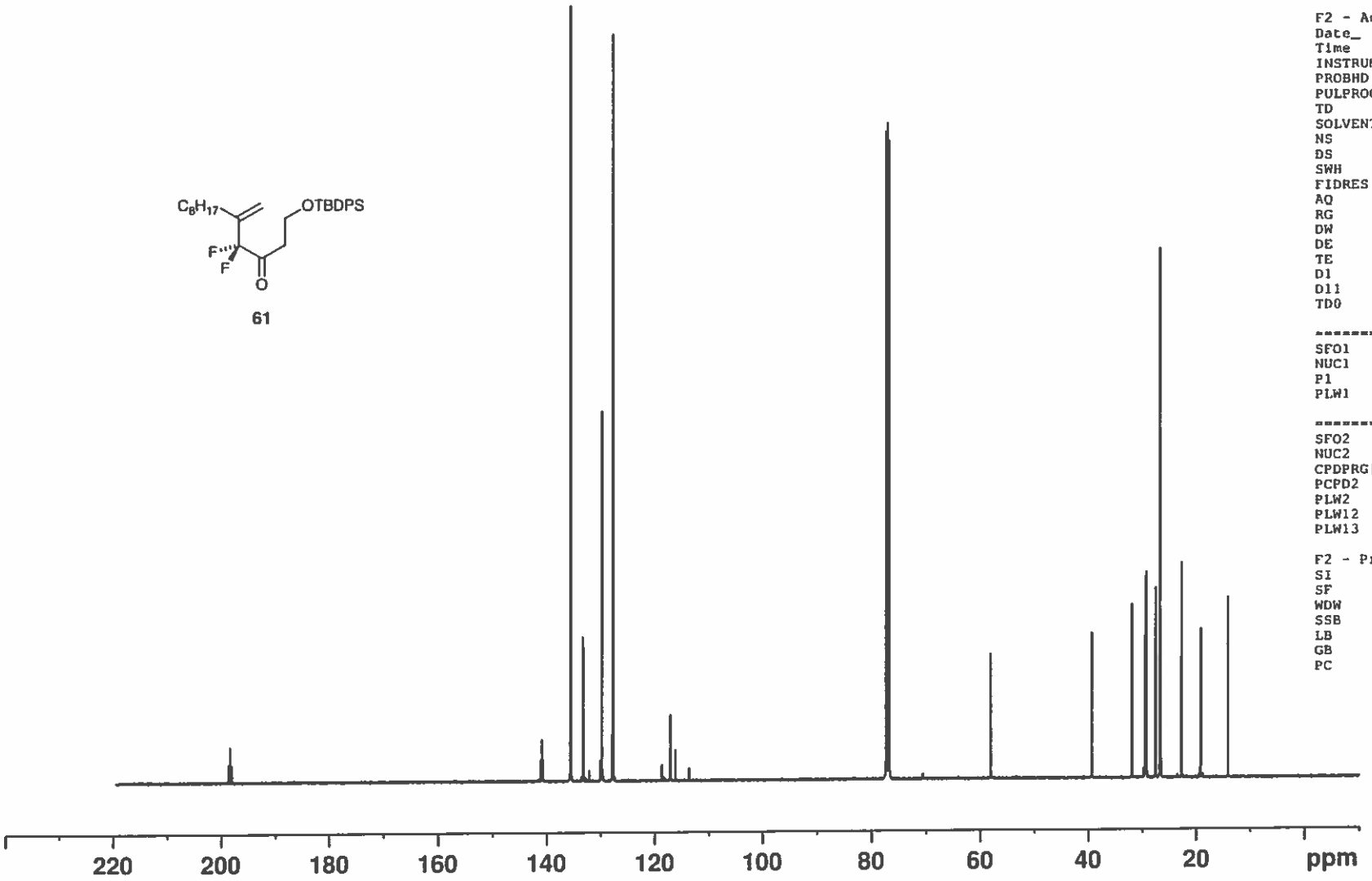


NAME	2014-03-03-ejt-28
EXPNO	10
PROCNO	1
Date_	20140303
Time	14.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	228
DW	48.400 usec
DE	13.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300498 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

EJT-PRM132 f11-19 55mg
mCARBON_B CDCl3 {e:\bruk400cdata\2014\Mar\ejt-34



61

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Current Data Parameters
NAME      2014-03-05-ejt-34
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140306
Time                   2.59
INSTRUM               spect
PROBHD    5 mm CPPBBO BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    45.2
DW                20.800 usec
DE                41.77 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6077379 MHz
NUC1                   13C
P1                 10.00 usec
PLW1          33.00000000 W

======== CHANNEL f2 ========
SFO2          400.0716003 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2              80.00 usec
PLW2           7.40000010 W
PLW12          0.17209999 W
PLW13          0.11014000 W

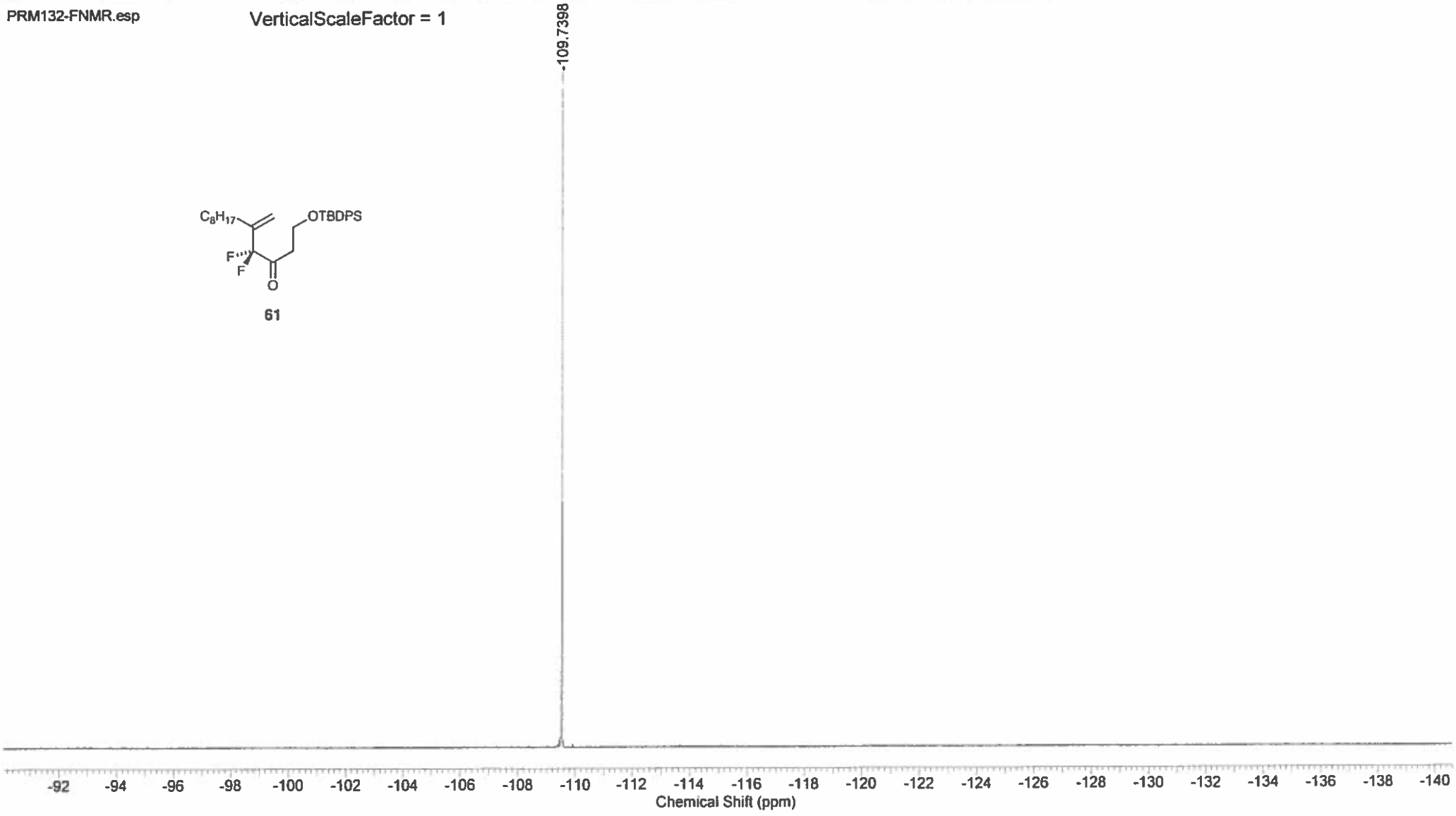
F2 - Processing parameters
SI                    32768
SF            100.5976815 MHz
WDW                      EM
SSB       0
LB                 1.00 Hz
GB        0
PC                    1.40
```

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM132 f5-10 7mg m19F CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 28				
Date	03 Mar 2014 14:21:52	*Date Stamp*	03 Mar 2014 14:21:52				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\MAR\DATA\EJT\NMR\2014-03-03-EJT-28\11\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgflqn
Receiver Gain	362.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	27.000		

PRM132-FNMR.esp

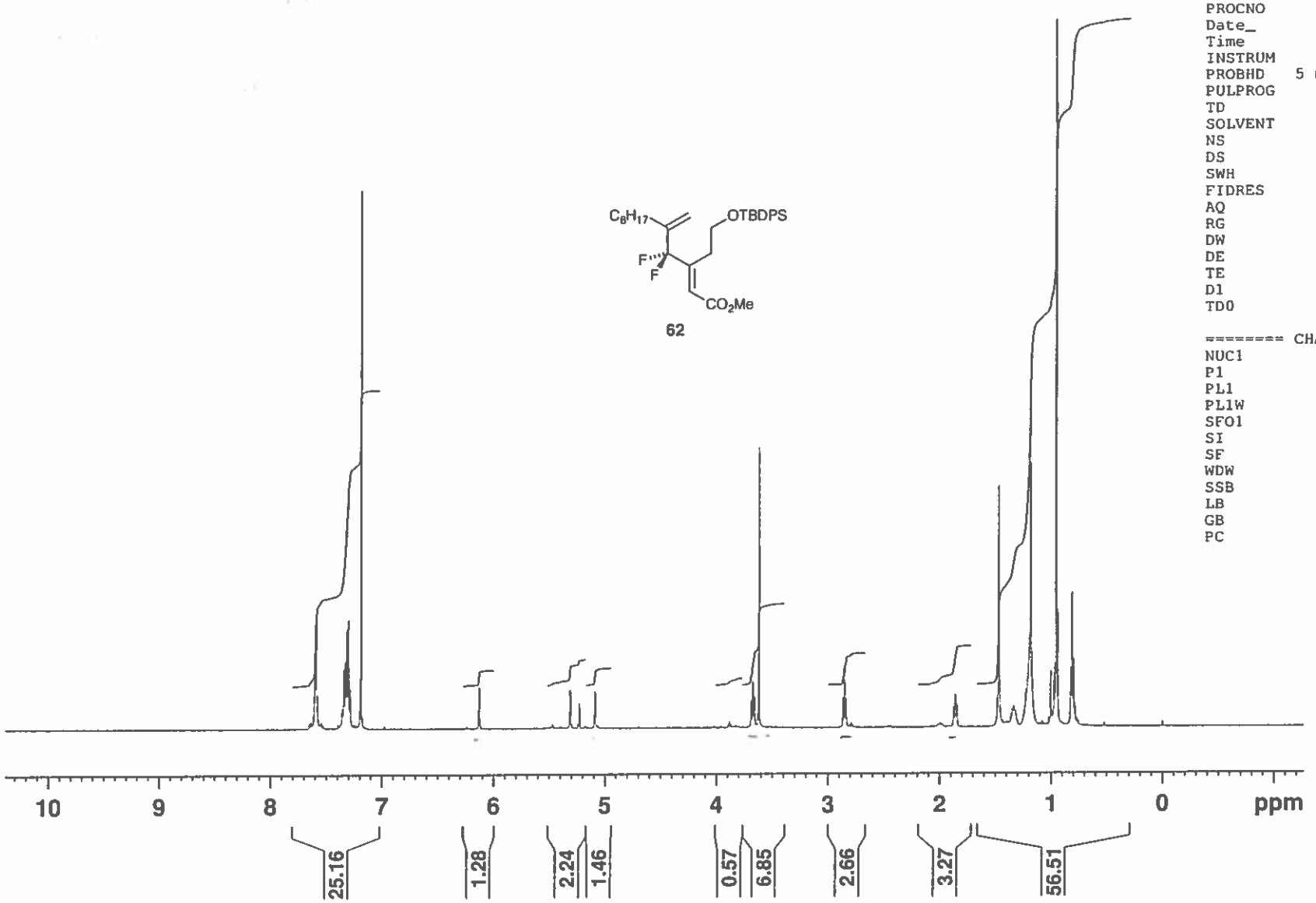
VerticalScaleFactor = 1

61



EJT-PRM133 f16-21 4mg
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 7

62



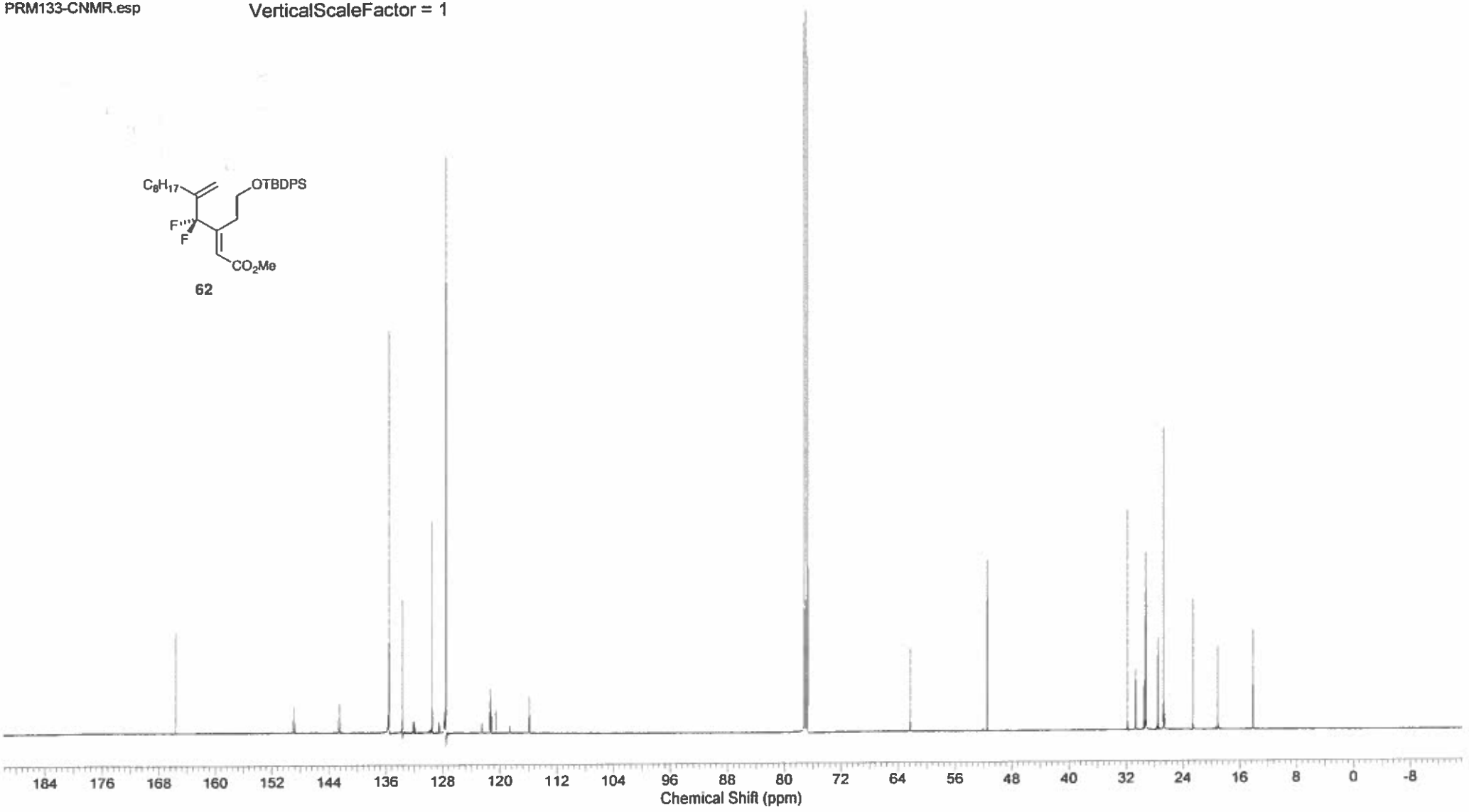
NAME	2014-03-07-ejt-7
EXPNO	10
PROCNO	1
Date_	20140307
Time	15.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDC13
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	287
DW	48.400 usec
DE	13.00 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300487 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Acquisition Time (sec)	1.1010	*Comment*	P. Mears EJT-PRM133prod 0614-032 mCARBON CDCl3 {E:\bruk500cdata\2014\Jun} staff 42				
Date	20 Jun 2014 07:19:44	*Date Stamp*	20 Jun 2014 07:19:44				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2014\Jun\data\staff\nmr\2014-06-19-staff-42\12\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10240	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12568.6943	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.159				

PRM133-CNMR.esp

VerticalScaleFactor = 1

62

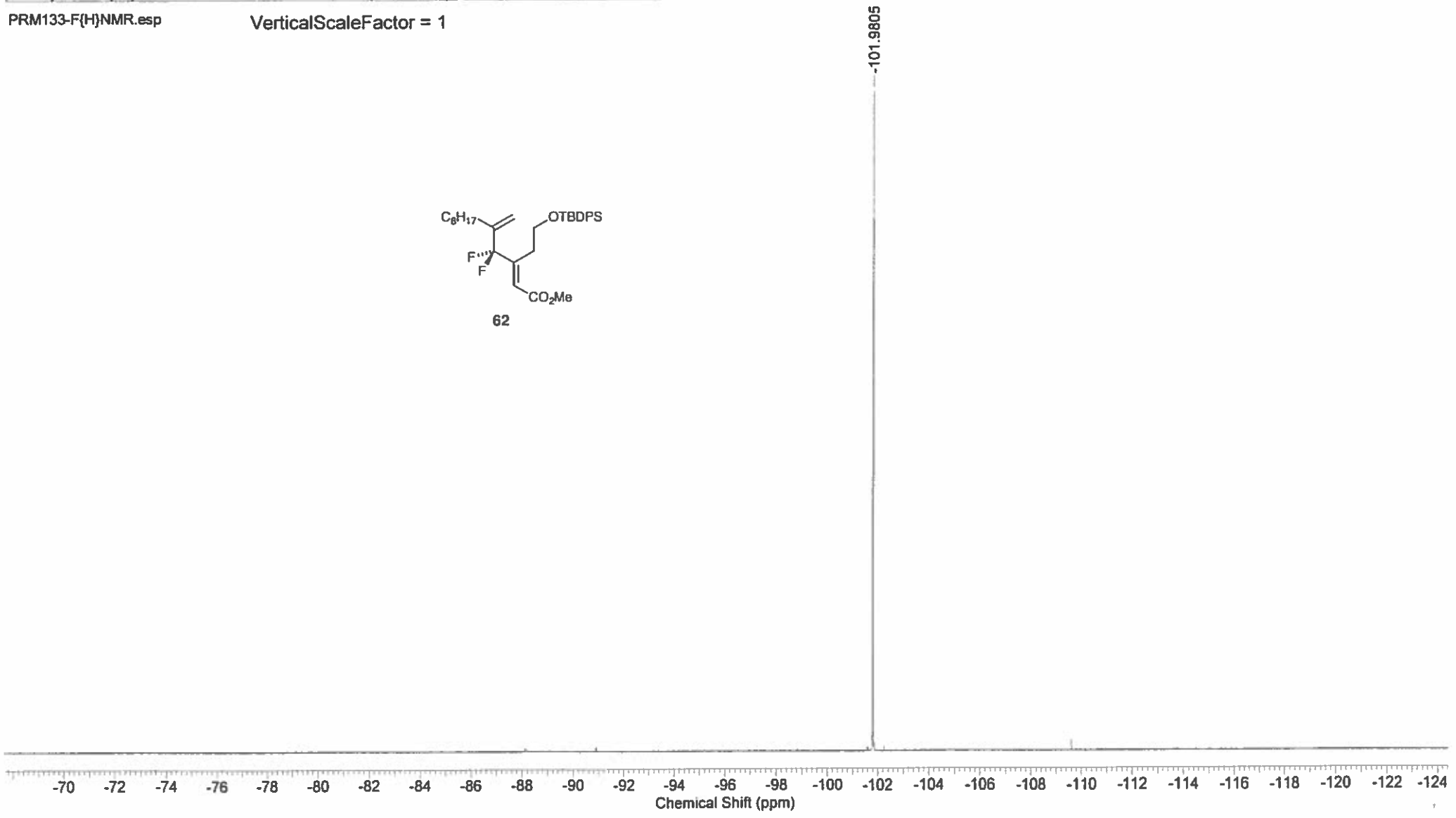


Acquisition Time (sec)	0.7340	***Comment***	EJT-PRM133 f14-21 17mg mF19CPD CDCl3 (e:\bruk400adata\2014\Jun) ejt 28				
Date	17 Jun 2014 12:50:24			***Date Stamp***	17 Jun 2014 12:50:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2014\Jun\data\ejt\nmr\2014-06-17-ejt-28\12\fid					***Frequency (MHz)***	376.50
Nucleus	19F	***Number of Transients***	16	***Origin***	AV400	***Original Points Count***	65536
Owner	nmrsu	***Points Count***	65536	***Pulse Sequence***	zgig	***Receiver Gain***	2050.00
SW(cyclical) (Hz)	89285.71	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	-37649.5977	***Spectrum Type***	STANDARD
Sweep Width (Hz)	89284.35	***Temperature (degree C)***	22.400				

PRM133-F{H}NMR.esp

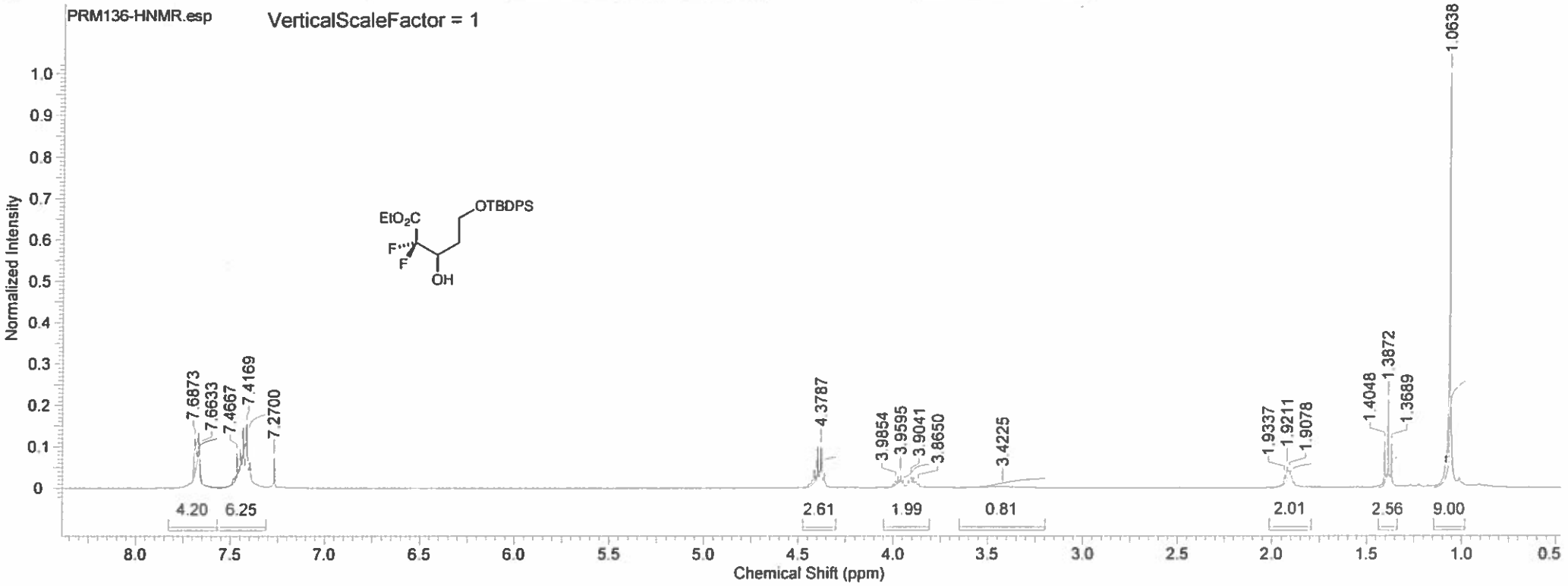
VerticalScaleFactor = 1

62



02/04/2014 17:04:51

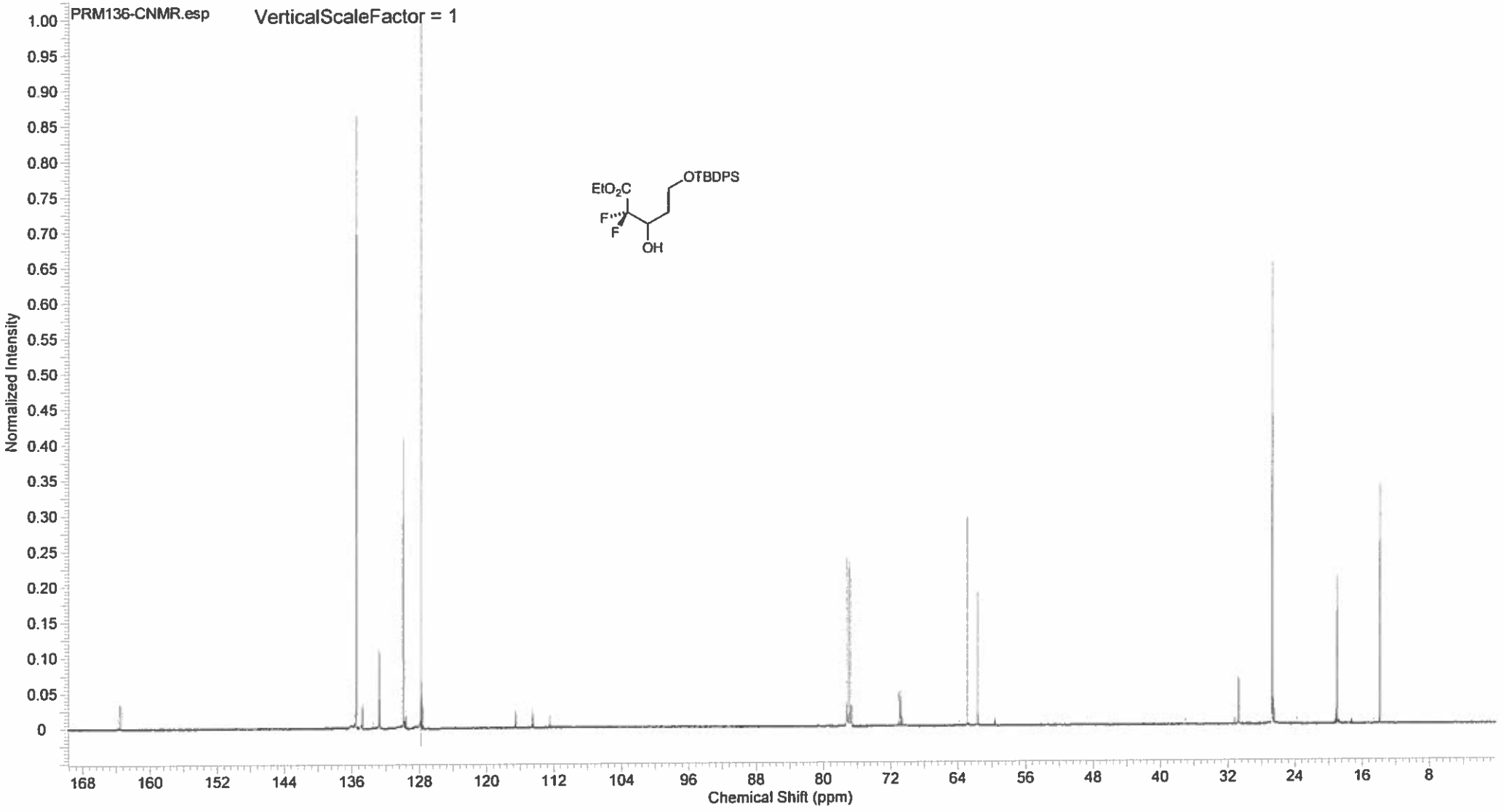
Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM136 prod mPROTON CDCl3 {e:\bruk400data\2014\Mar} ejt 44			*Date*	14 Mar 2014 11:46:08
Date Stamp	14 Mar 2014 11:46:08	*File Name*	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\MAR\DATA\EJT\NMR\2014-03-14-EJT-44\10\PDATA\1\1R				
Frequency (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	128.00	*SW(cyclical) (Hz)*	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.6750
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8264.21	*Temperature (degree C)*	21.400		



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	9815 .. 1.148	8.99984264	1.72771696e+8	8.99984264
2	3378 .. 1.432	2.56114244	4.91667400e+7	2.56114244
3	7934 .. 2.012	2.00694013	3.85276120e+7	2.00694013
4	1978 .. 3.650	0.80761468	1.55039330e+7	0.80761468
5	3076 .. 4.04	1.98614478	3.81284000e+7	1.98614478
6	3008 .. 4.472	2.61058092	5.01158200e+7	2.61058092
7	3095 .. 7.566	6.25181770	1.20017336e+8	6.25181770
8	5699 .. 7.824	4.19923115	8.06134400e+7	4.19923115

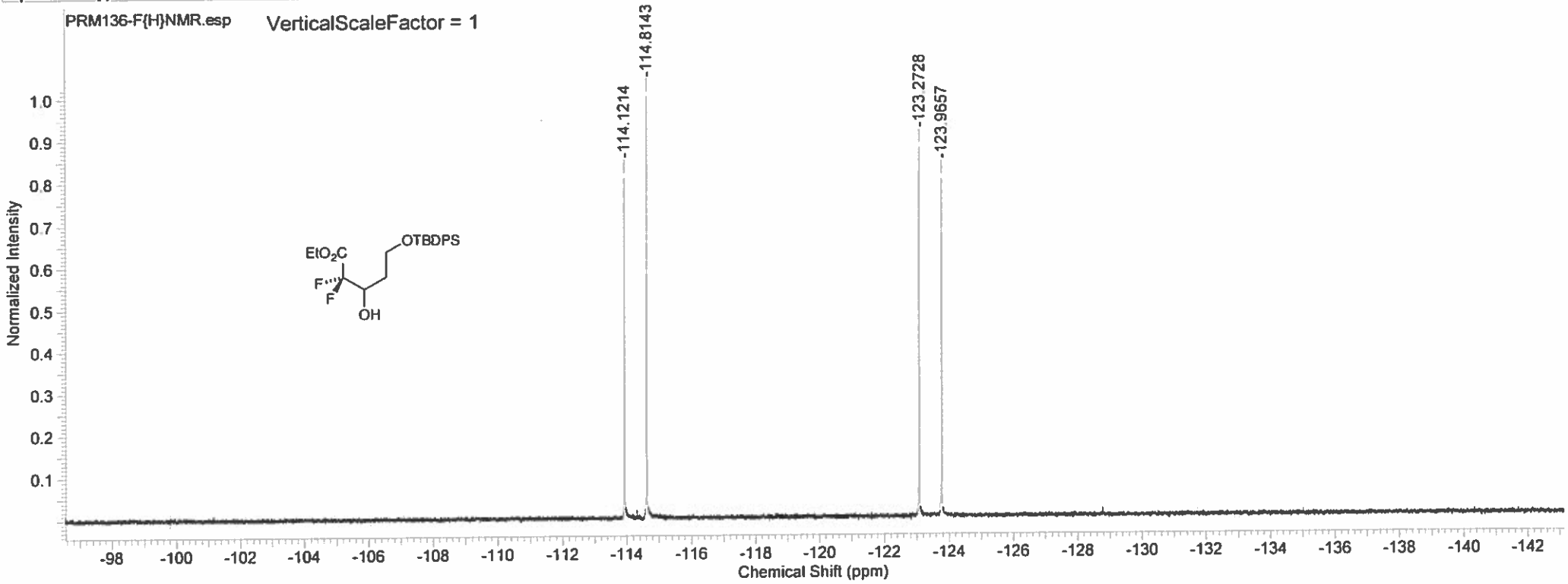
02/04/2014 16:39:43

Acquisition Time (sec)	1.0912	*Comment*	EJT-PRM136 Prod data mCARBONnight CDCl3 {F:\bruk500_b_data\2014\Mar} ejt 59				
Date	21 Mar 2014 21:41:20	*Date Stamp*	21 Mar 2014 21:41:20				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500bdata\2014\Mar\data\ejt\nmr\2014-03-21-ejt-59\10\fid					*Frequency (MHz)*	125.76
Nucleus	13C	*Number of Transients*	3096	*Origin*	spect	*Original Points Count*	32768
Owner	Administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	5792.60
SW(cyclical) (Hz)	30030.03	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12566.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				



02/04/2014 17:33:27

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM136 prod mF19CPD CDCl3 {e:\bruk400data\2014\Mar} ejt 44			*Date*	14 Mar 2014 11:46:08
Date Stamp	14 Mar 2014 11:46:08	*File Name*	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\MAR\DATA\EJT\NMR\2014-03-14-EJT-44\11\PDATA\1\1R				
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	21.600		

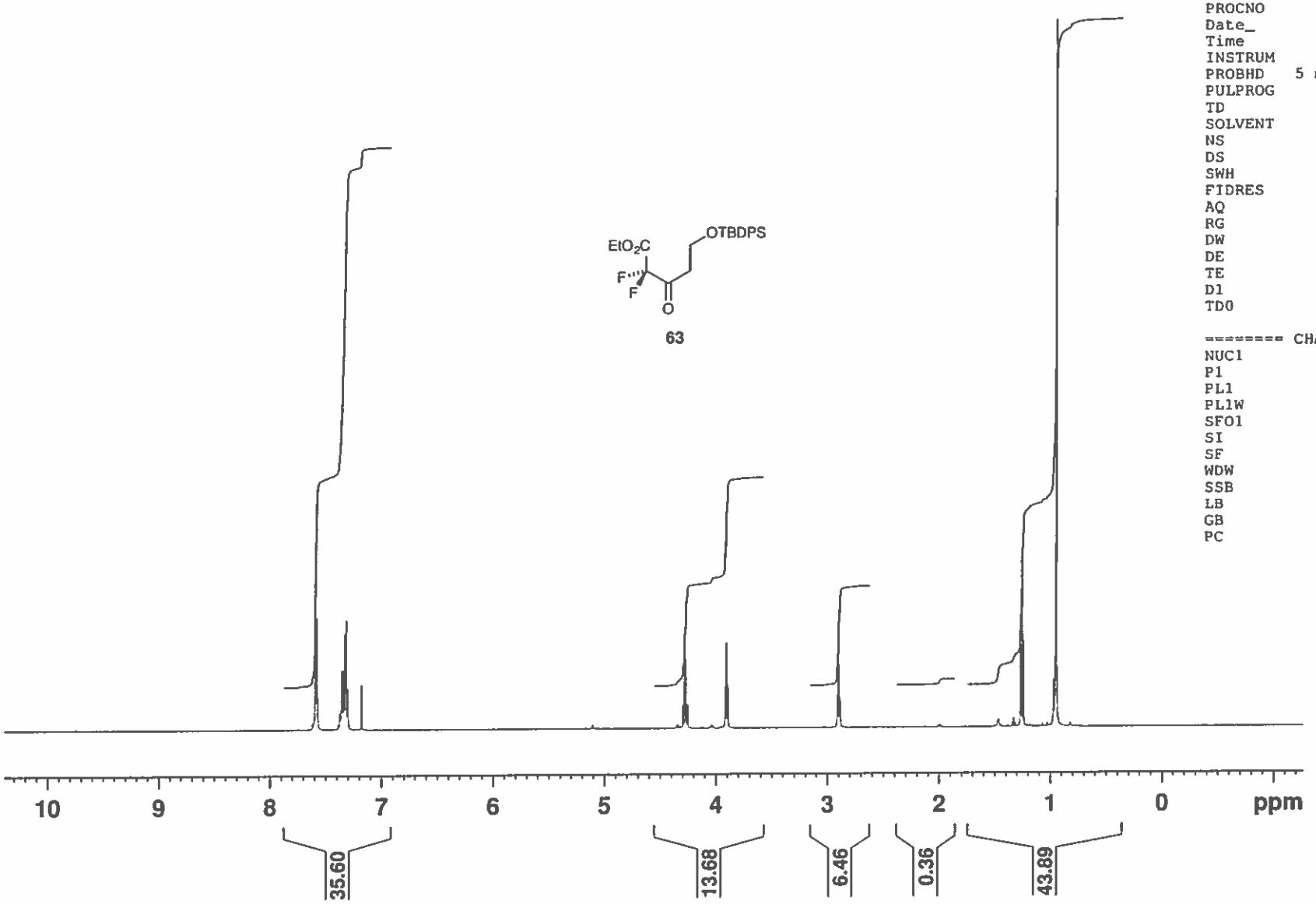


No.	(ppm)	(Hz)	Height
1	-123.97	-46672.9	0.8015
2	-123.27	-46412.0	0.8765
3	-114.81	-43227.4	1.0000
4	-114.12	-42966.5	0.8086

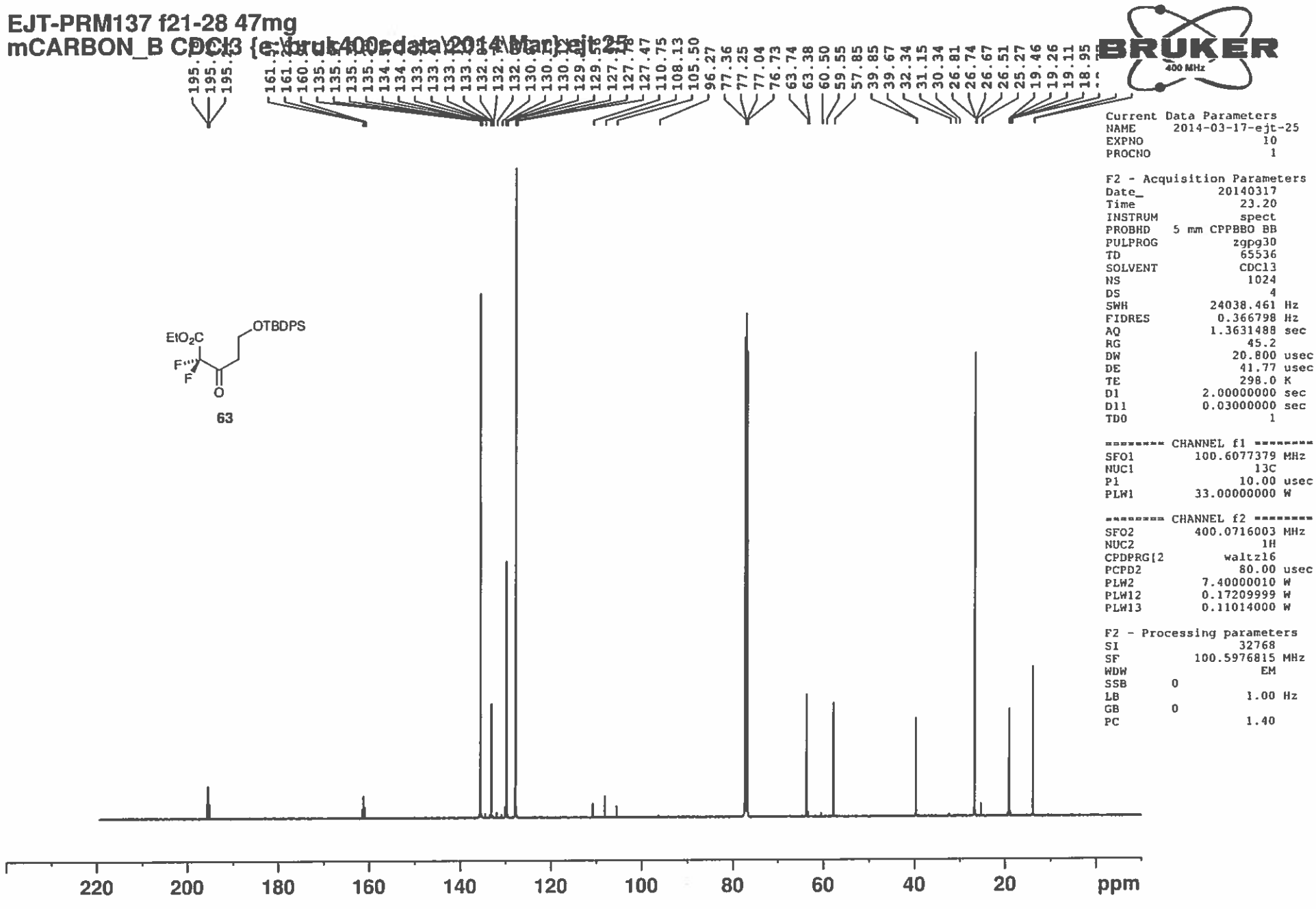
EJT–PRM137 DMP f21–26 22mg
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 56

63

NAME	2014-03-14-ejt-56
EXPNO	10
PROCNO	1
Date_	20140314
Time	15.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	90.5
DW	48.400 usec
DE	13.00 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-0.10 dB
PL1W	26.21803665 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300535 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



EJT-PRM137 f21-28 47mg
mCARBON_B CDCl3 {e:\bruk400edata\2014\Mar\ejt25



Current Data Parameters
NAME 2014-03-17-ejt-25
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140317
Time 23.20
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 41.77 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

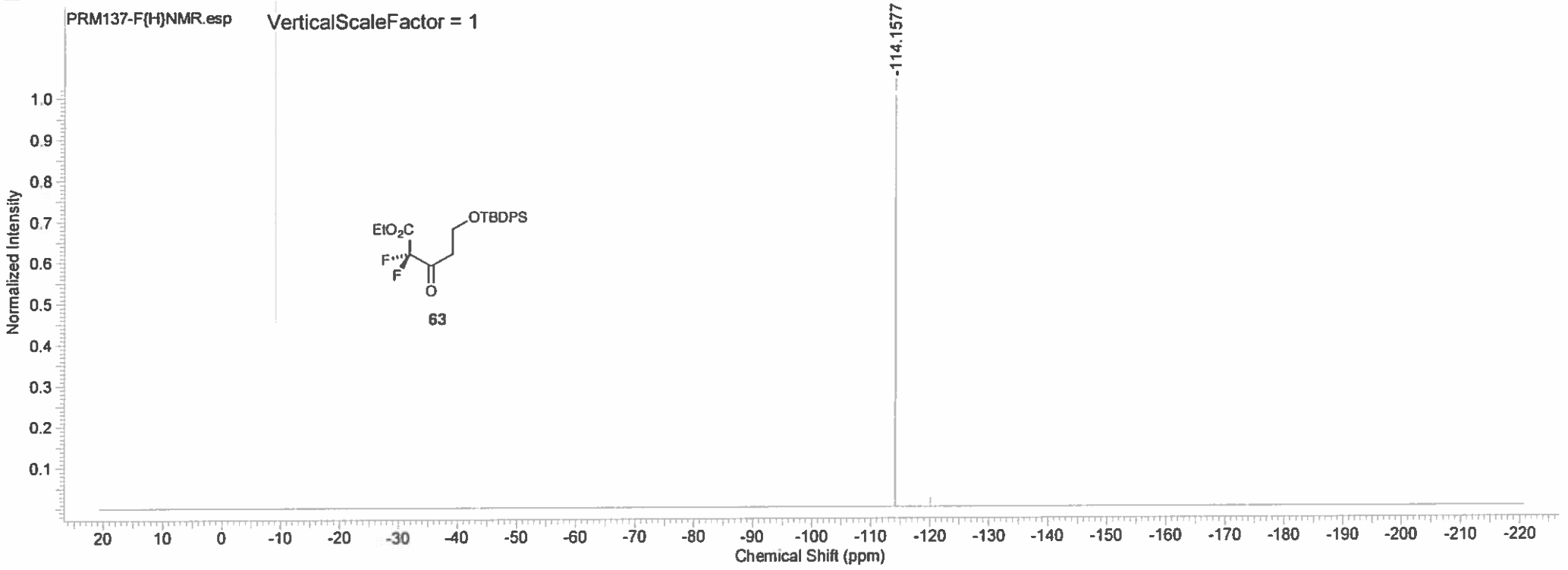
======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

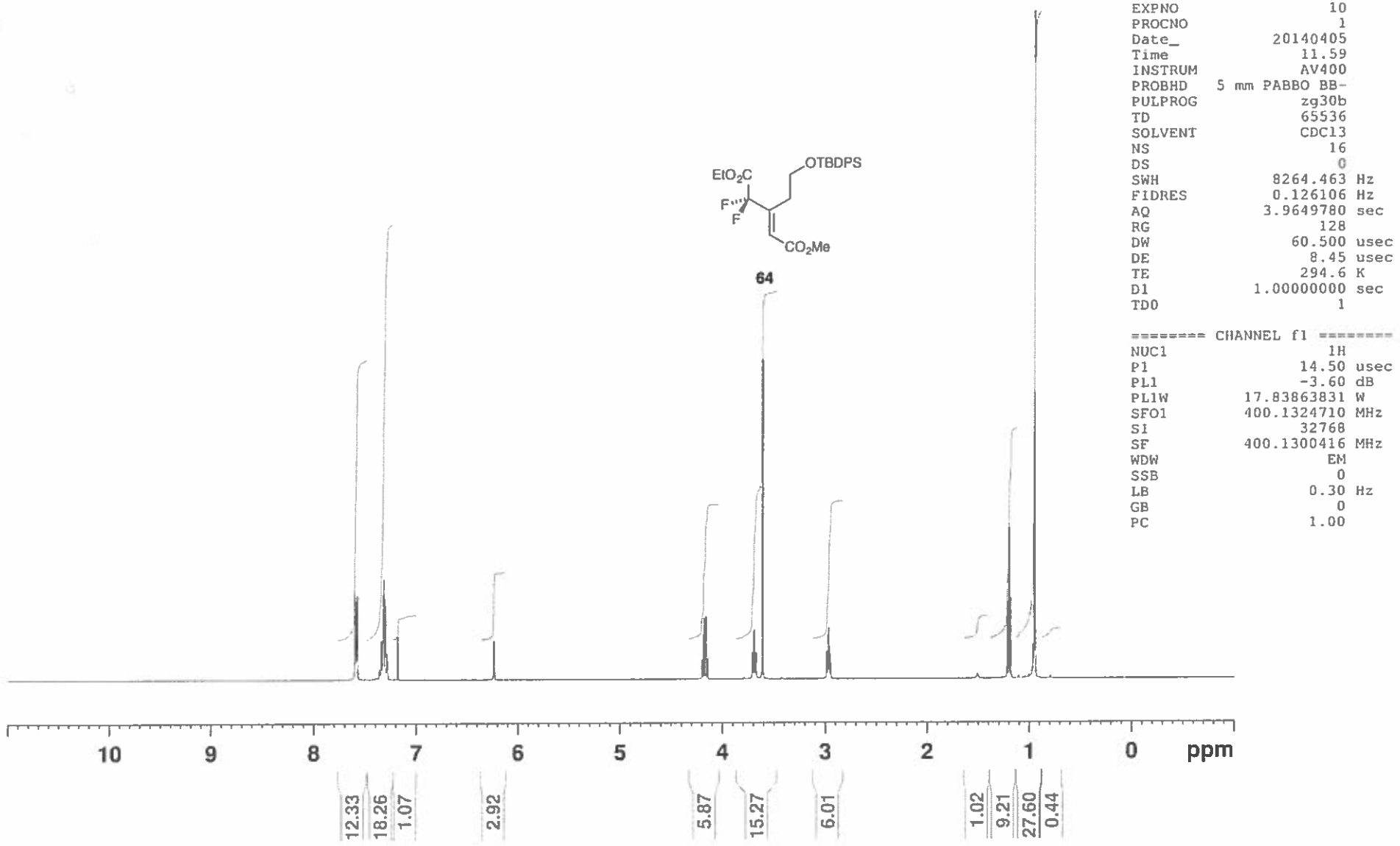
07/04/2014 11:10:45

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM137 DMP f21-26 22mg m19FCPD CDCl3 /opt/oldbruk500data.11vii11/2014/Mar ejt 56				
Date	14 Mar 2014 15:08:48	*Date Stamp*	14 Mar 2014 15:08:48				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK500DATA\BRUK500DATA\2014\MAR\DATA\EJT\NMR\2014-03-14-EJT-56\12\PDATA\1\1R						
Frequency (MHz)	470.59	*Nucleus*	19F	*Number of Transients*	16	*Origin*	spect
Original Points Count	65536	*Owner*	vnmr1	*Points Count*	65536	*Pulse Sequence*	zgfhigqn
Receiver Gain	912.00	*SW(cyclical) (Hz)*	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234
Spectrum Type	STANDARD	*Sweep Width (Hz)*	113634.63	*Temperature (degree C)*	27.000		



No.	(ppm)	(Hz)	Height
1	-114.16	-53721.7	1.0000

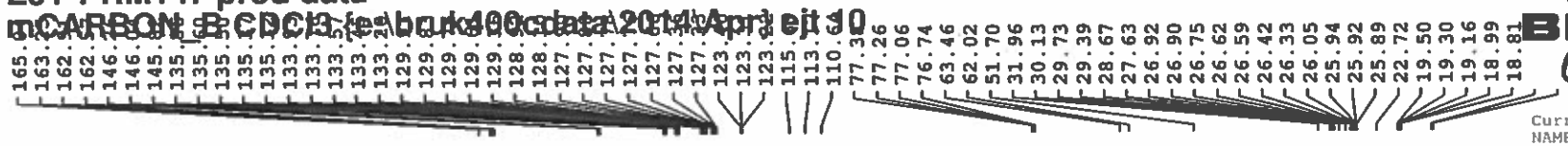
EJT-PRM147 f17-27 31mg
mPROTON CDCl3 {e:\bruk400data\2014\Apr} ejt 50



NAME	2014-04-05-ejt-50
EXPNO	10
PROCNO	1
Date_	20140405
Time	11.59
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	128
DW	60.500 usec
DE	8.45 usec
TE	294.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300416 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

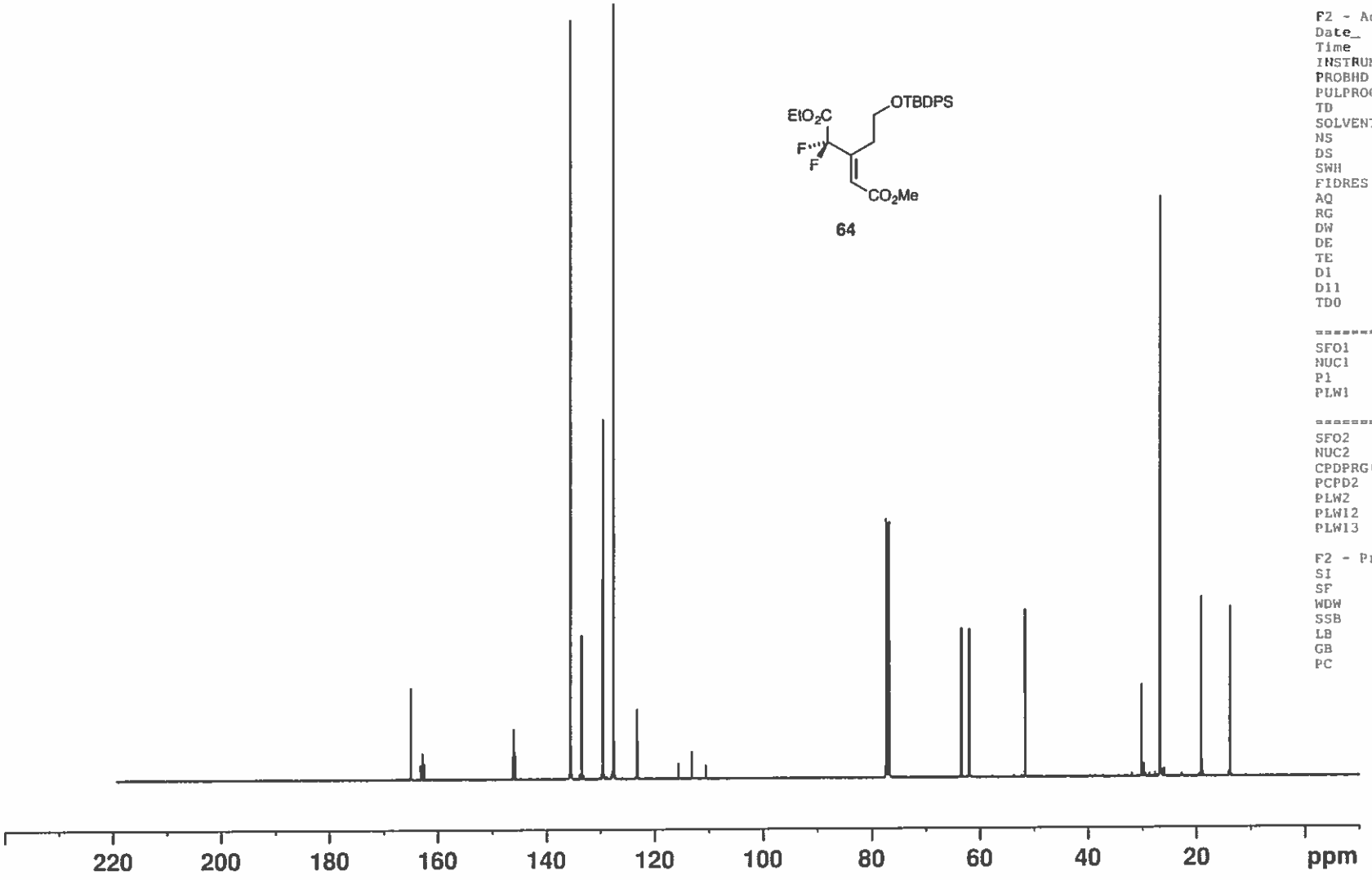
EJT-PRM147 prod data

mCARBON BCDCl3 /e/bruk400/data 2014/Apr/ ejt 10



BRUKER 400 MHz

64




```
Current Data Parameters
NAME      2014-04-06-ejt-10
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_           20140406
Time                20.53
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  45.2
DW                20.800 usec
DE                41.77 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

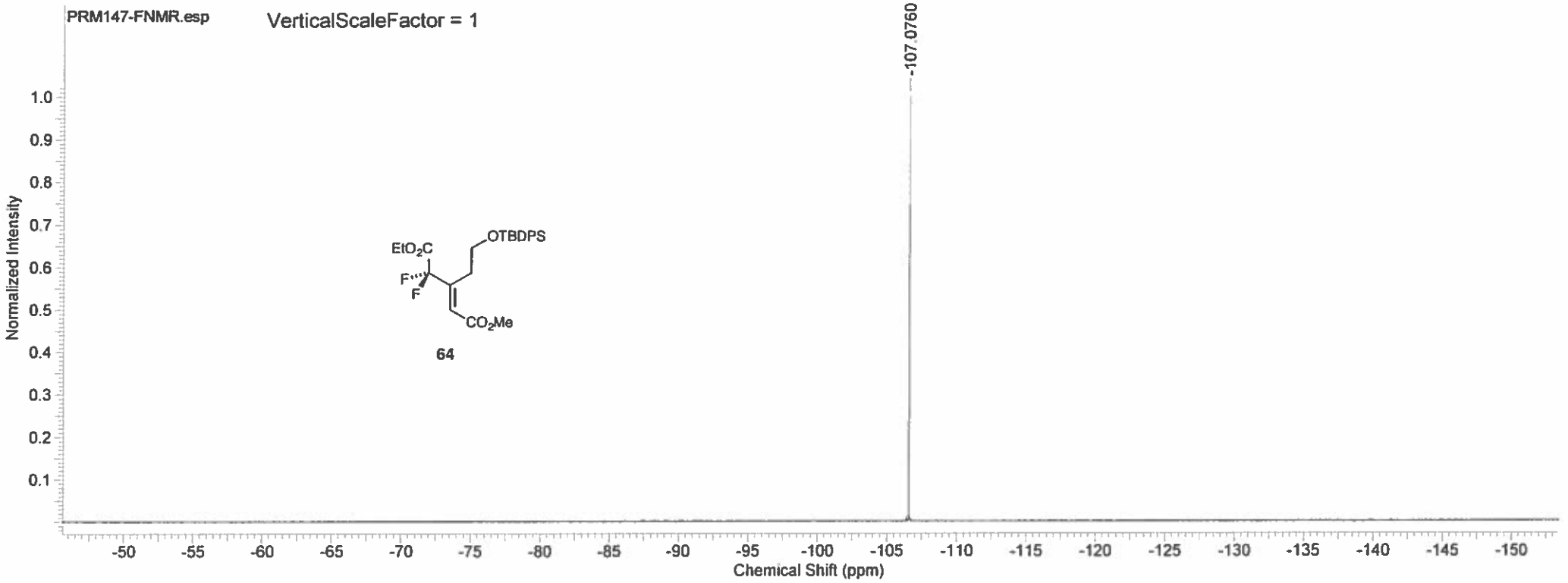
======== CHANNEL f1 ========
SFO1         100.6077379 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         33.00000000 W

======== CHANNEL f2 ========
SFO2         400.0716003 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          7.40000010 W
PLW12         0.17209999 W
PLW13         0.11014000 W

F2 - Processing parameters
SI                  32768
SF           100.5976815 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

