

# Supporting Information

## Cyclic dinuclear organotin cations stabilized by bulky substituents

Michael Wagner,<sup>a</sup> Bernhard Zobel,<sup>a</sup> Christina Dietz,<sup>a</sup> Dieter Schollmeyer,<sup>b</sup> Klaus Jurkschat<sup>a,\*</sup>

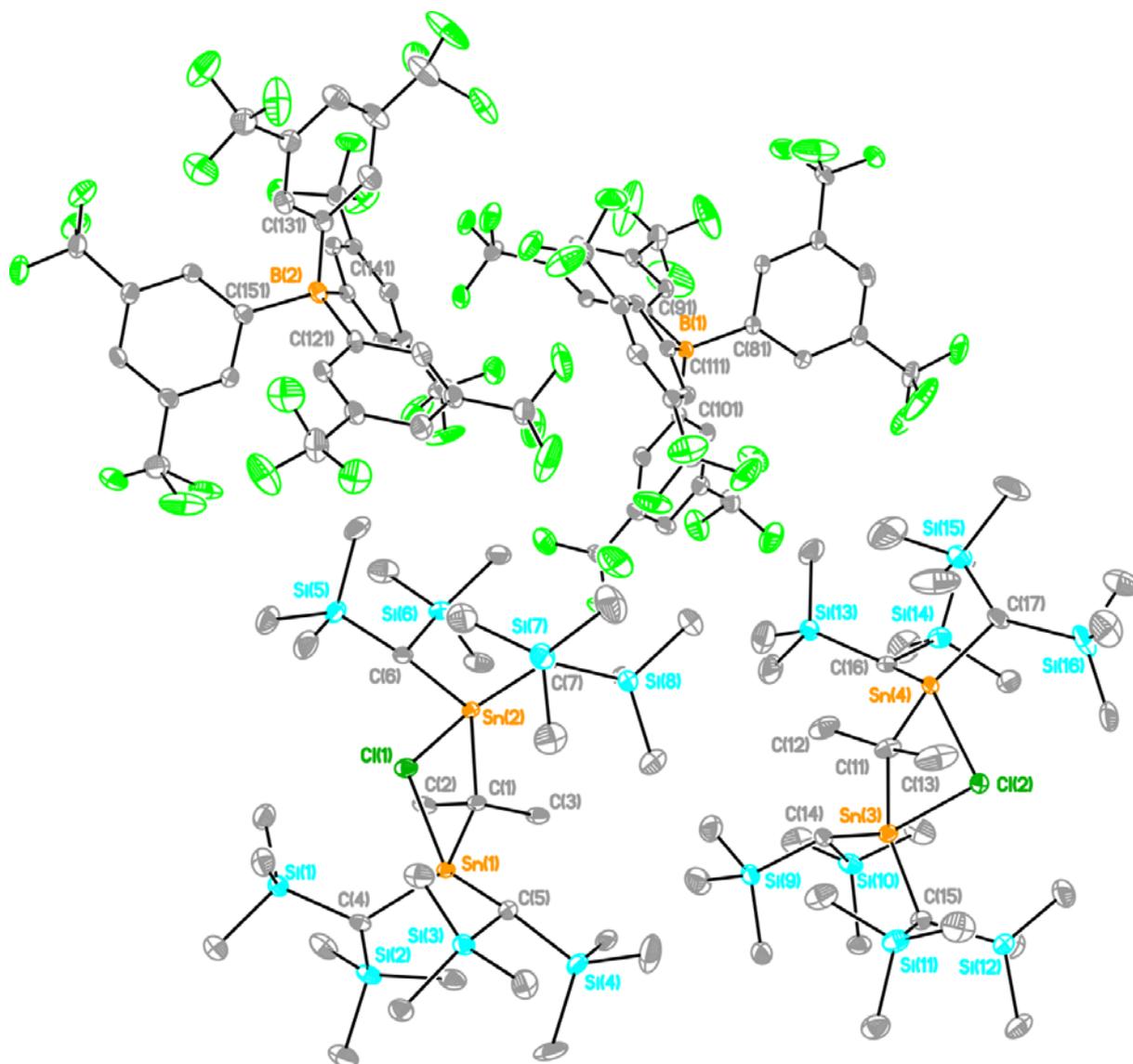
<sup>a</sup>Lehrstuhl für Anorganische Chemie II, Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany, E-mail: [klaus.jurkschat@tu-dortmund.de](mailto:klaus.jurkschat@tu-dortmund.de)

<sup>b</sup>Johannes Gutenberg-Universität Mainz, Institut für Organische Chemie, Duesbergweg 10-14, 55099 Mainz

