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Approaches to the total synthesis of chaetochalasin A

Eric J. Thomas*[a] and Mark Willis[a]

Supplementary data – ^{1}H and ^{13}C NMR spectra of key compounds.

Acquisition Time (sec)	3.9649	***Comment***	MWB092pp mPROTON CDCl3 {e:\bruk400data\2009\Aug} ejt 48			***Date***	03 Aug 2009 13:20:00
Date Stamp	03 Aug 2009 13:20:00			***File Name***	I:\Chemistry\NMR\Year 1\Data\Compound21\MWB092pp\MWB092pp_000000fid		
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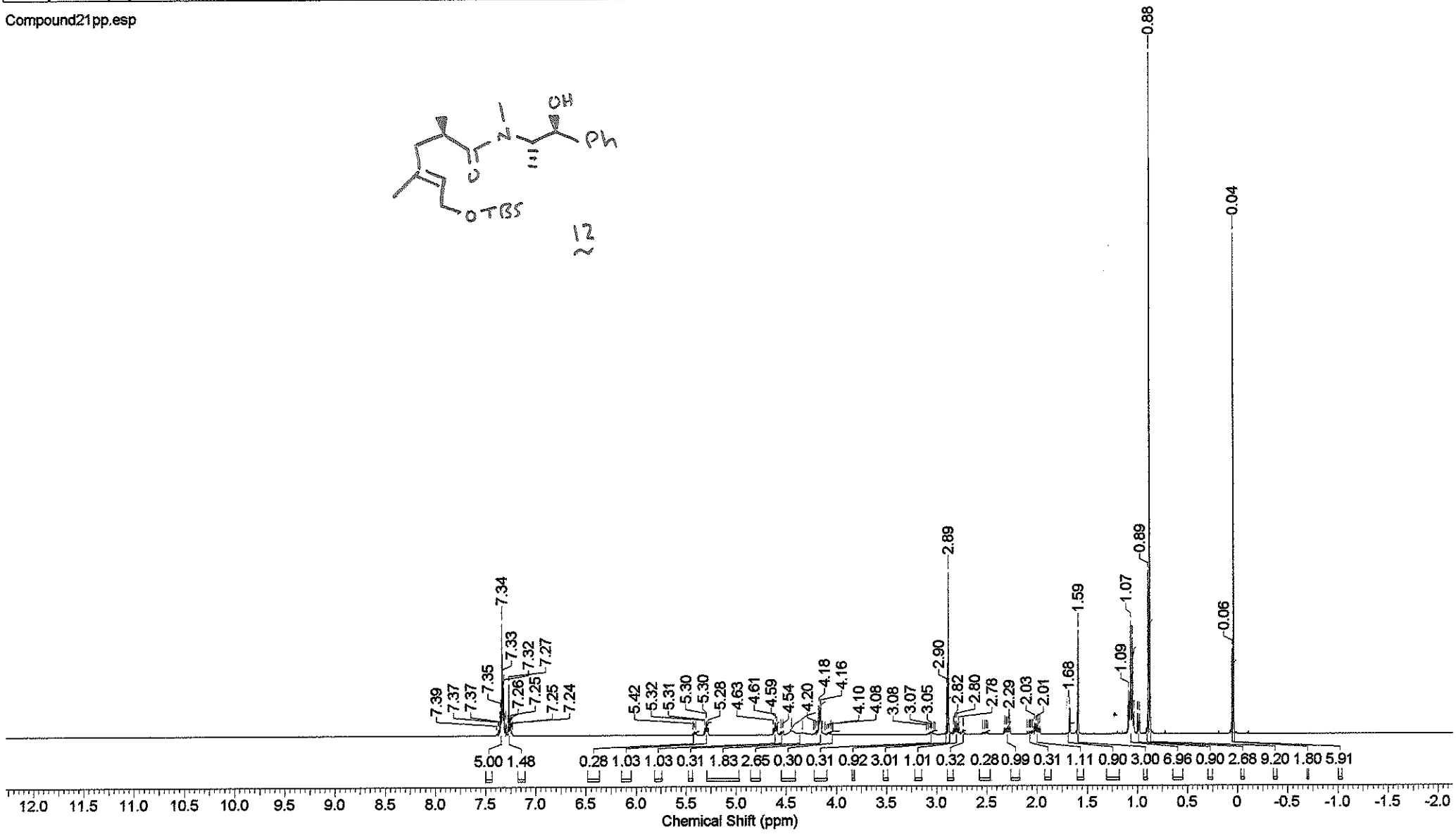
Receiver Gain	64.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.1973
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.200				

Compound21pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWB092pc mCARBON CDCl3 {e:\bruk400data\2009\Aug} ejt 49			***Date***	03 Aug 2009 13:45:36
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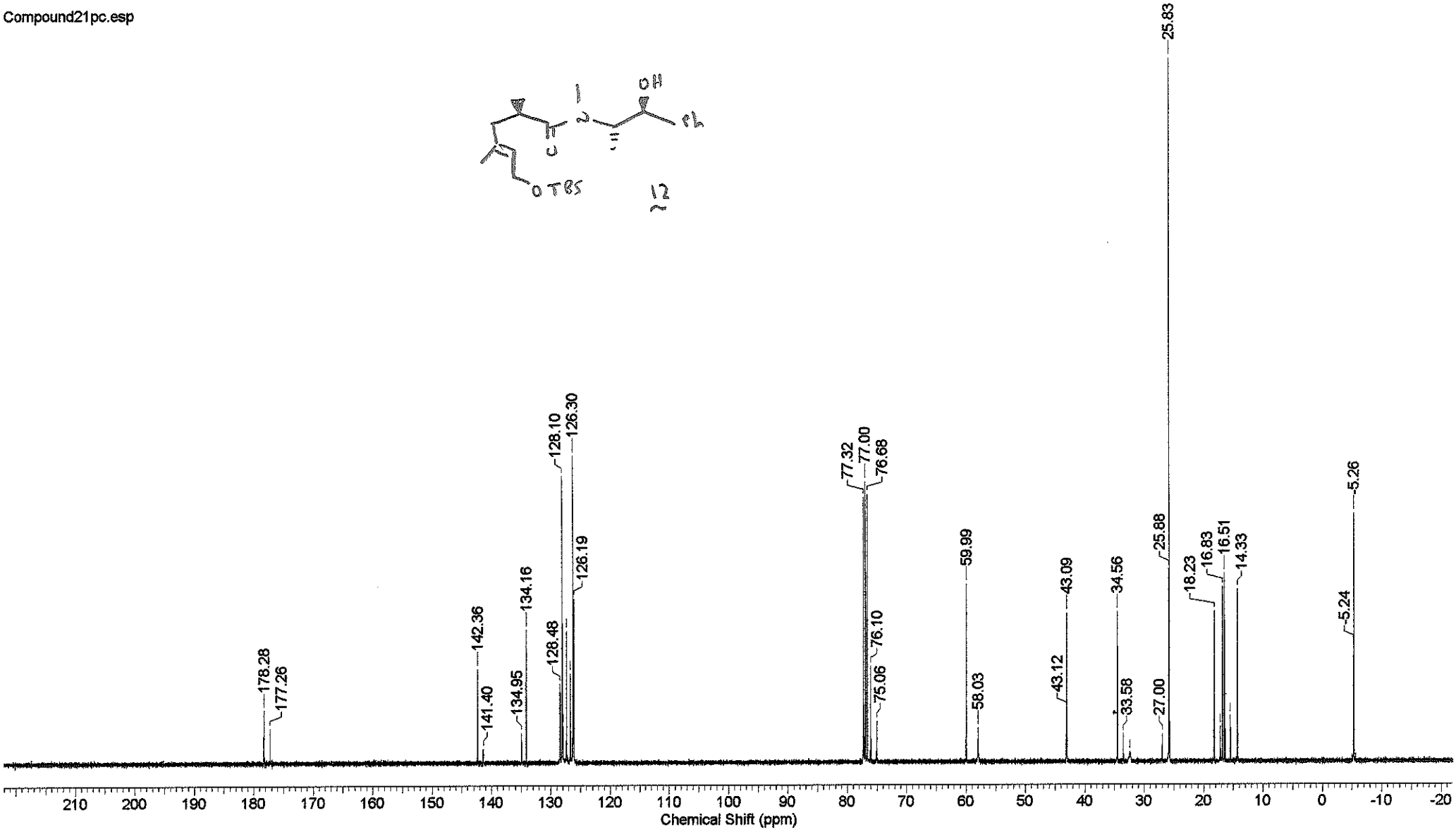
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11320.2314
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.900				

Compound21pc.esp

12



05/05/2012 15:06:13

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Date Stamp	15 Apr 2009 07:21:36			***File Name***	C:\Users\Mark\Documents\Chemistry\NMR\Data\MWB036pp\MWB036pp_000000fid		
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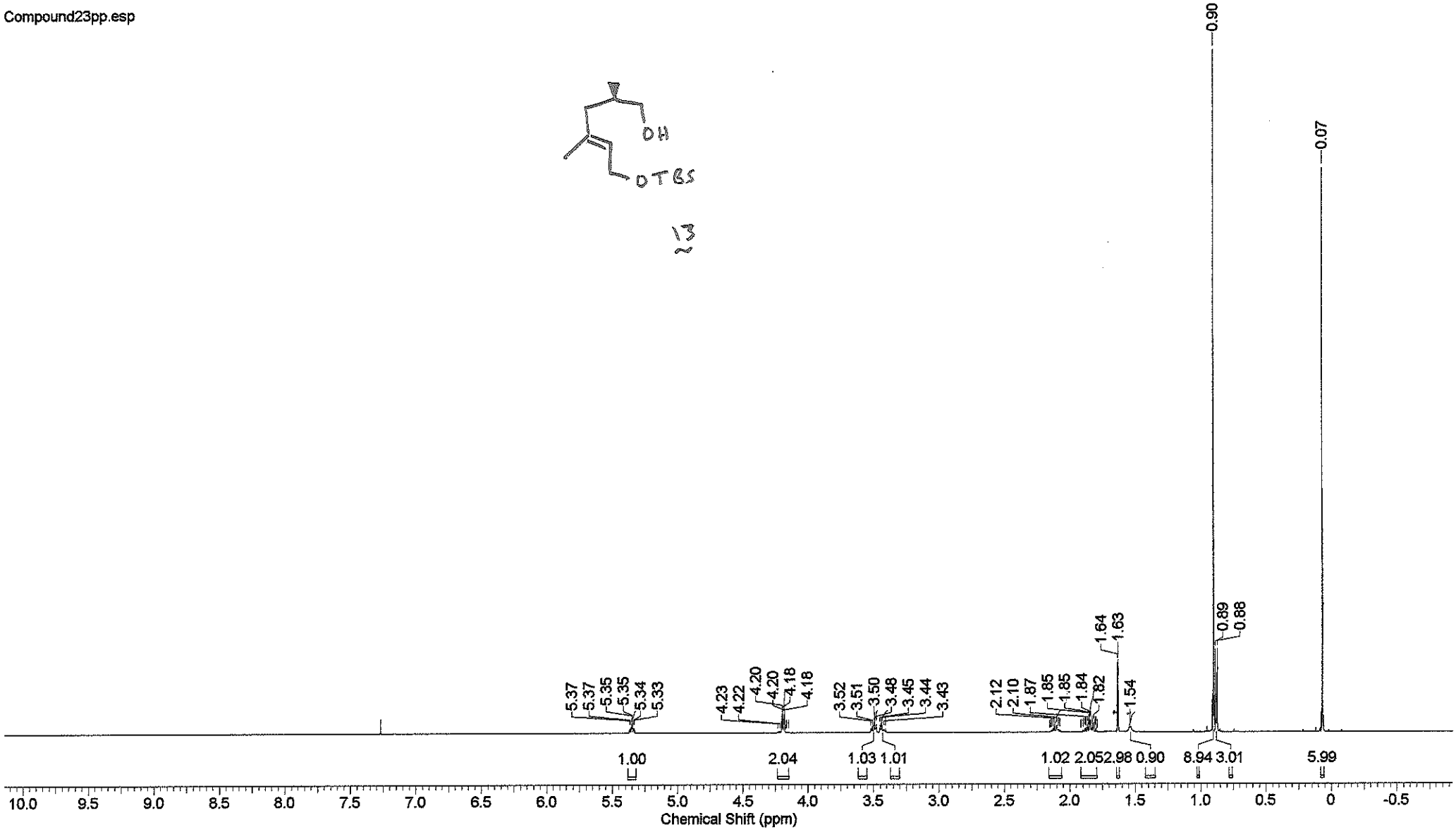
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	101.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2464.9451
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	22.000				

Compound23pp.esp



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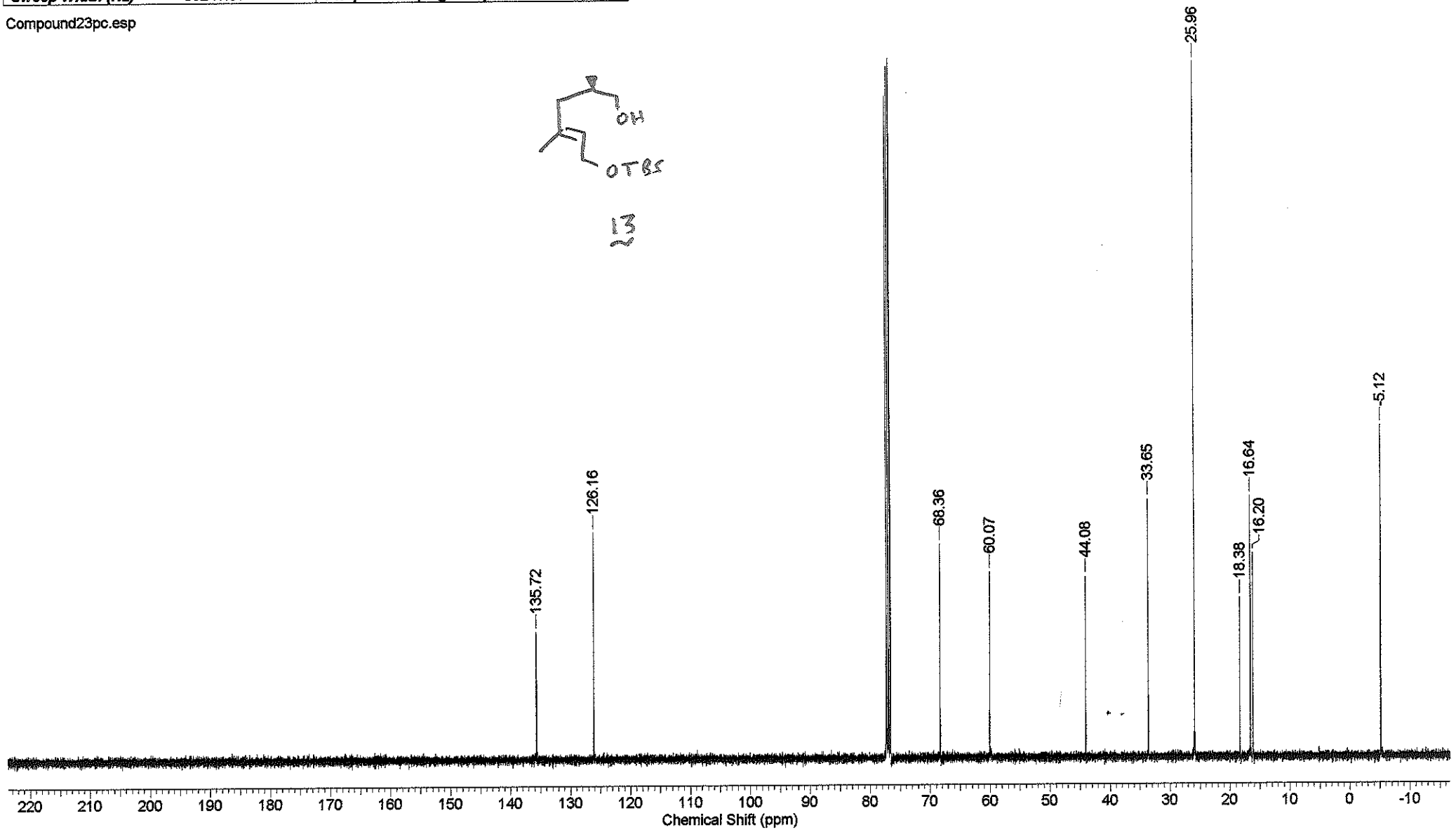
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2295
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	22.400				

Compound23pc.esp

13



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Date Stamp	17 Apr 2009 07:28:00			***File Name***	C:\Users\Mark\Documents\Chemistry\NMR\Data\MWB041pp\MWB041pp_000000fid		
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	161.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2464.9451
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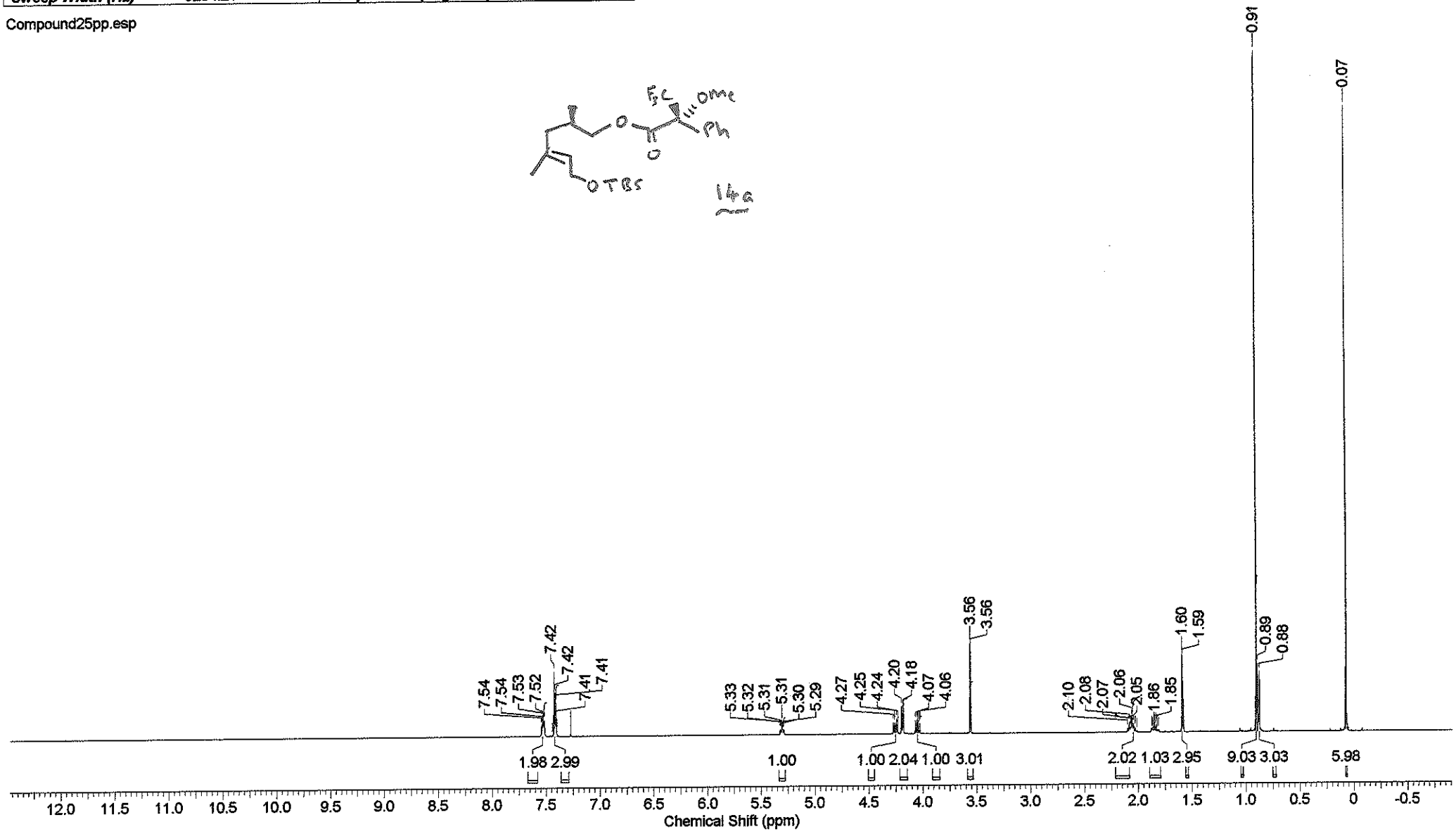
Compound25pp.esp

14a



06/05/2012 11:38:54

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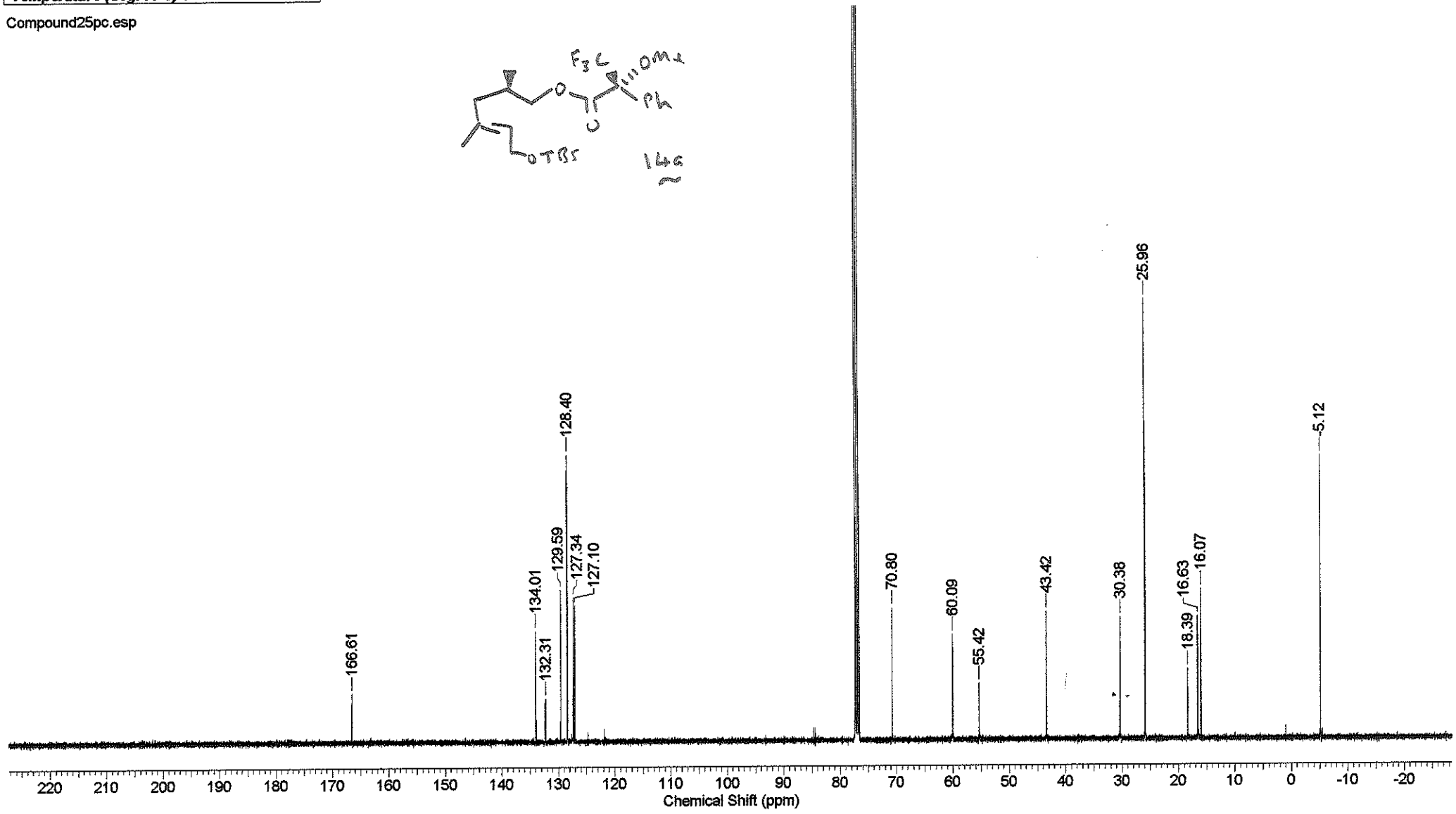
Nucleus	13C	***Number of Transients***	1024	***Origin***	AV400	***Original Points Count***	32768
Owner	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	512.00
SW(cyclical) (Hz)	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11333.1611	***Sweep Width (Hz)***	30241.01
Temperature (degree C)	21.800						

Compound25pc.esp



05/05/2012 16:30:35

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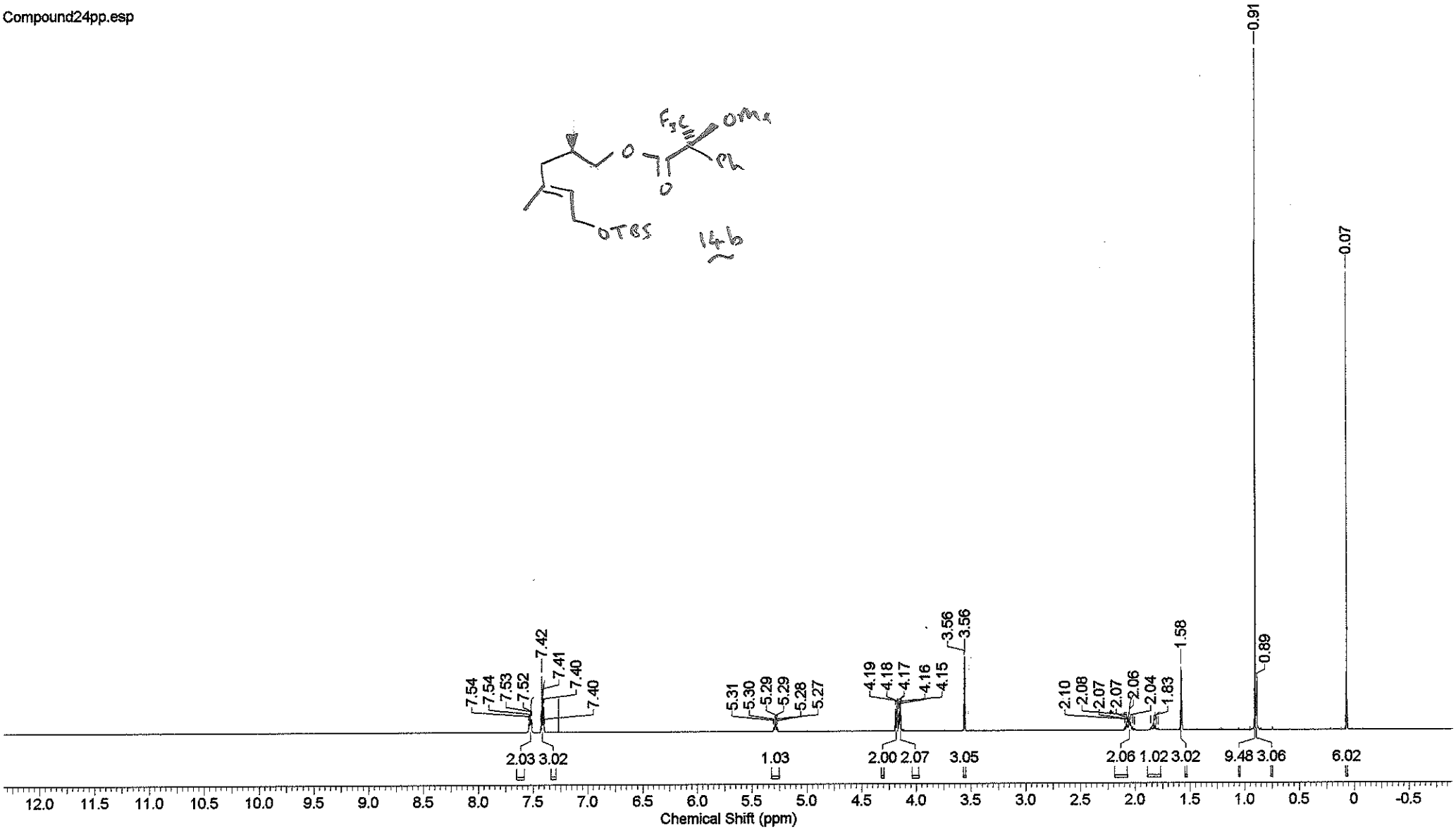
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	203.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2464.9451
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.900				

Compound24pp.esp



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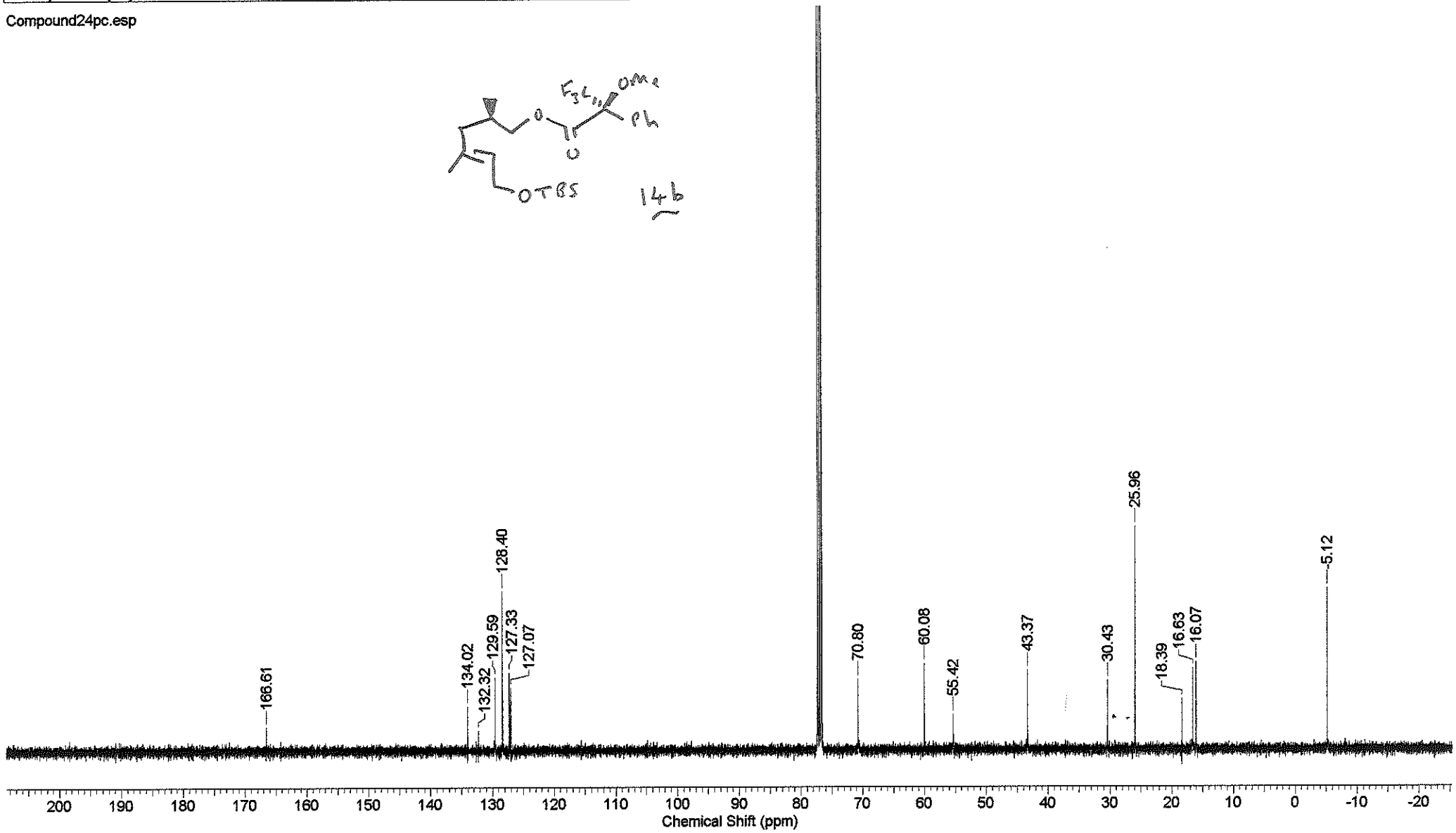
Date Stamp	16 Apr 2009 13:41:20			***File Name***	C:\Users\Mark\Documents\Chemistry\NMR\Data\MWB040pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11333.1523
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.500				

Compound24pc.esp



Acquisition Time (sec)	3.9649	***Comment***	MWB048pp mPROTON CDCl3 {e:\bruk400data\2009\Apr} ejt 21			***Date***	27 Apr 2009 08:08:32
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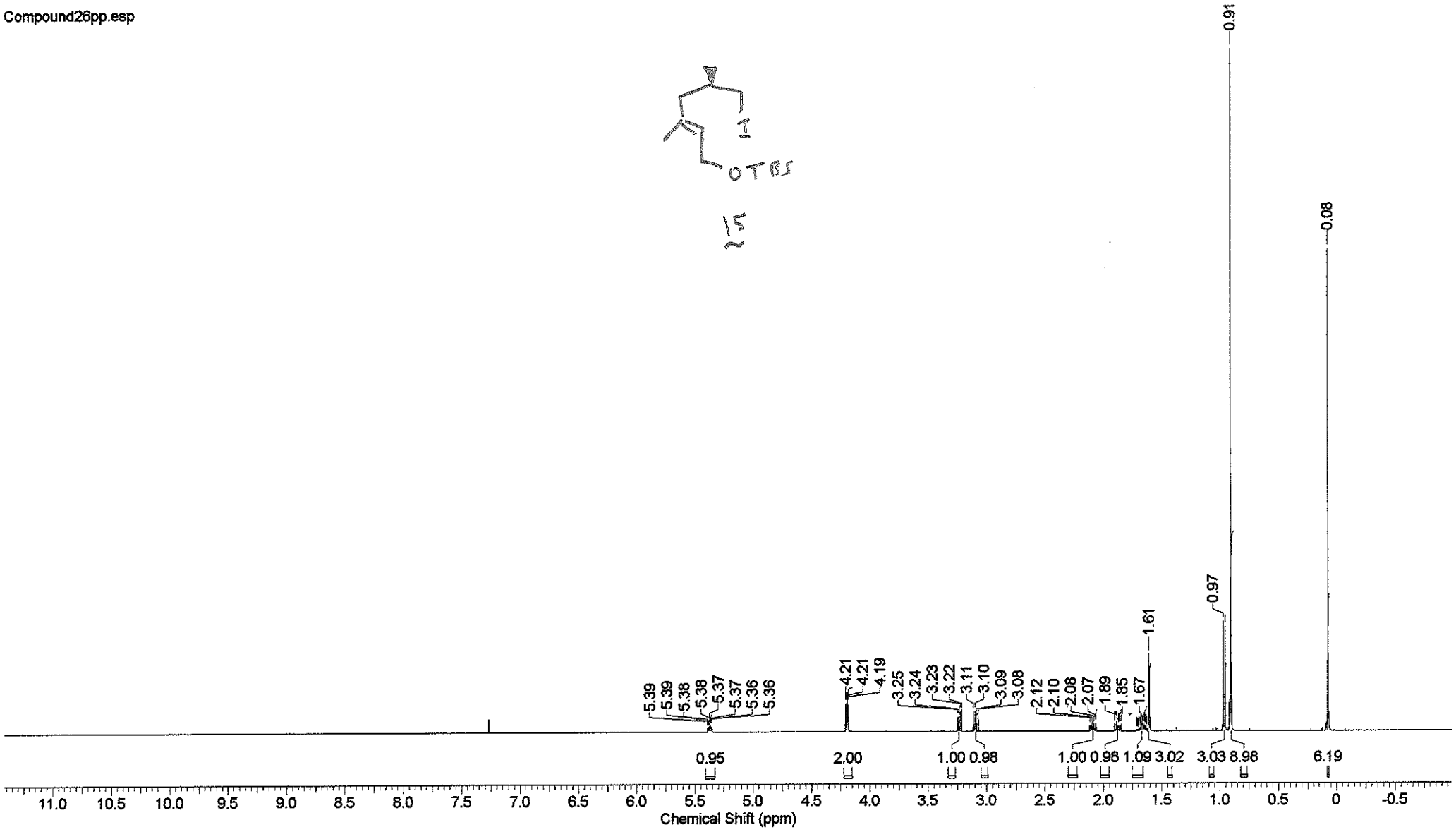
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	101.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2464.9451
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	22.000				

Compound26pp.esp



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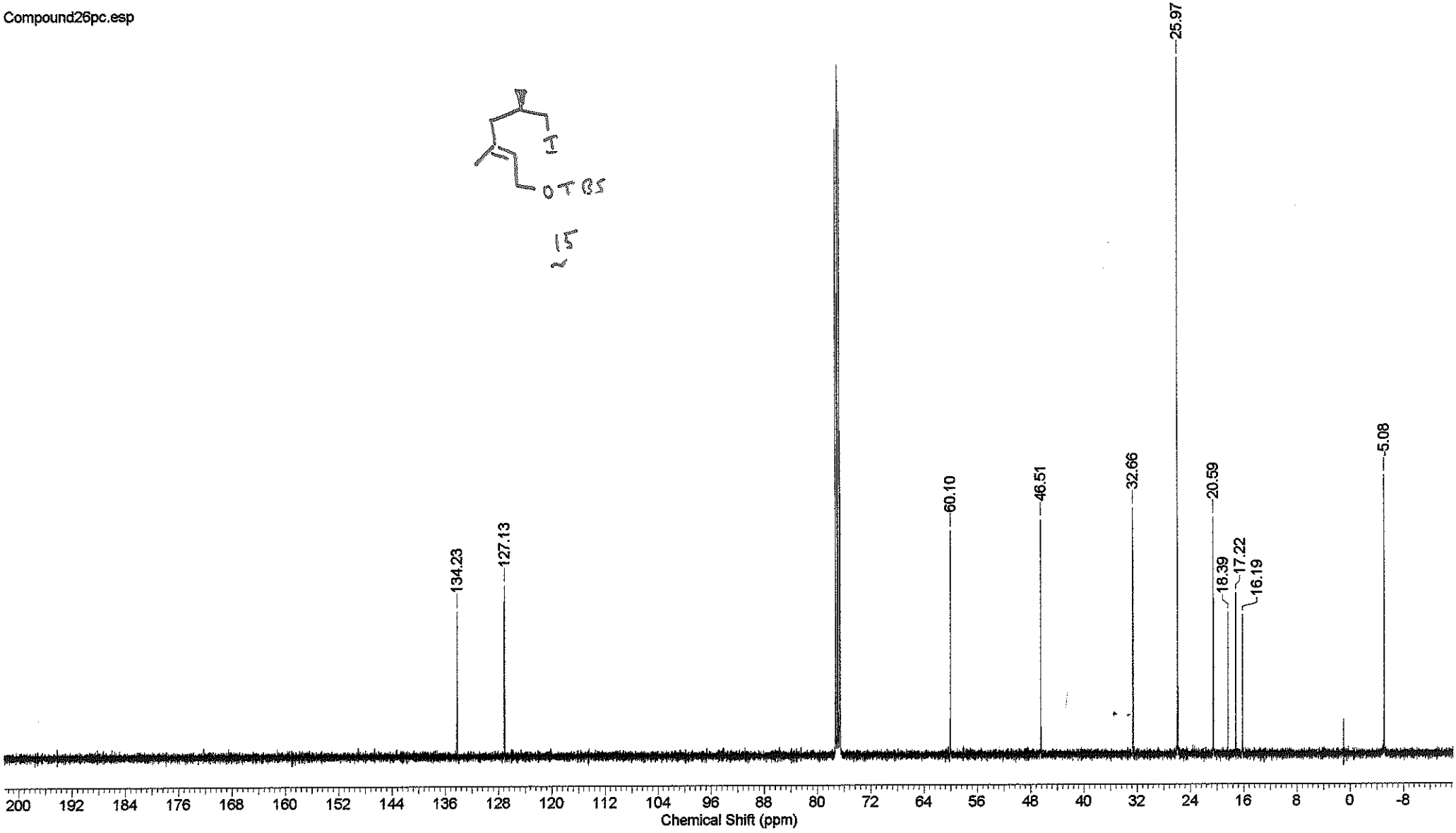
Date Stamp	27 Apr 2009 08:32:00			***File Name***	C:\Users\Mark\Documents\Chemistry\NMR\Data\MWB048pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2383
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	22.700				

Compound26pc.esp



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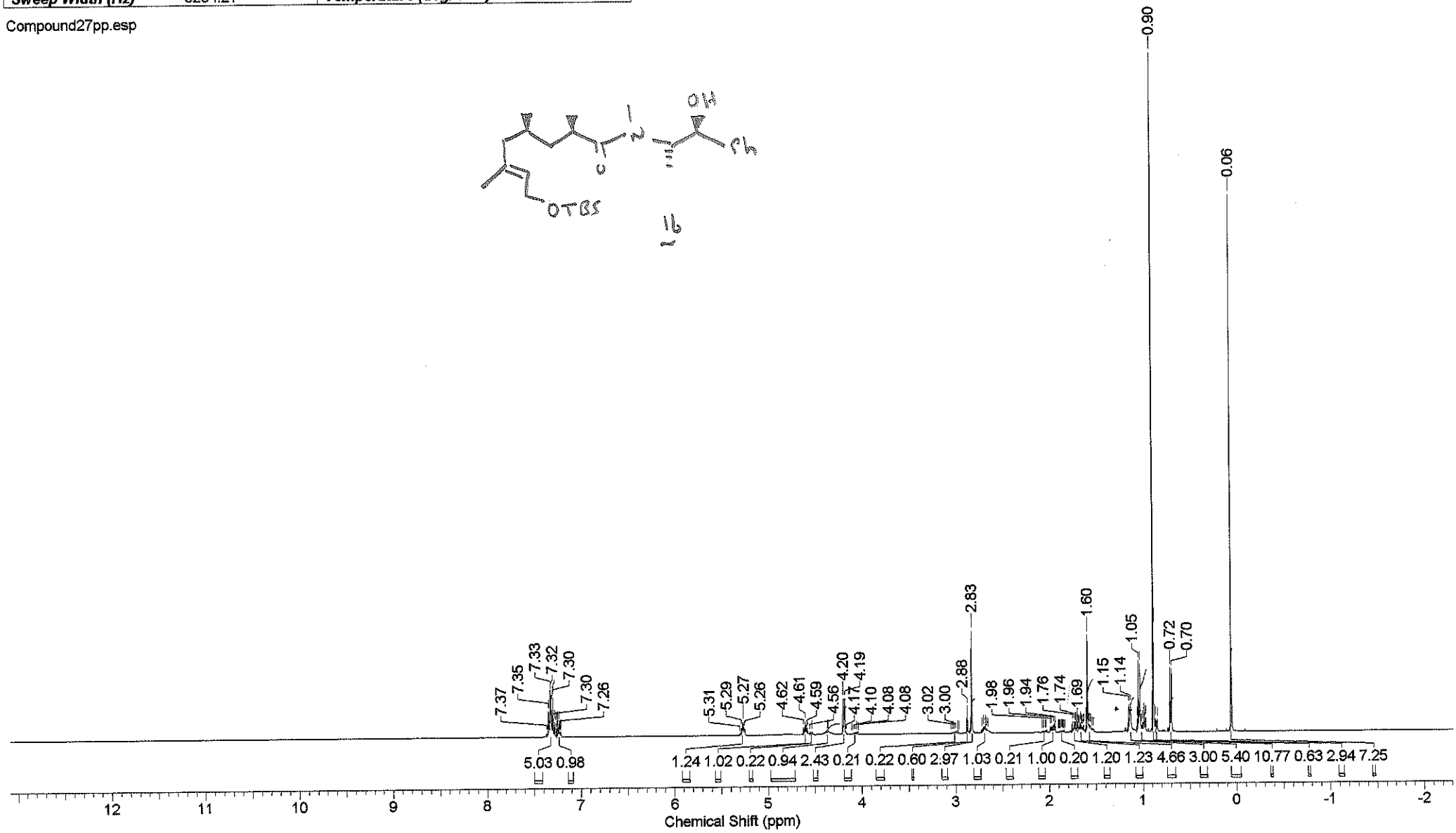
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	36.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2464.9451
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.100				