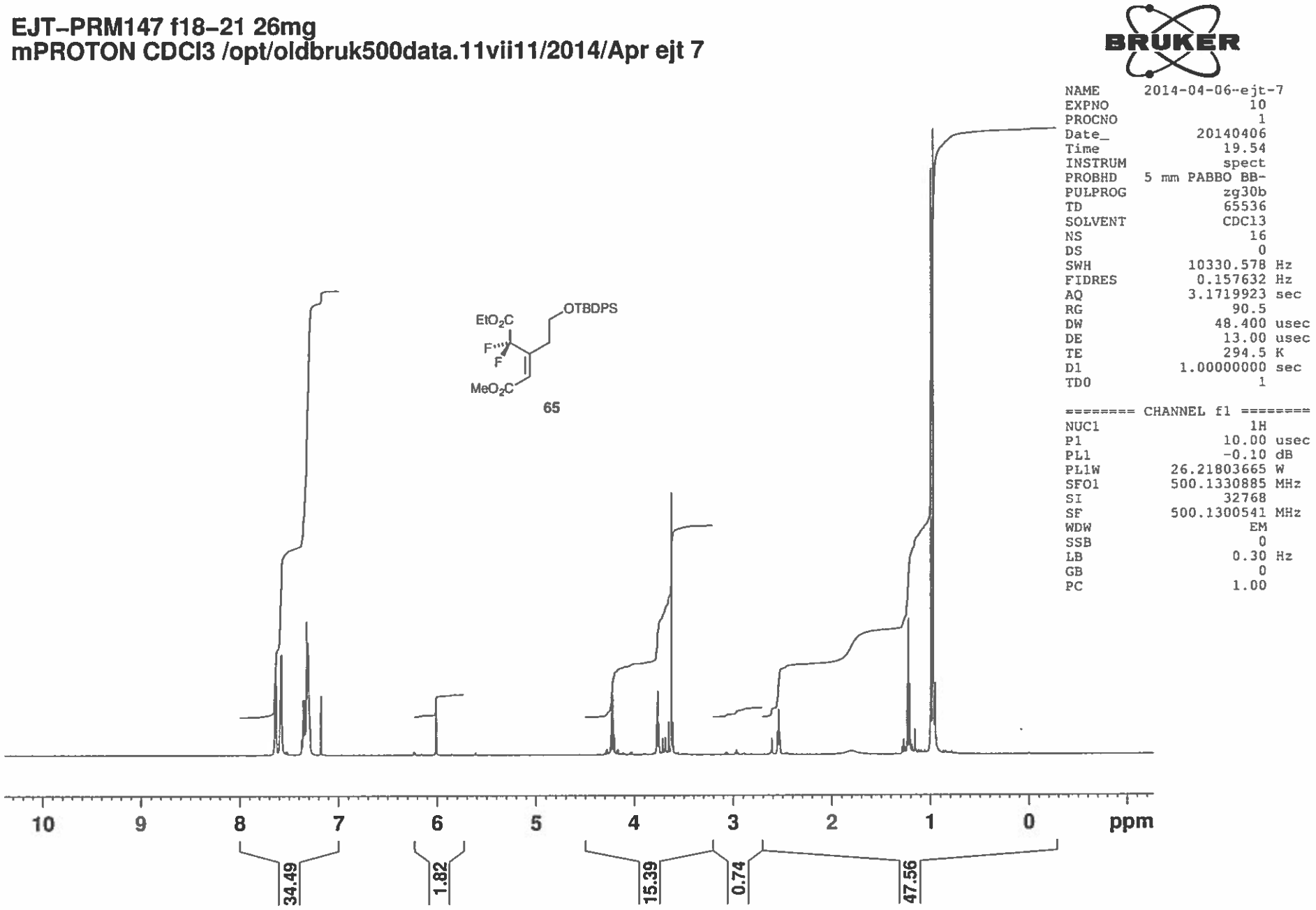
07/04/2014 17:01:40

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM147 f17-27 31mg mF19 CDCl3 {e:\bruk400data\2014\Apr} ejt 50			*Date*	05 Apr 2014 12:01:20
Date Stamp	05 Apr 2014 12:01:20	*File Name*	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\APR\DATA\EJT\NMR\2014-04-05-EJT-50\12\PDATA\1\1R				
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zg
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	21.700		



No.	(ppm)	(Hz)	Height
1	-107.08	-40313.9	1.0000

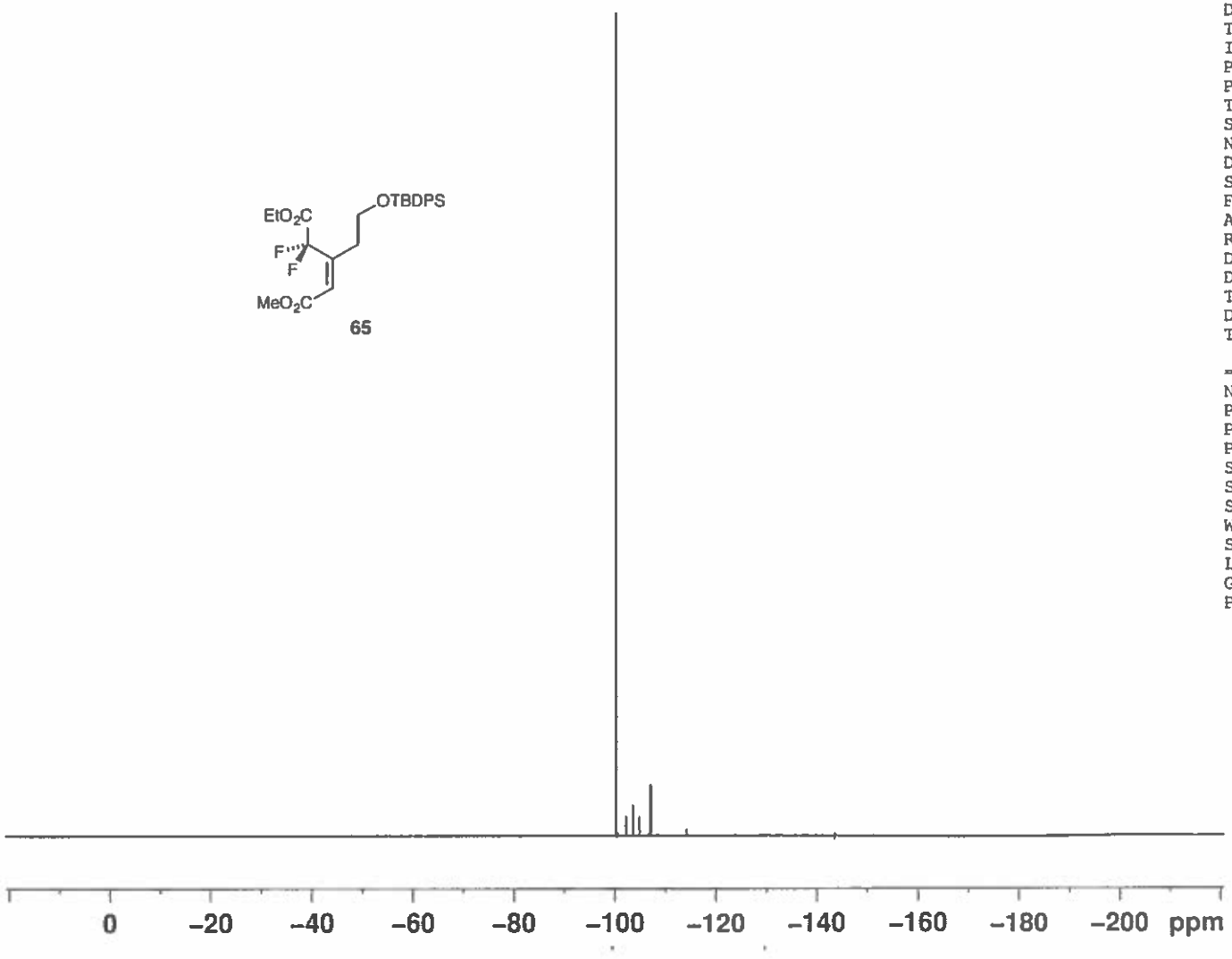
EJT-PRM147 f18-21 26mg
mPROTON CDCl3 /opt/oldbruk500data.11vii11/2014/Apr ejt 7



EJT-PRM147 f18-21 26mg
m19F CDCl3 /opt/oldbruk500data.11vii11/2014/Apr ejt 7

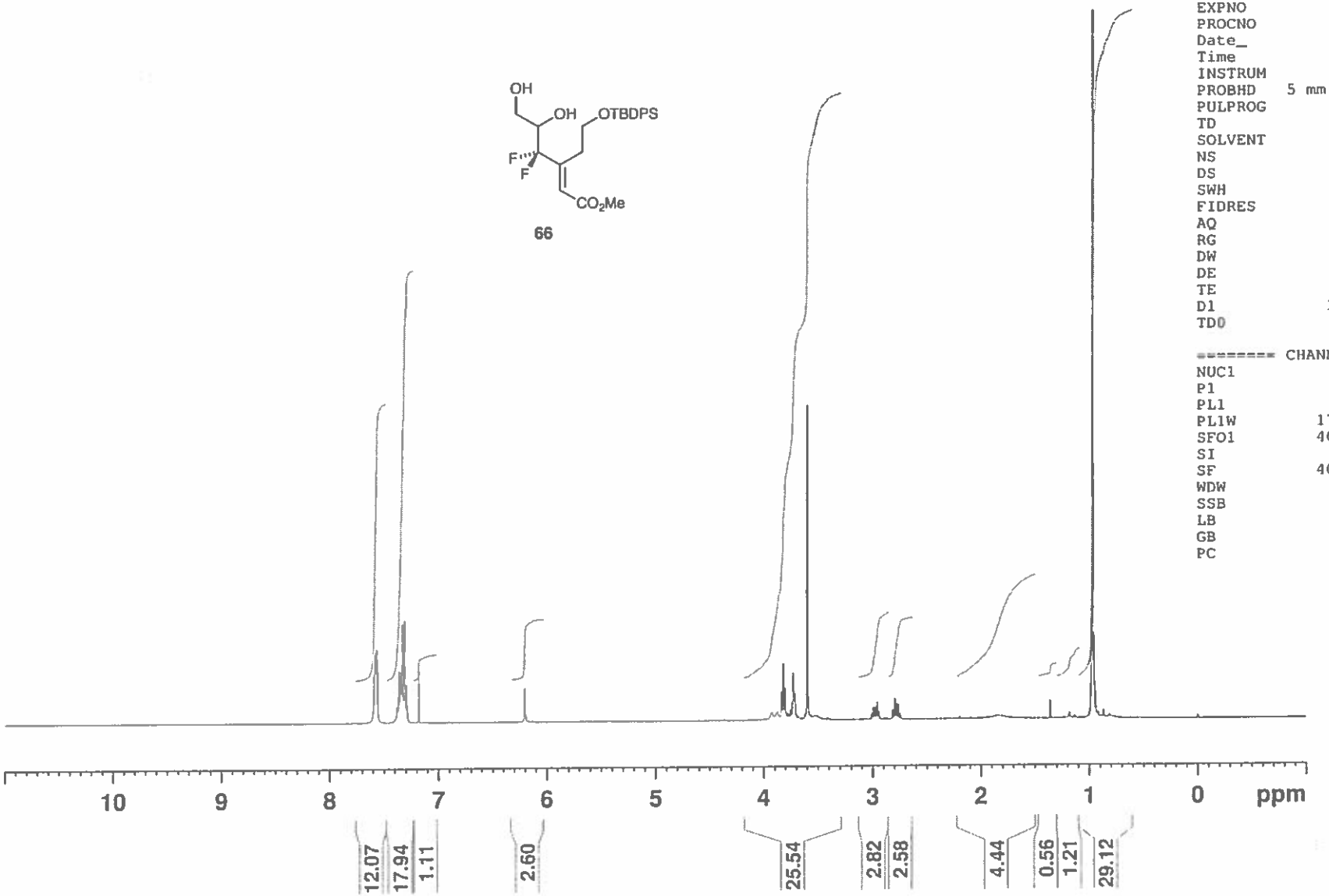
65

NAME	2014-04-06-ejt-7
EXPNO	11
PROCNO	1
Date_	20140406
Time	19.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	113636.367 Hz
FIDRES	0.866977 Hz
AQ	0.5767668 sec
RG	406
DW	4.400 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	12.38 usec
PL1	-0.10 dB
PL1W	25.70395851 W
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



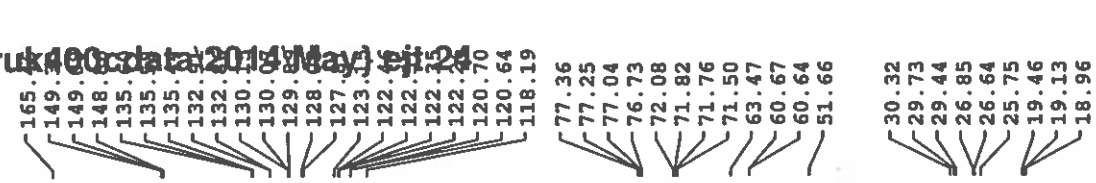
EJT–PRM149F f17–34 38mg
mPROTON CDCl3 {e:\bruk400data\2014\May} ejt 54

66

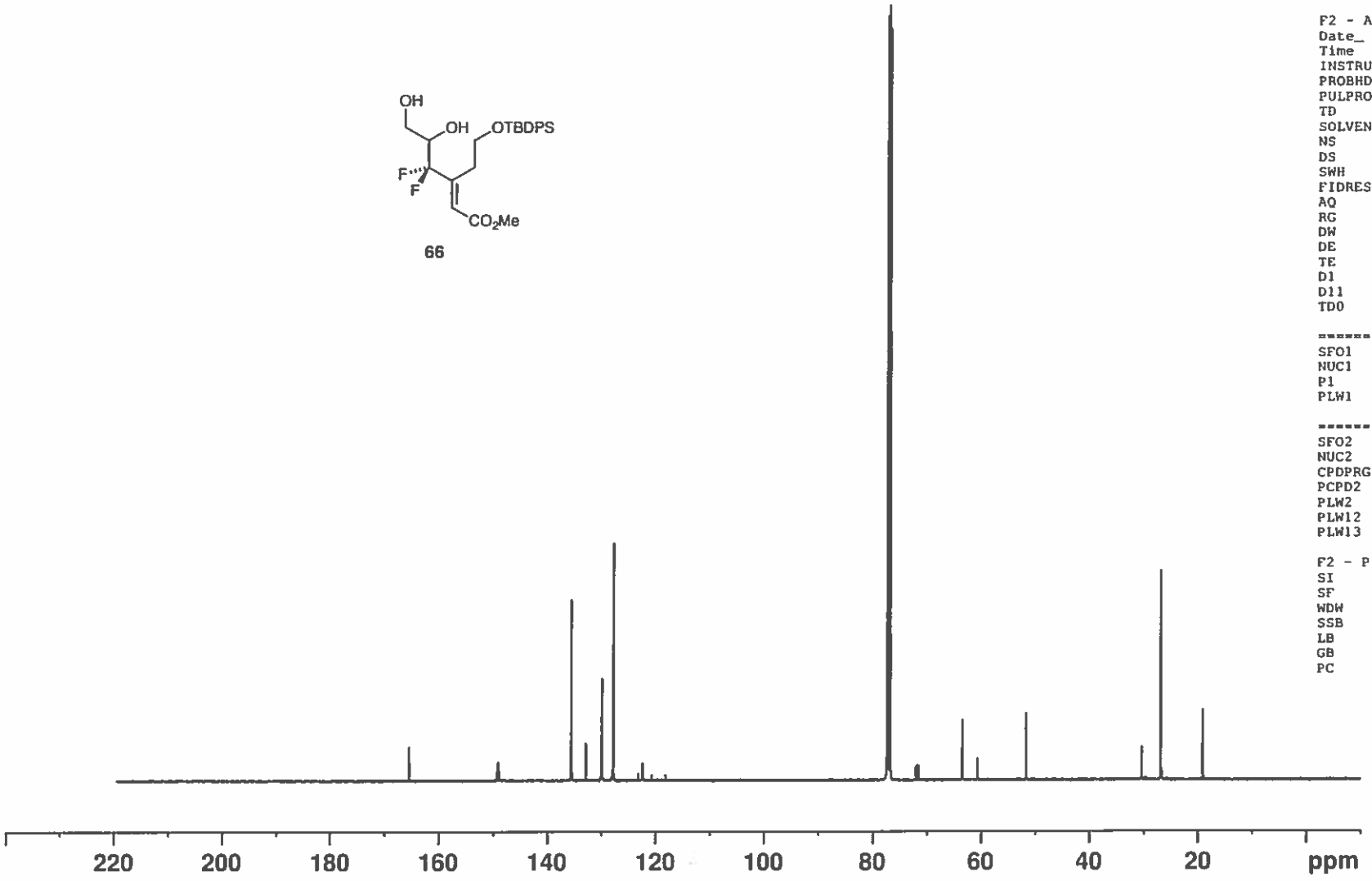


NAME	2014-05-09-ejt-54
EXPNO	10
PROCNO	1
Date_	20140509
Time	13.20
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	128
DW	60.500 usec
DE	8.45 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300407 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

EJT-PRM149 Prod data
mCARBON_B CDCl3 {e:\bruk400\data\2014May} ejt-24



66



BRUKER 400 MHz

```
Current Data Parameters
NAME      2014-05-12-ejt-24
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140513
Time                  22.51
INSTRUM               spect
PROBHD   5 mm CPPBBO BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                    71.8
DW                20.800 usec
DE                41.77 usec
TE                295.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

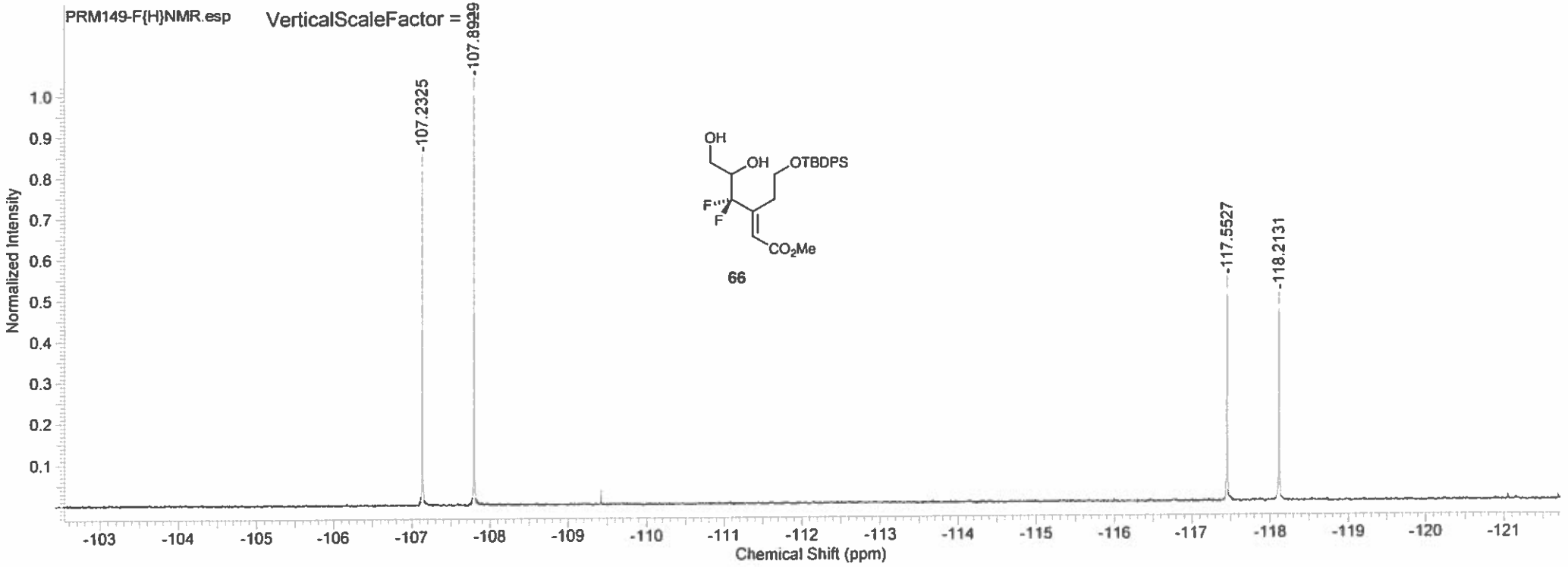
======== CHANNEL f1 ========
SFO1         100.6077379 MHz
NUC1                  13C
P1                 10.00 usec
PLW1         33.00000000 W

======== CHANNEL f2 ========
SFO2         400.0716003 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          7.40000010 W
PLW12         0.17209999 W
PLW13         0.11014000 W

F2 - Processing parameters
SI                   32768
SF           100.5976815 MHz
WDW                     EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

21/05/2014 12:04:27

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM149F f17-34 38mg mF19CPD CDCl3 (e:\bruk400data\2014\May) ejt 54				
Date	09 May 2014 13:22:24	*Date Stamp*	09 May 2014 13:22:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\MAY\DATA\EJT\NMR\2014-05-09-EJT-54\11\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	22.200		



No.	(ppm)	(Hz)	Height
1	-118.21	-44507.0	0.4667
2	-117.55	-44258.4	0.5046
3	-107.89	-40621.5	1.0000
4	-107.23	-40372.8	0.8148

EJT–PRM150 Zn allylation f5–15 20mg
mPROTON CDCl3 {e:\bruk400data\2014\May} ejt 11

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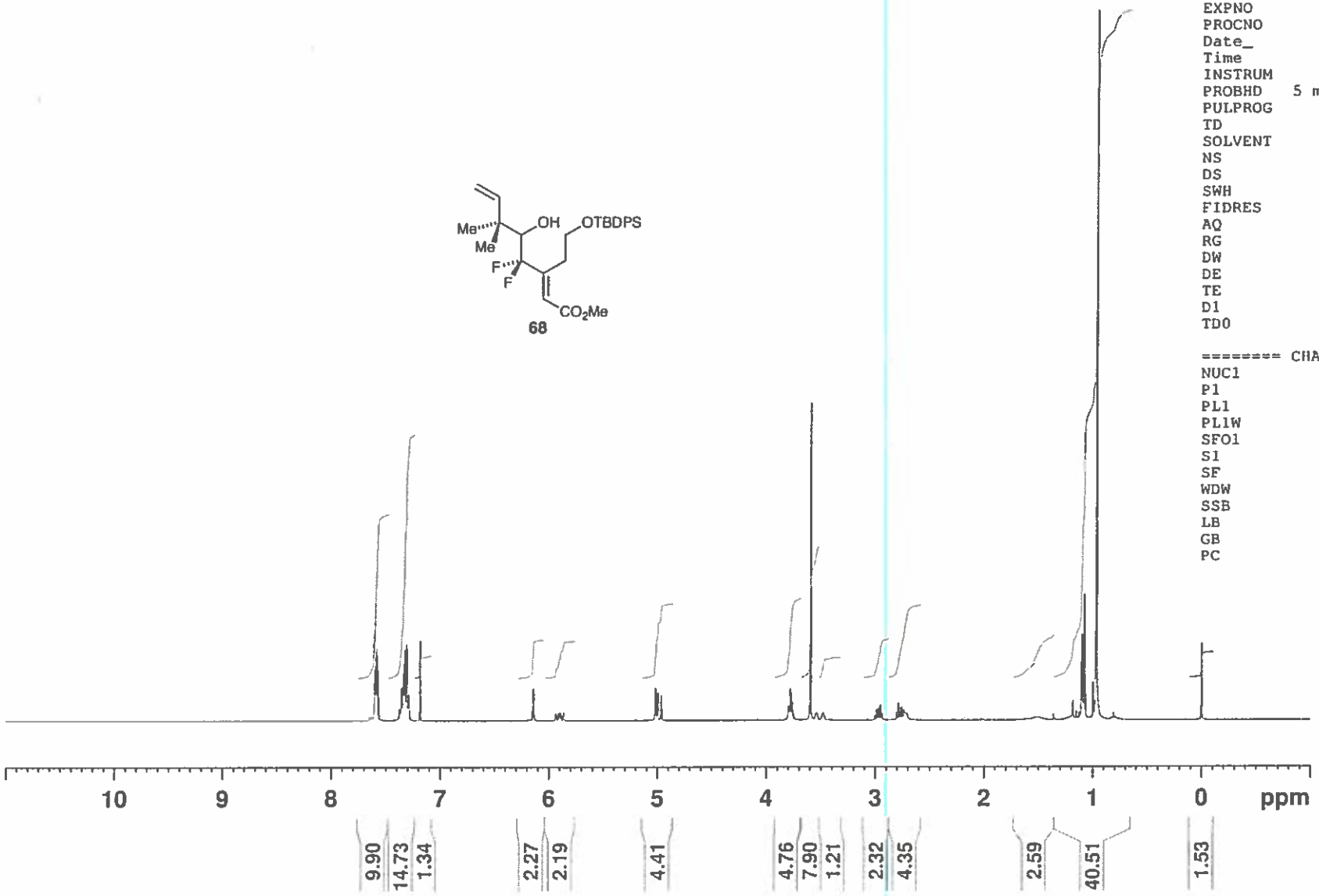
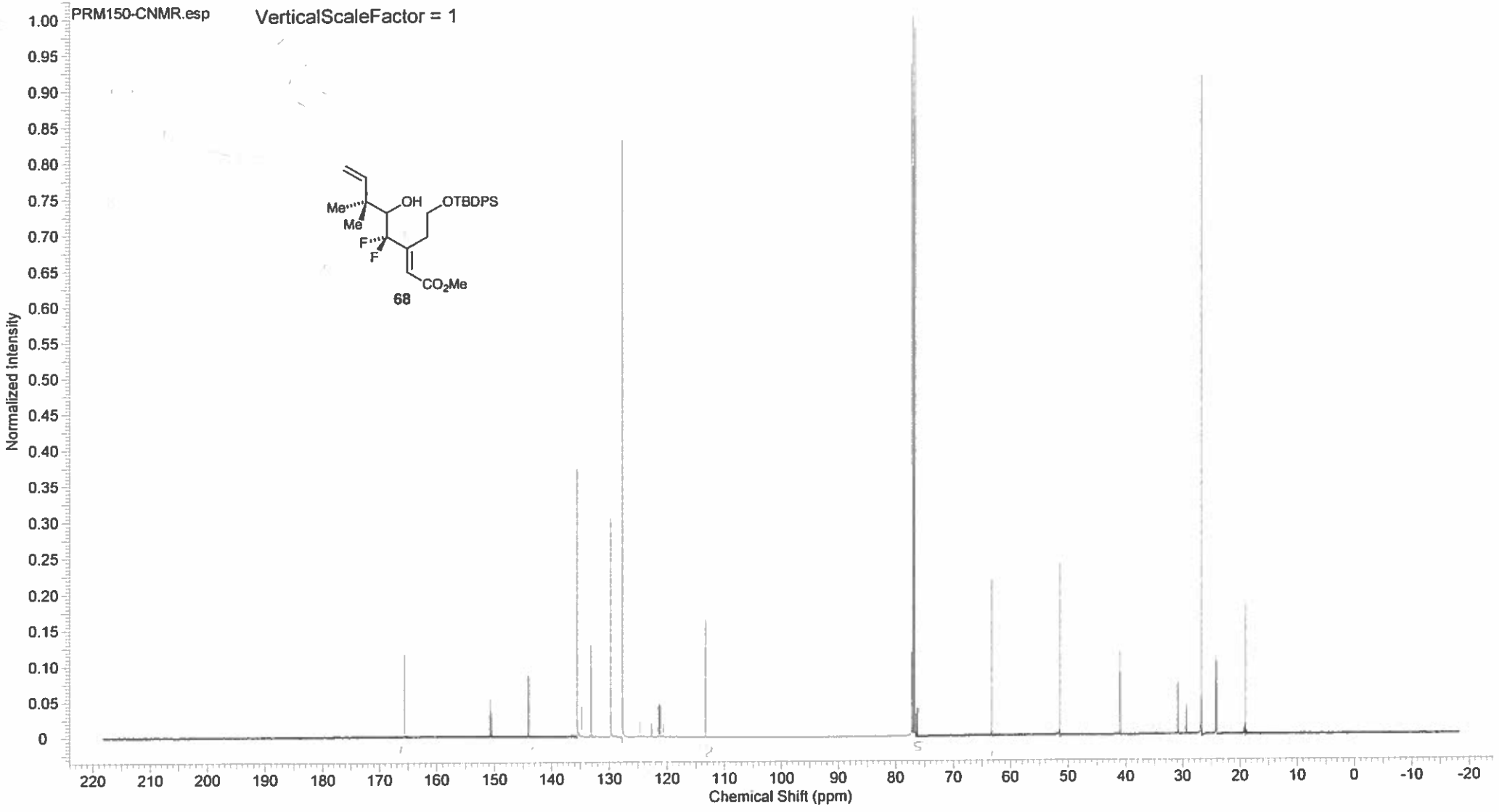
NAME	2014-05-16-ejt-11
EXPNO	10
PROCNO	1
Date_	20140516
Time	15.29
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	144
DW	60.500 usec
DE	8.45 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300394 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

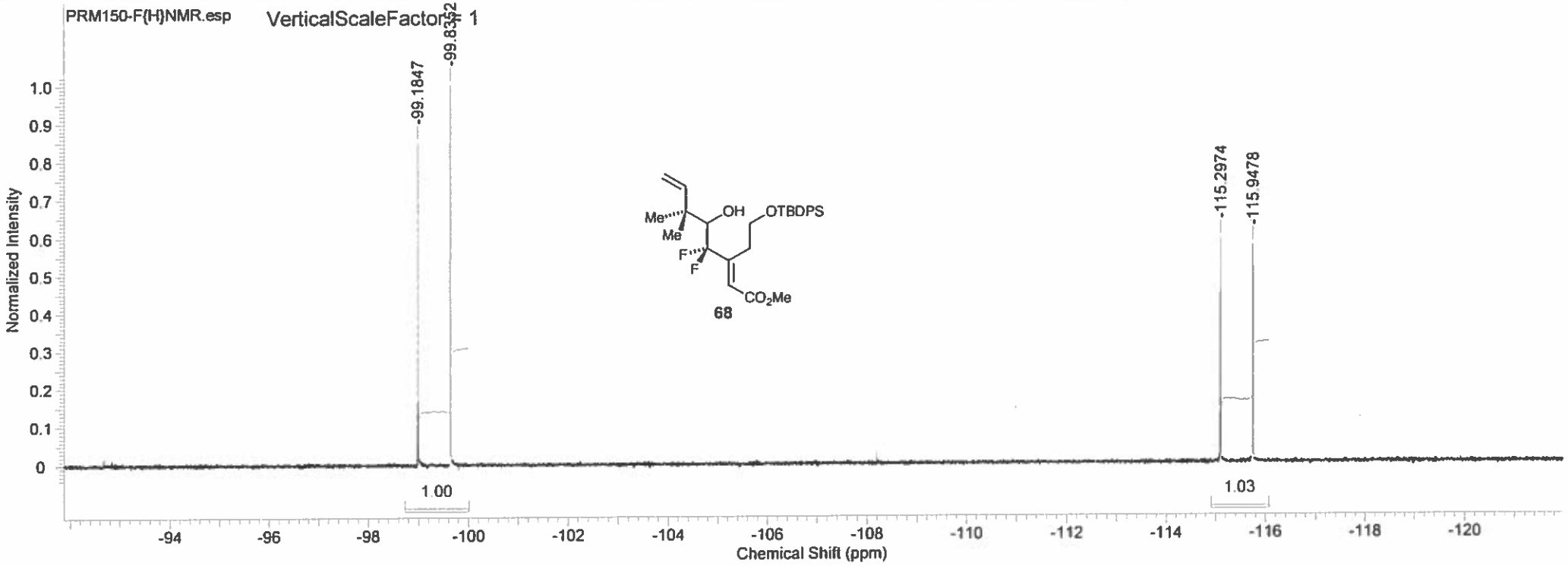
23/05/2014 19:19:14

Acquisition Time (sec)	1.1010	*Comment*	P. Mears EJT-PRM150 Prod 0514-049 mCARBON CDCl3 {E:\bruk500cdata\2014\May} staff 17				
Date	21 May 2014 15:30:24	*Date Stamp*	21 May 2014 15:30:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2014\May\data\staff\nmr\2014-05-21-staff-17\12\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	2048	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12568.6943	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.160				



28/05/2014 17:03:52

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM150 Zn allylation f5-15 20mg mF19CPD CDCl3 {e:\bruk400data\2014\May} ejt 11				
Date	16 May 2014 15:30:24	*Date Stamp*	16 May 2014 15:30:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\MAY\DATA\EJT\NMR\2014-05-16-EJT-11\11\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	22.200		



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2702 .. -1151	1.03150678	1.04263719e+6	1.03150678
2	2075 .. -98.0	0.99985164	1.01064050e+6	0.99985164

No.	(ppm)	(Hz)	Height
1	-115.95	-43654.2	0.5707
2	-115.30	-43409.3	0.5886
3	-99.84	-37587.8	1.0000
4	-99.18	-37342.9	0.8471

EJT-PRM151 f4-12 11mg
mPROTON CDCl3 {E:\bruk500adata\2014\May} ejt 7

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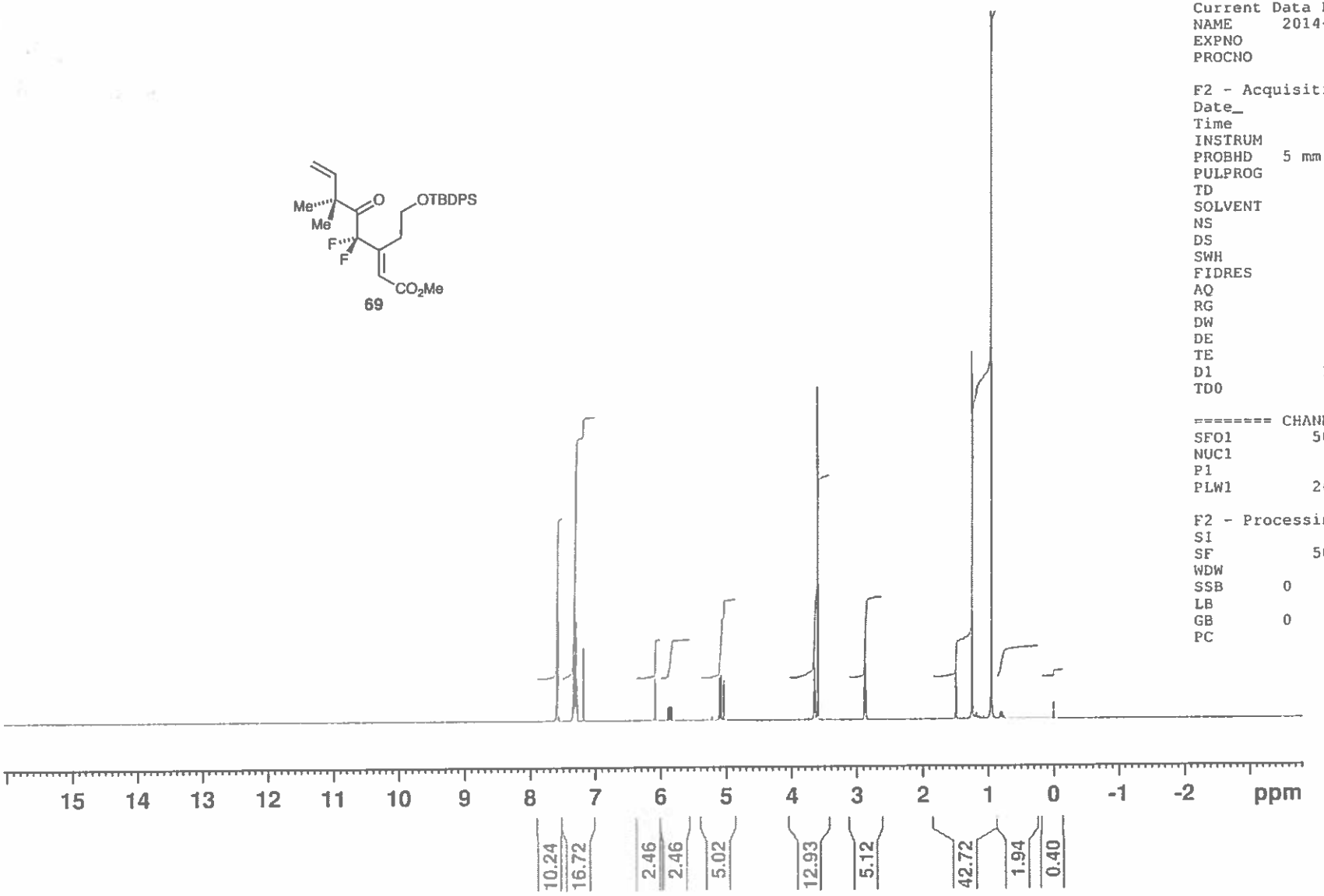


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Current Data Parameters
NAME      2014-05-17-ejt-7
EXPNO                   20
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140517
Time                  15.18
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH              10330.578 Hz
FIDRES           0.157632 Hz
AQ               3.1719425 sec
RG                     144
DW                48.400 usec
DE                13.00 usec
TE                293.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                    1H
P1                10.00 usec
PLW1          26.21800041 W

F2 - Processing parameters
SI                   32768
SF            500.1300481 MHz
WDW                     EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

P. Mears
EJT151 prod data
0614-017
2048 scans
mCARBON CDCl3 {E:\bruk500cdata\2014\Jun} staff 16

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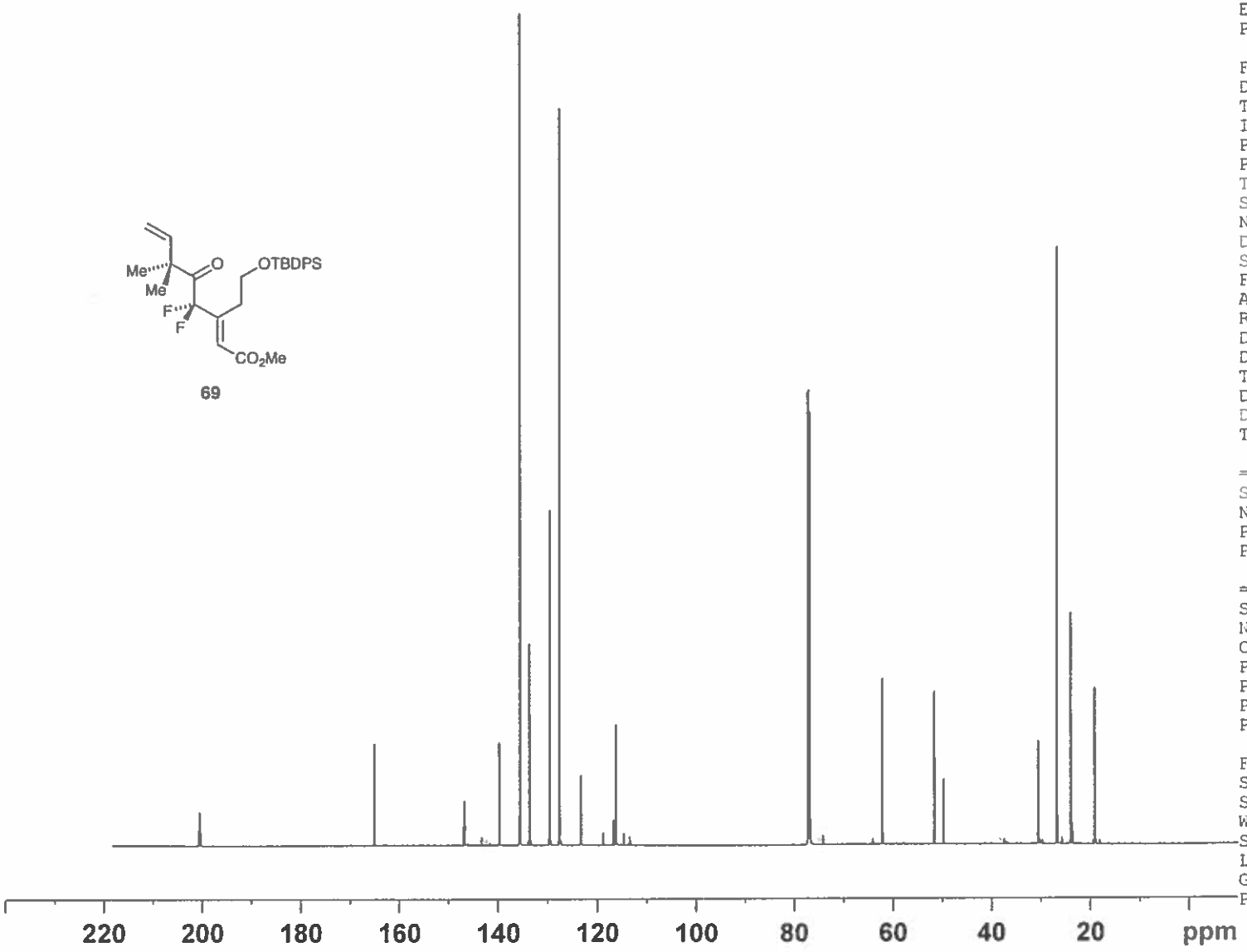


Current Data Parameters
NAME 2014-06-11-staff-16
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140611
Time 15.58
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 184.4
DW 16.800 usec
DE 102.82 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7854504 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.59999847 W

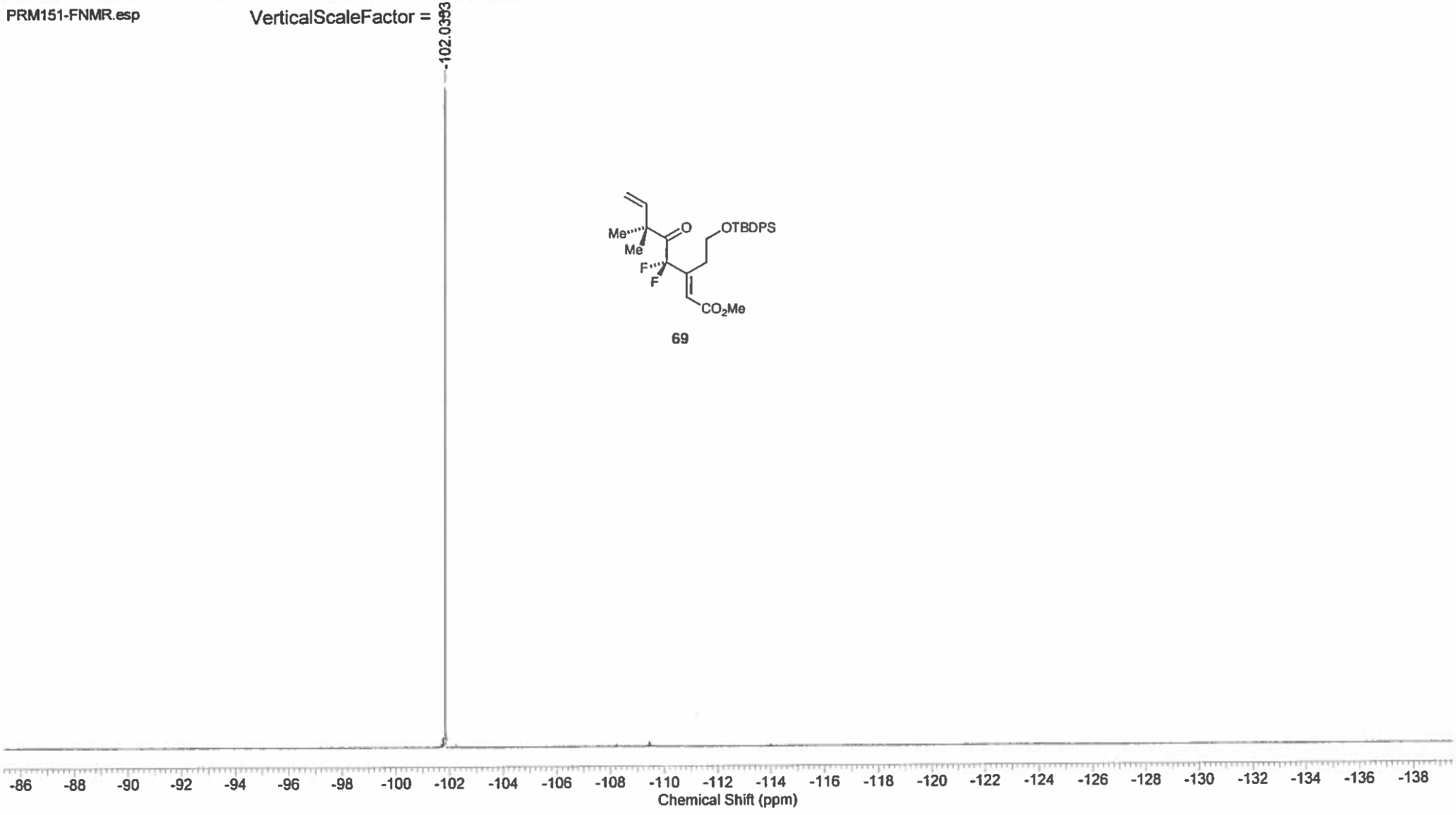
======== CHANNEL f2 ========
SFO2 500.1920008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.28622001 W
PLW13 0.18318000 W

F2 - Processing parameters
SI 32768
SF 125.7728760 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM151 f4-12 11mg m19F CDCl3 {E:\bruk500adata\2014\May} ejt 7				
Date	17 May 2014 15:21:52			*Date Stamp*	17 May 2014 15:21:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2014\May\data\ejt\nmr\2014-05-17-ejt-7\22\fid					*Frequency (MHz)*	470.59
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgflqn	*Receiver Gain*	362.00
SW(cyclical) (Hz)	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	113634.63	*Temperature (degree C)*	20.000				

PRM151-FNMR.esp

VerticalScaleFactor = 3

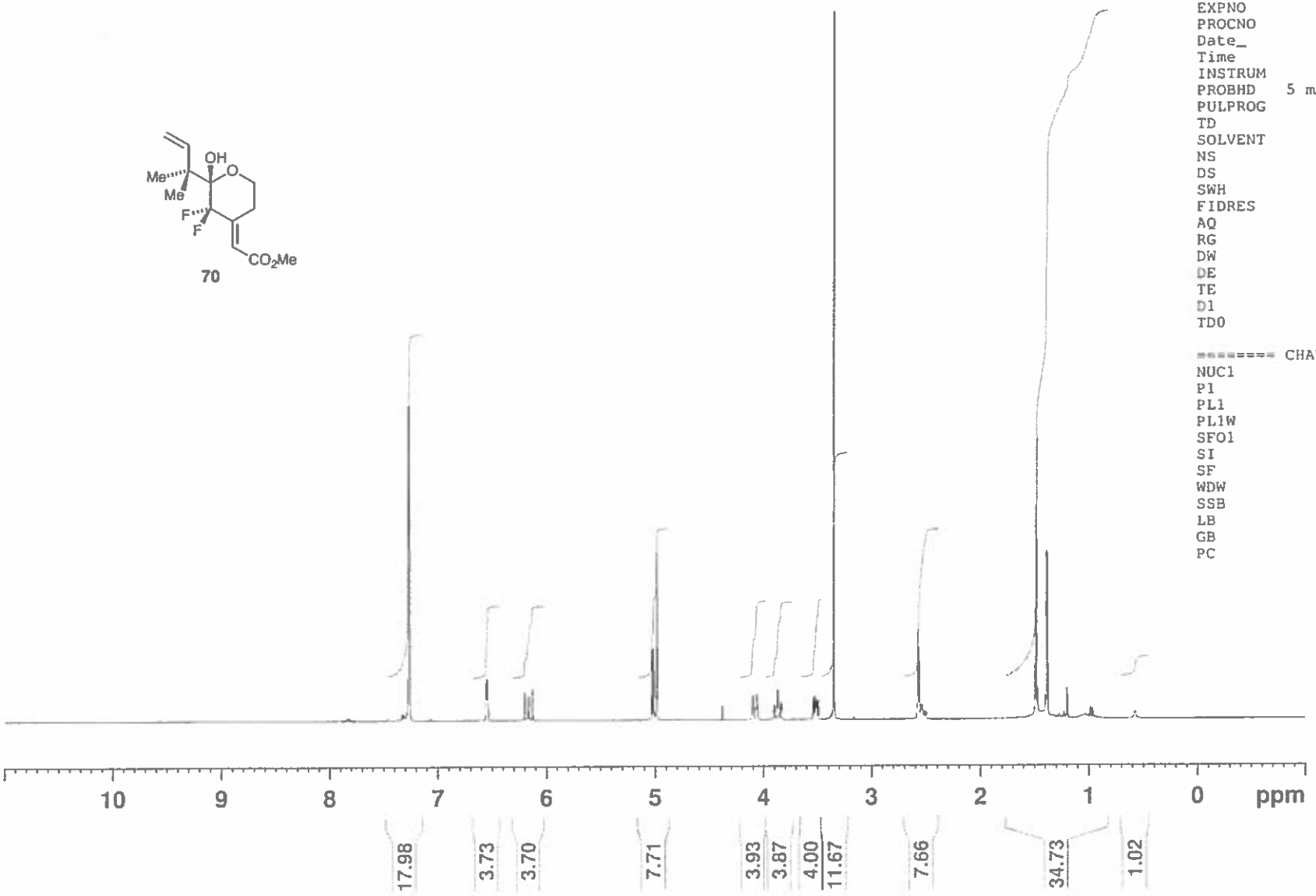


69

EJT–PRM152 HF.py f3–11 15mg
mPROTON C6D6 {e:\bruk400data\2014\May} ejt 2

70

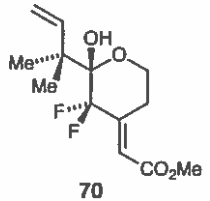
NAME	2014-05-23-ejt-2
EXPNO	10
PROCNO	1
Date_	20140523
Time	12.12
INSTRUM	AV400
PROBHD	5 mm PABBO BB-
PULPROG	zg30b
TD	65536
SOLVENT	C6D6
NS	16
DS	0
SWH	8264.463 Hz
FIDRES	0.126106 Hz
AQ	3.9649780 sec
RG	144
DW	60.500 usec
DE	8.45 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 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



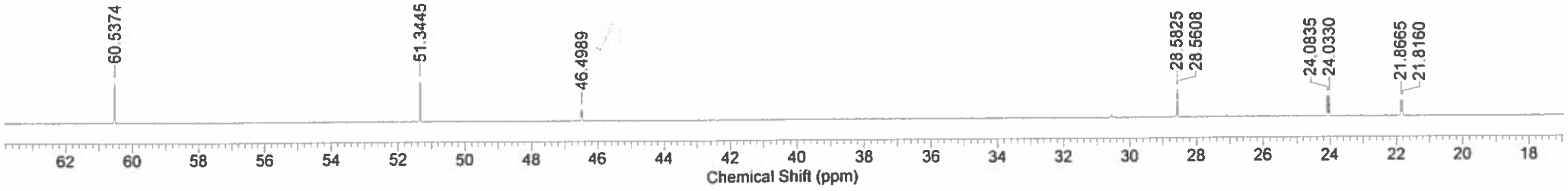
Acquisition Time (sec)	1.1010	*Comment*	P. Mears EJT-PRM152 HF.py 83-11 0514-053 mCARBON C6D6 {E:\bruk500cdata\2014\May} staff 28				
Date	23 May 2014 20:35:28	*Date Stamp*	23 May 2014 20:35:28				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2014\May\data\staff\nmr\2014-05-23-staff-28\12\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5120	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12662.5273	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	25.149				

PRM152-C13NMR.esp

VerticalScaleFactor = 1



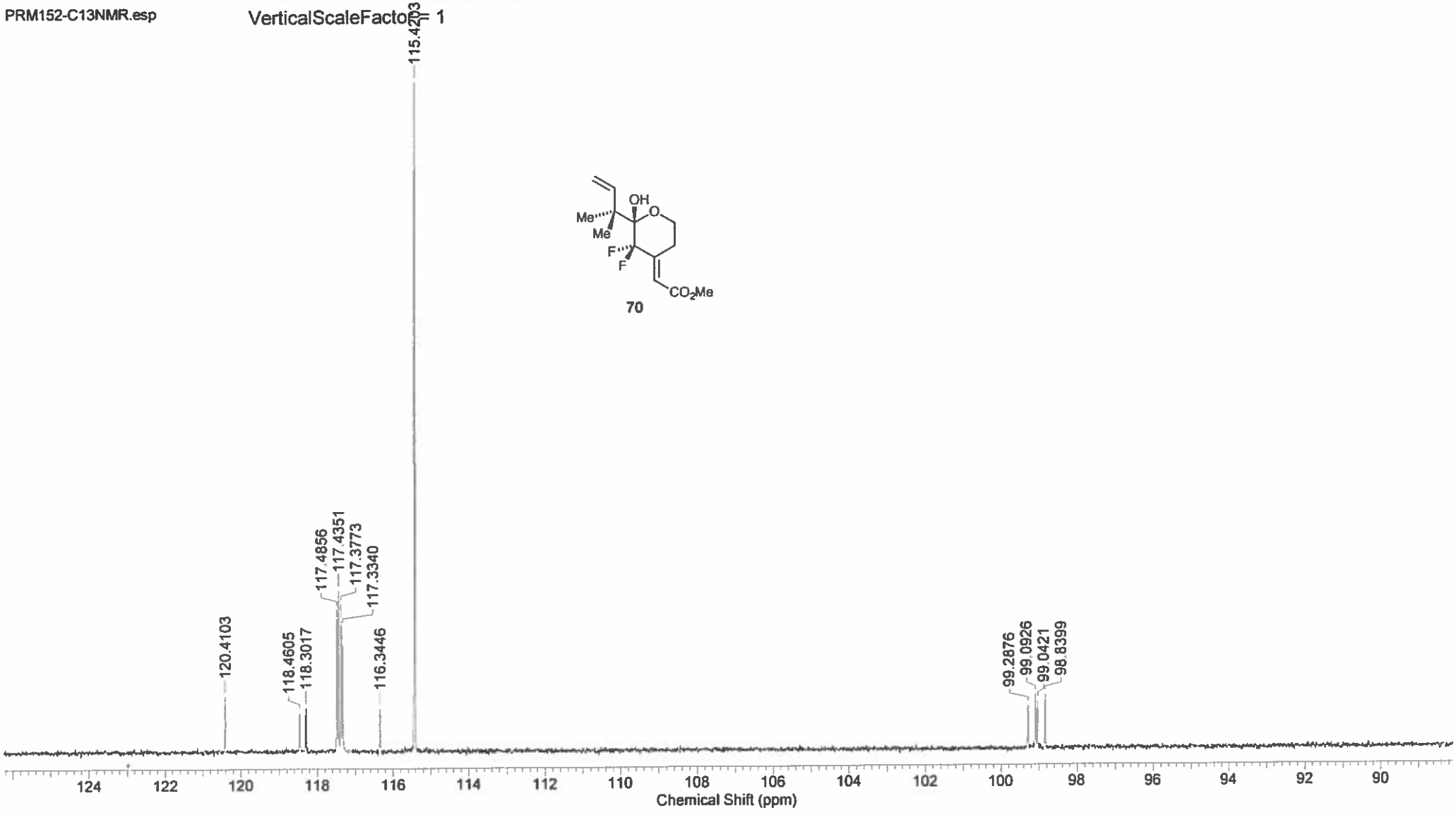
70



Acquisition Time (sec)	1.1010	*Comment*	P. Mears EJT-PRM152 HF.py 83-11 0514-053 mCARBON C6D6 (E:\bruk500cdata\2014\May) staff 28				
Date	23 May 2014 20:35:28	*Date Stamp*	23 May 2014 20:35:28				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2014\May\data\staff\nmr\2014-05-23-staff-28\12\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5120	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12662.5273	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	25.149				

PRM152-C13NMR.esp

VerticalScaleFactor[3] = 1

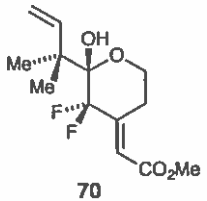


70

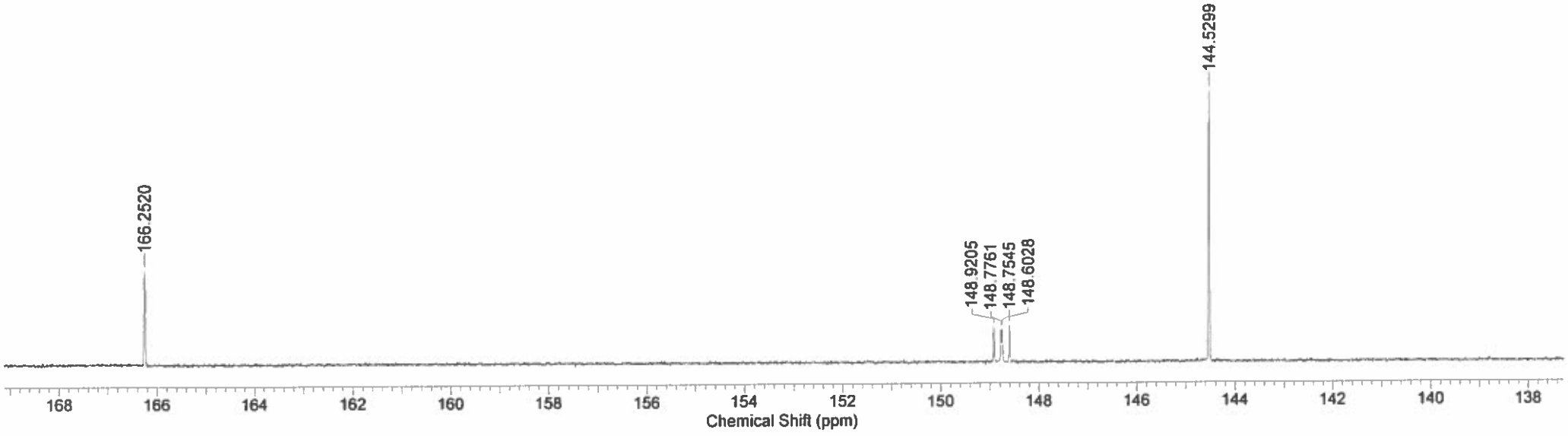
Acquisition Time (sec)	1.1010	*Comment*	P. Mears EJT-PRM152 HF.py 83-11 0514-053 mCARBON C6D6 (E:\bruk500cdata\2014\May) staff 28				
Date	23 May 2014 20:35:28	*Date Stamp*	23 May 2014 20:35:28				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2014\May\data\staff\nmr\2014-05-23-staff-28\12\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5120	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12662.5273	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	25.149				

PRM152-C13NMR.esp

VerticalScaleFactor = 1

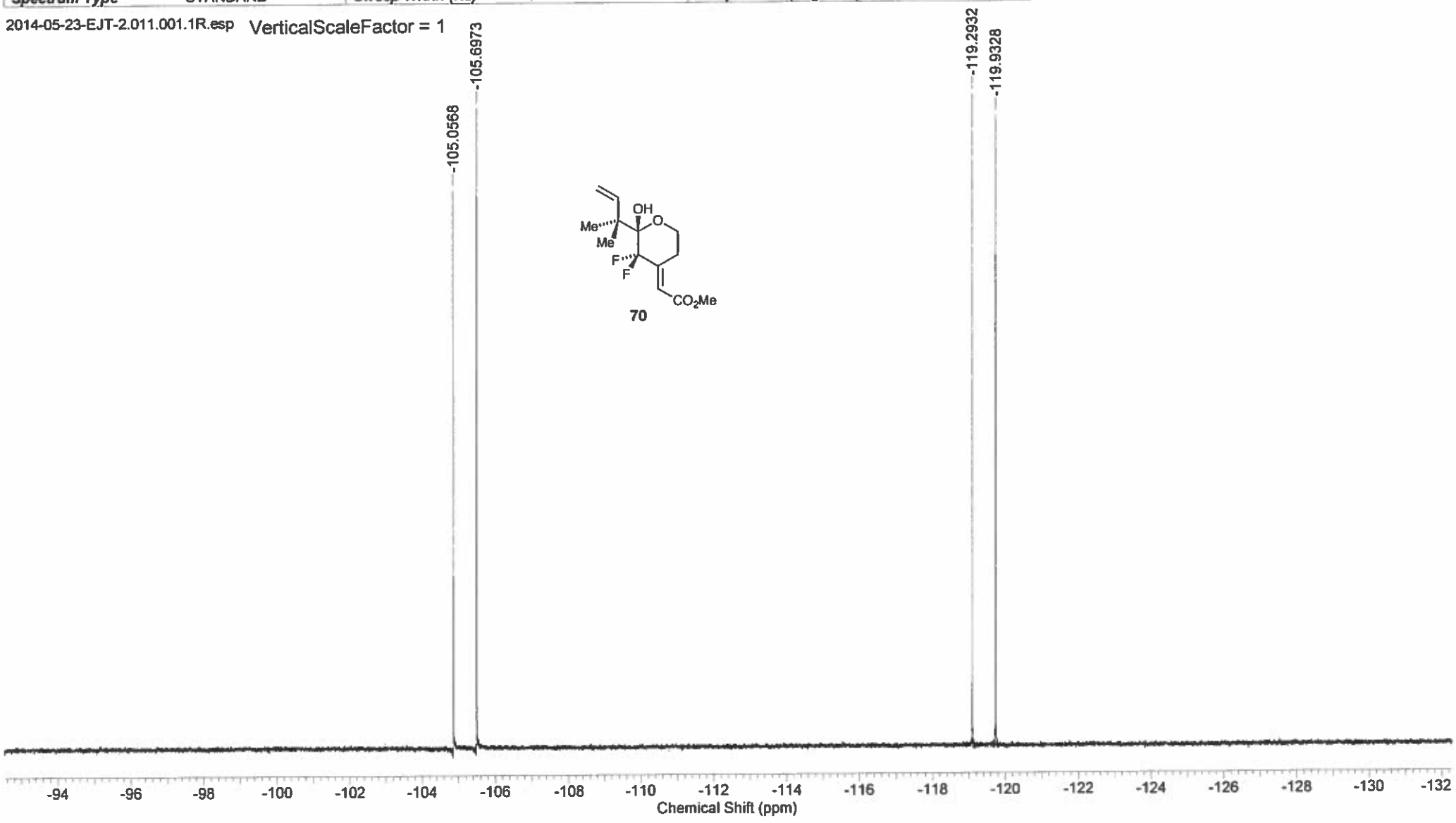


70



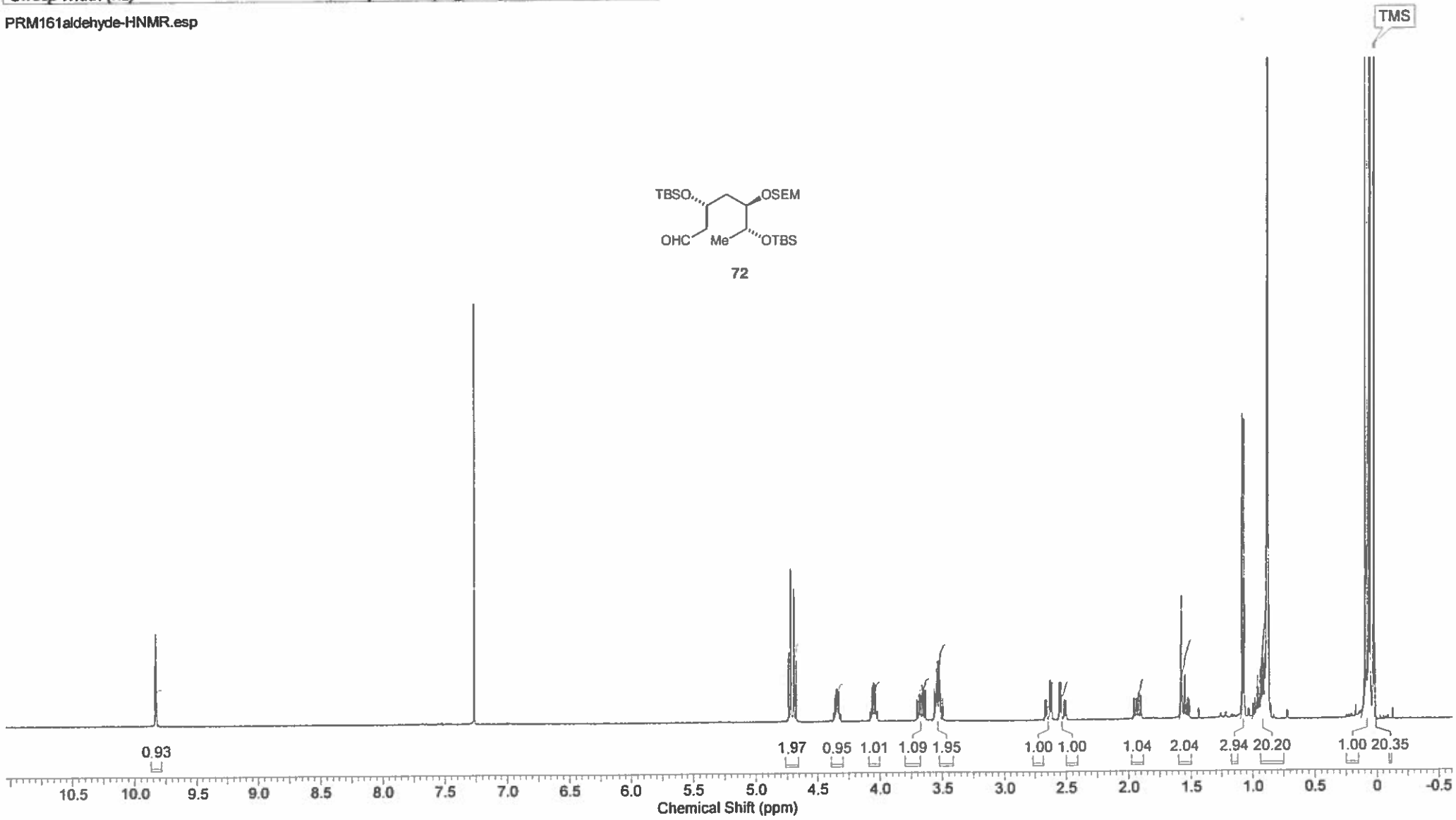
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM152 HF.py f3-11 15mg mF19CPD C6D6 {e:\bruk400data\2014\May} ejt 2				
Date	23 May 2014 12:14:08	*Date Stamp*	23 May 2014 12:14:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\VOL3\USERS\SNMRDATA\BRUK400DATA\2014\MAY\DATA\EJT\NMR\2014-05-23-EJT-2\11\PDATA\1\1R						
Frequency (MHz)	376.50	*Nucleus*	19F	*Number of Transients*	16	*Origin*	AV400
Original Points Count	65536	*Owner*	Administrator	*Points Count*	262144	*Pulse Sequence*	zgig
Receiver Gain	4100.00	*SW(cyclical) (Hz)*	89285.71	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-37649.5977
Spectrum Type	STANDARD	*Sweep Width (Hz)*	89285.37	*Temperature (degree C)*	22.300		

2014-05-23-EJT-2.011.001.1R.esp VerticalScaleFactor = 1



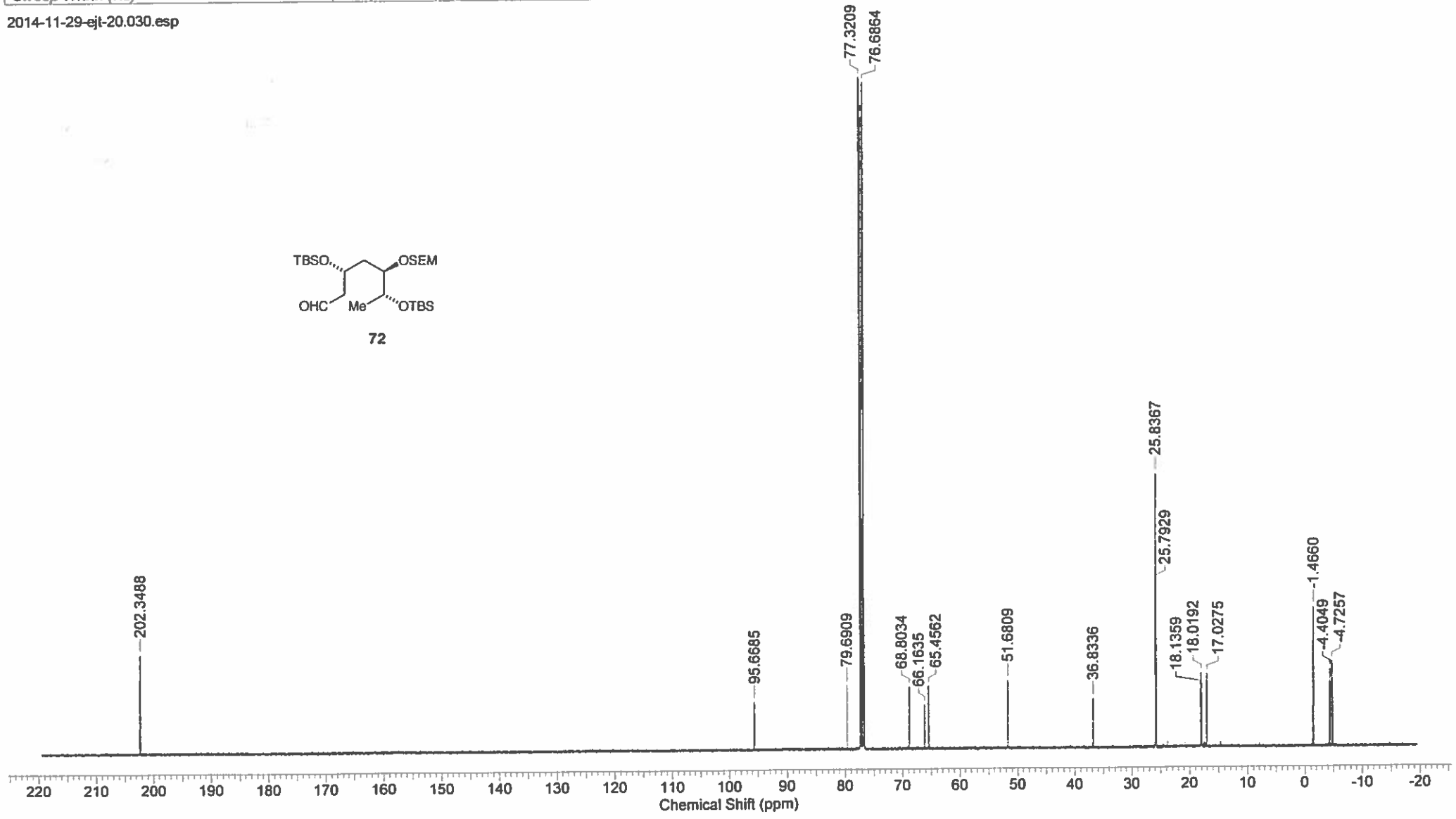
Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM161 f15-35 289mg mPROTON CDCl3 (e:\bruk400adata\2015\Feb) ejt 22				
Date	25 Feb 2015 16:36:16			*Date Stamp*	25 Feb 2015 16:36:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Feb\data\ejt\nmr\2015-02-25-ejt-22\10\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	144.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.6748	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	19.900				

PRM161aldehyde-HNMR.esp



Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM161 aldehyde mCARBON_B CDCl3 (e:\bruk400cdata\2014\Nov) ejt 20				
Date	29 Nov 2014 17:23:12			*Date Stamp*	29 Nov 2014 17:23:12		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2014\Nov\data\ejt\nmr\2014-11-29-ejt-20\30\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10053.5352	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	23.149				

2014-11-29-ejt-20.030.esp



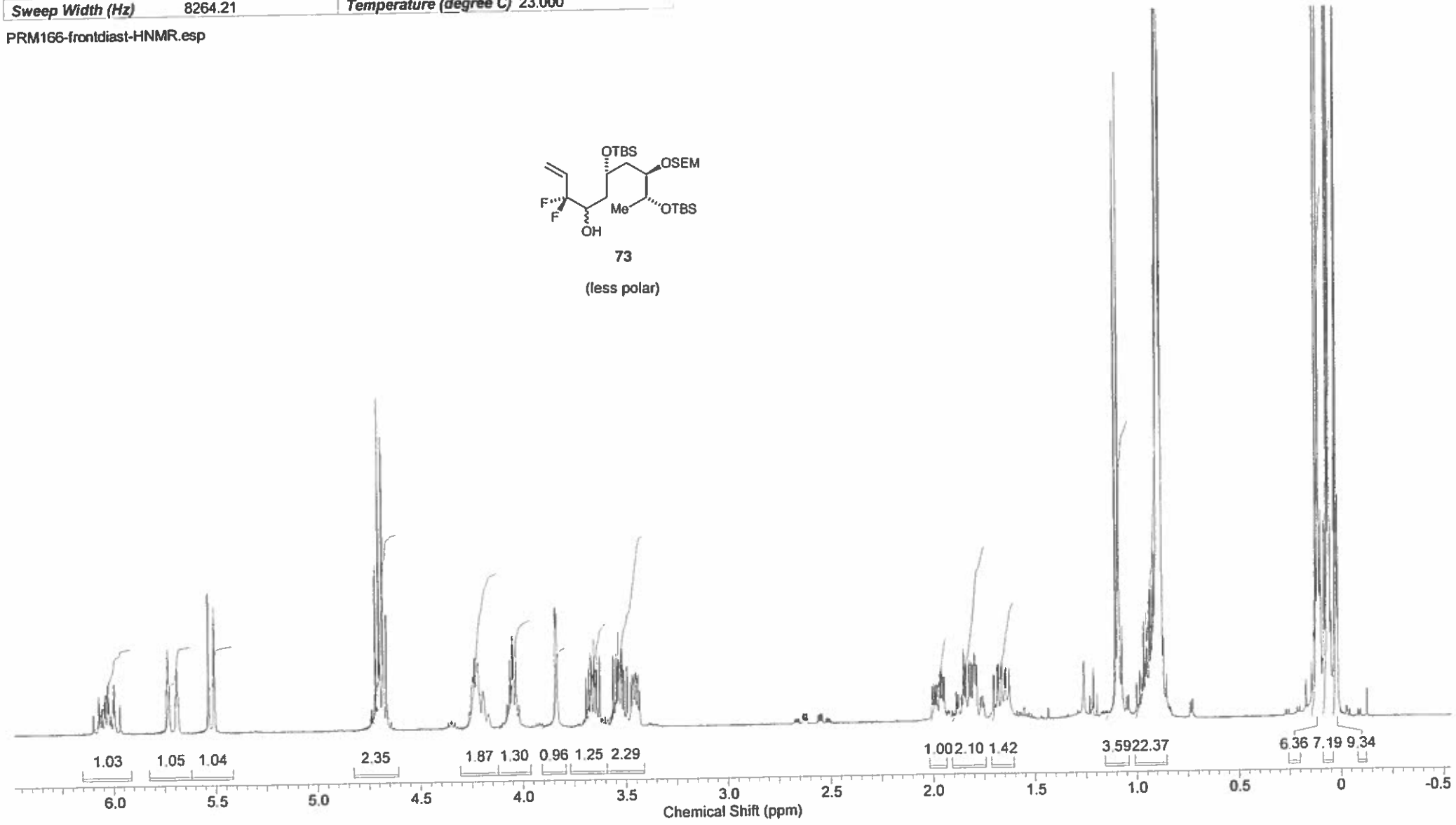
72

Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM166 f12+13 34mg clean front diastereomer? mPROTON CDCl3 {e:\bruk400adata\2015\Jan} ejt 2				
Date	08 Jan 2015 13:17:52	*Date Stamp*	08 Jan 2015 13:17:52				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-08-ejt-2\13\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	101.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9270	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	23.000				

PRM166-frontdiast-HNMR.esp

73

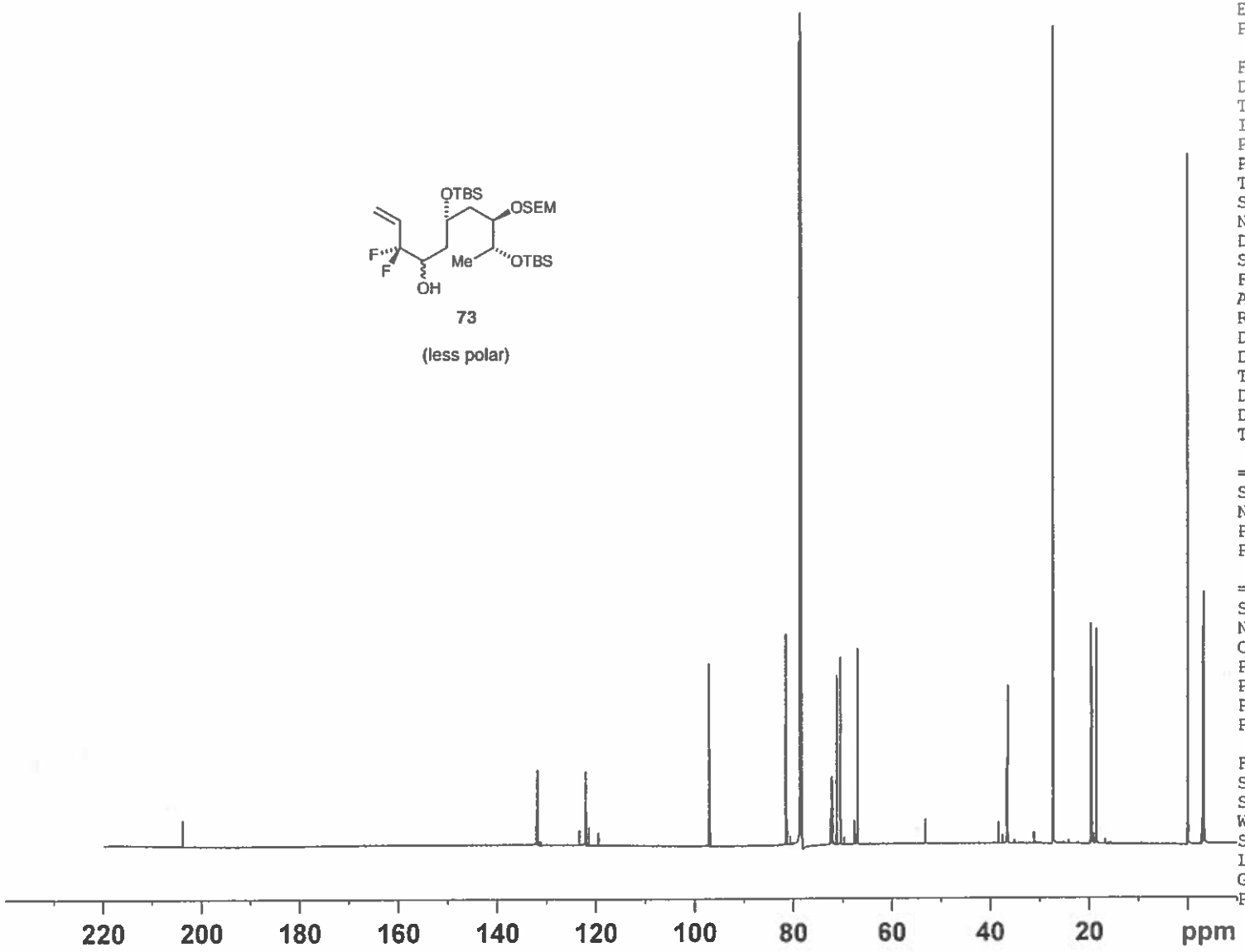
(less polar)



P.Mears EJT-PRM166 F1243 34mg 0115060
mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 7

73

(less polar)



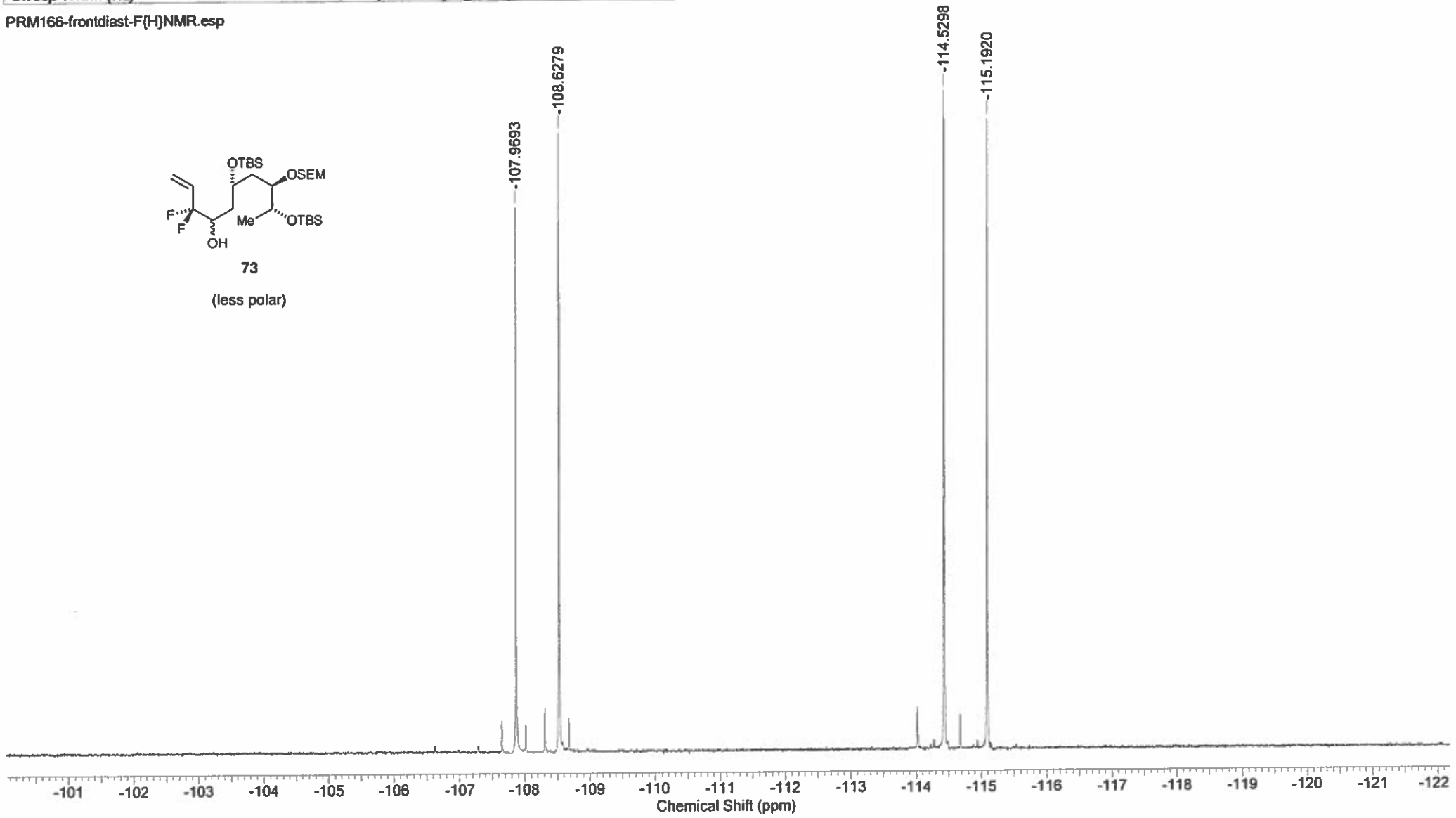