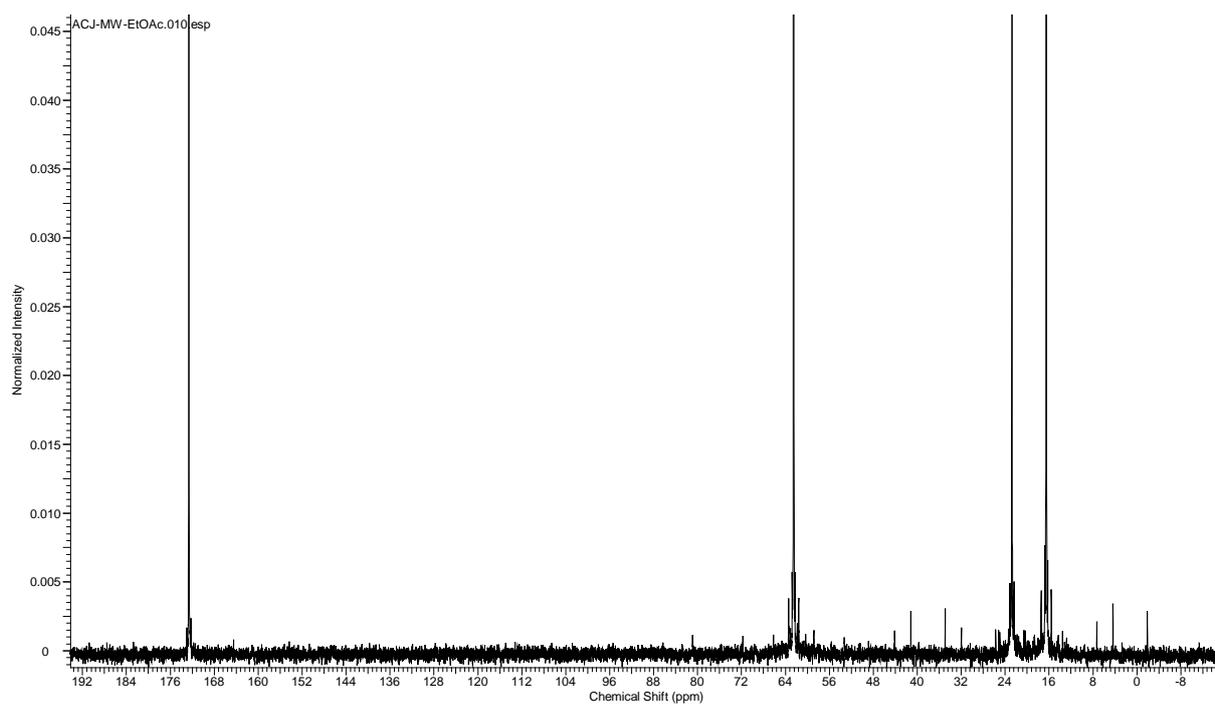
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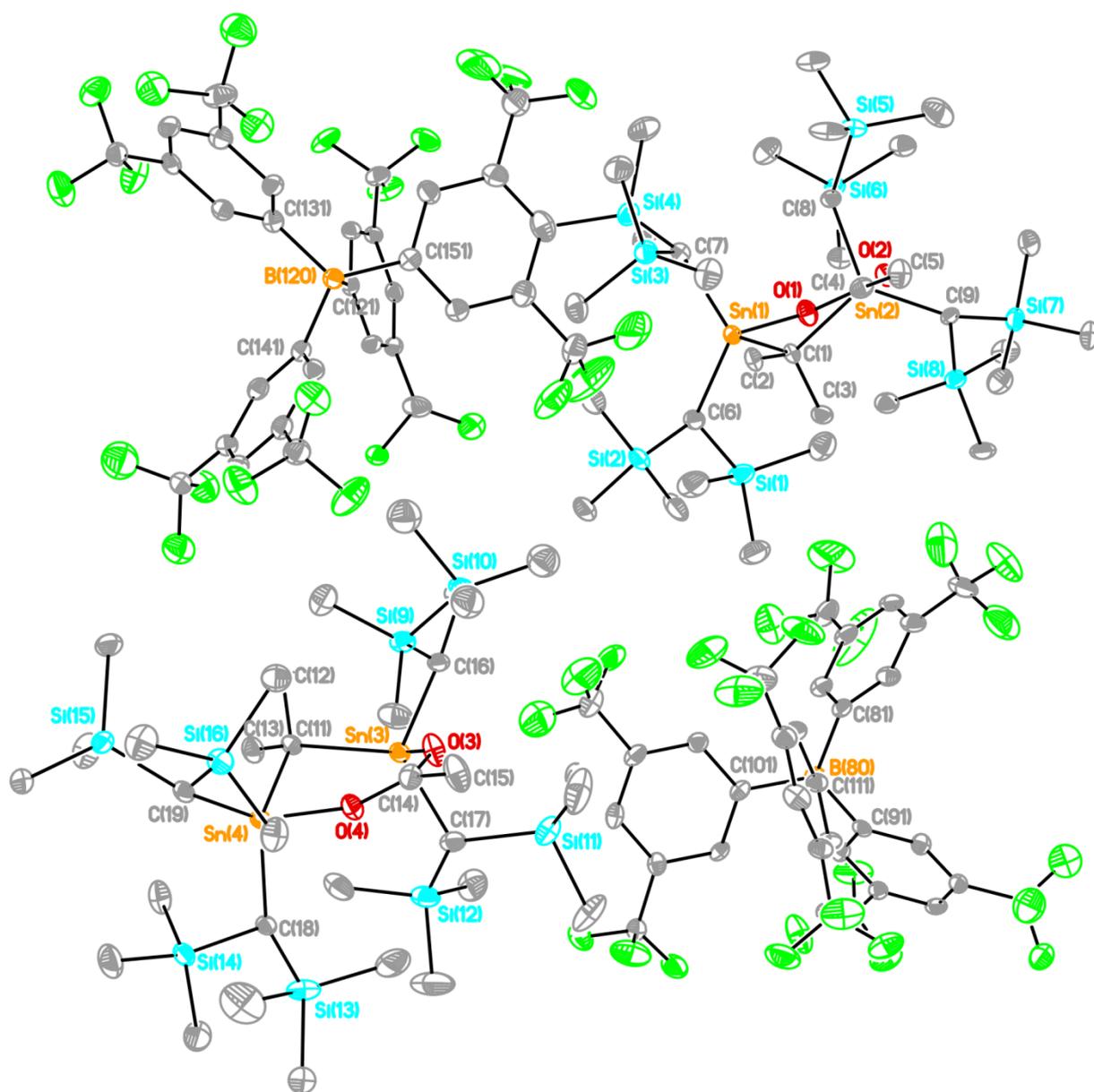
## 1. Figures



**Figure S1.** Asymmetric unit of compound **2** with 30% probability ellipsoids, the disorder is not shown. Selected selected interatomic distances (Å) and angles (°): Sn(3)-Cl(2) 2.5465(12), Sn(4)-Cl(2) 2.5725(13), Sn(3)-Cl(2)-Sn(4) 83.71(4), C(11)-Sn(4)-Cl(2) 81.44(13),