Compound27pp.esp



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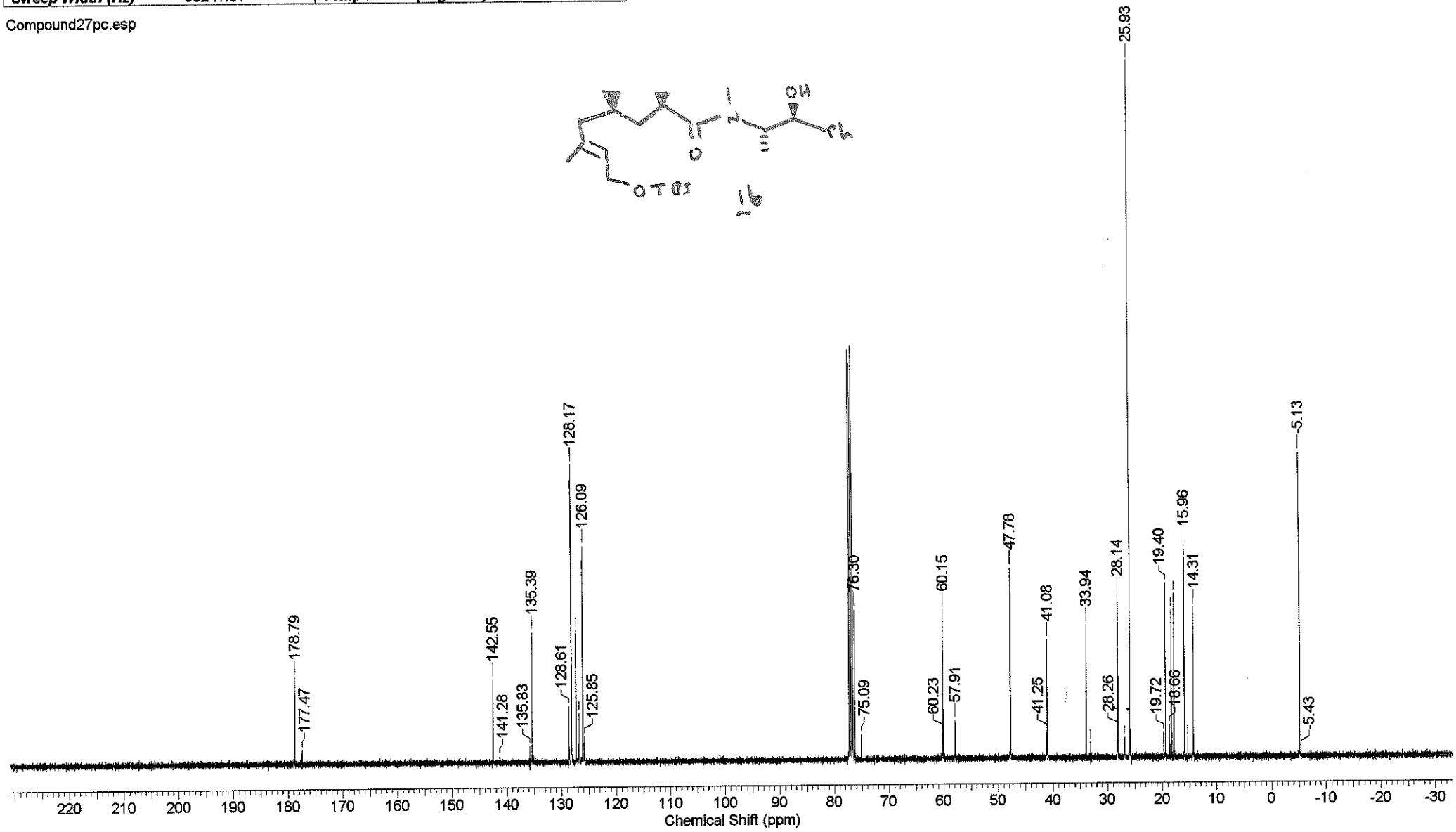
Date Stamp	09 Oct 2009 16:17:04			***File Name***	I:\Chemistry\NMR\Year 1\Data\Compound27\MWC023pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11325.7686
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.600				

Compound27pc.esp



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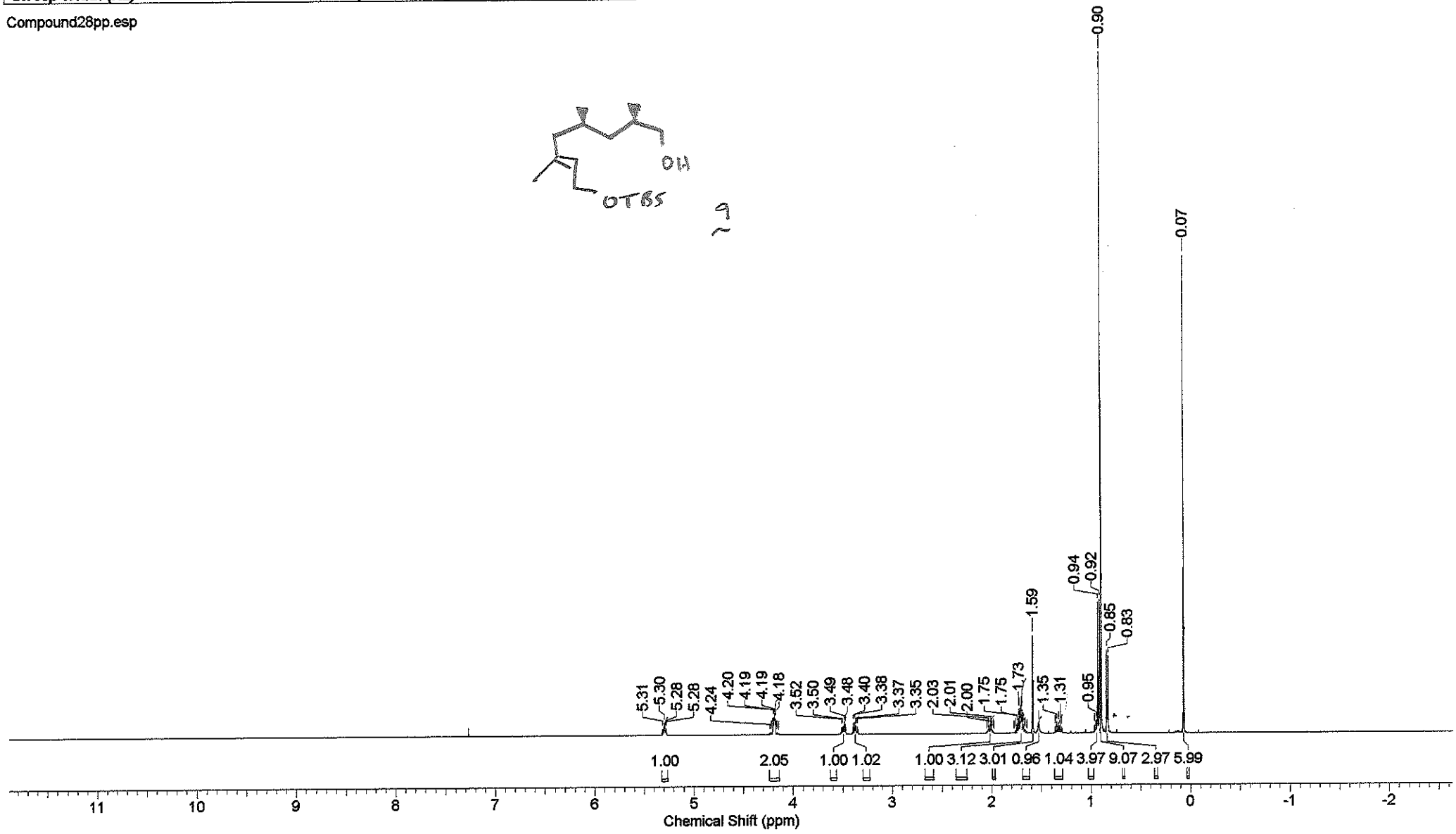
Date Stamp	11 May 2009 10:46:24			***File Name***	C:\Users\Mark\Documents\Chemistry\NMR\Data\MWB055pp\MWB055pp_000000fid		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	64.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.1973
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.300				

Compound28pp.esp



07/05/2012 09:52:16

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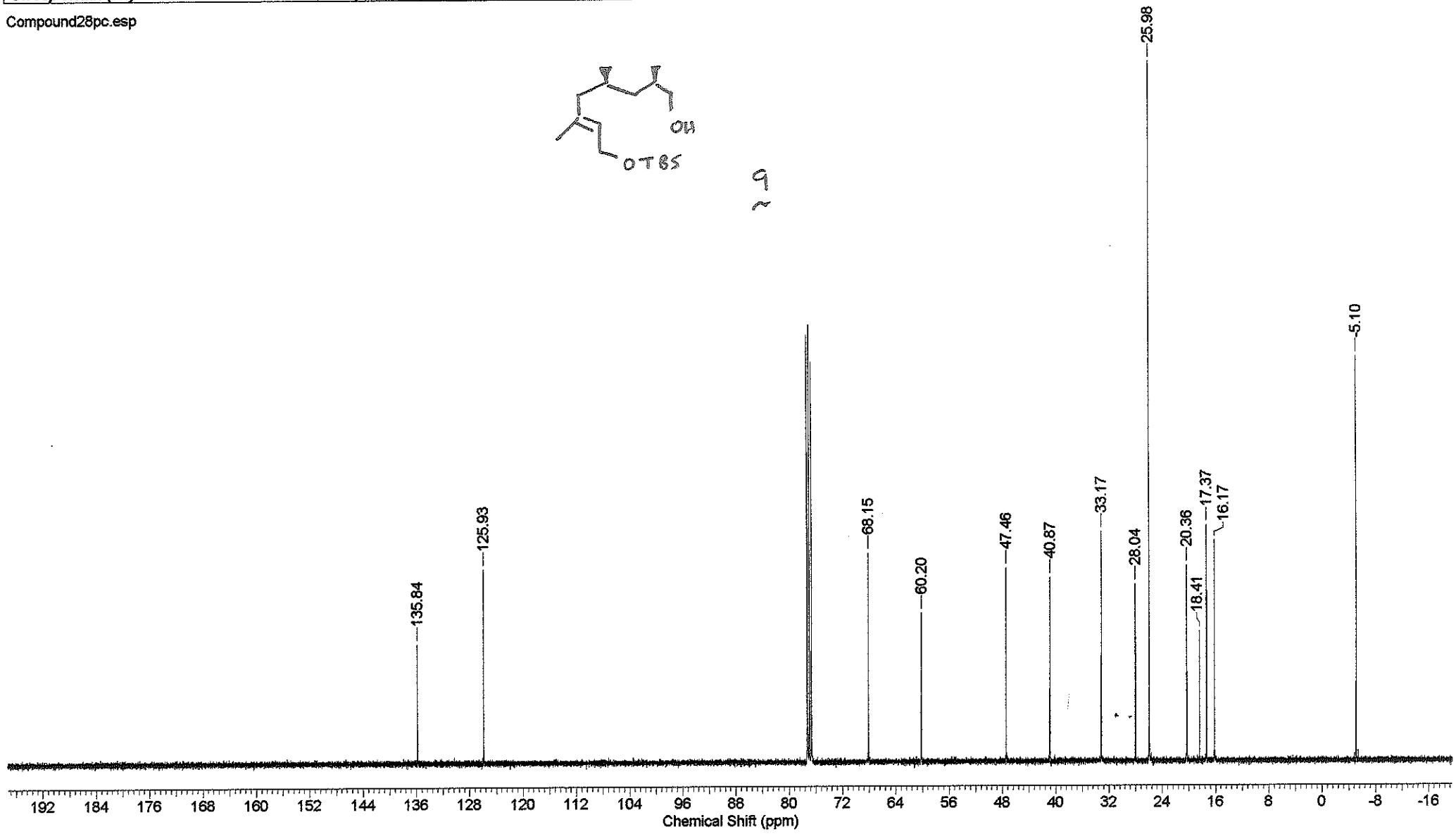
Date Stamp	11 May 2009 11:09:52			***File Name***	C:\Users\Mark\Documents\Chemistry\NMR\Data\MWB055pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2295
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.900				

Compound28pc.esp



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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	20.20	***SW(cyclical) (Hz)***	10330.58	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	3052.8643
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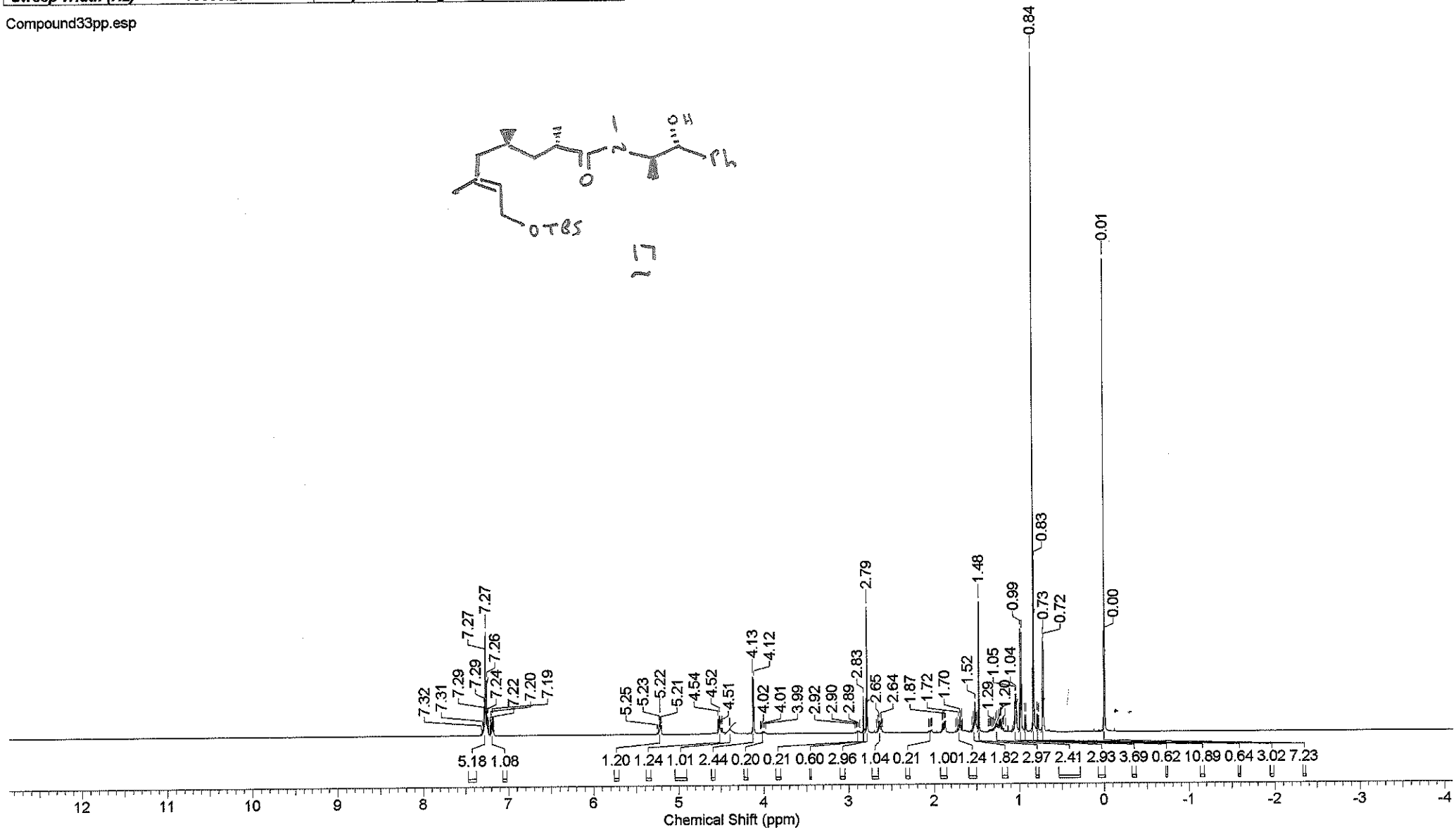
Compound33pp.esp



07/08/2012 12:14:09

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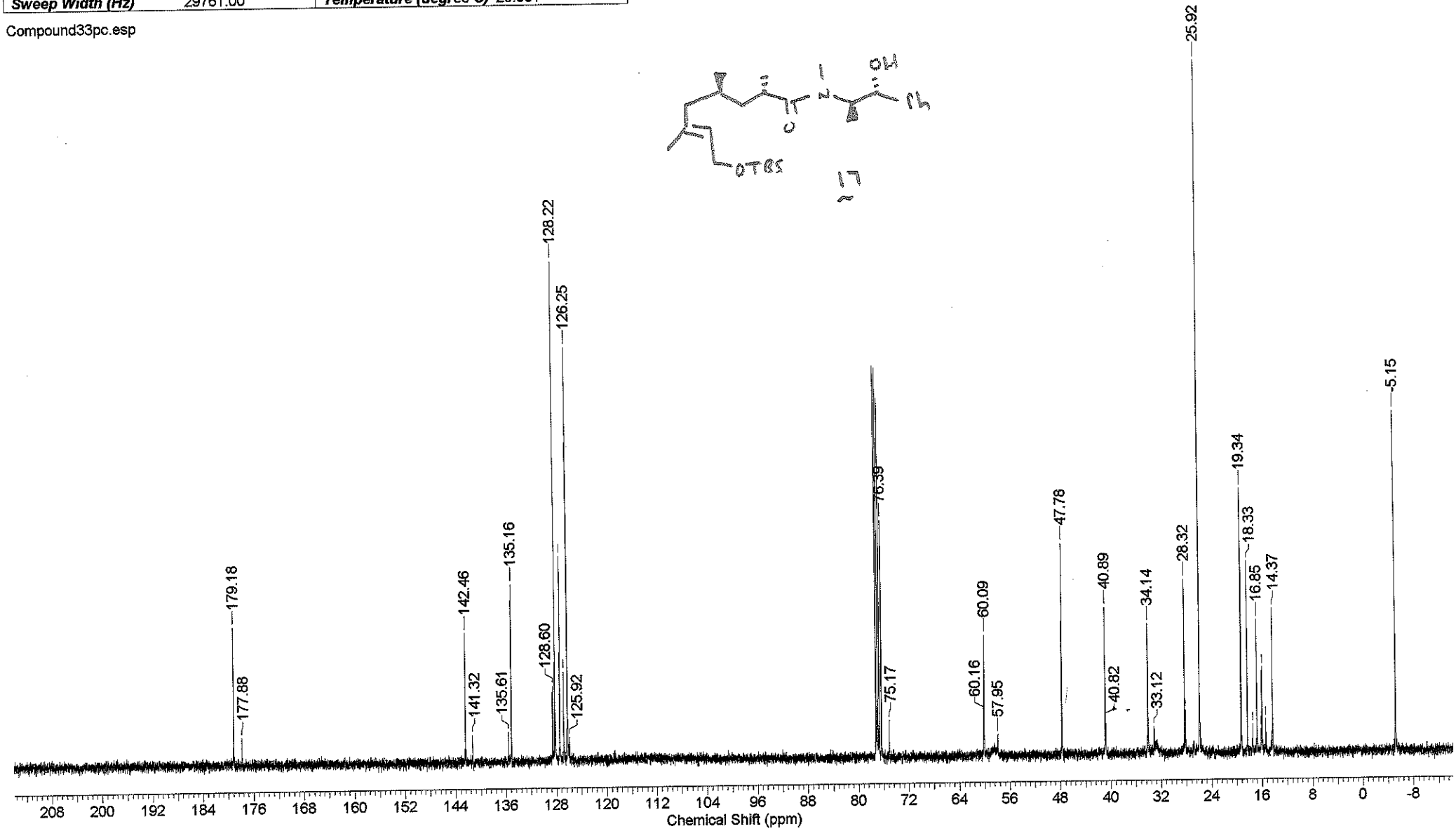
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12563.9004
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	20.001				

Compound33pc.esp



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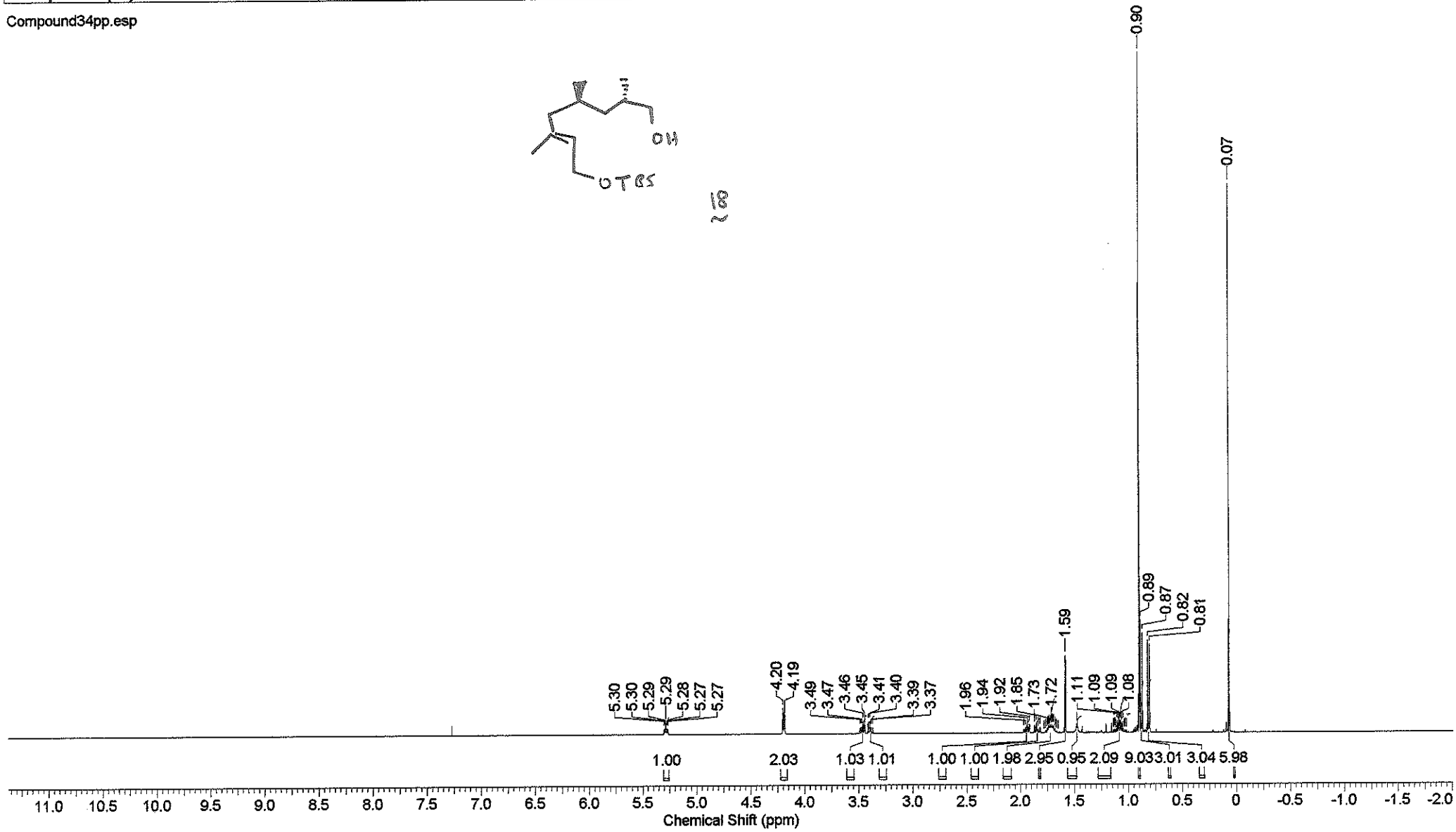
Date Stamp	26 Nov 2009 09:48:48			***File Name***	I:\Chemistry\NMR\Year 1\Data\Compound34\MWC053pp\MWC053pp_000000fid		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	71.80	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2464.9451
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.900				

Compound34pp.esp



08/05/2012 11:34:35

Acquisition Time (sec)	1.0835	***Comment***	MWVC053pc mCARBON CDCl3 {e:\bruk400data\2009\Nov} ejt 26			***Date***	26 Nov 2009 10:12:16
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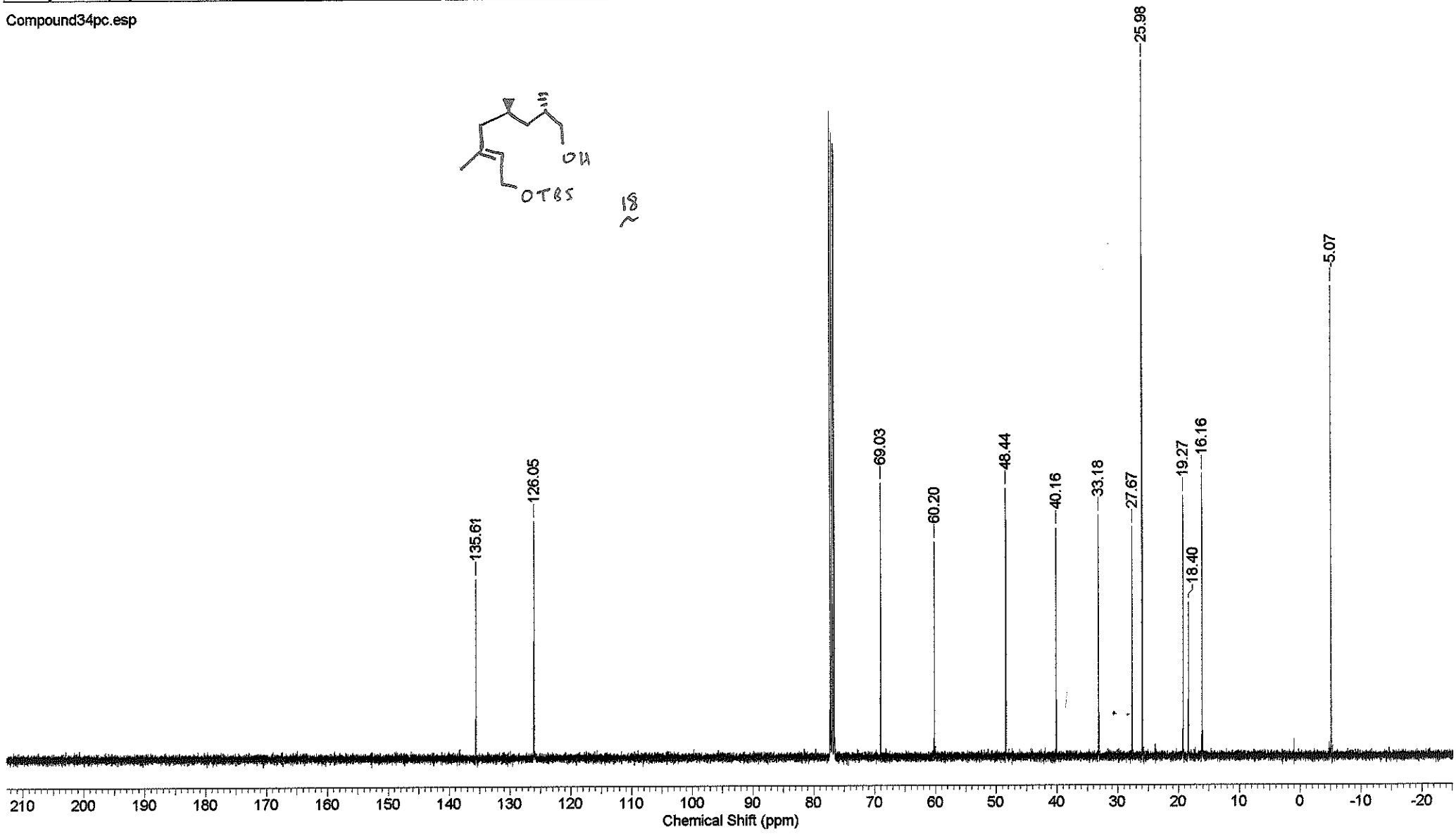
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2383
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.500				

Compound34pc.esp



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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	18.00	***SW(cyclical) (Hz)***	10330.58	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	3079.6616
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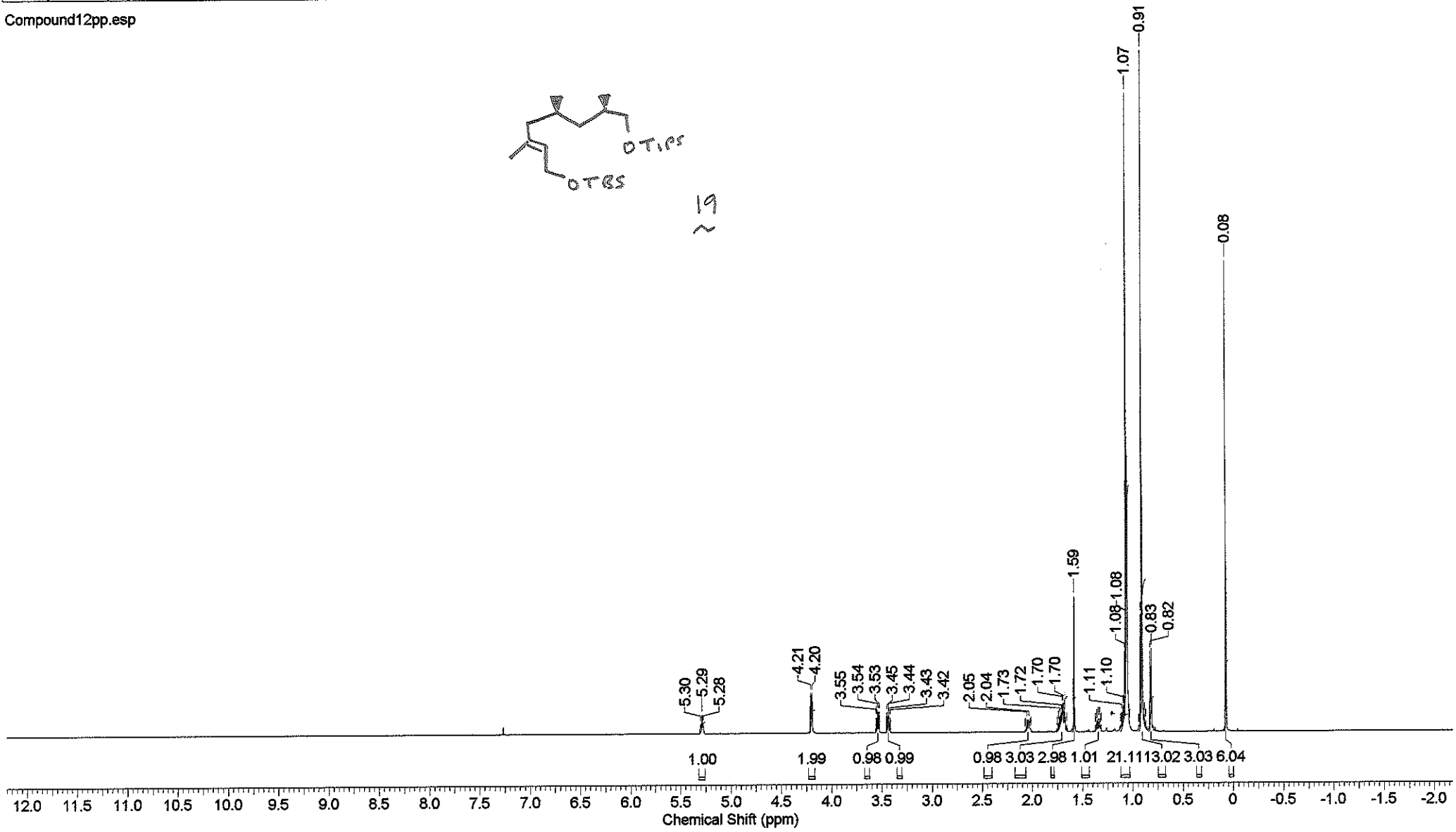
Compound12pp.esp



15/05/2012 14:58:35

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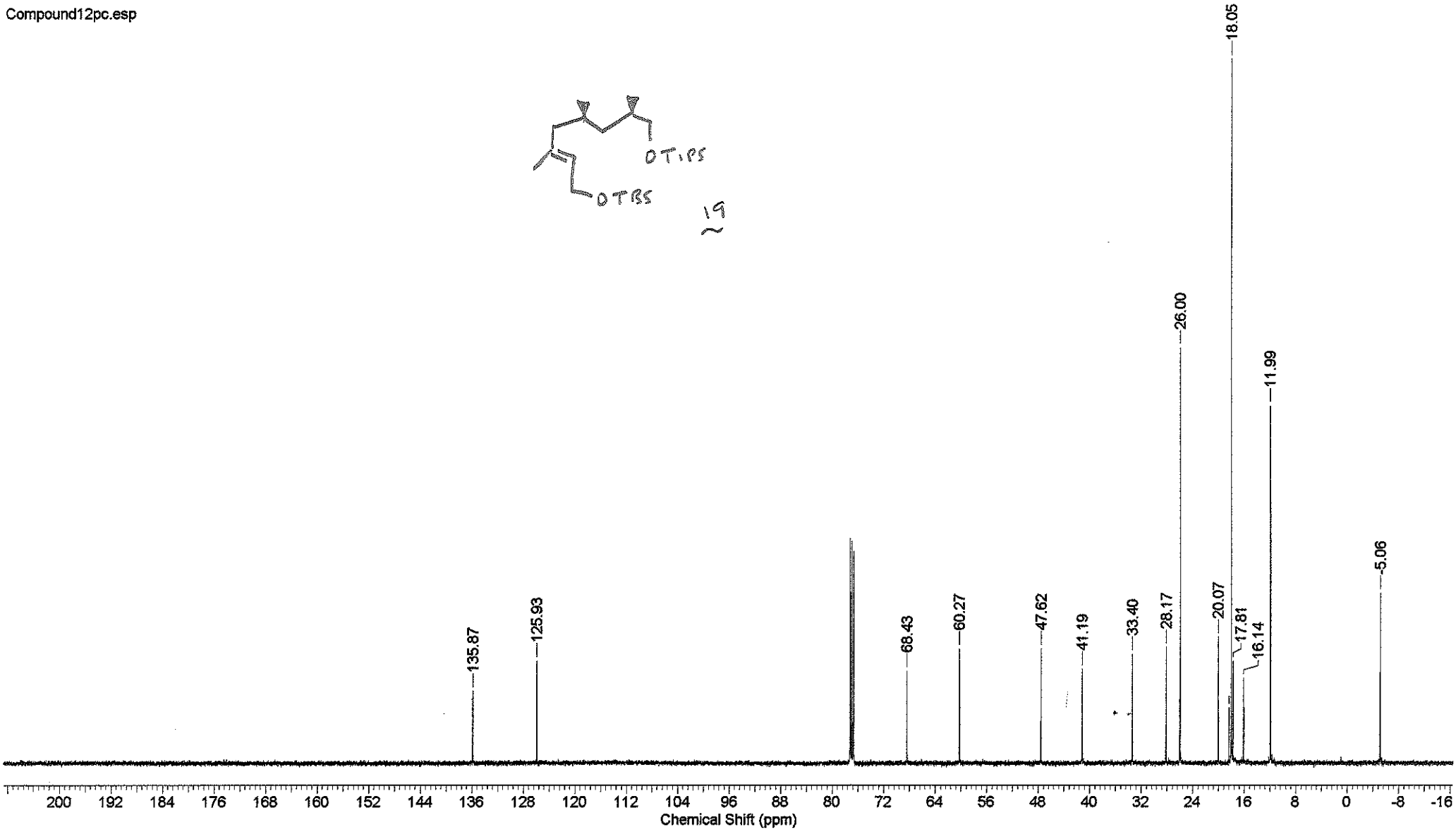
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12572.9824
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	21.933				

Compound12pc.esp

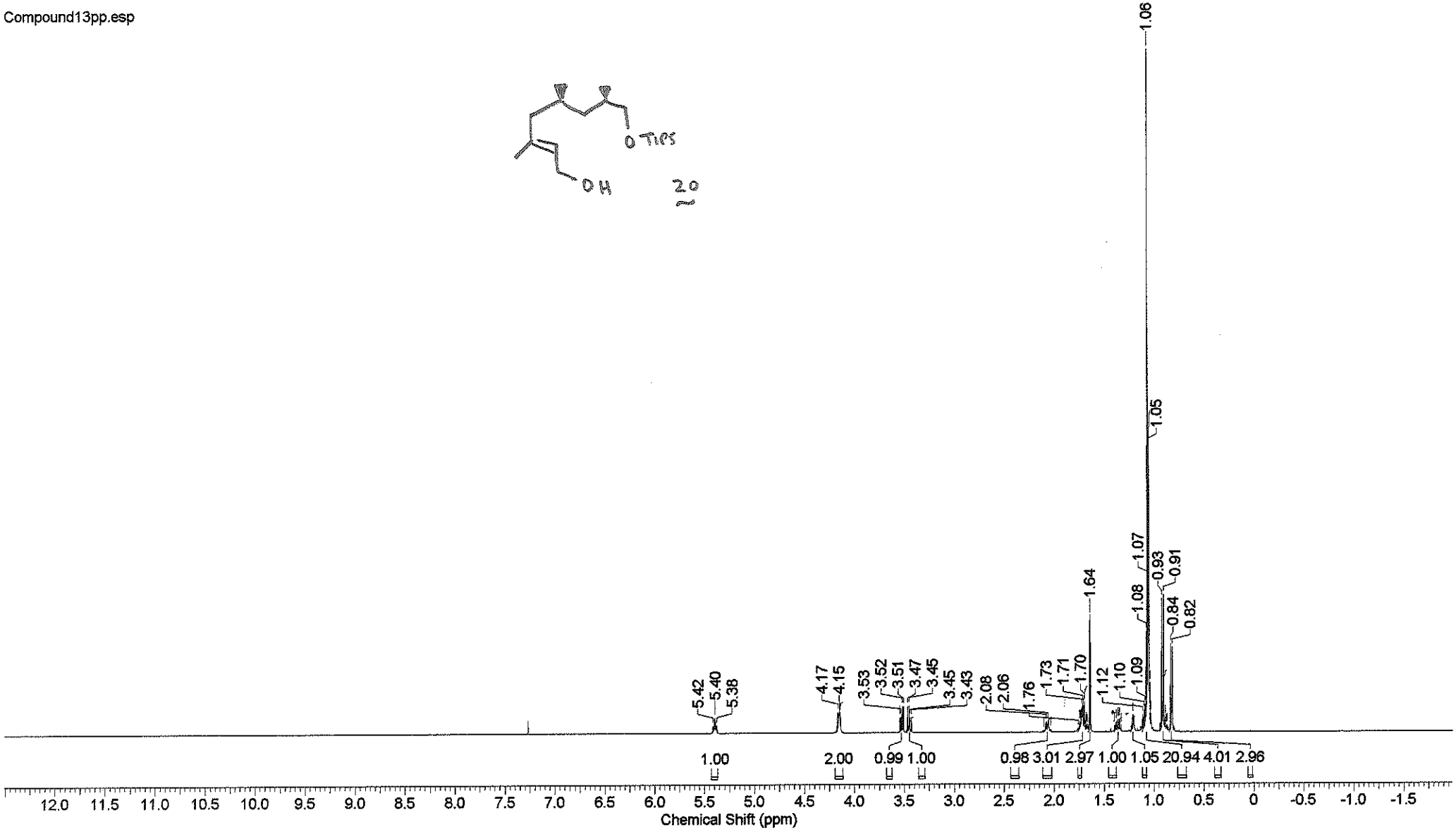
19



15/05/2012 16:26:40

Acquisition Time (sec)	3.9649	***Comment***	MWE087pp mPROTON CDCl3 {e:\bruk400data\2011\Mar} ejt 15	***Date***	10 Mar 2011 08:42:40		
Date Stamp	10 Mar 2011 08:42:40			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 13\MWE087pp_000001r		
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)***	2465.1794
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.100				