```
Current Data Parameters
NAME      2015-01-09-staff-7
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150109
Time                  18.18
INSTRUM               spect
PROBHD    5 mm CPPBBO BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    5000
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                    184.4
DW                 16.800 usec
DE                 102.82 usec
TE                   298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          125.7854504 MHz
NUC1                    13C
P1                  10.00 usec
PLW1          53.59999847 W

======== CHANNEL f2 ========
SFO2          500.1920008 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2          16.00000000 W
PLW12          0.28622001 W
PLW13          0.18318000 W

F2 - Processing parameters
SI                    32768
SF            125.7726921 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM166 f12+13 34mg clean front diastereomer? mF19CPD CDCl3 (e:\bruk400adata\2015\Jan) ejt 2				
Date	08 Jan 2015 13:22:08	*Date Stamp*	08 Jan 2015 13:22:08				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-08-ejt-2\15\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	2050.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	23.000				

PRM166-frontdiast-F{H}NMR.esp

73

(less polar)

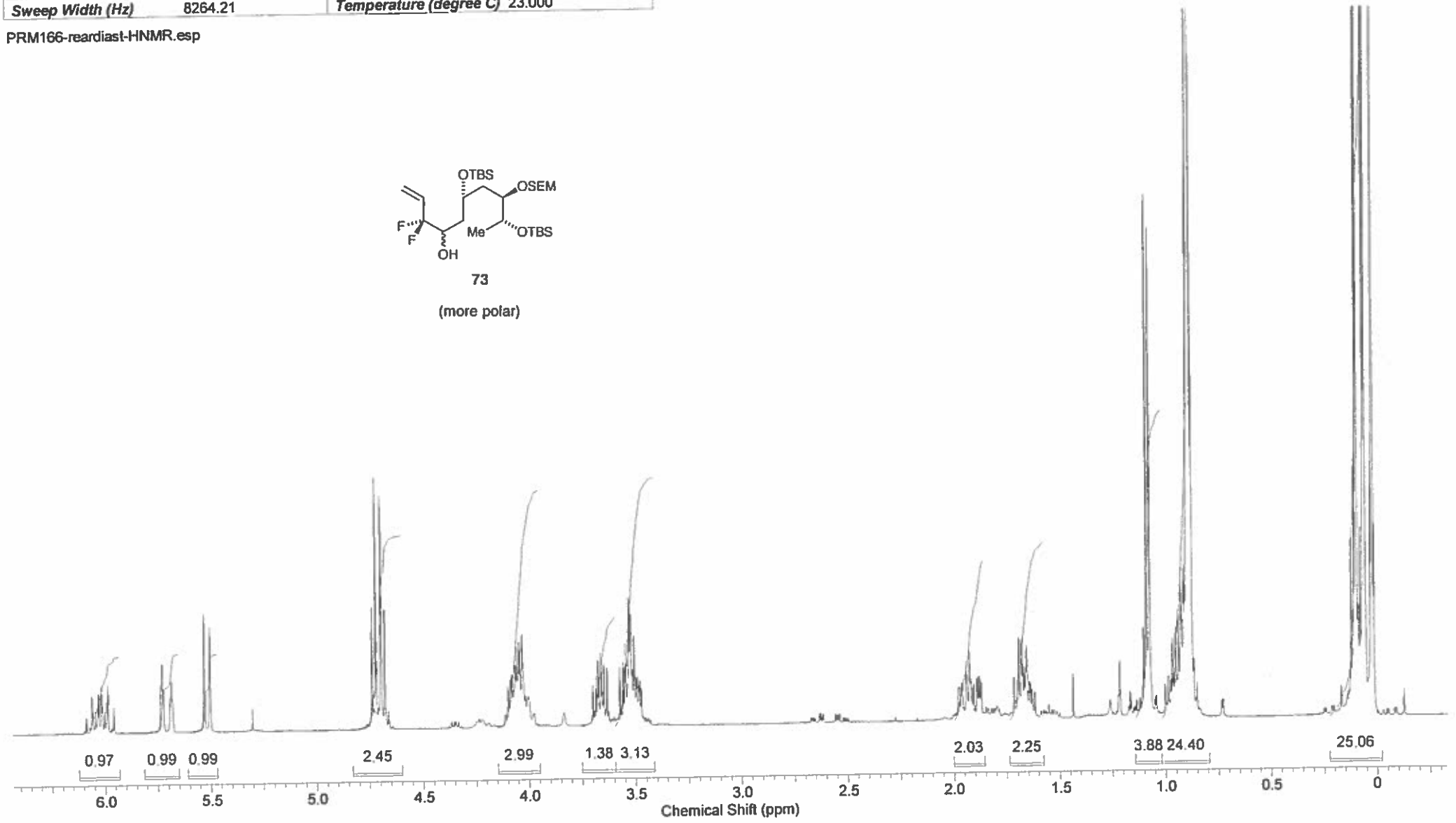


Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM166 f39-43 40mg mPROTON CDCl3 (e:\bruk400adata\2015\Jan) ejt 34				
Date	16 Jan 2015 11:35:28			*Date Stamp*	16 Jan 2015 11:35:28		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-16-ejt-34\10\fid			*Origin*	AV400	*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Pulse Sequence*	zg30b	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Spectrum Offset (Hz)*	2464.9272	*Receiver Gain*	80.60
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d			*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	23.000				

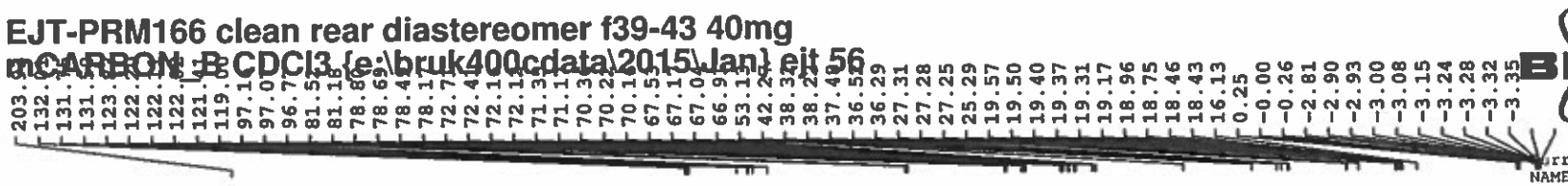
PRM166-reardiast-HNMR.esp

73

(more polar)

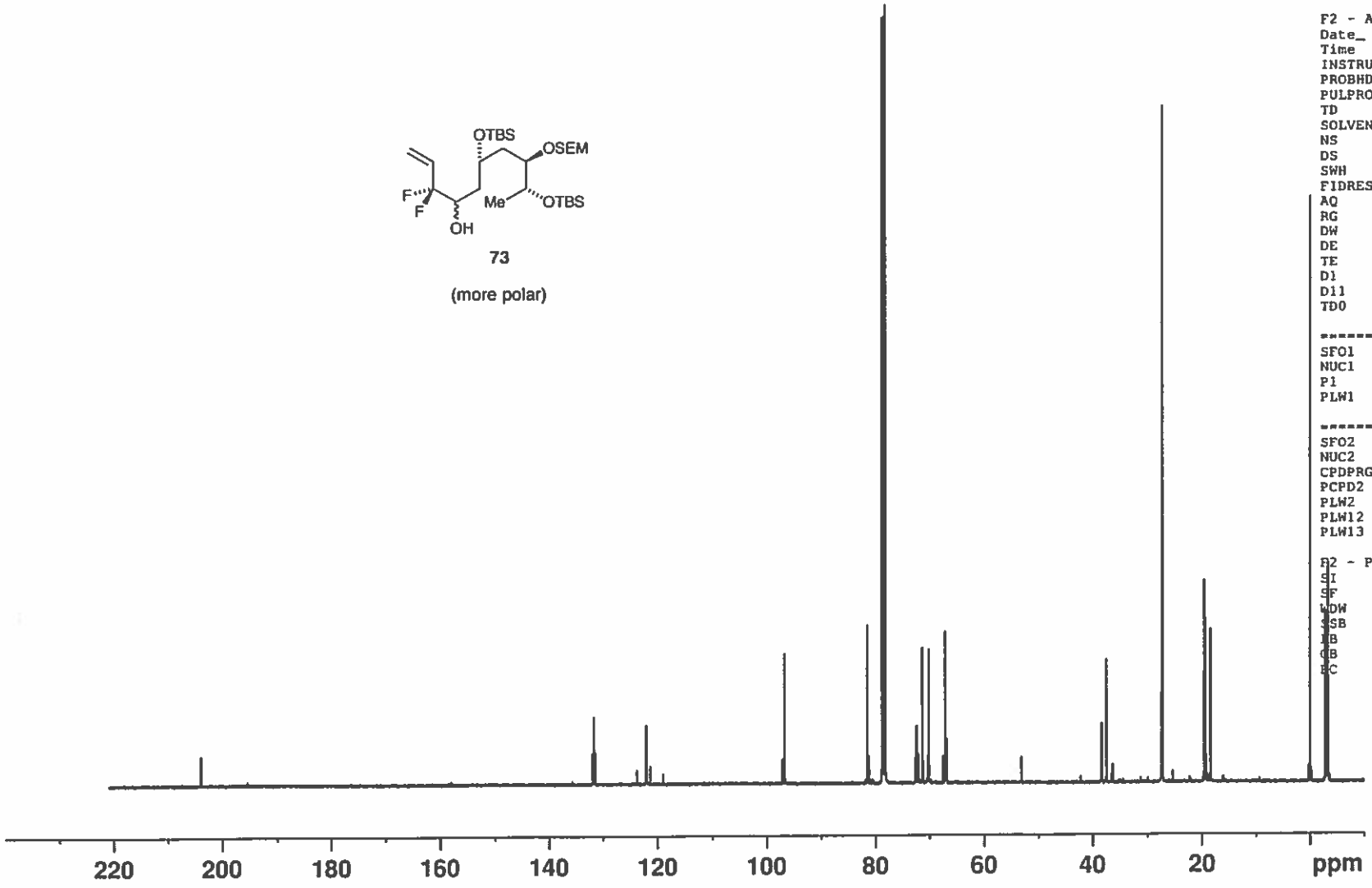


EJT-PRM166 clean rear diastereomer f39-43 40mg
mCARBON - B CDCl3 {e:\bruk400cdata\2015\Jan} ejt 56



73

(more polar)

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Current Data Parameters
NAME      2015-01-16-ejt-56
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150116
Time                 22.49
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    45.2
DW                 20.800 usec
DE                 41.77 usec
TE                 287.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

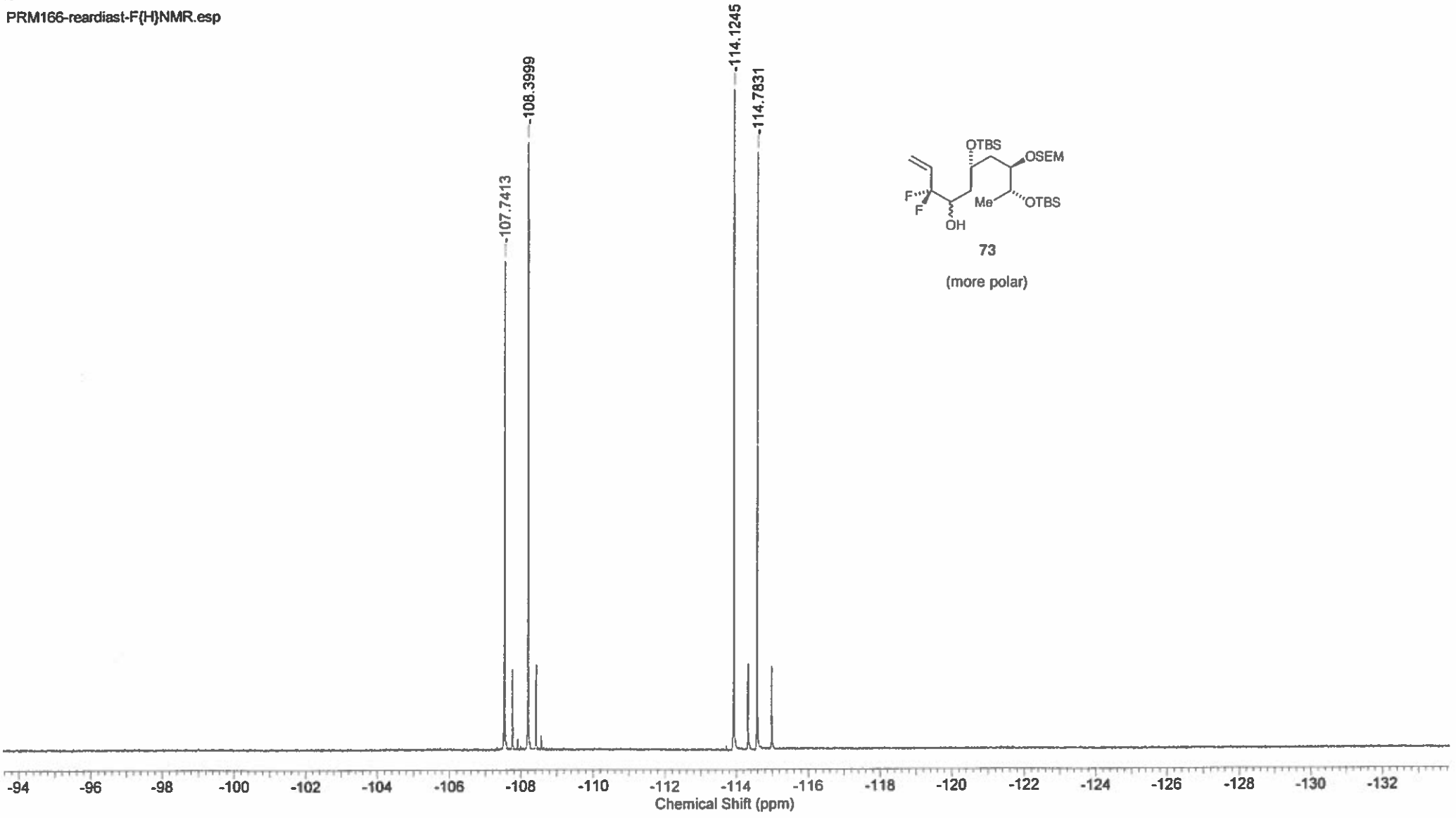
======== CHANNEL f1 ========
SFO1          100.6077379 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          33.00000000 W

======== CHANNEL f2 ========
SFO2          400.0716003 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2              80.00 usec
PLW2           7.40000010 W
PLW12          0.17209999 W
PLW13          0.11014000 W

F2 - Processing parameters
SI                    32768
SF            100.5975375 MHz
WDW                     EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM166 f39-43 40mg mF19CPD CDCl3 (e:\bruk400adata\2015\Jan) ejt 34				
Date	16 Jan 2015 11:39:44			*Date Stamp*	16 Jan 2015 11:39:44		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-16-ejt-34\12\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	322.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	23.000				

PRM166-reardiast-F{H}NMR.esp

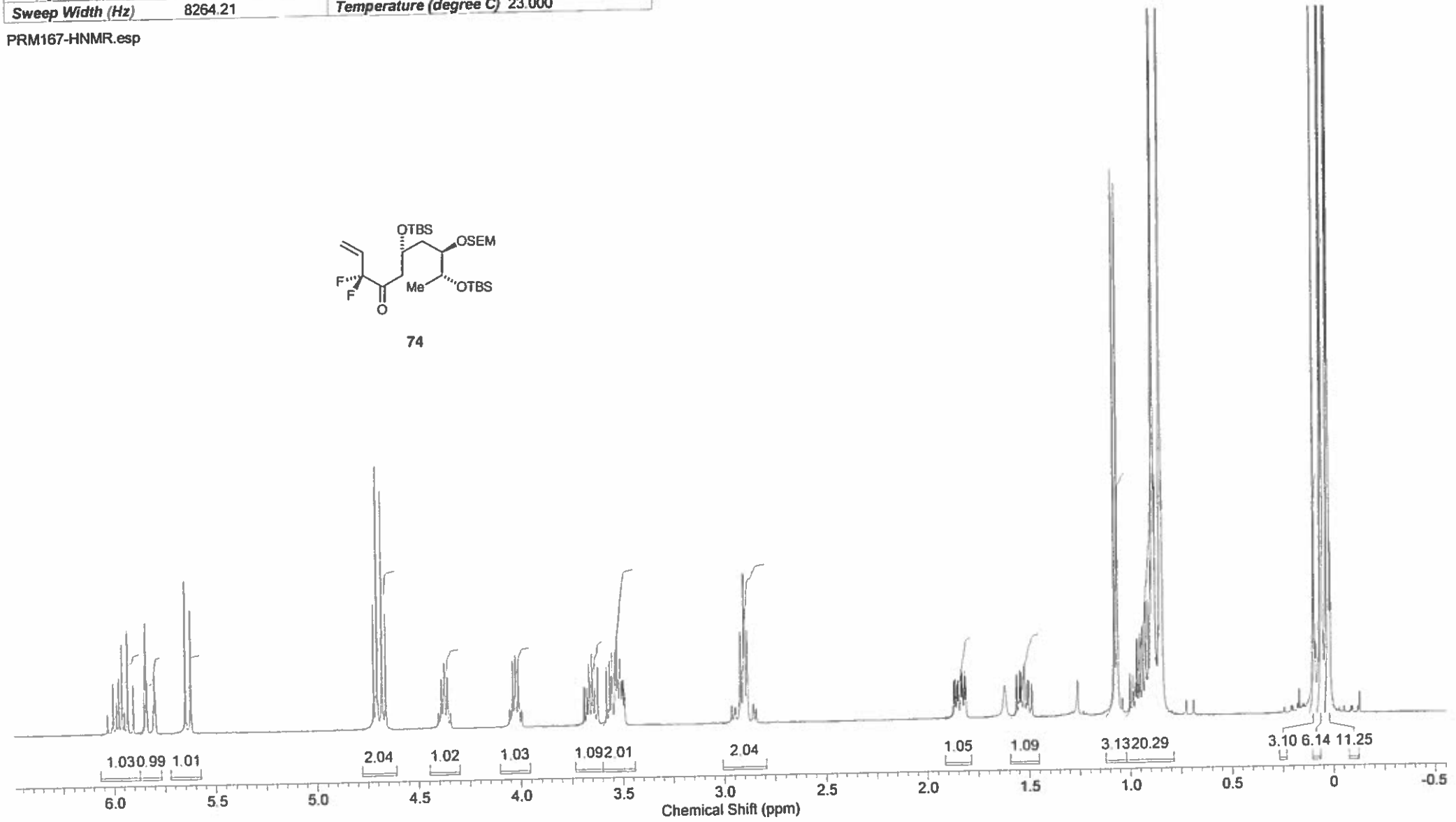


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

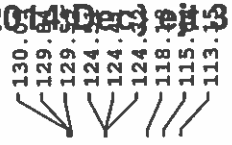
Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM167 f8-22 47mg mPROTON CDCl3 (e:\bruk400adata\2014\Dec) ejt 59				
Date	18 Dec 2014 14:13:20			*Date Stamp*	18 Dec 2014 14:13:20		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2014\Dec\data\ejt\nmr\2014-12-18-ejt-59\10\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	90.50
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9270	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	23.000				

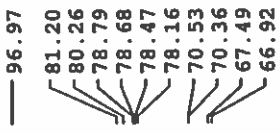
PRM167-HNMR.esp

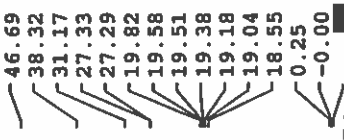
74



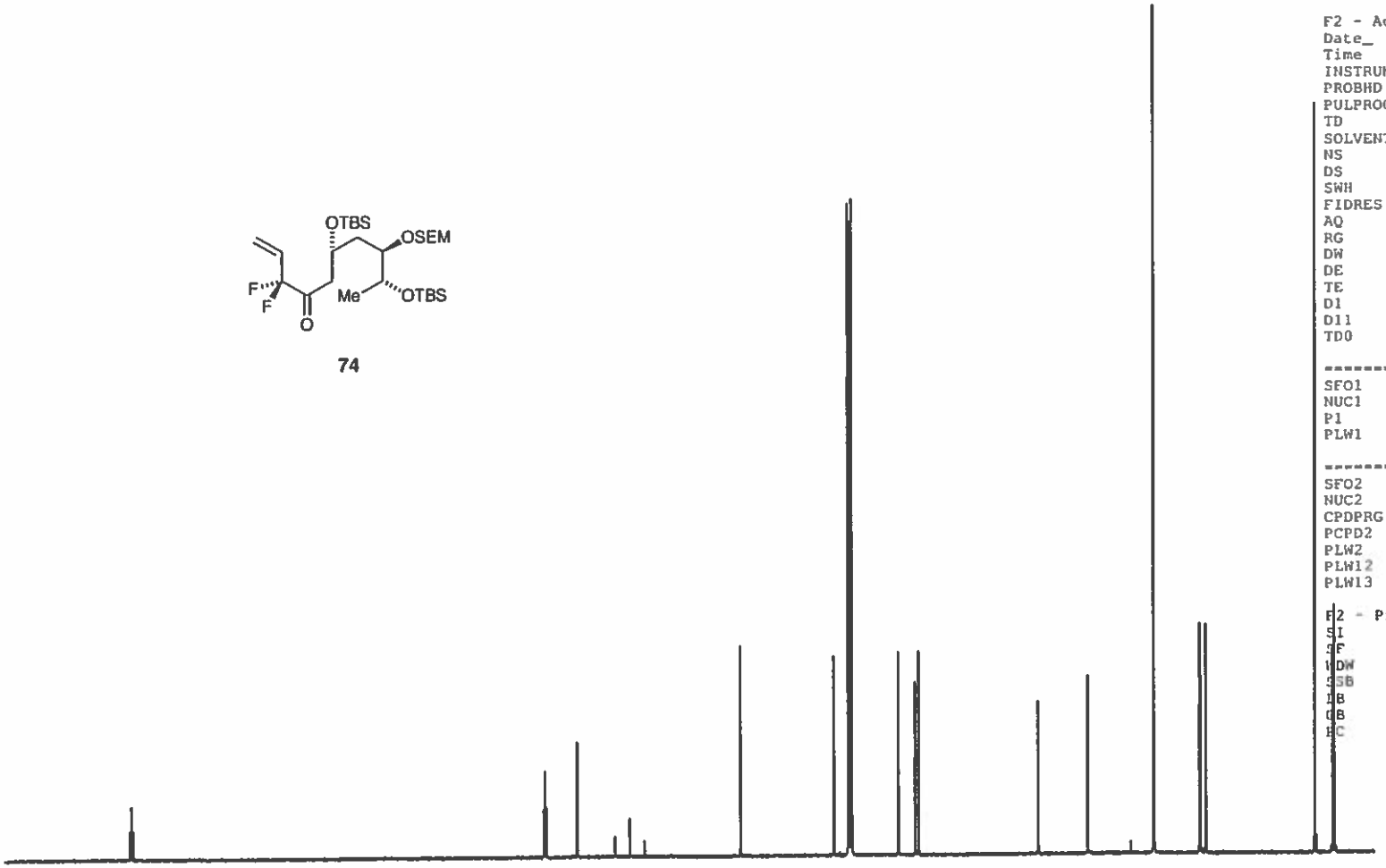
EJT-PRM167 f8-22 47mg
mCARBON_B CDCl3 {e:\bruk400cdata\2014Dec} ejt-3

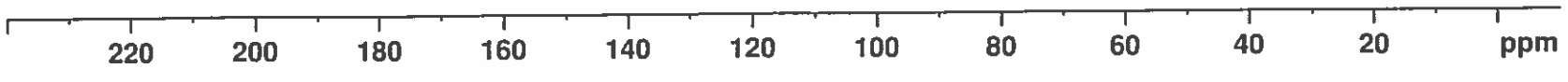






74



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Current Data Parameters
NAME      2014-12-18-ejt-3
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20141218
Time                 22.00
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    45.2
DW                 20.800 usec
DE                 41.77 usec
TE                 296.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6077379 MHz
NUC1                   13C
P1                  10.00 usec
PLW1         33.00000000 W

======== CHANNEL f2 ========
SFO2          400.0716003 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              80.00 usec
PLW2           7.40000010 W
PLW12          0.17209999 W
PLW13          0.11014000 W