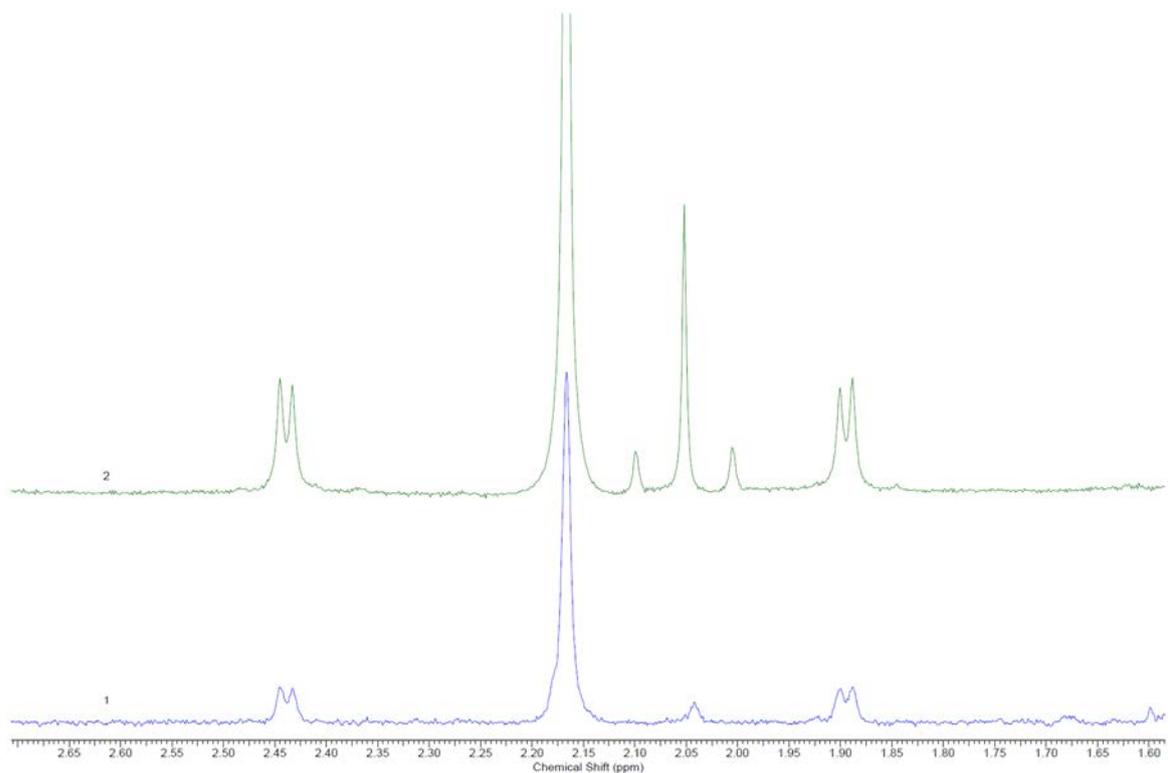


**Figure S2.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$  capillary) of the ethyl acetate used for the reaction with compound **2**.



**Figure S3.** Molecular structure of compound **3** with 30% ellipsoid probability. Disorder and the hydrogen atoms are omitted for clarity.





**Figure S6.** Part of the <sup>1</sup>H NMR spectrum of the organotin hydroxide **4** (top), after addition of D<sub>2</sub>O (bottom)

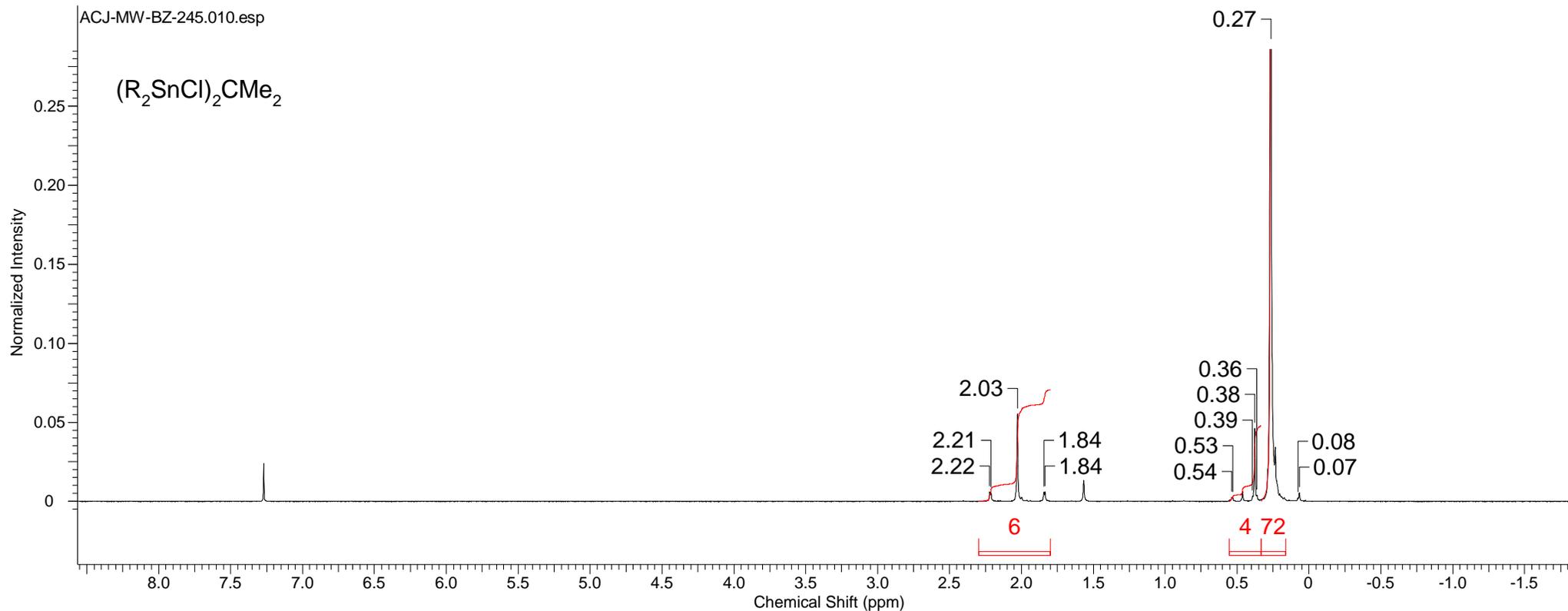
**Table S1.** Crystallographic data for compound **1**·0.5C<sub>3</sub>H<sub>6</sub>O, **2**, **3**.