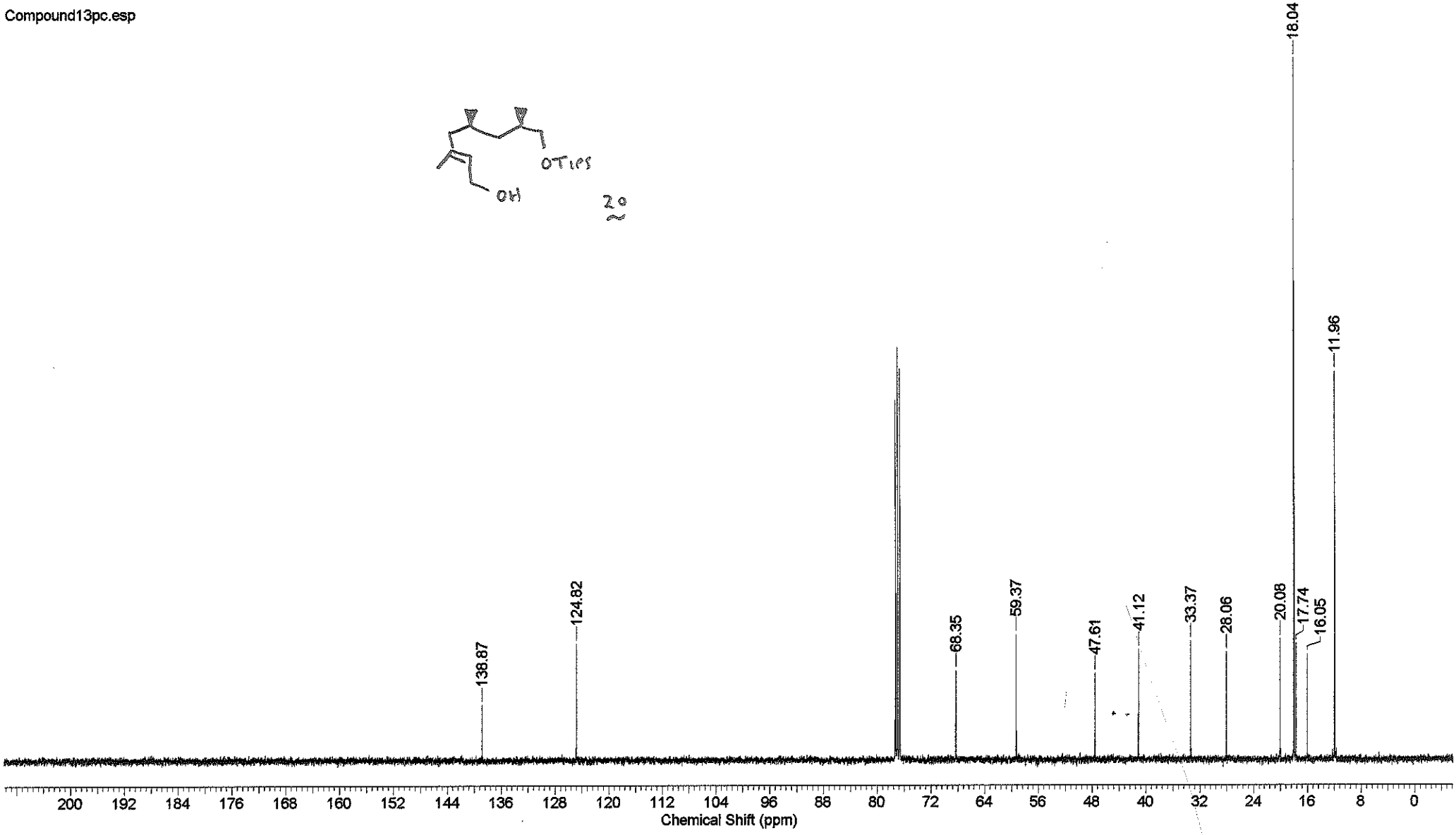
Compound13pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWE087pc mCARBON CDCl3 {e:\bruk400data\2011\Mar} ejt 15			***Date***	10 Mar 2011 09:06:08
Date Stamp	10 Mar 2011 09:06:08			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 13\MWE087pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2295
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.700				

Compound13pc.esp

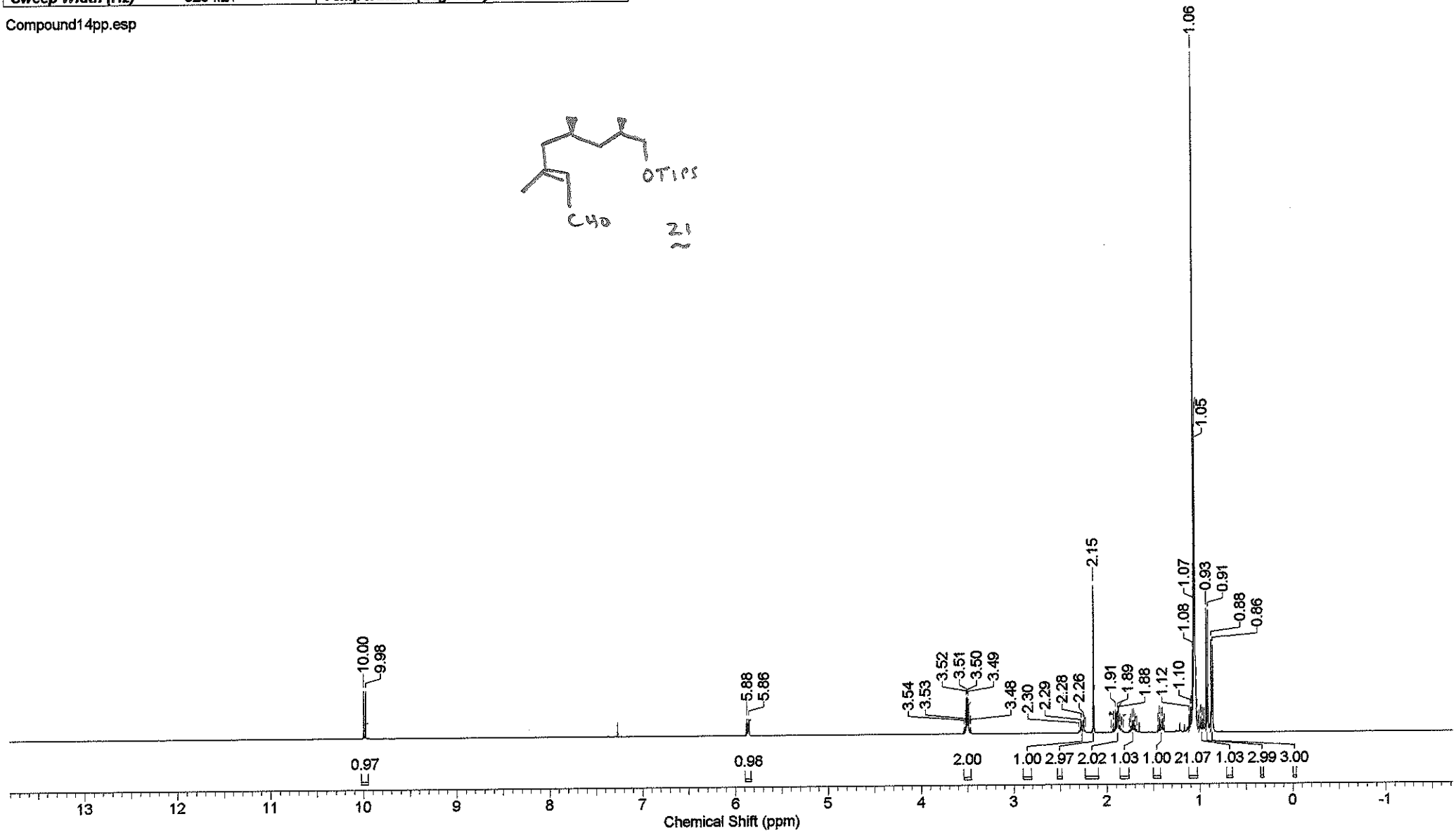
20



16/05/2012 12:43:19

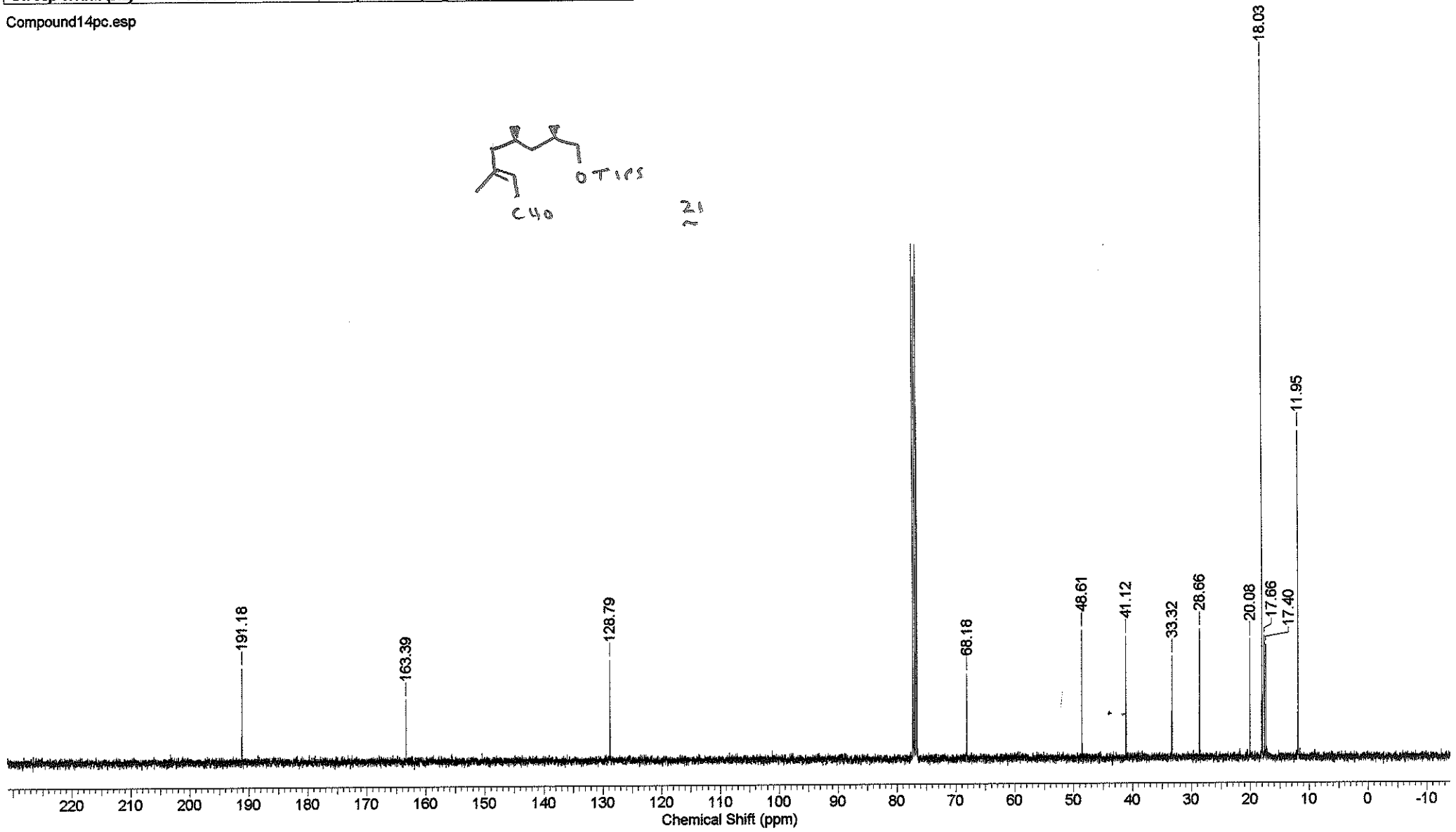
Acquisition Time (sec)	3.9649	***Comment***	MWE089pp mPROTON CDCl3 {e:\bruk400data\2011\Mar} ejt 7			***Date***	11 Mar 2011 09:01:52
Date Stamp	11 Mar 2011 09:01:52			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 14\MWE089pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	101.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.1794
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.200				

Compound14pp.esp



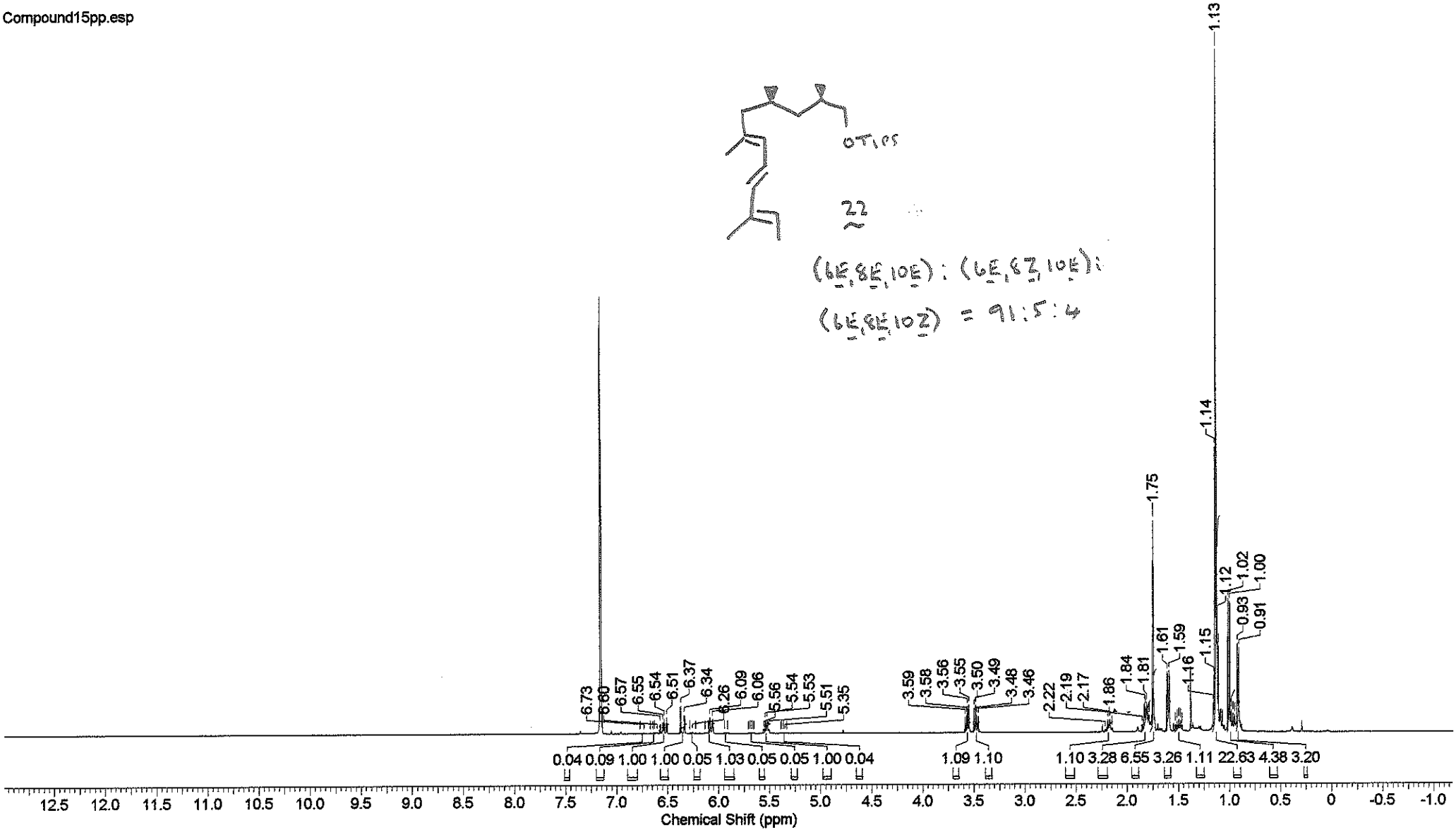
Acquisition Time (sec)	1.0835	***Comment***	MWE089pc mCARBON CDCl3 {e:\bruk400data\2011\Mar} ejt 7			***Date***	11 Mar 2011 09:25:20
Date Stamp	11 Mar 2011 09:25:20			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 14\MWE089pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2295
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.800				

Compound14pc.esp



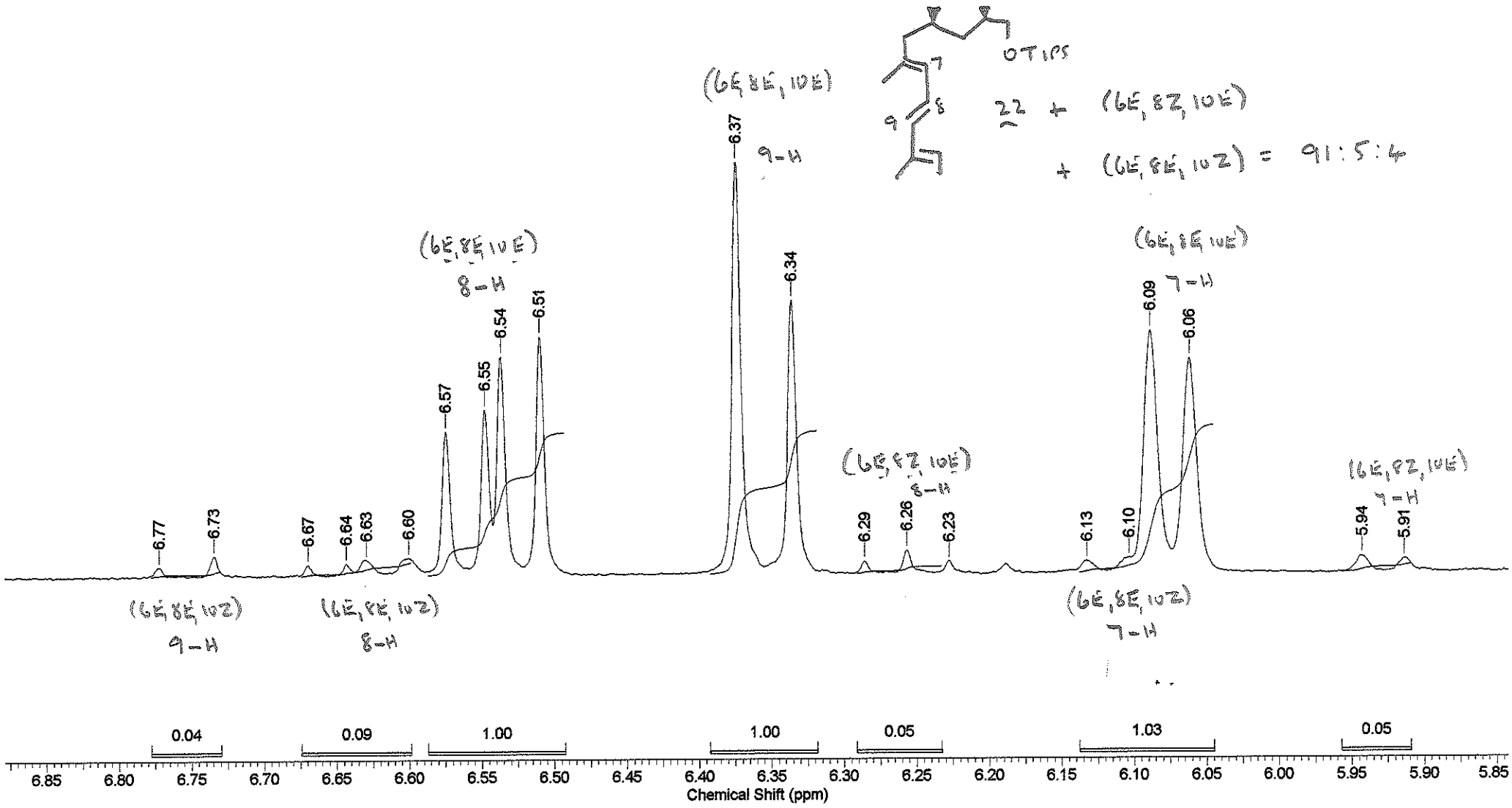
Acquisition Time (sec)	3.9649	***Comment***	MWF010pp mPROTON C6D6 {e:\bruk400data\2011\Apr} ejt 41	***Date***	14 Apr 2011 09:57:20		
Date Stamp	14 Apr 2011 09:57:20			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 15\MWF010pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	203.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2425.7051
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.600				

Compound15pp.esp



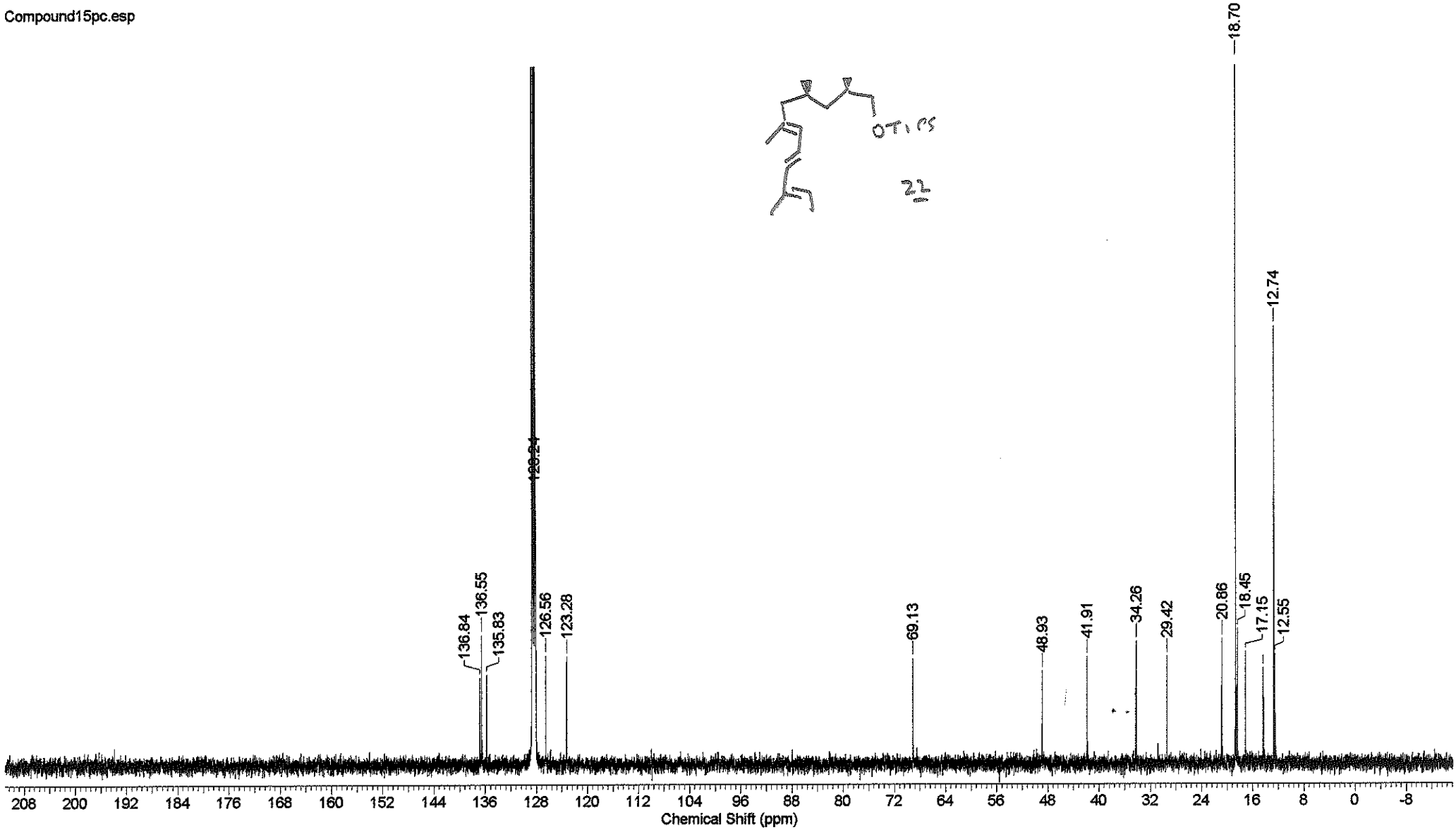
Acquisition Time (sec)	3.9649	***Comment***	MWF010pp mPROTON C6D6 {e:\bruk400data\2011\Apr} ejt 41			***Date***	14 Apr 2011 09:57:20
Date Stamp	14 Apr 2011 09:57:20			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 15\MWF010pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	203.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2425.7051
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.600				

Compound15pp.esp



Acquisition Time (sec)	1.0835	***Comment***	mCARBON C6D6 {e:\bruk400data\2011\Apr} ejt 45			***Date***	14 Apr 2011 11:41:52
Date Stamp	14 Apr 2011 11:41:52			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 15\MWF010pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11394.4072
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	22.400				

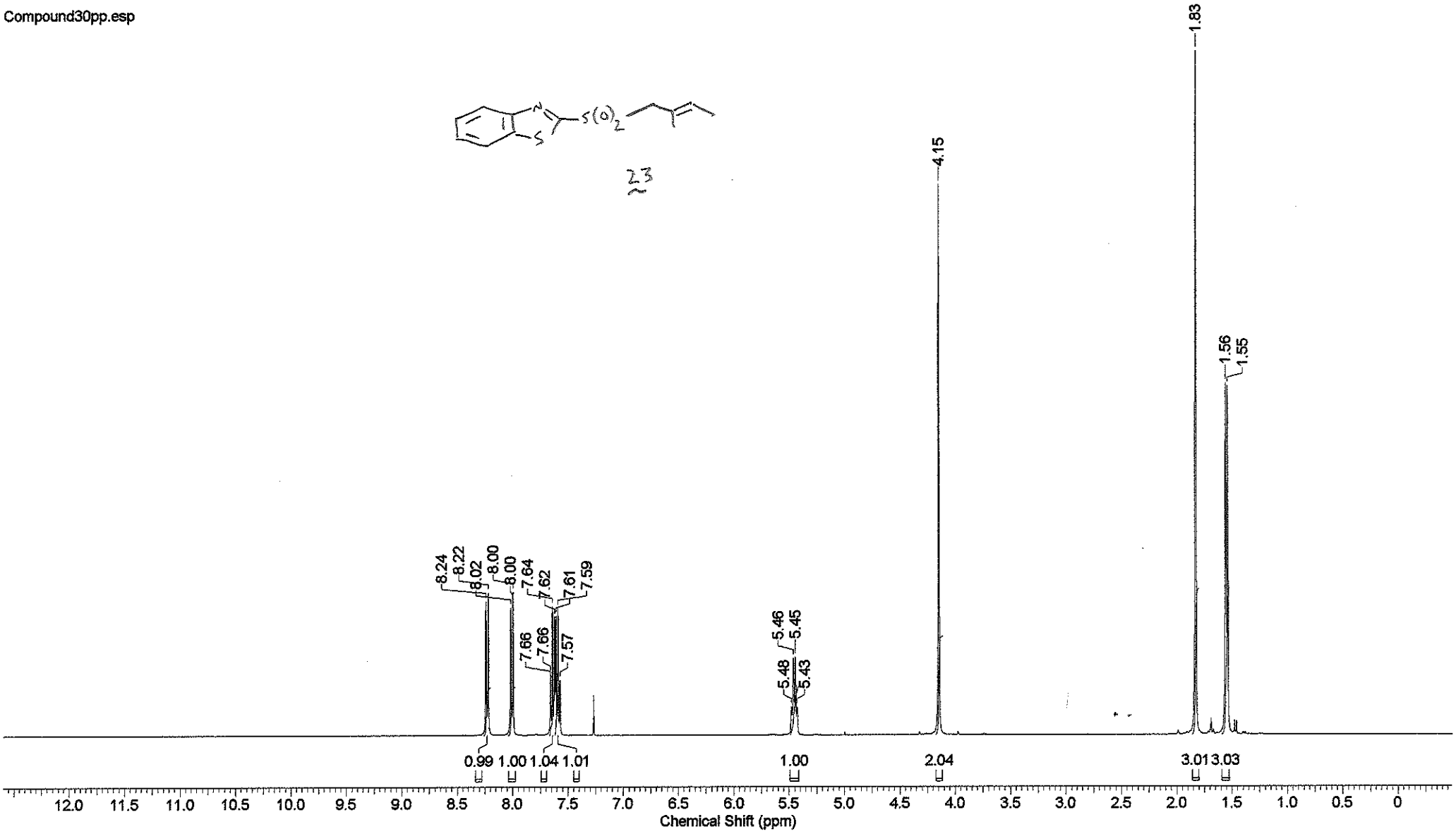
Compound15pc.esp



07/05/2012 11:04:21

Acquisition Time (sec)	3.9649	***Comment***	MWB066pp mPROTON CDCl3 {e:\bruk400data\2011\Feb} ejt 25			***Date***	01 Feb 2011 09:44:32
Date Stamp	01 Feb 2011 09:44:32			***File Name***	F:\Chemistry\Year 1 data\NMR data\Data\Compound30\MWB066pp_000001r		
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)***	2465.4316
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.400				

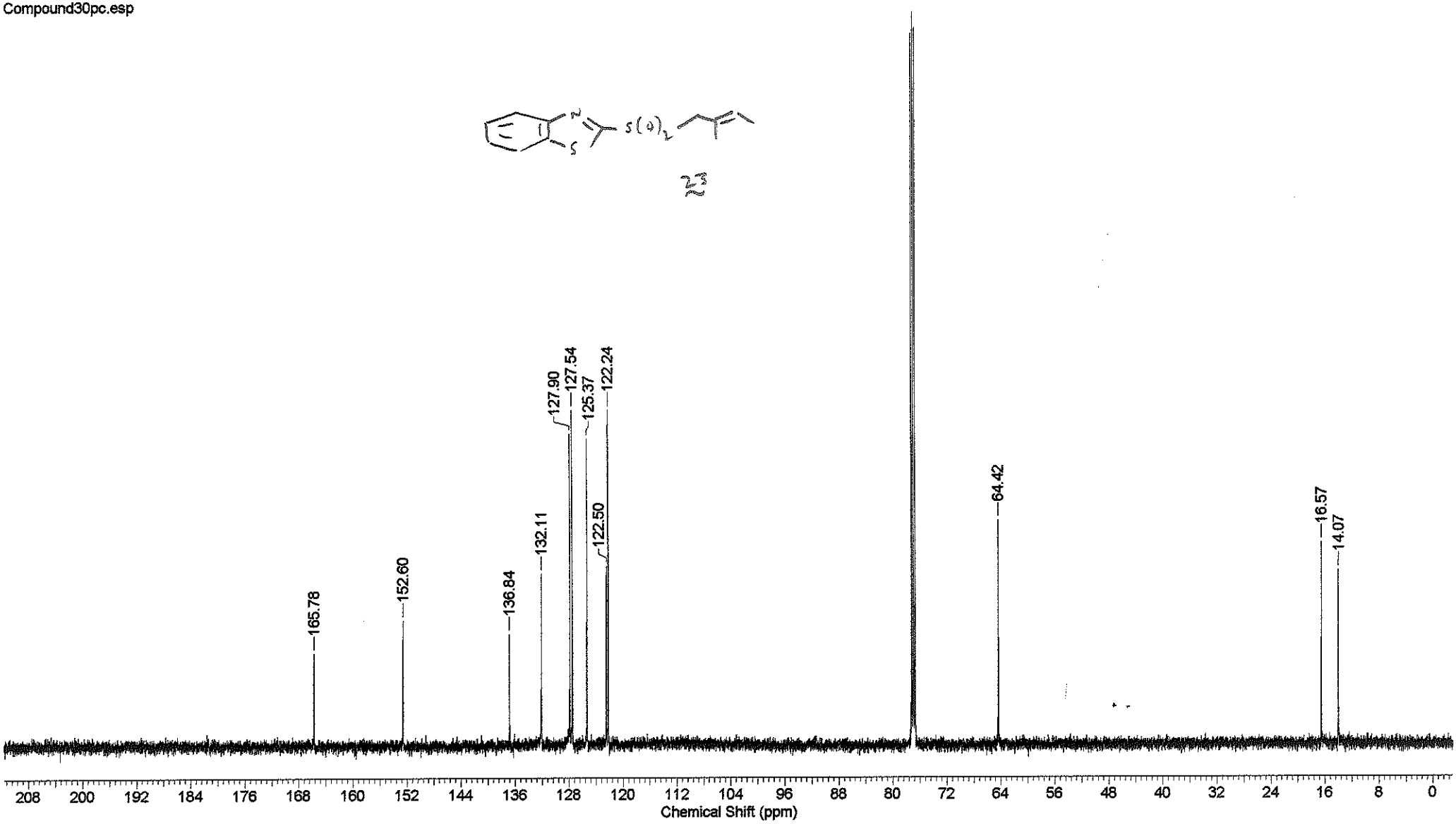
Compound30pp.esp



Acquisition Time (sec)	1.1010	***Comment***	MWC066pc mCARBON CDCl3 /opt/bruk500data/2011/Jan ejt 6			***Date***	01 Feb 2011 08:40:32
Date Stamp	01 Feb 2011 08:40:32			***File Name***	F:\Chemistry\Year 1 data\NMR data\Data\Compound30\MWB066pc_000001r		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***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)***	12564.8096
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	20.750				

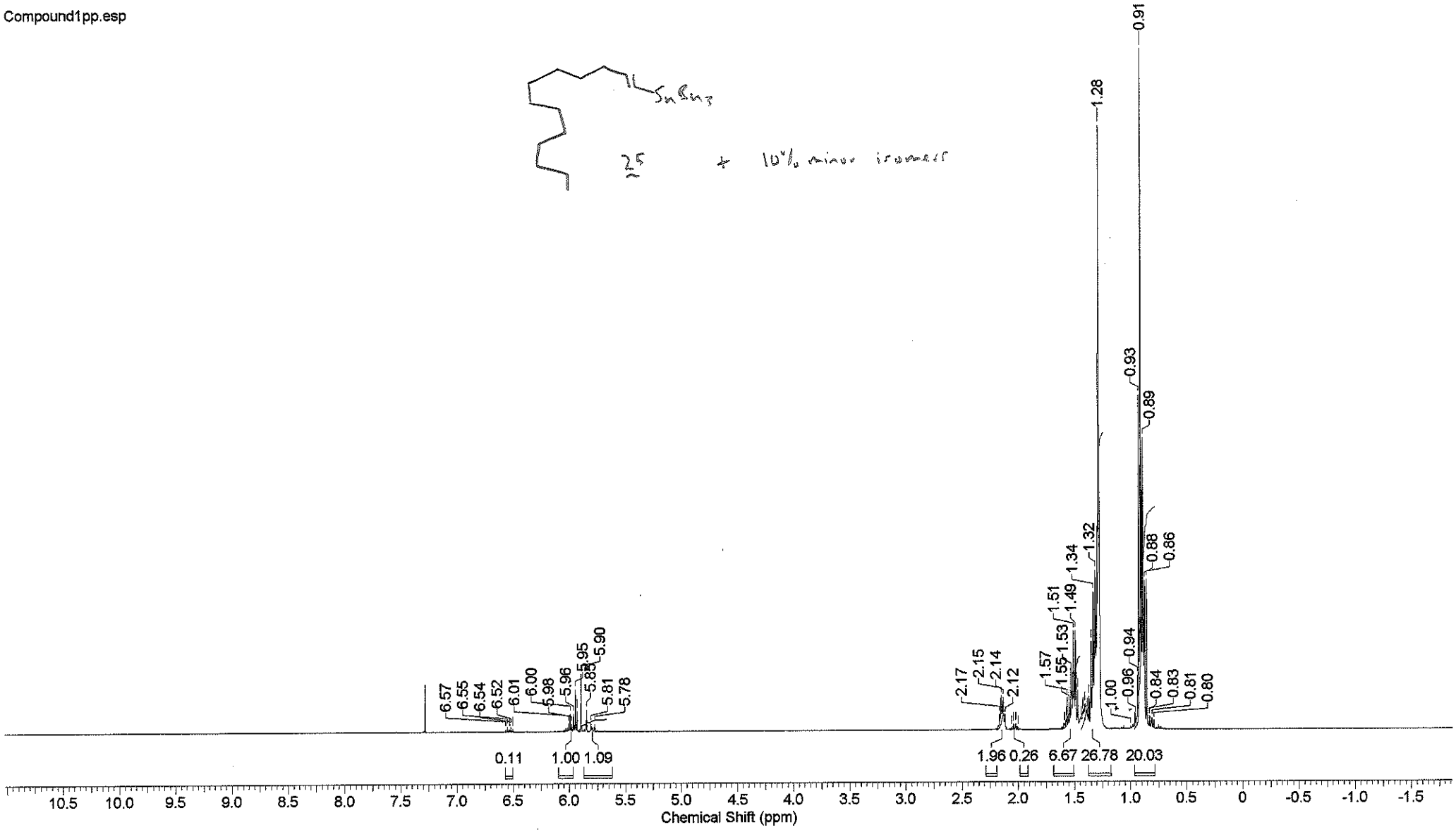
Compound30pc.esp

23



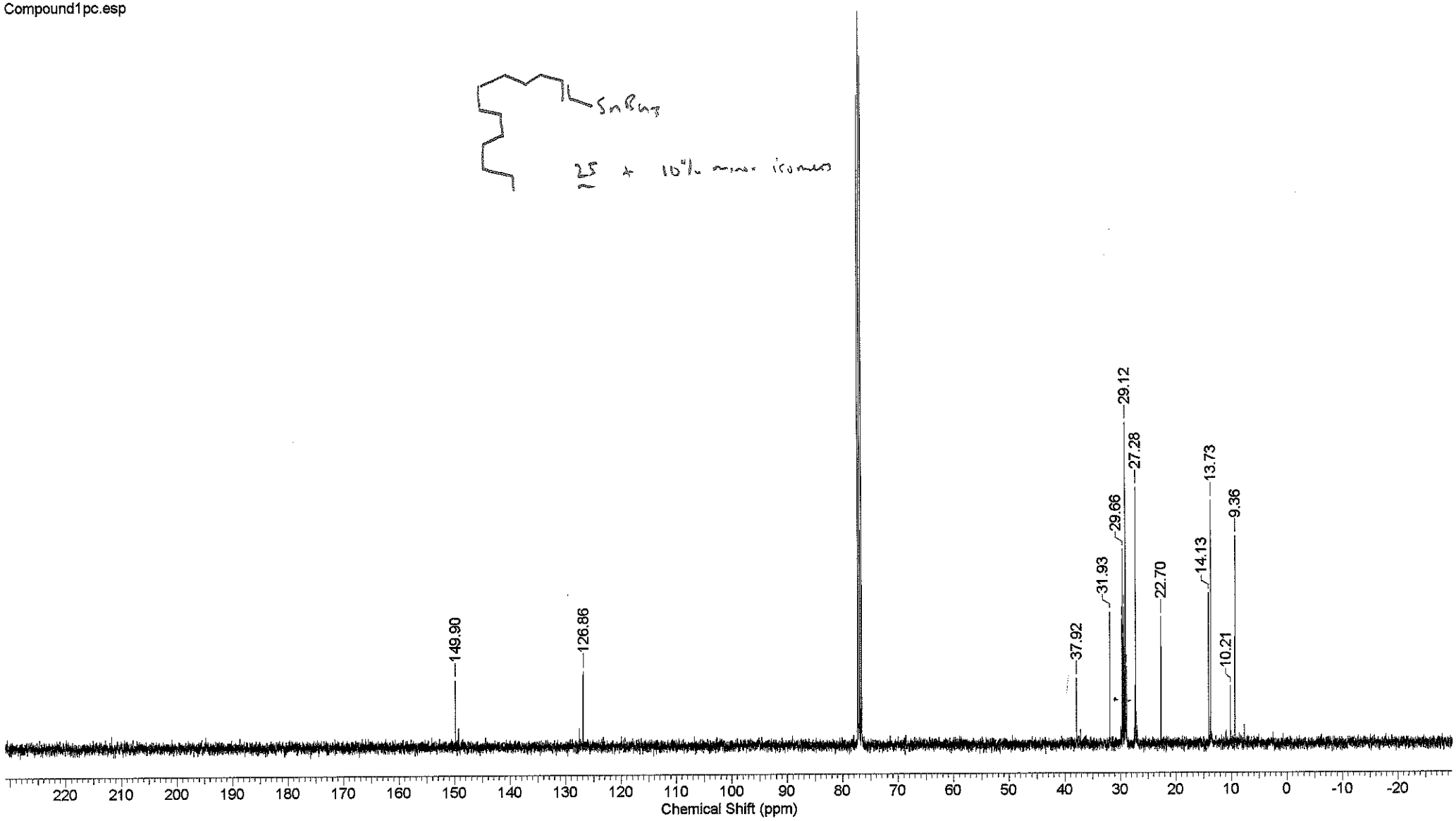
Acquisition Time (sec)	3.9649	***Comment***	MWC057pp mPROTON CDCl3 {e:\bruk400data\2009\Dec} ejt 22	***Date***	04 Dec 2009 10:16:32		
Date Stamp	04 Dec 2009 10:16:32			***File Name***	F:\Chemistry\Year 2 data\NMR data\Data\Compound1\MWC057pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number 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)***	2470.9661
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.400				

Compound1pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWC057pc mCARBON CDCl3 {e:\bruk400data\2009\Dec} ejt 48			***Date***	04 Dec 2009 13:17:52
Date Stamp	04 Dec 2009 13:17:52			***File Name***	F:\Chemistry\Year 2 data\NMR data\Data\Compound1\MWC057pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11333.1523
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.200				