F2 - Processing parameters
SI                    32768
SF           100.5975350 MHz
WDW                     EM
SSB          0
LB                  1.00 Hz
GB           0
PC                  1.40
```
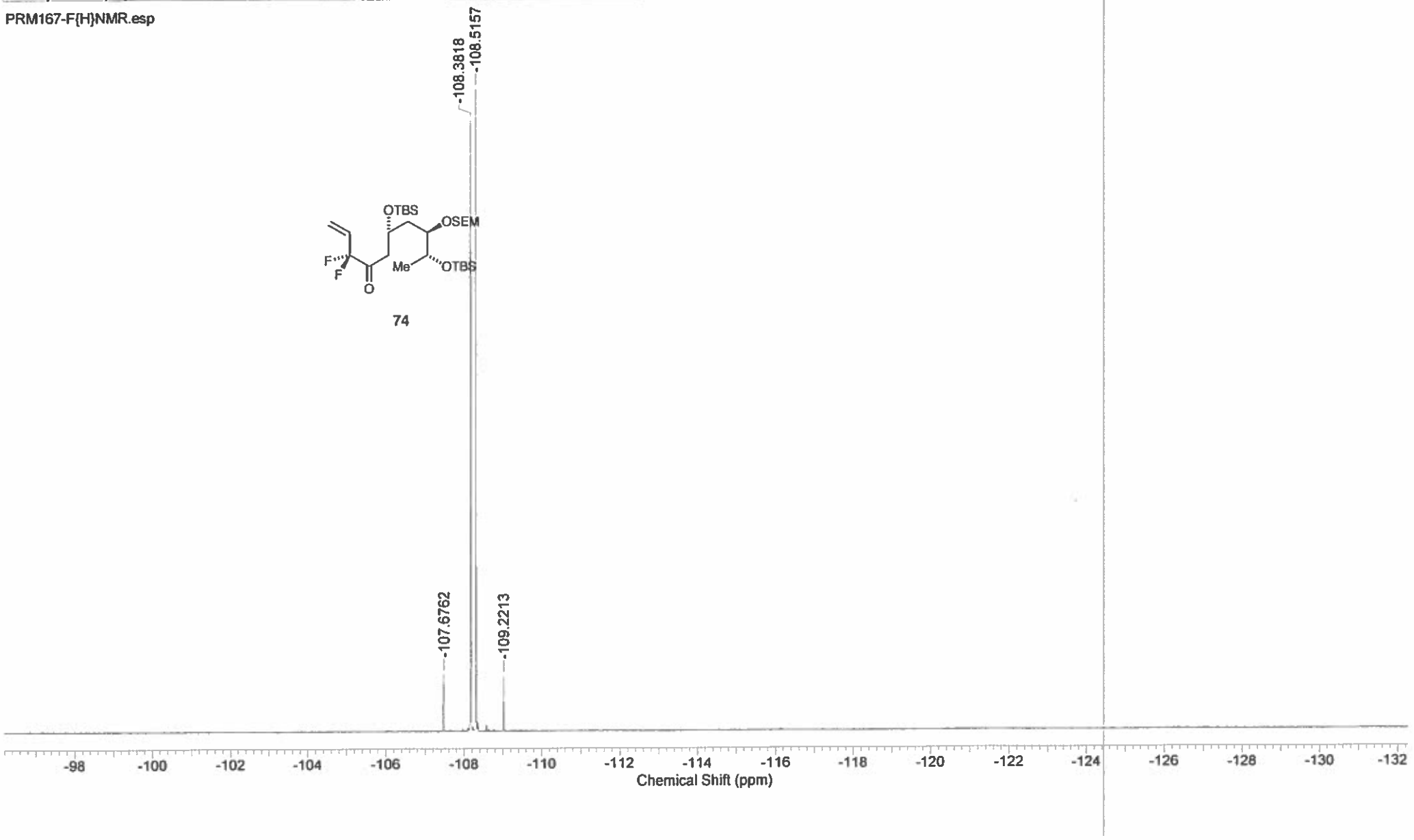
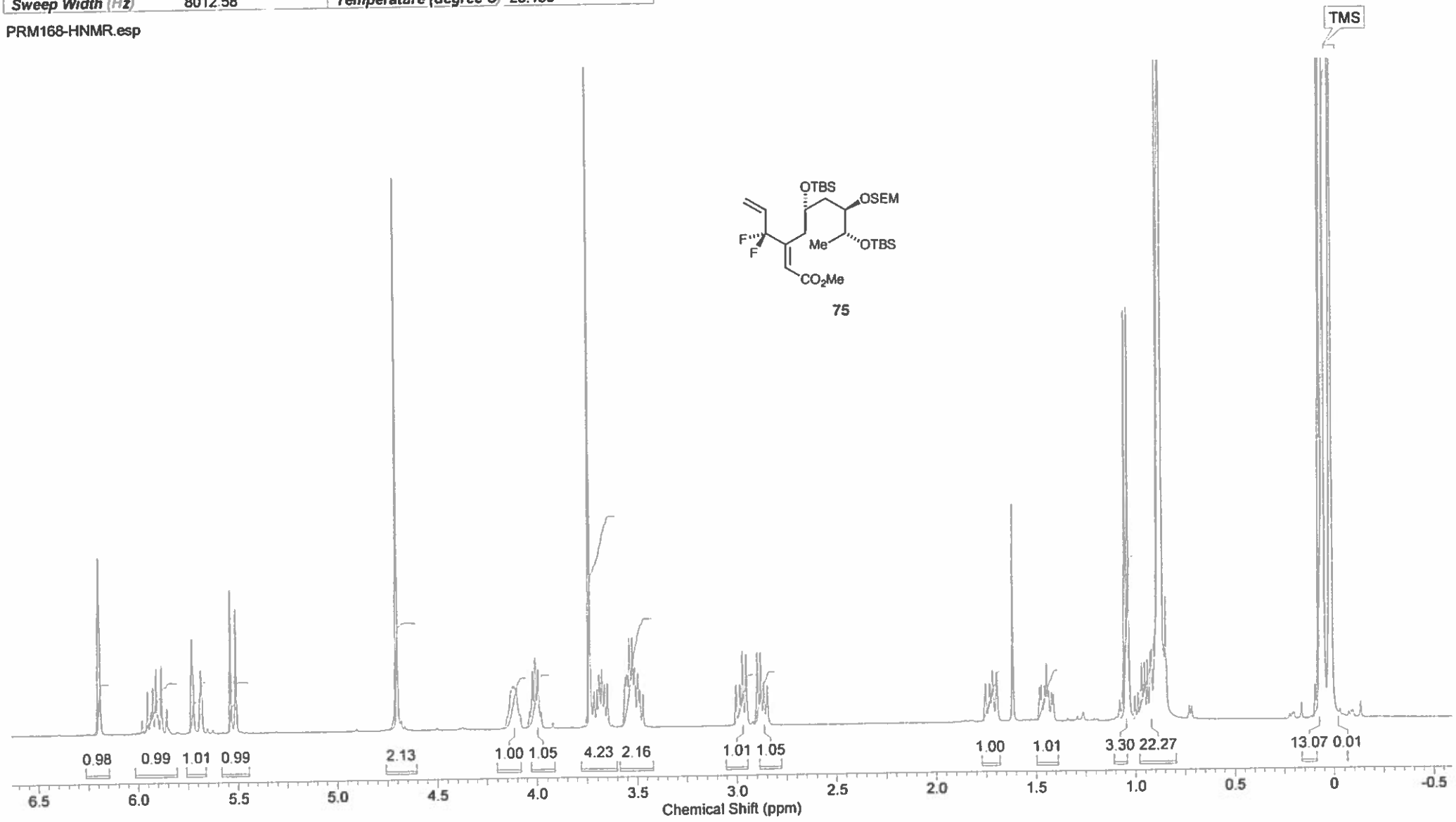

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM167 f8-22 47mg mF19CPD CDCl3 (e:\bruk400adata\2014\Dec) ejt 59				
Date	18 Dec 2014 14:17:36			*Date Stamp*	18 Dec 2014 14:17:36		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2014\Dec\data\ejt\nmr\2014-12-18-ejt-59\12\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	2050.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	27.000				

PRM167-F{H}NMR.esp



Acquisition Time (sec)	4.0894	*Comment*	EJT-PRM168 f7-9 38mg mPROTON_A CDCl3 (e:\bruk400cdata\2015\Jan) ejt 10				
Date	07 Jan 2015 16:34:08			*Date Stamp*	07 Jan 2015 16:34:08		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Jan\data\ejt\nmr\2015-01-07-ejt-10\10\fid					*Frequency (MHz)*	400.07
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	64.00
SW(cyclical) (Hz)	8012.82	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	1894.5574	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8012.58	*Temperature (degree C)*	23.150				

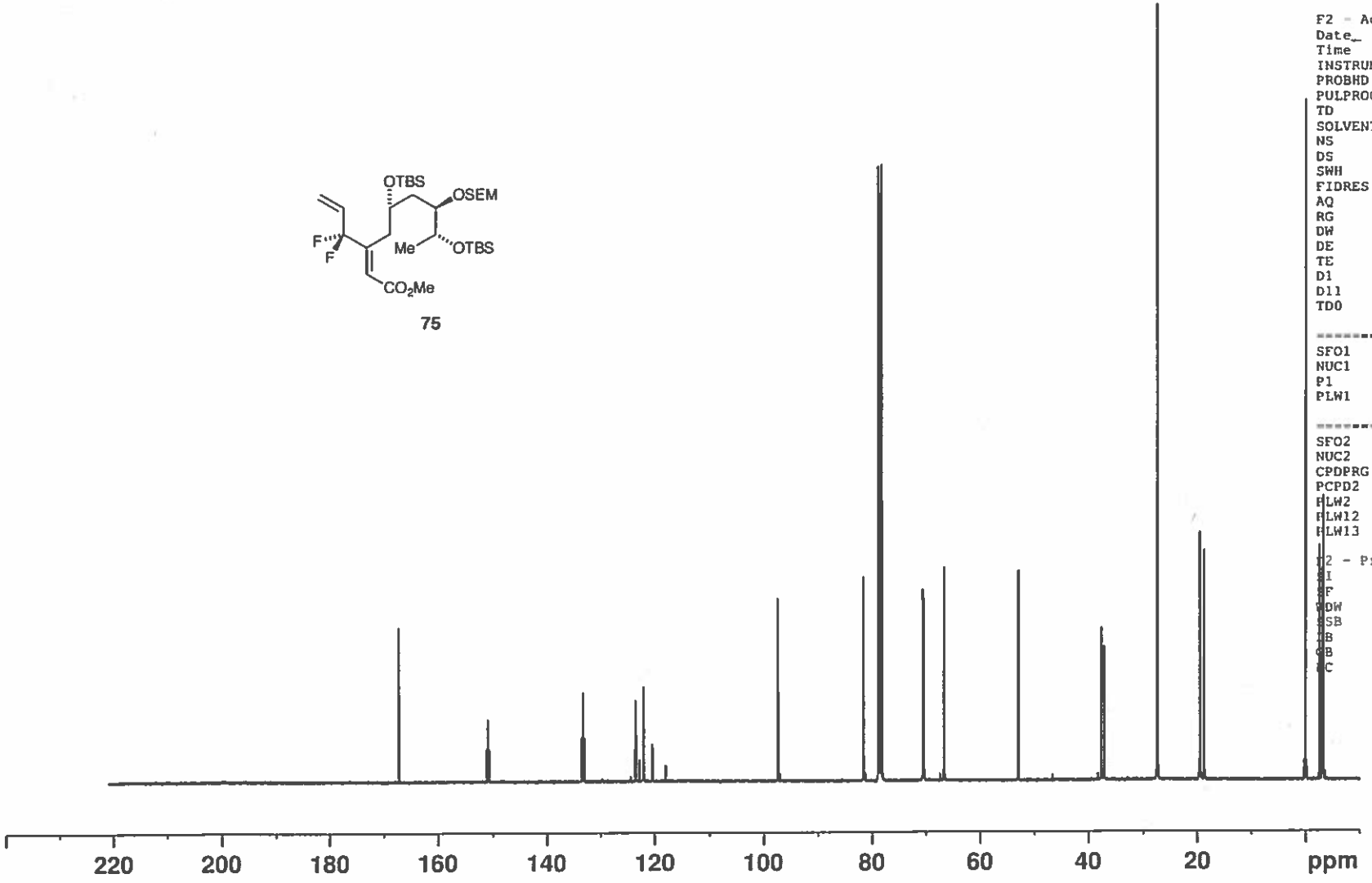
PRM168-HNMR.esp



EJT-PRM168 Prod data

mCARBON_B CDCl3 [e:\bruk400cdata\2015\Jan] ejt 26

75



Current Data Parameters

NAME	2015-01-11-ejt-26
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20150112
Time	19.11
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631488 sec
RG	71.8
DW	20.800 usec
DE	41.77 usec
TE	288.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

SFO1	100.6077379 MHz
NUC1	13C
P1	10.00 usec
PLW1	33.00000000 W

======== CHANNEL f2 ========

SFO2	400.0716003 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	7.40000010 W
PLW12	0.17209999 W
PLW13	0.11014000 W

F2 - Processing parameters

SI	32768
SF	100.5975370 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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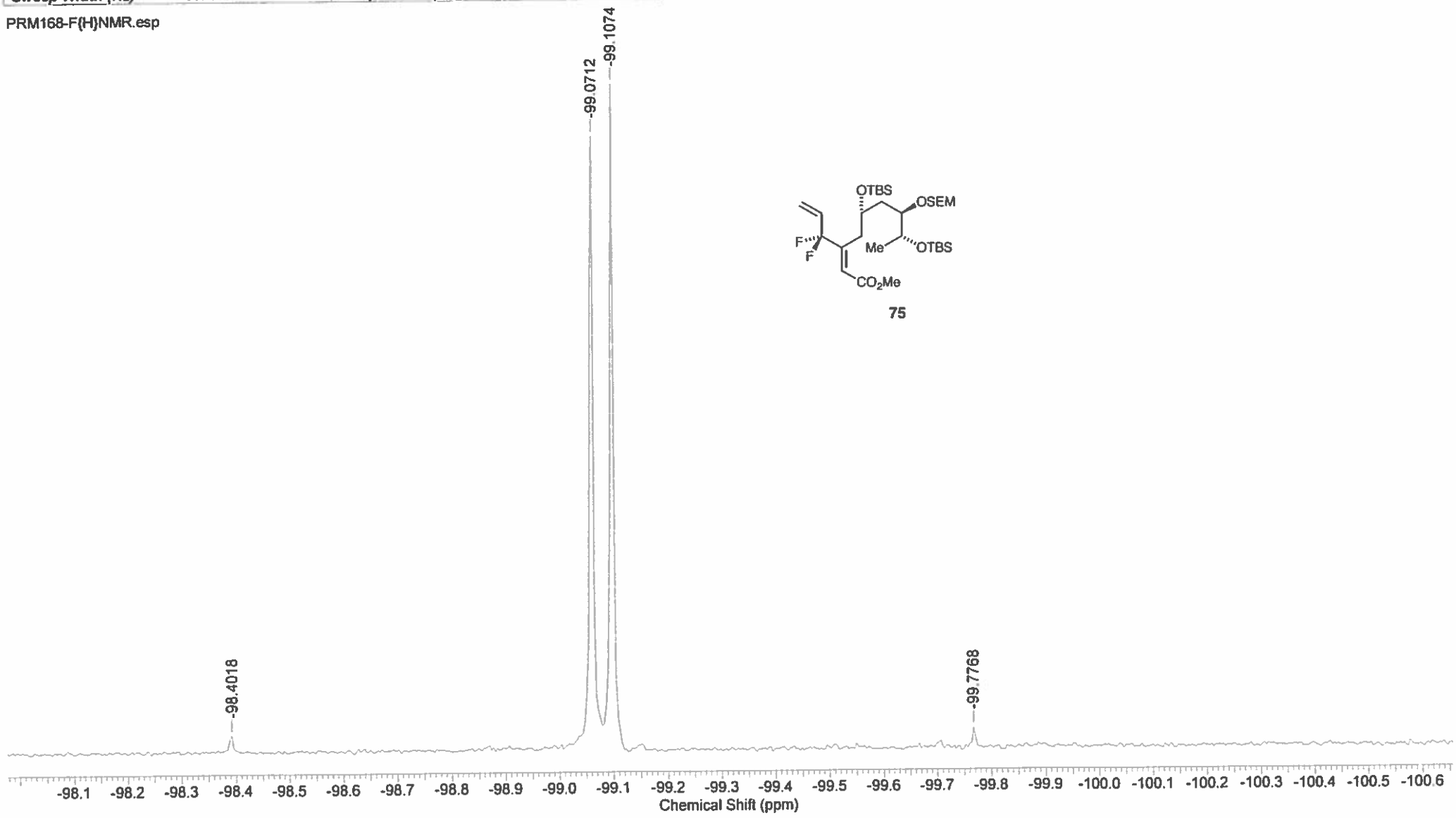
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM169 f17-33 124mg mF19CPD CDCl3 (e:\bruk400adata\2015\Jan) ejt 29				
Date	10 Jan 2015 15:32:16			*Date Stamp*	10 Jan 2015 15:32:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-10-ejt-29\12\fid			*Origin*	AV400	*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Pulse Sequence*	zgig	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Spectrum Offset (Hz)*	-37649.5977	*Receiver Gain*	287.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d			*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	23.000				

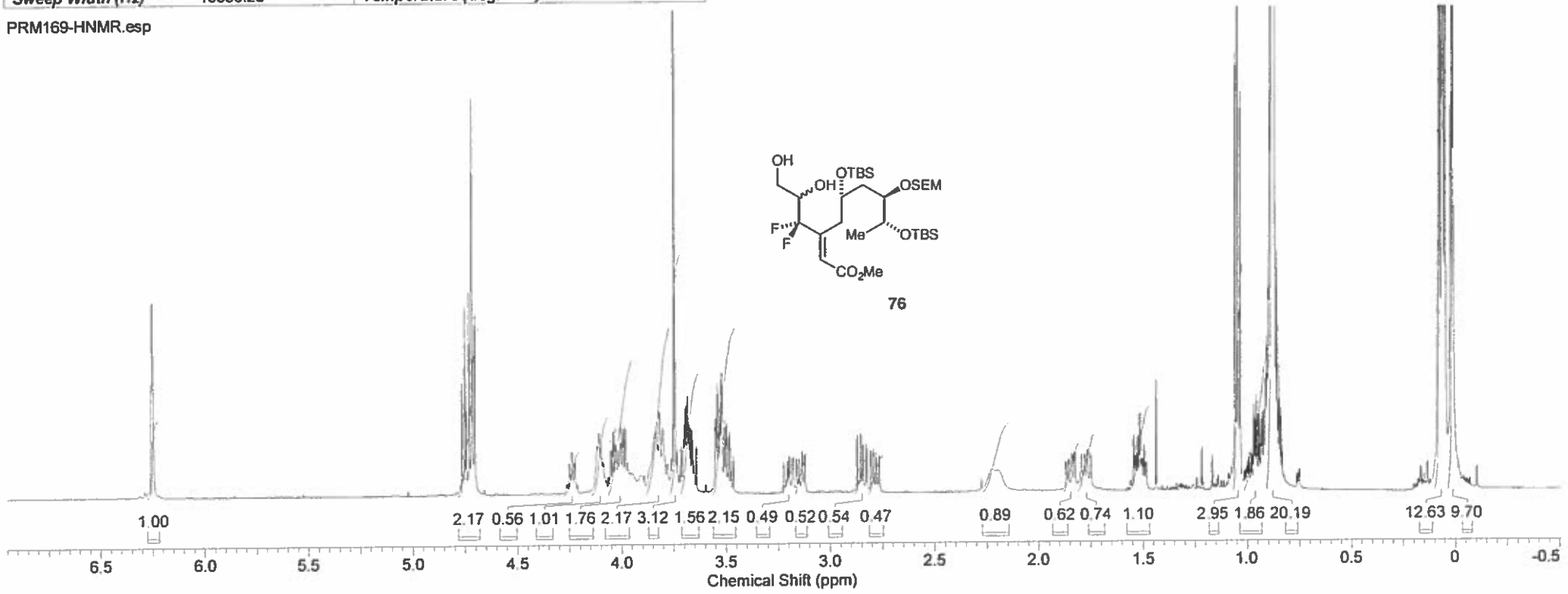
PRM168-F{H}NMR.esp



75

Acquisition Time (sec)	3.1719	*Comment*	EJT-PRM169 f28-36 44mg mPROTON CDCl3 (E:\bruk500adata\2015\Jan) ejt 10				
Date	12 Jan 2015 13:05:04			*Date Stamp*	12 Jan 2015 13:05:04		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2015\Jan\data\ejt\nmr\2015-01-12-ejt-10\20\fid					*Frequency (MHz)*	500.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	50.80
SW(cyclical) (Hz)	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3081.5532	*Spectrum Type*	STANDARD
Sweep Width (Hz)	10330.26	*Temperature (degree C)*	20.400				

PRM169-HNMR.esp



76

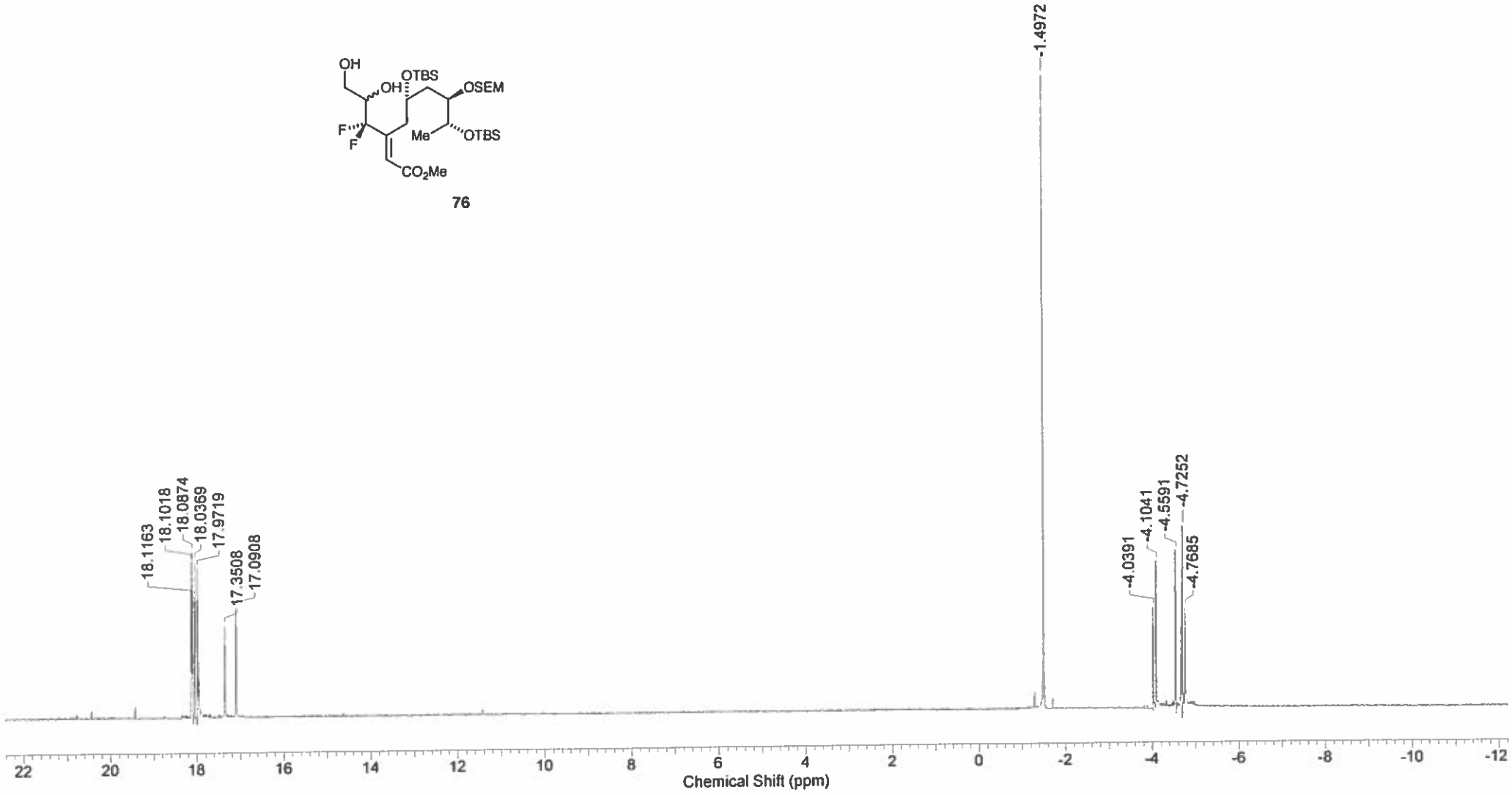
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	0087 .. 0.039	.70469666	1.55986125e+10	9.70469666
2	0363 .. 0.10	2.6314582	2.03028726e+10	12.63145828
3	3486 .. 0.900	0.1898193	3.24516250e+10	20.18981934
4	9102 .. 1.011	.85710049	2.98496614e+9	1.85710049
5	0235 .. 1.062	.95424557	4.74843597e+9	2.95424557
6	4679 .. 1.571	.09587038	1.76142106e+9	1.09587038
7	7343 .. 1.800	.74124676	1.19142528e+9	0.74124676
8	3096 .. 1.880	.62363493	1.00238470e+9	0.62363493
9	1451 .. 2.270	.89462709	1.43795750e+9	0.89462709
10	7469 .. 2.810	.47494268	7.63387776e+8	0.47494268
11	3156 .. 2.880	.53880036	8.66027904e+8	0.53880036

No.	(ppm)	Value	Absolute Value	Non-Negative Value
12	1107 .. 3.160	.51732343	8.31507520e+8	0.51732343
13	1687 .. 3.230	.49489146	7.95451968e+8	0.49489146
14	4552 .. 3.562	.15453339	3.46303770e+9	2.15453339
15	5323 .. 3.711	.56468415	2.51495782e+9	1.56468415
16	7205 .. 3.763	.11513853	5.00704358e+9	3.11513853
17	7679 .. 3.882	.17377329	3.49396250e+9	2.17377329
18	9501 .. 4.061	.75517964	2.82114611e+9	1.75517964
19	0657 .. 4.141	.01384950	1.62958682e+9	1.01384950
20	1993 .. 4.280	.56165135	9.02756928e+8	0.56165135
21	3814 .. 4.782	.17071009	3.48903910e+9	2.17071009
22	2189 .. 6.271	.00053573	1.60818714e+9	1.00053573

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM 169 f28-36 44mg 0115 062 mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 10				
Date	14 Jan 2015 02:48:32	*Date Stamp*	14 Jan 2015 02:48:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Jan\data\staff\nmr\2015-01-13-staff-10\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.4053	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	24.997				

PRM169-CNMR.esp

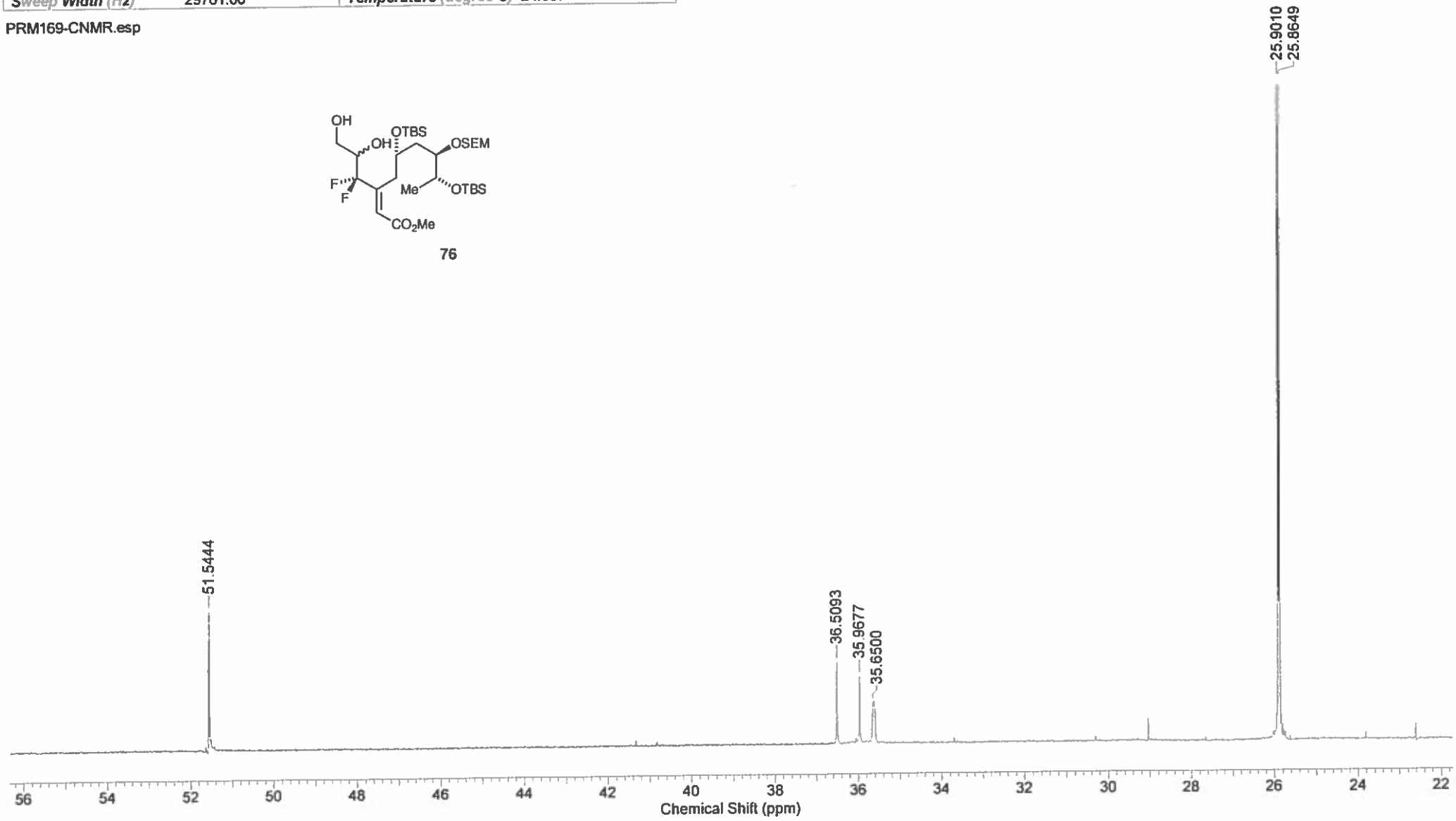
76



Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM 169 f28-36 44mg 0115 062 mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 10				
Date	14 Jan 2015 02:48:32	*Date Stamp*	14 Jan 2015 02:48:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Jan\data\staff\nmr\2015-01-13-staff-10\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.4053	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	24.997				

PRM169-CNMR.esp

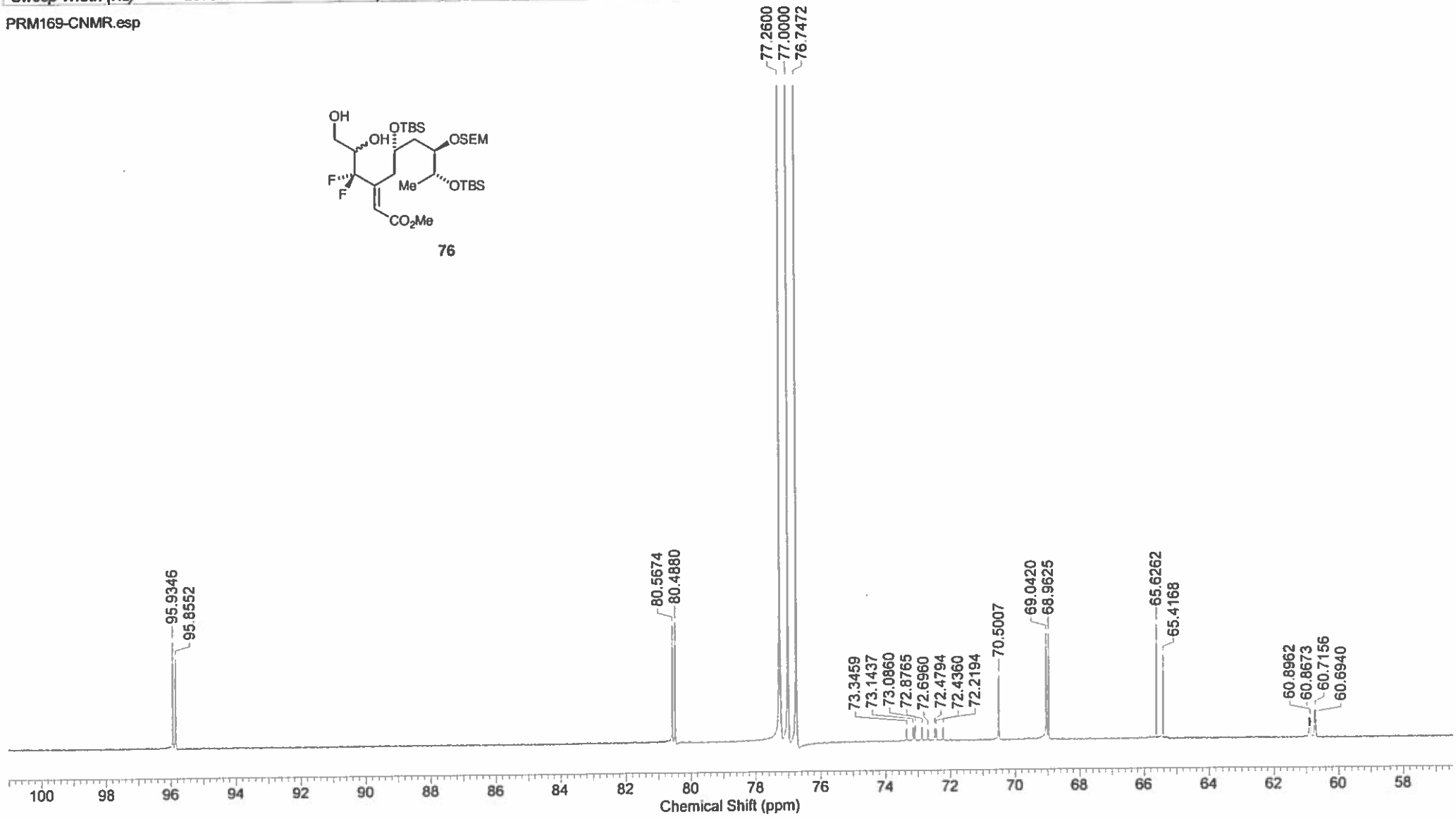
76



Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM 169 f28-36 44mg 0115 062 mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 10				
Date	14 Jan 2015 02:48:32	*Date Stamp*	14 Jan 2015 02:48:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Jan\data\staff\nmr\2015-01-13-staff-10\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.4053	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	24.997				

PRM169-CNMR.esp

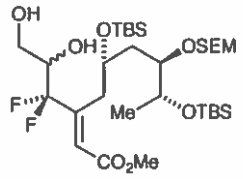
76



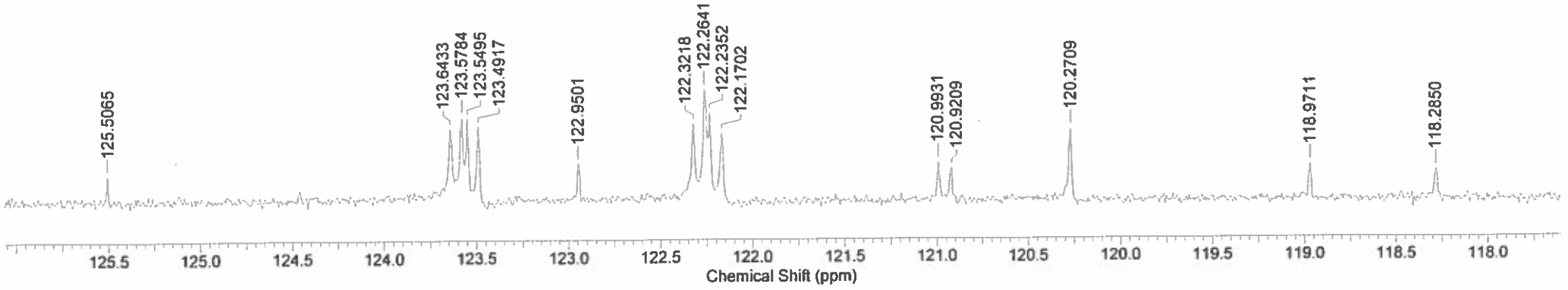
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM 169 f28-36 44mg 0115 062 mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 10				
Date	14 Jan 2015 02:48:32	*Date Stamp*	14 Jan 2015 02:48:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Jan\data\staff\nmr\2015-01-13-staff-10\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.4053	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	24.997				

PRM169-CNMR.esp



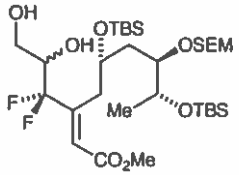
76



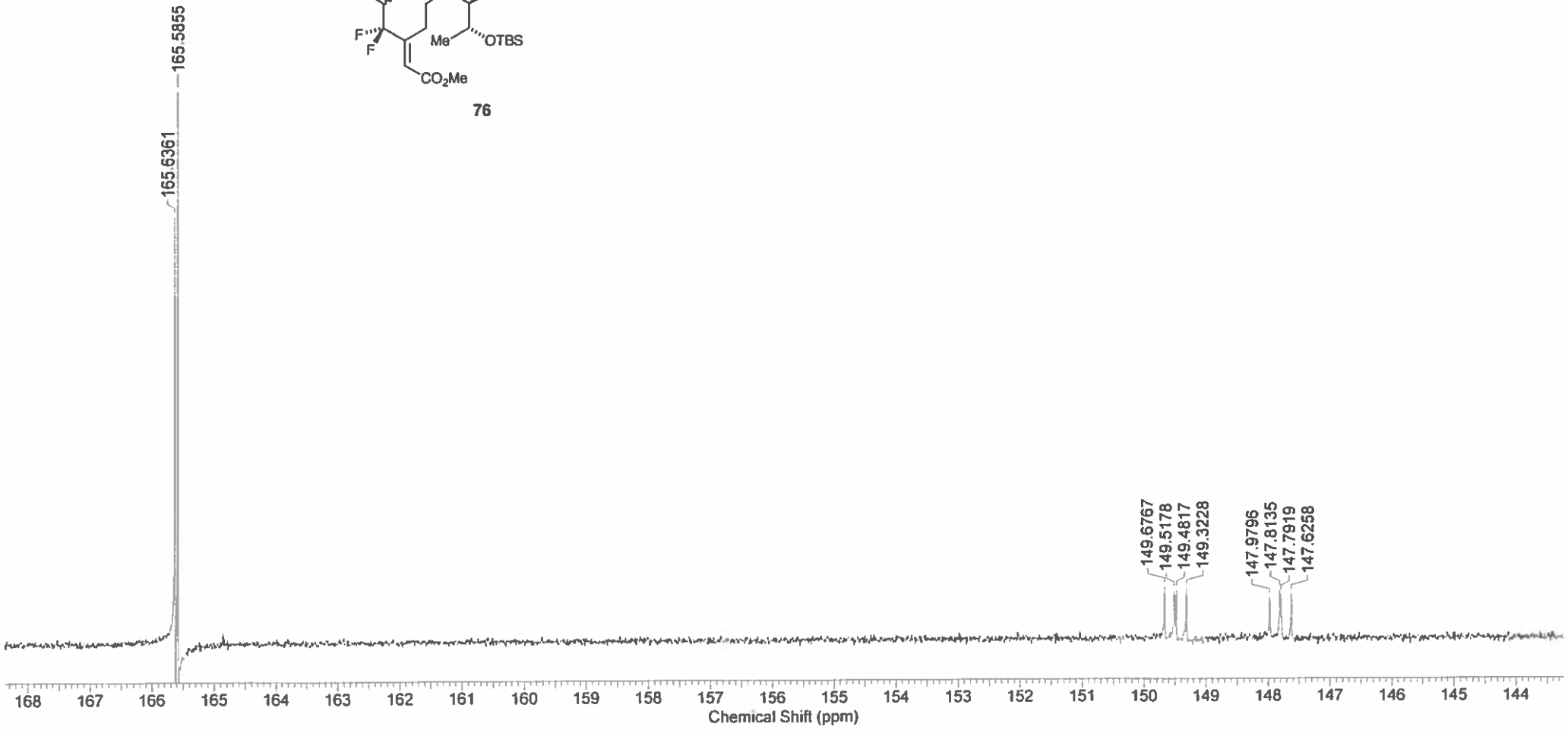
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	EJT-PRM 169 f28-36 44mg 0115 062 mCARBON CDCl3 (E:\bruk500cdata\2015\Jan) staff 10				
Date	14 Jan 2015 02:48:32	*Date Stamp*	14 Jan 2015 02:48:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Jan\data\staff\nmr\2015-01-13-staff-10\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	5000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	12571.4053	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	24.997				

PRM169-CNMR.esp



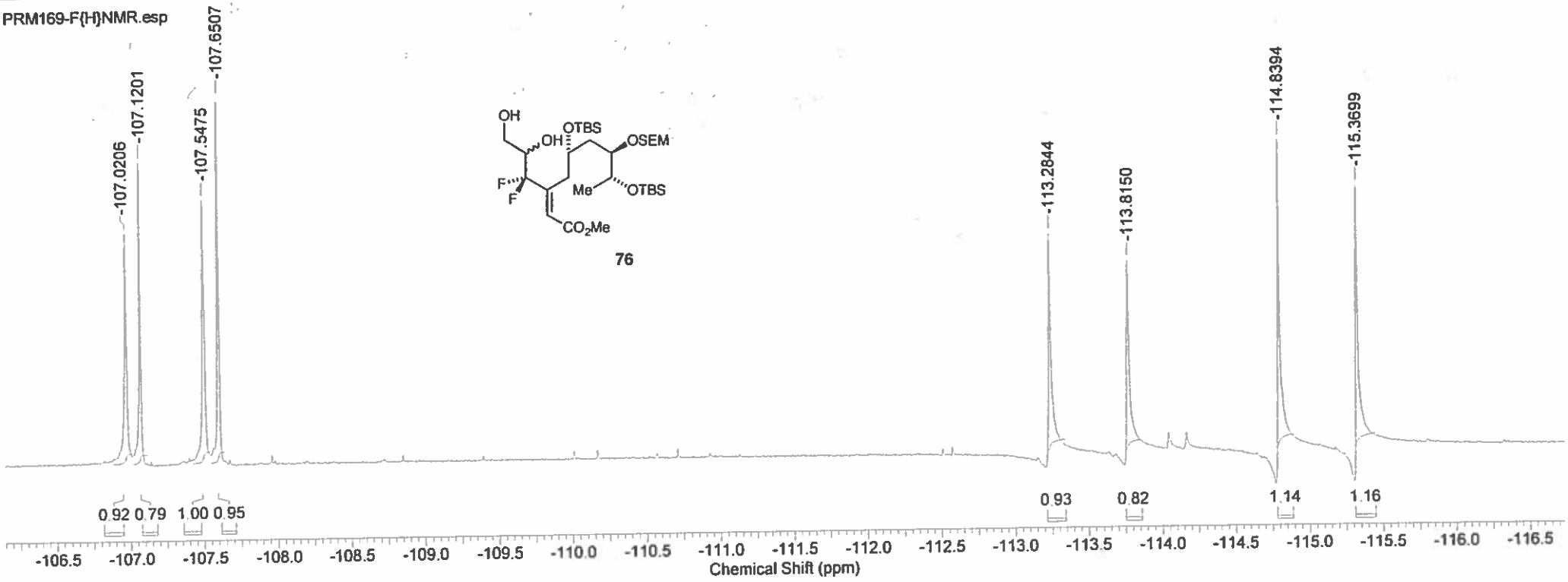
76



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM169 f28-36 44mg m19FCPD CDCl3 {E:\bruk500adata\2015\Jan} ejt 10				
Date	12 Jan 2015 13:09:20			*Date Stamp*	12 Jan 2015 13:09:20		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2015\Jan\data\ejt\nmr\2015-01-12-ejt-10\23\fid					*Frequency (MHz)*	470.59
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgfhigqn	*Receiver Gain*	575.00
SW(cyclical) (Hz)	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	113634.63	*Temperature (degree C)*	20.500				

PRM169-F{H}NMR.esp



76

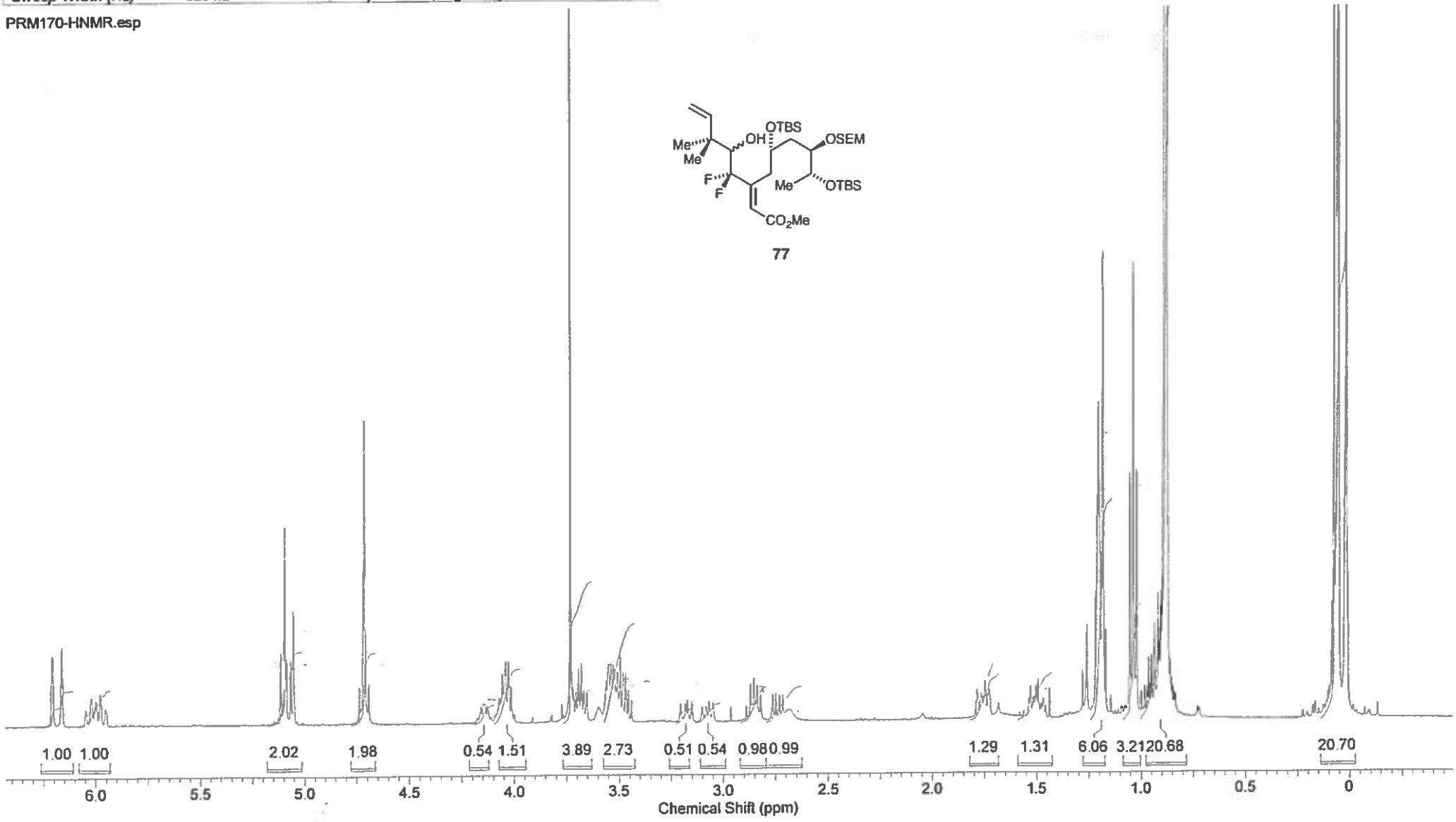
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	4979 .. -1151	1.16230905	2.03938675e+9	1.16230905
2	9359 .. -1141	1.13637888	1.99388979e+9	1.13637888
3	9101 .. -1130	0.82051349	1.43967245e+9	0.82051349
4	3913 .. -1130	0.92547381	1.62383578e+9	0.92547381
5	3915 .. -1070	0.94717634	1.66191501e+9	0.94717634
6	5948 .. -1070	0.99769104	1.75054810e+9	0.99769104
7	1681 .. -1070	0.79453856	1.39409690e+9	0.79453856
8	0656 .. -1060	0.92355108	1.62046221e+9	0.92355108

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM170 f75-87 27mg mPROTON CDCl3 (e:\bruk400adata\2015\Jan) ejt 38				
Date	21 Jan 2015 14:06:56			*Date Stamp*	21 Jan 2015 14:06:56		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-21-ejt-38\10\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	101.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9270	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	23.000				

PRM170-HNMR.esp

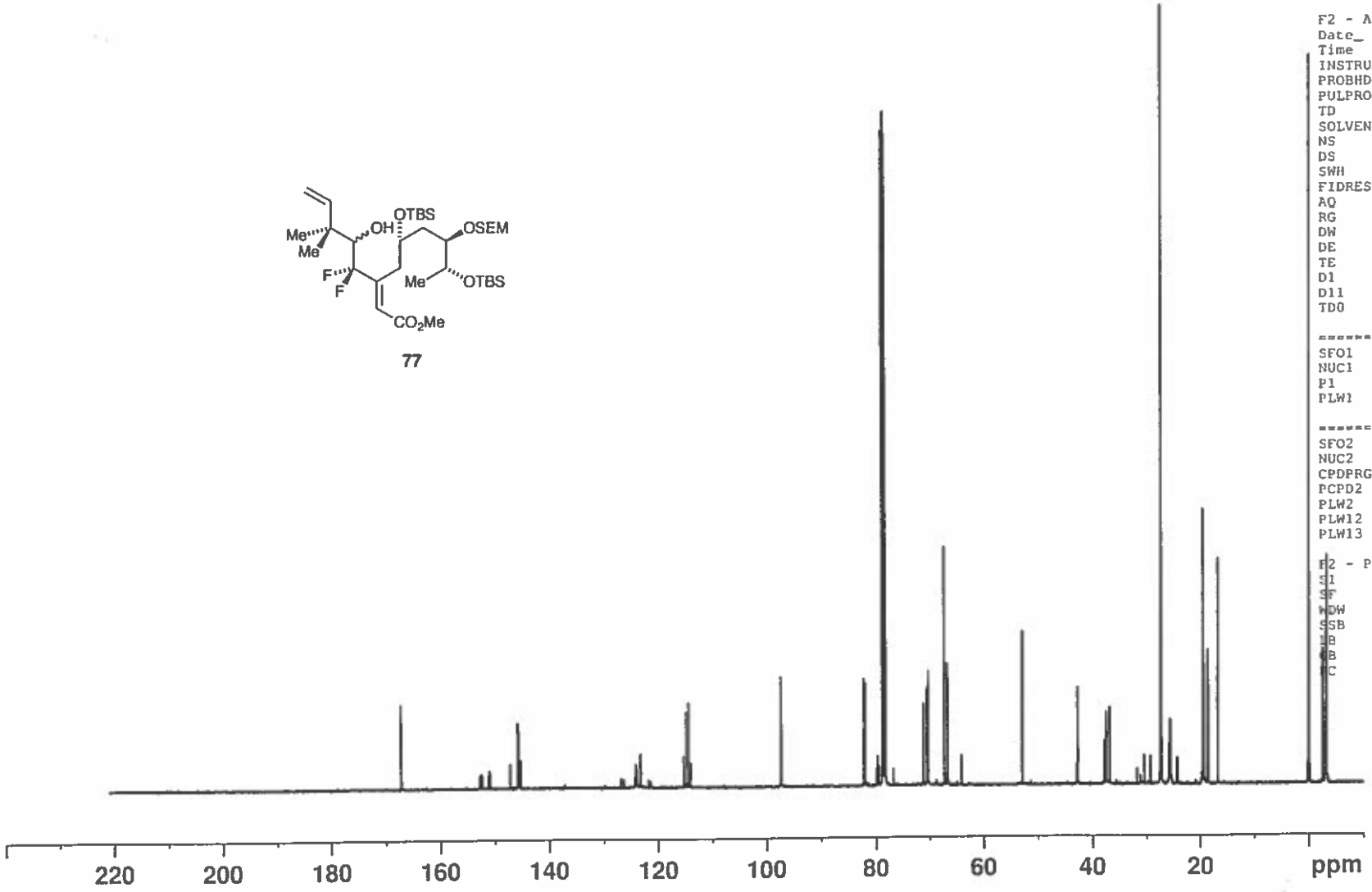
77



EJT-PRM170 Prod

mCARBON, B CDCl3 {e:\bruk400cdata\2015\Jan} ejt 16

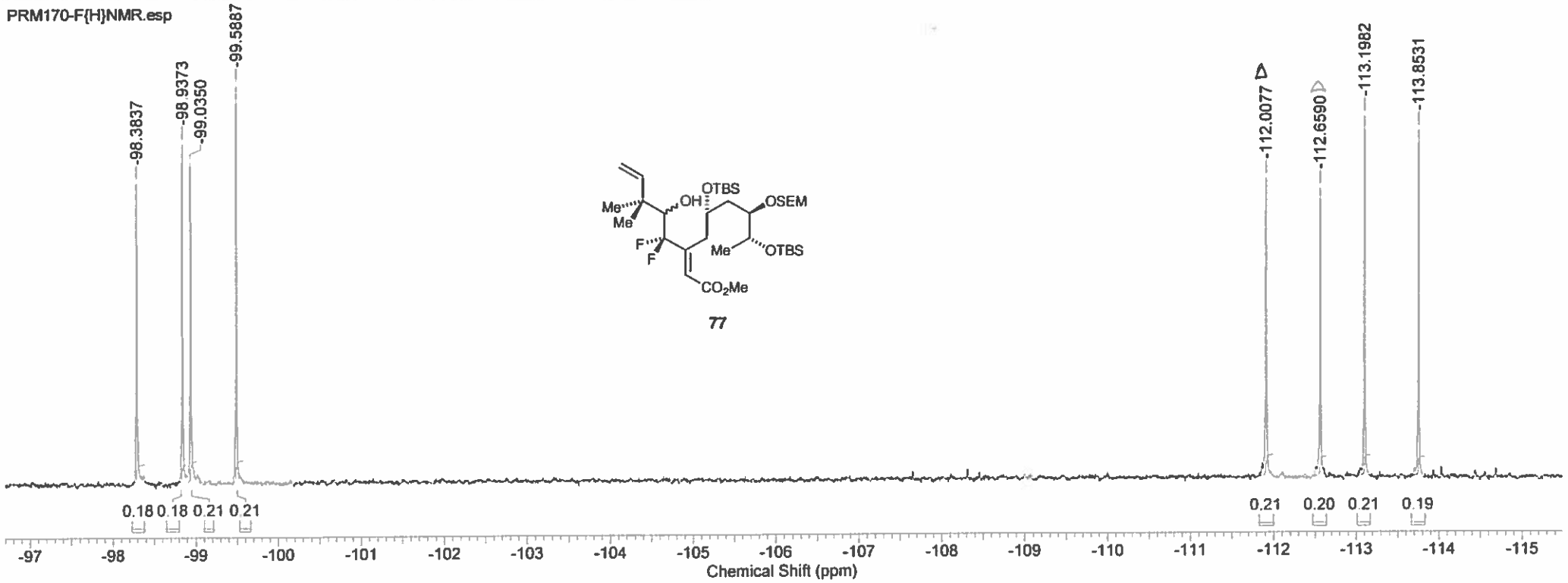
77



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM170 f75-87 27mg mF19CPD CDCl3 (e:\bruk400adata\2015\Jan) ejt 38				
Date	21 Jan 2015 14:11:12			*Date Stamp*	21 Jan 2015 14:11:12		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jan\data\ejt\nmr\2015-01-21-ejt-38\12\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	406.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	23.000				

PRM170-F{H}NMR.esp



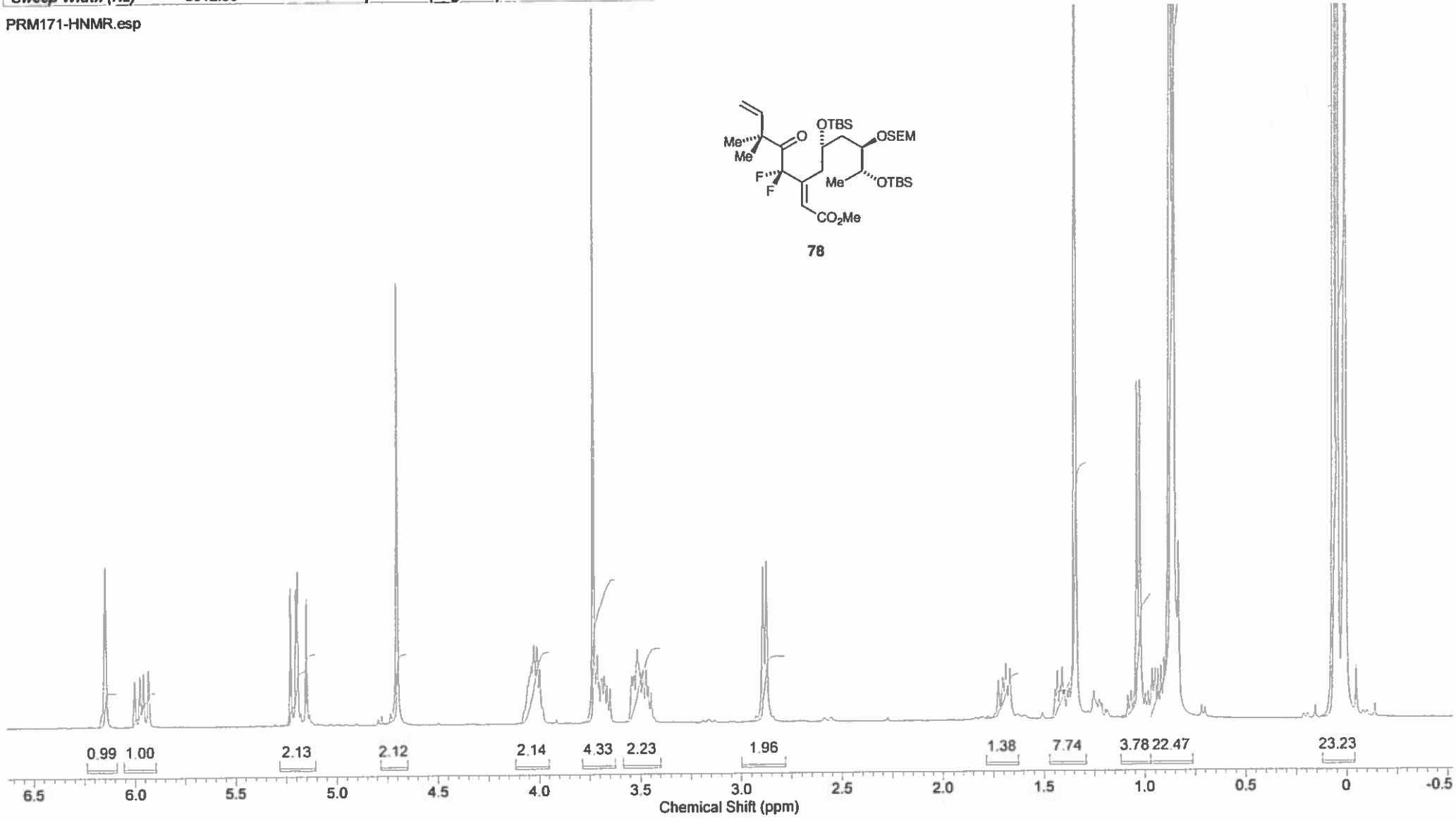
77

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	9327 .. -1130	0.18757442	3.96218432e+8	0.18757442
2	2709 .. -1130	0.20678121	4.36789440e+8	0.20678121
3	7358 .. -1120	0.19675171	4.15603872e+8	0.19675171
4	0951 .. -1110	0.21439180	4.52865504e+8	0.21439180
5	6717 .. -99.50	0.21261145	4.49104832e+8	0.21261145
6	1085 .. -98.90	0.20801891	4.39403872e+8	0.20801891
7	9958 .. -98.80	0.18103851	3.82412448e+8	0.18103851
8	4783 .. -98.30	0.17934489	3.78834976e+8	0.17934489

Acquisition Time (sec)	4.0894	*Comment*	EJT-PRM171 f3-9 50mg mPROTON_A CDCl3 (e:\bruk400cdata\2015\Feb) ejt 6				
Date	04 Feb 2015 16:06:24			*Date Stamp*	04 Feb 2015 16:06:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-02-04-ejt-6\10\fid					*Frequency (MHz)*	400.07
Nucleus	1H	*Number of Transients*	4	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	32.00
SW(cyclical) (Hz)	8012.82	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	1894.0684	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8012.58	*Temperature (degree C)*	14.793				

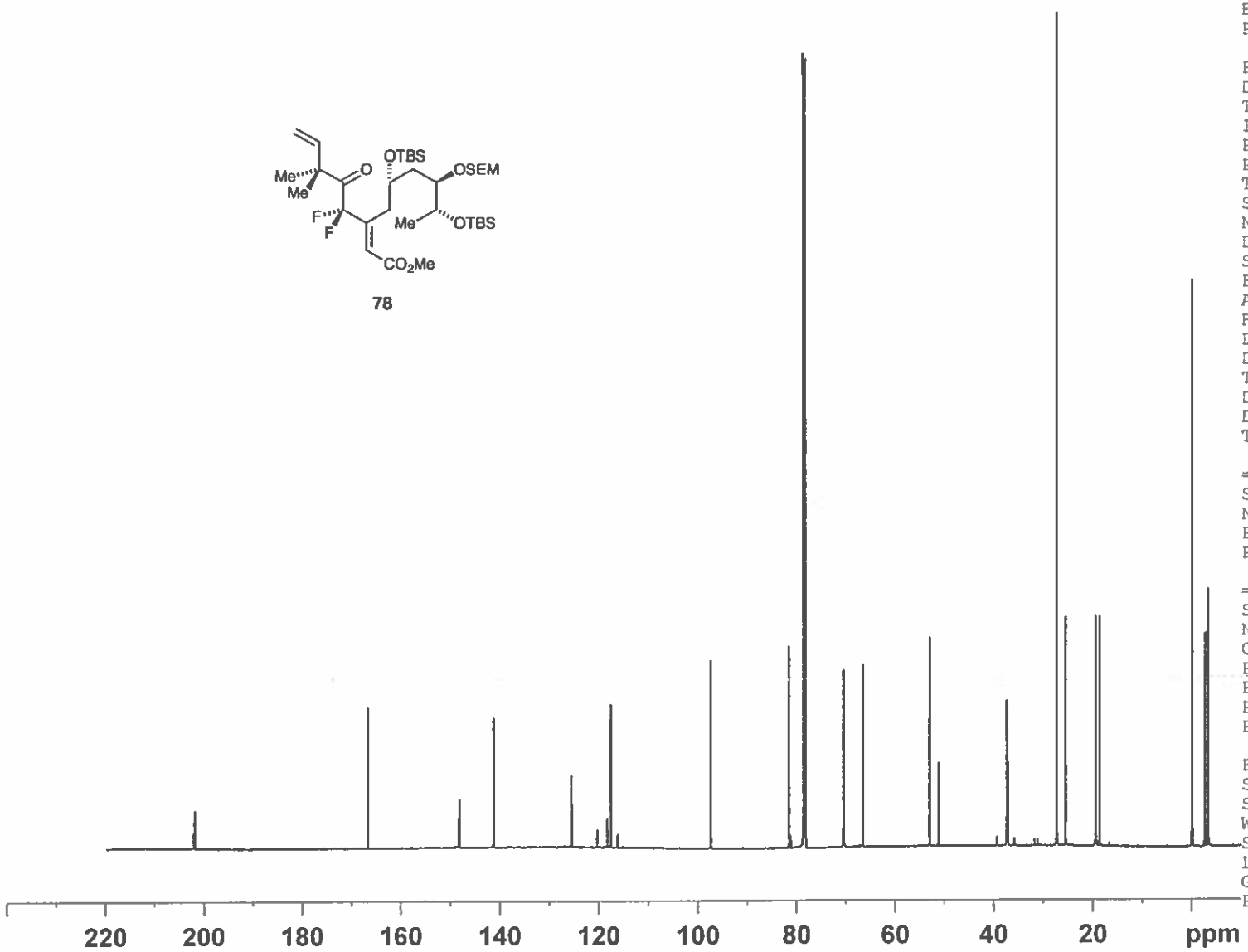
PRM171-HNMR.esp

78



0215-106
Mears P.
EJT-PRM 171 f3-9
50 mg
mCARBON CDCl3 (E:\bruk500cdata\2015\Feb) staff-22

78



Current Data Parameters
NAME 2015-02-04-staff-22
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150205
Time 0.34
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 184.4
DW 16.800 usec
DE 102.82 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7854504 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.59999847 W

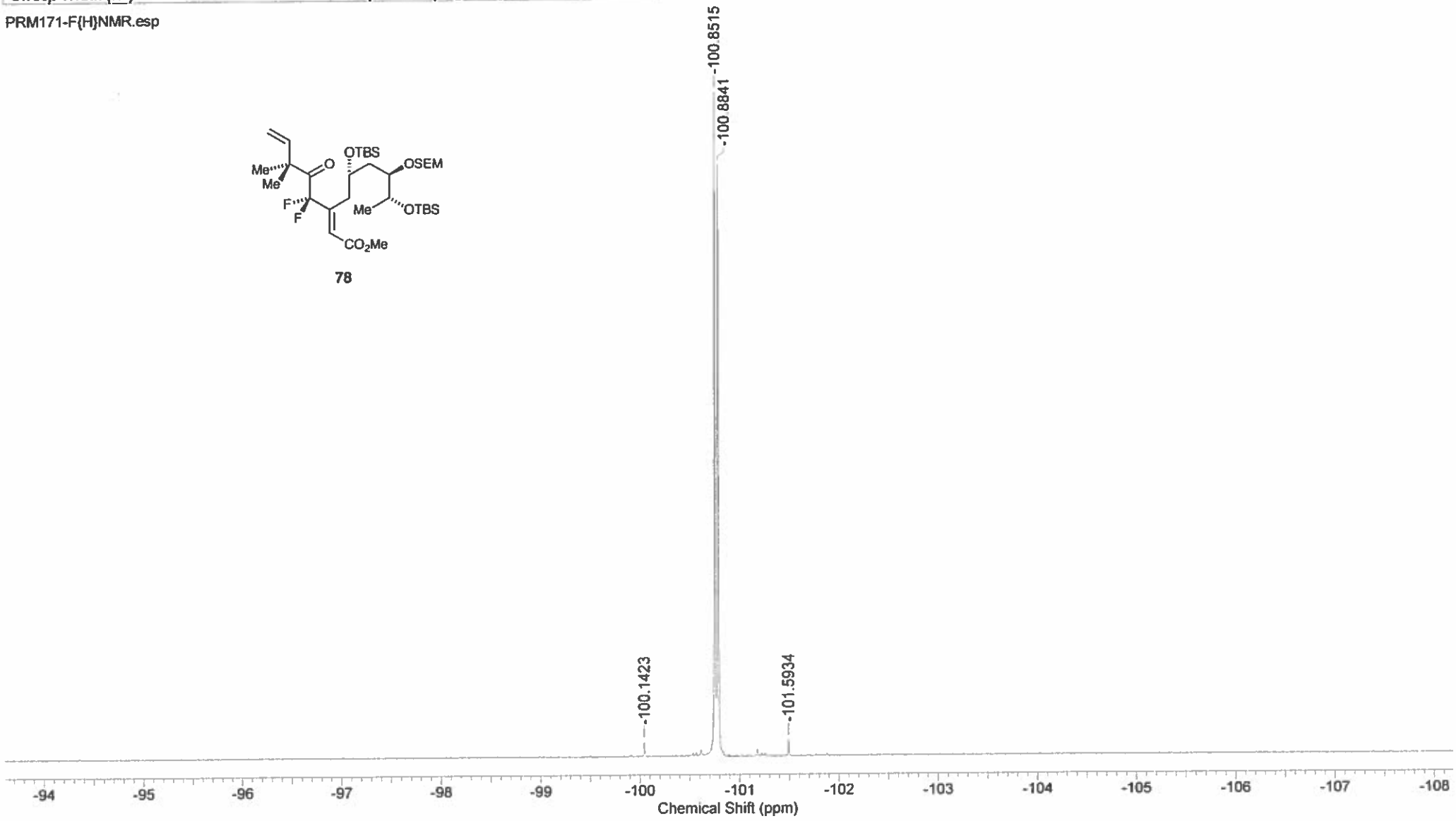
======== CHANNEL f2 ========
SFO2 500.1920008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.28622001 W
PLW13 0.18318000 W

F2 - Processing parameters
SI 32768
SF 125.7726934 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM171 f4-18 57mg mF19CPD CDCl3 {e:\bruk400adata\2015\Feb} ejt 55				
Date	02 Feb 2015 12:45:52			*Date Stamp*	02 Feb 2015 12:45:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Feb\data\ejt\nmr\2015-02-02-ejt-55\13\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	203.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	23.000				

PRM171-F{H}NMR.esp

78



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	4.0894	*Comment*	EJT-PRM173 f6-22 29mg mPROTON_A CDCl3 {e:\bruk400cdata\2015\Feb} ejt 14				
Date	12 Feb 2015 16:00:00			*Date Stamp*	12 Feb 2015 16:00:00		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-02-12-ejt-14\10\fid					*Frequency (MHz)*	400.07
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	32.00
SW(cyclical) (Hz)	8012.82	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	1893.8241	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8012.58	*Temperature (degree C)*	14.915				

PRM173-HNMR.esp

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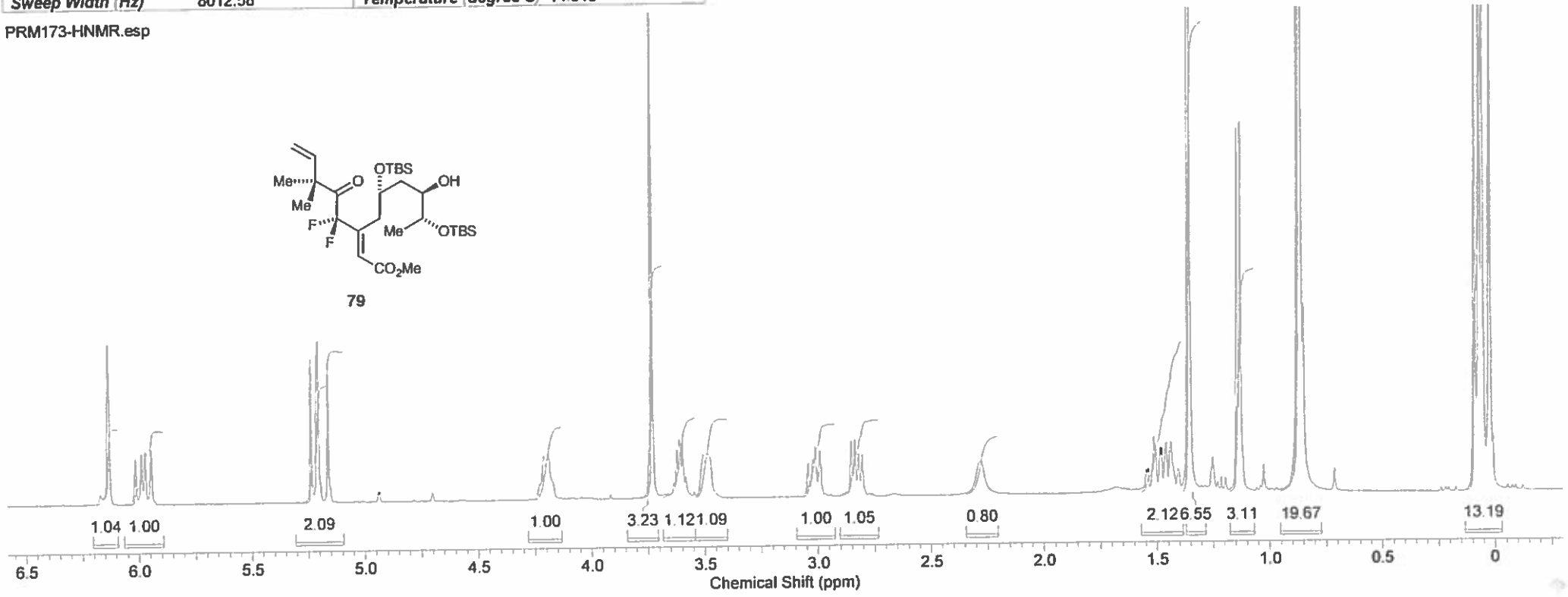
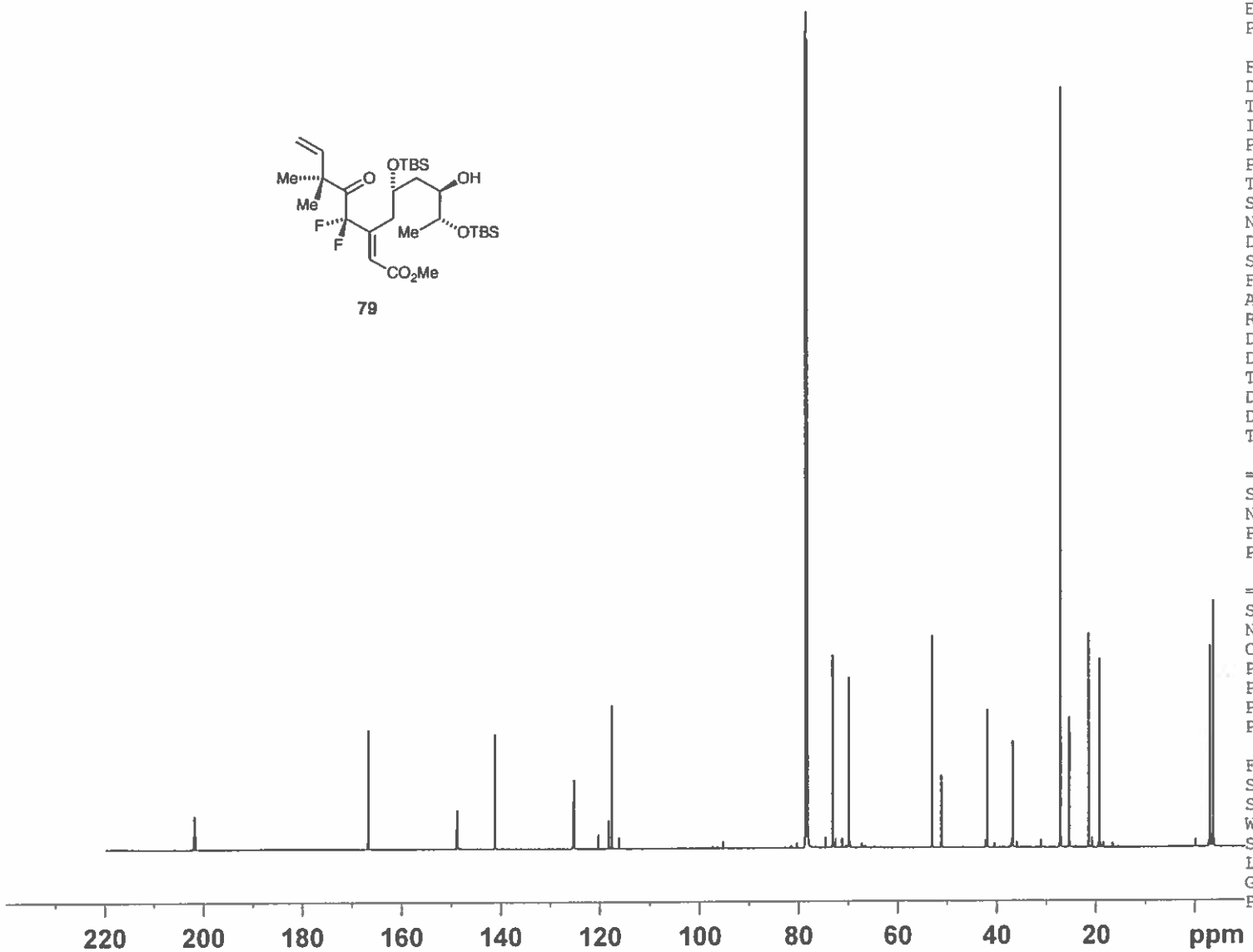


No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	0300 .. 0.13	3.19273376	2.20347003e+10	13.19273376
2	7731 .. 0.95	19.67392731	3.28596849e+10	19.67392731
3	0681 .. 1.17	3.11152554	5.19691622e+9	3.11152554
4	2976 .. 1.38	6.54978418	1.09395466e+10	6.54978418
5	3850 .. 1.57	2.12479234	3.54885965e+9	2.12479234
6	2045 .. 2.34	0.80205345	1.33960154e+9	0.80205345
7	7344 .. 2.90	1.04649985	1.74787955e+9	1.04649985
8	9256 .. 3.09	0.99720508	1.66554675e+9	0.99720508

No.	(ppm)	Value	Absolute Value	Non-Negative Value
9	4009 .. 3.54	1.08516133	1.81245261e+9	1.08516133
10	5430 .. 3.68	1.11831653	1.86782886e+9	1.11831653
11	5850 .. 3.82	3.23063946	5.39586202e+9	3.23063946
12	1330 .. 4.28	0.99953032	1.66943040e+9	0.99953032
13	0945 .. 5.30	2.08711100	3.48592358e+9	2.08711100
14	3922 .. 6.06	0.99999589	1.67020800e+9	0.99999589
15	0943 .. 6.20	1.03641319	1.73103270e+9	1.03641319

EJT-PRM173 f6-22 29mg
mCARBON CDCl3 {E:\bruk500cdata\2015\Feb} staff 57

79