	<b>1</b> ·0.5C <sub>3</sub> H <sub>6</sub> O	<b>2</b>	<b>3</b>
Empirical formula	C <sub>32.5</sub> H <sub>85</sub> Cl <sub>2</sub> O <sub>0.5</sub> Si <sub>8</sub> Sn <sub>2</sub>	C <sub>63</sub> H <sub>94</sub> BClF <sub>24</sub> Si <sub>8</sub> Sn <sub>2</sub>	C <sub>65</sub> H <sub>97</sub> BF <sub>24</sub> O <sub>2</sub> Si <sub>8</sub> Sn <sub>2</sub>
Formula mass [g mol <sup>-1</sup> ]	1017.00	1815.74	1839.33
$\lambda$ [Å]	0.71073	0.71073	0.71073
<i>T</i> [K]	173(2)	173(2)	173(2)
Crystal system	orthorhombic	triclinic	triclinic
Crystal size [mm]	0.31x0.25x0.08	0.43x0.18x0.13	0.33x0.15x0.07
Space group	<i>Pbcn</i>	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> [Å]	28.4631(10)	18.0884(5)	21.0297(7)
<i>b</i> [Å]	23.2026(5)	19.9197(6)	21.3202(8)
<i>c</i> [Å]	16.3645(4)	25.3597(8)	22.2151(9)
$\alpha$ [°]	90	95.528(2)	62.979(4)
$\beta$ [°]	90	100.315(3)	80.751(3)
$\gamma$ [°]	90	110.312(3)	85.767(3)
<i>V</i> [Å <sup>3</sup> ]	10807.4(5)	8305.5(5)	8757.7(6)
<i>Z</i>	8	4	4
$\rho_{\text{calcd.}}$ [Mgm <sup>-3</sup> ]	1.250	1.452	1.395
$\mu$ [mm <sup>-1</sup> ]	1.221	0.838	0.768
<i>F</i> (000)	4240	3688	3744
$\theta$ range [°]	2.265-25.242	2.185-25.499	2.169-25.50
Index ranges	-38 ≤ <i>h</i> ≤ 38 -30 ≤ <i>k</i> ≤ 31 -22 ≤ <i>l</i> ≤ 22	-21 ≤ <i>h</i> ≤ 21 -24 ≤ <i>k</i> ≤ 24 -30 ≤ <i>l</i> ≤ 30	-25 ≤ <i>h</i> ≤ 25 -25 ≤ <i>k</i> ≤ 25 -26 ≤ <i>l</i> ≤ 26
No. of reflections collected	118841	113070	101867
Completeness of $\theta_{\text{max}}$ [%]	99.9	99.9	99.9
No. of independent reflections / <i>R</i> <sub>int</sub>	13761 / 0.0650	30901 / 0.0528	32571 / 0.0666
No. of reflections observed with [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	10334	23326	21793
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
<i>T</i> <sub>max</sub> / <i>T</i> <sub>min</sub>	1.0/0.83029	1.0/0.92877	1.0/0.81355
No. of refined parameters/restraints	405/1	1949/180	1904/295
GoF( <i>F</i> <sup>2</sup> )	0.960	1.065	0.976
<i>R</i> <sub>1</sub> ( <i>F</i> ) [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	0.0483	0.0566	0.0600
w <i>R</i> <sub>2</sub> ( <i>F</i> <sup>2</sup> ) (all data)	0.1477	0.1635	0.1699
( $\Delta/\sigma$ ) <sub>max</sub>	0.001	0.007	0.008
Largest difference peak/hole [eÅ <sup>-3</sup> ]	0.996 / -0.818	3.307 / -1.457	1.956 / -1.016
CCDC number	1409484	1409485	1409486

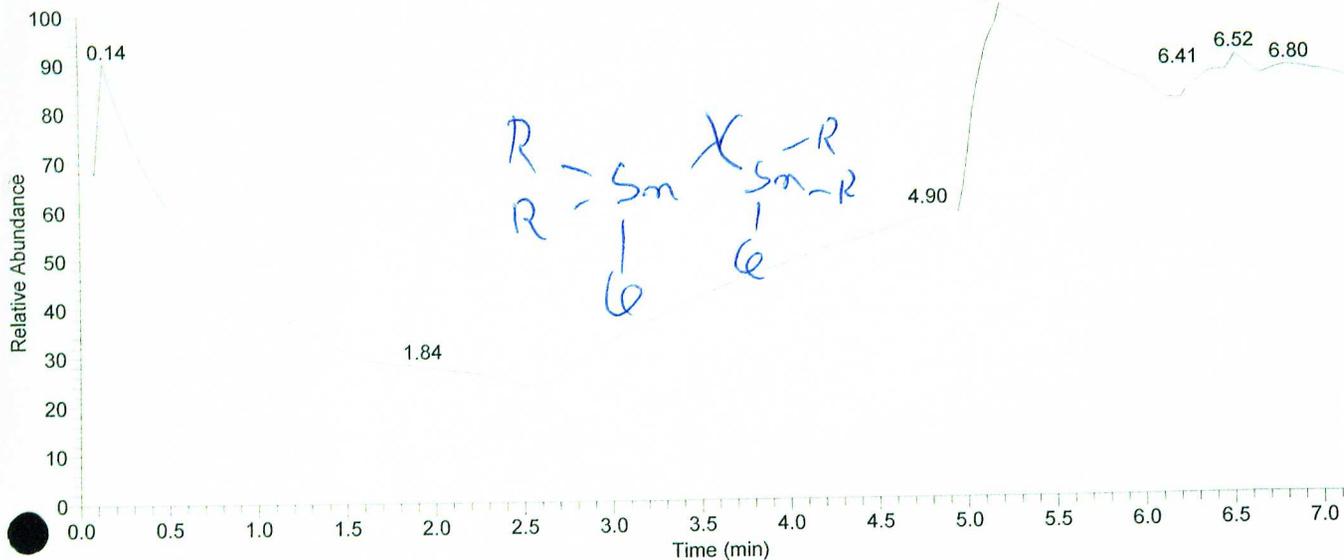
**Table S2.** Crystallographic data for compound **4**, **5**.