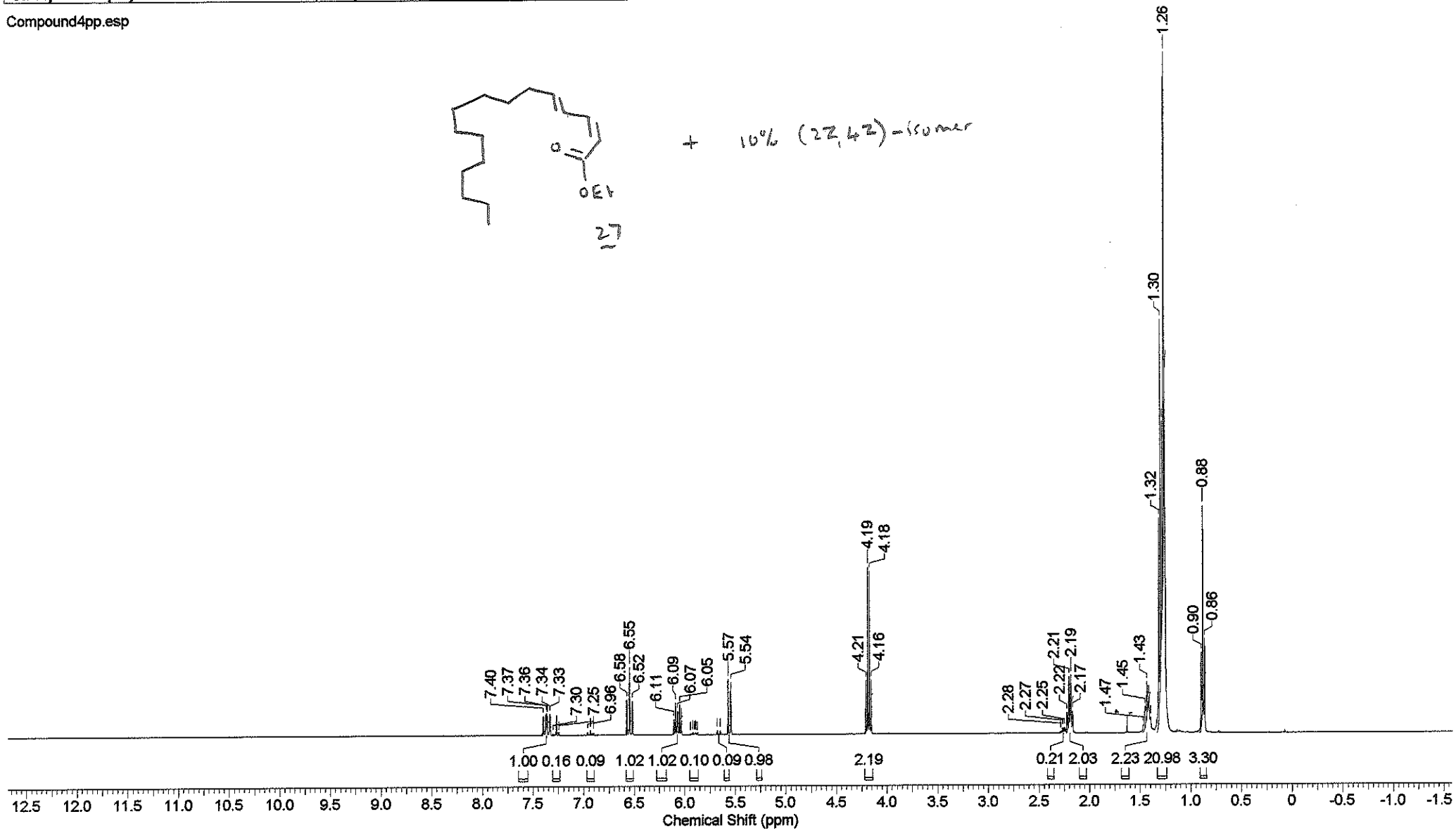
Compound1pc.esp



11/05/2012 12:47:30

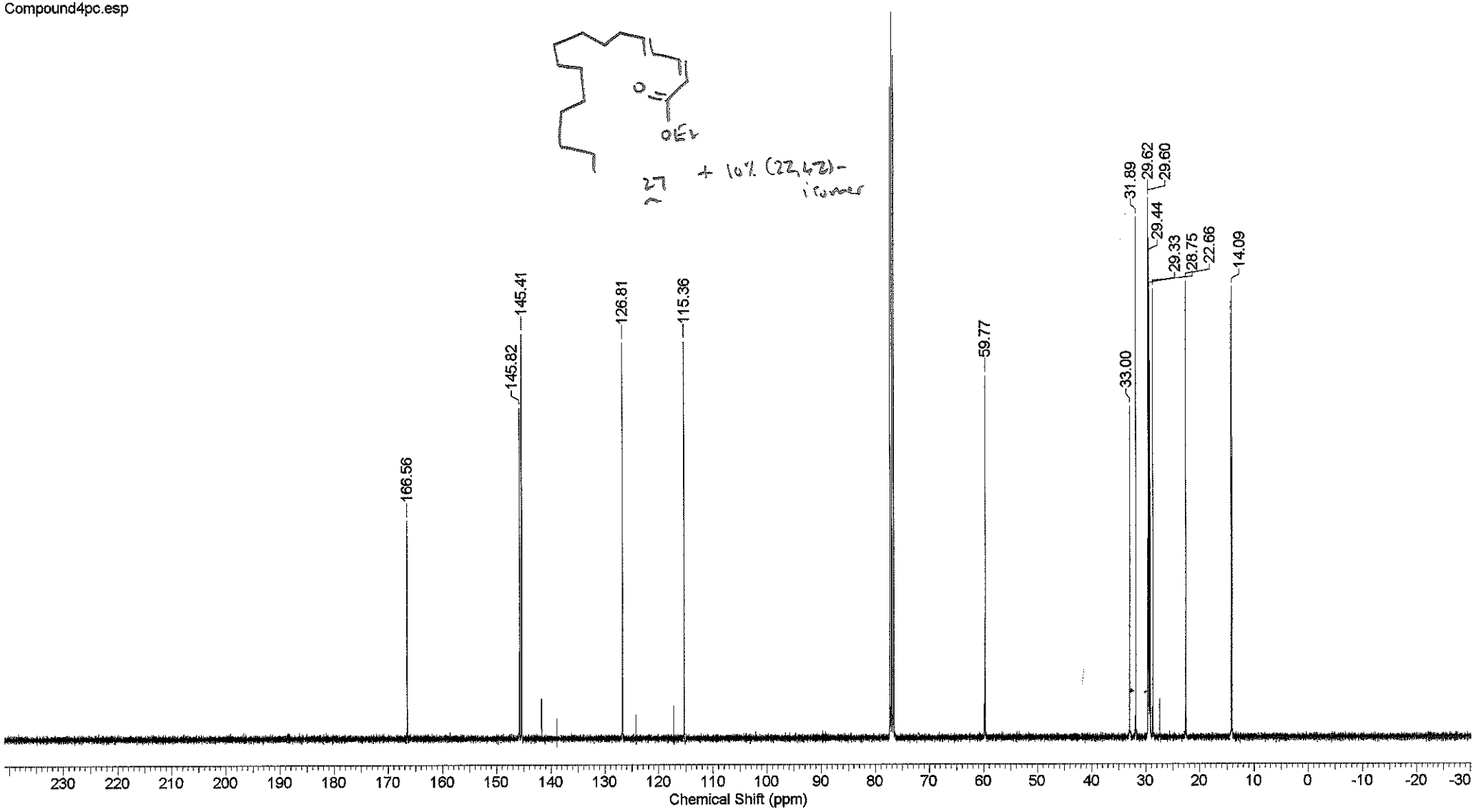
Acquisition Time (sec)	3.9649	***Comment***	MWC056app mPROTON CDCl3 {e:\bruk400data\2009\Dec} ejt 51			***Date***	08 Dec 2009 08:06:24
Date Stamp	08 Dec 2009 08:06:24			***File Name***	I:\Chemistry\Year 2 data\NMR data\Data\Compound4\MWC056pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	64.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.1794
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.700				

Compound4pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWC056pp mCARBONnight CDCl3 {e:\bruk400data\2010\Jan} ejt 21				
Date	07 Jan 2010 17:33:52			***Date Stamp***	07 Jan 2010 17:33:52		
File Name	I:\Chemistry\Year 2 data\NMR data\Data\Compound4\MWC056pc_000001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	512	***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	***Sweep Width (Hz)***	30241.01
Temperature (degree C)	19.000						

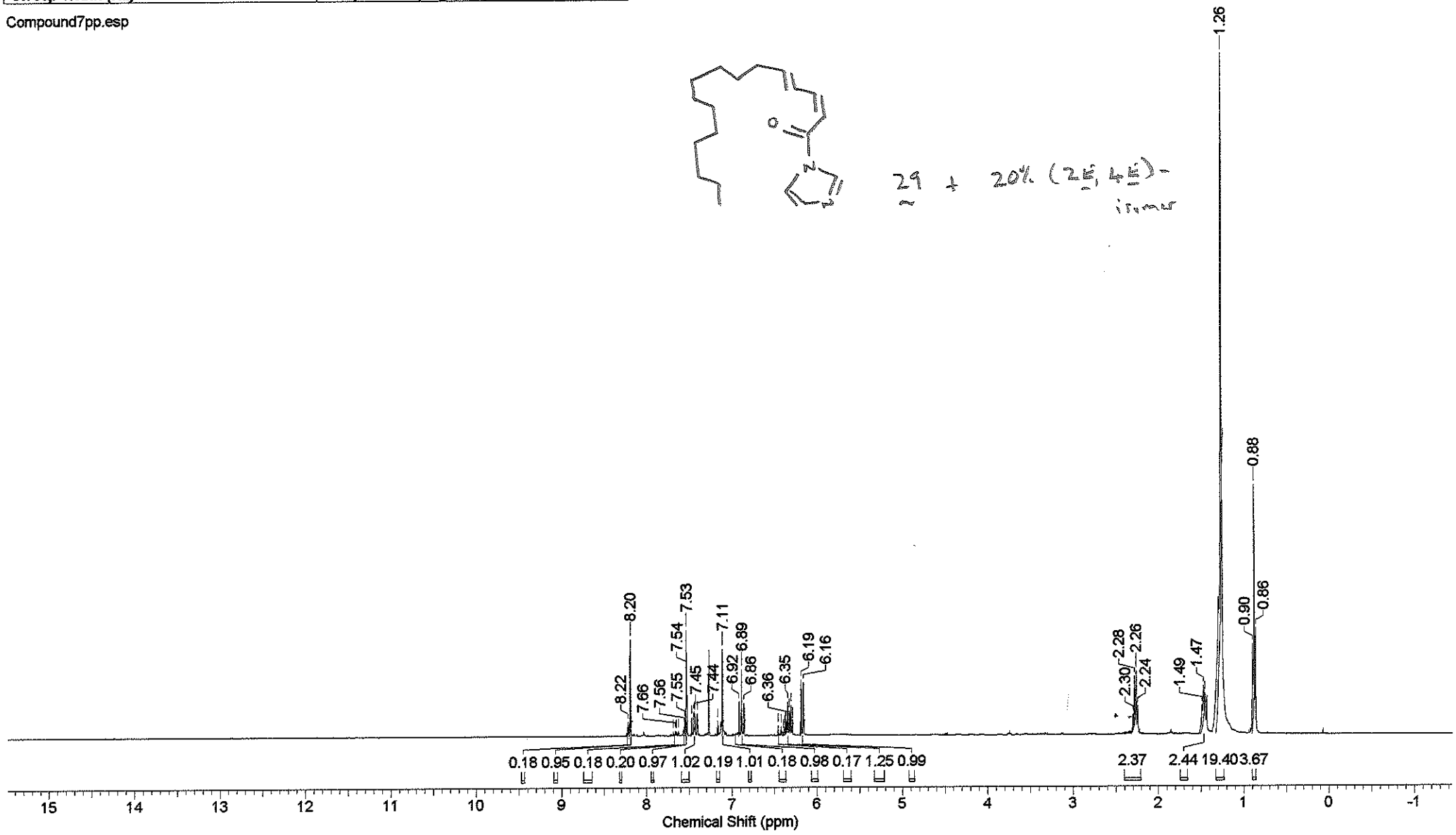
Compound4pc.esp



Acquisition Time (sec)	3.9649	***Comment***	MWC069pp mPROTON CDCl3 {e:\bruk400data\2010\Jan} ejt 20			***Date***	22 Jan 2010 11:39:44
Date Stamp	22 Jan 2010 11:39:44			***File Name***	F:\Chemistry\Year 2 data\NMR data\Data\Compound7\MWC069pp_000001r		
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	181.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.1794
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.600				

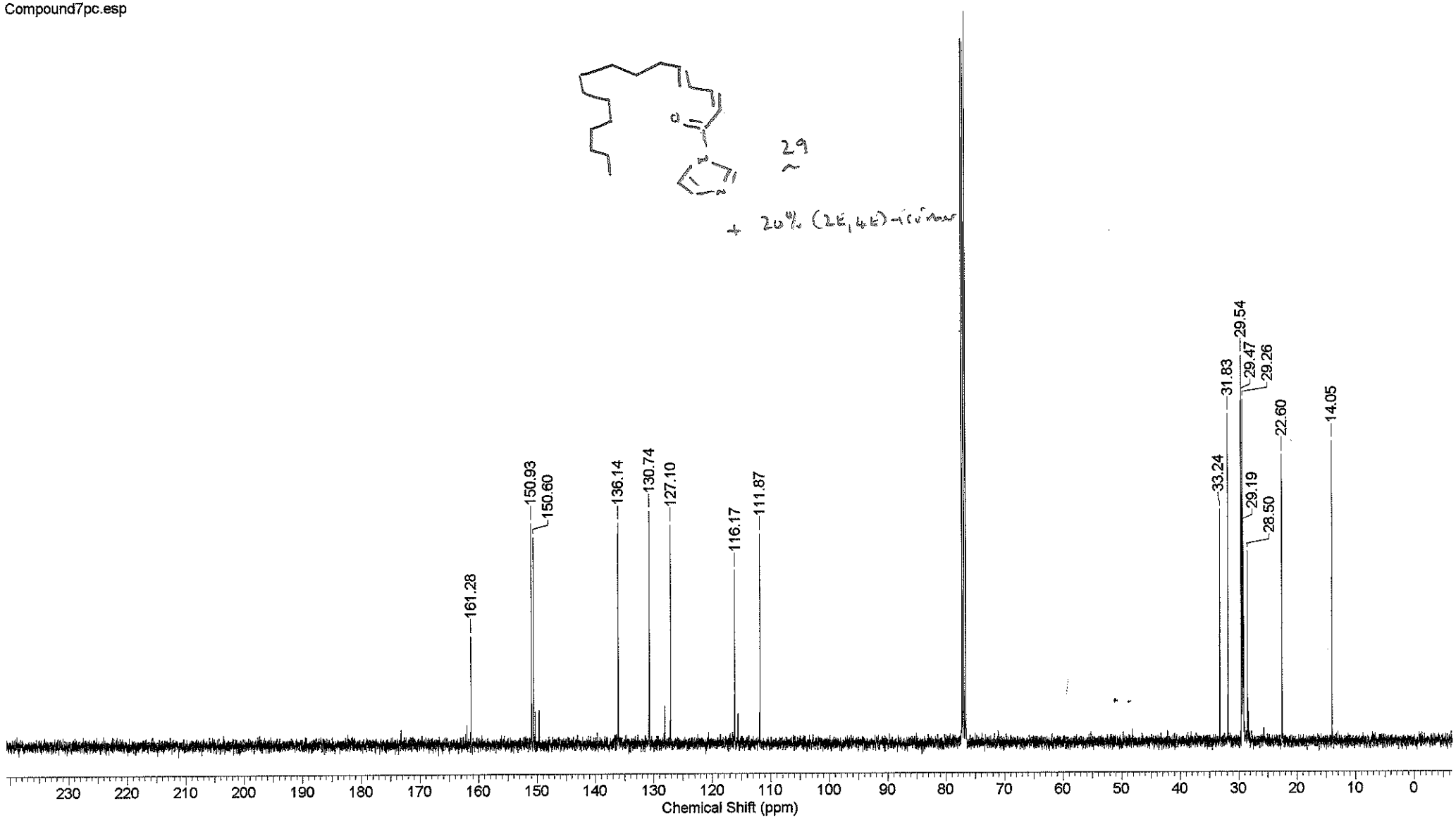
Compound7pp.esp

29 + 20% (2E, 4E)-
isomer



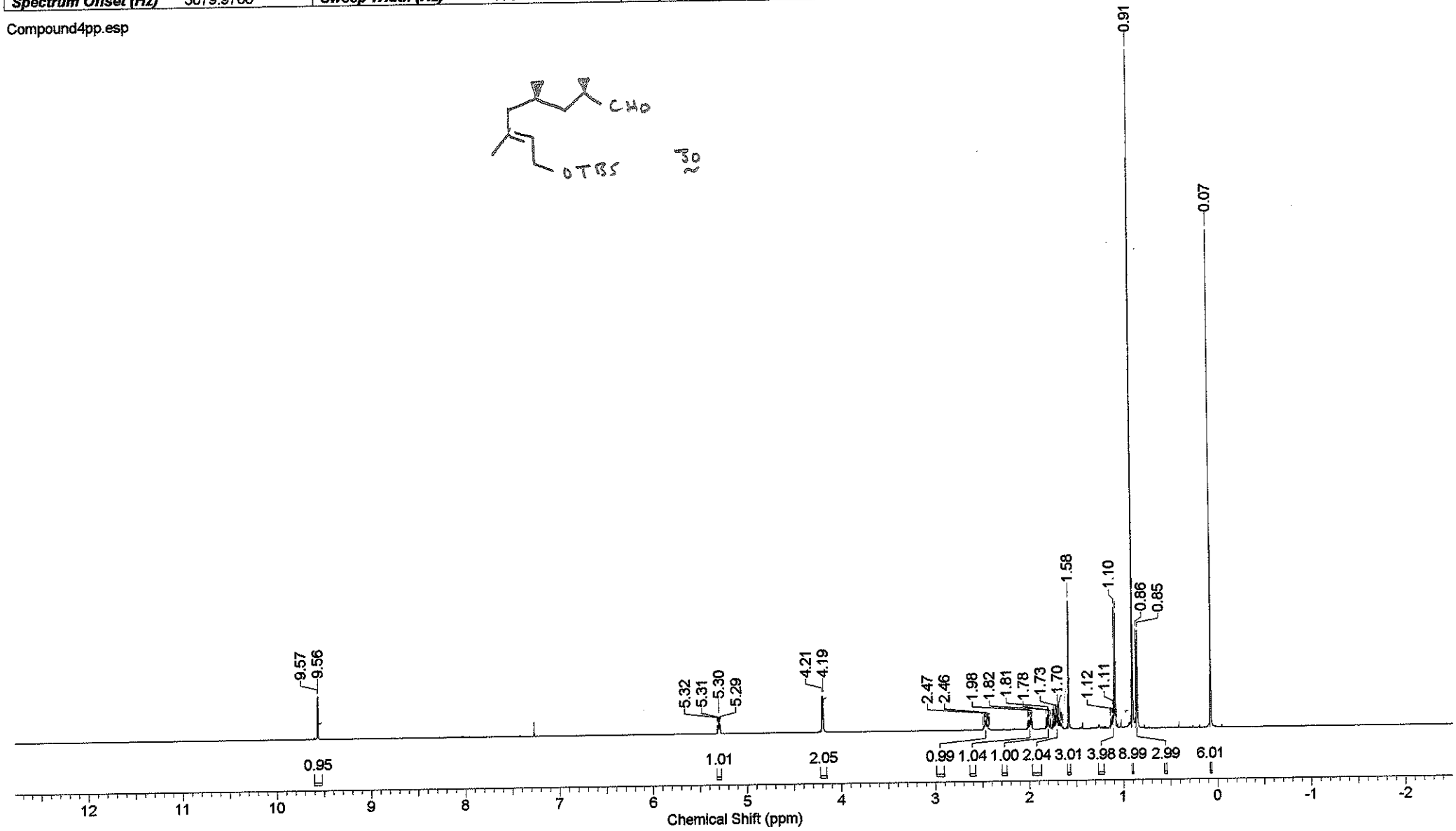
Acquisition Time (sec)	1.0835	***Comment***	MWC069pc mCARBON CDCl3 {e:\bruk400data\2010\Jan} ejt 34			***Date***	26 Jan 2010 14:19:44
Date Stamp	26 Jan 2010 14:19:44			***File Name***	F:\Chemistry\Year 2 data\NMR data\Data\Compound7\MWC069pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11327.6152
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.600				

Compound7pc.esp



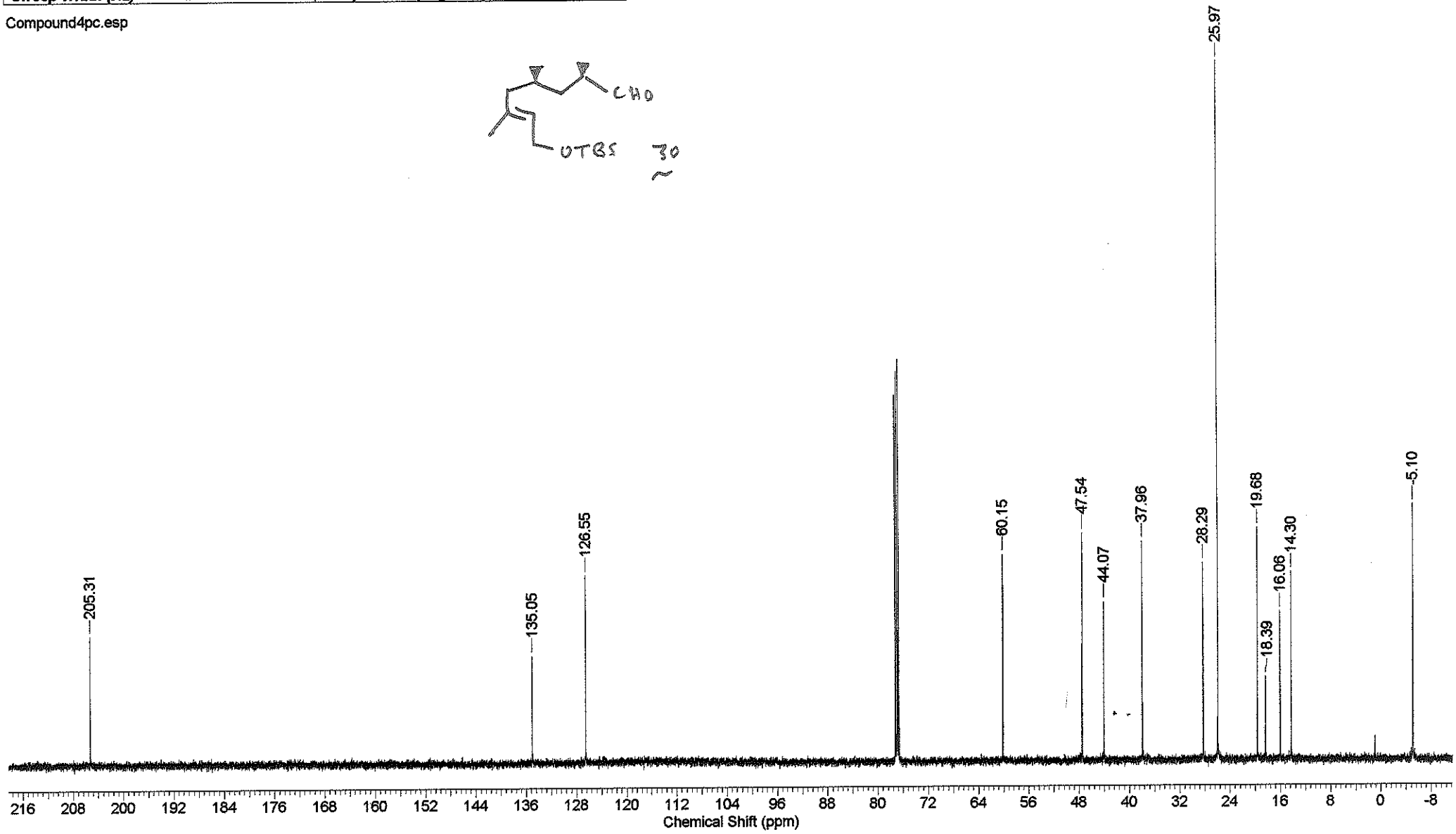
Acquisition Time (sec)	3.1719	***Comment***	MWE019pp mPROTON CDCl3 /opt/bruk500data/2010/Oct ejt 41	***Date***	12 Oct 2010 07:28:00		
Date Stamp	12 Oct 2010 07:28:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 4\MWE019pp_000001r		
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	57.00	***SW(cyclical) (Hz)***	10330.58	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	3079.9768	***Sweep Width (Hz)***	10330.26	***Temperature (degree C)***	21.282		

Compound4pp.esp



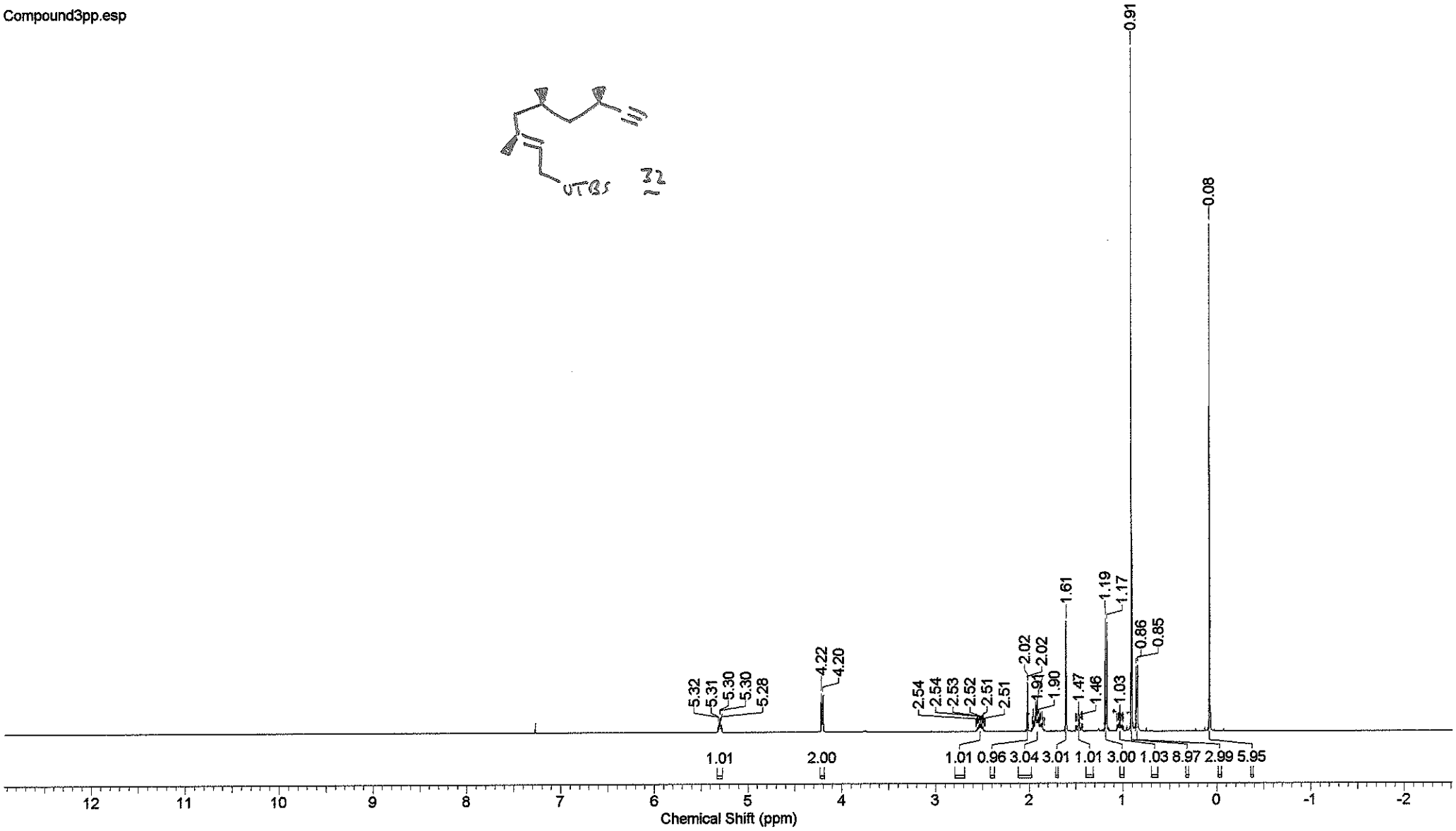
Acquisition Time (sec)	1.1010	***Comment***	MWE019pc mCARBON CDCl3 /opt/bruk500data/2010/Oct ejt 7	***Date***	11 Oct 2010 13:47:44		
Date Stamp	11 Oct 2010 13:47:44			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 4\MWE019pc_000001r		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***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)***	12571.1768
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	21.677				

Compound4pc.esp



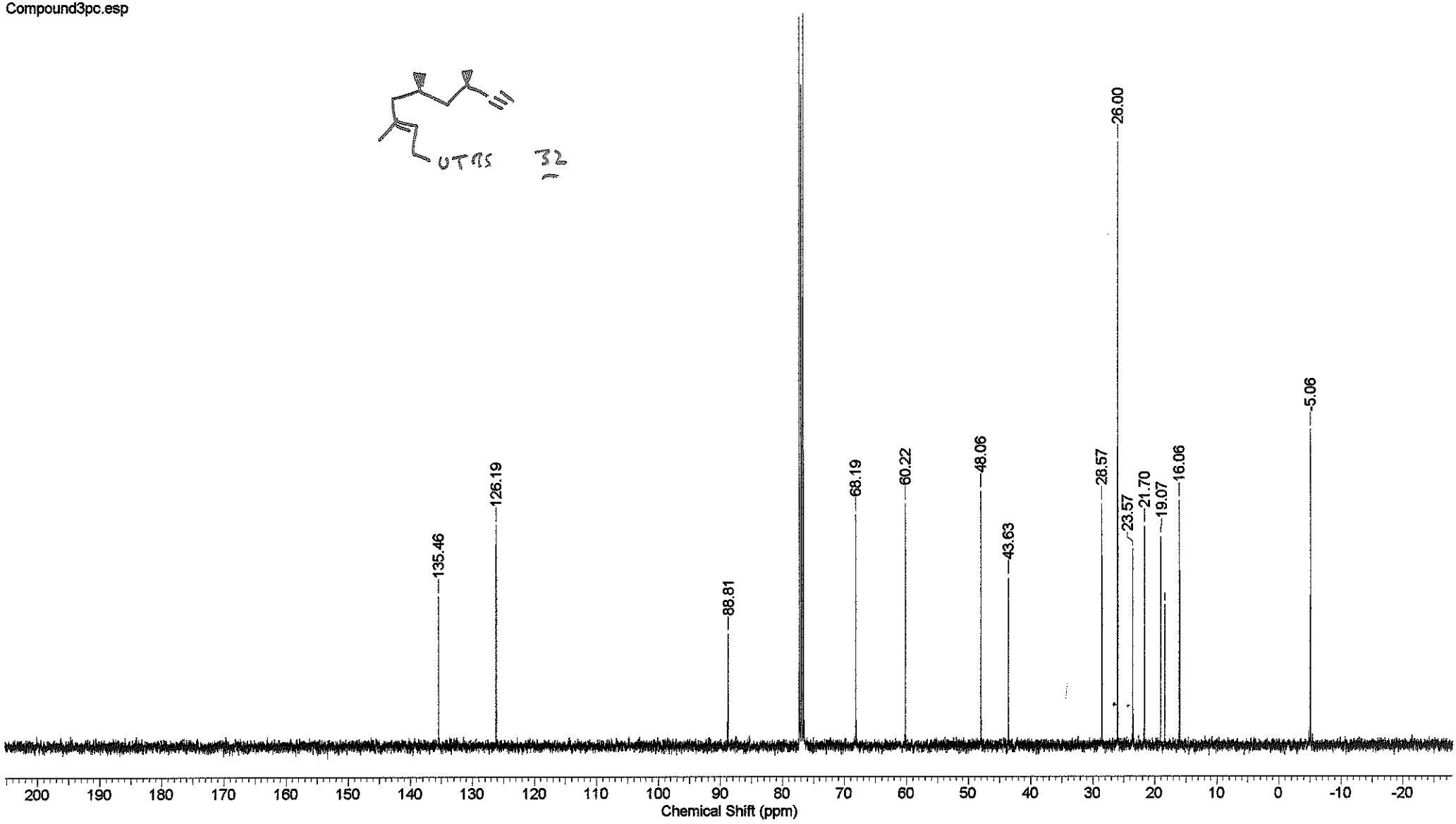
Acquisition Time (sec)	3.9649	***Comment***	MWE021pp mPROTON CDCl3 {e:\bruk400data\2010\Oct} ejt 35			***Date***	14 Oct 2010 13:52:00
Date Stamp	14 Oct 2010 13:52:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 3\MWE021pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number 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)***	2465.4316
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.400				

Compound3pp.esp



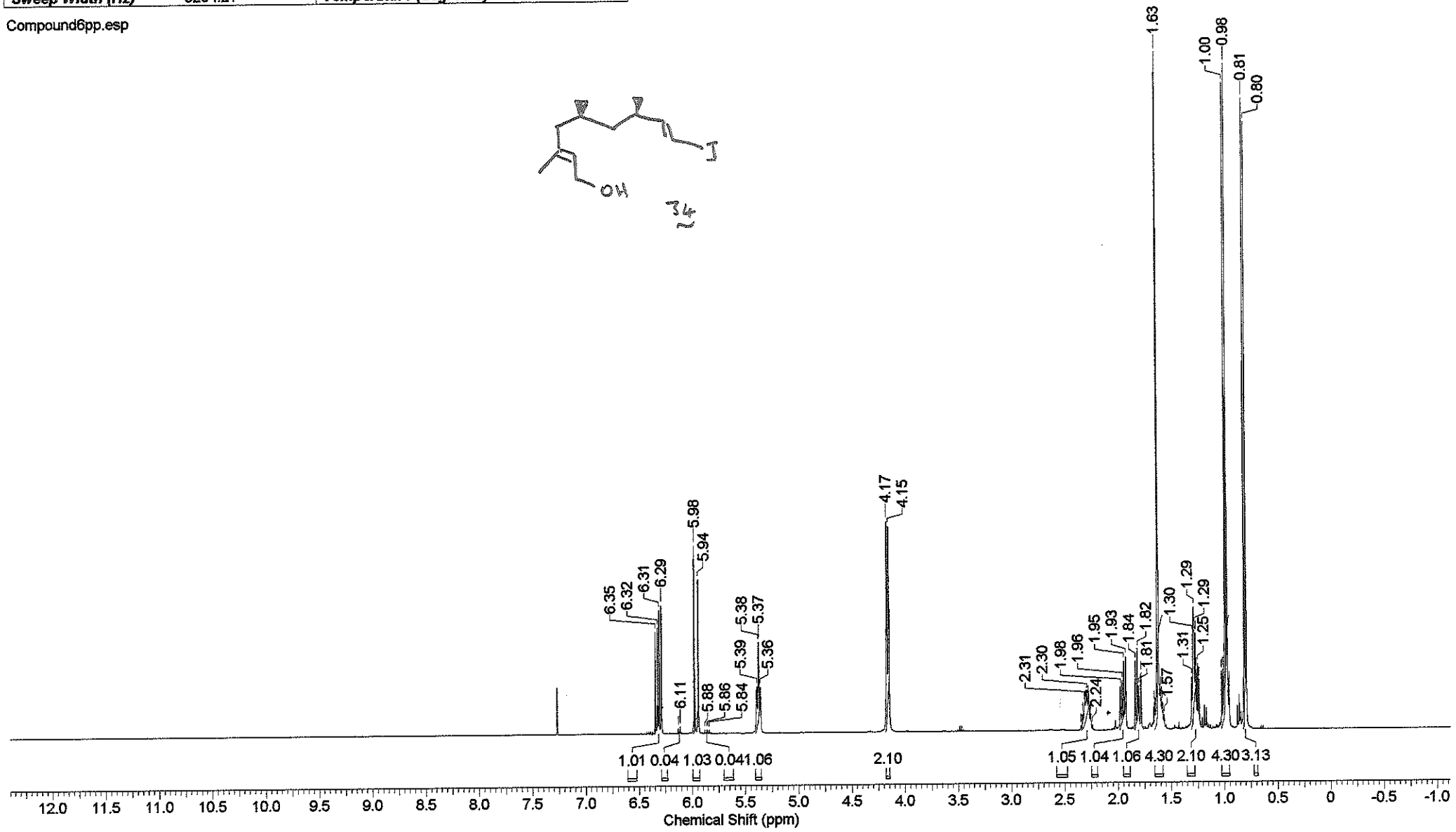
Acquisition Time (sec)	1.0835	***Comment***	MWE021pc mCARBON CDCl3 {e:\bruk400data\2010\Oct} ejt 35			***Date***	14 Oct 2010 14:15:28
Date Stamp	14 Oct 2010 14:15:28			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 3\MWE021pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11332.2295
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.200				

Compound3pc.esp



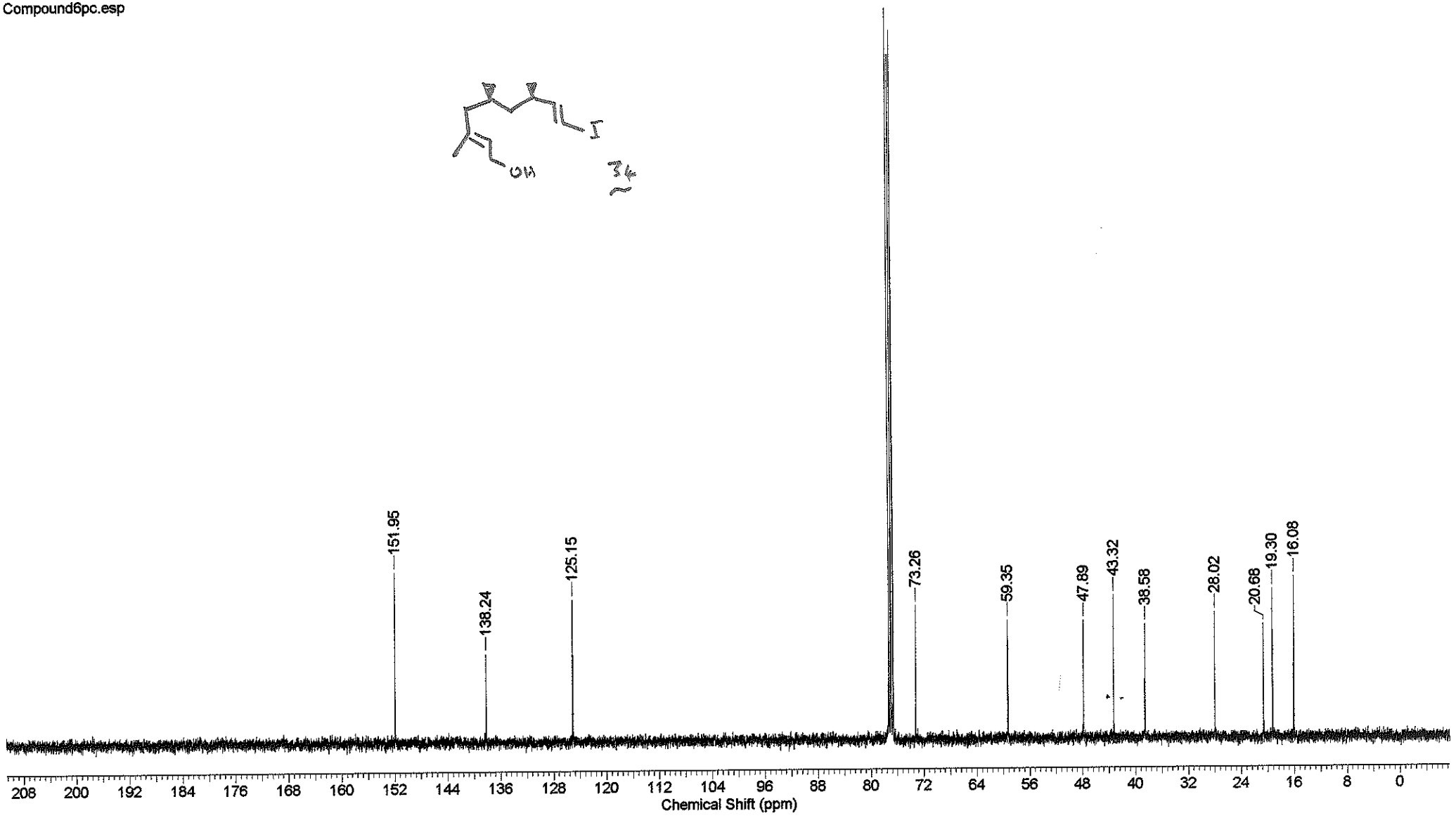
Acquisition Time (sec)	3.9649	***Comment***	MWE036pp mPROTON CDCl3 {e:\bruk400data\2010\Nov} ejt 13			***Date***	17 Nov 2010 17:08:16
Date Stamp	17 Nov 2010 17:08:16			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 6\MWE036pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	114.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.1794
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.300				

Compound6pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWE036pc mCARBON CDCl3 {e:\bruk400data\2010\Nov} ejt 23	***Date***	17 Nov 2010 13:30:40		
Date Stamp	17 Nov 2010 13:30:40			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 6\MWE036pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	11331.3076
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.900				

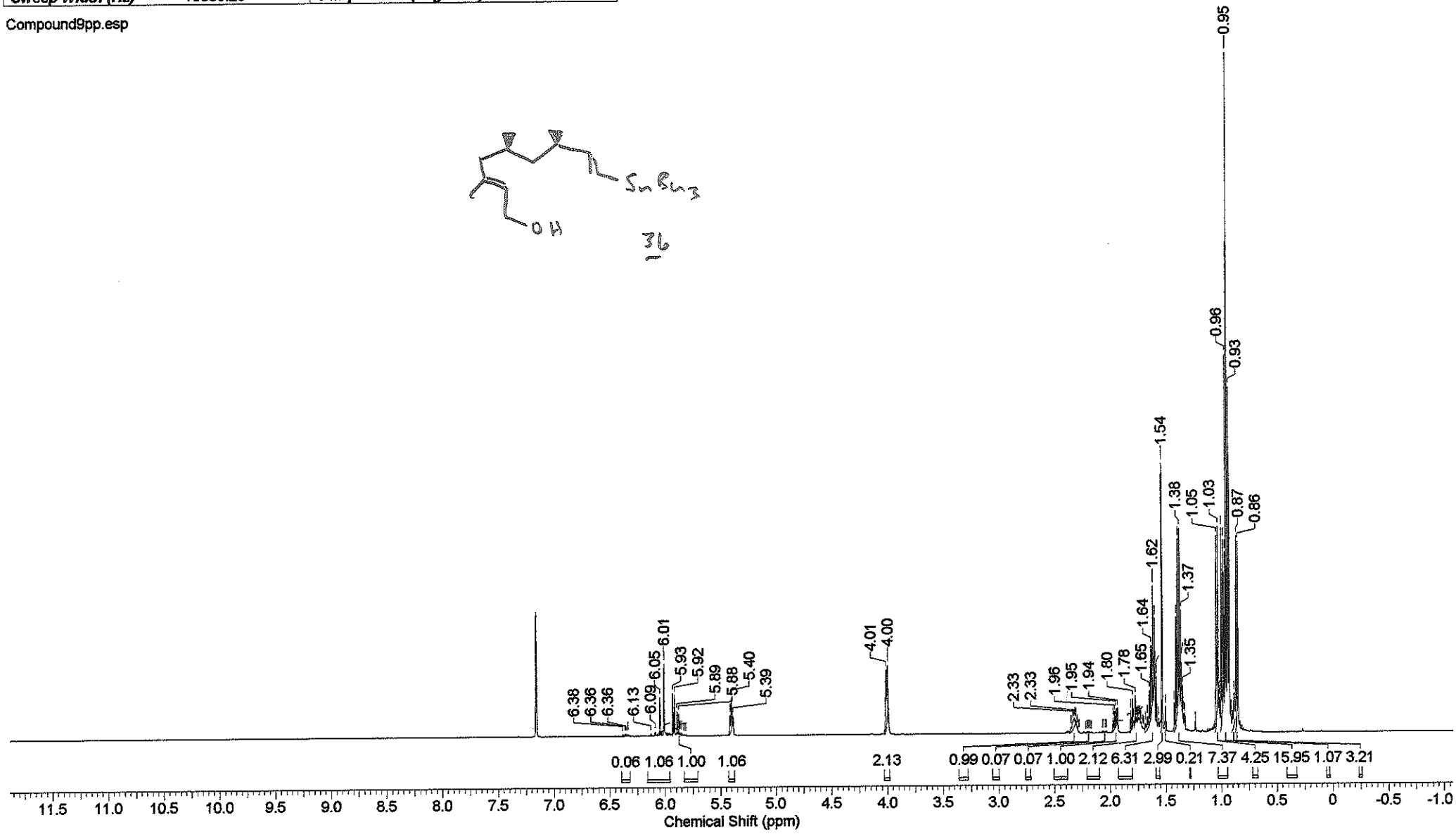
Compound6pc.esp



06/06/2012 12:37:46

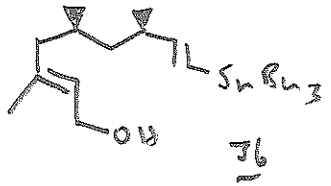
Acquisition Time (sec)	3.1719	***Comment***	MWF023pp mPROTON C6D6 /opt/bruk500data/2011/Apr ejt 6			***Date***	26 Apr 2011 09:55:12
Date Stamp	26 Apr 2011 09:55:12			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 9\MWE057pp_000001r		
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	20.20	***SW(cyclical) (Hz)***	10330.58	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	3031.5835
Sweep Width (Hz)	10330.26	***Temperature (degree C)***	25.187				