```
Current Data Parameters
NAME      2015-02-13-staff-57
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150214
Time                  17.32
INSTRUM               spect
PROBHD    5 mm CPPBBO BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   30000
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                   184.4
DW                 16.800 usec
DE                 102.82 usec
TE                  295.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          125.7854504 MHz
NUC1                    13C
P1                  10.00 usec
PLW1          53.59999847 W

======== CHANNEL f2 ========
SFO2          500.1920008 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2          16.00000000 W
PLW12          0.28622001 W
PLW13          0.18318000 W

F2 - Processing parameters
SI                   32768
SF            125.7726936 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM173 f6-22 29mg mF19_cryo_zgbs CDCl3 (e:\bruk400cdata\2015\Feb) ejt 14				
Date	12 Feb 2015 16:02:08			*Date Stamp*	12 Feb 2015 16:02:08		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-02-12-ejt-14\11\fid					*Frequency (MHz)*	376.44
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgbs	*Receiver Gain*	7.12
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37644.8594	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	14.924				

PRM173-FNMR.esp

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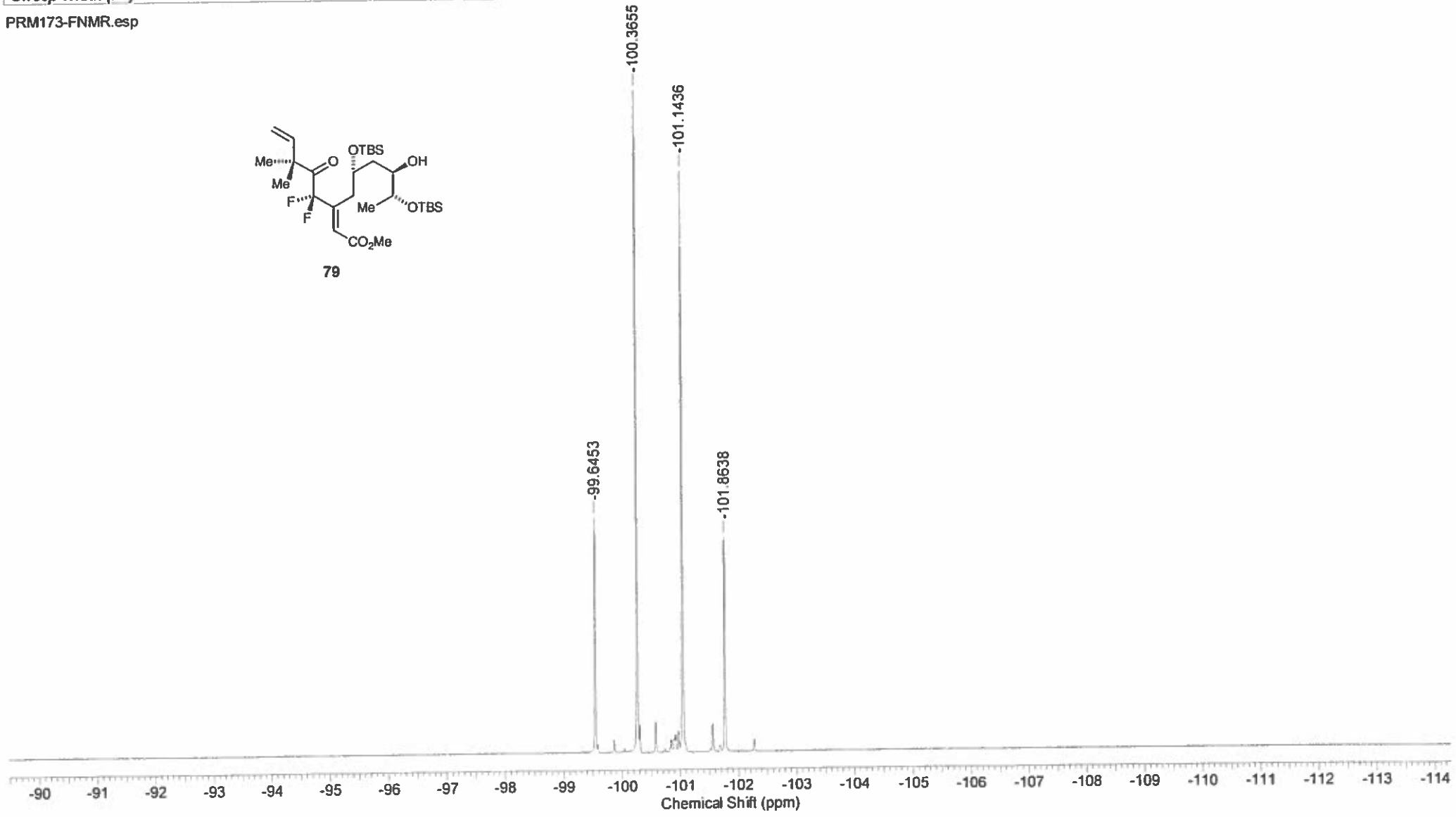
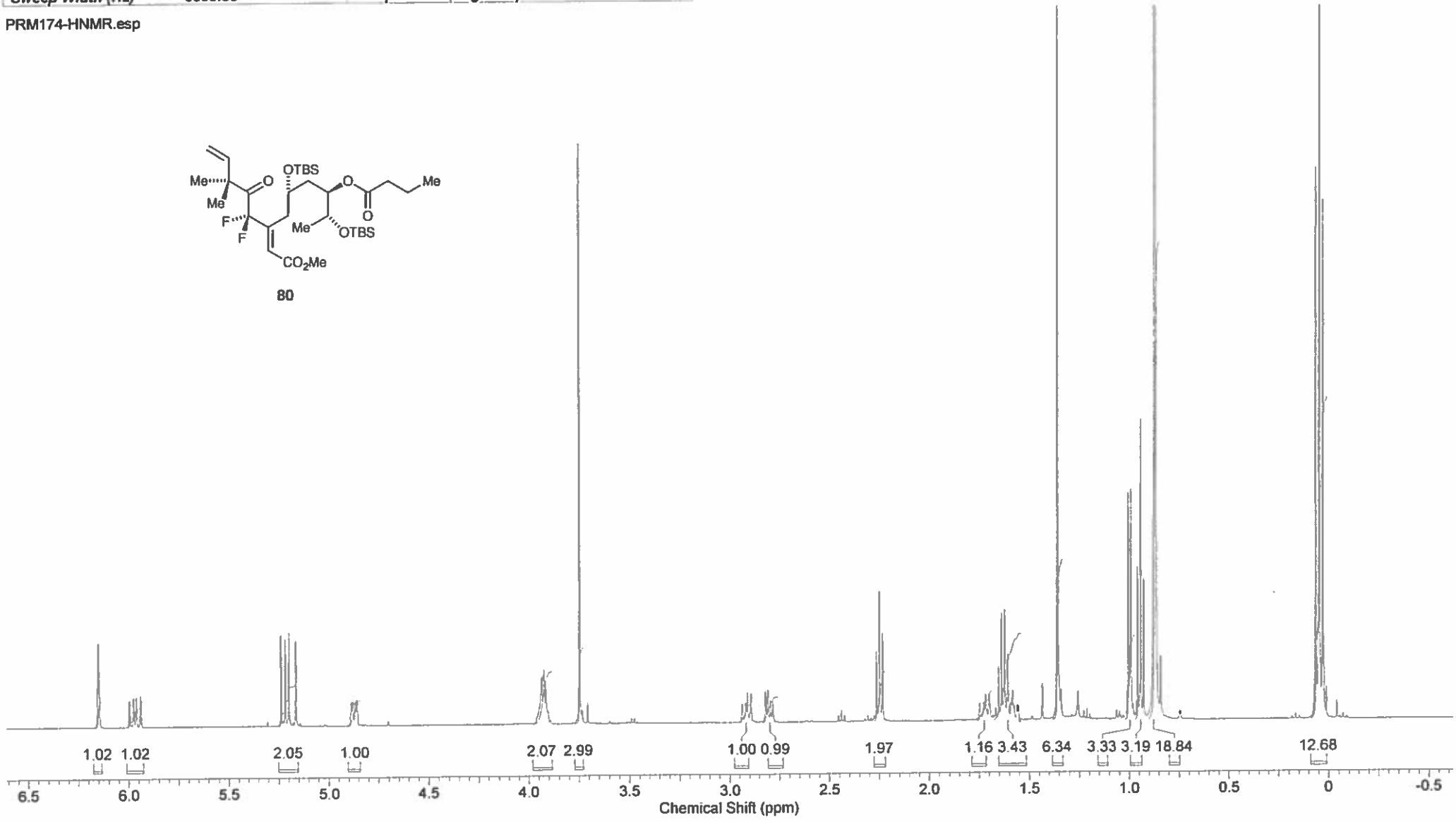


Acquisition Time (sec)	3.2768	*Comment*	0215 121 Mears P EJT-PRM174 F5-15 26 mg in CDCl3 mPROTON CDCl3 {E:\bruk500cdata\2015\Feb} staff 39				
Date	24 Feb 2015 02:14:24	*Date Stamp*	24 Feb 2015 02:14:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-23-staff-39\10\PDATA\1\1r					*Frequency (MHz)*	500.19
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zg30	*Receiver Gain*	30.53
SW(cyclical) (Hz)	10000.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3081.8008	*Spectrum Type*	STANDARD
Sweep Width (Hz)	9999.85	*Temperature (degree C)*	22.154				

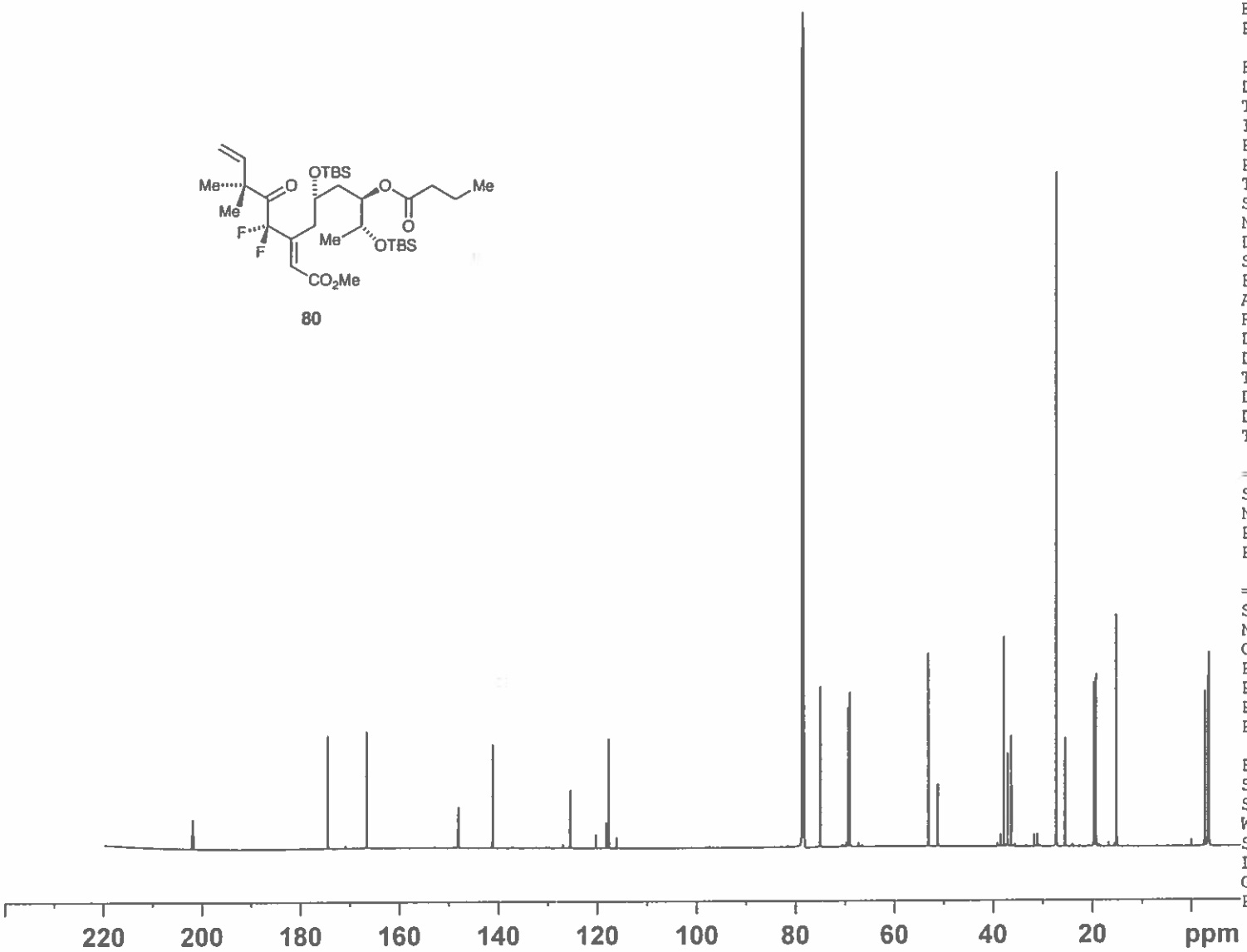
PRM174-HNMR.esp

80



0215 121
Mears P
EJT-PRM174 F5-15
26 mg in CDCl3
mCARBON CDCl3 {E:\bruk500cdata\2015\Feb}_staff_39

80



BRUKER 500 MHz

Current Data Parameters
NAME 2015-02-23-staff-39
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150224
Time 10.14
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9223
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 184.4
DW 16.800 usec
DE 102.82 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7854504 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.59999847 W

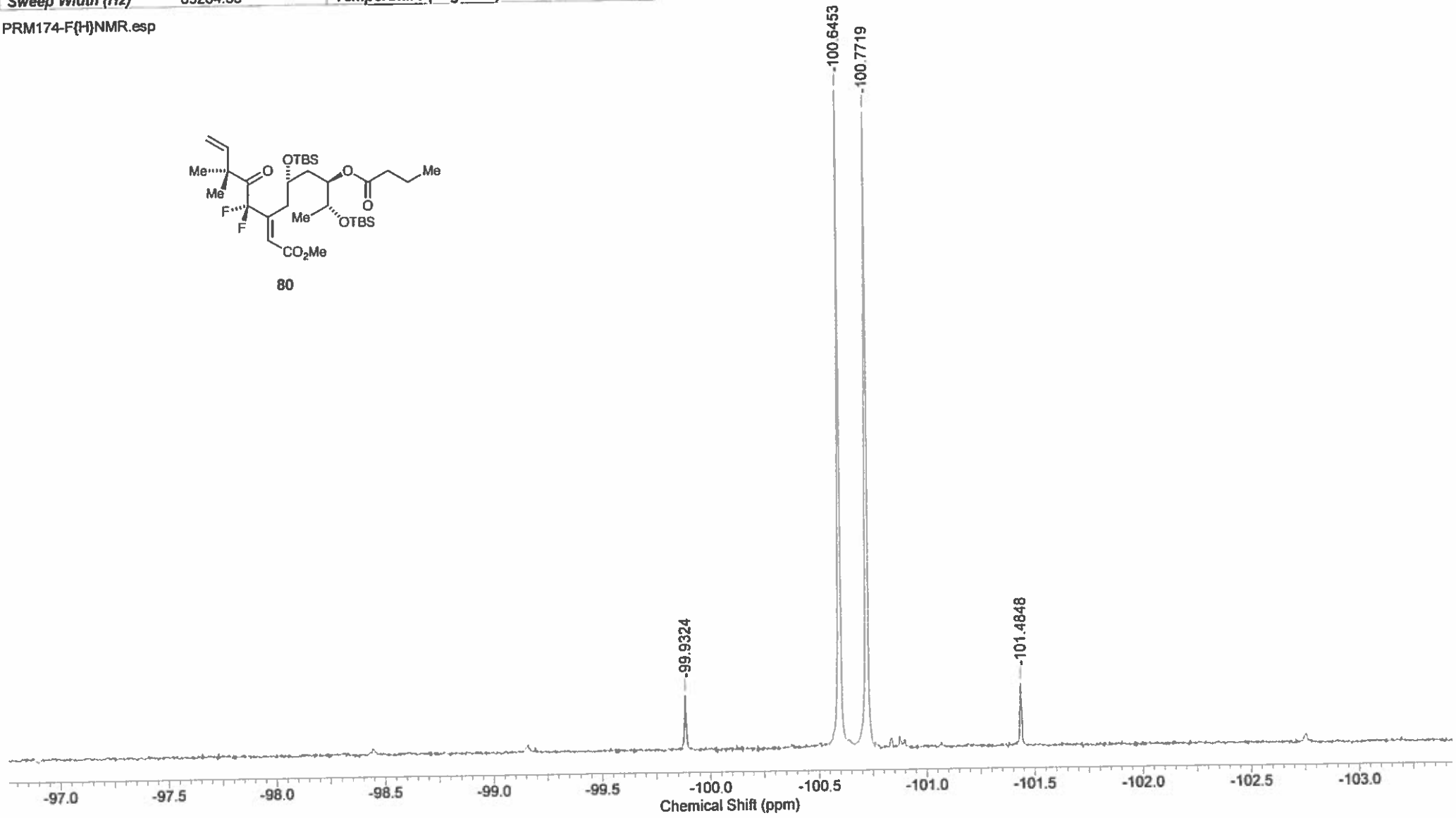
======== CHANNEL f2 ========
SFO2 500.1920008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.28622001 W
PLW13 0.18318000 W

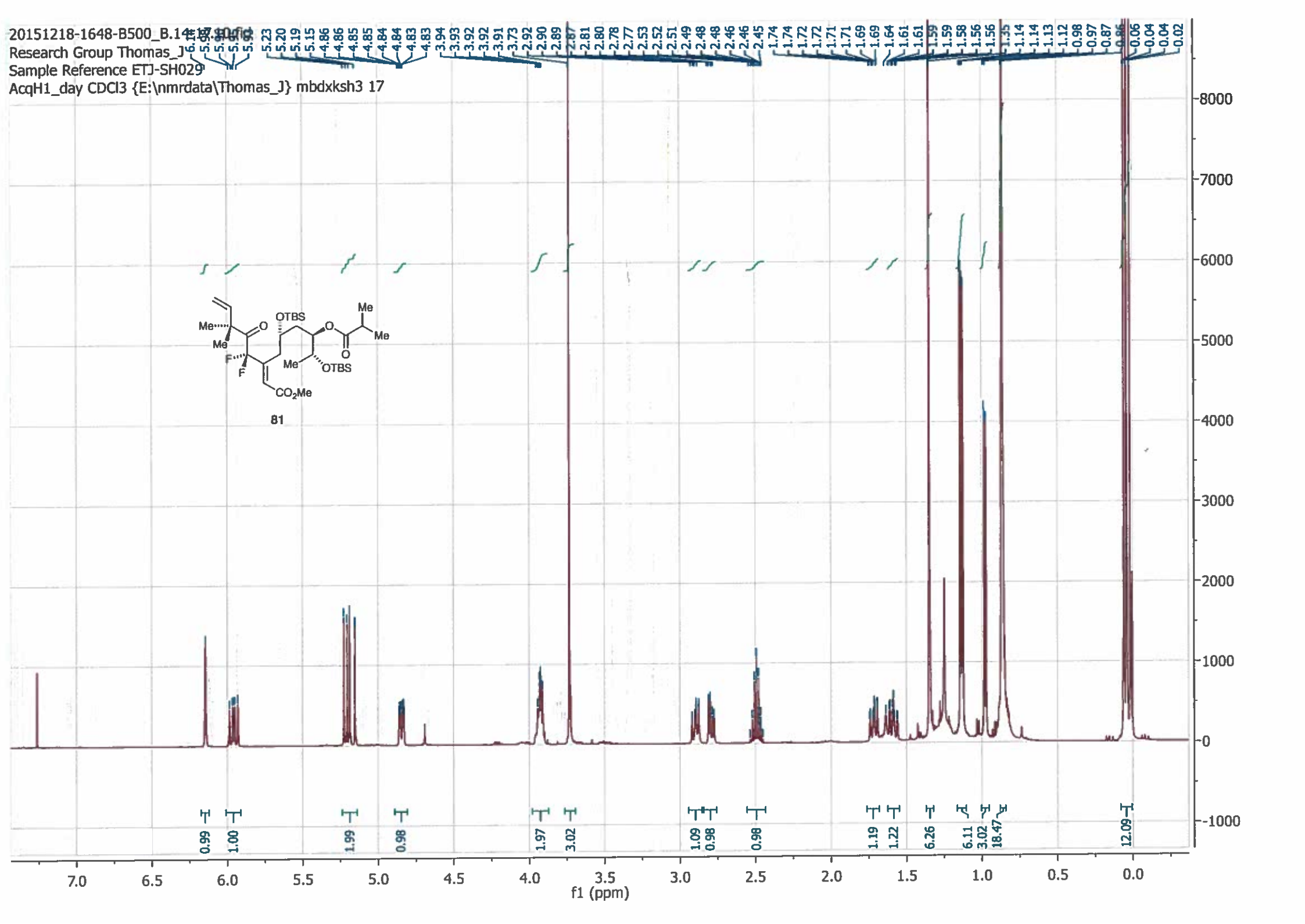
F2 - Processing parameters
SI 32768
SF 125.7726933 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM174 f5-15 26mg mF19CPD CDCl3 (e:\bruk400adata\2015\Feb) ejt 58				
Date	23 Feb 2015 15:30:08			*Date Stamp*	23 Feb 2015 15:30:08		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Feb\data\ejt\nmr\2015-02-23-ejt-58\12\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	203.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	19.900				

PRM174-F{H}NMR.esp

80




20151218-1648-B500_B.14.17.10.fid
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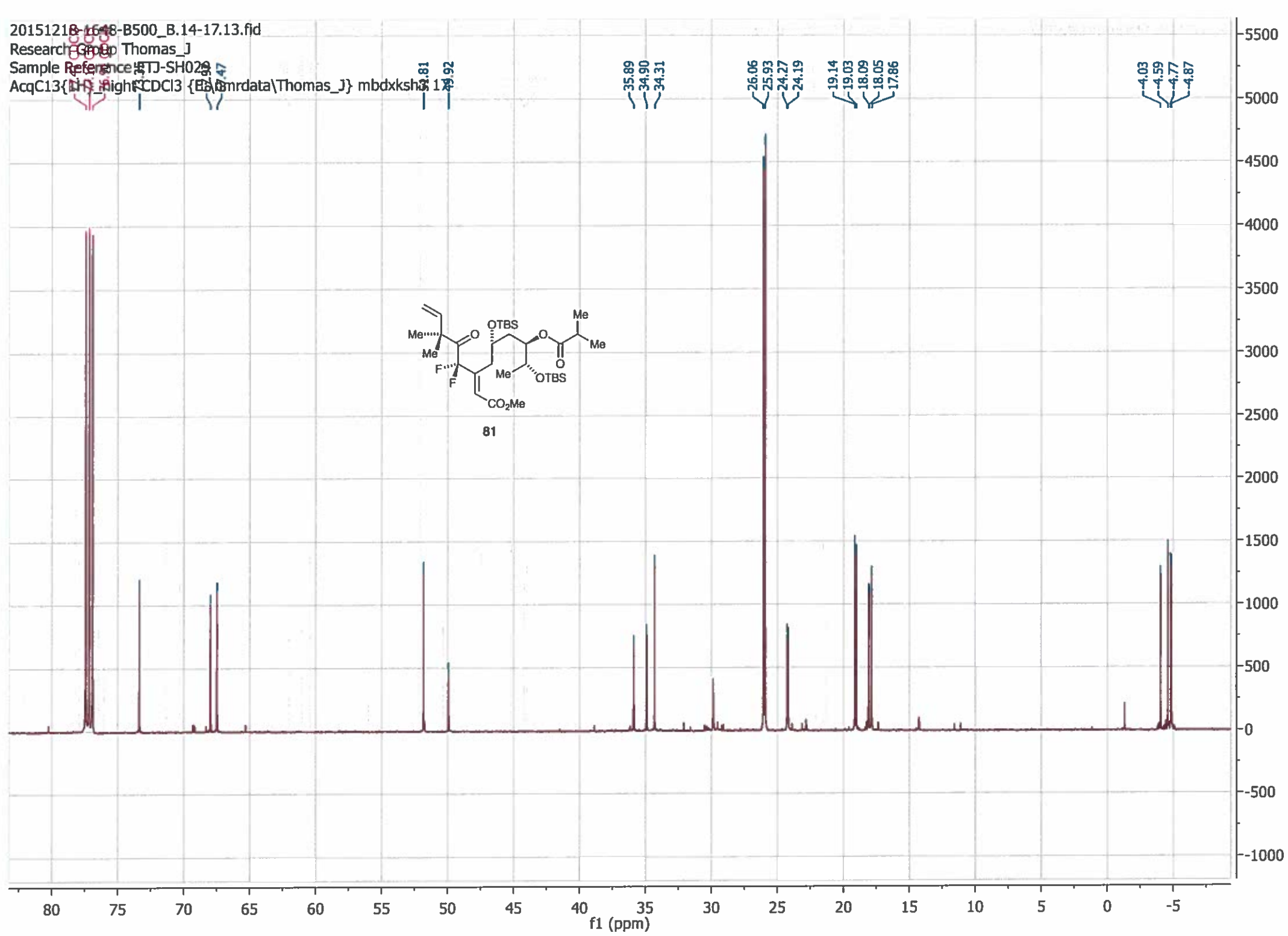
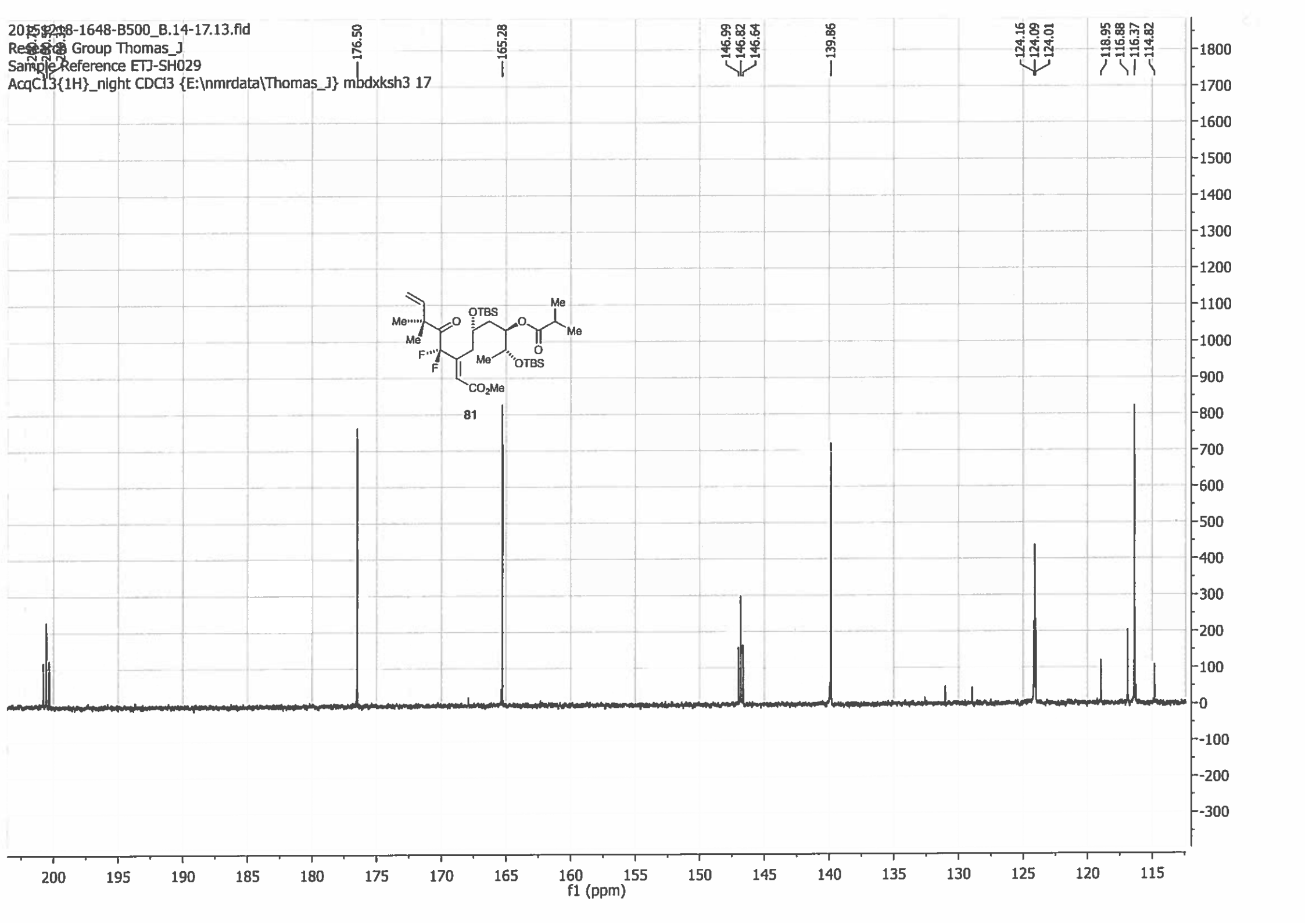
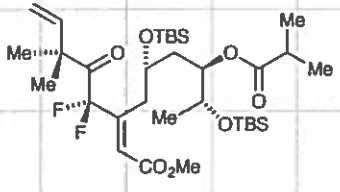
Sample Reference ETJ-SH029
AcqH1_day CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 17
81
f1 (ppm)


20151218-1648-B500_B.14-17.13.fid
Research Group Thomas_J
Sample Reference: RTJ-SH029
AcqC13{1H}_high CDCl3 {Ea\Bmrdata\Thomas_J} mbdxksh 3.17
35.89
34.90
34.31
26.06
25.93
24.27
24.19
19.14
19.03
18.09
18.05
17.86
4.03
4.59
4.77
4.87
OTBS
Me
Me
O
O
Me
Me
F
F
Me
OTBS
CO2Me
81
f1 (ppm)


176.50
165.28
146.99
146.82
146.64
139.86
124.16
124.09
124.01
118.95
116.88
116.37
114.82
Me
OTBS
Me
Me
O
O
Me
F
F
Me
OTBS
CO2Me
81
f1 (ppm)

20151221-1708-B400_B.12-35.11.fid
Research Group Thomas_J
Sample Reference EJT-SH029Fluorine
mF19CPD CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 35

-99.90
-100.61
-100.72
-101.43



81

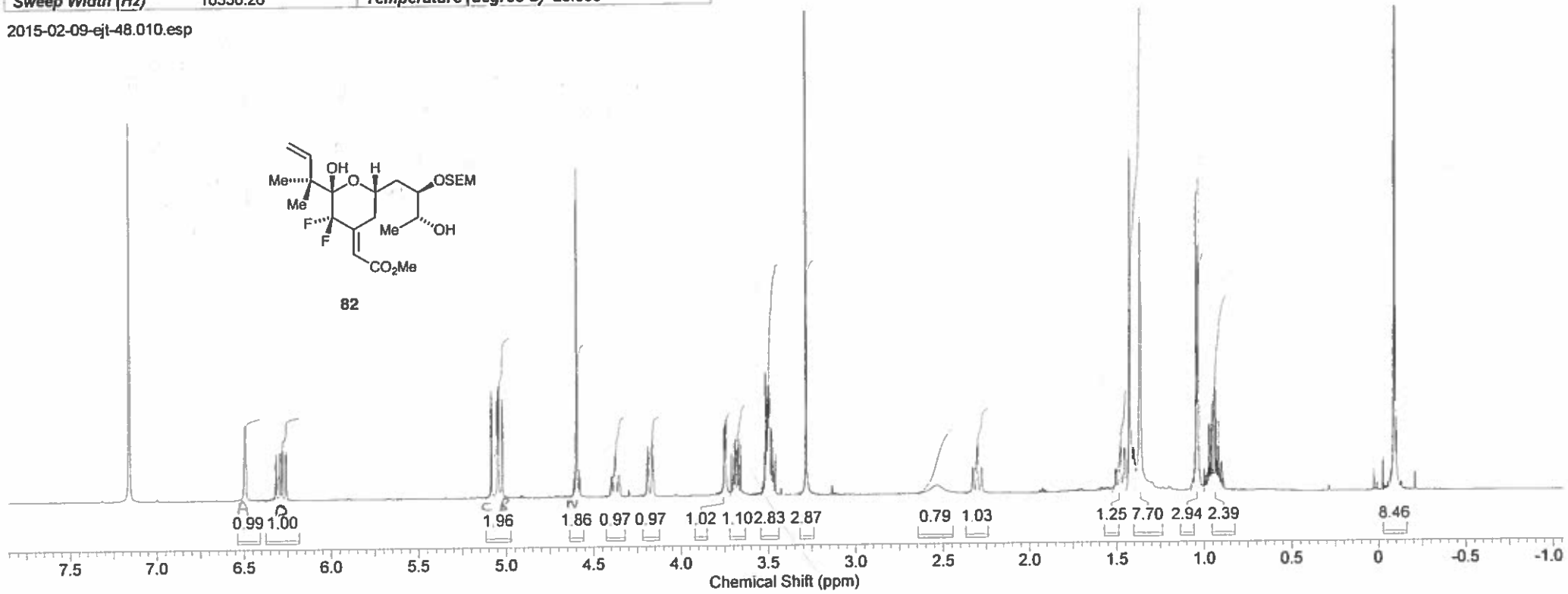
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.1719	*Comment*	EJT-PRM172 bis-TBS deprot. 24mg mPROTON C6D6 {E:\bruk500adata\2015\Feb} ejt 48				
Date	09 Feb 2015 14:24:00			*Date Stamp*	09 Feb 2015 14:24:00		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2015\Feb\data\ejt\nmr\2015-02-09-ejt-48\10\fid					*Frequency (MHz)*	500.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	90.50
SW(cyclical) (Hz)	10330.58	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	3093.0591	*Spectrum Type*	STANDARD
Sweep Width (Hz)	10330.26	*Temperature (degree C)*	25.000				

2015-02-09-ejt-48.010.esp



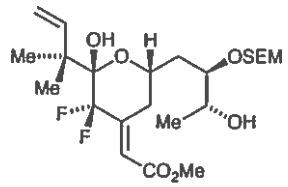
No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1599 .. -0.02	8.45782185	2.23010775e+10	8.45782185
2	3718 .. 1.002	2.39459229	6.31391744e+9	2.39459229
3	0027 .. 1.082	2.94357920	7.76145357e+9	2.94357920
4	2804 .. 1.447	7.70429850	2.03142328e+10	7.70429850
5	4463 .. 1.521	1.24665987	3.28711808e+9	1.24665987
6	2401 .. 2.361	1.03409398	2.72663706e+9	1.03409398
7	4444 .. 2.640	0.78715116	2.07551309e+9	0.78715116
8	2388 .. 3.312	2.86838222	7.56317850e+9	2.86838222
9	4414 .. 3.542	2.82843184	7.45783962e+9	2.82843184

No.	(ppm)	Value	Absolute Value	Non-Negative Value
10	5335 .. 3.721	1.10219407	2.90619930e+9	1.10219407
11	7208 .. 3.791	1.01866615	2.68595789e+9	1.01866615
12	1260 .. 4.220	0.96806675	2.55254042e+9	0.96806675
13	3233 .. 4.420	0.97044659	2.55881549e+9	0.97044659
14	5590 .. 4.631	1.86019683	4.90485555e+9	1.86019683
15	9744 .. 5.111	1.95728326	5.16084736e+9	1.95728326
16	1829 .. 6.370	0.99992341	2.63653811e+9	0.99992341
17	4099 .. 6.540	0.99473357	2.62285389e+9	0.99473357

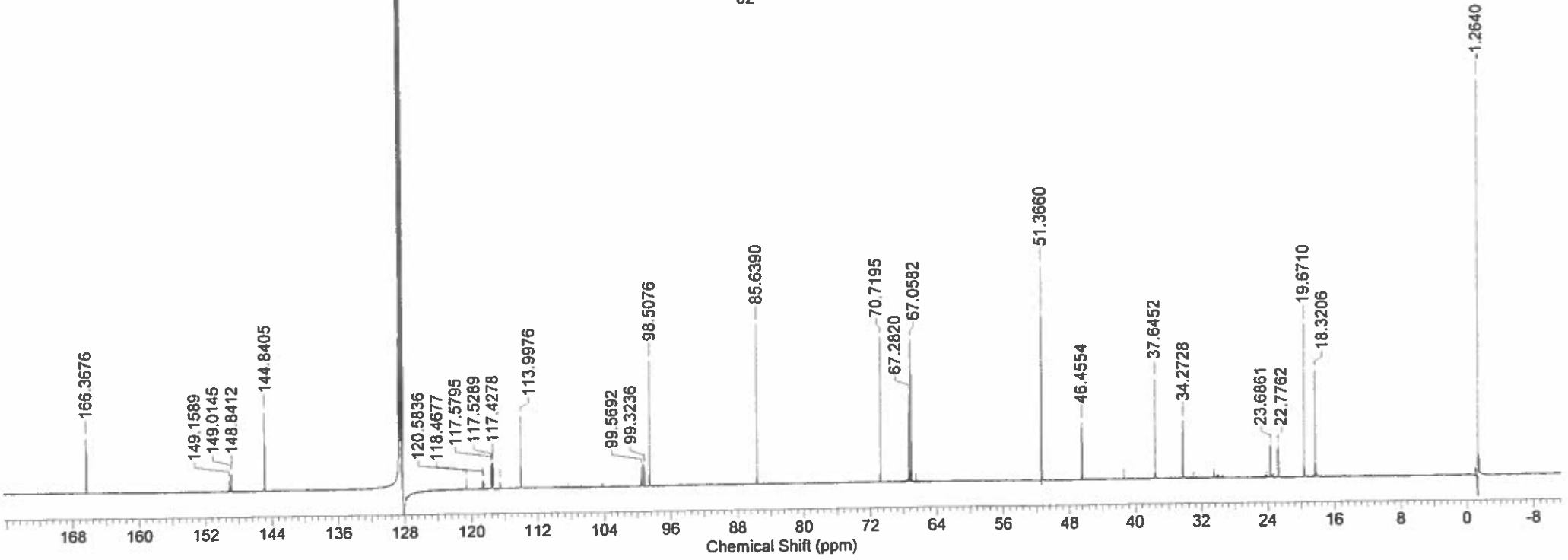
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	P.Mears EJT-PRM172 bis-TBS deprot mCARBON C6D6 (E:\bruk500cdata\2015\Feb) staff 26				
Date	10 Feb 2015 01:44:32	*Date Stamp*	10 Feb 2015 01:44:32				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-09-staff-26\21\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12661.5830	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.161				

PRM172-columnedX3-CNMR-C6D6.esp

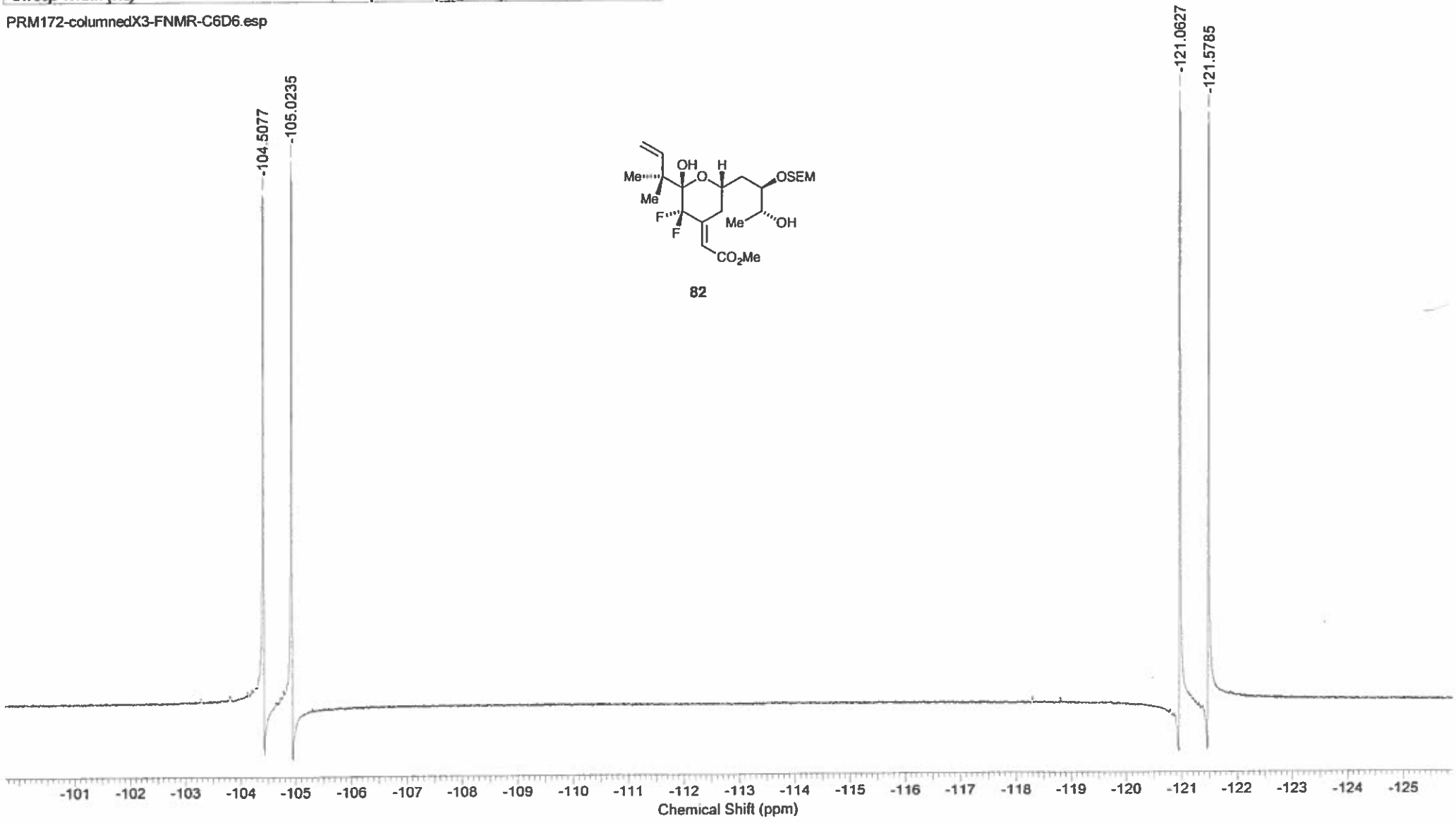


82



Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM172 bis-TBS deprot. 24mg m19F C6D6 (E:\bruk500adata\2015\Feb) ejt 48				
Date	09 Feb 2015 14:34:40			*Date Stamp*	09 Feb 2015 14:34:40		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2015\Feb\data\ejt\nmr\2015-02-09-ejt-48\12\fid					*Frequency (MHz)*	470.59
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgflqn	*Receiver Gain*	406.00
SW(cyclical) (Hz)	113636.37	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-47059.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	113634.63	*Temperature (degree C)*	25.000				

PRM172-columnedX3-FNMR-C6D6.esp



82

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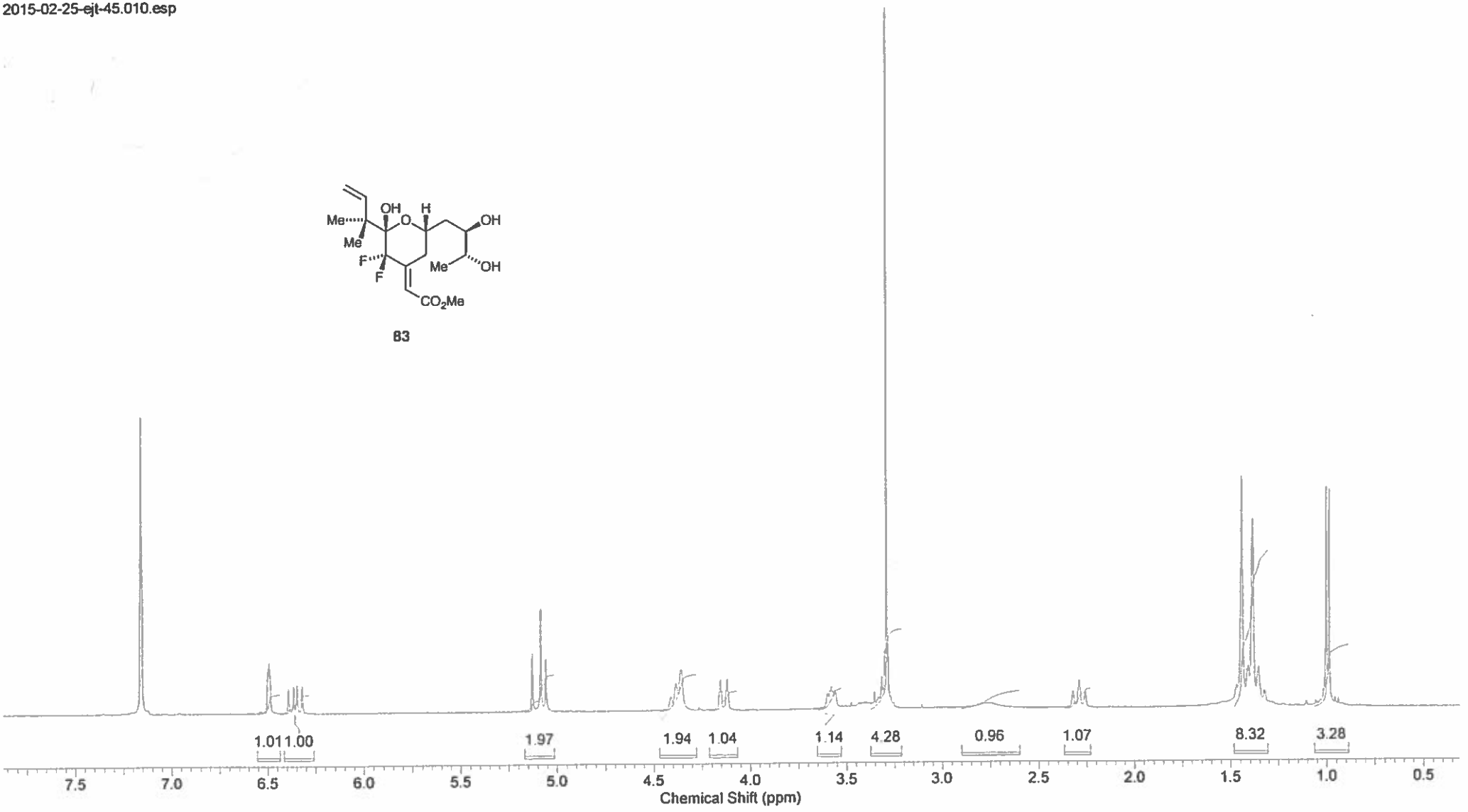
Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM175 f6-28 11mg mPROTON C6D6 {e:\bruk400adata\2015\Feb} ejt 45				
Date	25 Feb 2015 18:31:28			*Date Stamp*	25 Feb 2015 18:31:28		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Feb\data\ejt\nmr\2015-02-25-ejt-45\10\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	128.00
SW(cyclical) (Hz)	8264.46	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	2473.8770	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	19.800				

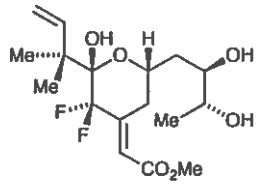
2015-02-25-ejt-45.010.esp

83



Acquisition Time (sec)	1.1010						
Comment	Research Group EJT Acad/Staff/PDRA/PG/UG PDRA 0215 129 EJT-PRM175 F6-28 11mg Mears P. mCARBON C6D6 (E:\bruk500cdata\2015\Feb) staff 53						
Date	28 Feb 2015 19:50:24	*Date Stamp*	28 Feb 2015 19:50:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-27-staff-53\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	8192	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12660.7109	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.153				