	<b>4</b>	<b>5</b>
Empirical formula	C <sub>63</sub> H <sub>95</sub> BOF <sub>24</sub> Si <sub>8</sub> Sn <sub>2</sub>	C <sub>31</sub> H <sub>82</sub> OSi <sub>8</sub> Sn <sub>2</sub>
Formula mass [g mol <sup>-1</sup> ]	1797.29	933.06
$\lambda$ [Å]	0.71073	1.54178
$T$ [K]	173(2)	296(2)
Crystal system	triclinic	monoclinic
Crystal size [mm]	0.28x0.21x0.17	0.58x0.42x0.22
Space group	$P\bar{1}$	$C2/c$
$a$ [Å]	14.6916(4)	21.800(6)
$b$ [Å]	17.9511(6)	9.4970(4)
$c$ [Å]	18.3180(5)	25.406(3)
$\alpha$ [°]	113.362(3)	90
$\beta$ [°]	97.832(2)	106.313(15)
$\gamma$ [°]	104.520(3)	90
$V$ [Å <sup>3</sup> ]	4139.6(2)	5048.2(16)
$Z$	2	4
$\rho_{\text{calcd.}}$ [Mgm <sup>-3</sup> ]	1.442	1.228
$\mu$ [mm <sup>-1</sup> ]	0.810	9.833
$F(000)$	1828	1952
$\theta$ range [°]	2.252-25.500	3.625-74.642
Index ranges	-17 $\leq h \leq$ 17 -21 $\leq k \leq$ 21 -22 $\leq l \leq$ 22	0 $\leq h \leq$ 27 0 $\leq k \leq$ 11 -31 $\leq l \leq$ 31
No. of reflections collected	47920	5174
Completeness of $\theta_{\text{max}}$ [%]	99.9	99.9
No. of independent reflections / $R_{\text{int}}$	15405 / 0.0240	5174 / n. d.
No. of reflections observed with $[I > 2\sigma(I)]$	13353	4633
Absorption correction	Semi-empirical from equivalents	psi scan
$T_{\text{max}}/T_{\text{min}}$	1.0/0.86424	0.217/ 0.069
No. of refined parameters/restraints	999/170	228/82
GoF( $F^2$ )	1.032	1.019
$R_1(F)$ [ $I > 2\sigma(I)$ ]	0.0507	0.0807
$wR_2(F^2)$ (all data)	0.1442	0.2277
$(\Delta/\sigma)_{\text{max}}$	0.002	0.001
Largest difference peak/hole [eÅ <sup>-3</sup> ]	1.310 / -0.951	2.262 / -2.217
CCDC number	1409487	1409488