Compound9pp.esp



Acquisition Time (sec)	1.1010	***Comment***	MWF023pc mCARBON C6D6 /opt/bruk500data/2011/Apr ejt 6	***Date***	26 Apr 2011 10:08:00		
Date Stamp	26 Apr 2011 10:08:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 9\MWE057pc_000001r		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	12650.5957
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	25.187				

Compound9pc.esp



156.10
137.33
129.30
125.85
59.67
48.92
44.58
40.58
29.98
28.04
22.16
19.85
16.41
14.34
10.16

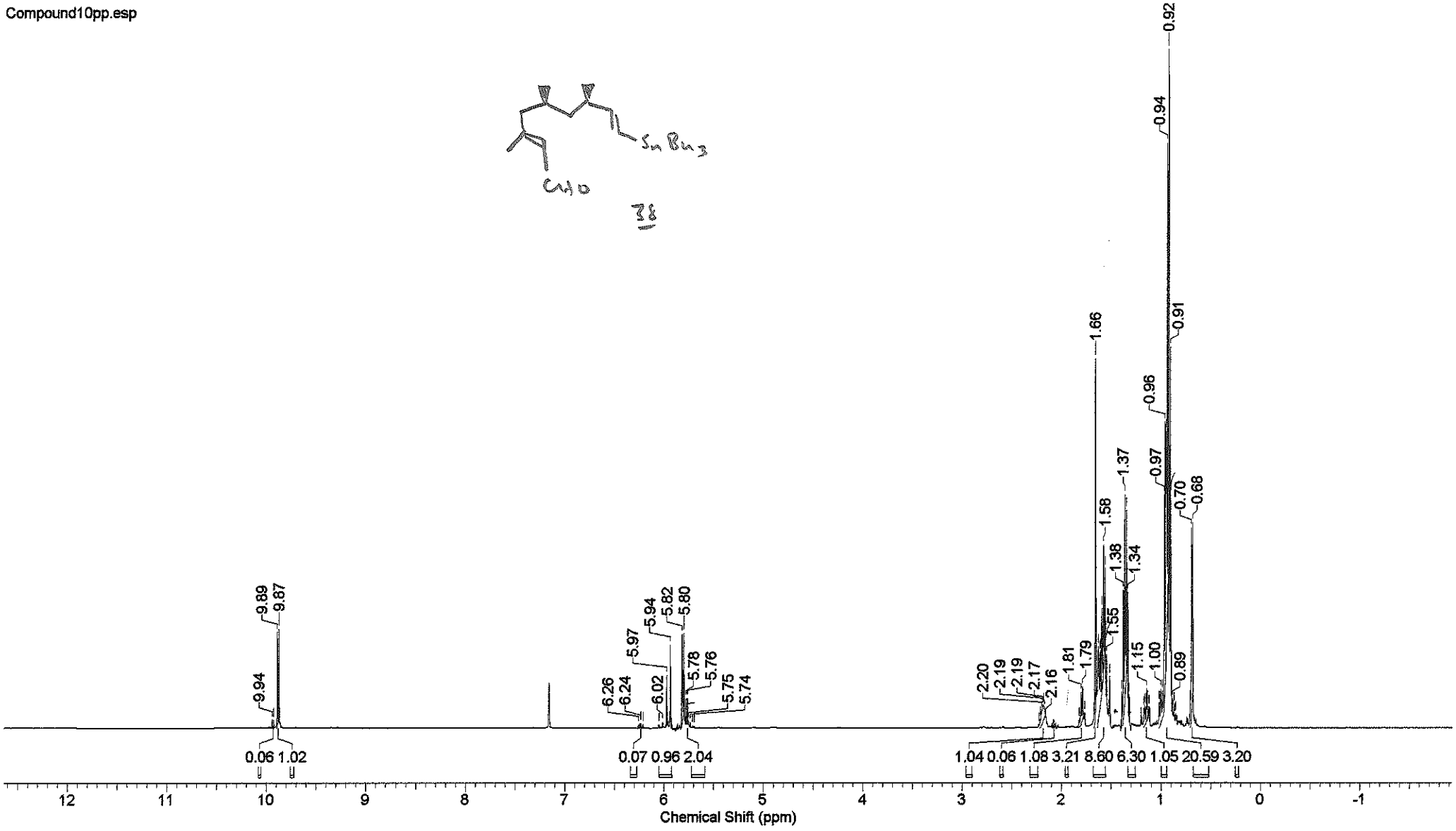
192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0

Chemical Shift (ppm)

06/06/2012 16:05:39

Acquisition Time (sec)	3.1719	***Comment***	MWF026pp mPROTON C6D6 /opt/bruk500data/2011/May ejt 3			***Date***	03 May 2011 09:44:32
Date Stamp	03 May 2011 09:44:32			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 10\MWE058pp_000001r		
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	8.00	***SW(cyclical) (Hz)***	10330.58	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	3031.5837
Sweep Width (Hz)	10330.26	***Temperature (degree C)***	22.623				

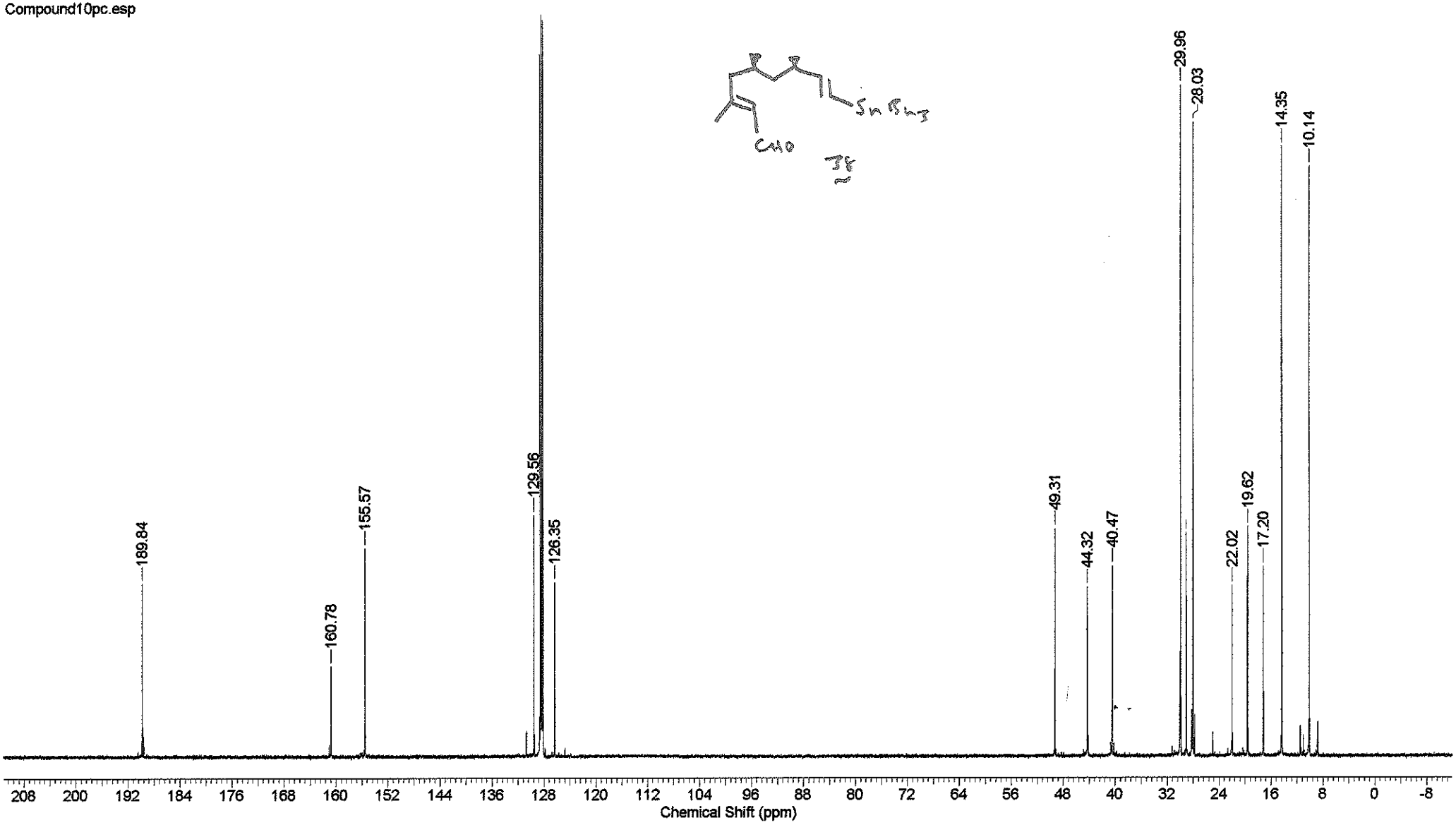
Compound10pp.esp



06/06/2012 16:14:06

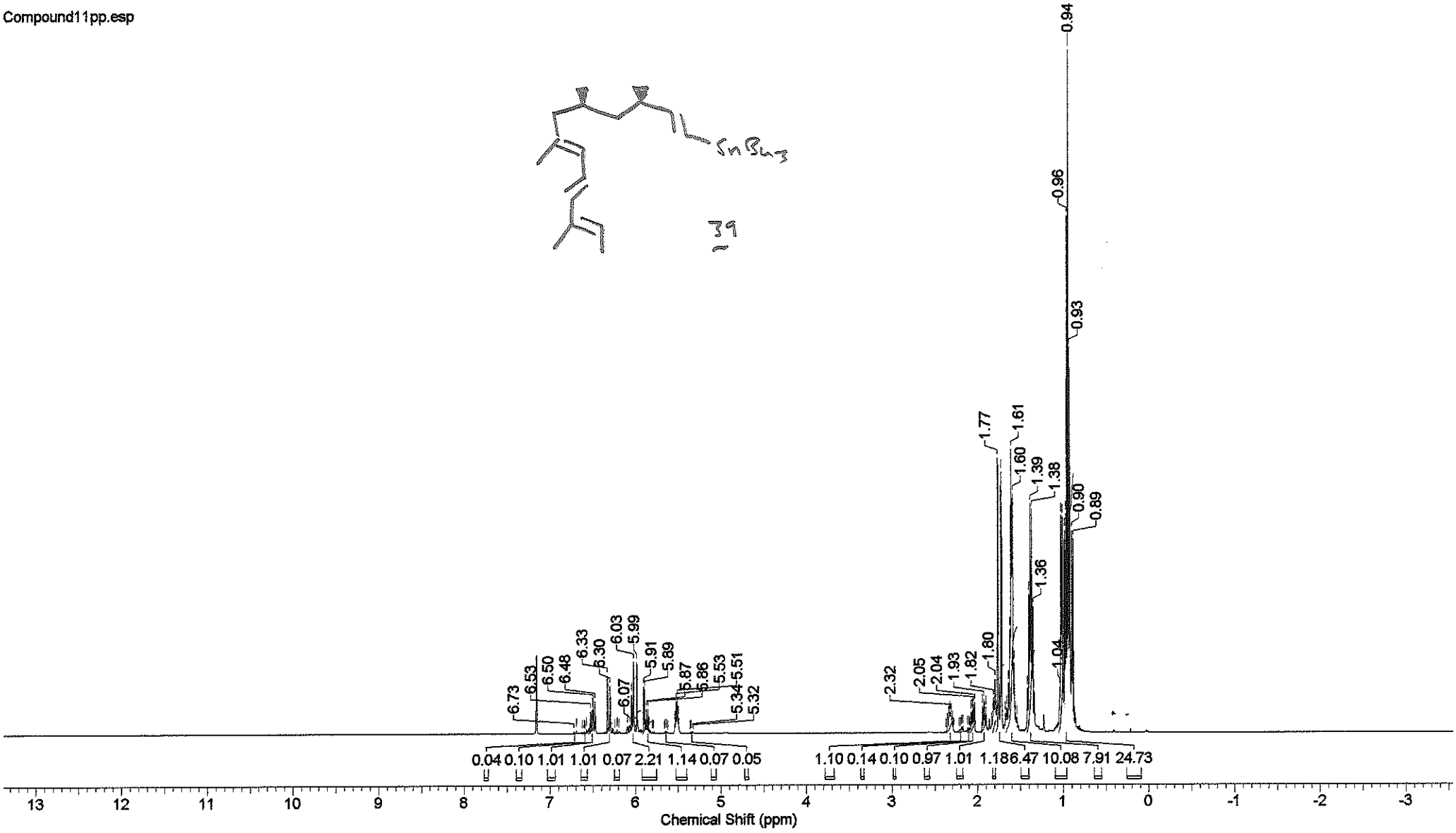
Acquisition Time (sec)	1.1010	***Comment***	MWF026pc mCARBON C6D6 /opt/bruk500data/2011/May ejt 3	***Date***	03 May 2011 09:57:20		
Date Stamp	03 May 2011 09:57:20			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 10\MWE058pc_000001r		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	12654.2275
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	23.116				

Compound10pc.esp



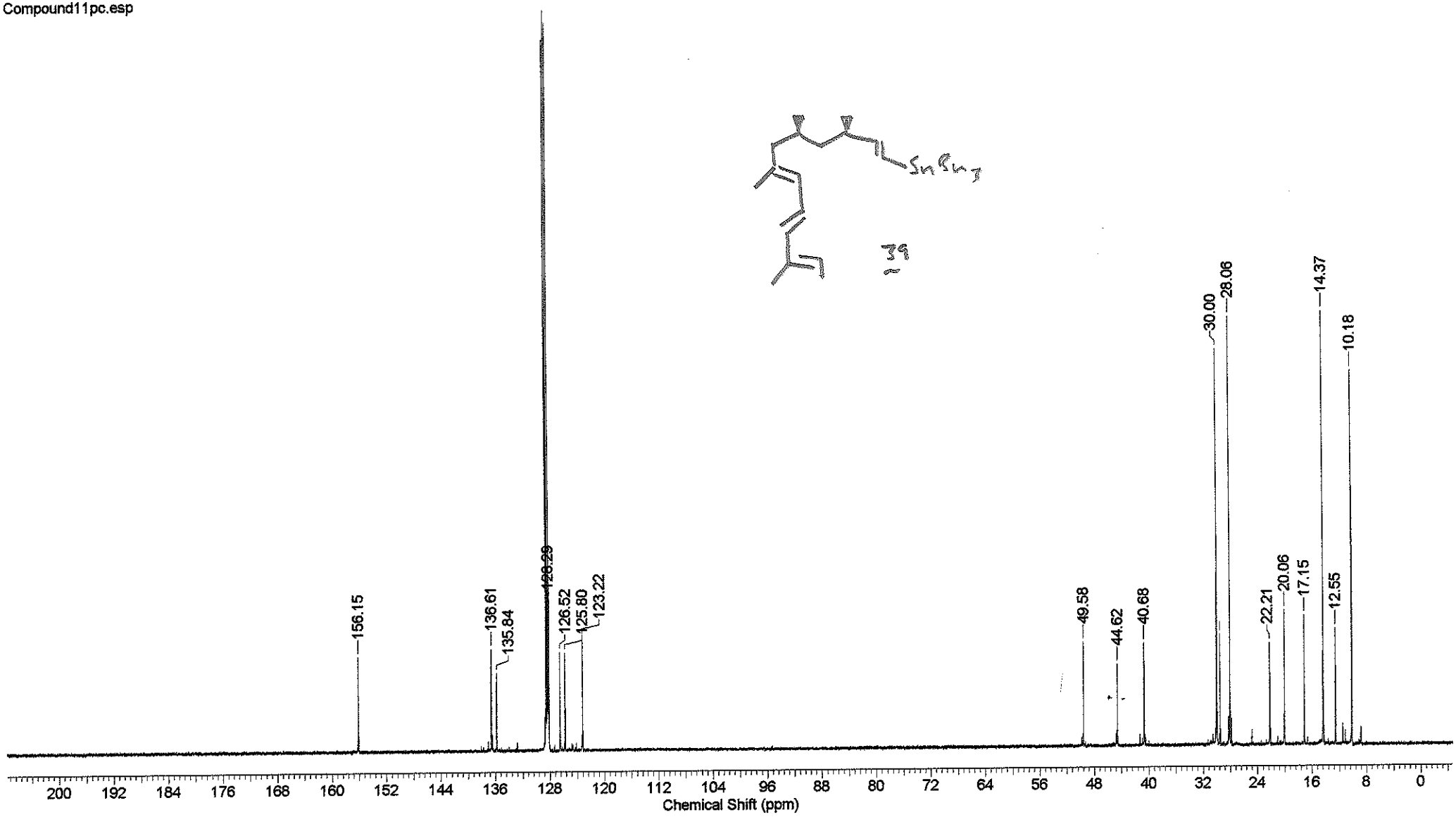
Acquisition Time (sec)	3.1719	***Comment***	MWF029pp mPROTON C6D6 /opt/bruk500data/2011/May ejt 5	***Date***	10 May 2011 08:57:36		
Date Stamp	10 May 2011 08:57:36			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 11\MWF029pp_000001r		
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	9.00	***SW(cyclical) (Hz)***	10330.58	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	3031.2683
Sweep Width (Hz)	10330.26	***Temperature (degree C)***	25.187				

Compound11pp.esp



Acquisition Time (sec)	1.1010	***Comment***	MWF029pc mCARBON C6D6 /opt/bruk500data/2011/May ejt 5			***Date***	10 May 2011 09:10:24
Date Stamp	10 May 2011 09:10:24			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 11\MWF029pc_000001r		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	12654.2275
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	25.187				

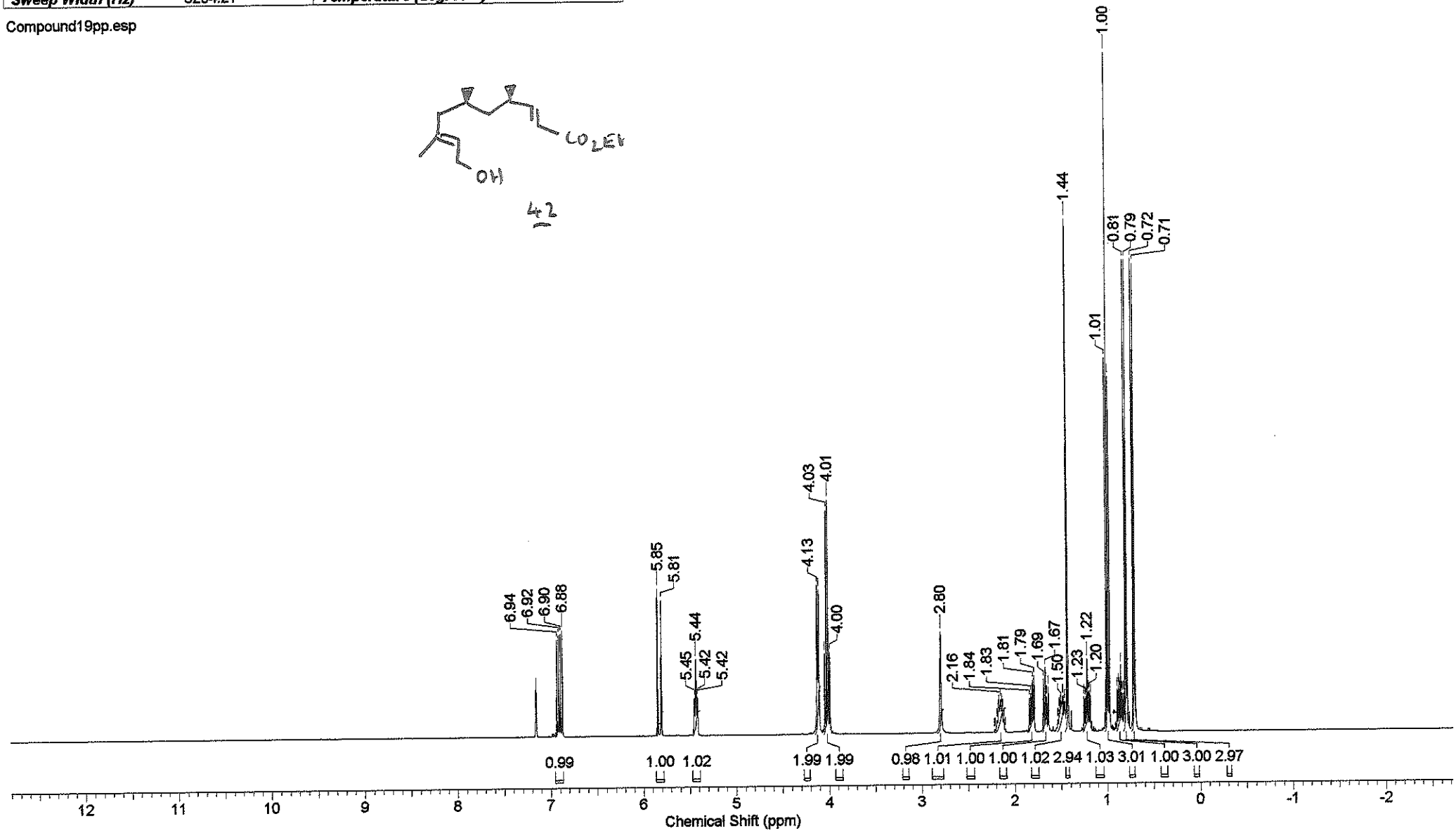
Compound11pc.esp



Acquisition Time (sec)	3.9649	***Comment***	MWF066pp mPROTON C6D6 {e:\bruk400data\2011\Jun} ejt 21			***Date***	30 Jun 2011 12:48:00
Date Stamp	30 Jun 2011 12:48:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 19\MWF066pp_000001r		
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	22.60	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2425.7046
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.900				

Compound19pp.esp

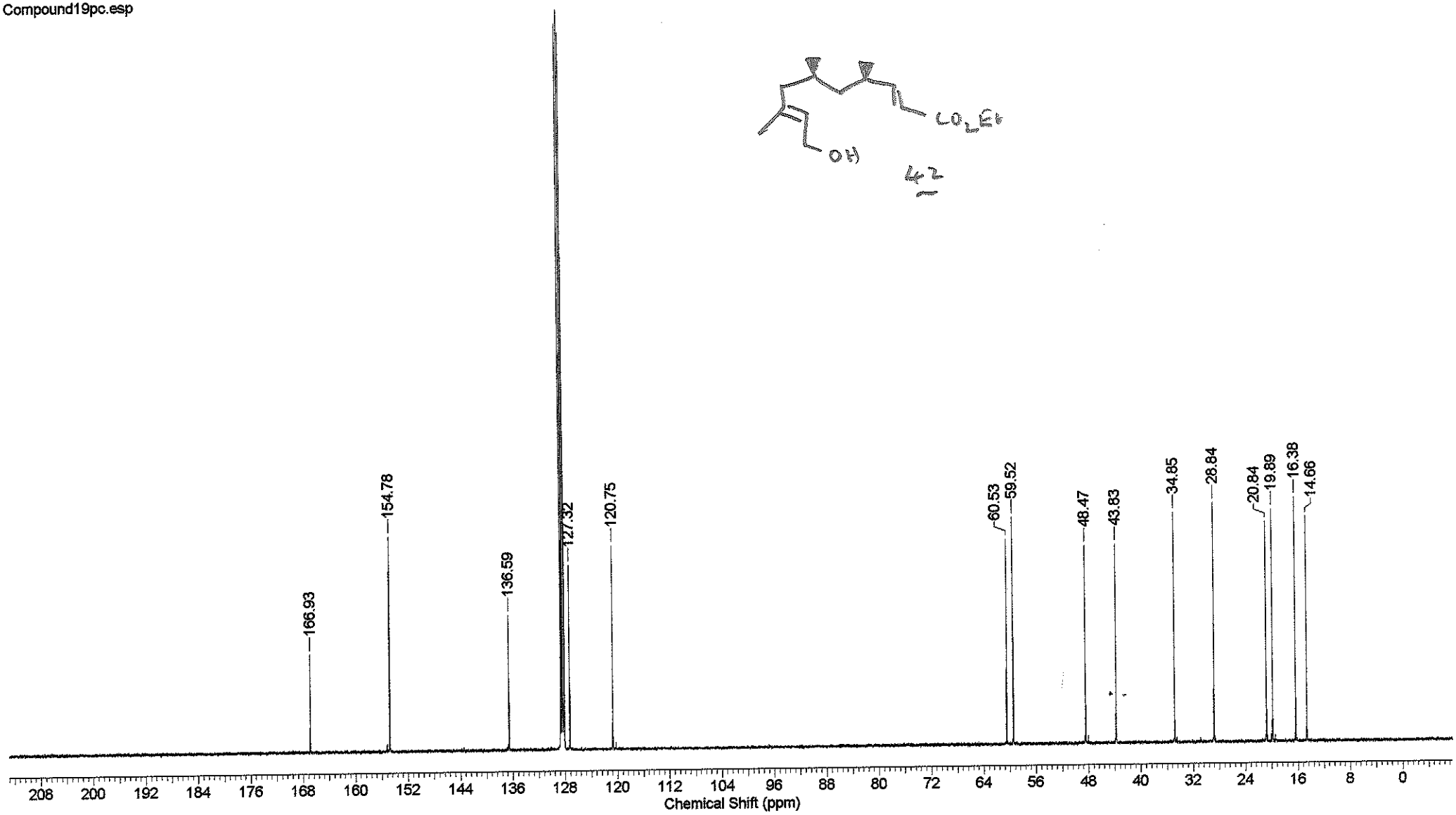
42



Acquisition Time (sec)	1.0835	***Comment***	MWF066pc mCARBON C6D6 {e:\bruk400data\2011\Jun} ejt 18			***Date***	30 Jun 2011 12:39:28
Date Stamp	30 Jun 2011 12:39:28			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 19\MWF066pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11395.3301
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.500				

Compound19pc.esp

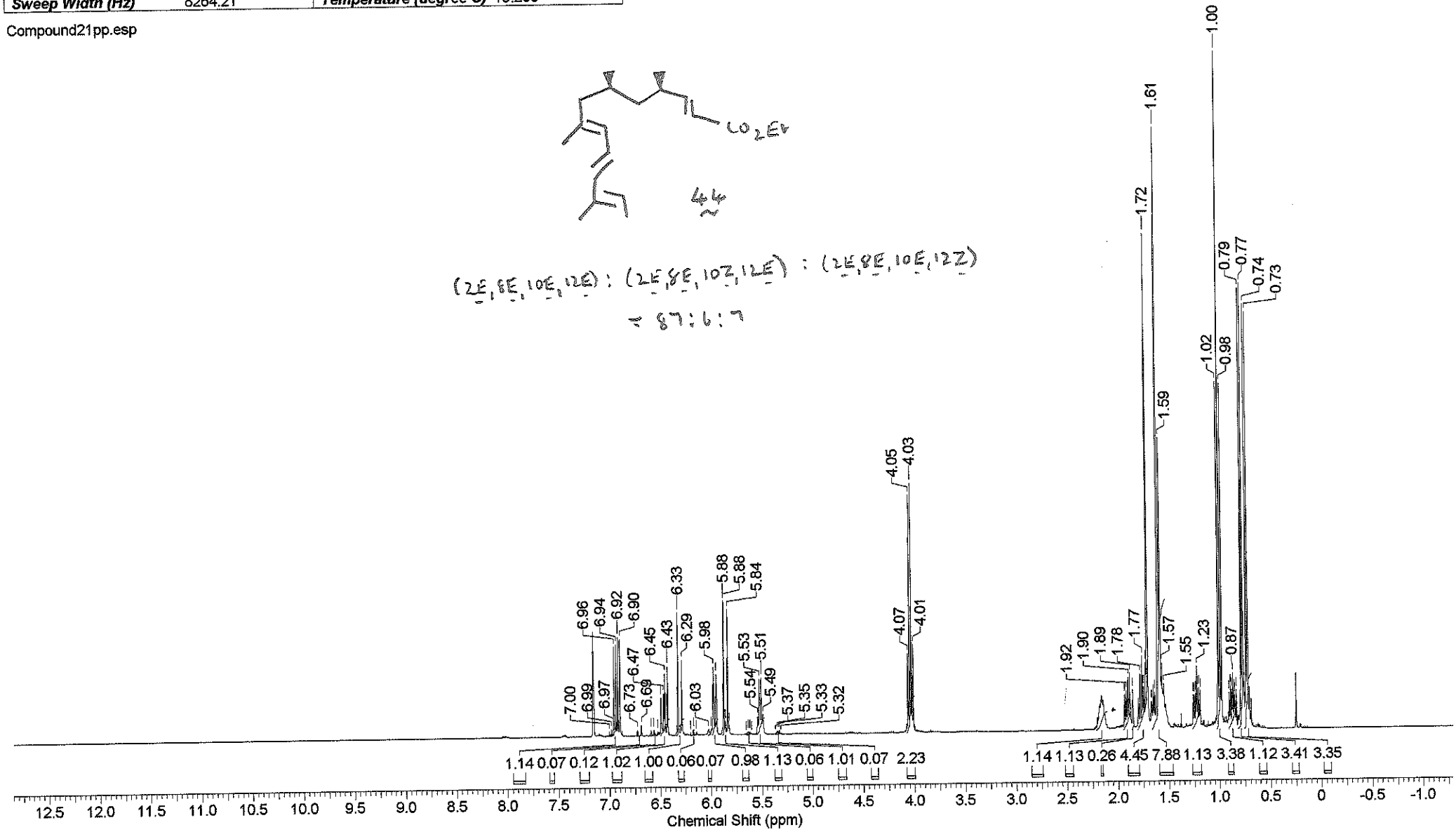
42



14/07/2012 10:43:52

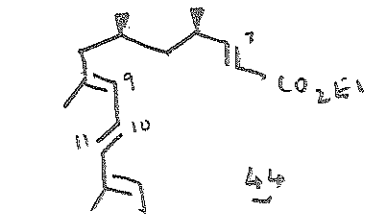
Acquisition Time (sec)	3.9649	***Comment***	MWF048pp mPROTON C6D6 {e:\bruk400data\2011\May} ejt 36			***Date***	01 Jun 2011 06:38:56
Date Stamp	01 Jun 2011 06:38:56			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 21\MWF048pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	36.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2432.7671
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.200				

Compound21pp.esp



Acquisition Time (sec)	3.9649	***Comment***	MWF048pp mPROTON C6D6 {e:\bruk400data\2011\May} ejt 36	***Date***	01 Jun 2011 06:38:56		
Date Stamp	01 Jun 2011 06:38:56			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 21\MWF048pp_000001r		
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	36.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2432.7671
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.200				

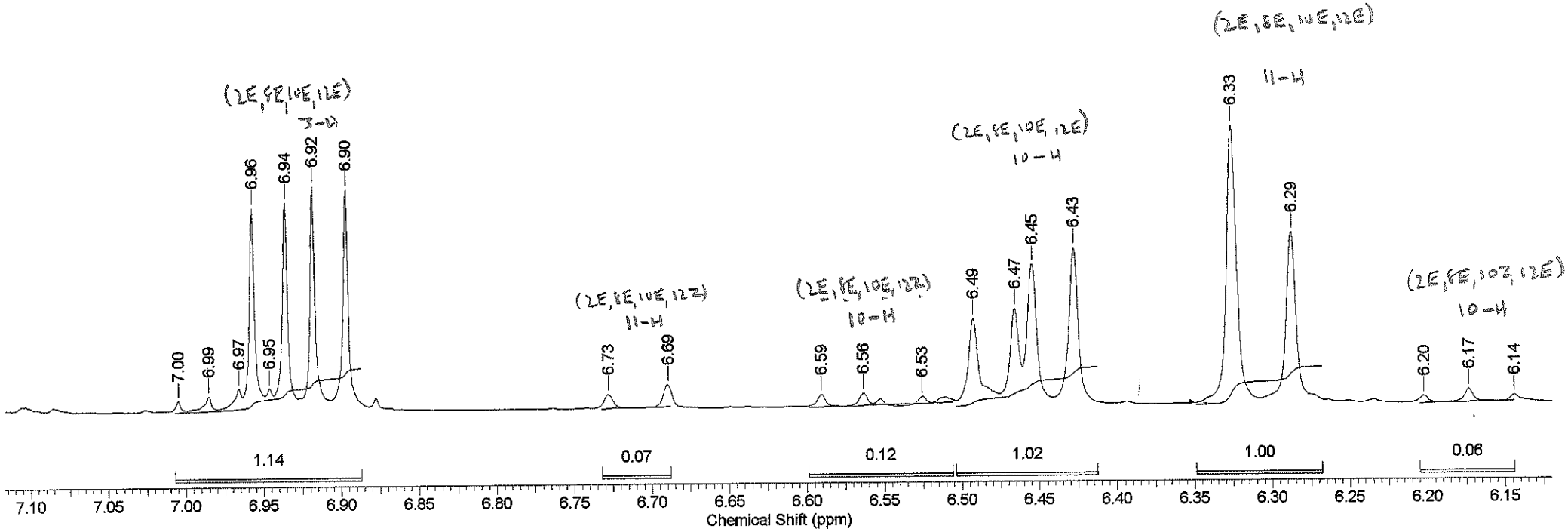
Compound21pp.esp



44

(2E,8E,10E,12E) : (2E,8E,10Z,12E) : (2E,8E,10E,12Z)

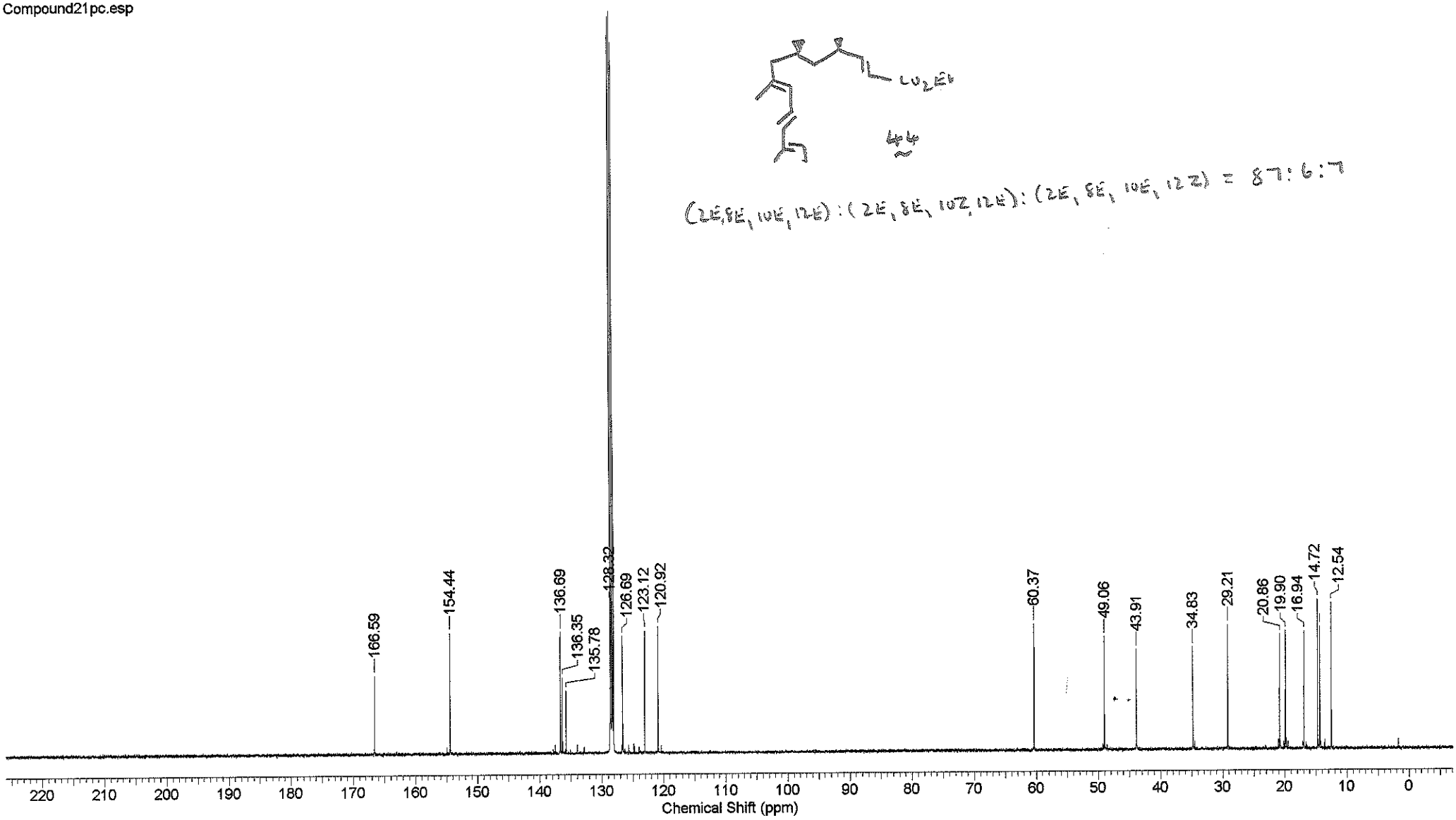
= 87:6:7



Acquisition Time (sec)	1.0835	***Comment***	MWF048pc mCARBON C6D6 {e:\bruk400data\2011\May} ejt 36			***Date***	01 Jun 2011 07:10:56
Date Stamp	01 Jun 2011 07:10:56			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 21\MWF048pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11397.1934
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.100				

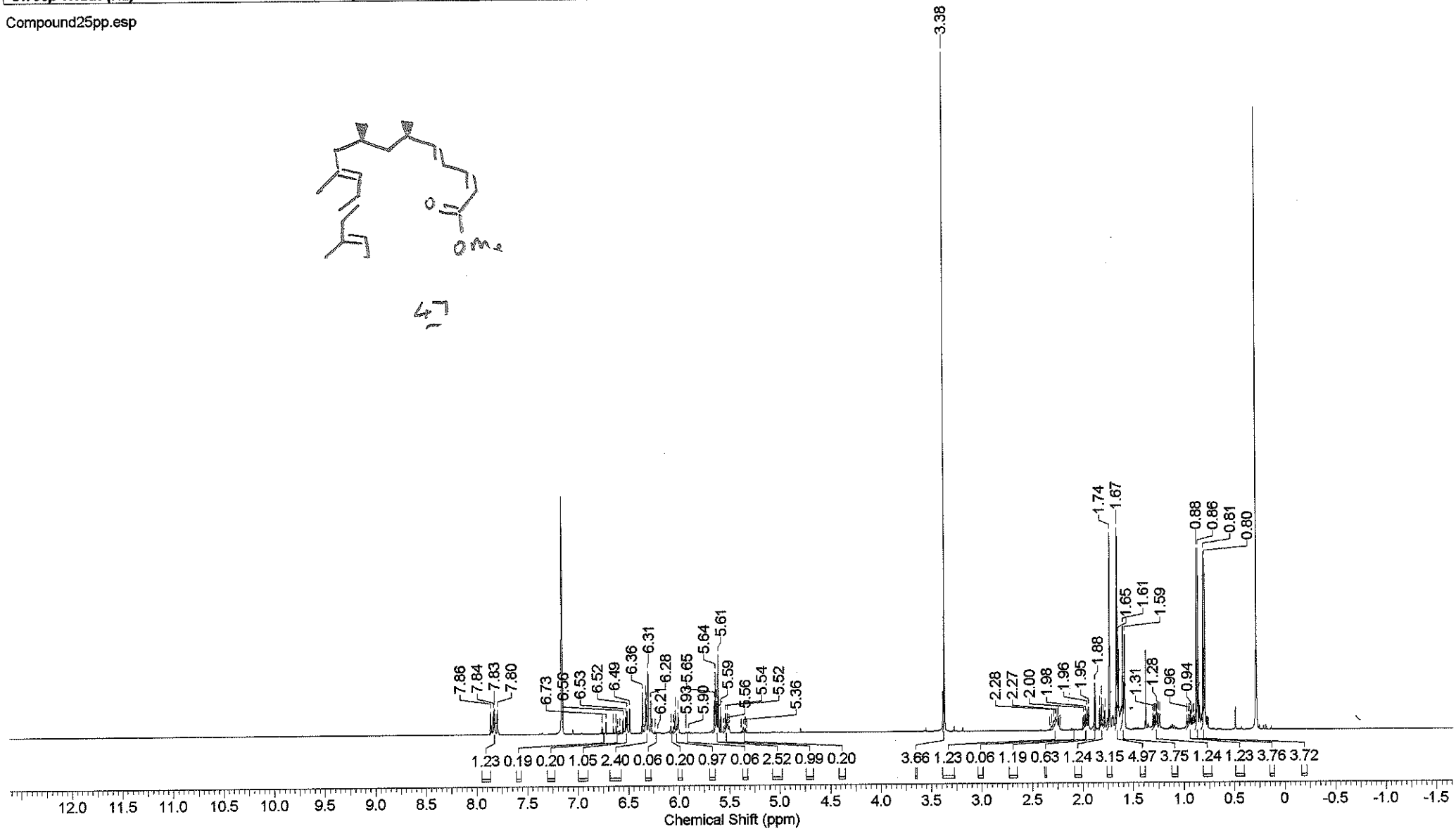
Compound21pc.esp

(2E,8E,10E,12E) : (2E,8E,10Z,12E) : (2E,8E,10E,12Z) = 87 : 6 : 7



Acquisition Time (sec)	3.9649	***Comment***	MWG064pp mPROTON C6D6 {e:\bruk400data\2012\Apr} ejt 18	***Date***	23 Apr 2012 08:51:12		
Date Stamp	23 Apr 2012 08:51:12			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 25\MWH048pp_000001r		
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	101.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2092
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.800				