PRM175-CNMR.esp



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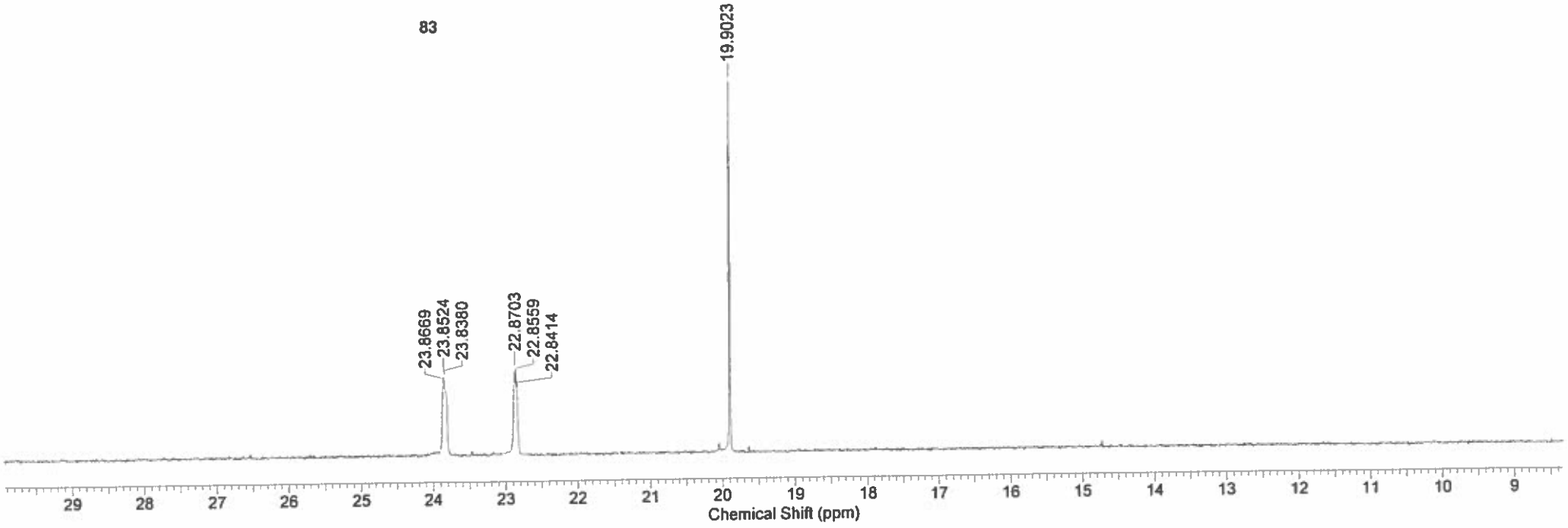
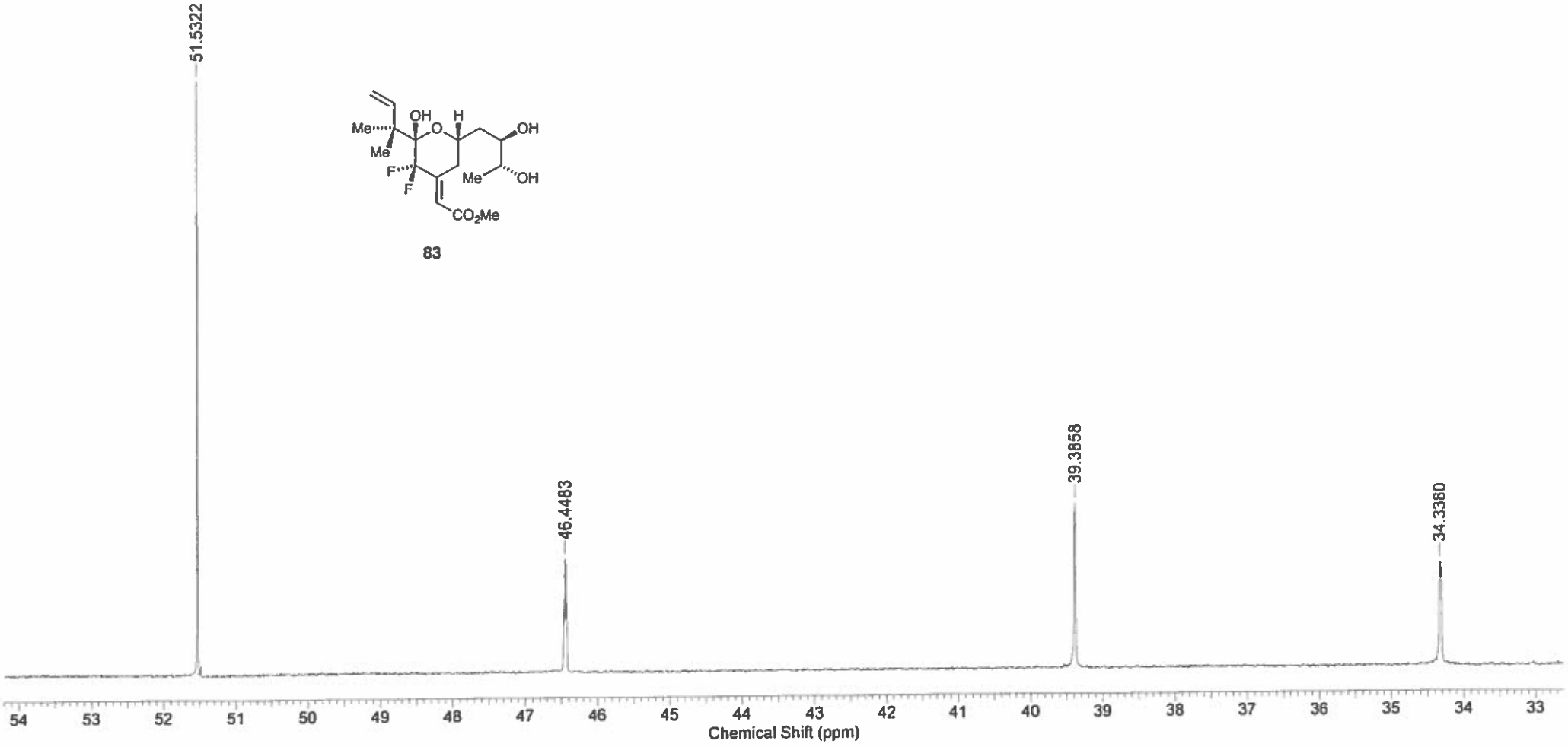


Acquisition Time (sec)	1.1010						
Comment	Research Group EJT Acad/Staff/PDRA/PG/UG PDRA 0215 129 EJT-PRM175 F6-28 11mg Mears P. mCARBON C6D6 (E:\bruk500cdata\2015\Feb) staff 53						
Date	28 Feb 2015 19:50:24	*Date Stamp*	28 Feb 2015 19:50:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-27-staff-53\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	8192	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12660.7109	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.153				

PRM175-CNMR.esp



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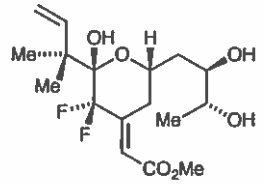
Acquisition Time (sec)	1.1010						
Comment	Research Group EJT Acad/Staff/PDRA/PG/UG PDRA 0215 129 EJT-PRM175 F6-28 11mg Mears P. mCARBON C6D6 {E:\bruk500cdata\2015\Feb} staff 53						
Date	28 Feb 2015 19:50:24	*Date Stamp*	28 Feb 2015 19:50:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-27-staff-53\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	8192	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12660.7109	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.153				

PRM175-CNMR.esp



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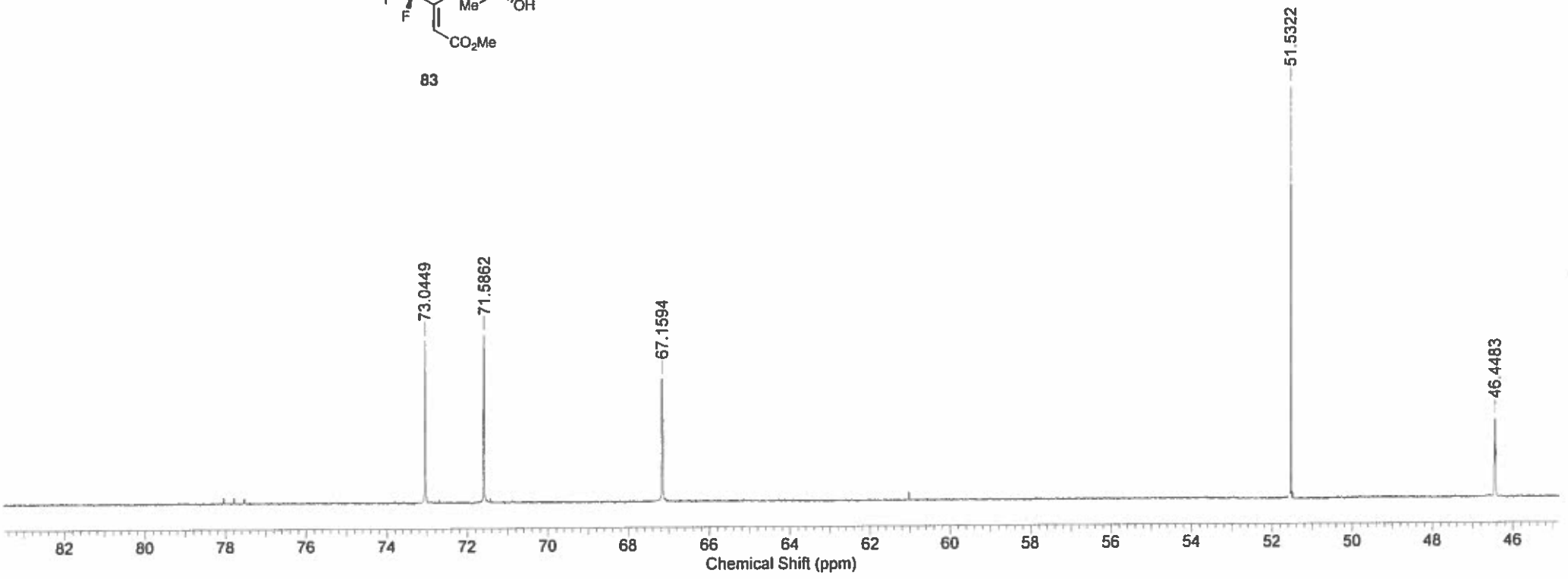
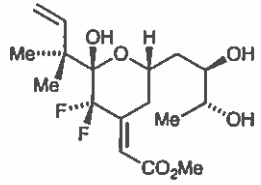


Acquisition Time (sec)	1.1010						
Comment	Research Group EJT Acad/Staff/PDRA/PG/UG PDRA 0215 129 EJT-PRM175 F6-28 11mg Mears P. mCARBON C6D6 {E:\bruk500cdata\2015\Feb} staff 53						
Date	28 Feb 2015 19:50:24	*Date Stamp*	28 Feb 2015 19:50:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-27-staff-53\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	8192	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12660.7109	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.153				

PRM175-CNMR.esp



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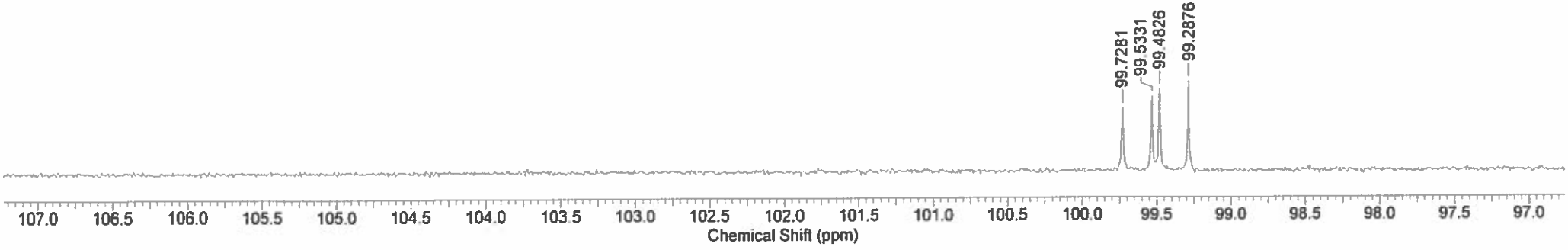

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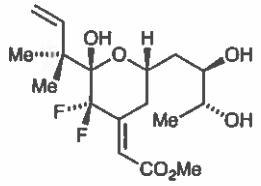
Acquisition Time (sec)	1.1010						
Comment	Research Group EJT Acad/Staff/PDRA/PG/UG PDRA 0215 129 EJT-PRM175 F6-28 11mg Mears P. mCARBON C6D6 {E:\bruk500cdata\2015\Feb} staff 53						
Date	28 Feb 2015 19:50:24	*Date Stamp*	28 Feb 2015 19:50:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-27-staff-53\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	8192	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12660.7109	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.153				

PRM175-CNMR.esp



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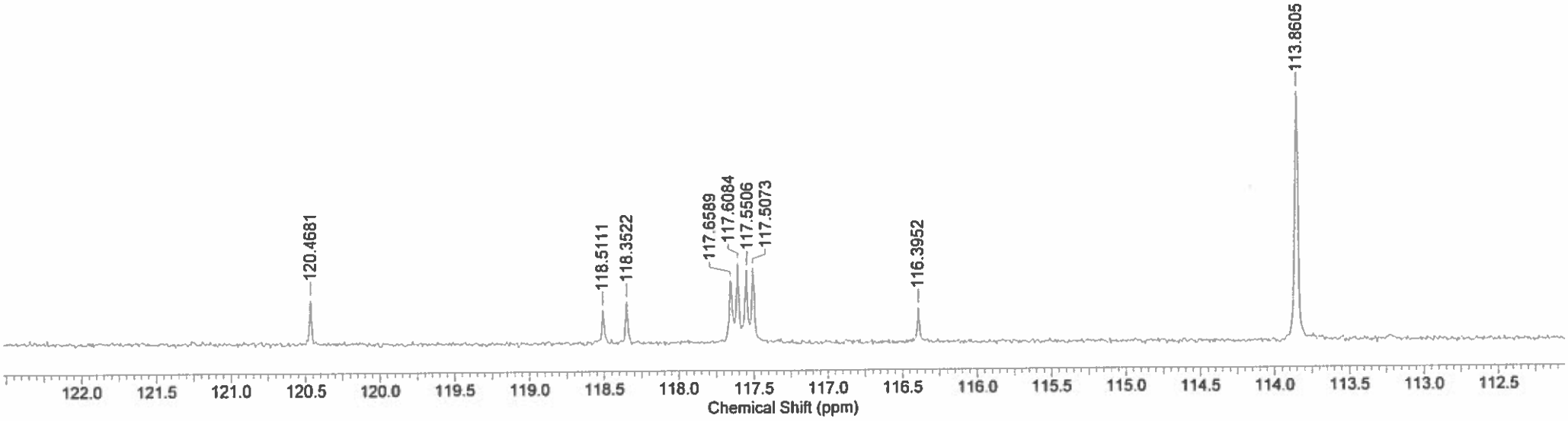
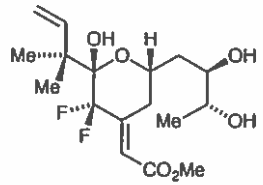


Acquisition Time (sec)	1.1010						
Comment	Research Group EJT Acad/Staff/PDRA/PG/UG PDRA 0215 129 EJT-PRM175 F6-28 11mg Mears P. mCARBON C6D6 (E:\bruk500cdata\2015\Feb) staff 53						
Date	28 Feb 2015 19:50:24	*Date Stamp*	28 Feb 2015 19:50:24				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Feb\data\staff\nmr\2015-02-27-staff-53\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	8192	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12660.7109	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.153				

PRM175-CNMR.esp



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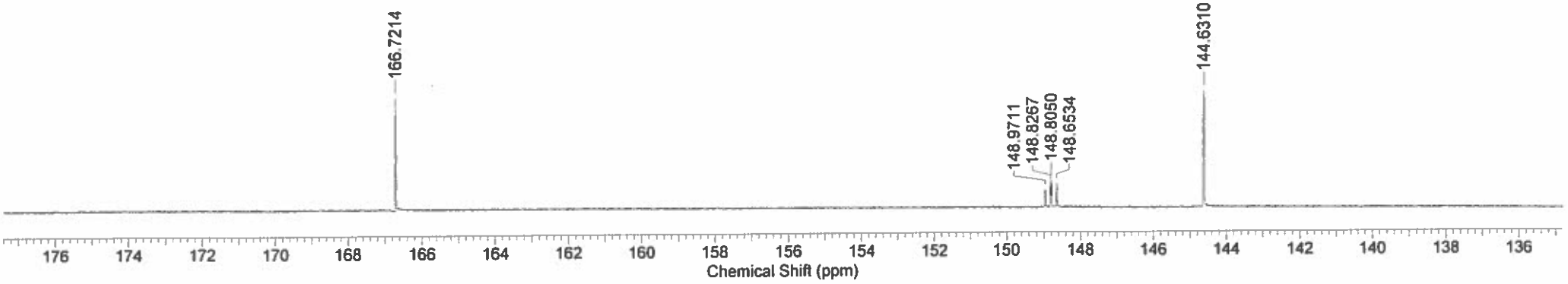
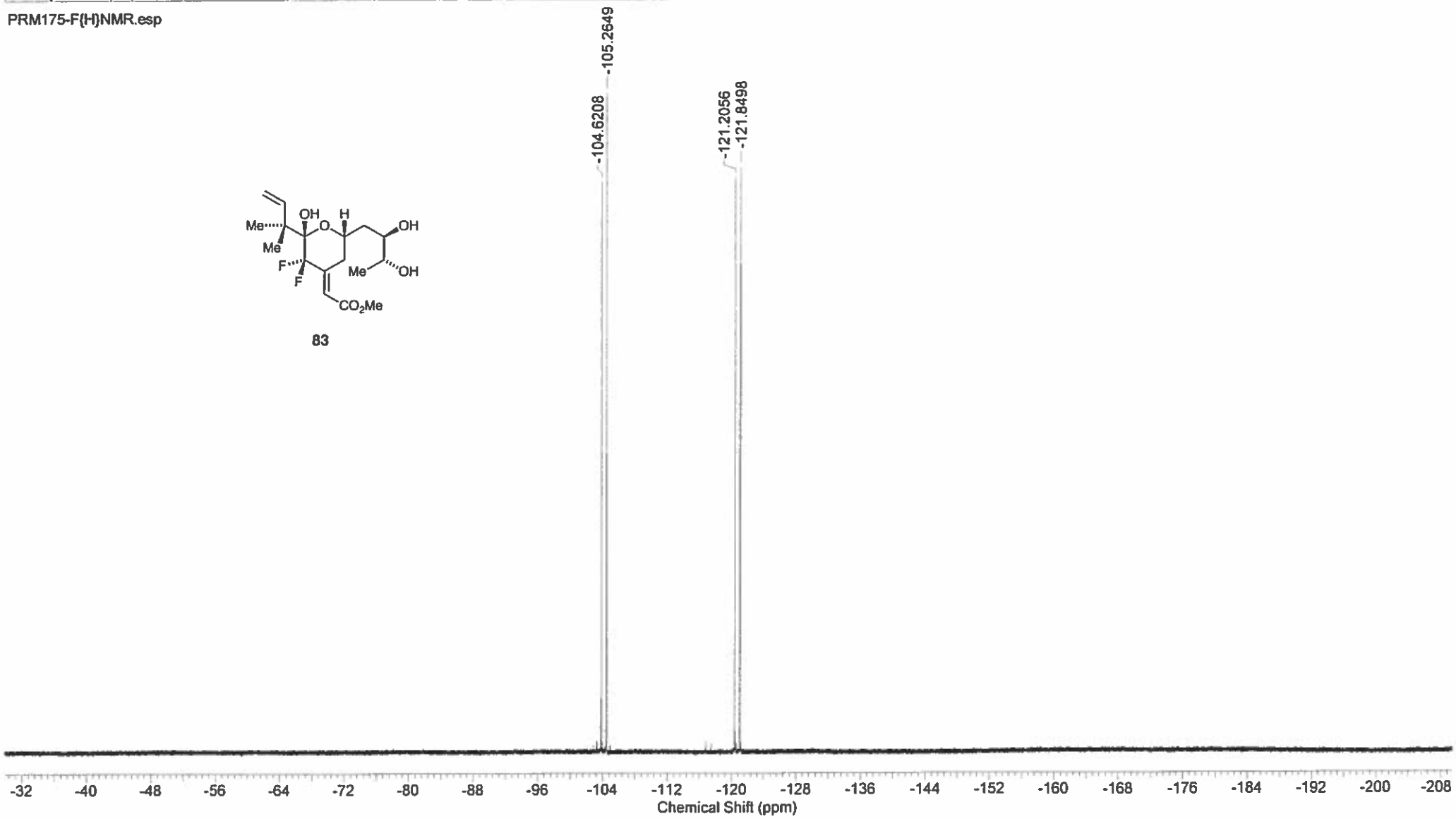


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM175 f6-28 11mg mF19CPD C6D6 (e:\bruk400adata\2015\Feb) ejt 45				
Date	25 Feb 2015 18:46:24			*Date Stamp*	25 Feb 2015 18:46:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Feb\data\ejt\nmr\2015-02-25-ejt-45\14\PDATA\1\1r					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	262144	*Pulse Sequence*	zgig	*Receiver Gain*	322.00
SW(cyclical) (Hz)	89285.71	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89285.37	*Temperature (degree C)*	19.900				

PRM175-F{H}NMR.esp



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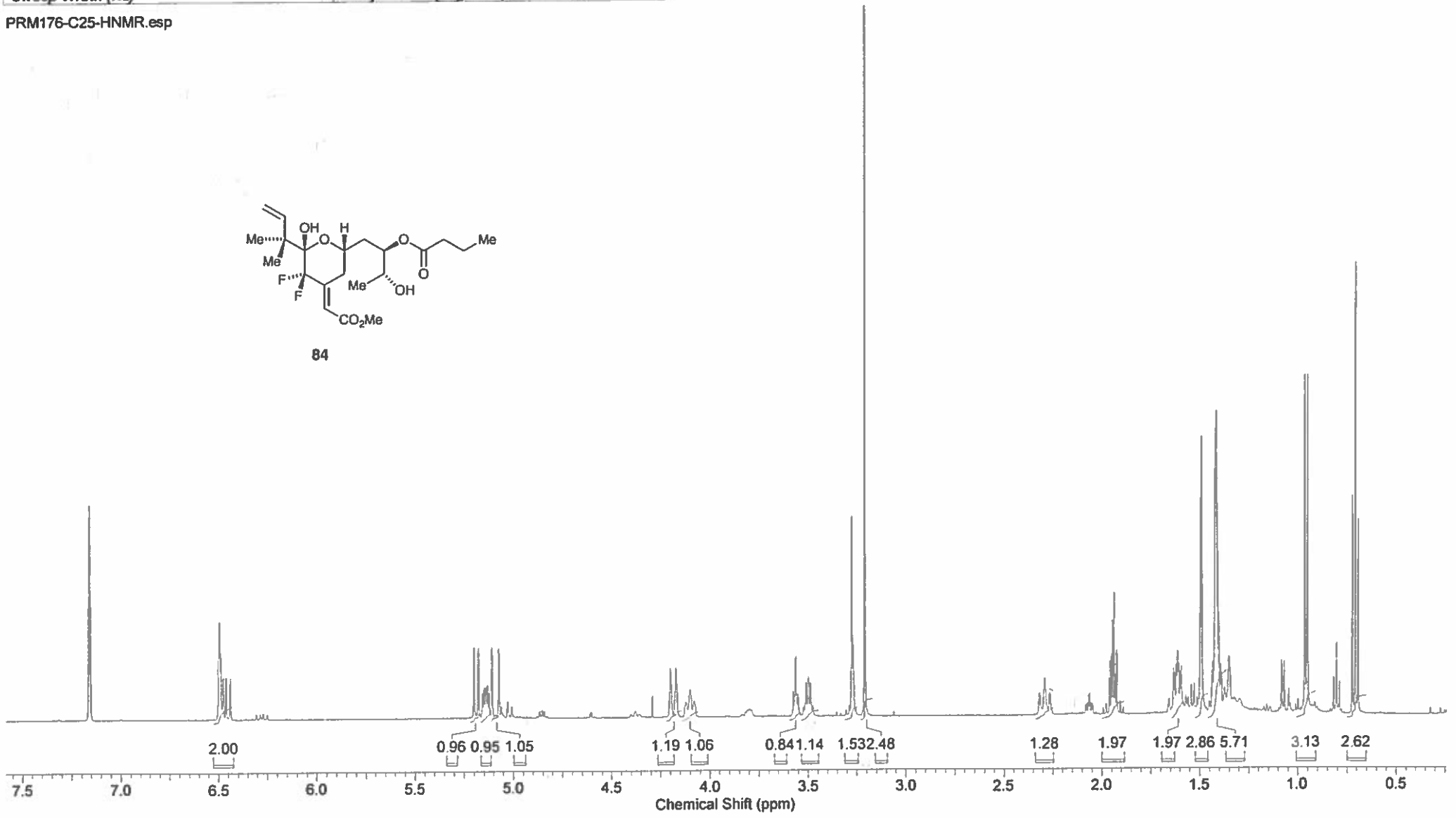
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.2768	*Comment*	0315 160 Mears P. EJT-PRM176 "C25" mPROTON C6D6 {E:\bruk500cdata\2015\Mar} staff 56				
Date	21 Mar 2015 20:43:44			*Date Stamp*	21 Mar 2015 20:43:44		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-56\10\fid					*Frequency (MHz)*	500.19
Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	61.38
SW(cyclical) (Hz)	10000.00	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	3092.6208	*Spectrum Type*	STANDARD
Sweep Width (Hz)	9999.70	*Temperature (degree C)*	22.153				

PRM176-C25-HNMR.esp

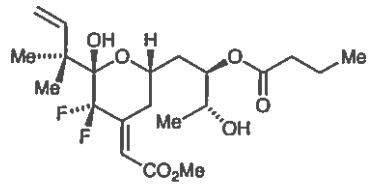
84



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 (E:\bruk500cdata\2015\Mar) staff 56				
Date	22 Mar 2015 05:45:36	*Date Stamp*	22 Mar 2015 05:45:36				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-56\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10240	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12661.6182	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.164				

PRM176-C25-CNMR.esp



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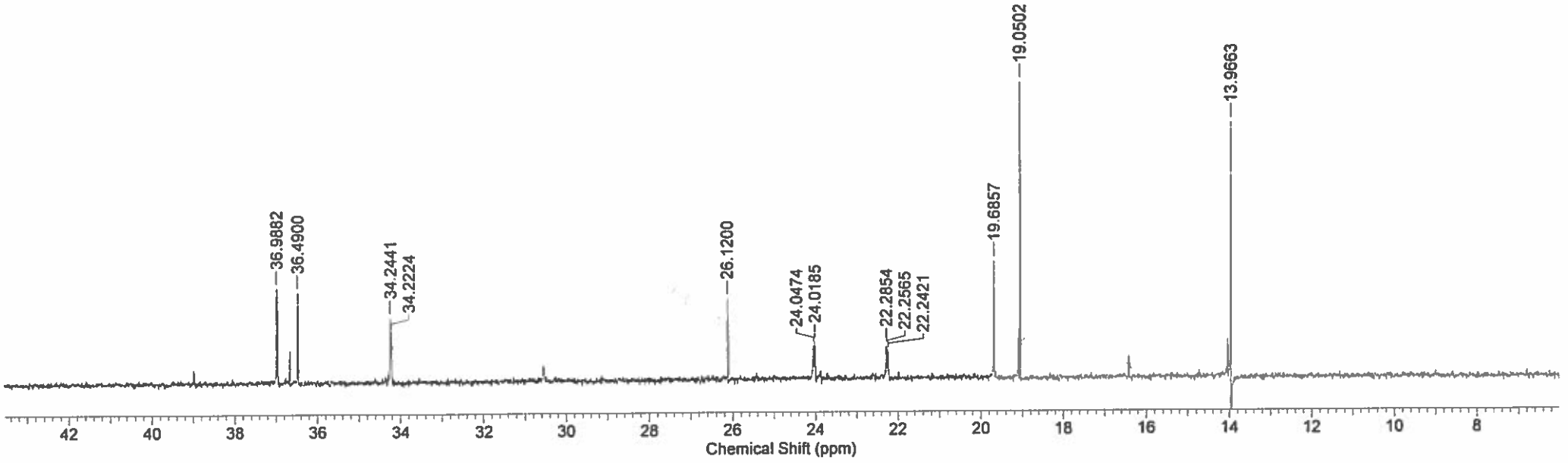
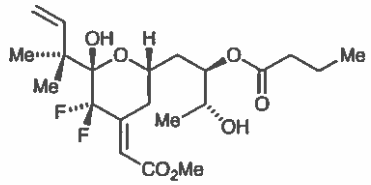


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 (E:\bruk500cdata\2015\Mar) staff 56				
Date	22 Mar 2015 05:45:36	*Date Stamp*	22 Mar 2015 05:45:36				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-56\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10240	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12661.6182	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.164				

PRM176-C25-CNMR.esp



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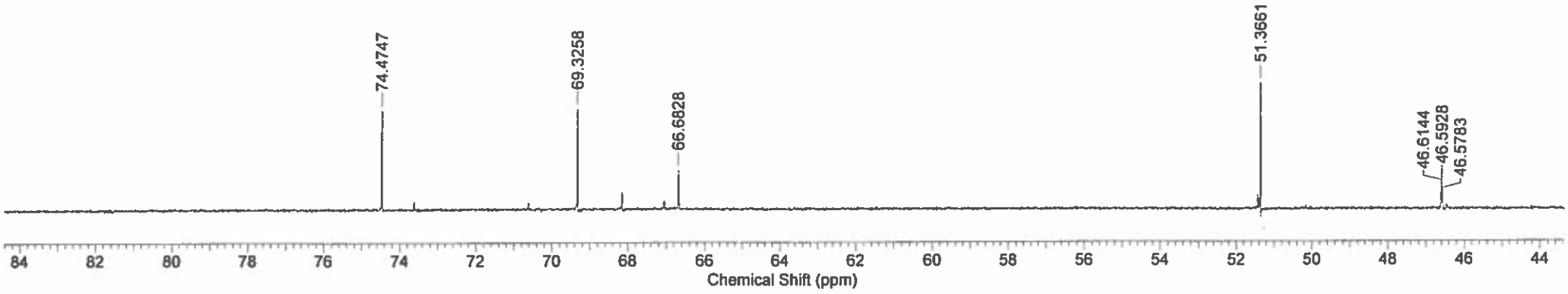
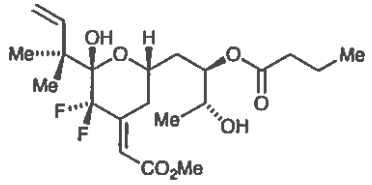


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 {E:\bruk500cdata\2015\Mar} staff 56				
Date	22 Mar 2015 05:45:36	*Date Stamp*	22 Mar 2015 05:45:36				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-56\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10240	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12661.6182	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.164				

PRM176-C25-CNMR.esp



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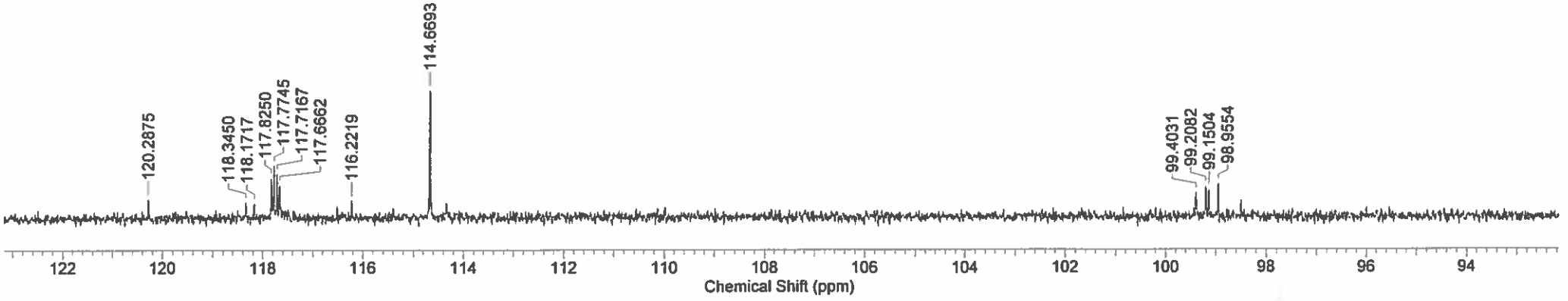
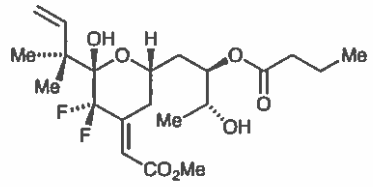


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	0315 160 Mears P. EJT-PRM176 "C25" mCARBON C6D6 {E:\bruk500cdata\2015\Mar} staff 56				
Date	22 Mar 2015 05:45:36	*Date Stamp*	22 Mar 2015 05:45:36				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-56\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10240	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12661.6182	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.164				

PRM176-C25-CNMR.esp



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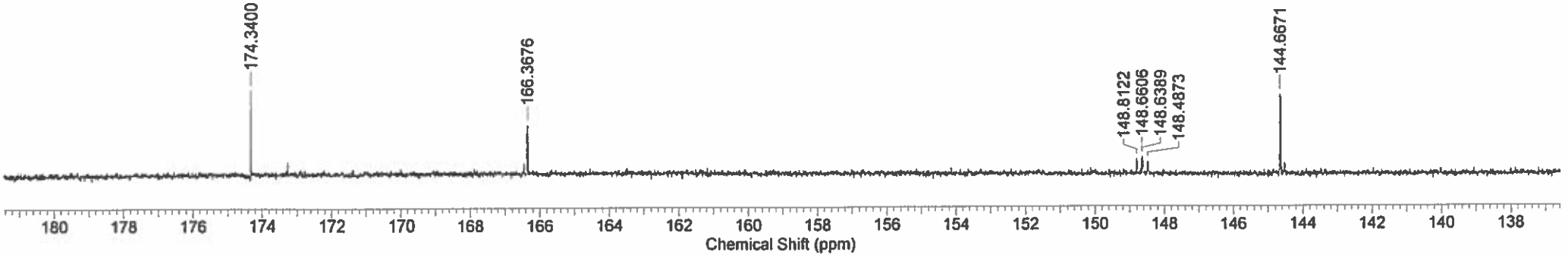

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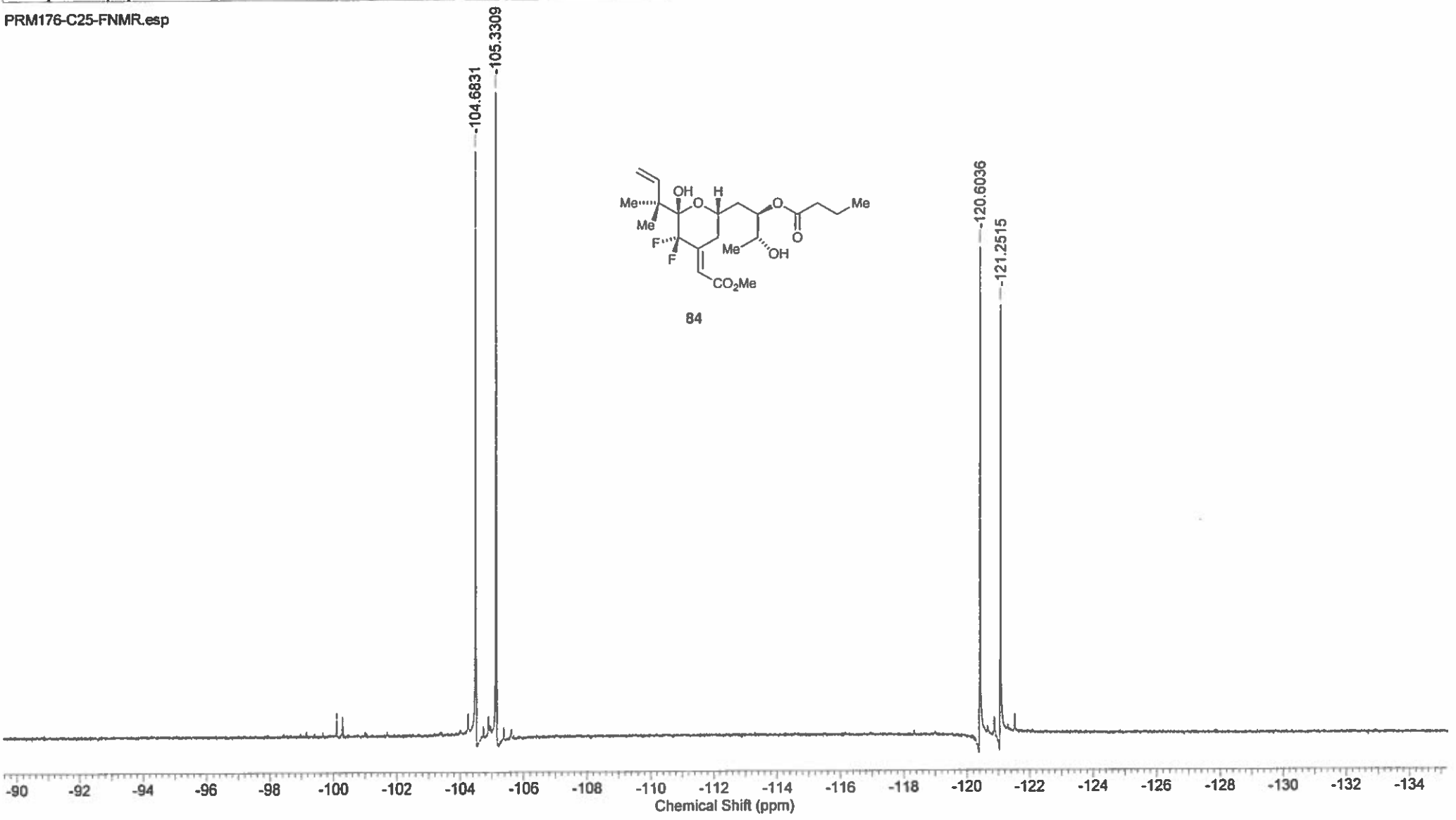
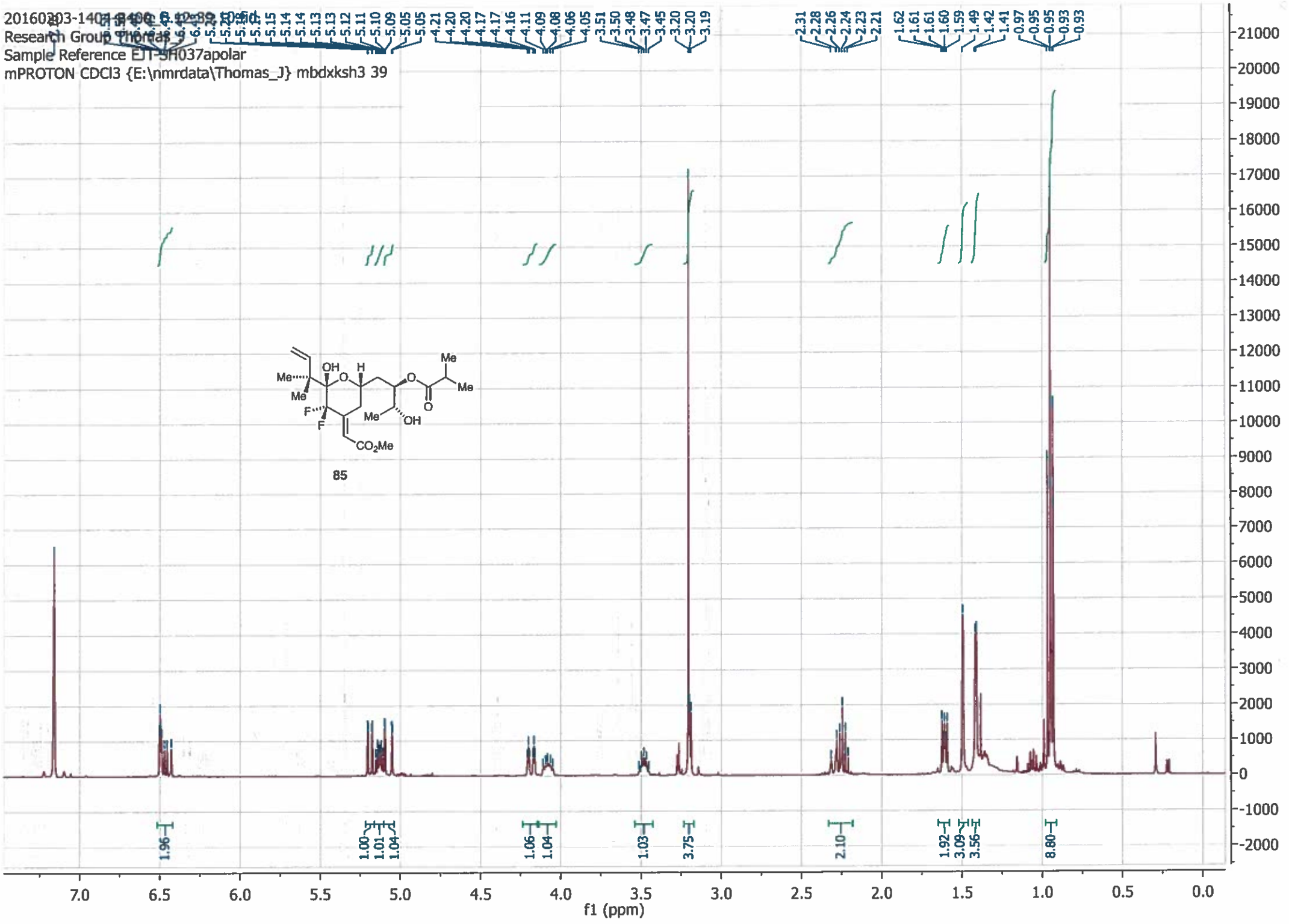
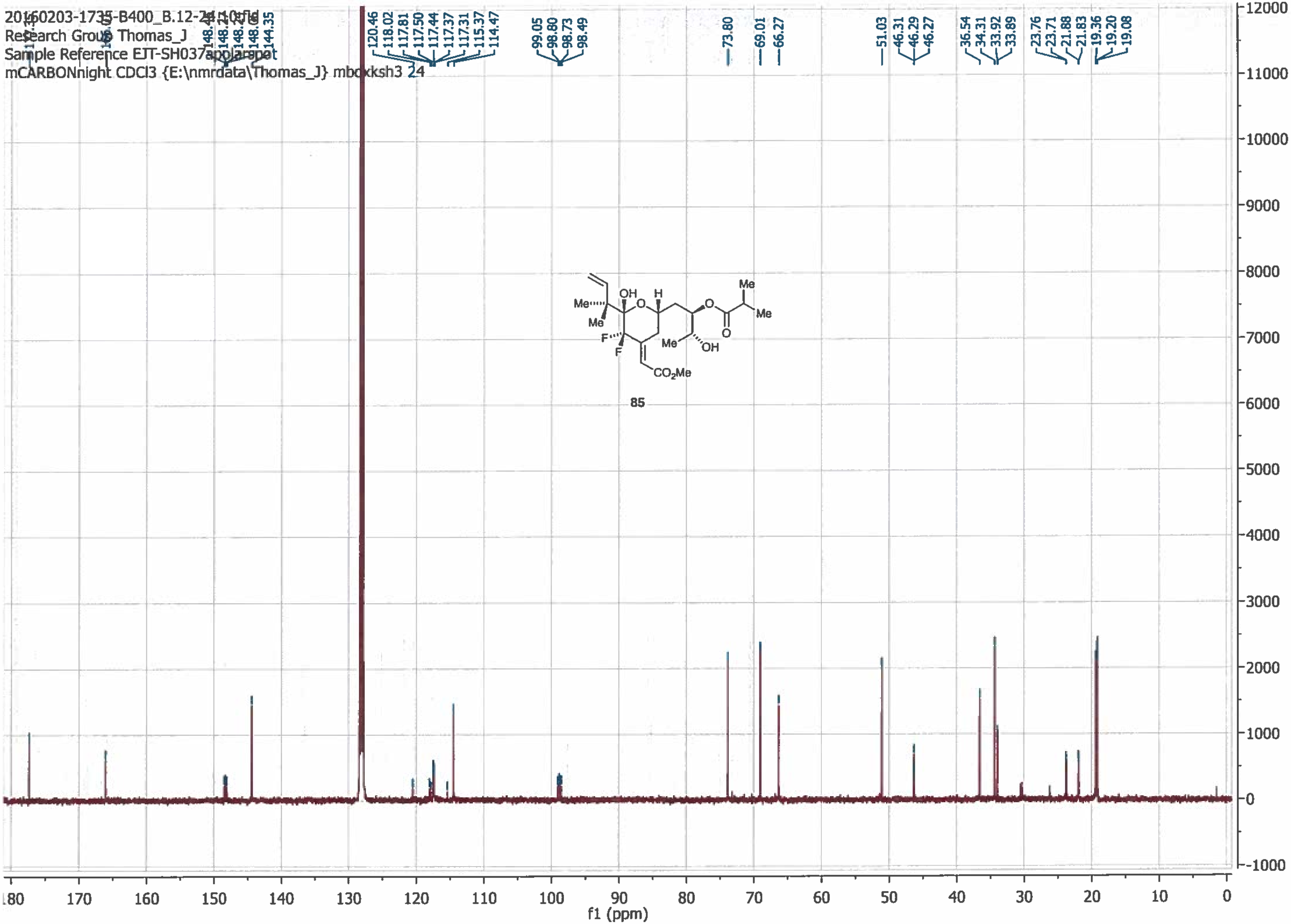
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM176 2nd re-col. f4-12 7mg mF19_cryo_zgbs C6D6 {e:\bruk400cdata\2015\Feb} ejt 44				
Date	05 Mar 2015 17:46:40			*Date Stamp*	05 Mar 2015 17:46:40		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-03-05-ejt-44\11\fid					*Frequency (MHz)*	376.44
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgbs	*Receiver Gain*	22.60
SW(cyclical) (Hz)	89285.71	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-37644.8594	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	15.742				

PRM176-C25-FNMR.esp



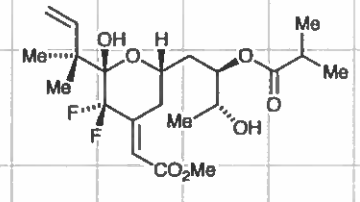
84


Research Group Thomas_J
Sample Reference EJT-5H037apolar
mPROTON CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 39
85
f1 (ppm)


20160203-1735-B400_B.12-24.10.fid
Research Group Thomas_J
Sample Reference EJT-SH037applarapat
mCARBONnight CDCl3 {E:\nmrdata\Thomas_J} mbokksh3 24
144.35
120.46
118.02
117.81
117.50
117.44
117.37
117.31
115.37
114.47
99.05
98.80
98.73
98.49
73.80
69.01
66.27
51.03
46.31
46.29
46.27
36.54
34.31
33.92
33.89
23.76
23.71
21.88
21.83
19.36
19.20
19.08
OH
H
O
Me
F
OH
CO_2Me
85
f1 (ppm)

20160203-1735-B400_B.12-24.11.fid
Research Group Thomas_J
Sample Reference EJT-SH037apolarspot
mF19 CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 24

-104.65
-105.30
-120.57
-121.21



85

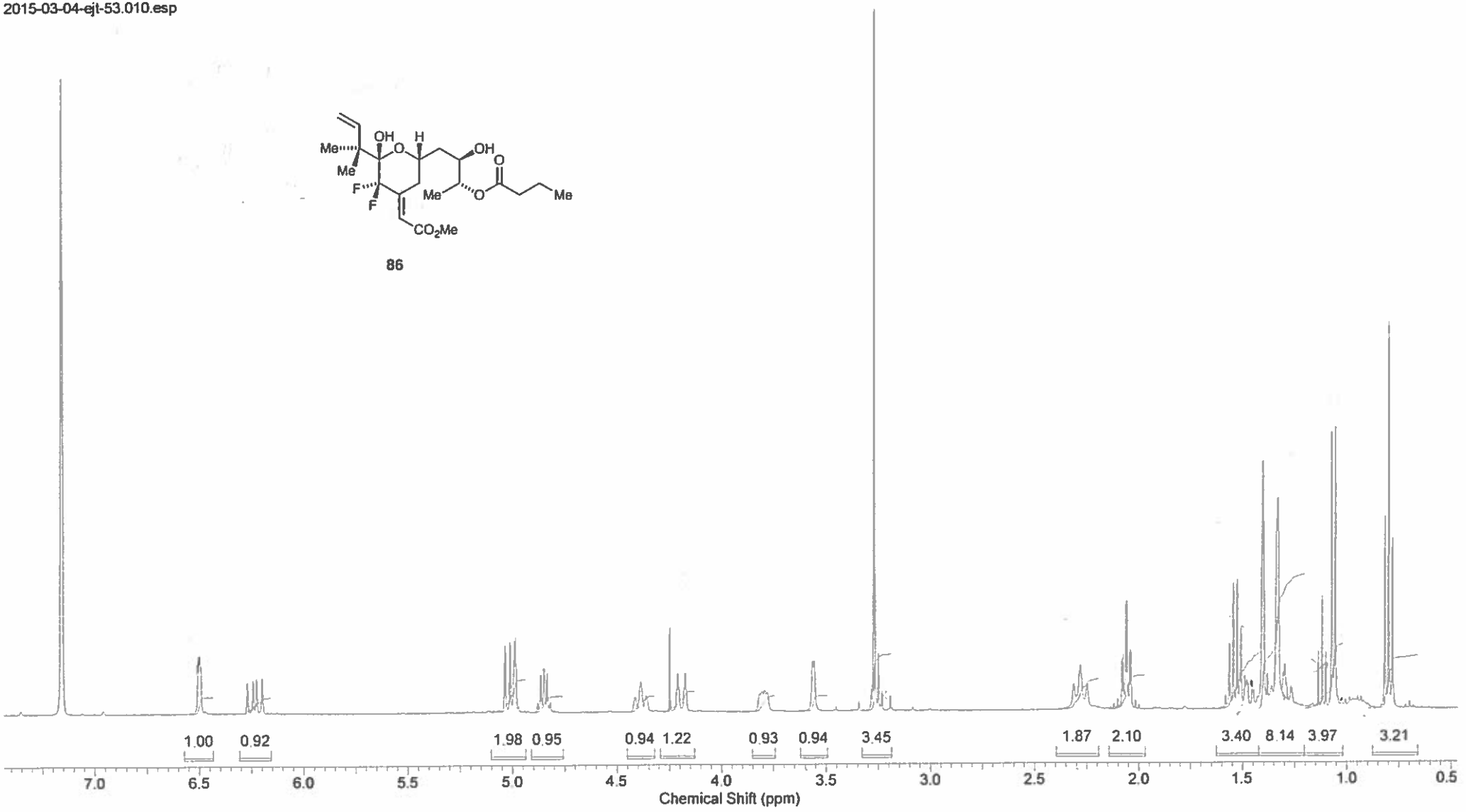
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

Acquisition Time (sec)	4.0894	*Comment*	EJT-PRM176 f6-17 6mg mPROTON_A C6D6 {e:\bruk400cdata\2015\Feb} ejt 53				
Date	04 Mar 2015 10:14:24			*Date Stamp*	04 Mar 2015 10:14:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-03-04-ejt-53\10\fid					*Frequency (MHz)*	400.07
Nucleus	1H	*Number of Transients*	4	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	161.00
SW(cyclical) (Hz)	8012.82	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	1903.3687	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8012.58	*Temperature (degree C)*	15.338				

2015-03-04-ejt-53.010.esp

86

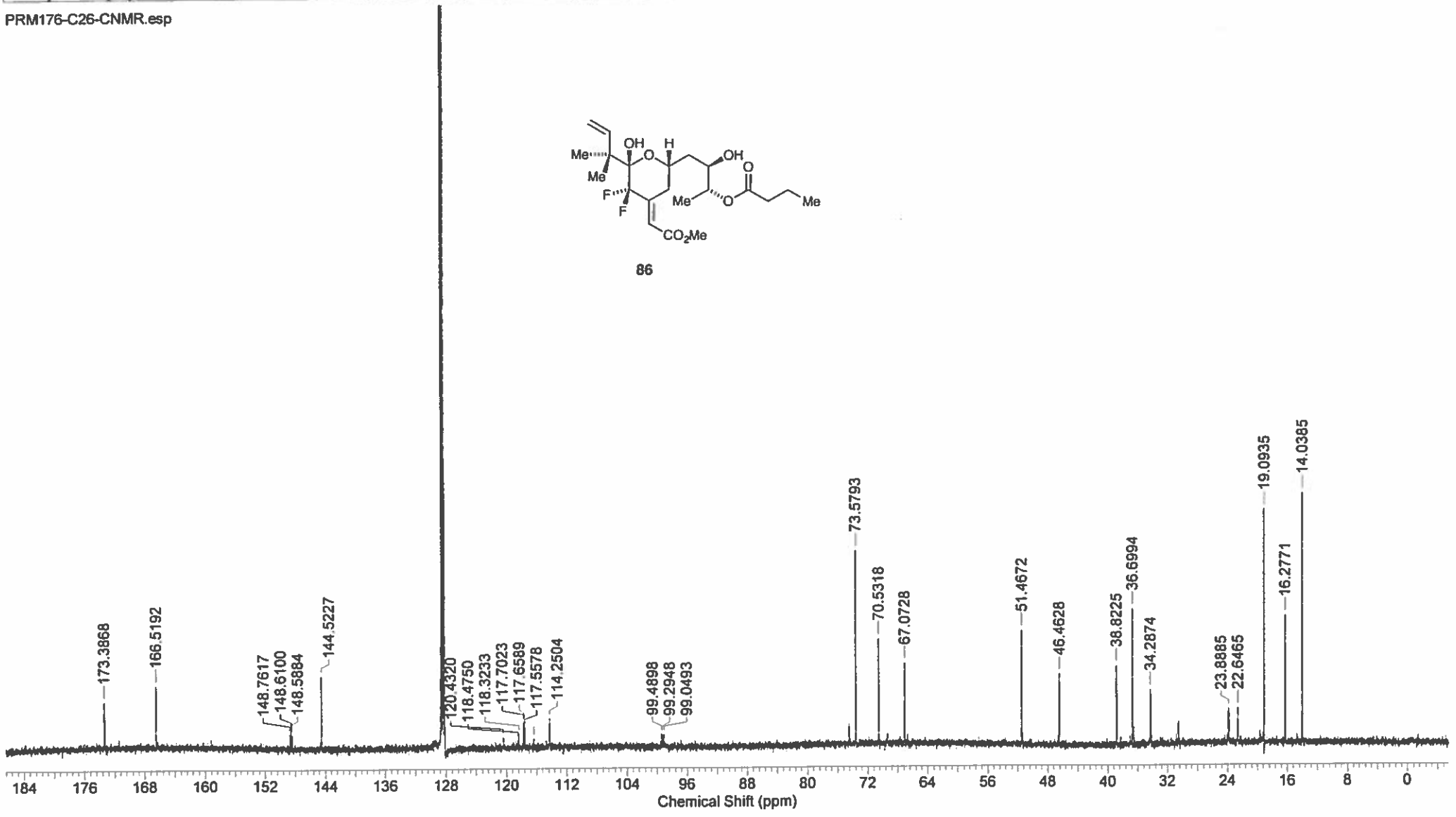


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.1010	*Comment*	0315 159 Mears P. EJT-PRM176 "C26" mCARBON C6D6 (E:\bruk500cdata\2015\Mar) staff 55				
Date	21 Mar 2015 19:39:44	*Date Stamp*	21 Mar 2015 19:39:44				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500cdata\2015\Mar\data\staff\nmr\2015-03-20-staff-55\11\fid					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10240	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	184.40
SW(cyclical) (Hz)	29761.90	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	12661.6182	*Spectrum Type*	STANDARD
Sweep Width (Hz)	29761.00	*Temperature (degree C)*	22.158				