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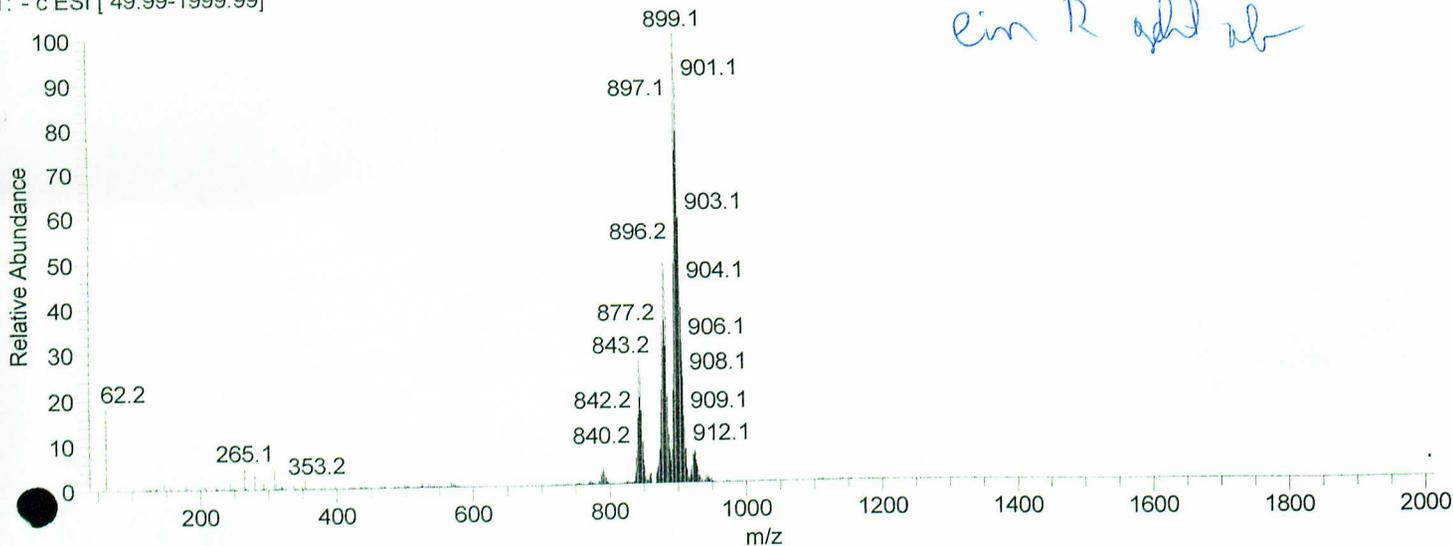
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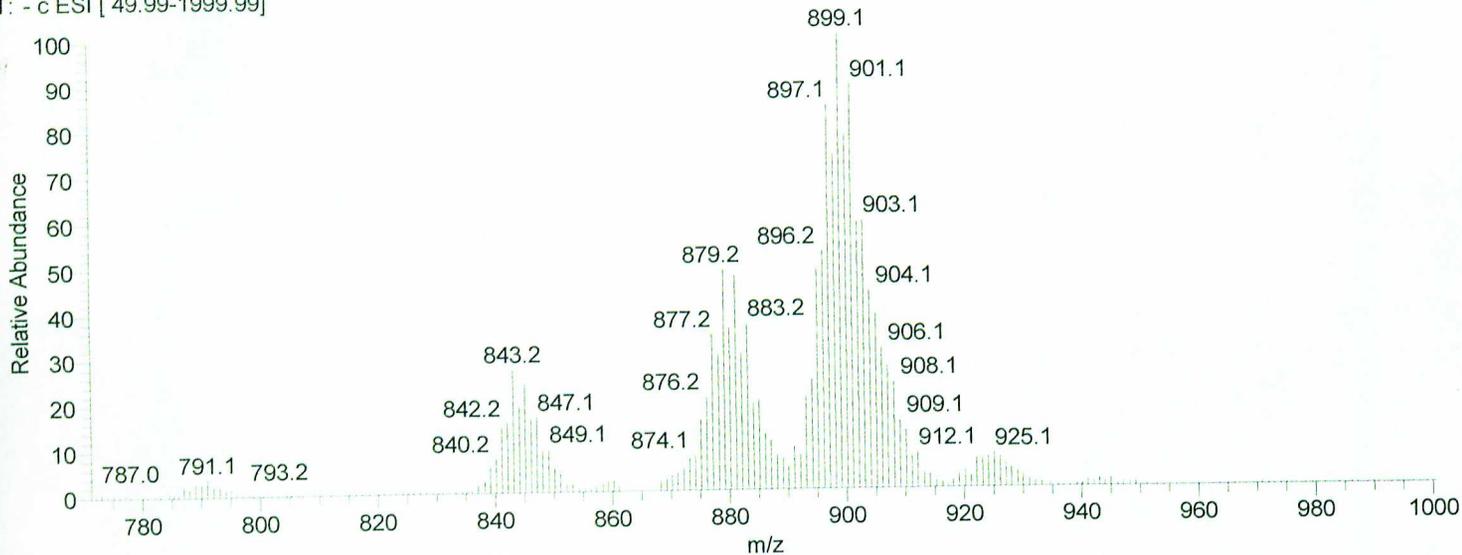
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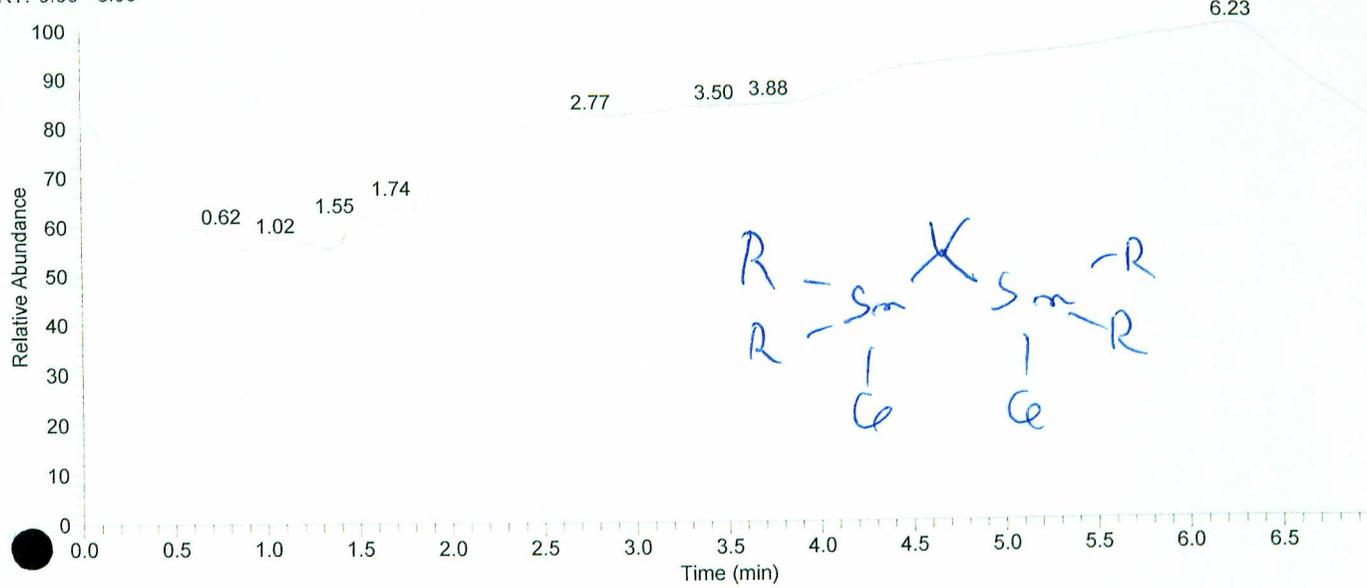