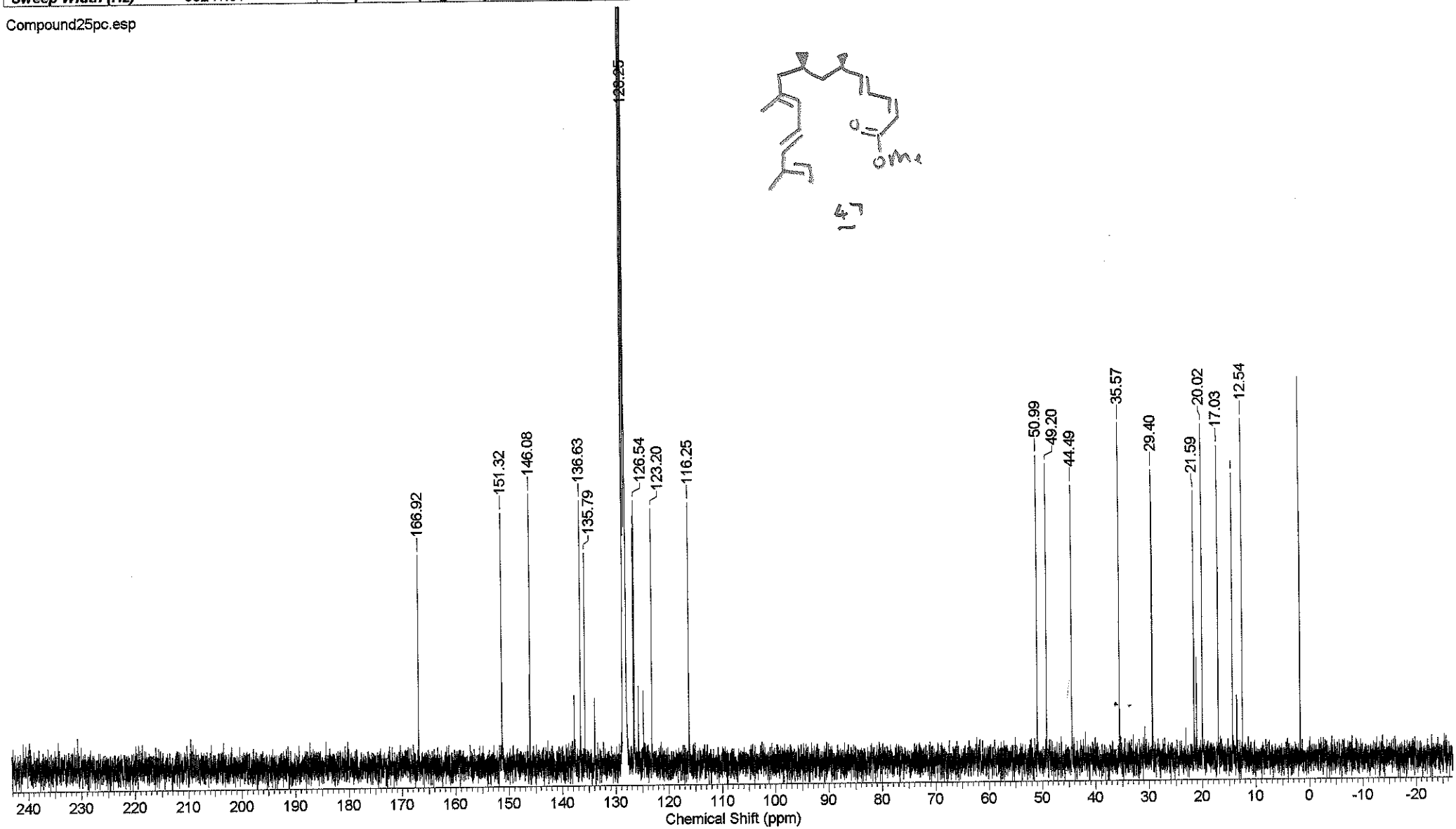
Compound25pp.esp



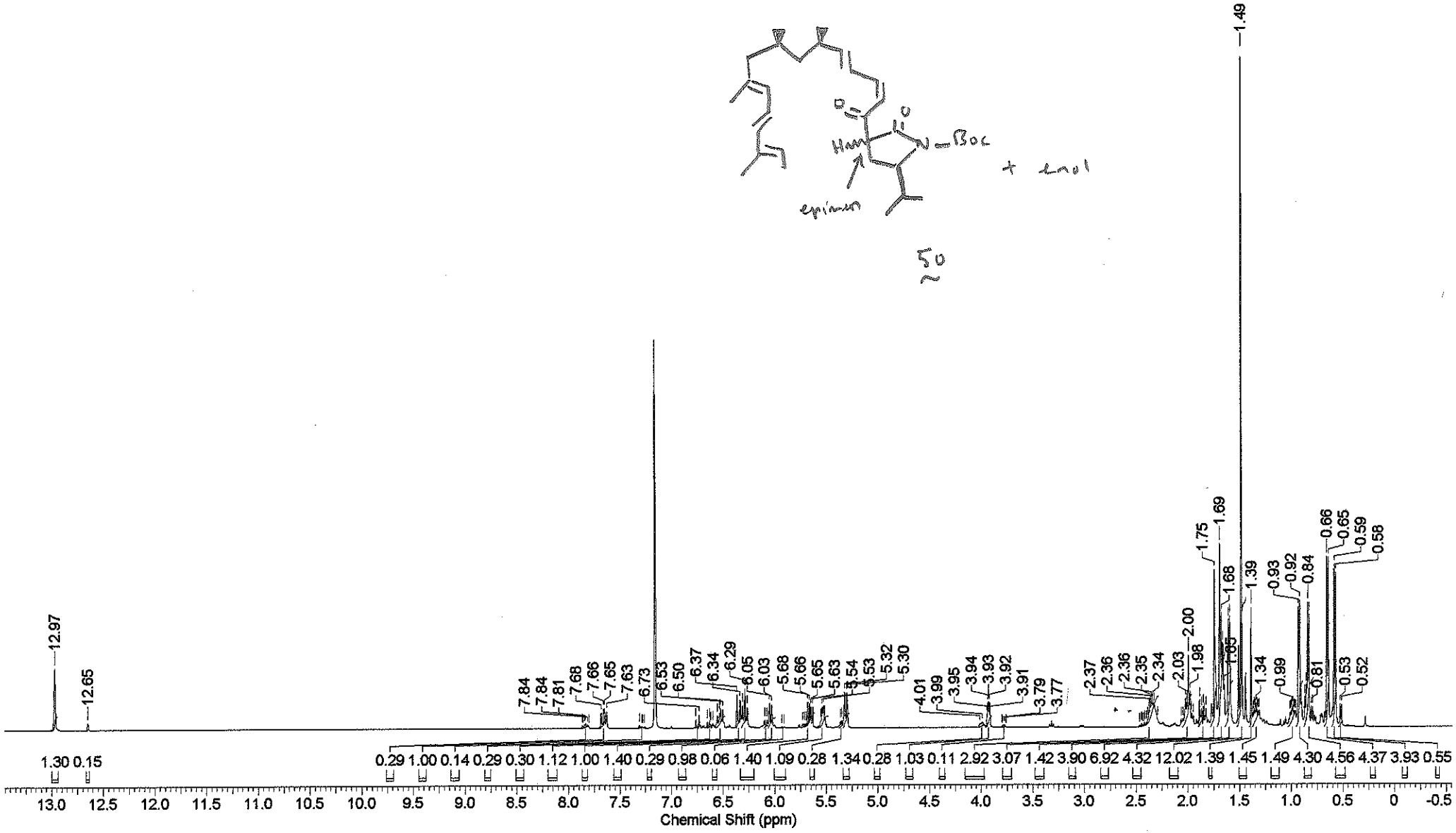
Acquisition Time (sec)	1.0835	***Comment***	MWG064pc mCARBON C6D6 {e:\bruk400data\2012\Apr} ejt 18			***Date***	23 Apr 2012 09:12:32
Date Stamp	23 Apr 2012 09:12:32			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 25\MWH048pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.5010
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.600				

Compound25pc.esp

47

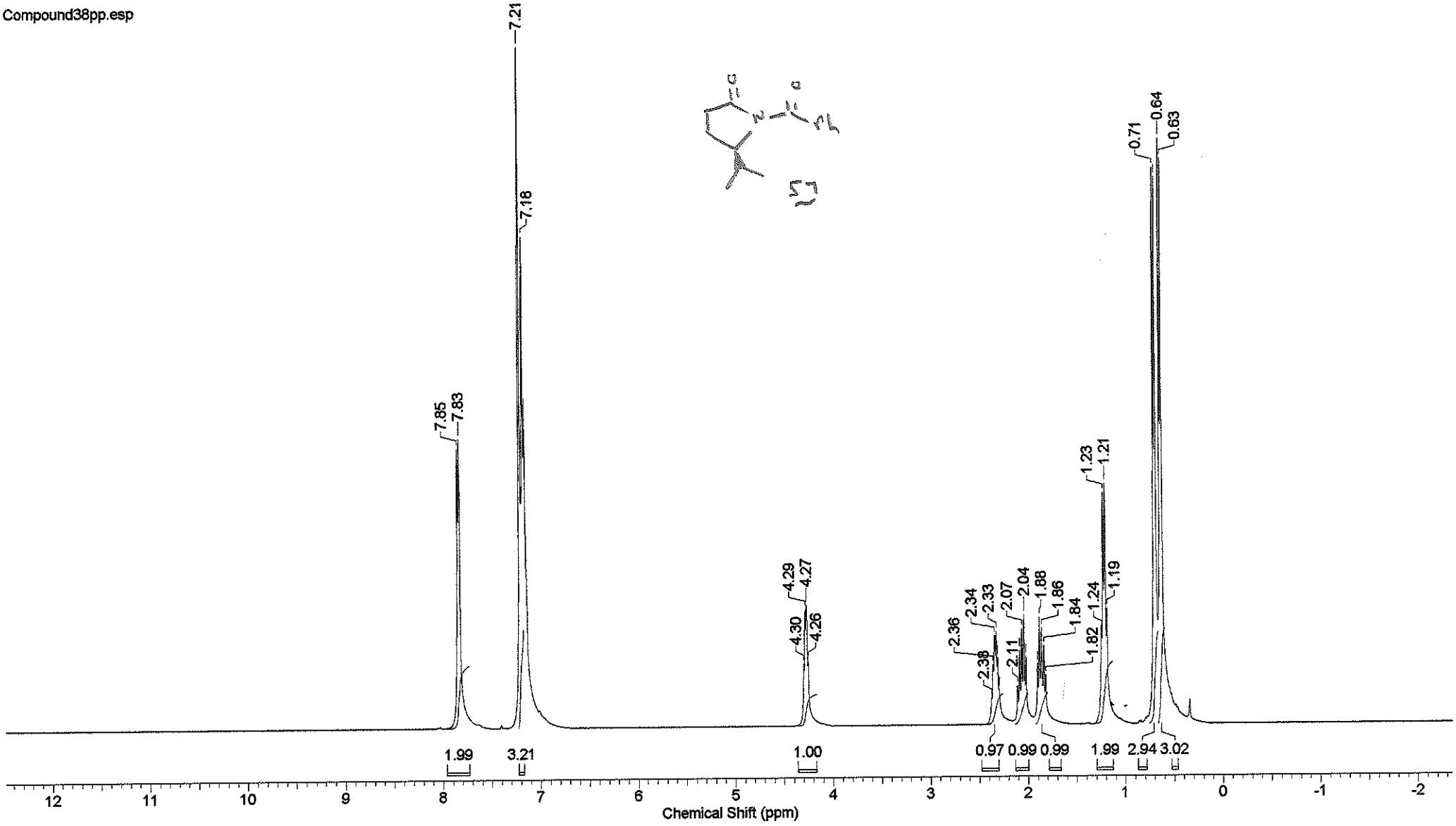


Acquisition Time (sec)	3.1719	***Comment***	MWF036pp mPROTON C6D6 /opt/bruk500data/2011/May ejt 27			***Date***	17 May 2011 16:06:24
Date Stamp	17 May 2011 16:06:24			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 28\MWF036pp_000001r		
Frequency (MHz)	500.13	***Nucleus***	1H	***Number 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***	BENZENE-d6	***Spectrum Offset (Hz)***	3031.5837
Sweep Width (Hz)	10330.26	***Temperature (degree C)***	22.032				



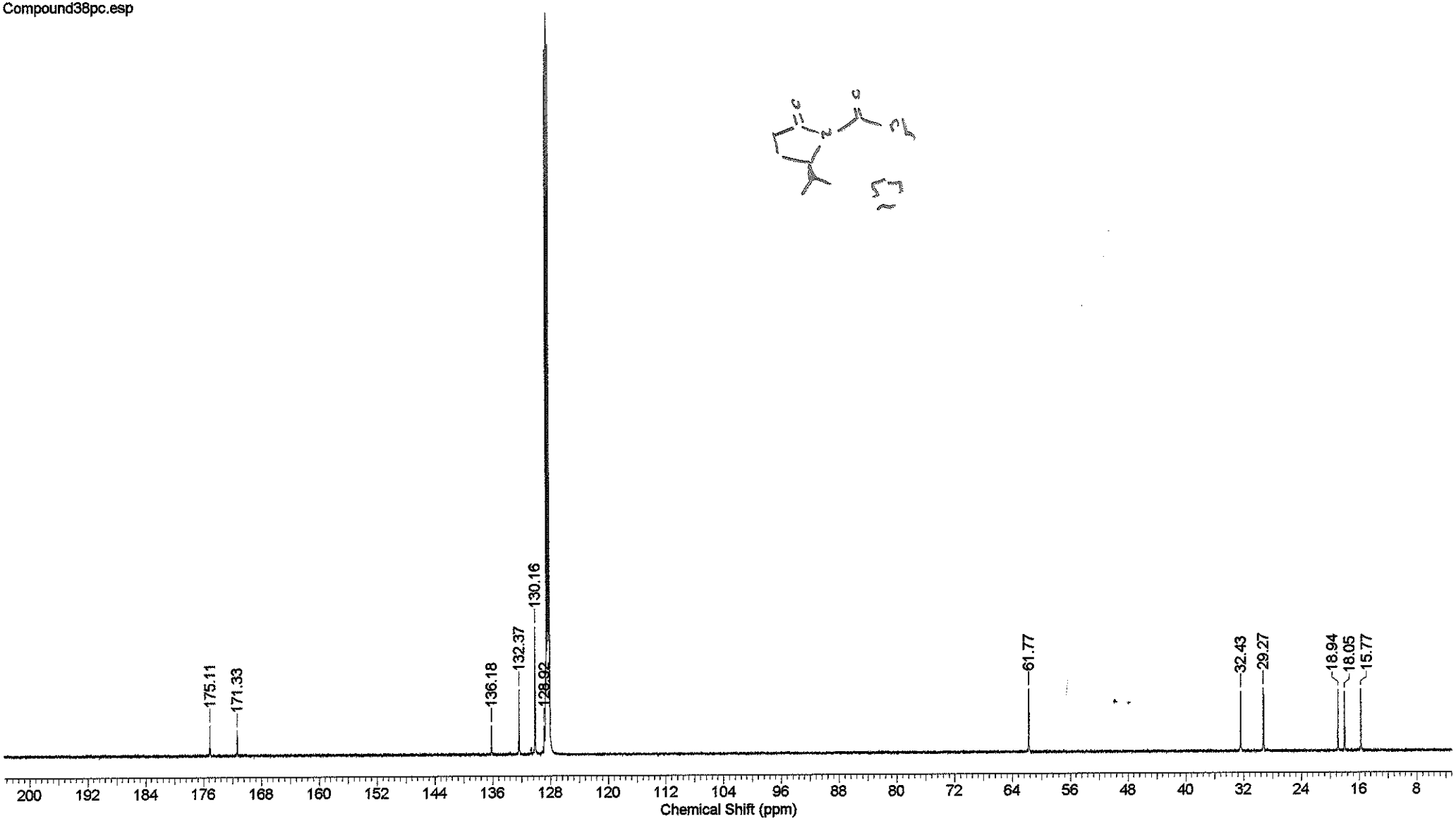
Acquisition Time (sec)	3.9649	***Comment***	MWG053pp mPROTON C6D6 {e:\bruk400data\2012\Jan} ejt 53	***Date***	09 Jan 2012 16:57:36		
Date Stamp	09 Jan 2012 16:57:36			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 38\MWG053pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	144.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2446.3857
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	22.700				

Compound38pp.esp



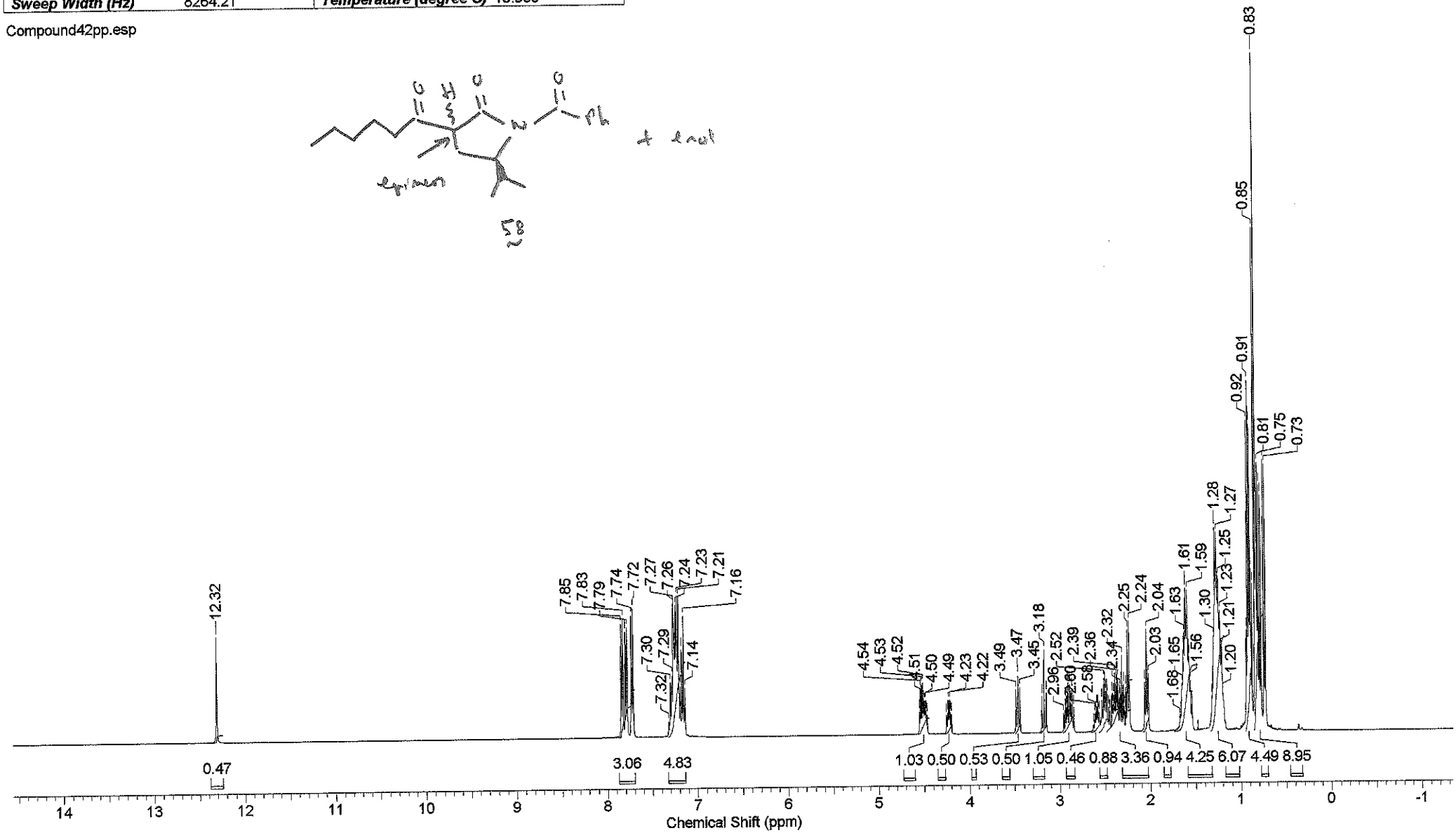
Acquisition Time (sec)	1.1010	***Comment***	MWG053pc mCARBON C6D6 /opt/bruk500data/2011/Nov ejt 15	***Date***	12 Nov 2011 12:18:08		
Date Stamp	12 Nov 2011 12:18:08			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 38\MWG053pc_000001r		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	256	***Origin***	spect
Original Points Count	32768	***Owner***	vnmr1	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	12646.0762
Sweep Width (Hz)	29761.00	***Temperature (degree C)***	20.198				

Compound38pc.esp



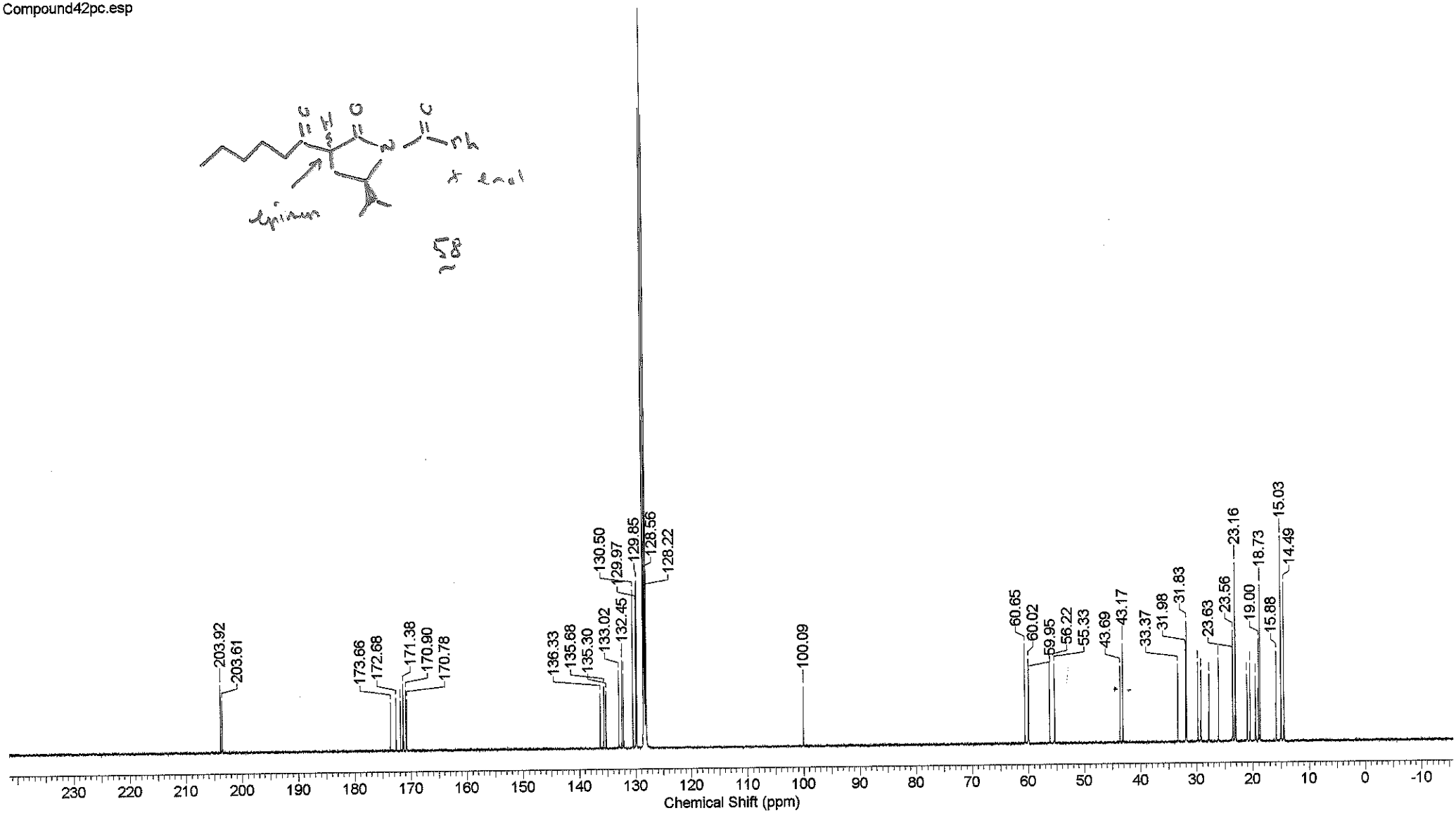
Acquisition Time (sec)	3.9649	***Comment***	MWG084pp mPROTON C6D6 {e:\bruk400data\2011\Dec} ejt 30	***Date***	19 Dec 2011 12:03:12		
Date Stamp	19 Dec 2011 12:03:12			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 42\MWG084pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	16.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2470.5981
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.900				

Compound42pp.esp



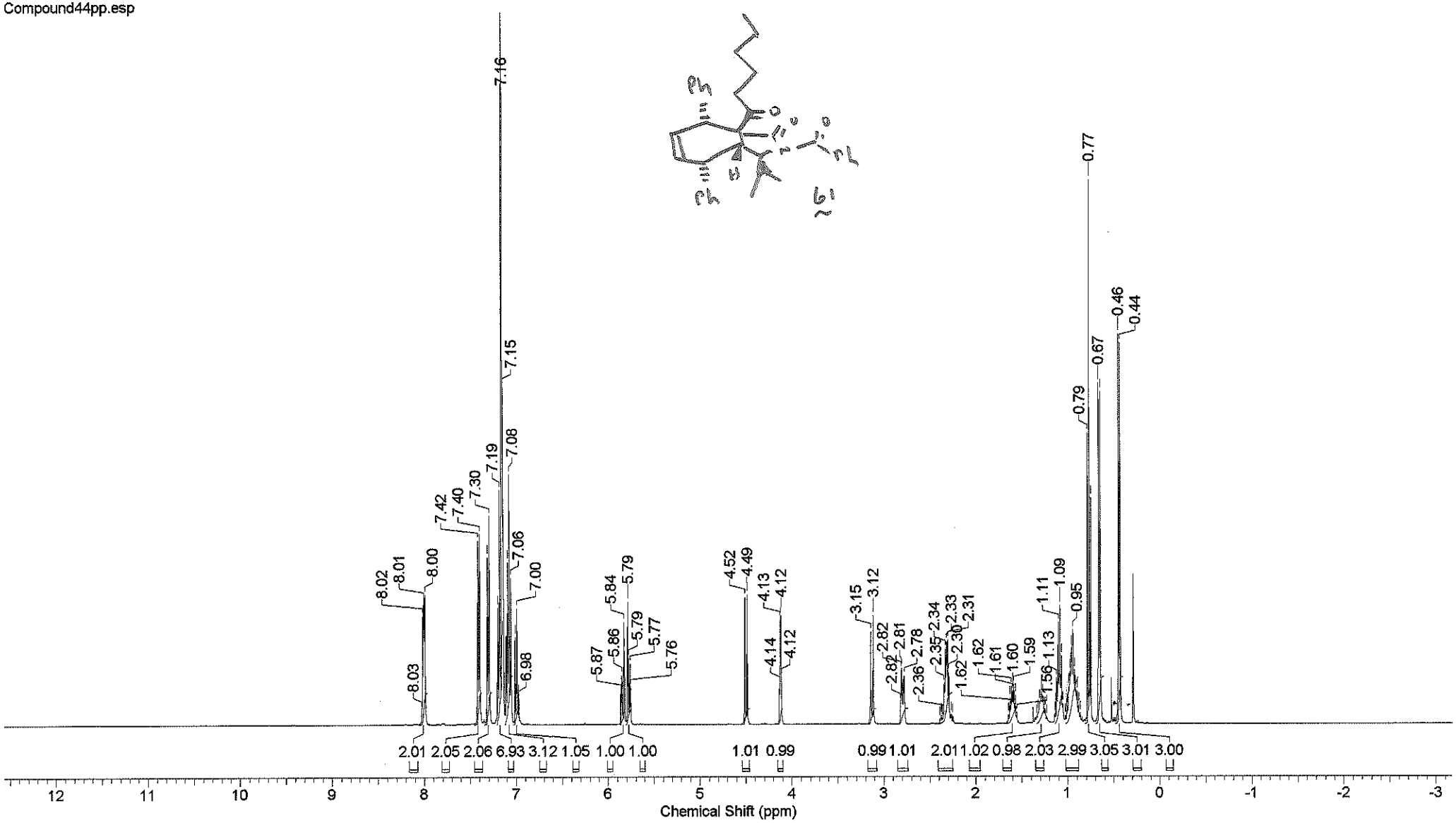
Acquisition Time (sec)	1.0835	***Comment***	MWG084pc mCARBON C6D6 {e:\bruk400data\2011\Dec} ejt 30	***Date***	19 Dec 2011 12:26:40		
Date Stamp	19 Dec 2011 12:26:40			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 42\MWG084pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.4844
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.600				

Compound42pc.esp



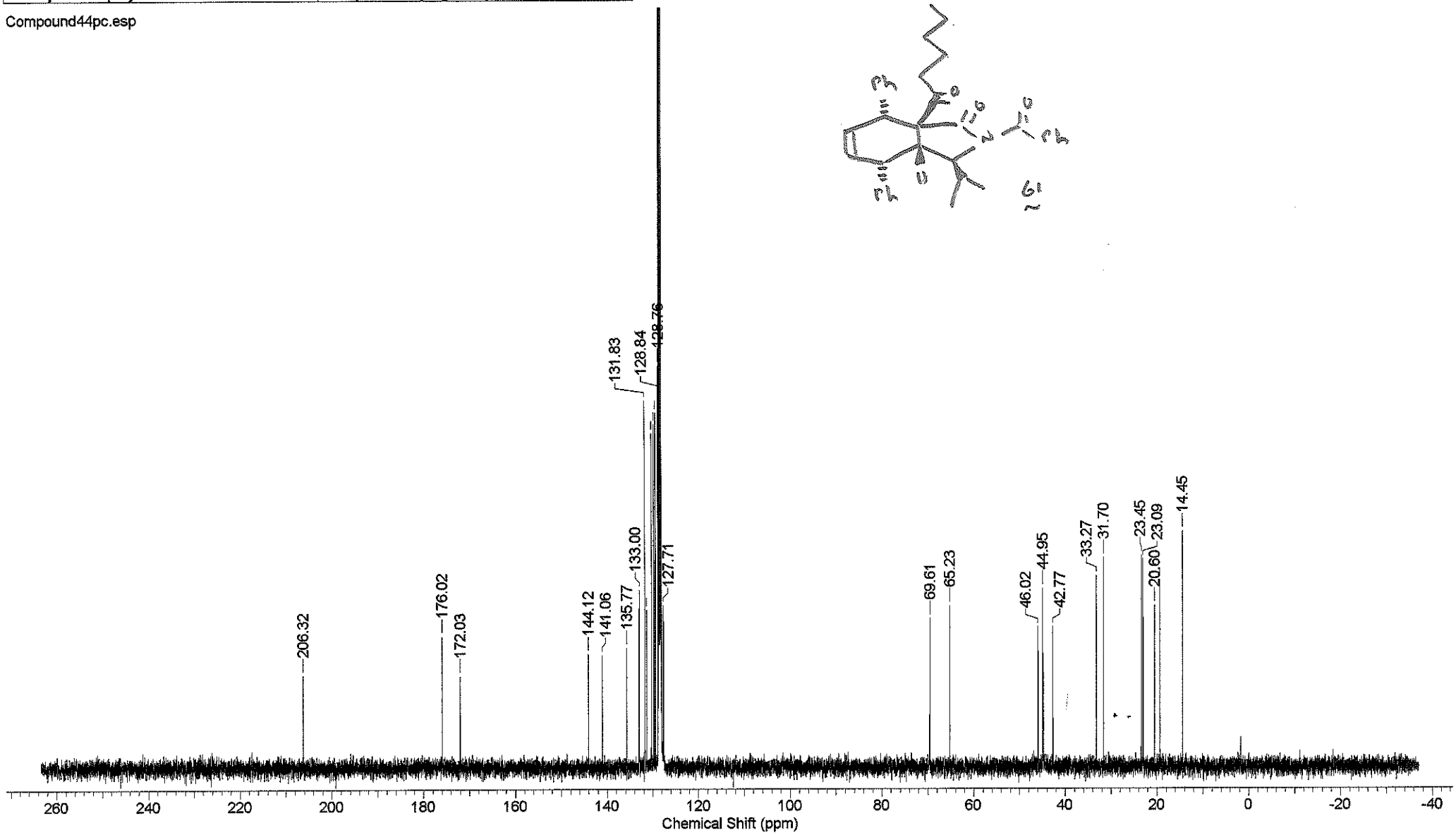
Acquisition Time (sec)	3.9649	***Comment***	MWG093pp mPROTON C6D6 {e:\bruk400data\2012\Jan} ejt 56			***Date***	20 Jan 2012 10:54:56
Date Stamp	20 Jan 2012 10:54:56			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 44\MWG093pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	101.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2425.9570
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.700				

Compound44pp.esp



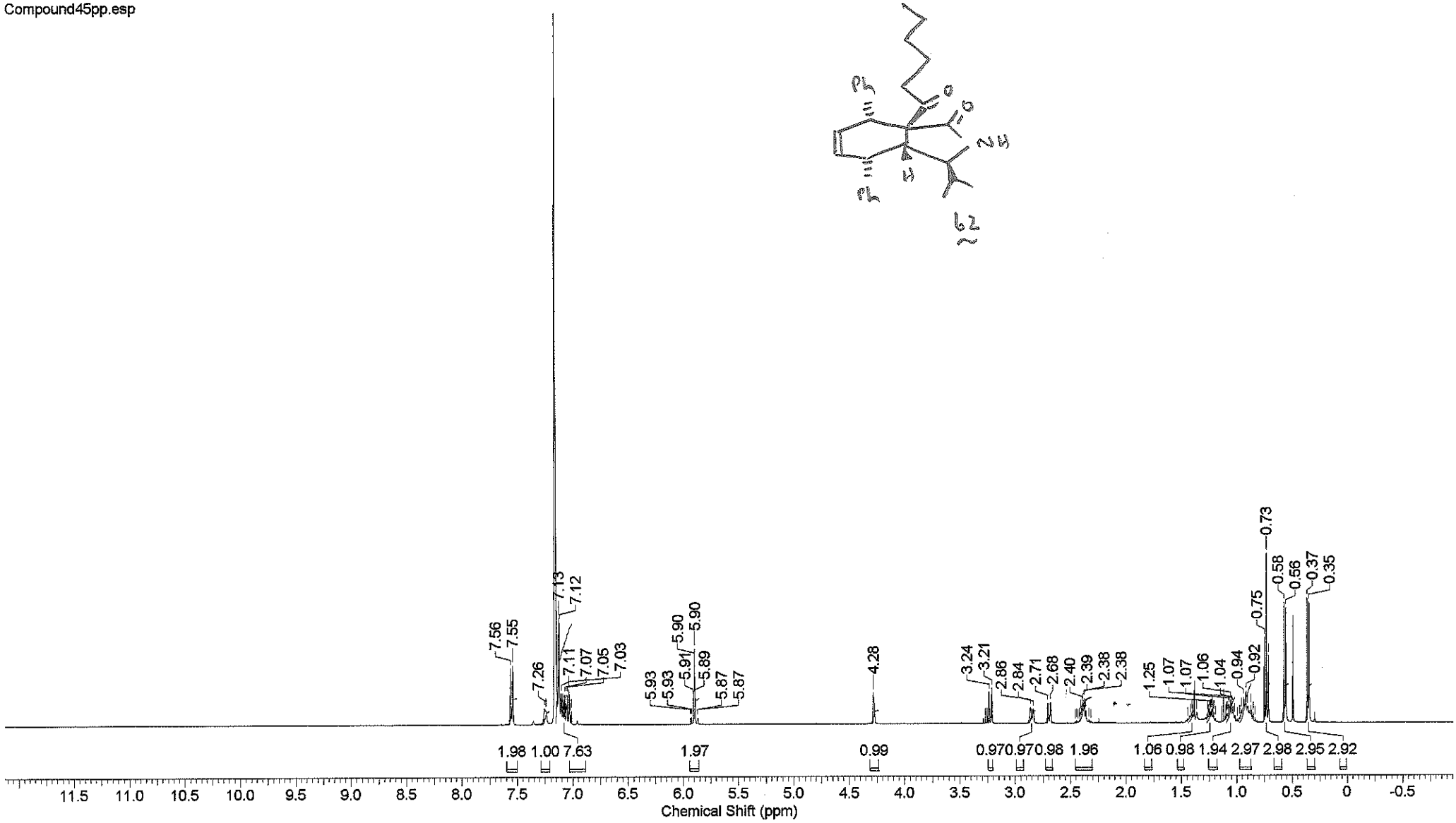
Acquisition Time (sec)	1.0835	***Comment***	MWG093pc mCARBON C6D6 {e:\bruk400data\2012\Jan} ejt 56			***Date***	20 Jan 2012 11:18:24
Date Stamp	20 Jan 2012 11:18:24			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 44\MWG093pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.5010
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	22.400				

Compound44pc.esp



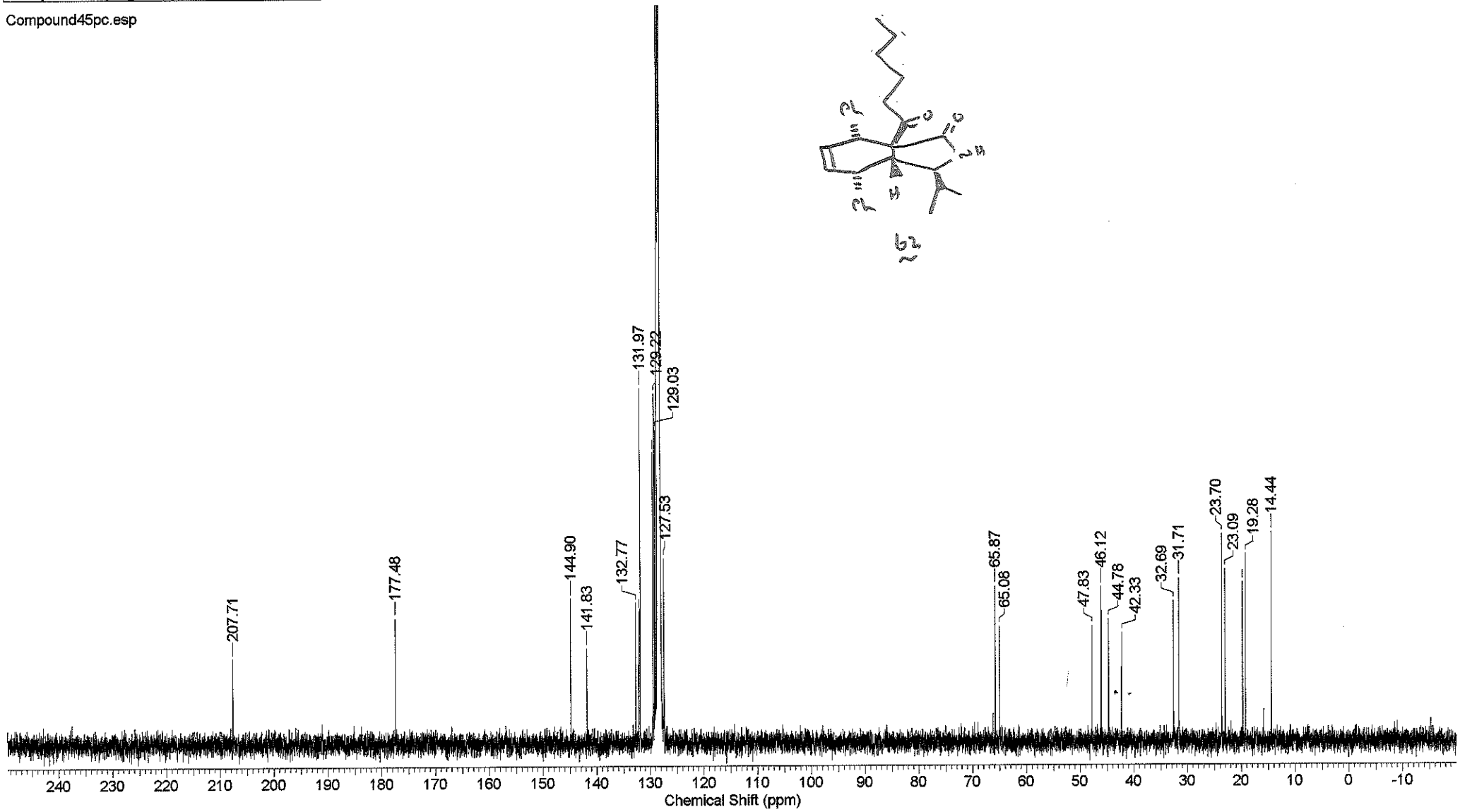
Acquisition Time (sec)	3.9649	***Comment***	MWG098pp mPROTON C6D6 {e:\bruk400data\2012\Jan} ejt 53			***Date***	23 Jan 2012 18:03:44
Date Stamp	23 Jan 2012 18:03:44			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 45\MWH018pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	256.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2097
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.400				

Compound45pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWH018pc mCARBONnight C6D6 {e:\bruk400data\2012\Mar} ejt 28				
Date	04 Mar 2012 05:22:08			***Date Stamp***	04 Mar 2012 05:22:08		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 45\MWH018pc_000001r					***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	3072	***Origin***	AV400	***Original Points Count***	32768
Owner	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	512.00
SW(cyclical) (Hz)	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.4844	***Sweep Width (Hz)***	30241.01
Temperature (degree C)	22.500						

Compound45pc.esp

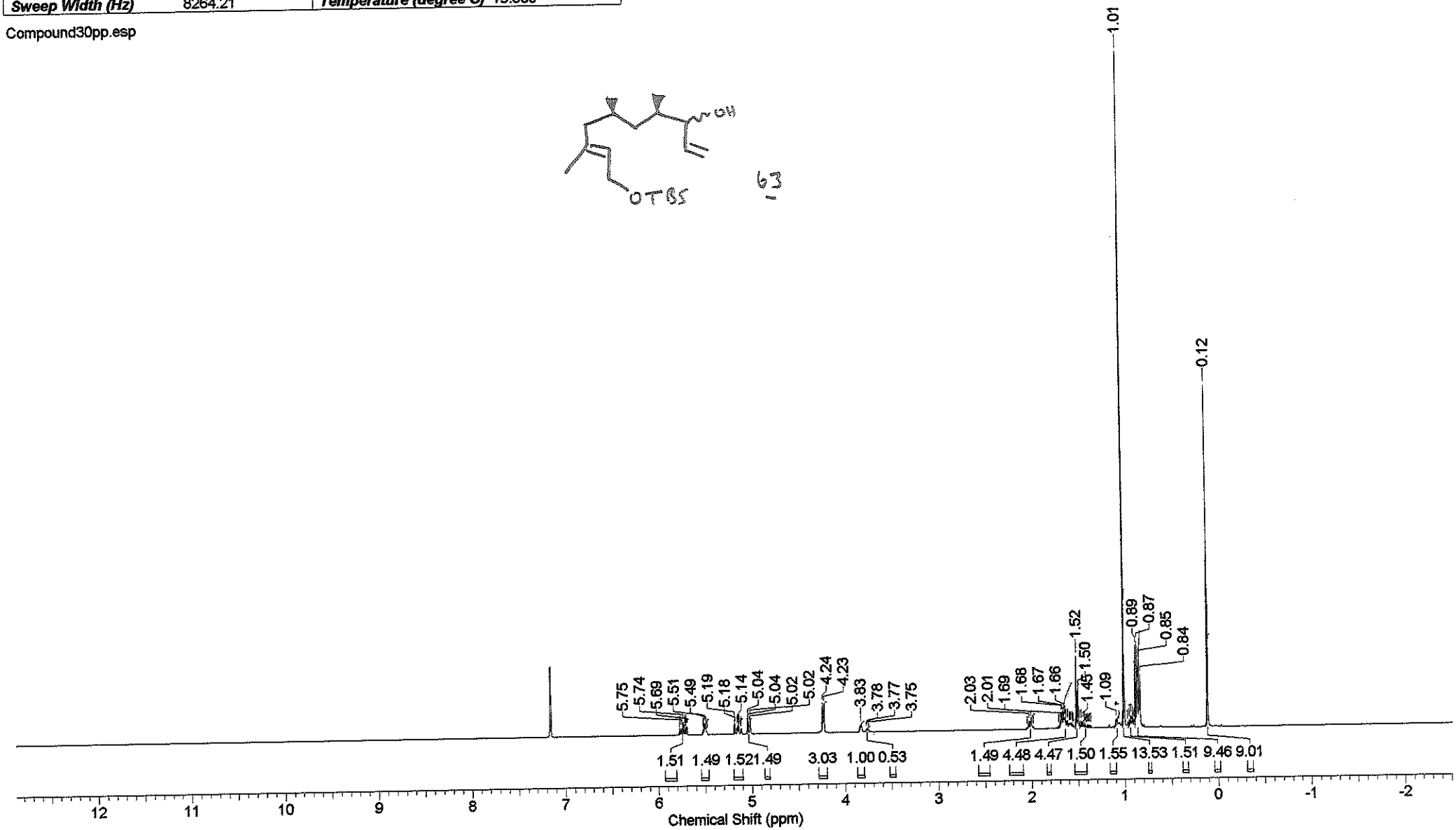


01/06/2012 15:20:51

Acquisition Time (sec)	3.9649	***Comment***	MWG005pp mPROTON C6D6 {e:\bruk400data\2011\Oct} ejt 37	***Date***	30 Oct 2011 13:20:00		
Date Stamp	30 Oct 2011 13:20:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 30\MWG005pp_000001r		
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***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2097
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.900				