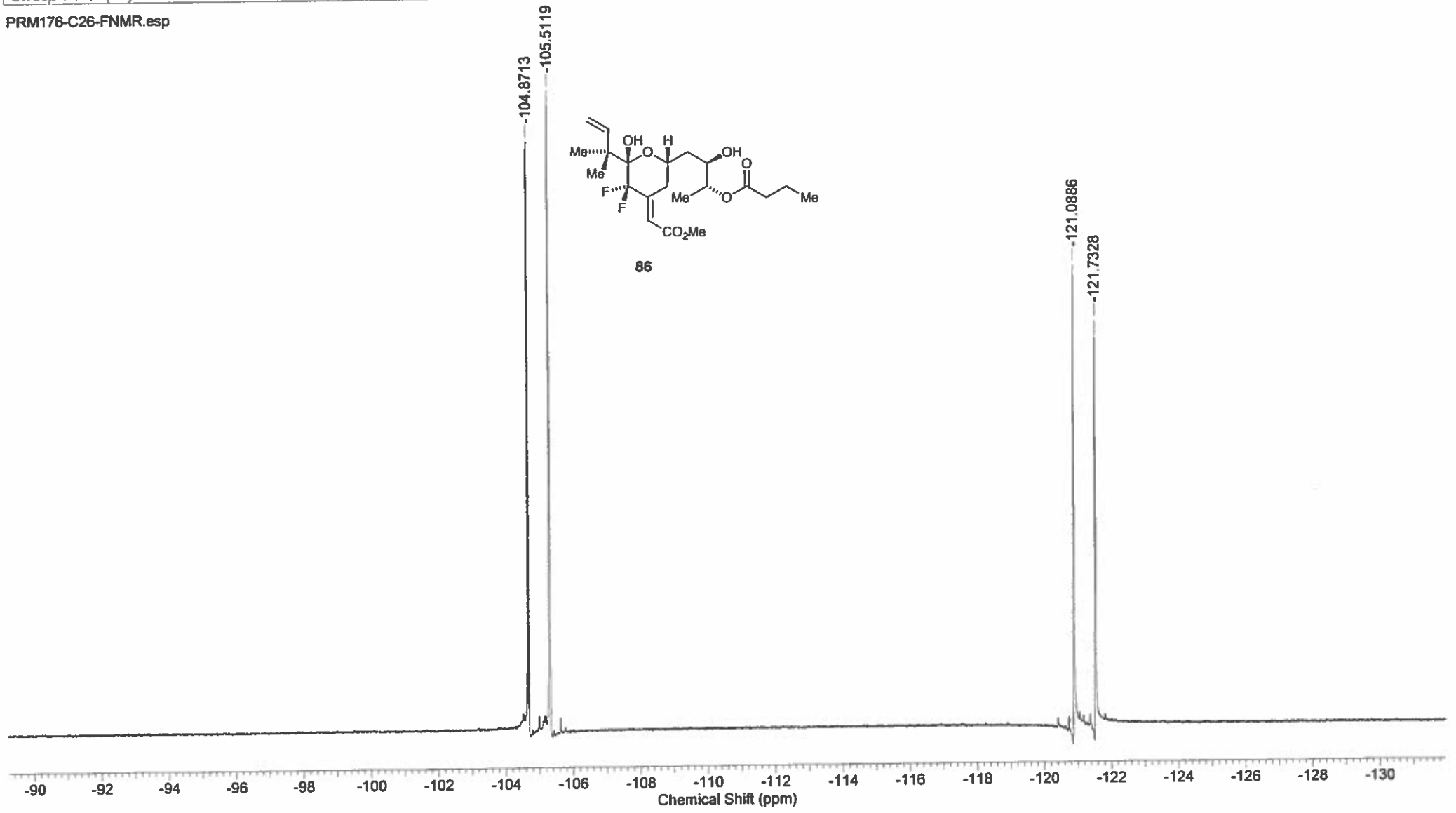
PRM176-C26-CNMR.esp

86

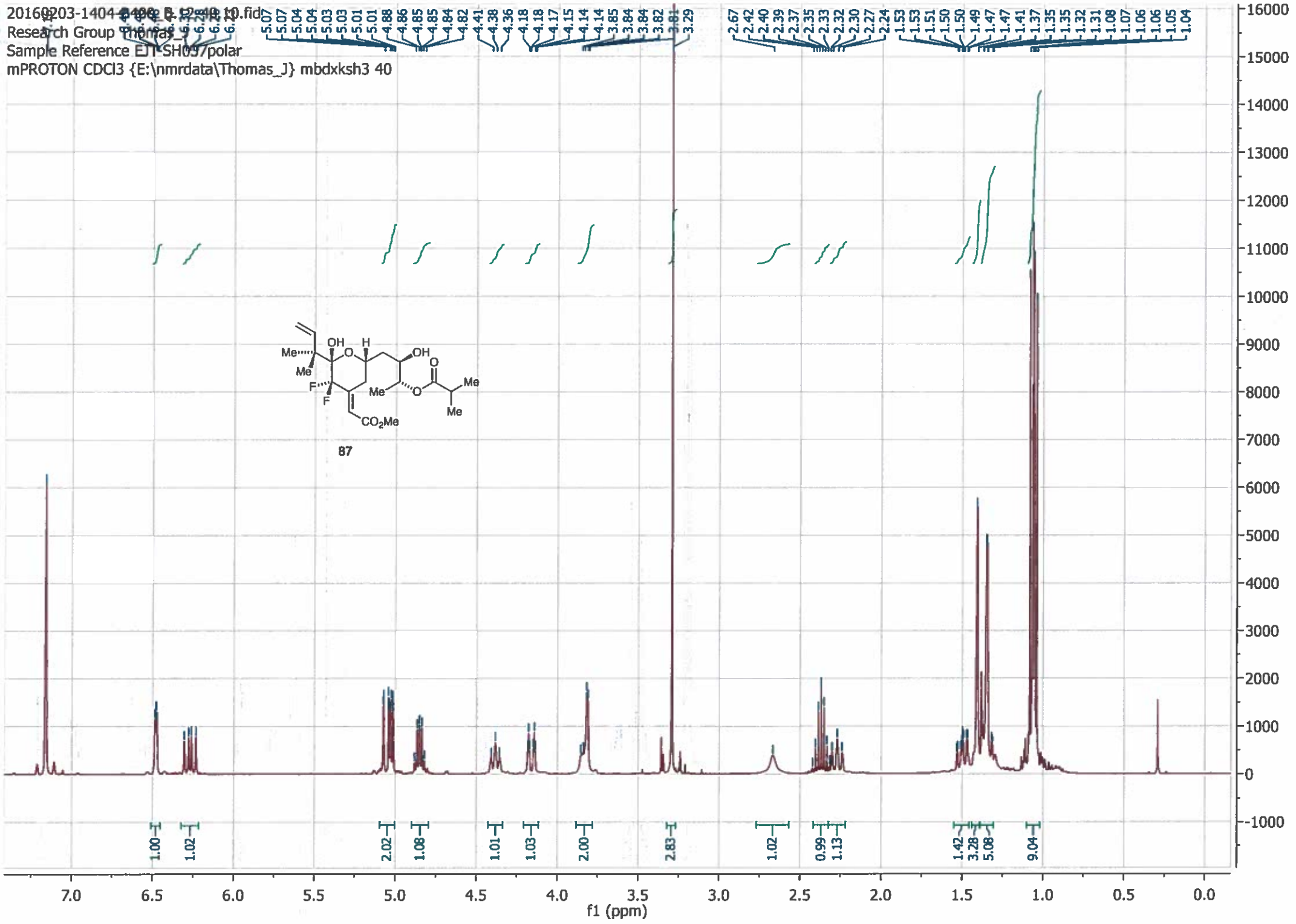


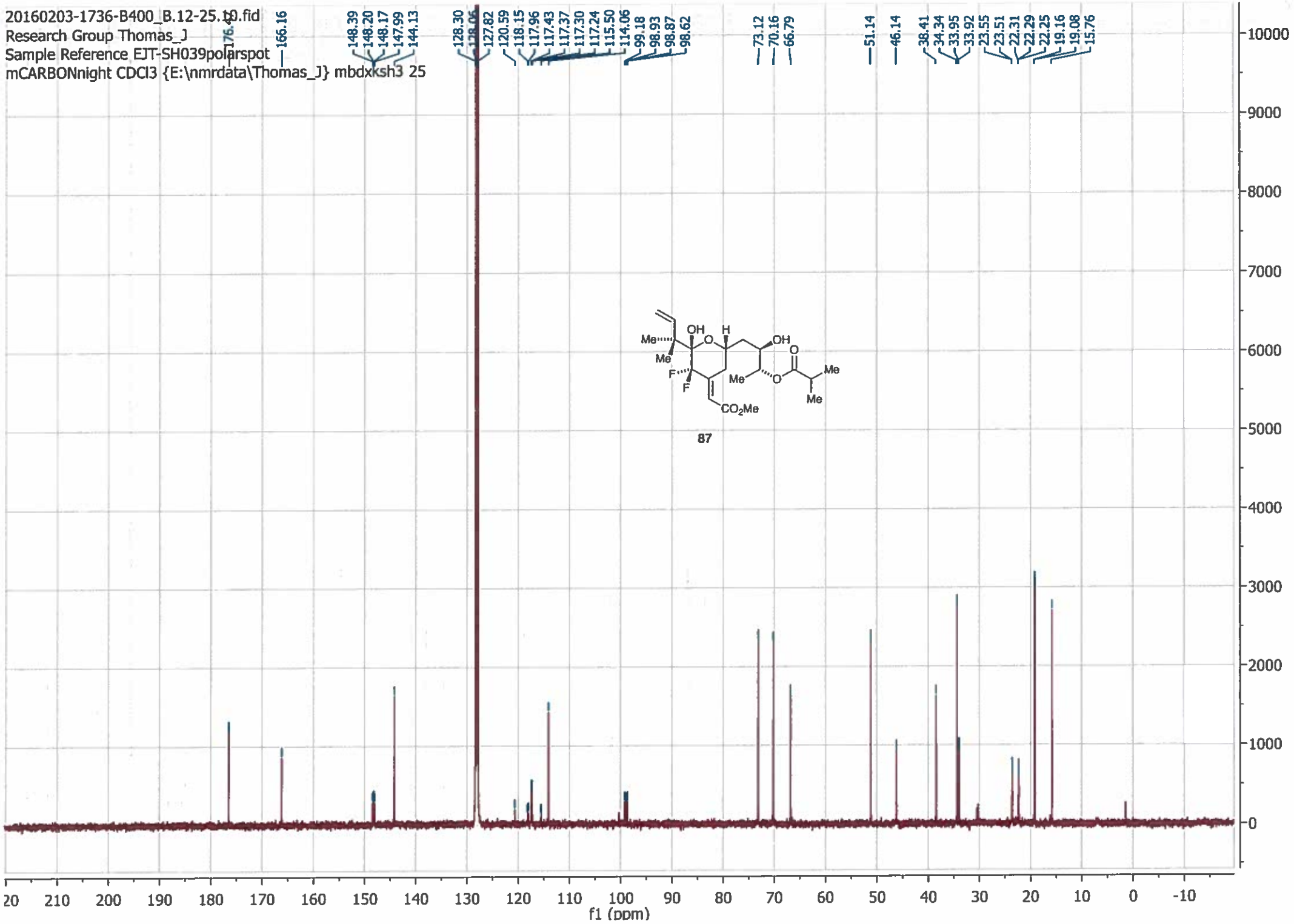
Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM176 f6-17 6mg mF19_cryo_zgbs C6D6 (e:\bruk400cdata\2015\Feb) ejt 53				
Date	04 Mar 2015 10:16:32			*Date Stamp*	04 Mar 2015 10:16:32		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Feb\data\ejt\nmr\2015-03-04-ejt-53\11\fid					*Frequency (MHz)*	376.44
Nucleus	19F	*Number of Transients*	16	*Origin*	specl	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgbs	*Receiver Gain*	20.20
SW(cyclical) (Hz)	89285.71	*Solvent*	BENZENE-d6	*Spectrum Offset (Hz)*	-37644.8594	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	15.336				

PRM176-C26-FNMR.esp



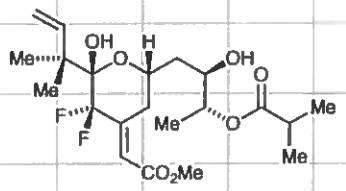
86


20160203-1404-8406 5 12 49 10.fid
Research Group Thomas_J
Sample Reference EJT-SH097polar
mPROTON CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 40
87
f1 (ppm)


20160203-1736-B400_B.12-25.10.fid
Research Group Thomas_J
Sample Reference EJT-SH039polarspot
mCARBONnight CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 25
176.40
166.16
148.39
148.20
148.17
147.99
144.13
128.30
128.06
127.82
120.59
118.15
117.96
117.43
117.37
117.30
117.24
115.50
114.06
99.18
98.93
98.87
98.62
73.12
70.16
66.79
51.14
46.14
38.41
34.34
33.95
33.92
23.55
23.51
22.31
22.29
22.25
19.16
19.08
15.76
Me
OH
O
H
OH
Me
F
F
Me
O
O
Me
Me
CO2Me
87
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

20160203-1736-B400_B.12-25.11.fid
Research Group Thomas_J
Sample Reference EJT-SH039polarspot
mF19 CDCl3 {E:\nmrdata\Thomas_J} mbdxksh3 25

104.65
105.30
121.04
121.69



87

9000 8500 8000 7500 7000 6500 6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0 -500 -1000

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)

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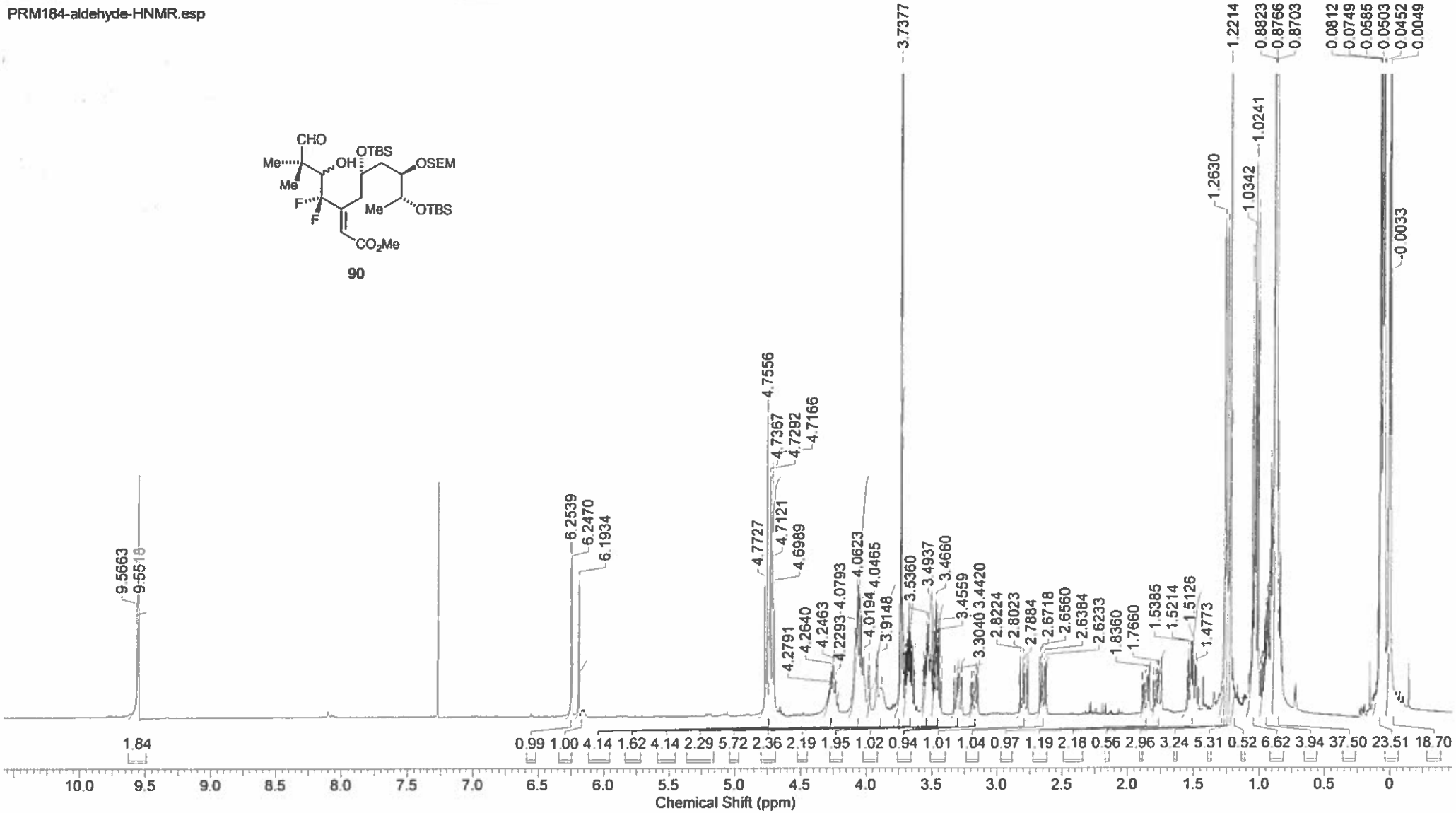
Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM184 f8-25 157mg mPROTON CDCl3 {e:\bruk400adata\2015\Jul} ejt 52				
Date	14 Jul 2015 19:25:04			*Date Stamp*	14 Jul 2015 19:25:04		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jul\data\ejt\nmr\2015-07-14-ejt-52\10\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	36.00
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2465.1792	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	21.300				

PRM184-aldehyde-HNMR.esp

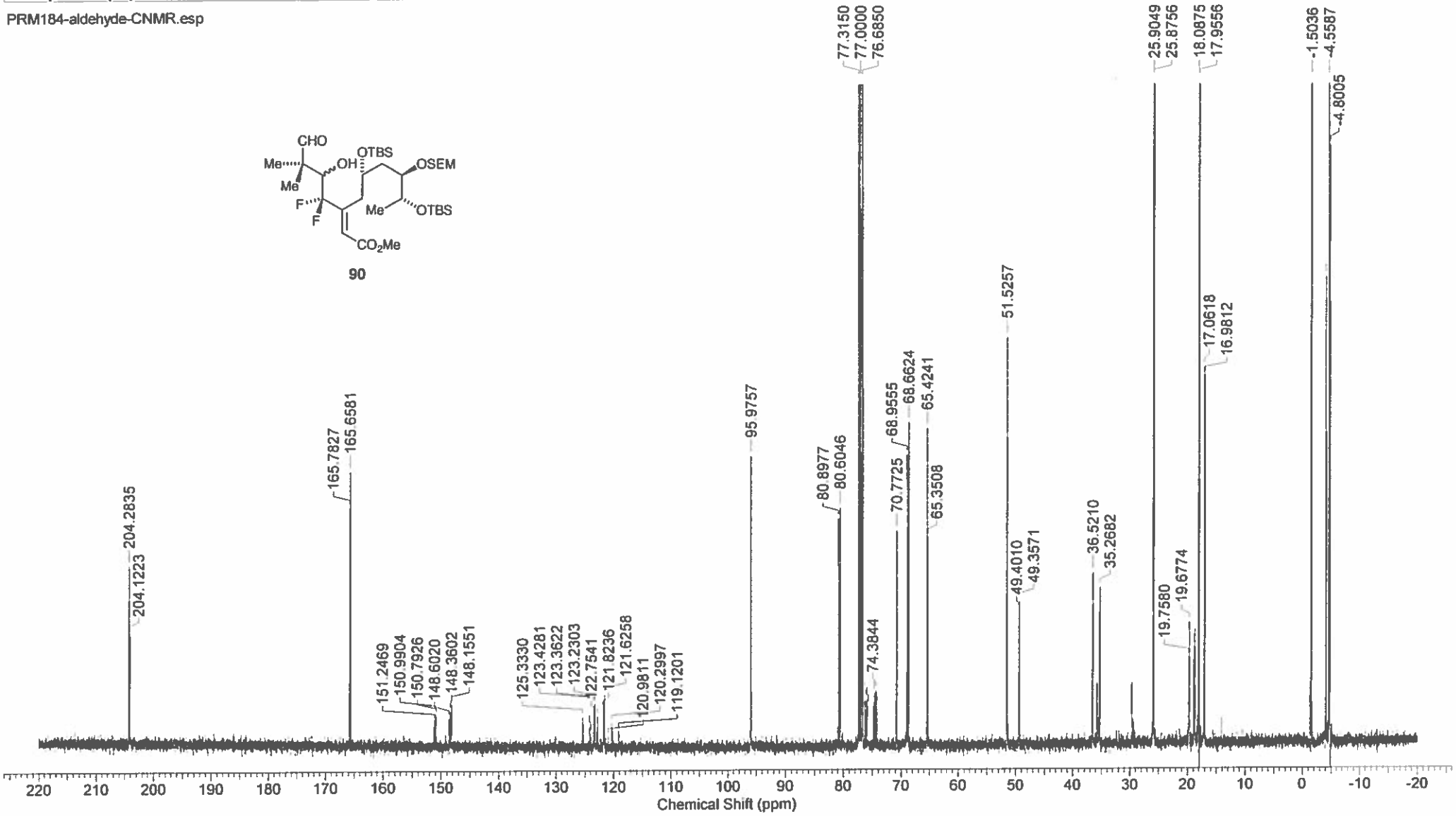
90



Acquisition Time (sec)	1.3566	*Comment*	EJT-PRM184 f8-25 157mg mCARBONnight CDCl3 {e:\bruk400adata\2015\Jul} ejt 52				
Date	14 Jul 2015 22:30:40	*Date Stamp*	14 Jul 2015 22:30:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jul\data\ejt\nmr\2015-07-14-ejt-52\13\fid					*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	3000	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	512.00
SW(cyclical) (Hz)	24154.59	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10059.2100	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24153.85	*Temperature (degree C)*	22.900				

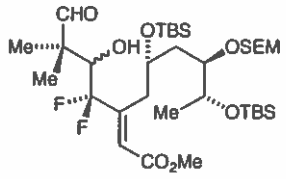
PRM184-aldehyde-CNMR.esp

90



Acquisition Time (sec)	1.3566	*Comment*	EJT-PRM184 f8-25 157mg mCARBONnight CDCl3 (e:\bruk400adata\2015\Jul) ejt 52				
Date	14 Jul 2015 22:30:40	*Date Stamp*	14 Jul 2015 22:30:40				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jul\data\ejt\nmr\2015-07-14-ejt-52\13\fid					*Frequency (MHz)*	100.61
Nucleus	13C	*Number of Transients*	3000	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	512.00
SW(cyclical) (Hz)	24154.59	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10059.2100	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24153.85	*Temperature (degree C)*	22.900				

PRM184-aldehyde-CNMR.esp



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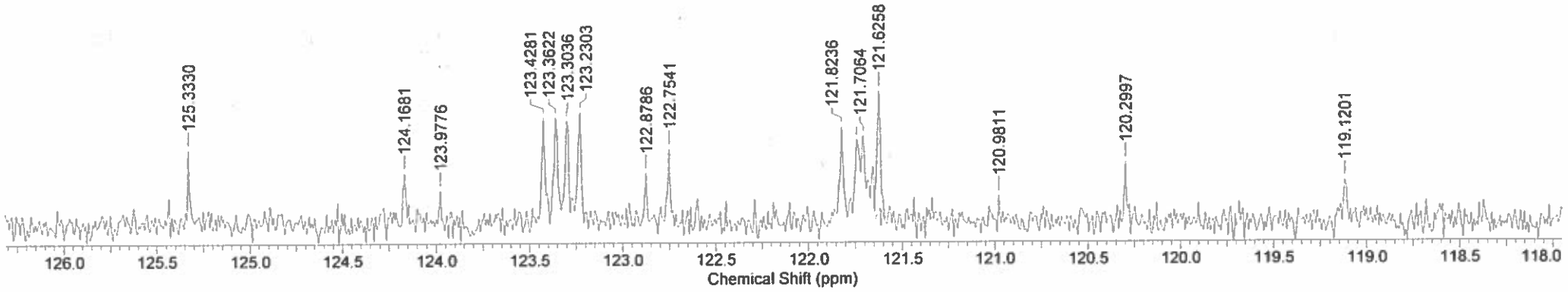
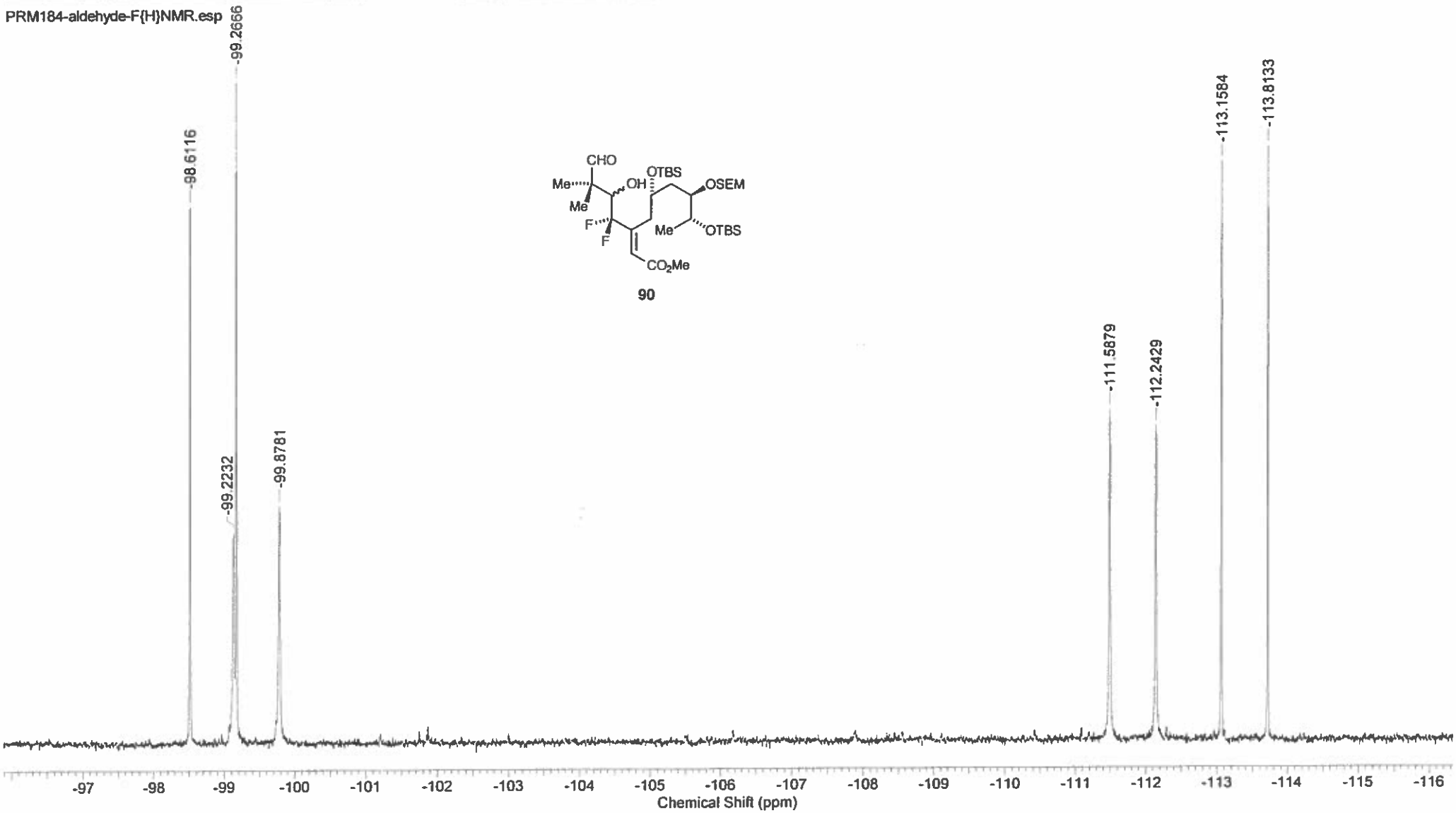


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM184 f8-25 157mg mF19CPD CDCl3 (e:\bruk400adata\2015\Jul) ejt 52				
Date	14 Jul 2015 19:29:20	*Date Stamp*	14 Jul 2015 19:29:20				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jul\data\ejt\nmr\2015-07-14-ejt-52\12\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	362.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	21.500				

PRM184-aldehyde-F{H}NMR.esp

90

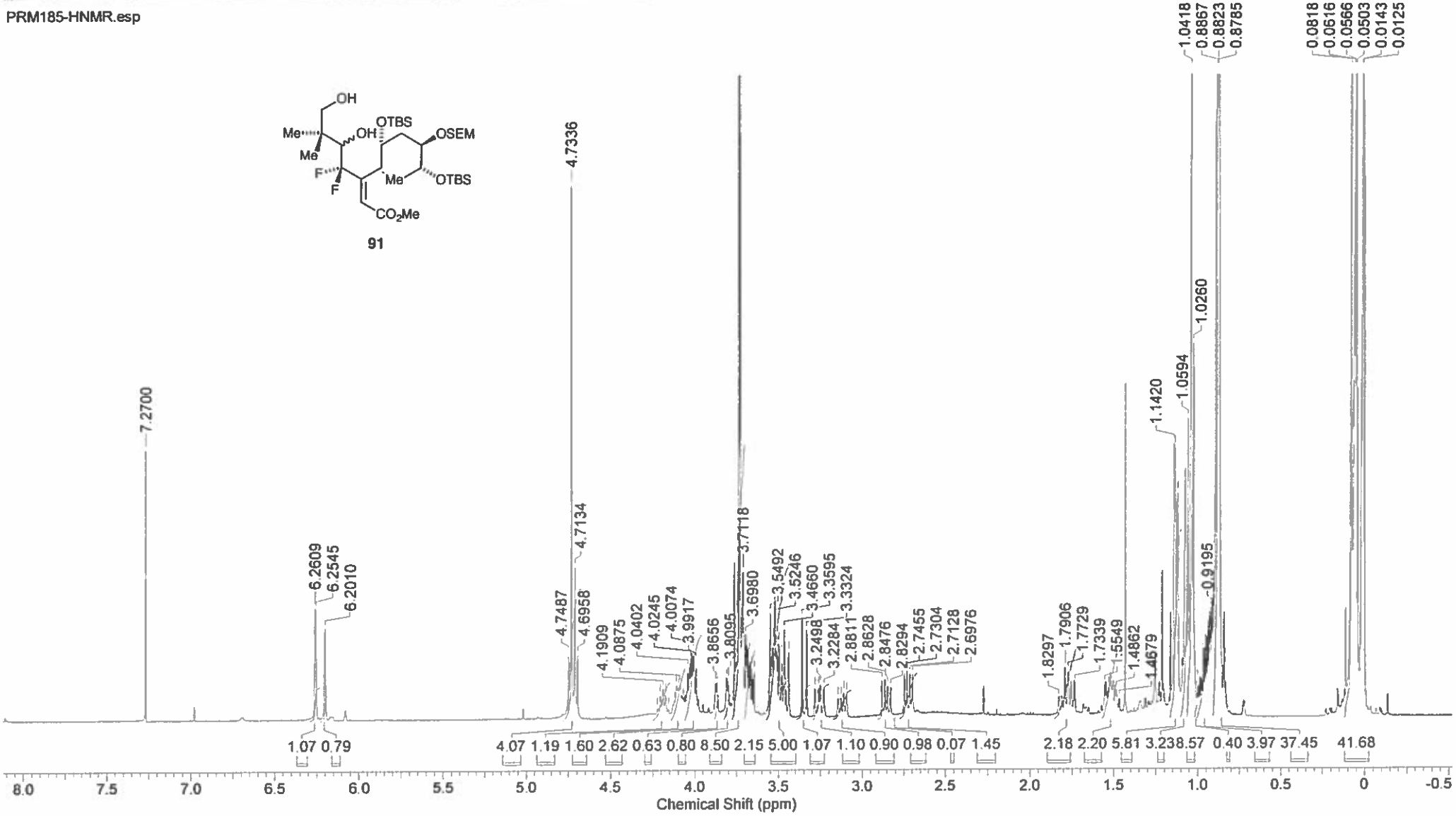


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	3.9649	*Comment*	EJT-PRM185 f15-33 118mg mPROTON CDCl3 {e:\bruk400adata\2015\Jul} ejt 40				
Date	16 Jul 2015 16:08:48			*Date Stamp*	16 Jul 2015 16:08:48		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jul\data\ejt\nmr\2015-07-16-ejt-40\10\fid					*Frequency (MHz)*	400.13
Nucleus	1H	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30b	*Receiver Gain*	80.60
SW(cyclical) (Hz)	8264.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2464.9270	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8264.21	*Temperature (degree C)*	21.500				

PRM185-HNMR.esp

91

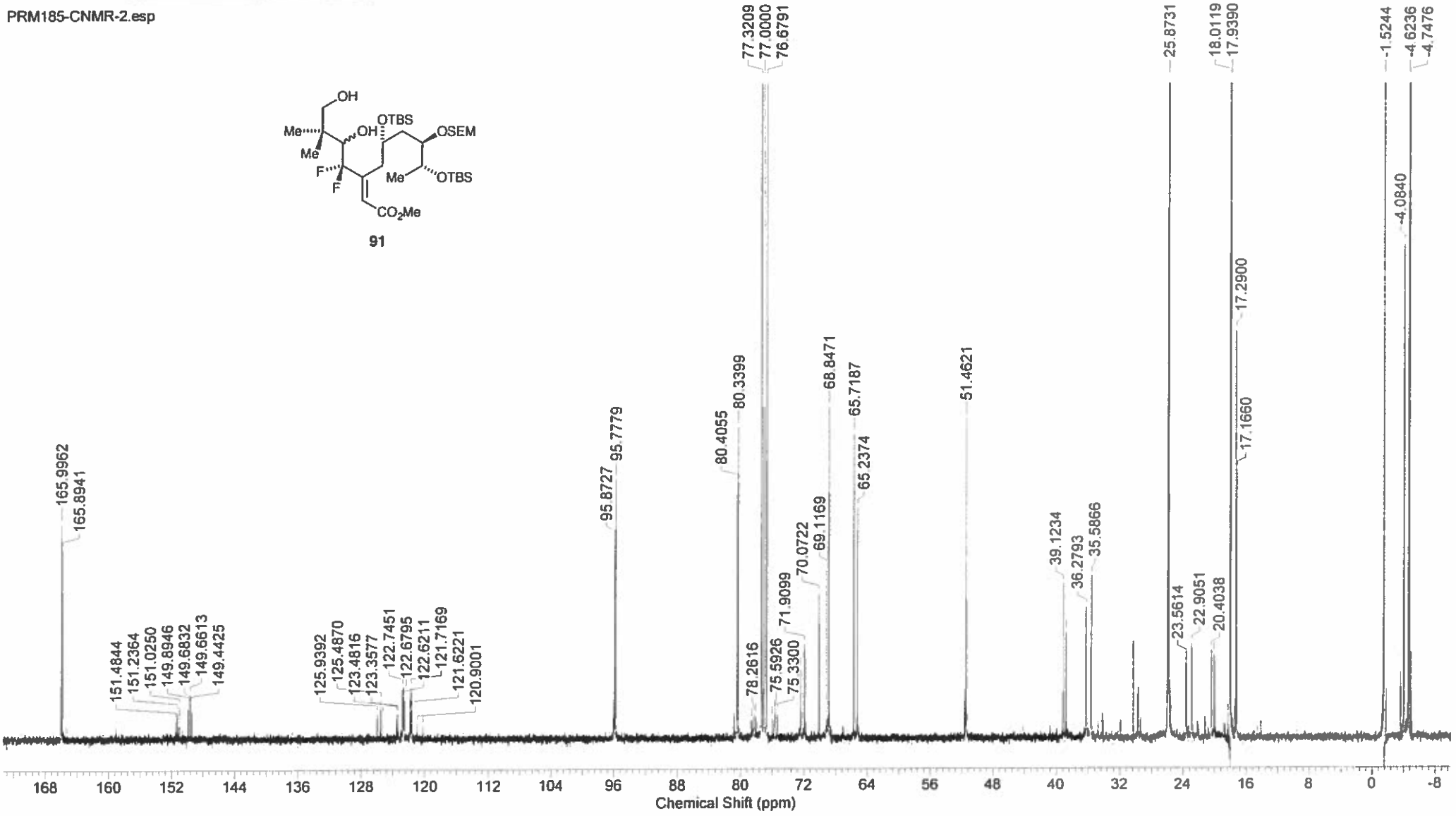


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM185 Prod mCARBON_B CDCl3 {e:\bruk400cdata\2015\Jul} ejt 20				
Date	22 Jul 2015 23:41:04			*Date Stamp*	22 Jul 2015 23:41:04		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Jul\data\ejt\nmr\2015-07-22-ejt-20\10\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10050.6006	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	17.967				

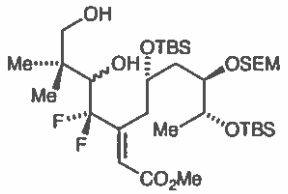
PRM185-CNMR-2.esp

91



Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM185 Prod mCARBON_B CDCl3 {e:\bruk400cdata\2015\Jul} ejt 20				
Date	22 Jul 2015 23:41:04			*Date Stamp*	22 Jul 2015 23:41:04		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Jul\data\ejt\nmr\2015-07-22-ejt-20\10\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1024	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10050.6006	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	17.967				

2015-07-22-ejt-20.010.esp



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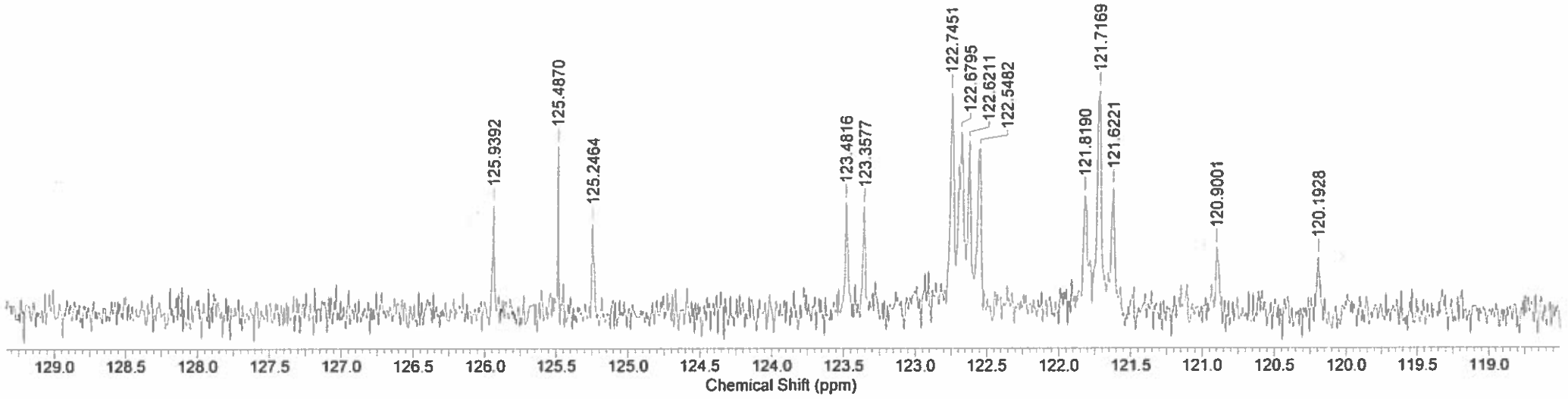
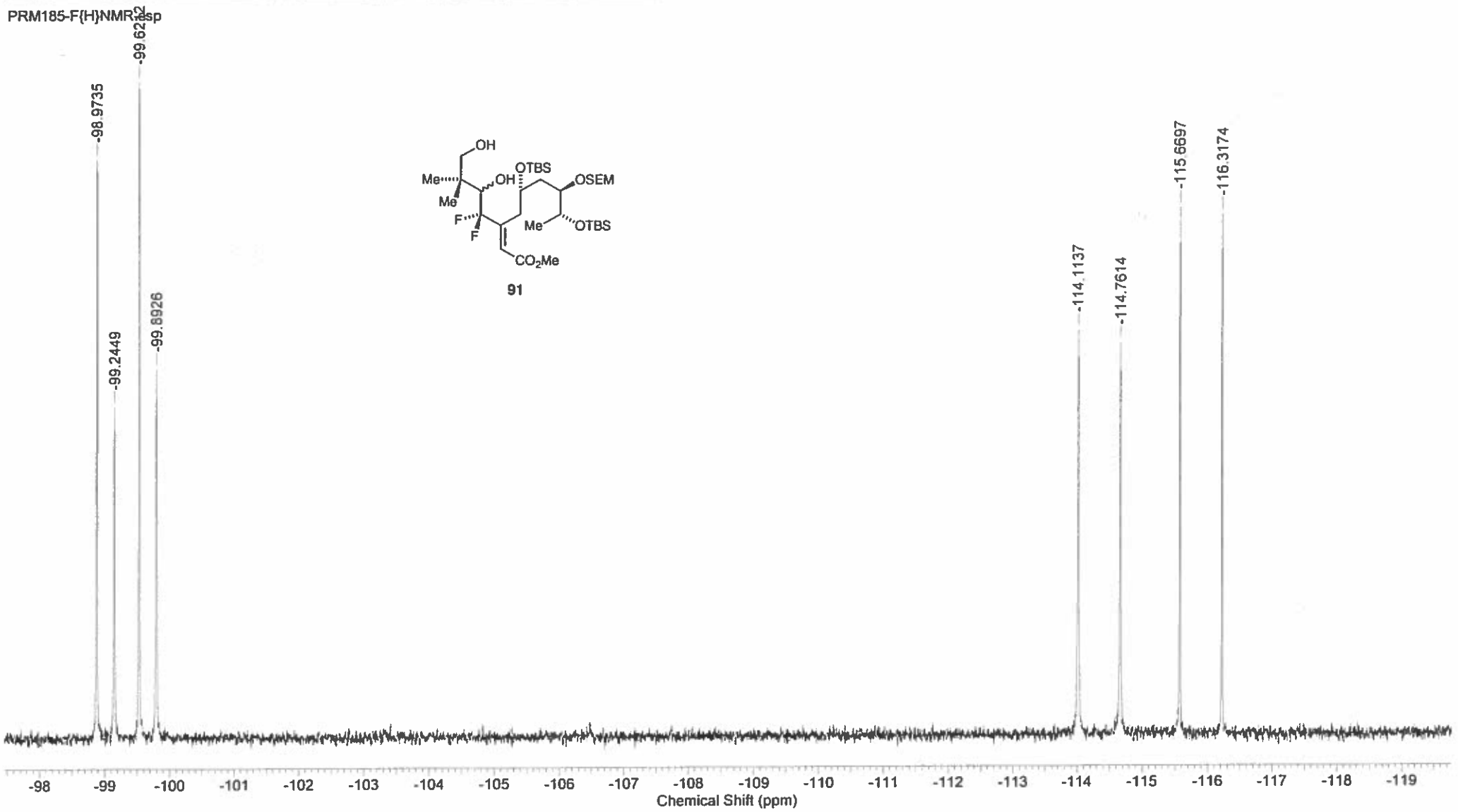


Acquisition Time (sec)	0.7340	*Comment*	EJT-PRM185 f15-33 118mg mF19CPD CDCl3 {e:\bruk400adata\2015\Jul} ejt 40				
Date	16 Jul 2015 16:13:04	*Date Stamp*	16 Jul 2015 16:13:04				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400adata\2015\Jul\data\ejt\nmr\2015-07-16-ejt-40\12\fid					*Frequency (MHz)*	376.50
Nucleus	19F	*Number of Transients*	16	*Origin*	AV400	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgig	*Receiver Gain*	362.00
SW(cyclical) (Hz)	89285.71	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-37649.5977	*Spectrum Type*	STANDARD
Sweep Width (Hz)	89284.35	*Temperature (degree C)*	21.700				

PRM185-F{H}NMR-esp

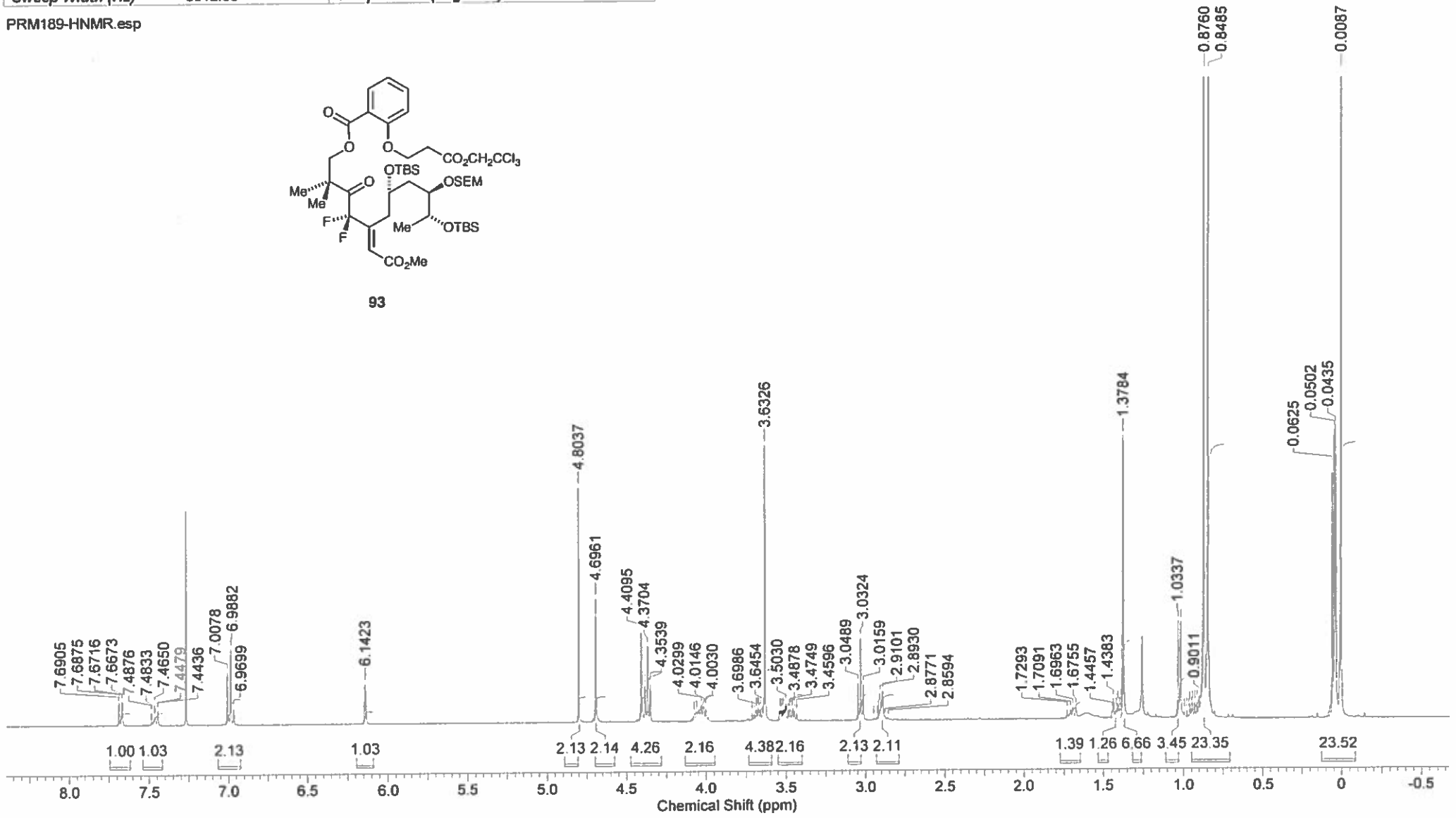


91

Acquisition Time (sec)	4.0894	*Comment*	EJT-PRM189 f3-15 16mg mPROTON_A CDCl3 (e:\bruk400cdata\2015\Jul) ejt 32				
Date	05 Aug 2015 12:46:08			*Date Stamp*	05 Aug 2015 12:46:08		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Jul\data\ejt\nmr\2015-08-05-ejt-32\10\fid					*Frequency (MHz)*	400.07
Nucleus	1H	*Number of Transients*	4	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	161.00
SW(cyclical) (Hz)	8012.82	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	1894.3132	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8012.58	*Temperature (degree C)*	18.208				

PRM189-HNMR.esp

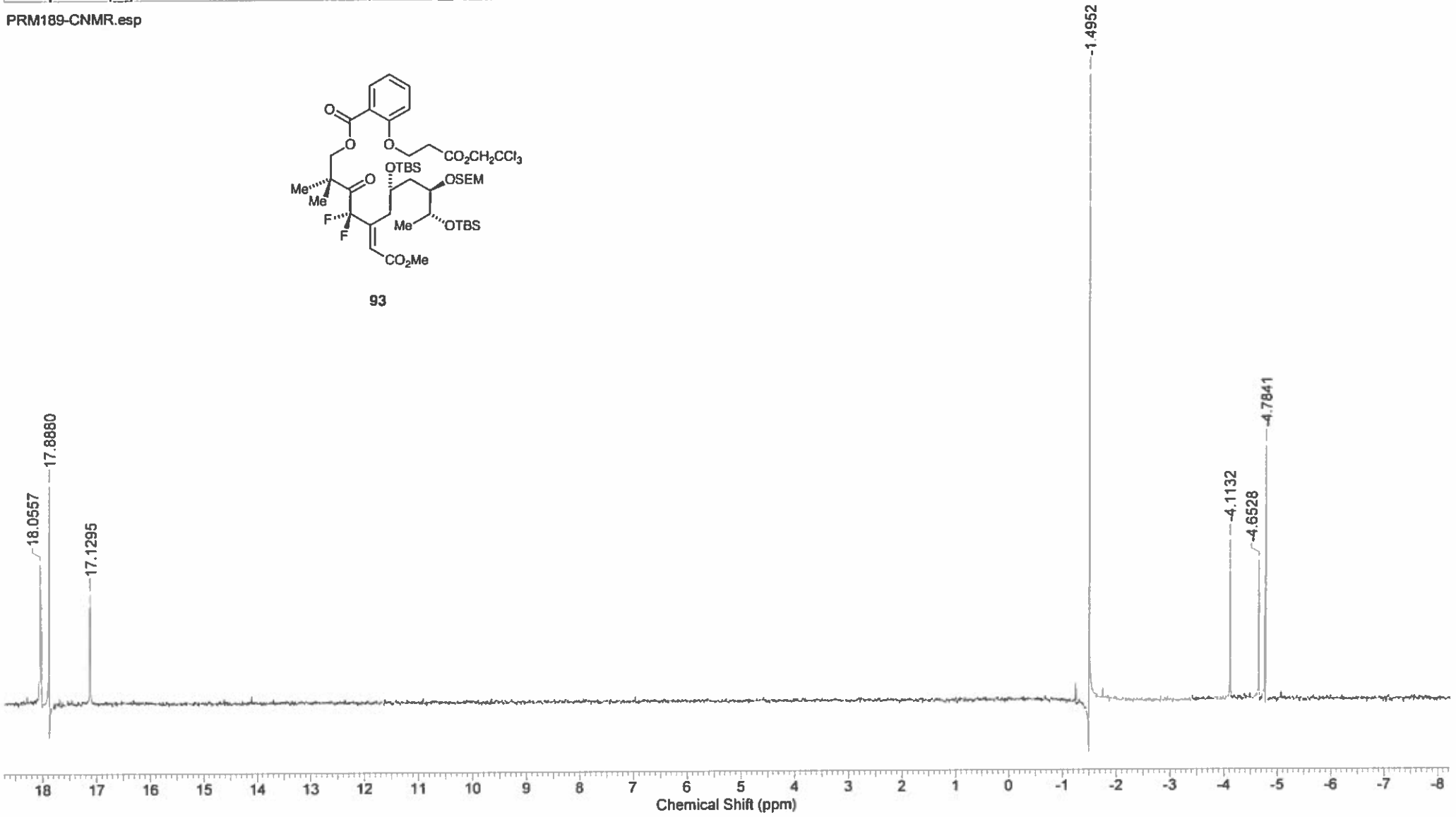
93



Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM189 prod mCARBON_A CDCl3 (e:\bruk400cdata\2015\Aug) ejt 54				
Date	20 Aug 2015 16:00:16			*Date Stamp*	20 Aug 2015 16:00:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-20-ejt-54\11\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	256	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	71.80
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8672	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.046				

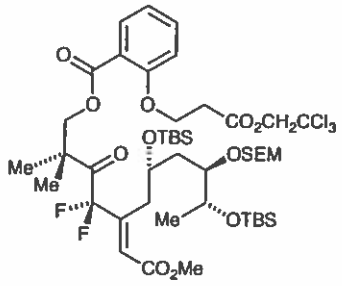
PRM189-CNMR.esp

93



Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM189 prod mCARBON_A CDCl3 (e:\bruk400cdata\2015\Aug) ejt 54				
Date	20 Aug 2015 16:00:16			*Date Stamp*	20 Aug 2015 16:00:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-20-ejt-54\11\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	256	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	71.80
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8672	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.046				

PRM189-CNMR.esp



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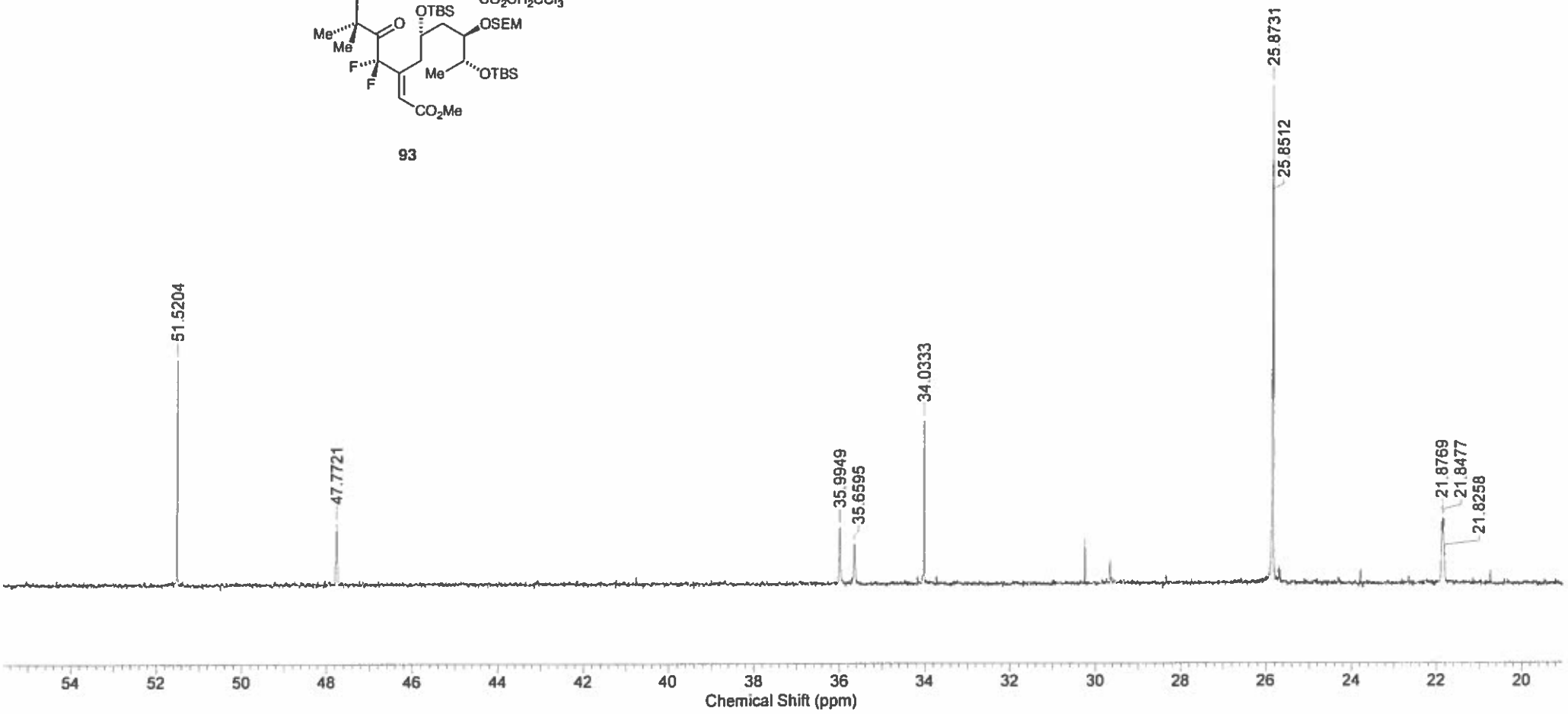
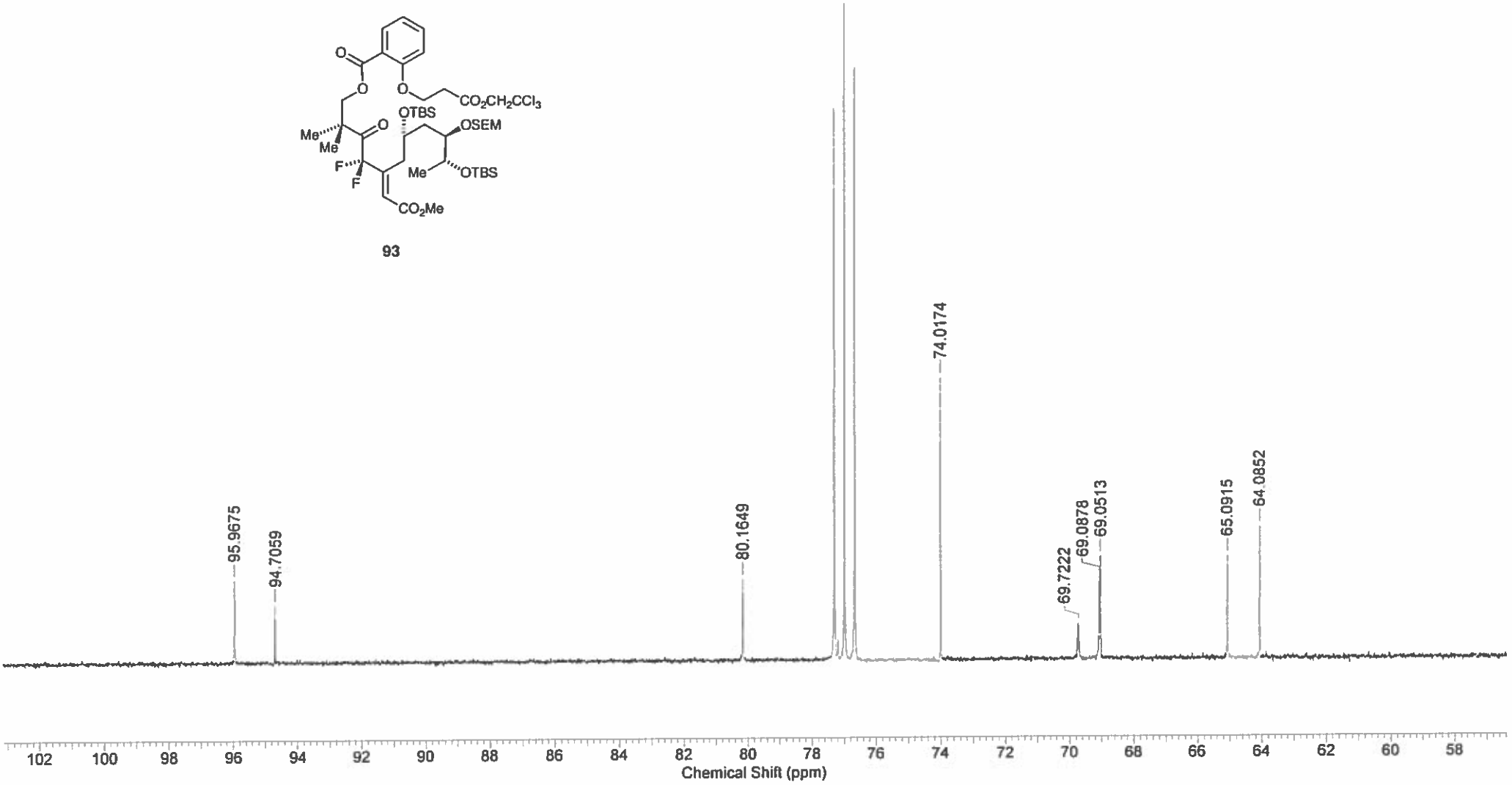


Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM189 prod mCARBON_A CDCl3 {e:\bruk400cdata\2015\Aug} ejt 54				
Date	20 Aug 2015 16:00:16			*Date Stamp*	20 Aug 2015 16:00:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-20-ejt-54\11\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	256	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	71.80
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8672	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.046				

PRM189-CNMR.esp

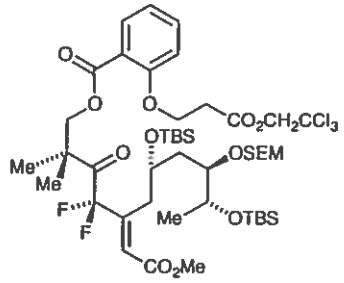
93



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM189 prod mCARBON_A CDCl3 {e:\bruk400cdata\2015\Aug} ejt 54				
Date	20 Aug 2015 16:00:16			*Date Stamp*	20 Aug 2015 16:00:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-20-ejt-54\11\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	256	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	71.80
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8672	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.046				

PRM189-CNMR.esp



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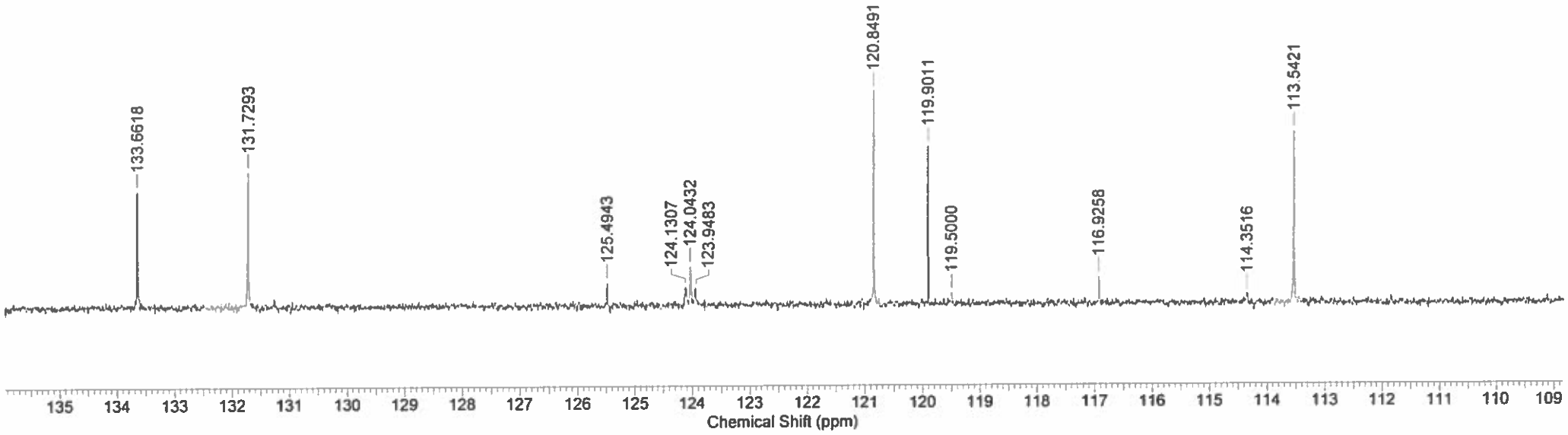
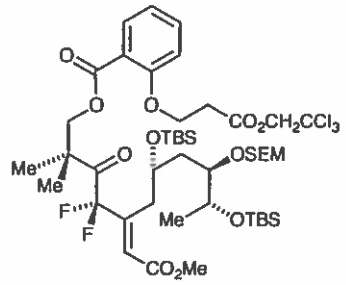


Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM189 prod mCARBON_A CDCl3 {e:\bruk400cdata\2015\Aug} ejt 54				
Date	20 Aug 2015 16:00:16			*Date Stamp*	20 Aug 2015 16:00:16		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-20-ejt-54\11\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	256	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	71.80
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8672	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.046				

PRM189-CNMR.esp



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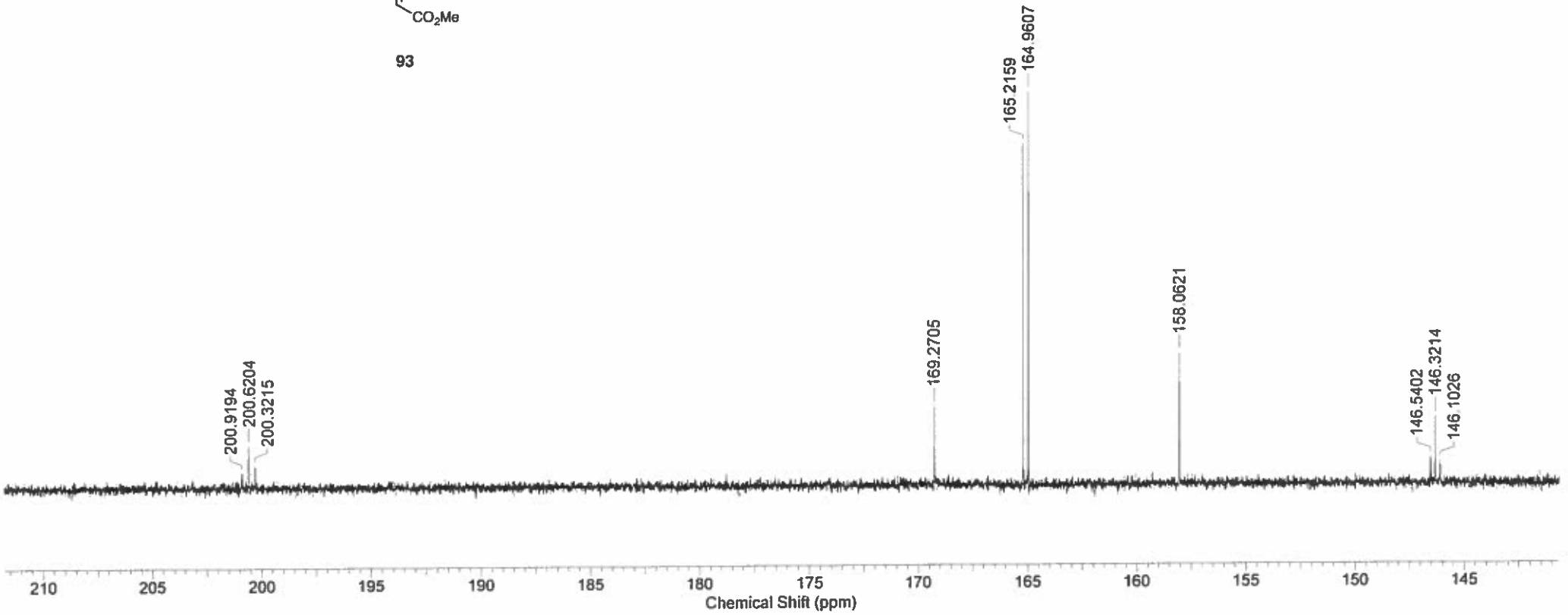
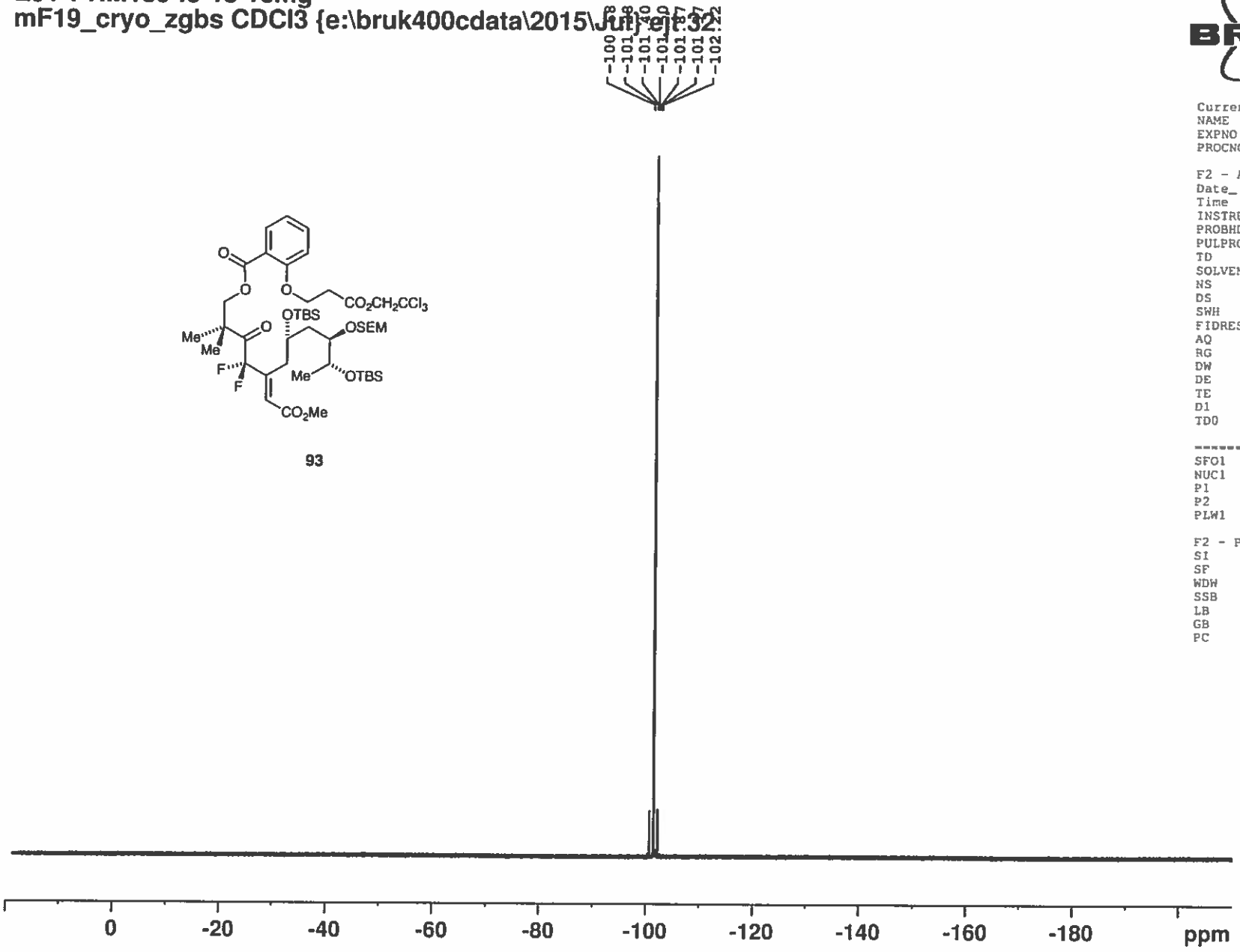


EJT-PRM189 f3-15 16mg
mF19_cryo_zgbs CDCl3 {e:\bruk400cdata\2015\Jul}-ejt-32

93

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Current Data Parameters
NAME      2015-08-05-ejt-32
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150805
Time                  12.50
INSTRUM               spect
PROBHD   5 mm CPPBBO BB
PULPROG                zgbs
TD                   131072
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               89285.711 Hz
FIDRES            0.681196 Hz
AQ                0.7340032 sec
RG                     7.12
DW                 5.600 usec
DE                 18.83 usec
TE                   291.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          376.4042649 MHz
NUC1                   19F
P1                  15.00 usec
P2                  30.00 usec
PLW1           3.79999995 W

F2 - Processing parameters
SI                    262144
SF            376.4419098 MHz
WDW                       EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   2.00
```

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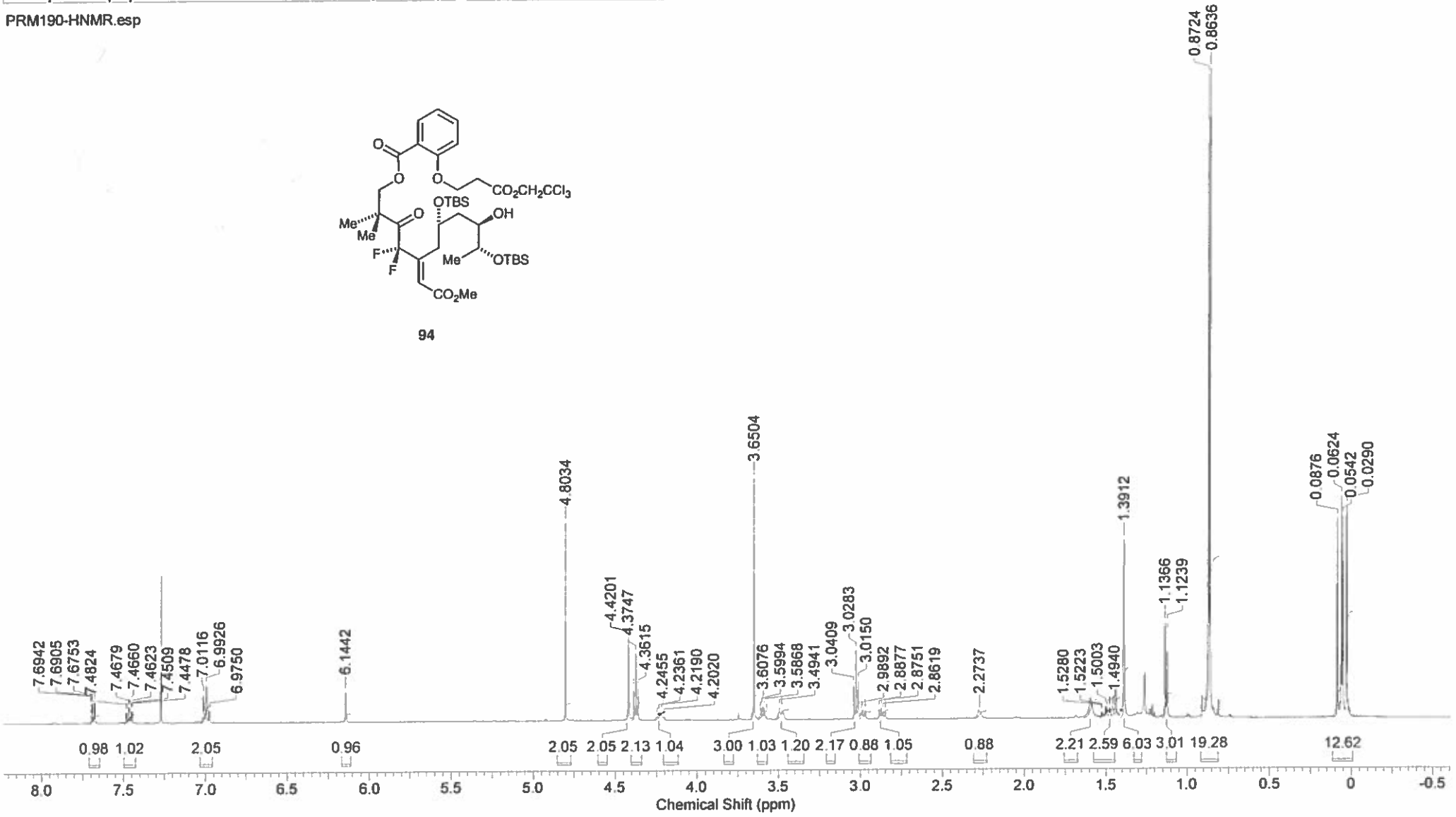
Acquisition Time (sec)	3.1719	*Comment*	EJT-PRM190 f7-19 11mg mPROTON CDCl3 {E:\bruk500adata\2015\Aug} ejt 43				
Date	13 Aug 2015 14:17:52			*Date Stamp*	13 Aug 2015 14:17:52		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2015\Aug\data\ejt\nmr\2015-08-13-ejt-43\10\PDATA\1\1r					*Frequency (MHz)*	500.13
Nucleus	1H	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	144.00
SW(cyclical) (Hz)	10330.58	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	3081.2380	*Spectrum Type*	STANDARD
Sweep Width (Hz)	10330.26	*Temperature (degree C)*	25.000				

PRM190-HNMR.esp

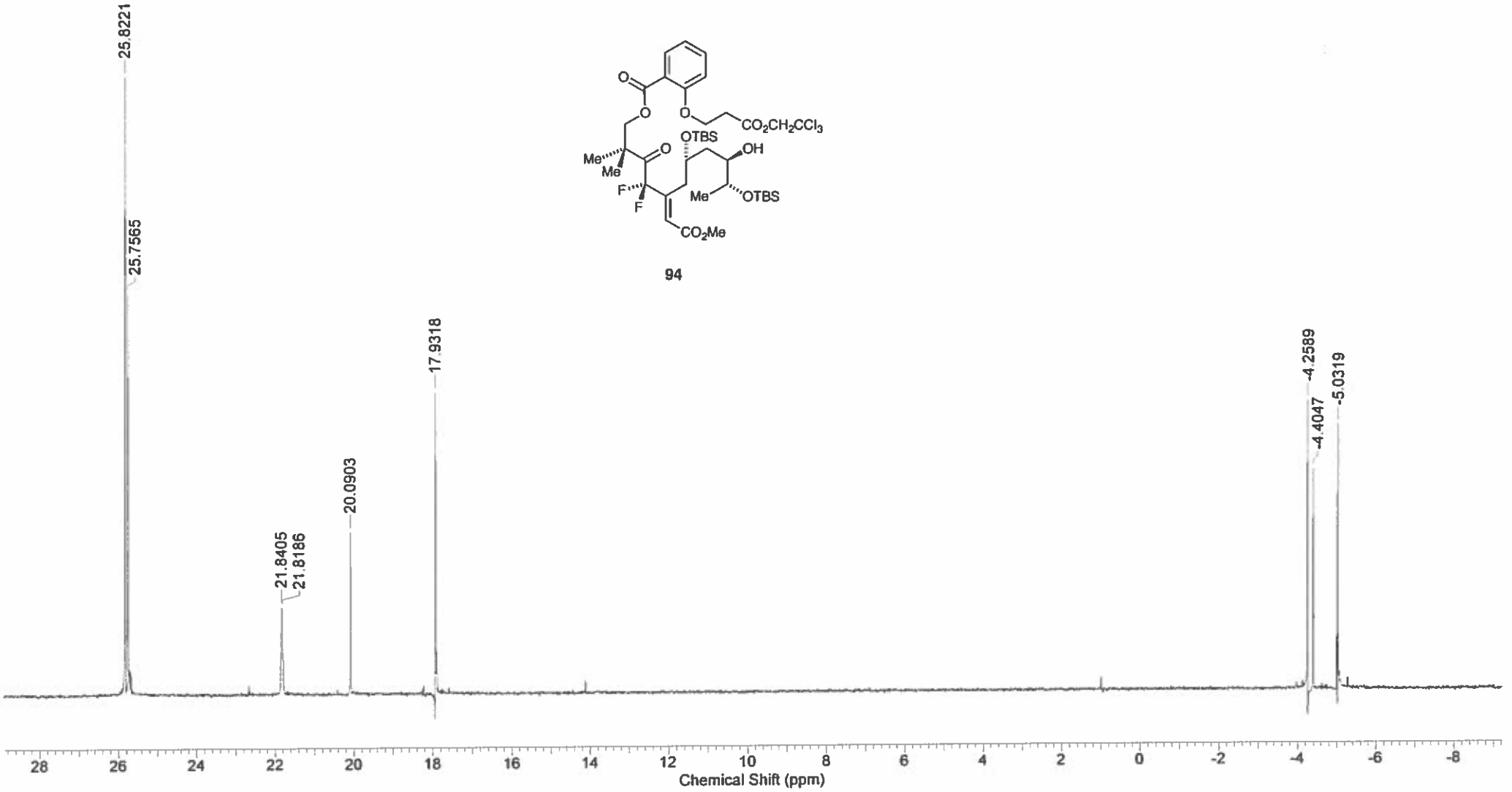
94



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 {e:\bruk400cdata\2015\Aug} ejt 6				
Date	21 Aug 2015 22:58:24			*Date Stamp*	21 Aug 2015 22:58:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-6\21\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8789	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.170				

PRM190-CNMR.esp



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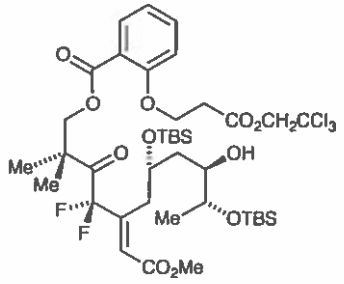
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 {e:\bruk400cdata\2015\Aug} ejt 6				
Date	21 Aug 2015 22:58:24			*Date Stamp*	21 Aug 2015 22:58:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-6\21\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8789	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.170				

PRM190-CNMR.esp



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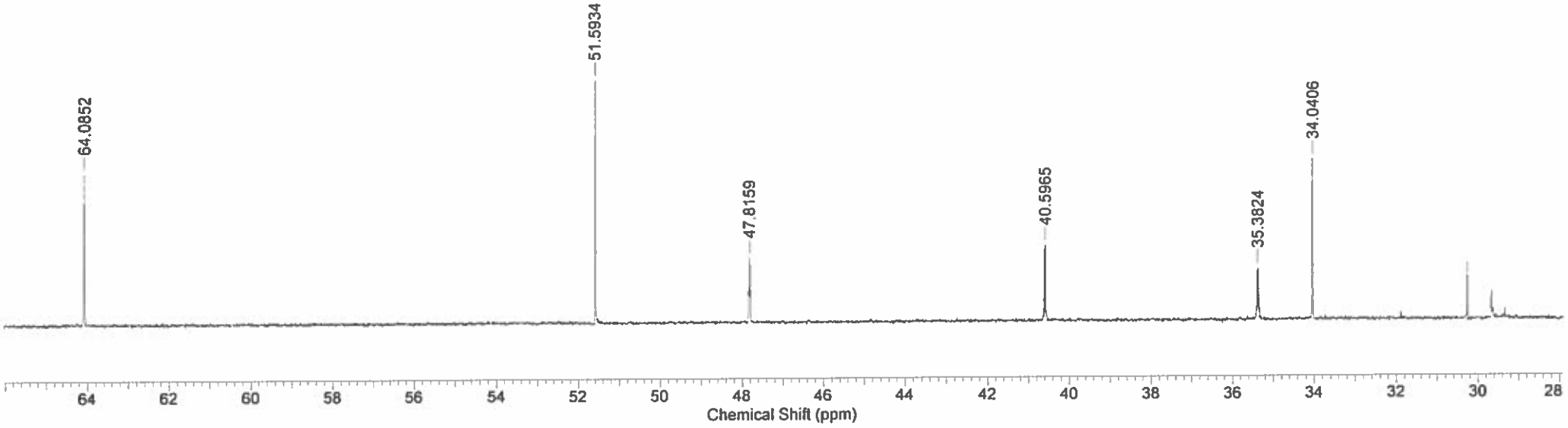
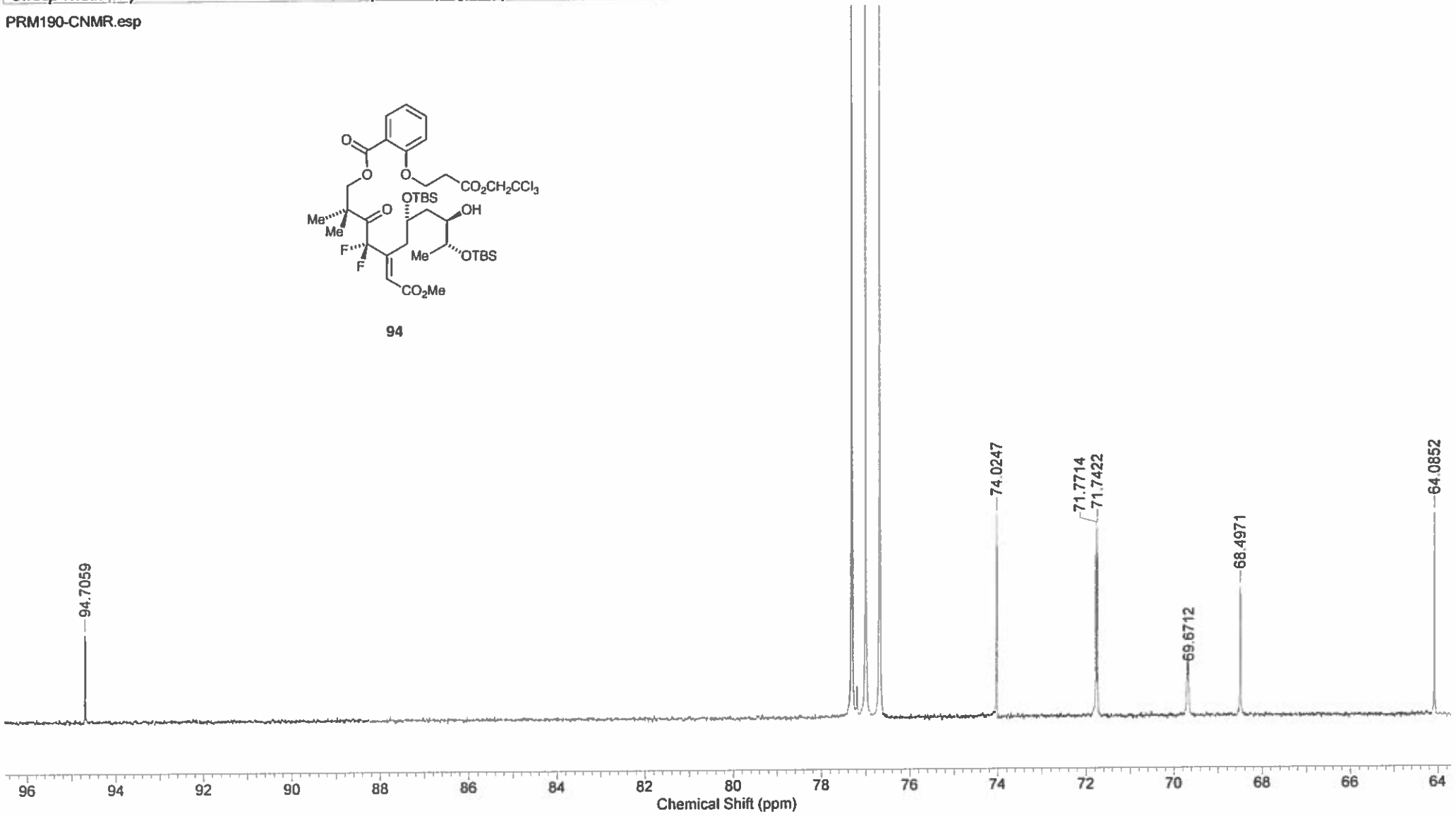


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug) ejt 6				
Date	21 Aug 2015 22:58:24			*Date Stamp*	21 Aug 2015 22:58:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-6\21\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8789	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.170				

PRM190-CNMR.esp

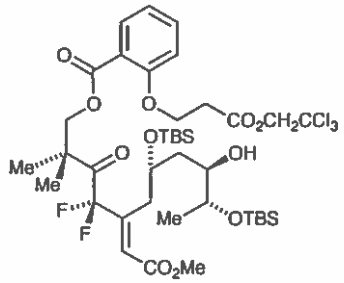
94



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug) ejt 6				
Date	21 Aug 2015 22:58:24			*Date Stamp*	21 Aug 2015 22:58:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-6\21\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8789	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.170				

PRM190-CNMR.esp



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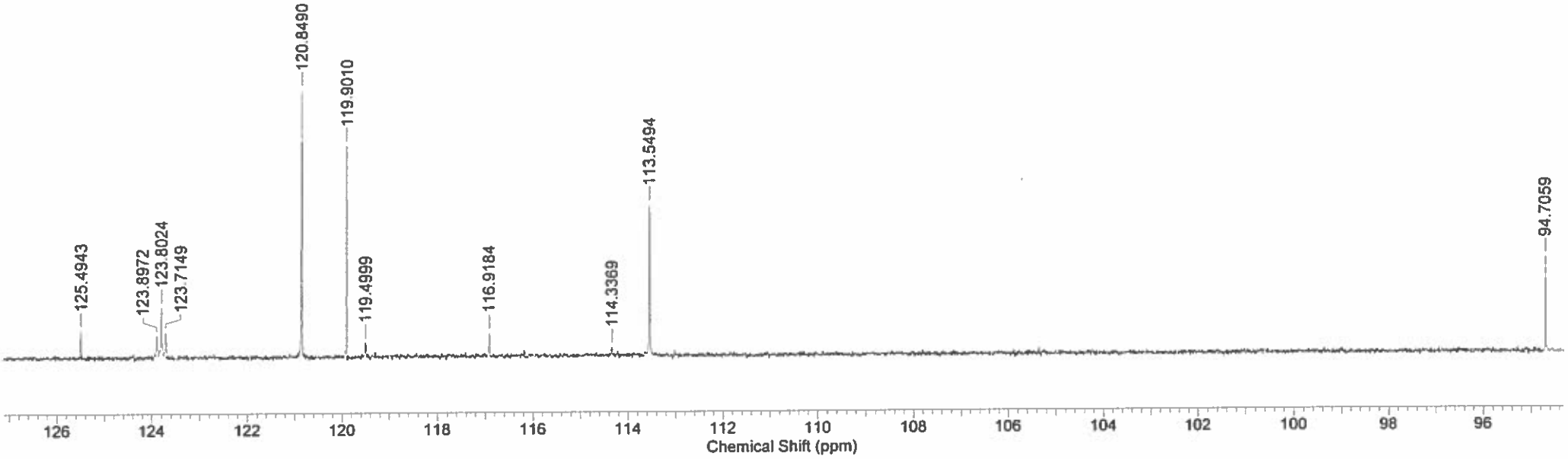
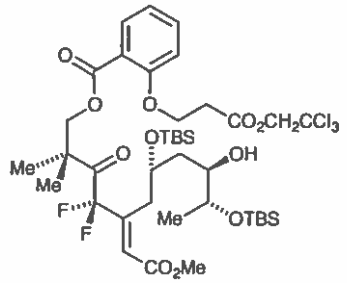


Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug) ejt 6				
Date	21 Aug 2015 22:58:24			*Date Stamp*	21 Aug 2015 22:58:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-6\21\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8789	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.170				

PRM190-CNMR.esp



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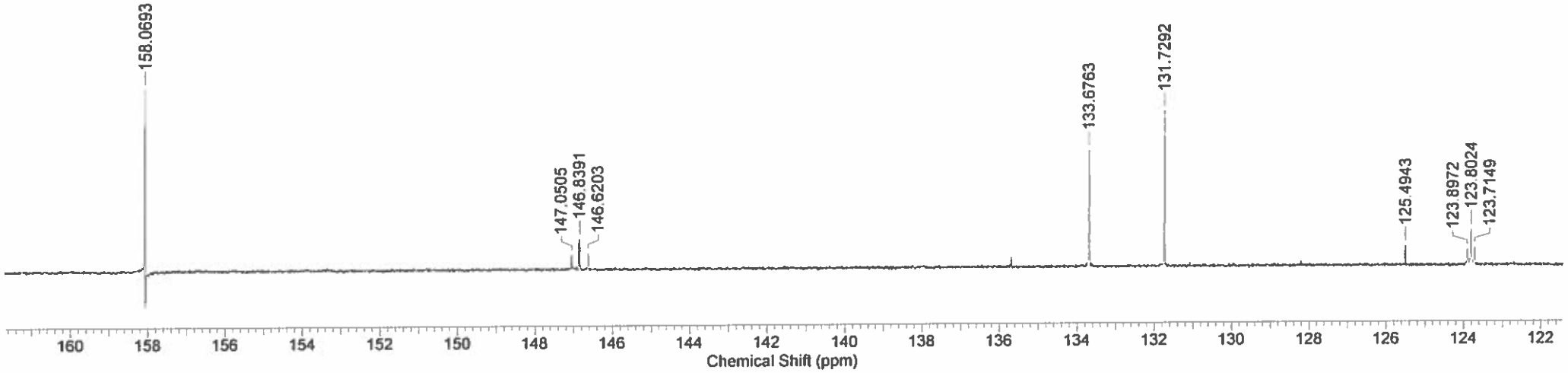
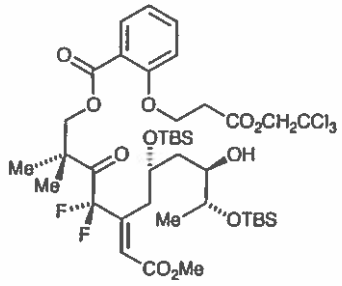


Acquisition Time (sec)	1.3631	*Comment*	EJT-PRM190 f13-46 54mg mCARBON_B CDCl3 (e:\bruk400cdata\2015\Aug) ejt 6				
Date	21 Aug 2015 22:58:24			*Date Stamp*	21 Aug 2015 22:58:24		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-6\21\fid					*Frequency (MHz)*	100.60
Nucleus	13C	*Number of Transients*	1000	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	45.20
SW(cyclical) (Hz)	24038.46	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	10049.8789	*Spectrum Type*	STANDARD
Sweep Width (Hz)	24037.73	*Temperature (degree C)*	18.170				

PRM190-CNMR.esp



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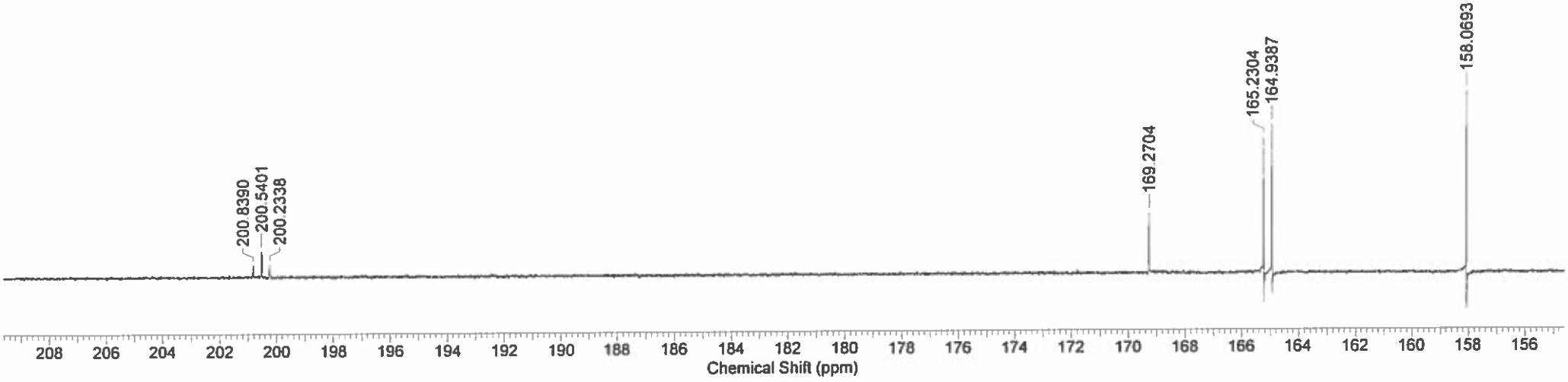
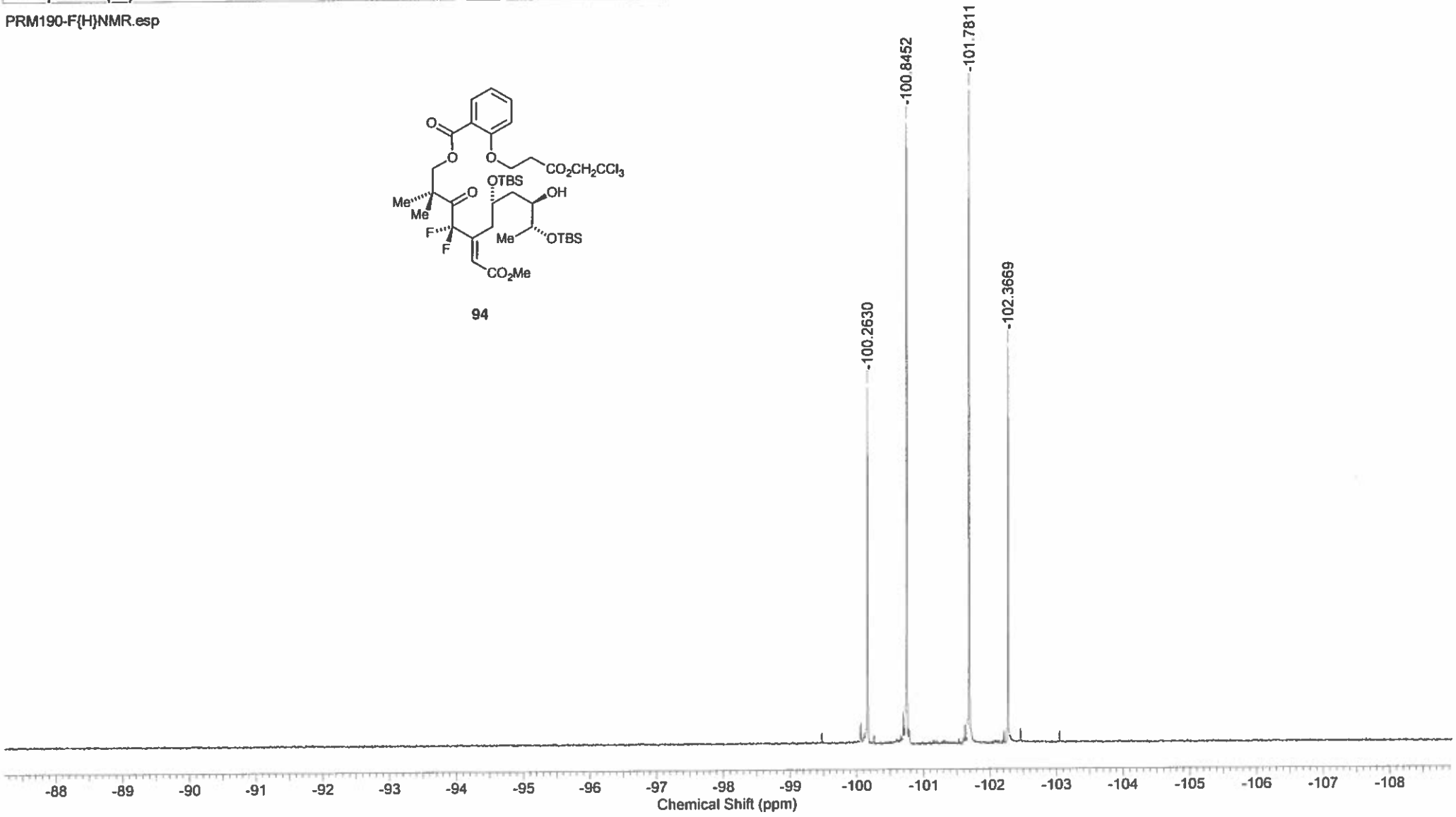


Acquisition Time (sec)	0.5767	*Comment*	EJT-PRM190 f7-19 11mg m19FCPD CDCl3 (E:\bruk500adata\2015\Aug) ejt 43				
Date	13 Aug 2015 14:32:48			*Date Stamp*	13 Aug 2015 14:32:48		
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk500adata\2015\Aug\data\ejt\nmr\2015-08-13-ejt-43\13\fid					*Frequency (MHz)*	470.59
Nucleus	19F	*Number of Transients*	16	*Origin*	spect	*Original Points Count*	65536
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zgfhigqn	*Receiver Gain*	575.00
SW(cyclical) (Hz)	113636.37	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	-47059.0234	*Spectrum Type*	STANDARD
Sweep Width (Hz)	113634.63	*Temperature (degree C)*	25.000				

PRM190-F{H}NMR.esp

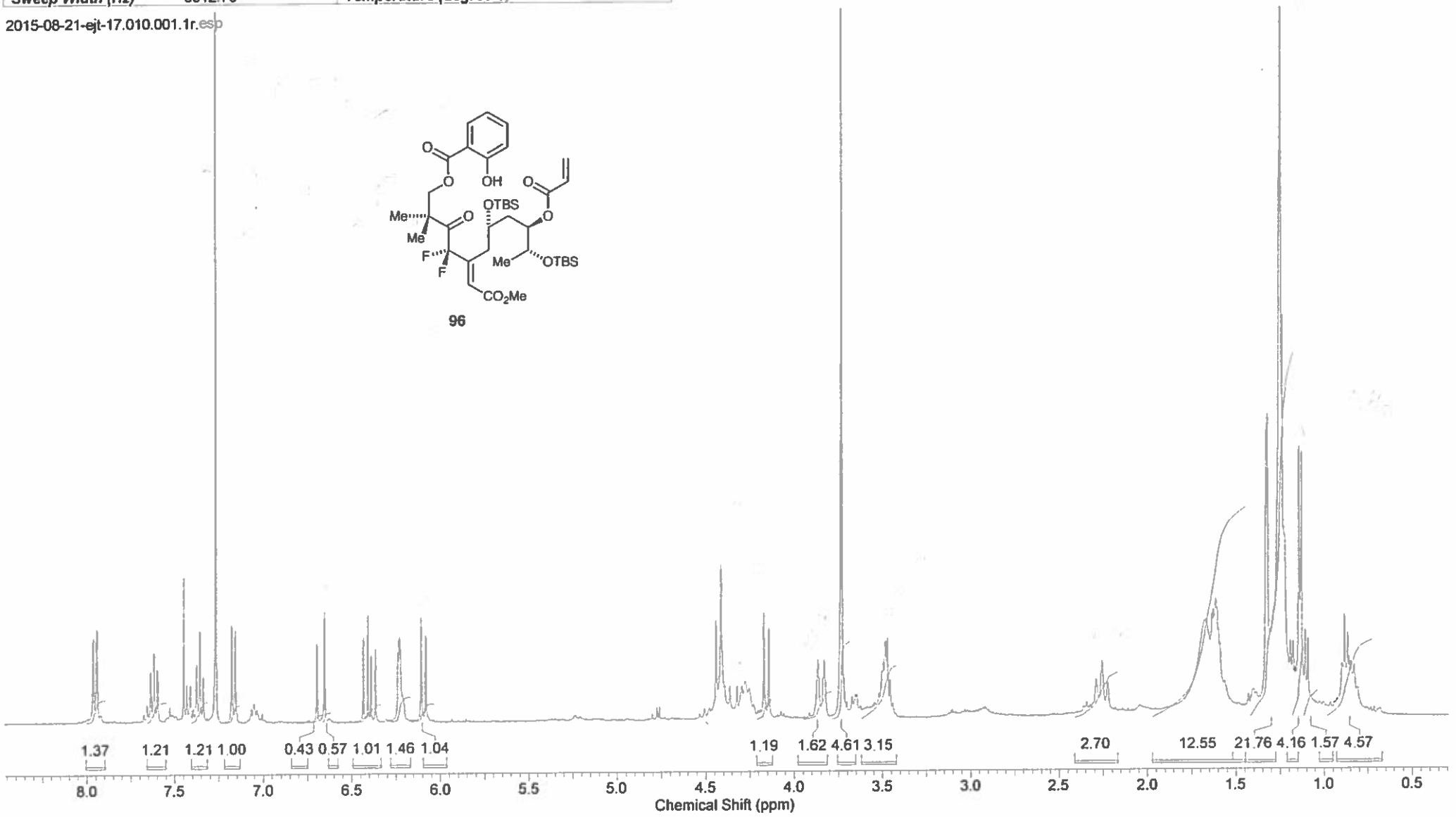
94



Acquisition Time (sec)	4.0894	*Comment*	EJT-PRM193 f11-18 5mg chloroform mPROTON_A CDCl3 {e:\bruk400cdata\2015\Aug} ejt 17				
Date	21 Aug 2015 15:56:00	*Date Stamp*	21 Aug 2015 15:56:00				
File Name	\\ss7a.ds.man.ac.uk\vol5\vol3\users\snmrdata\bruk400cdata\2015\Aug\data\ejt\nmr\2015-08-21-ejt-17\10\PDATA\1\1r					*Frequency (MHz)*	400.07
Nucleus	1H	*Number of Transients*	4	*Origin*	spect	*Original Points Count*	32768
Owner	nmrsu	*Points Count*	65536	*Pulse Sequence*	zg30	*Receiver Gain*	203.00
SW(cyclical) (Hz)	8012.82	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	1894.6188	*Spectrum Type*	STANDARD
Sweep Width (Hz)	8012.70	*Temperature (degree C)*	18.371				

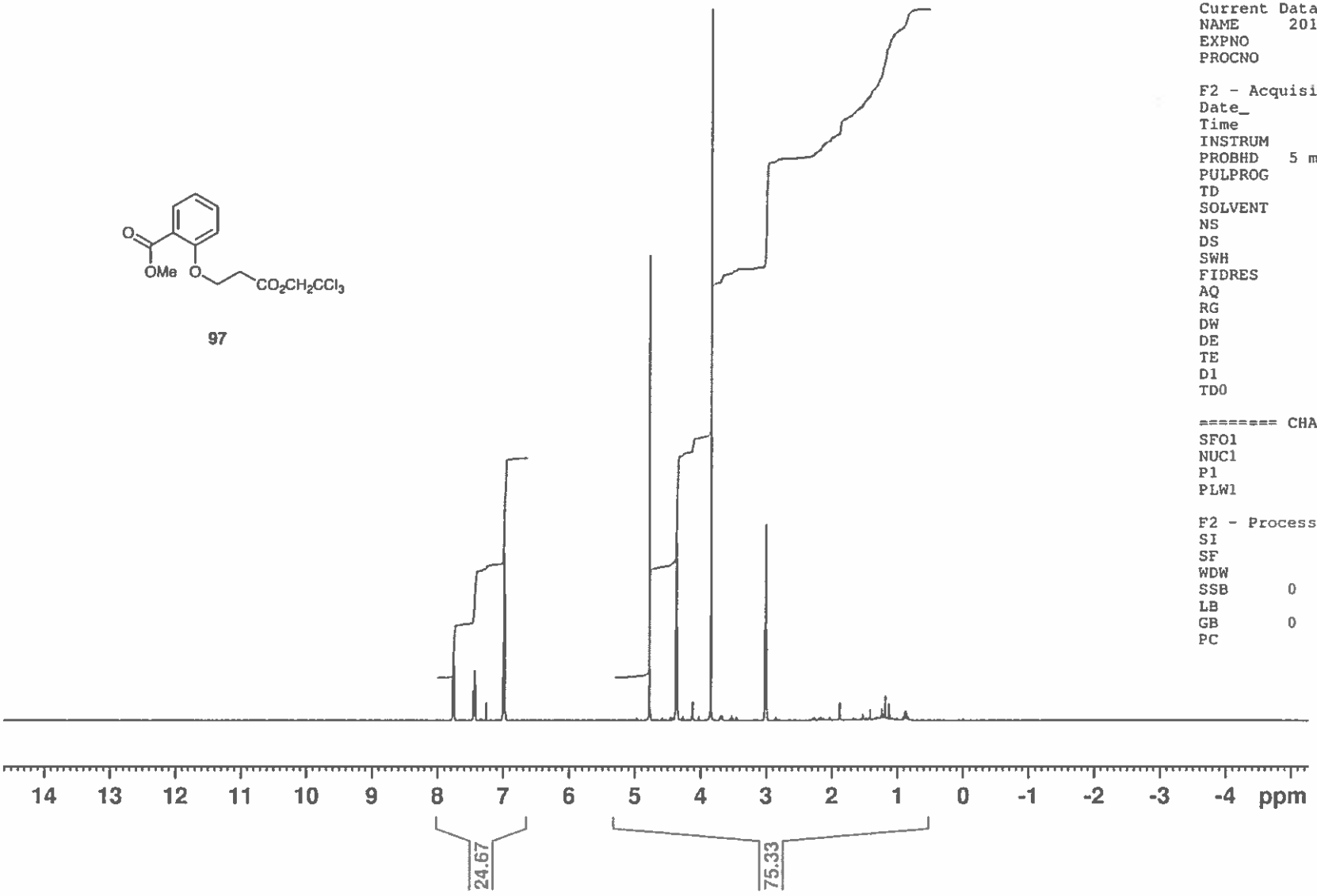
2015-08-21-ejt-17.010.001.1r.esp

96



EJT-PRM186 f19-32 155mg
mPROTON_A CDCl3 {e:\bruk400cdata\2015\Jul} ejt 44

97

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Current Data Parameters
NAME      2015-07-29-ejt-44
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150729
Time                 10.57
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     32
DW                  62.400 usec
DE                  10.00 usec
TE                  290.5 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1           400.0719003 MHz
NUC1                    1H
P1                   12.00 usec
PLW1            7.40000010 W

F2 - Processing parameters
SI                    65536
SF             400.0700087 MHz
WDW                      EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```
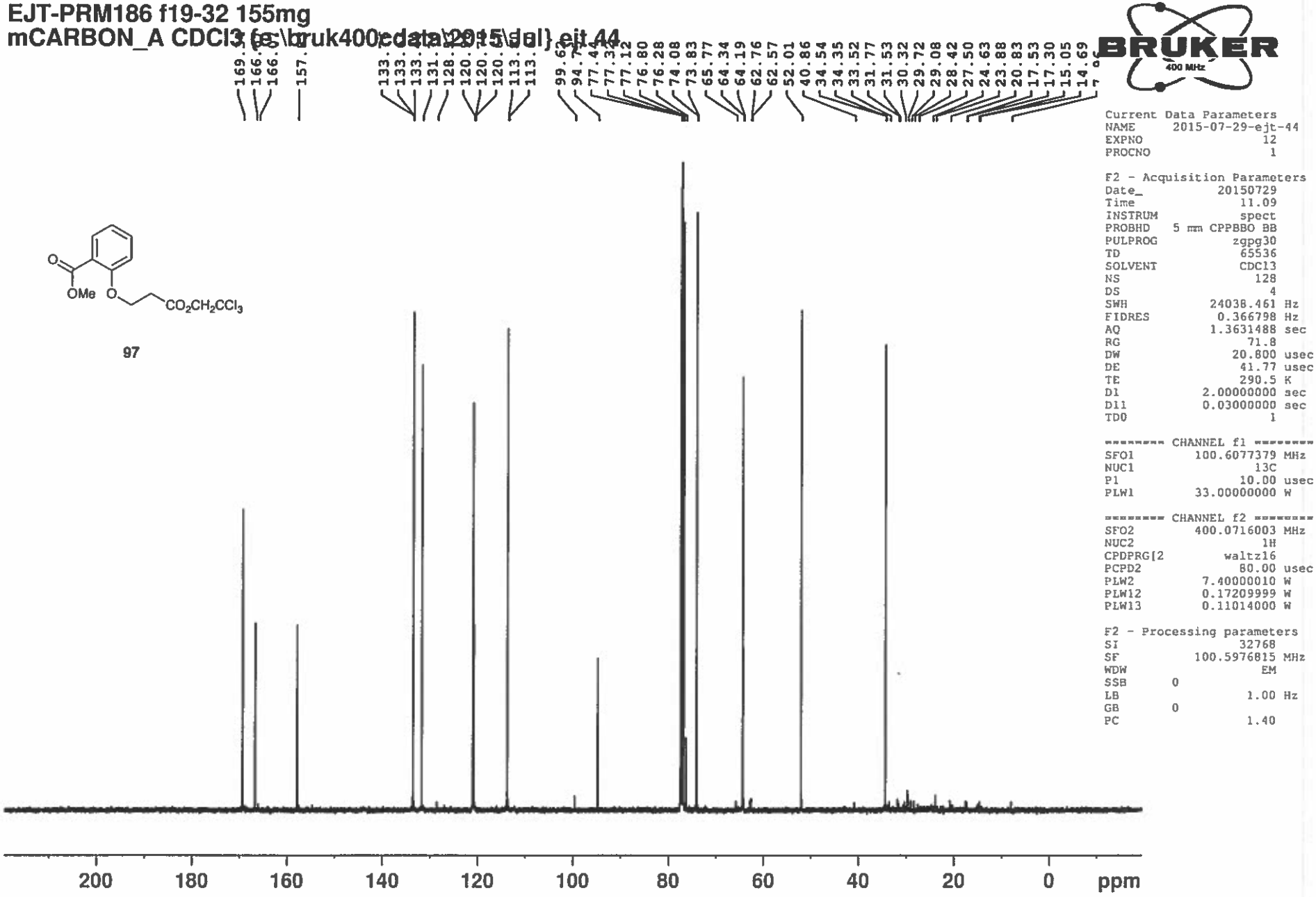

EJT-PRM186 f19-32 155mg
mCARBON_A CDCl3 (c:\bruk400\data\2015\dal) ejt 44



BRUKER 400 MHz

Current Data Parameters
NAME 2015-07-29-ejt-44
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150729
Time 11.09
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 71.8
DW 20.800 usec
DE 41.77 usec
TE 290.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

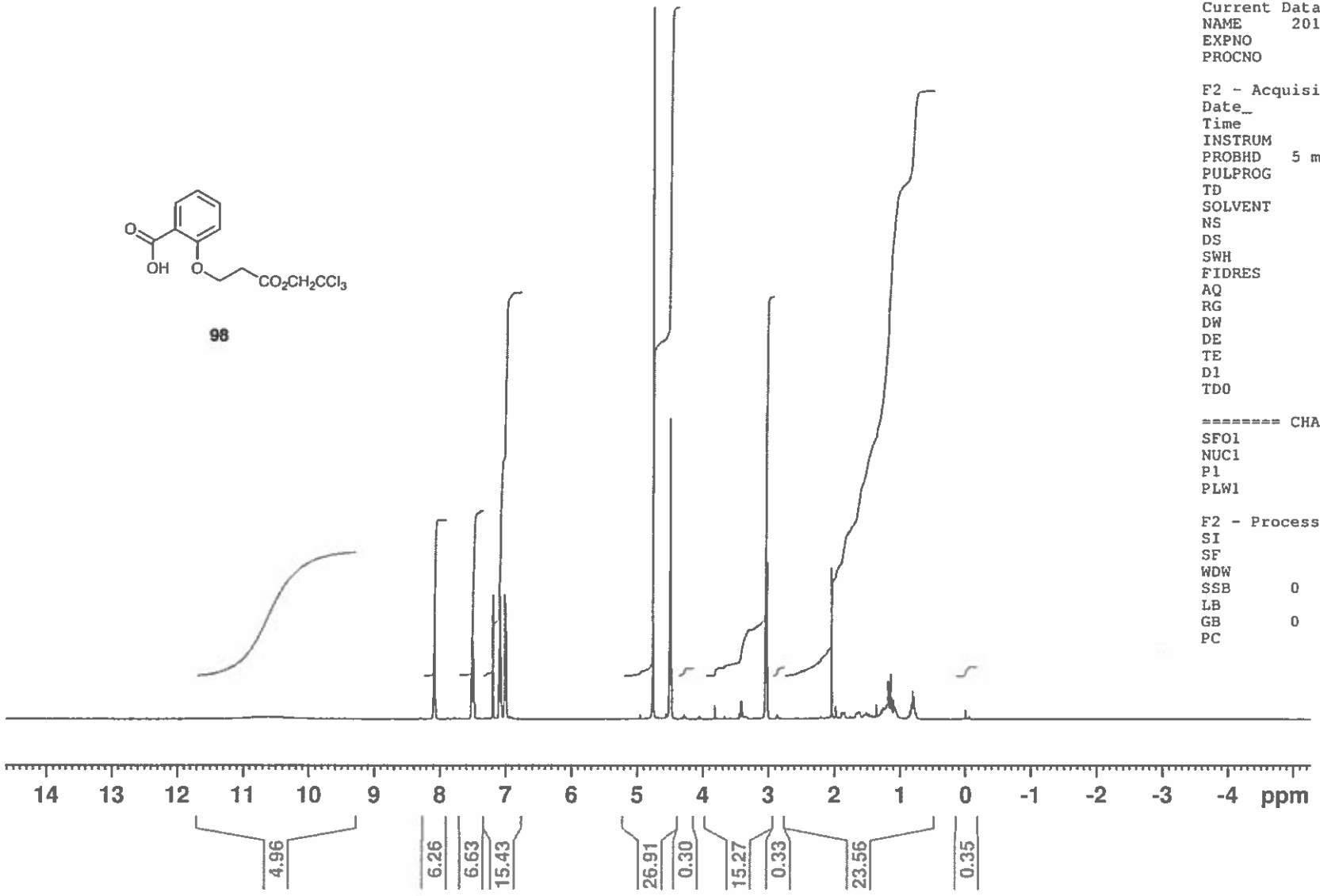
======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

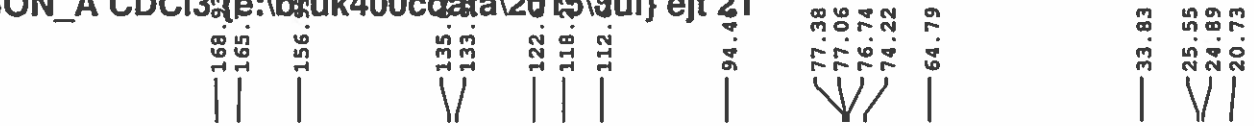
EJT-PRM187 f22-29 14mg
mPROTON_A CDCl3 {e:\bruk400cdata\2015\Jul} ejt 21

98

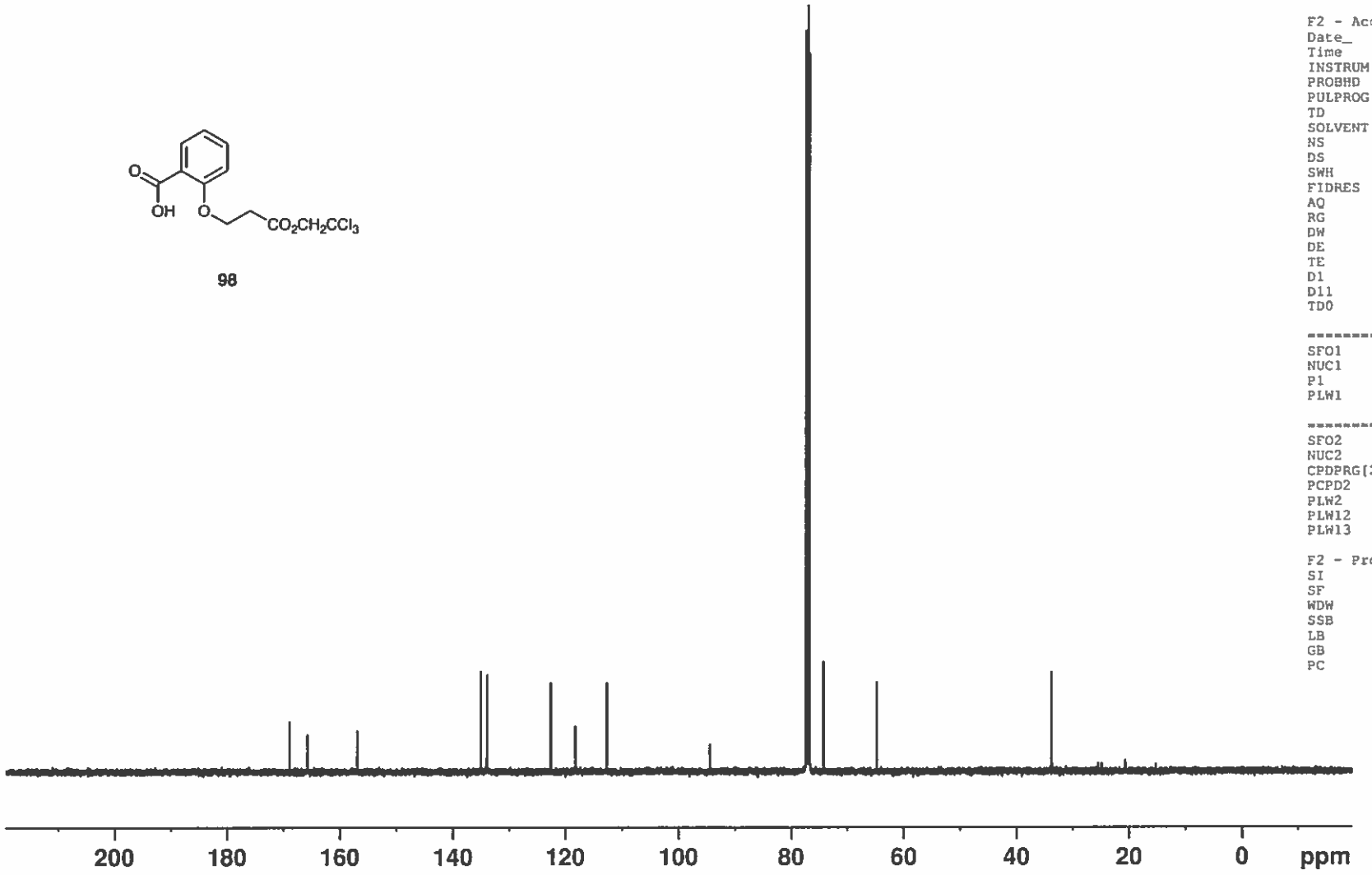



```
Current Data Parameters
NAME      2015-07-31-ejt-21
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150731
Time                 11.22
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     203
DW                  62.400 usec
DE                  10.00 usec
TE                  290.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.0719003 MHz
NUC1                   1H
P1                  12.00 usec
PLW1            7.40000010 W

F2 - Processing parameters
SI                   65536
SF             400.0700350 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

EJT-PRM187 f22-29 14mg
mCARBON_A CDCl3 {e:\bruk400cdata\2015\jul} ejt 21



98



BRUKER 400 MHz

Current Data Parameters
NAME 2015-07-31-ejt-21
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150731
Time 11.27
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 71.8
DW 20.800 usec
DE 41.77 usec
TE 290.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6077379 MHz
NUC1 13C
P1 10.00 usec
PLW1 33.00000000 W

======== CHANNEL f2 ========
SFO2 400.0716003 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 7.40000010 W
PLW12 0.17209999 W
PLW13 0.11014000 W

F2 - Processing parameters
SI 32768
SF 100.5976815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40