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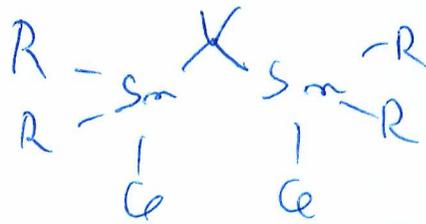
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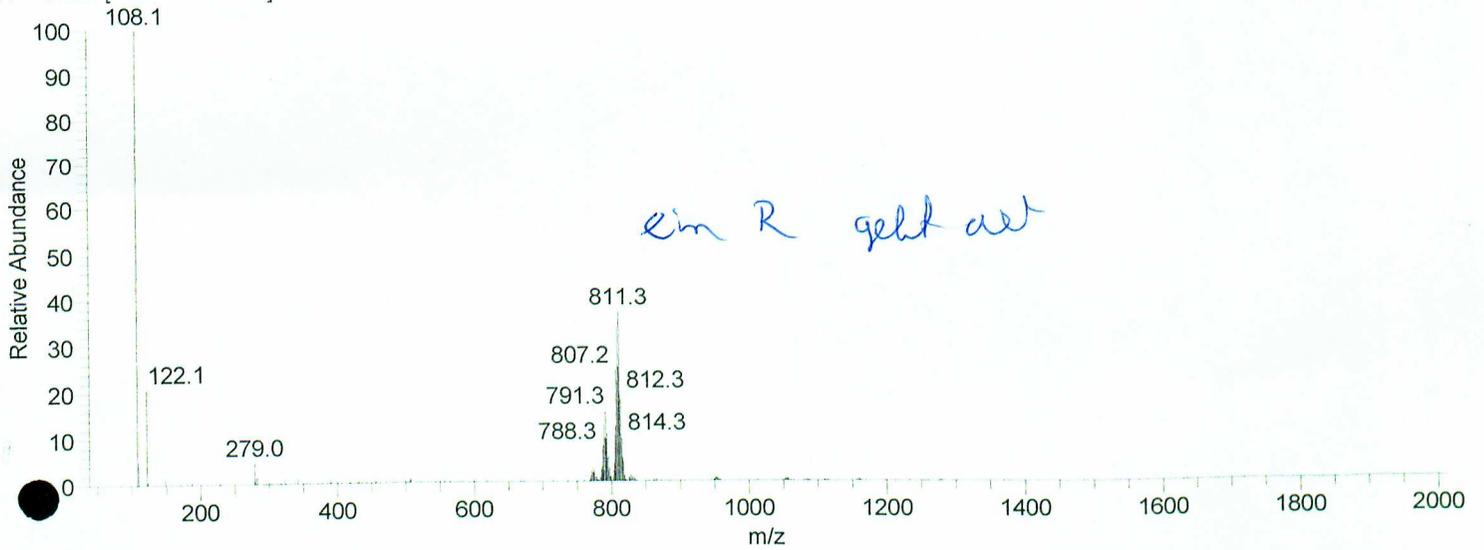
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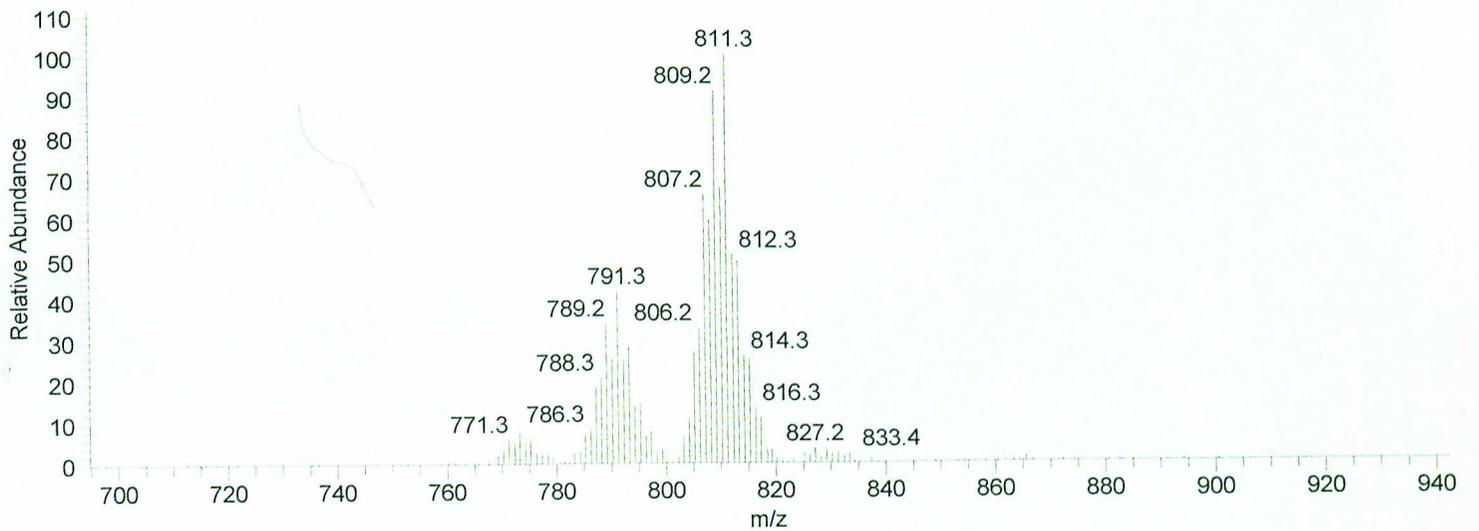


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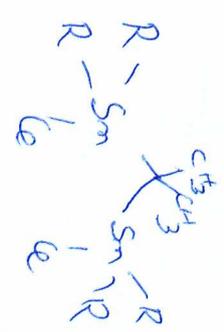
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MW-B2245