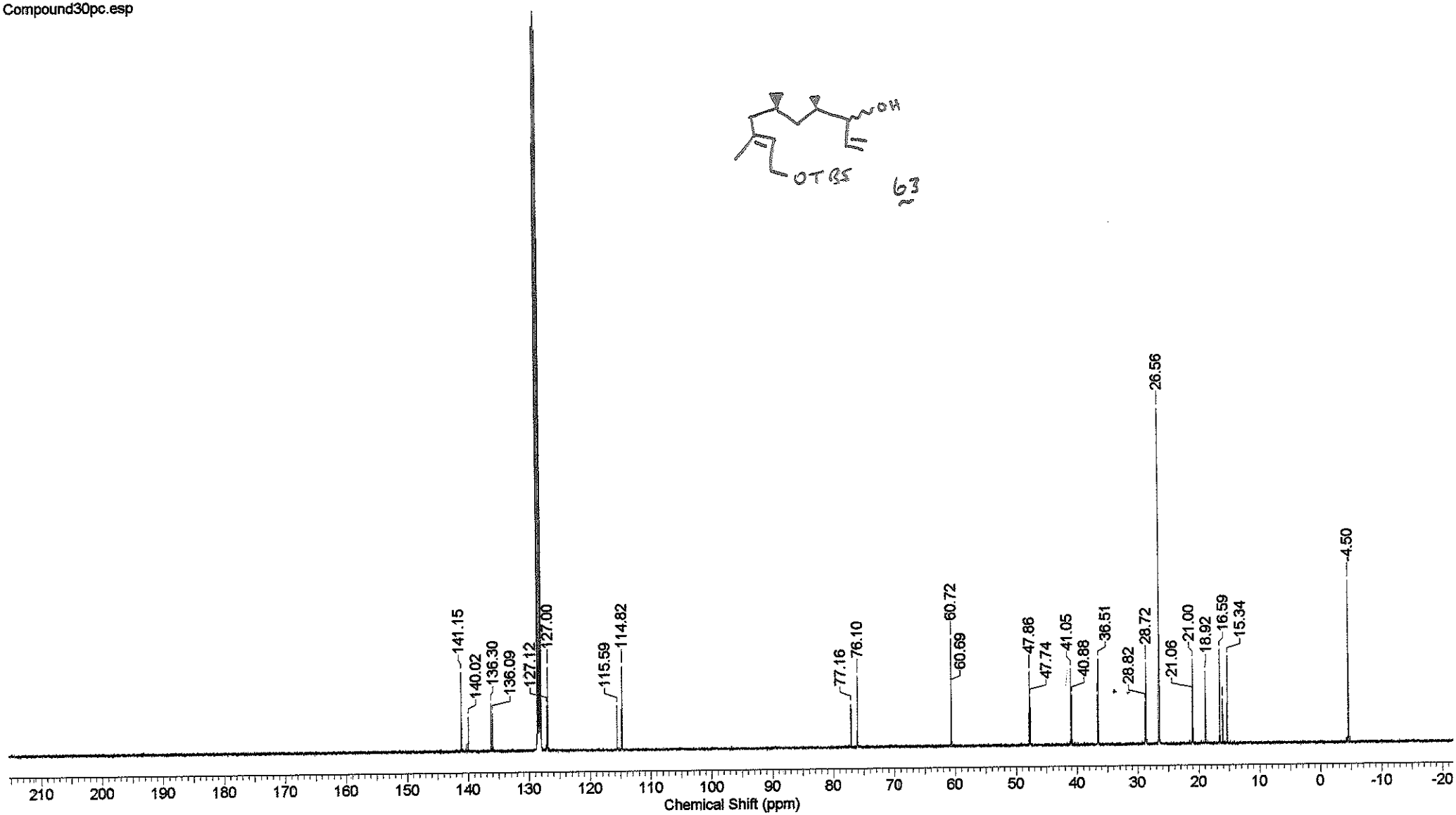
Compound30pp.esp

63



Acquisition Time (sec)	1.0835	***Comment***	MWG005pc mCARBON C6D6 {e:\bruk400data\2011\Sep} ejt 15			***Date***	27 Sep 2011 08:12:48
Date Stamp	27 Sep 2011 08:12:48			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 30\MWG005pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11395.3301
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.000				

Compound30pc.esp

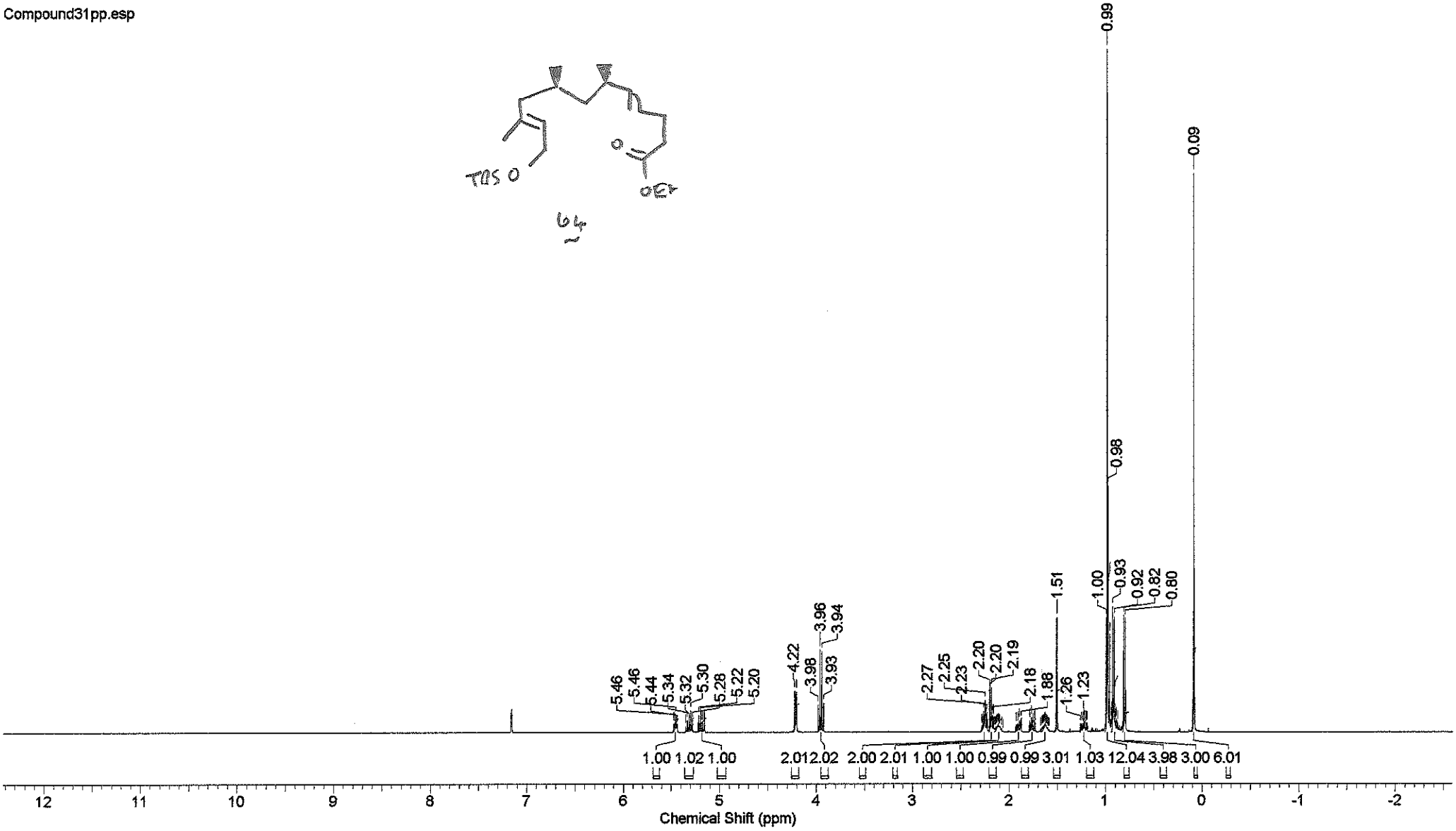


25/05/2012 11:41:07

Acquisition Time (sec)	3.9649	***Comment***	MWG006pp mPROTON C6D6 {e:\bruk400data\2011\Sep} ejt 53			***Date***	01 Oct 2011 19:44:00
Date Stamp	01 Oct 2011 19:44:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 31\MWG006pp_000001r		
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	22.60	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2425.9573
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.900				

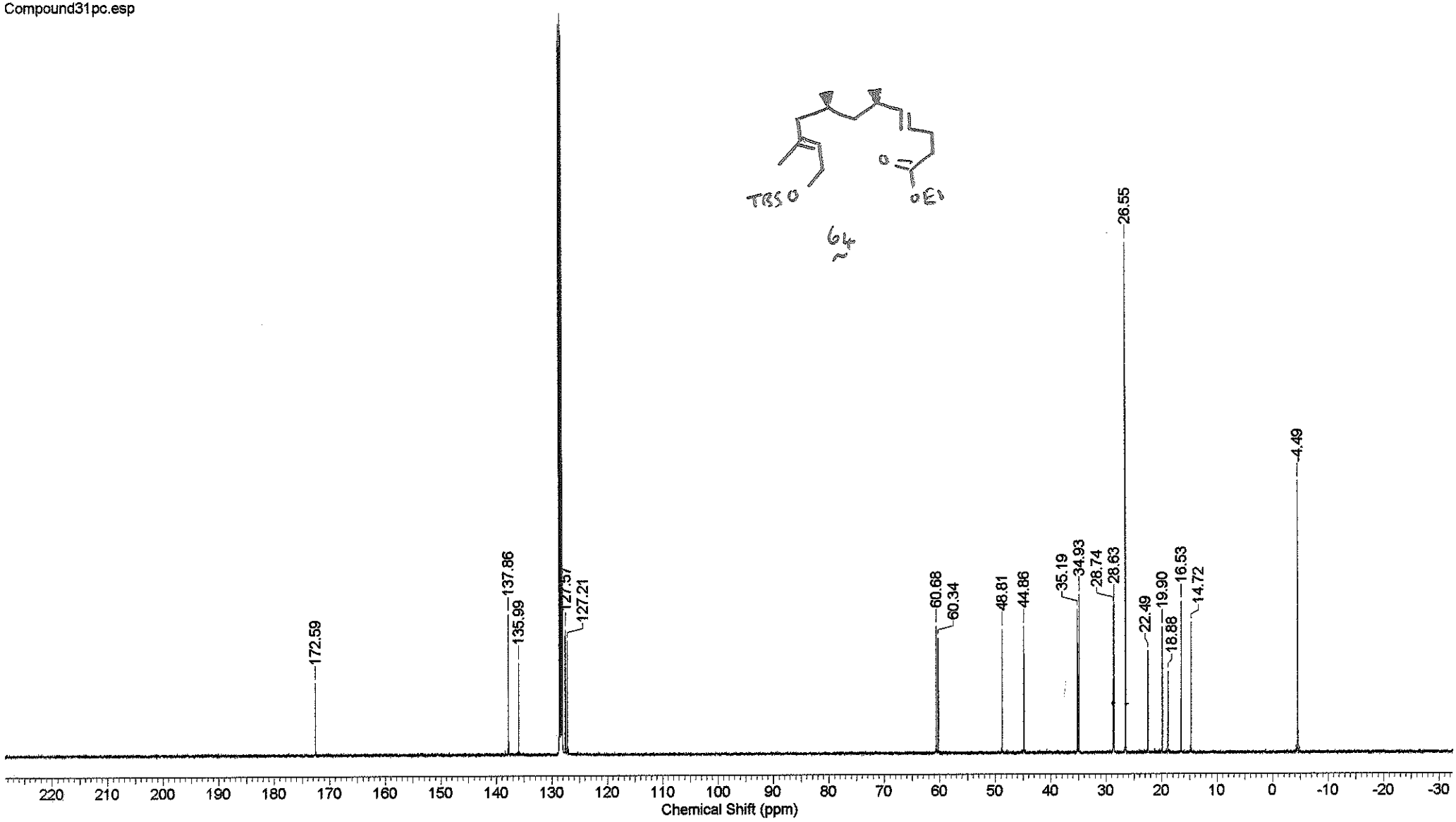
Compound31pp.esp

64



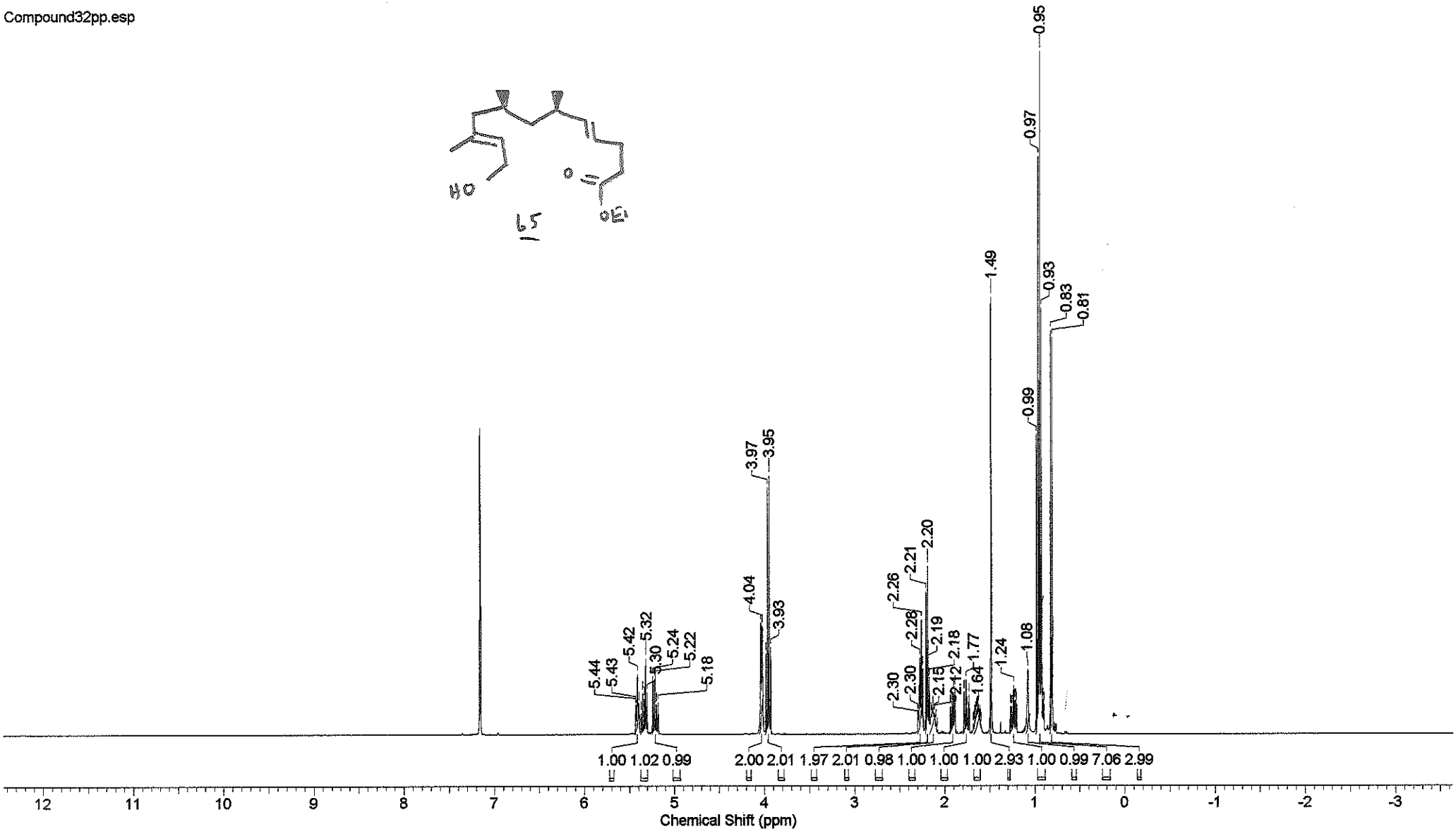
Acquisition Time (sec)	1.0835	***Comment***	MWG006pc mCARBON C6D6 {e:\bruk400data\2011\Sep} ejt 53			***Date***	01 Oct 2011 20:07:28
Date Stamp	01 Oct 2011 20:07:28			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 31\MWG006pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11397.1748
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.600				

Compound31pc.esp



Acquisition Time (sec)	3.9649	***Comment***	MWG009pp mPROTON C6D6 {e:\bruk400data\2011\Dec} ejt 16			***Date***	08 Dec 2011 14:53:52
Date Stamp	08 Dec 2011 14:53:52			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 32\MWG009pp_000001r		
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	101.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.4619
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	21.100				

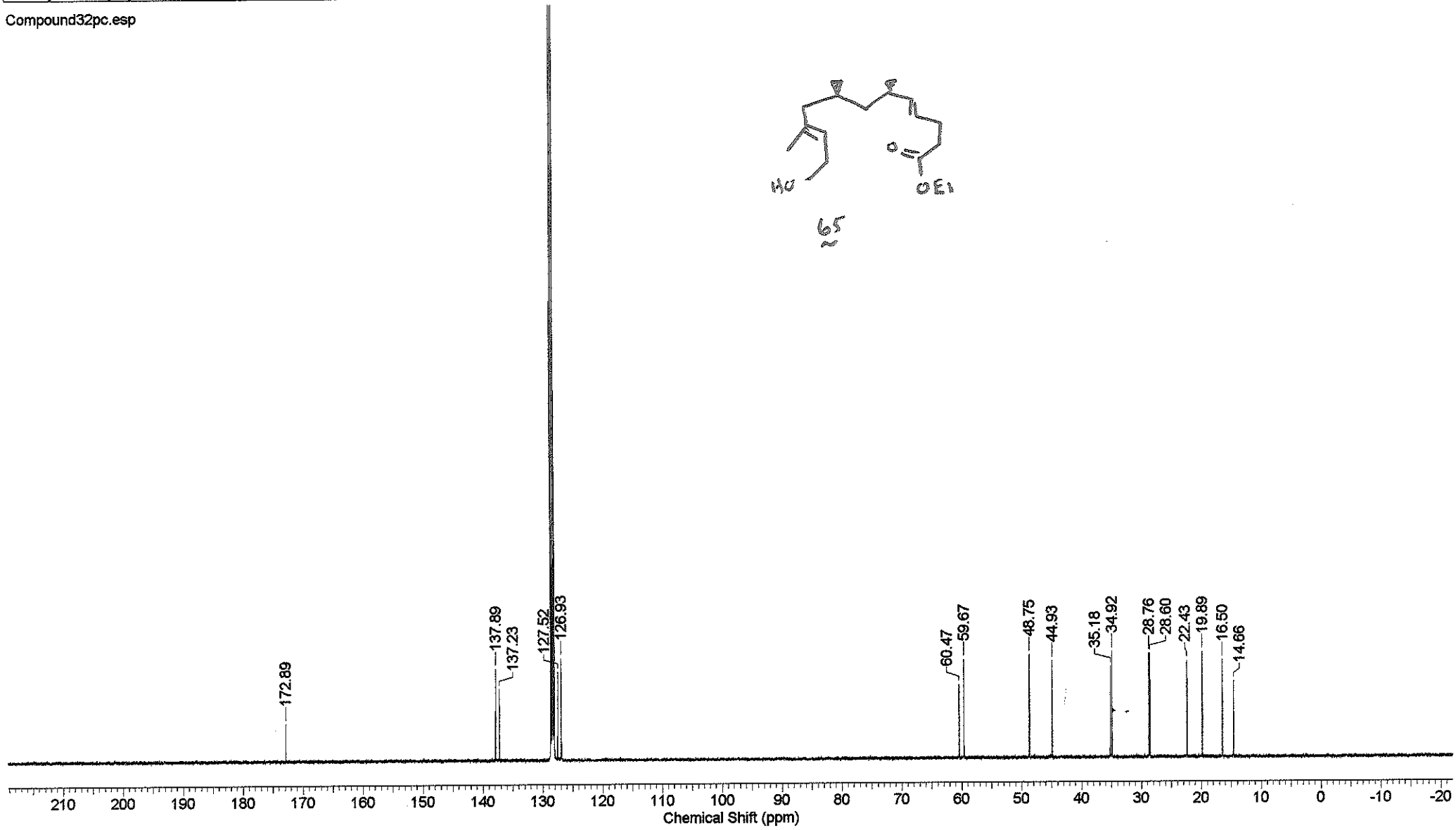
Compound32pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWG009pc mCARBON C6D6 {e:\bruk400data\2011\Oct} ejt 6			***Date***	10 Oct 2011 07:10:56
Date Stamp	10 Oct 2011 07:10:56			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 32\MWG009pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11394.4072
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	22.700				

Compound32pc.esp

65



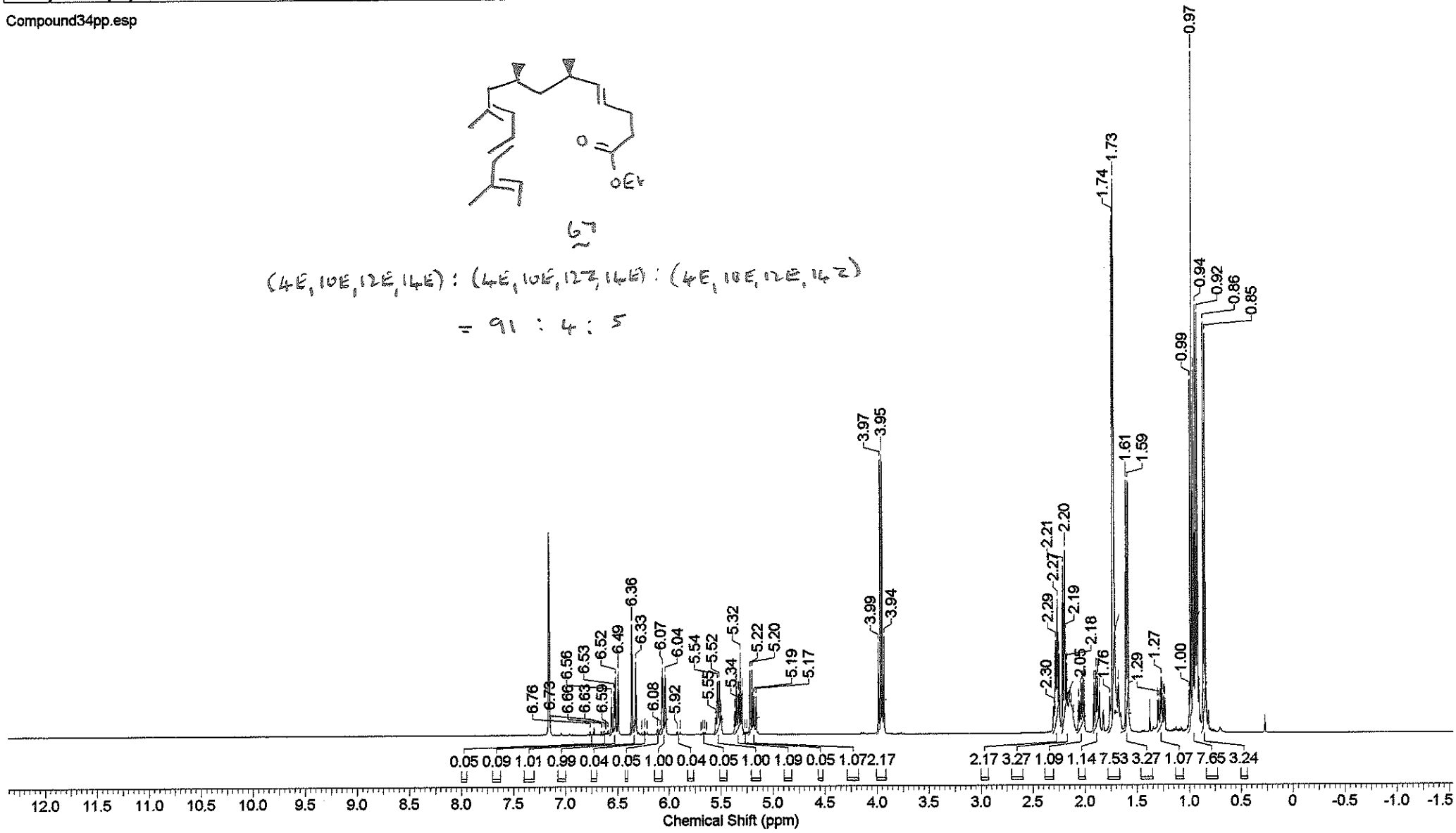
Acquisition Time (sec)	3.9649	***Comment***	MWG055pp mPROTON C6D6 {e:\bruk400data\2011\Nov} ejt 3			***Date***	08 Nov 2011 15:21:36
Date Stamp	08 Nov 2011 15:21:36			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 34\MWG055pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	36.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2097
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.900				

Compound34pp.esp

6j

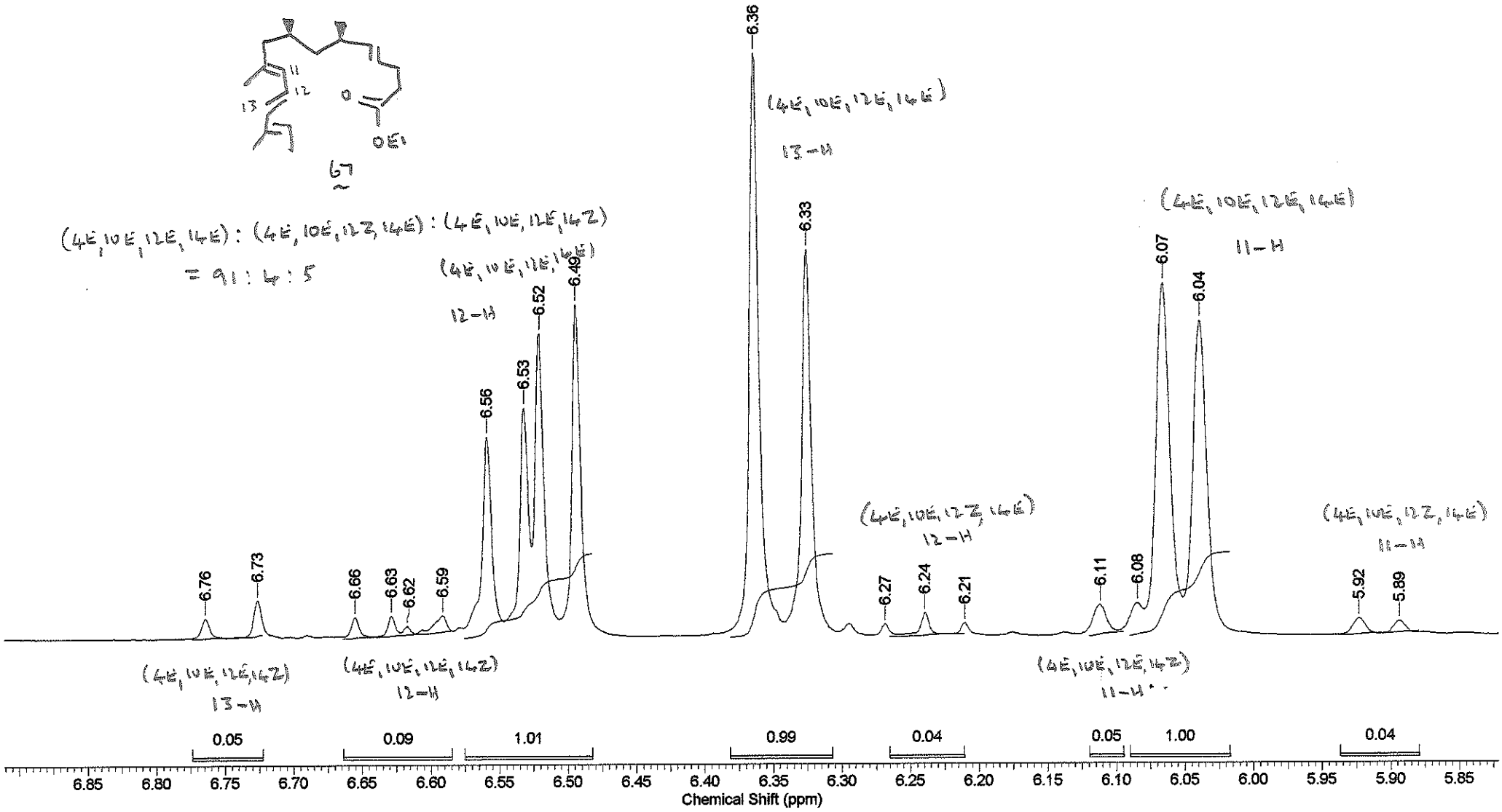
(4E,10E,12E,14E) : (4E,10E,12Z,14E) : (4E,10E,12E,14Z)

= 91 : 4 : 5



Acquisition Time (sec)	3.9649	***Comment***	MWG055pp mPROTON C6D6 {e:\bruk400data\2011\Nov} ejt 3			***Date***	08 Nov 2011 15:21:36
Date Stamp	08 Nov 2011 15:21:36			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 34\MWG055pp_000001r		
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	36.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2097
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.900				

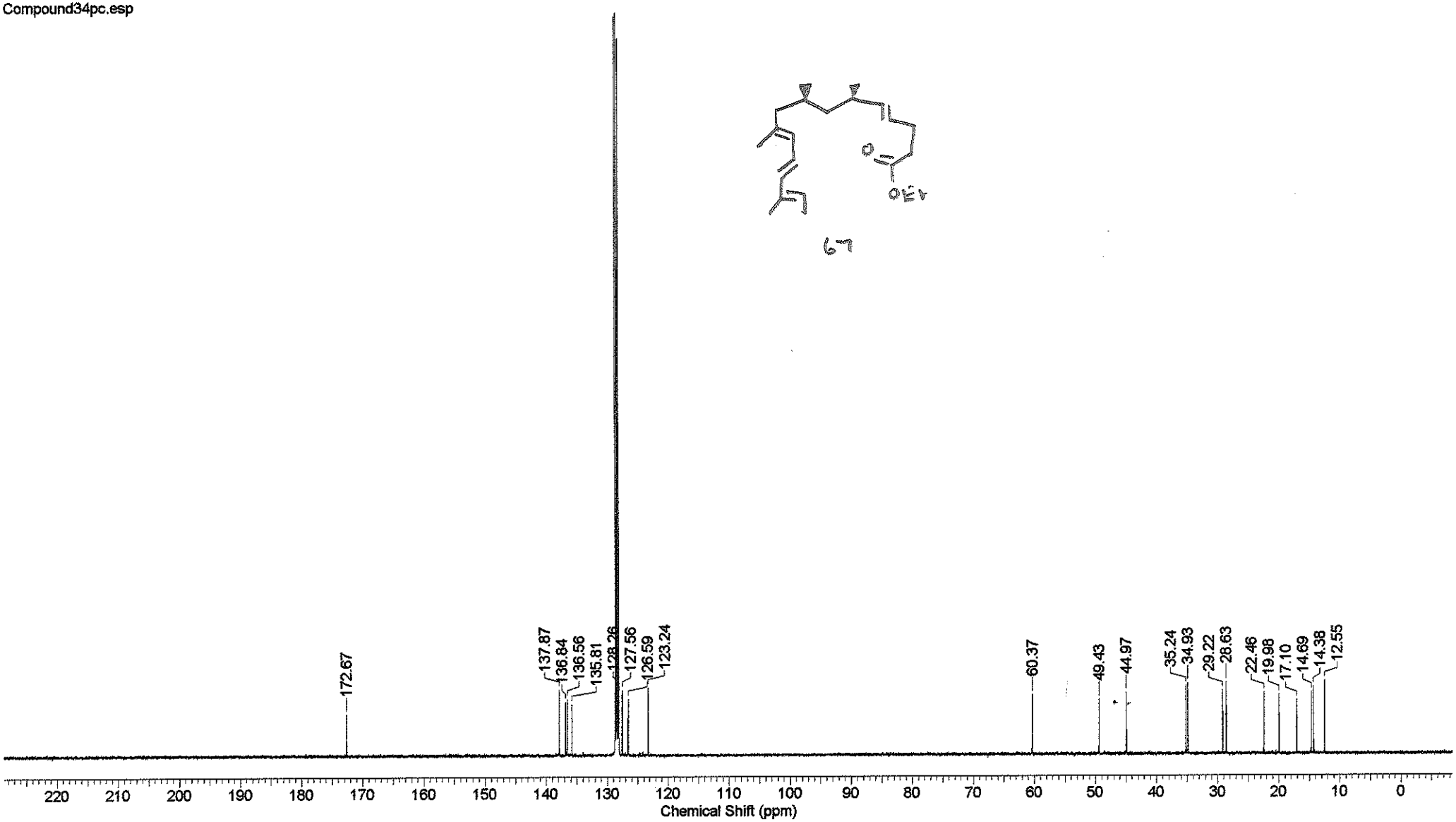
Compound34pp.esp



Acquisition Time (sec)	1.0835	***Comment***	MWG055pc mCARBON C6D6 {e:\bruk400data\2011\Nov} ejt 3			***Date***	08 Nov 2011 15:45:04
Date Stamp	08 Nov 2011 15:45:04			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 34\MWG055pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11394.4072
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.600				

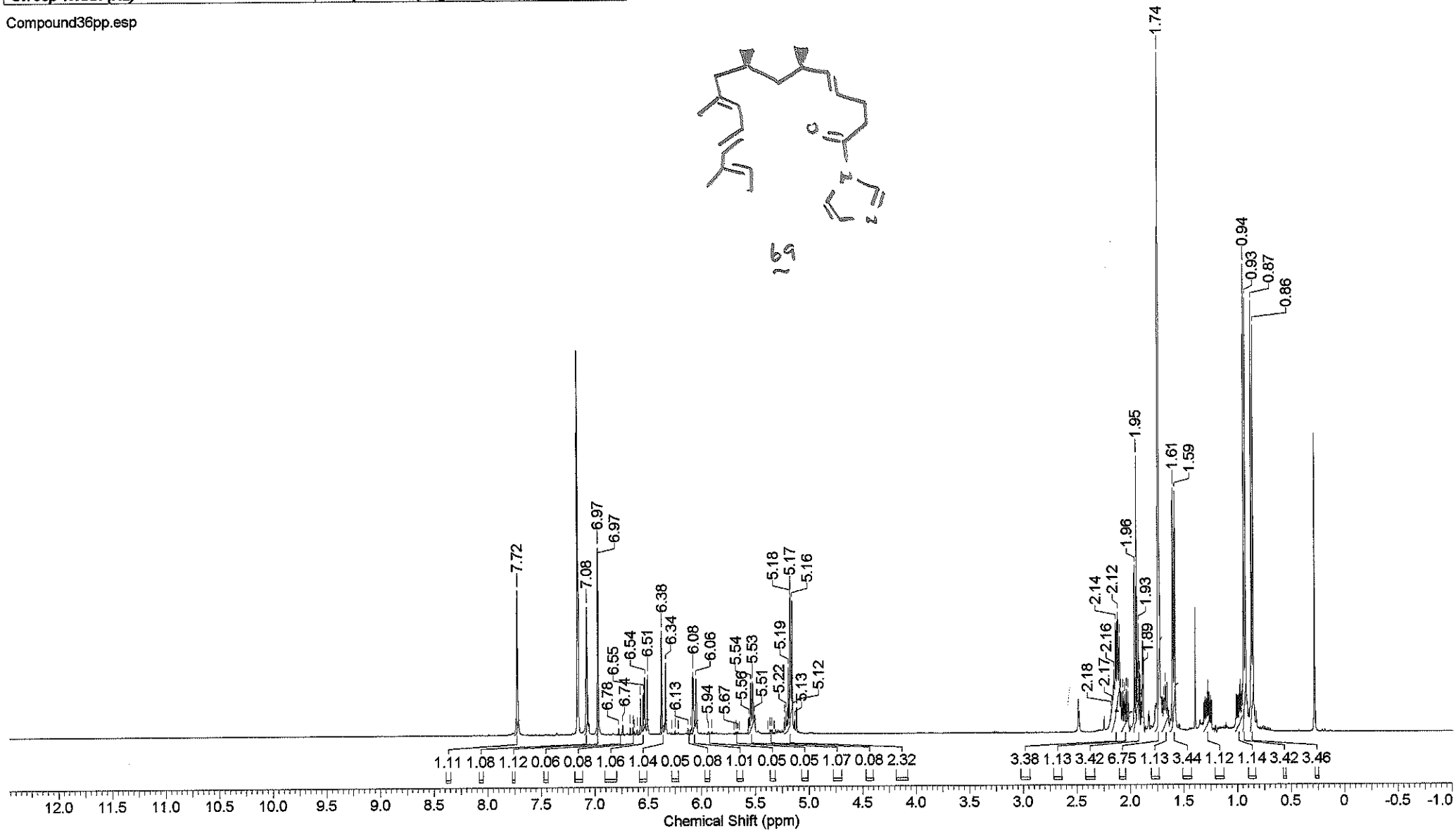
Compound34pc.esp

67



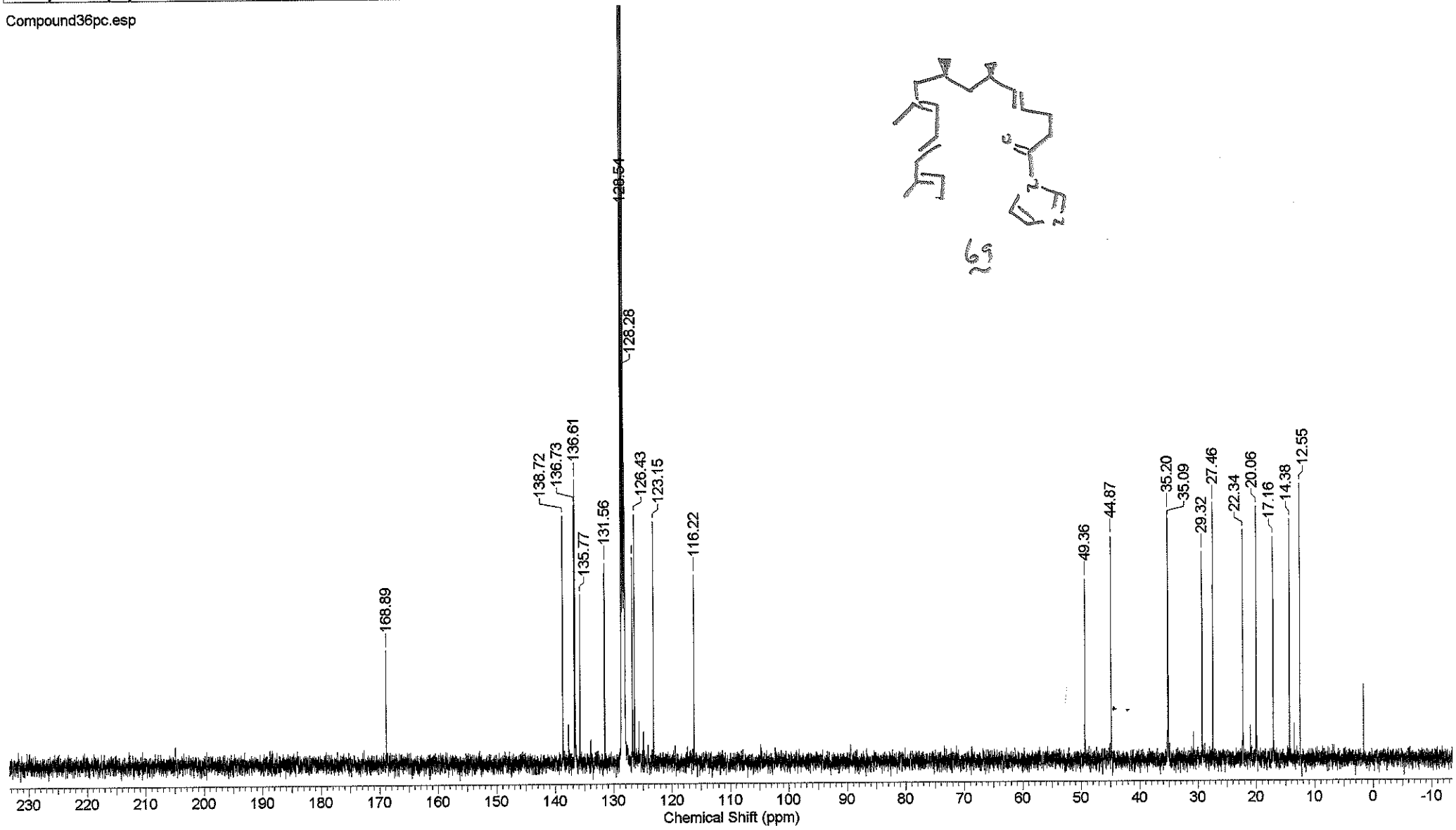
Acquisition Time (sec)	3.9649	***Comment***	MWG078pp mPROTON C6D6 {e:\bruk400data\2011\Dec} ejt 37	***Date***	08 Dec 2011 09:12:32		
Date Stamp	08 Dec 2011 09:12:32			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 36\MWG078pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	80.60	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.4619
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	20.900				

Compound36pp.esp



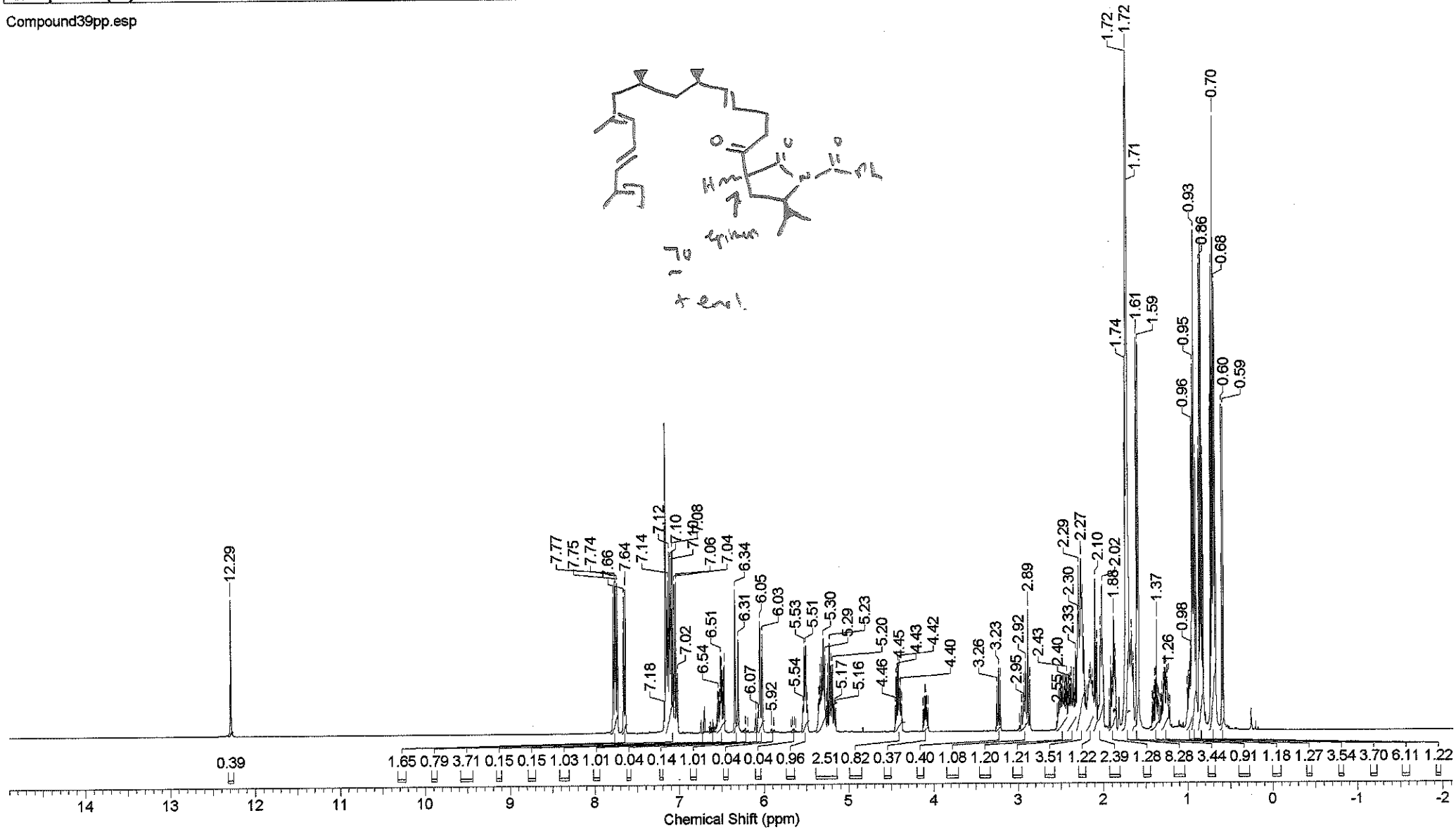
Acquisition Time (sec)	1.0835	***Comment***	MWG078pc mCARBON C6D6 {e:\bruk400data\2011\Dec} ejt 37			***Date***	08 Dec 2011 09:36:00
Date Stamp	08 Dec 2011 09:36:00			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 36\MWG078pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.5020
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.600				

Compound36pc.esp



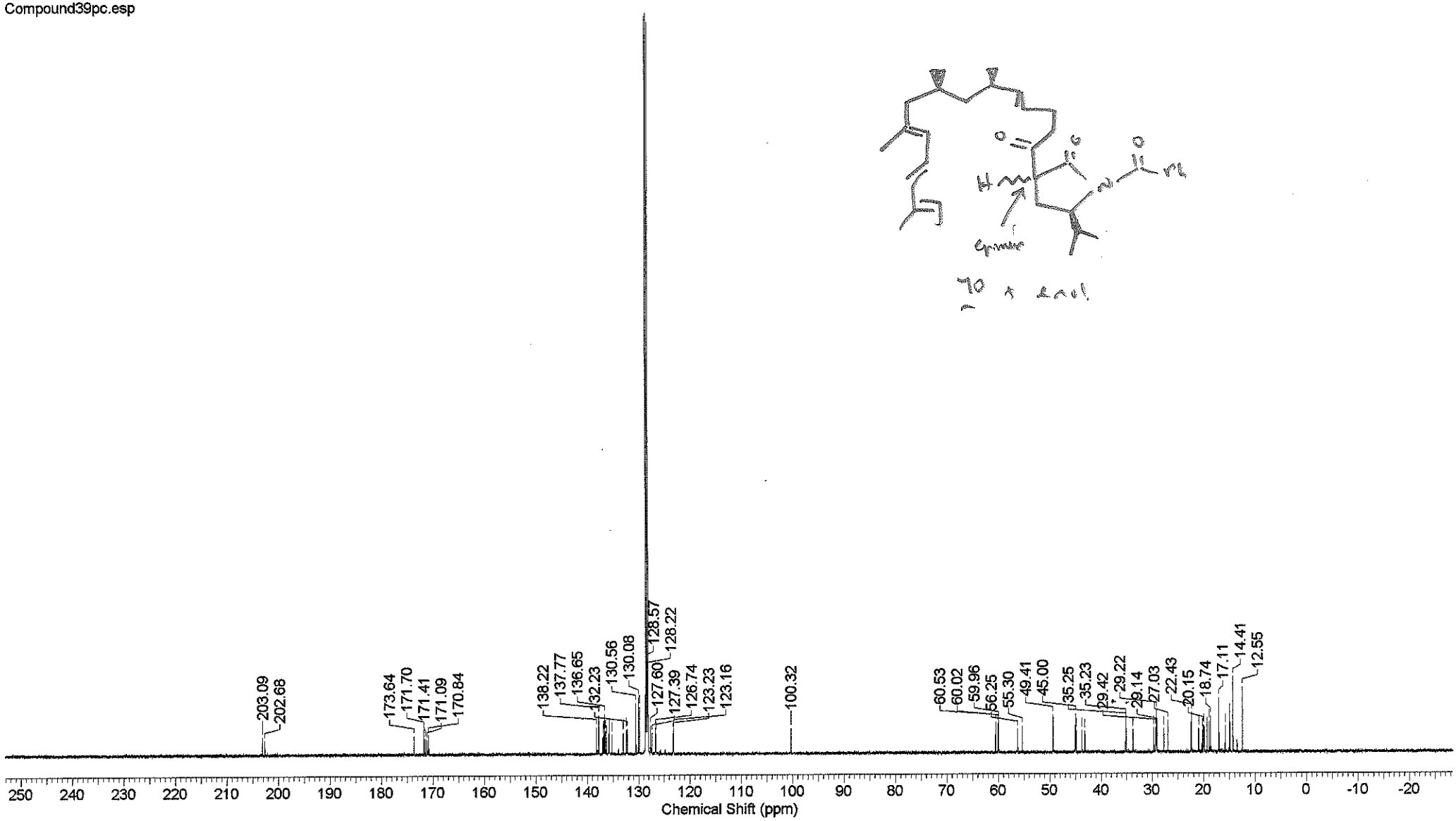
Acquisition Time (sec)	3.9649	***Comment***	MWG086pp mPROTON C6D6 {e:\bruk400data\2011\Dec} ejt 6	***Date***	19 Dec 2011 08:55:28		
Date Stamp	19 Dec 2011 08:55:28			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 39\MWG086pp_000001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30b
Receiver Gain	36.00	***SW(cyclical) (Hz)***	8264.46	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2092
Sweep Width (Hz)	8264.21	***Temperature (degree C)***	19.900				

Compound39pp.esp



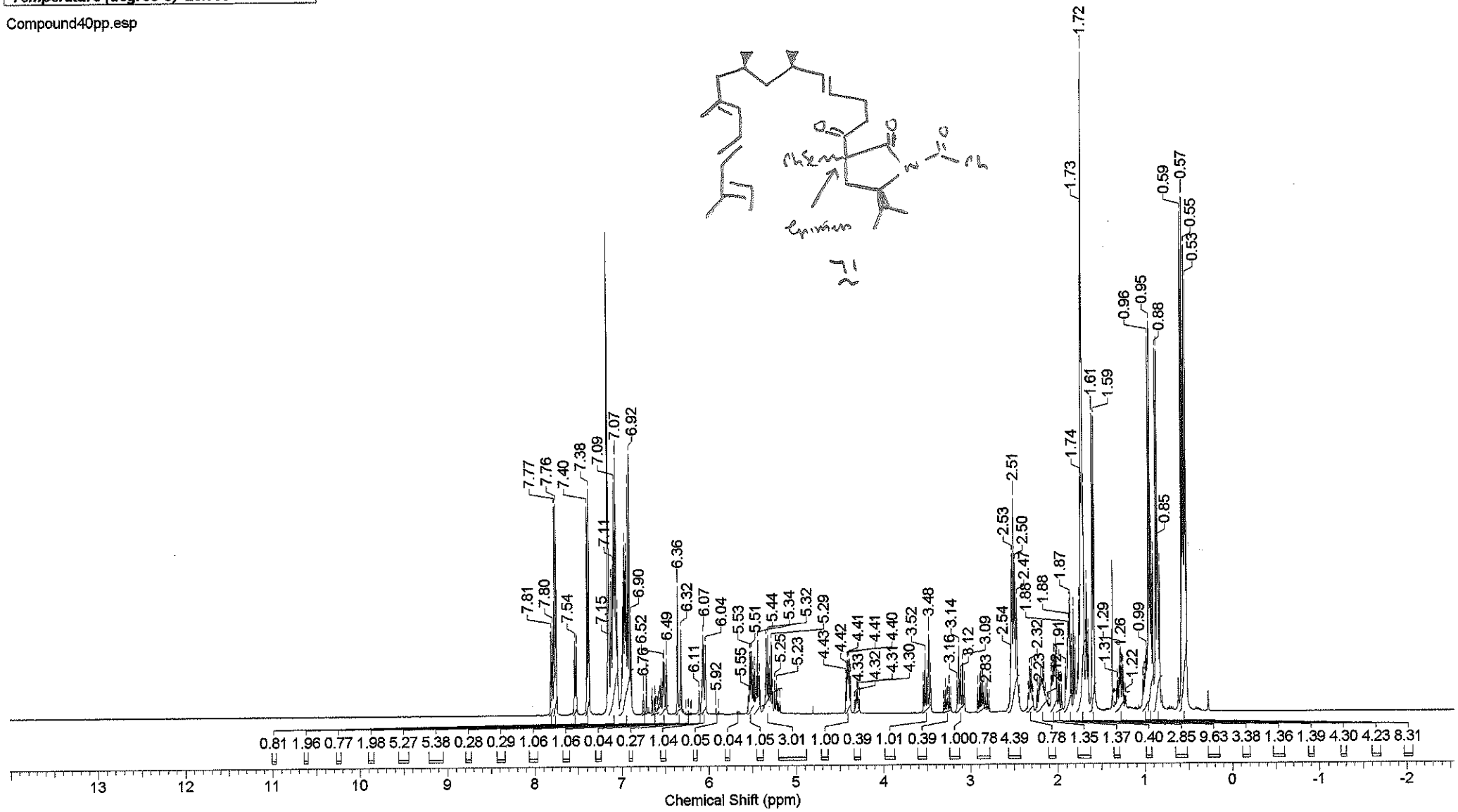
Acquisition Time (sec)	1.0835	***Comment***	MWG086pc mCARBON C6D6 {e:\bruk400data\2011\Dec} ejt 6			***Date***	19 Dec 2011 09:18:56
Date Stamp	19 Dec 2011 09:18:56			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 39\MWG086pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	256	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.4844
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	20.600				

Compound39pc.esp



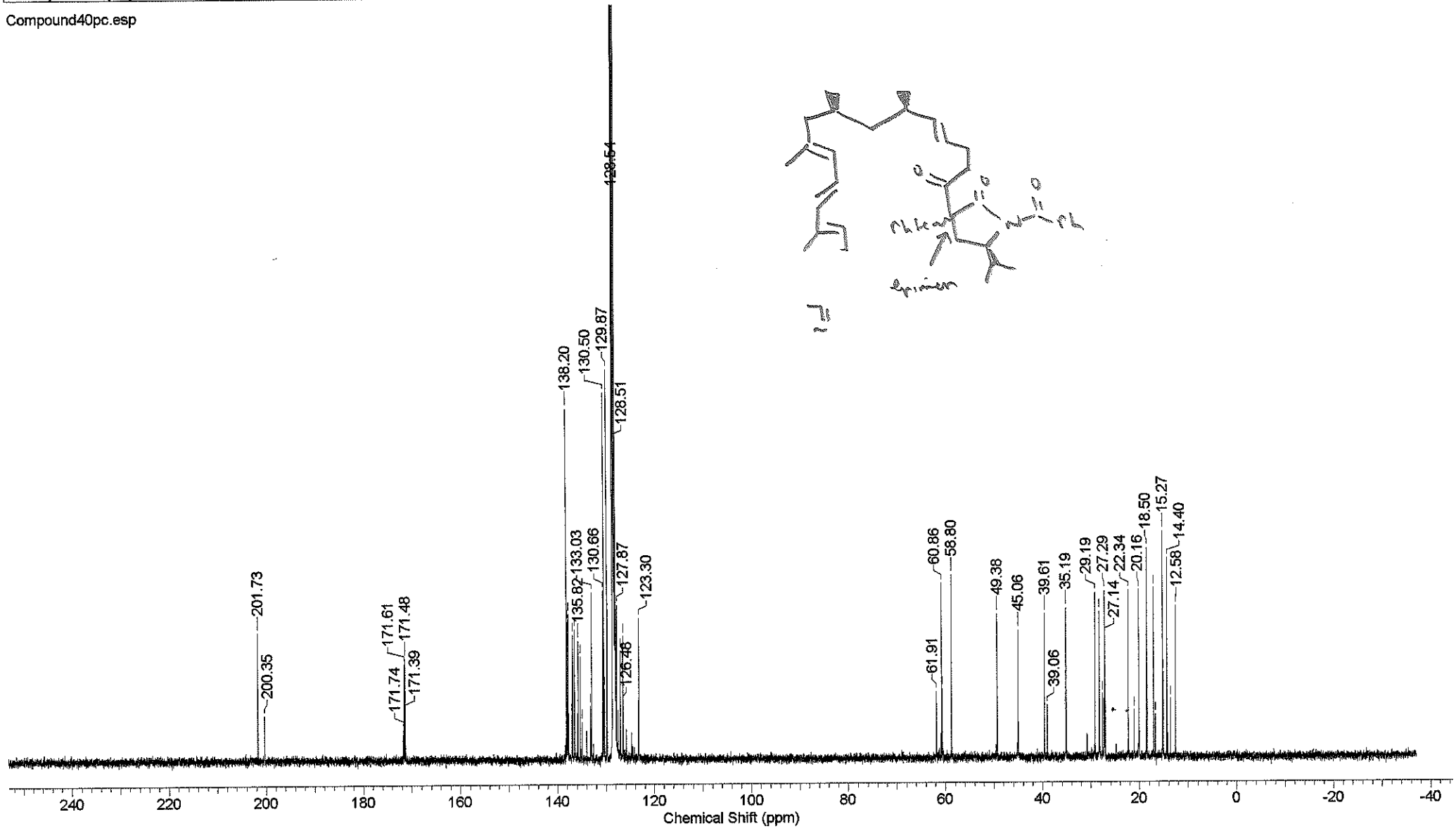
Acquisition Time (sec)	3.9649	***Comment***	MWH047pp mPROTONnight C6D6 {e:\bruk400data\2012\Apr} ejt 5				
Date	07 Apr 2012 04:54:24			***Date Stamp***	07 Apr 2012 04:54:24		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 40\MWH047pp_000001r					***Frequency (MHz)***	400.13
Nucleus	1H	***Number 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***	BENZENE-d6	***Spectrum Offset (Hz)***	2426.2097	***Sweep Width (Hz)***	8264.21
Temperature (degree C)	20.900						

Compound40pp.esp



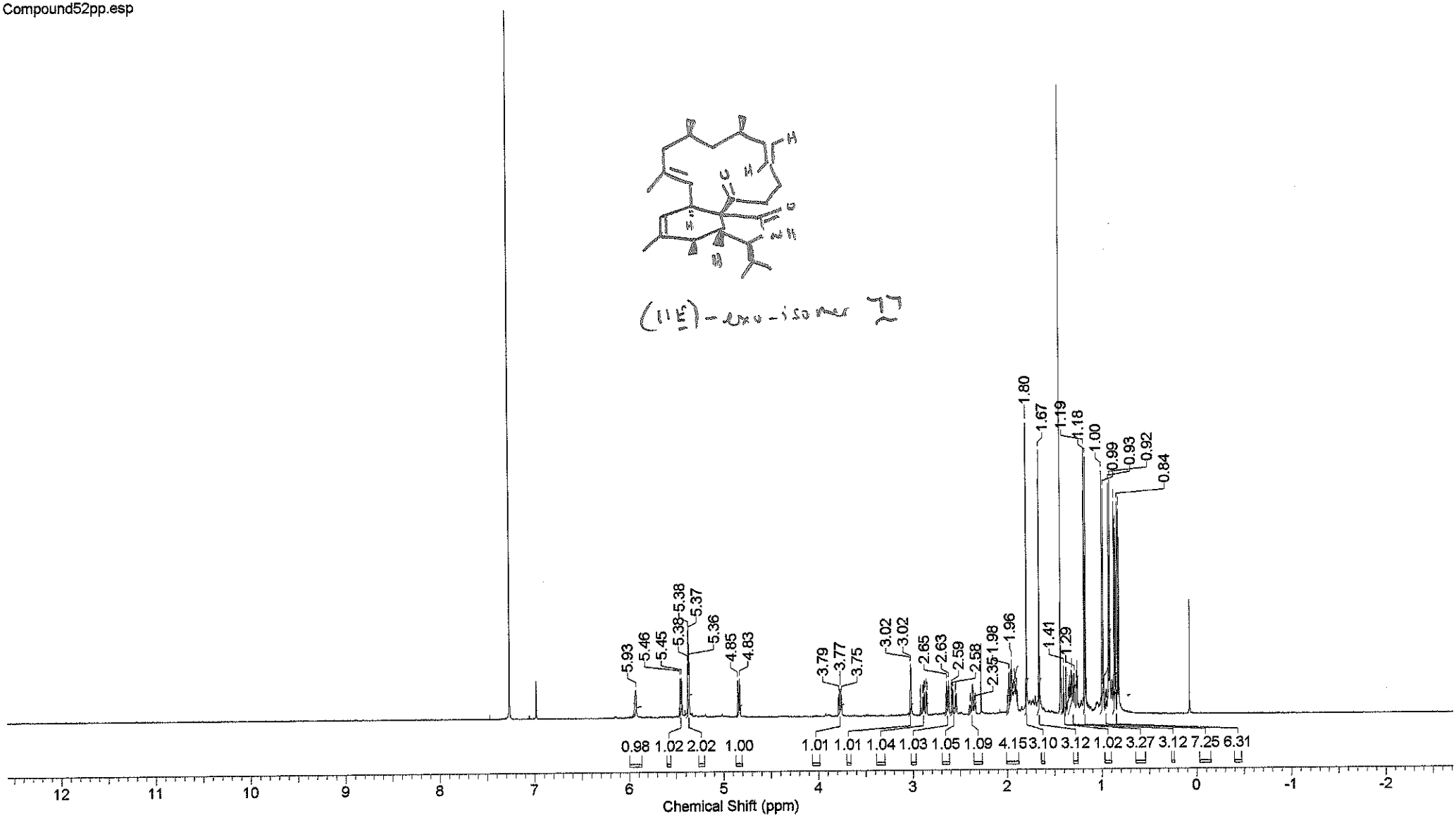
Acquisition Time (sec)	1.0835	***Comment***	MWH047pc mCARBONnight C6D6 {e:\bruk400data\2012\Apr} ejt 5	***Date***	07 Apr 2012 05:56:16		
Date Stamp	07 Apr 2012 05:56:16			***File Name***	F:\Chemistry\Year 3 data\NMR data\Data\Compound 40\MWH047pc_000001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1024	***Origin***	AV400
Original Points Count	32768	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	30241.94	***Solvent***	BENZENE-d6	***Spectrum Offset (Hz)***	11393.4844
Sweep Width (Hz)	30241.01	***Temperature (degree C)***	21.700				

Compound40pc.esp



Acquisition Time (sec)	3.1719	***Comment***	Mark Willis MWH064PPB mPROTON CDCl3 /opt/bruk500data/2012/Apr vnmr1 56				
Date	25 Apr 2012 07:45:04			***Date Stamp***	25 Apr 2012 07:45:04		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 52_010001r			***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***	228.00	***SW(cyclical) (Hz)***	10330.58
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	3079.9771	***Sweep Width (Hz)***	10330.26	***Temperature (degree C)***	25.128

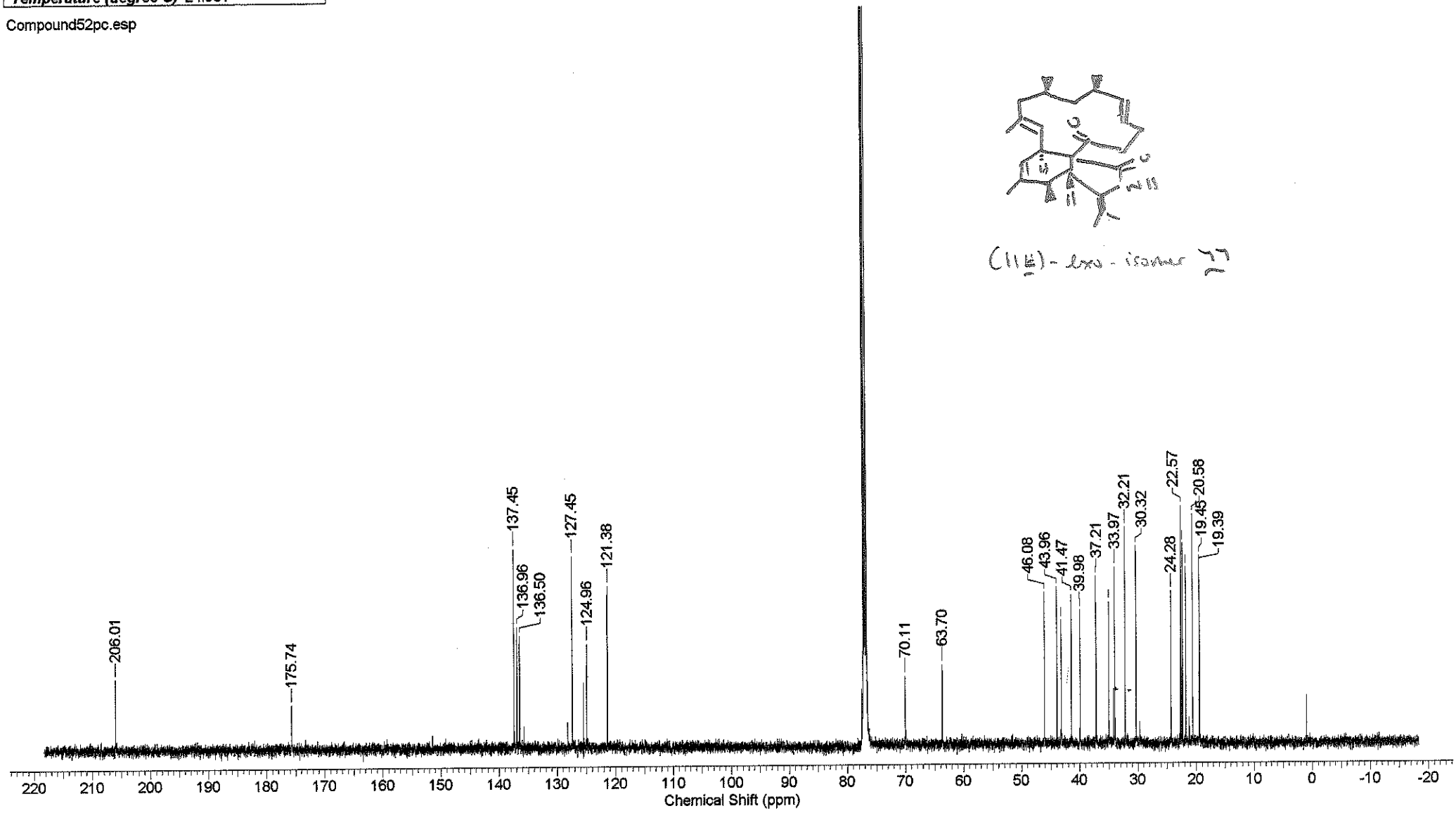
Compound52pp.esp



11/08/2012 17:2

Acquisition Time (sec)	1.1010	***Comment***	Mark Willis MWH064PPB mCARBON CDCl3 /opt/bruk500data/2012/Apr vnmr1 56				
Date	26 Apr 2012 04:28:48			***Date Stamp***	26 Apr 2012 04:28:48		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 52\MWH064pcb_000001r					***Frequency (MHz)***	125.76
Nucleus	13C	***Number of Transients***	18432	***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)***	12573.9014	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	24.931						

Compound52pc.esp



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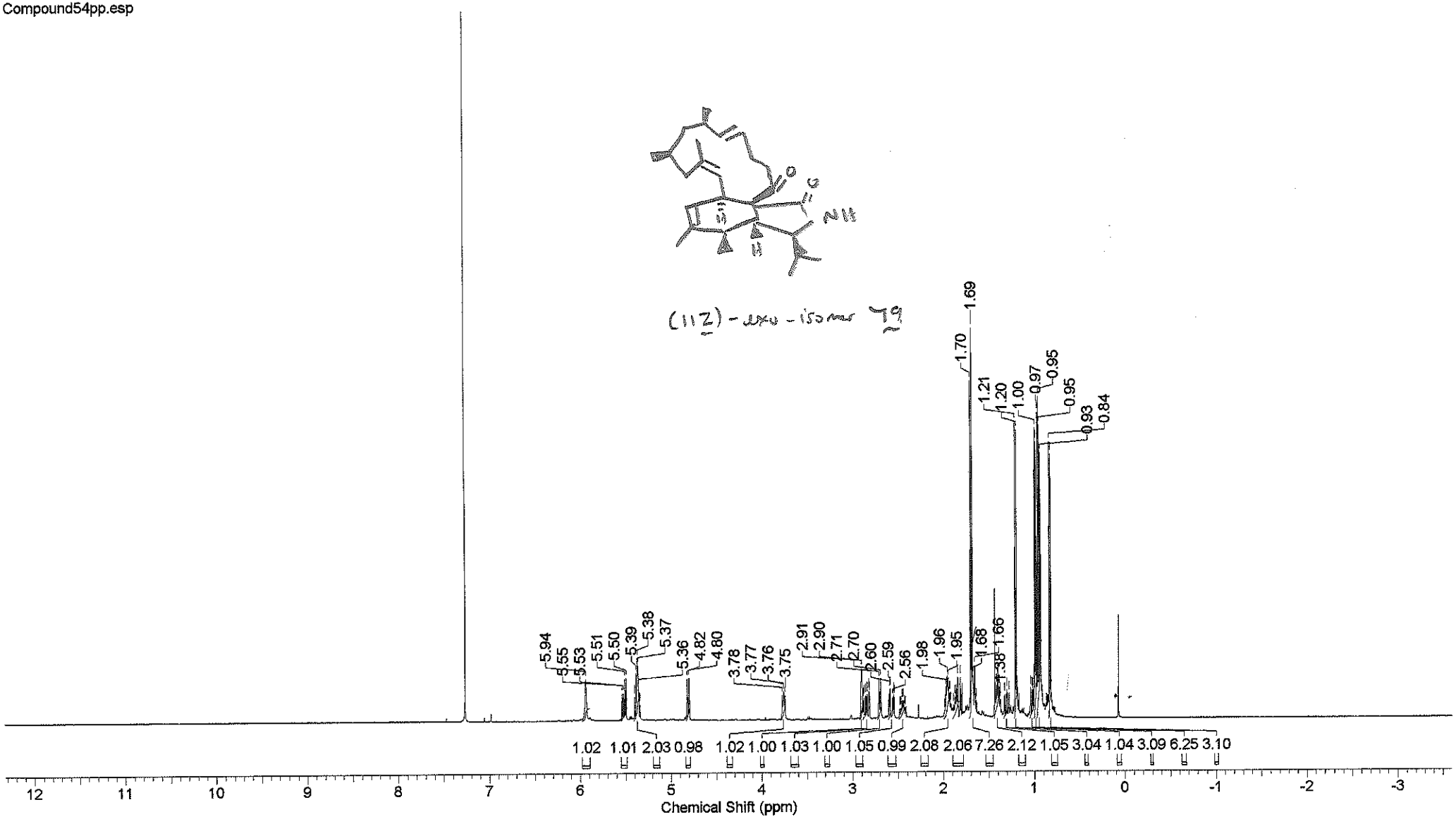
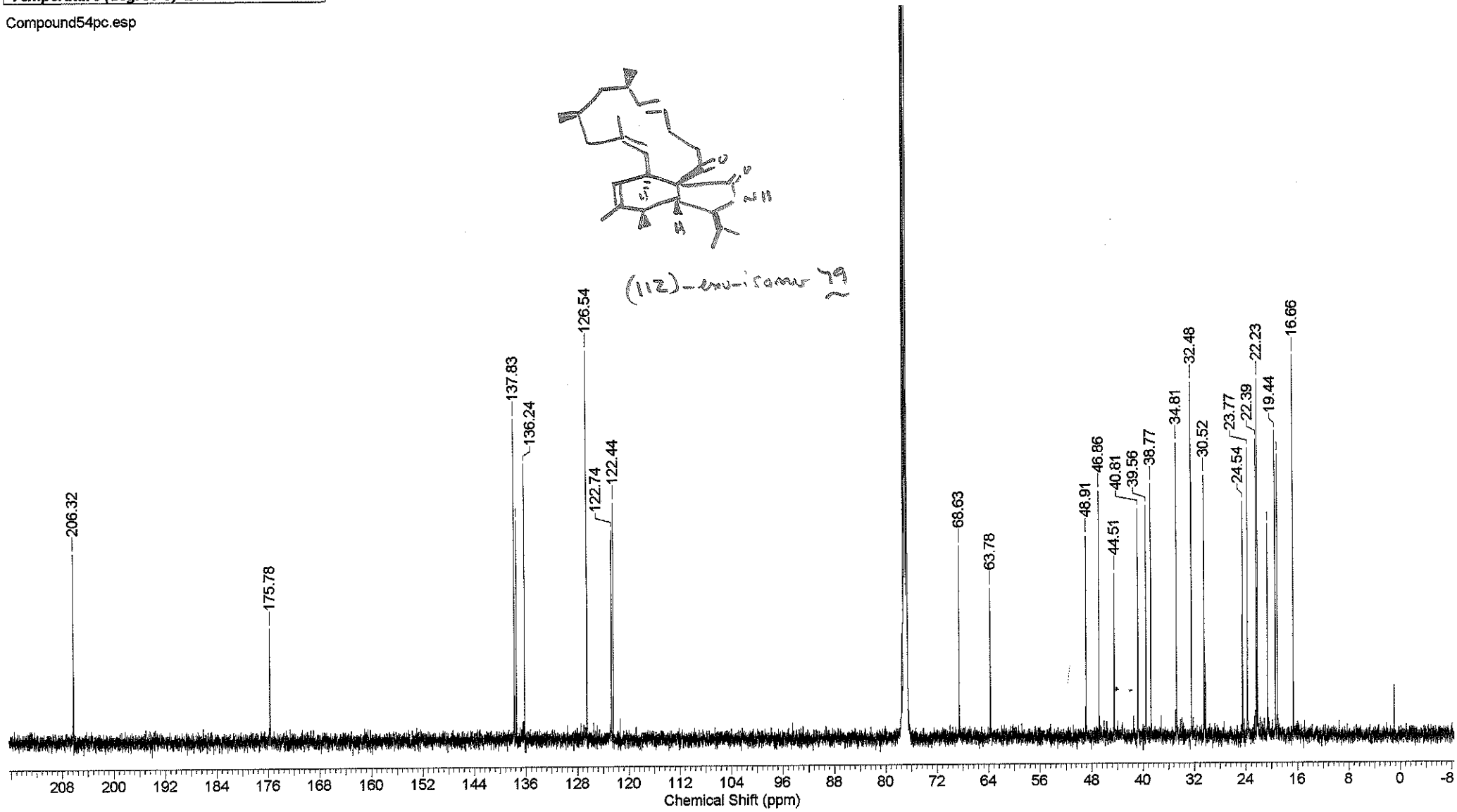
Acquisition Time (sec)	3.1719	***Comment***	Mark willis MWH066ppb mPROTON CDCl3 /opt/bruk500data/2012/Apr vnmr1 18				
Date	27 Apr 2012 08:55:28			***Date Stamp***	27 Apr 2012 08:55:28		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 54_010001r			***Frequency (MHz)***	500.13	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	vnmr1
Points Count	32768	***Pulse Sequence***	zg30b	***Receiver Gain***	228.00	***SW(cyclical) (Hz)***	10330.58
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	3079.9768	***Sweep Width (Hz)***	10330.26	***Temperature (degree C)***	25.029

Compound54pp.esp



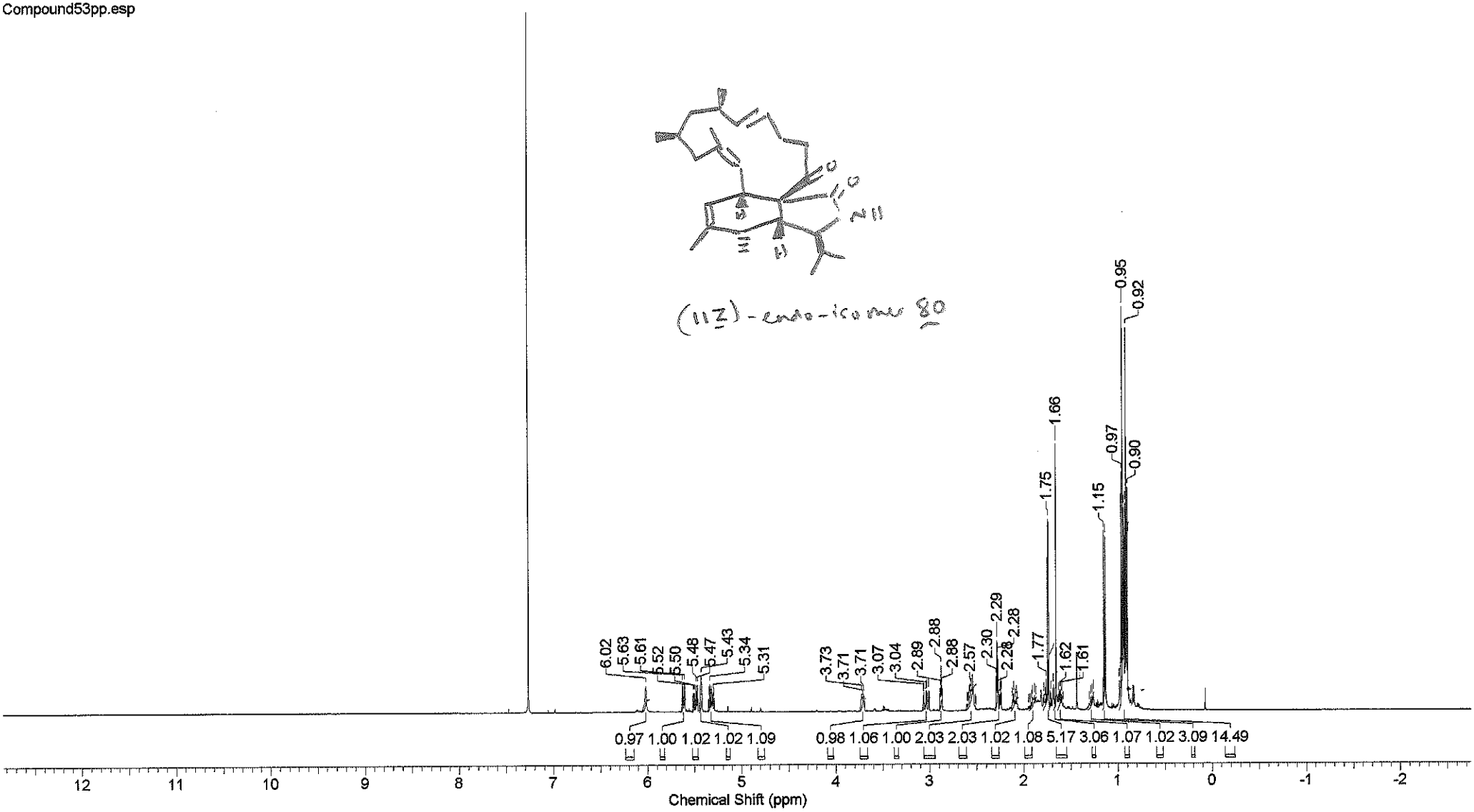
Acquisition Time (sec)	1.1010	***Comment***	Mark willis MWH066ppb mCARBON CDCl3 /opt/bruk500data/2012/Apr vnmr1 18				
Date	27 Apr 2012 10:18:40			***Date Stamp***	27 Apr 2012 10:18:40		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 54\MWH066pcb_000001r					***Frequency (MHz)***	125.76
Nucleus	13C	***Number of Transients***	18432	***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)***	12572.9922	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	25.029						

Compound54pc.esp

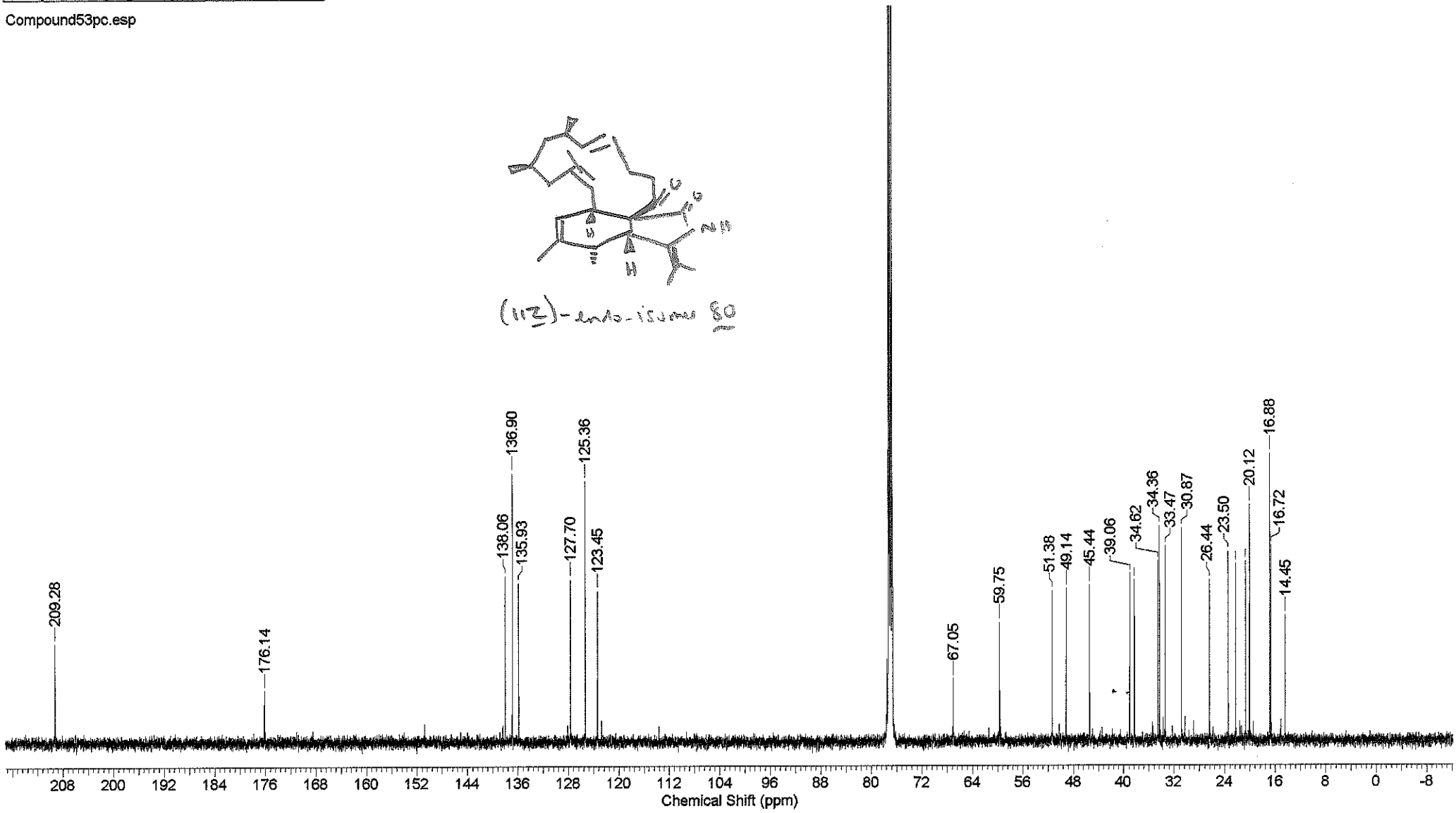


Acquisition Time (sec)	3.1719	***Comment***	Mark willis MWH066ppt mPROTON CDCl3 /opt/bruk500data/2012/Apr vnmr1 19				
Date	28 Apr 2012 06:06:56			***Date Stamp***	28 Apr 2012 06:06:56		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 53\MWH066ppt_000001r					***Frequency (MHz)***	500.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	vnmr1	***Points Count***	32768	***Pulse Sequence***	zg30b	***Receiver Gain***	256.00
SW(cyclical) (Hz)	10330.58	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	3079.9768	***Sweep Width (Hz)***	10330.26
Temperature (degree C)	25.029						

Compound53pp.esp



Acquisition Time (sec)	1.1010	***Comment***	Mark willis MWH066ppt mCARBON CDCl3 /opt/bruk500data/2012/Apr vnmr1 19				
Date	28 Apr 2012 22:51:44			***Date Stamp***	28 Apr 2012 22:51:44		
File Name	F:\Chemistry\Year 3 data\NMR data\Data\Compound 53\MWH066pct_000001r					***Frequency (MHz)***	125.76
Nucleus	13C	***Number of Transients***	18432	***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)***	12572.9824	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	24.931						

Compound53pc.esp

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