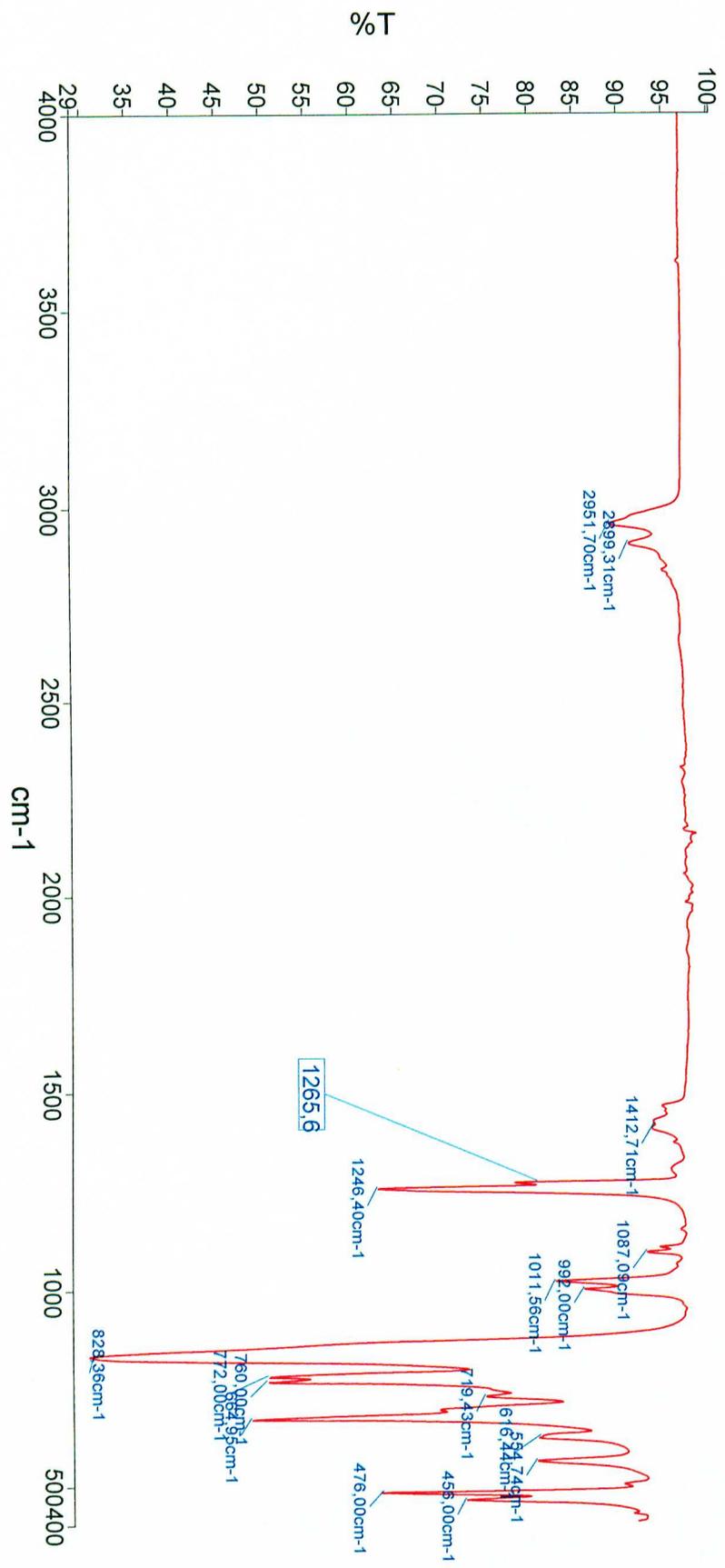
Kristalle



Anwender  
Datum/ Uhrzeit

Jurkschat  
Sonntag, 12. April 2015 12:23

PerkinElmer Spectrum Version 10.03.08  
Sonntag, 12. April 2015 12:23



jurkschat 210 Sample 210 By Jurkschat date Sonntag, April 12 2015

M.p. 167-170°C  
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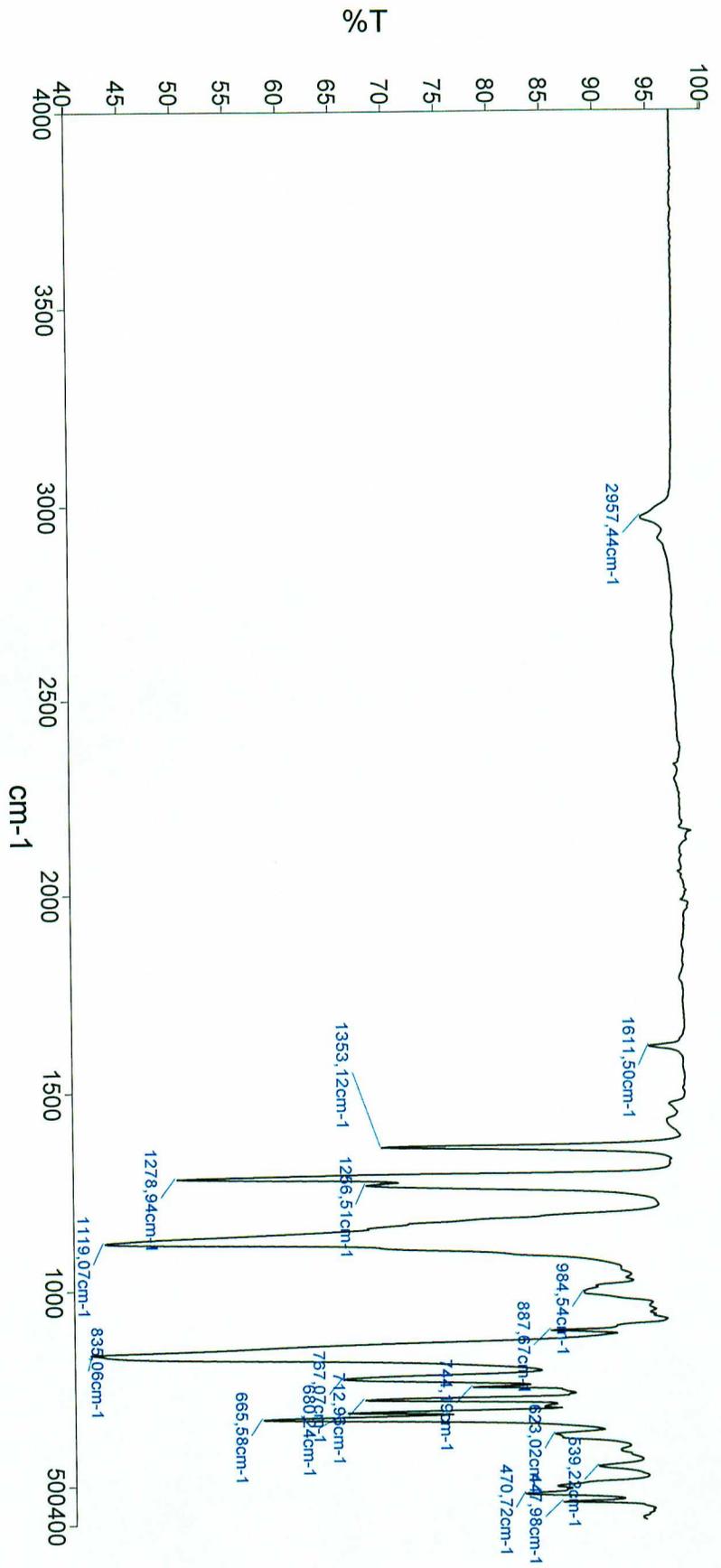


7+

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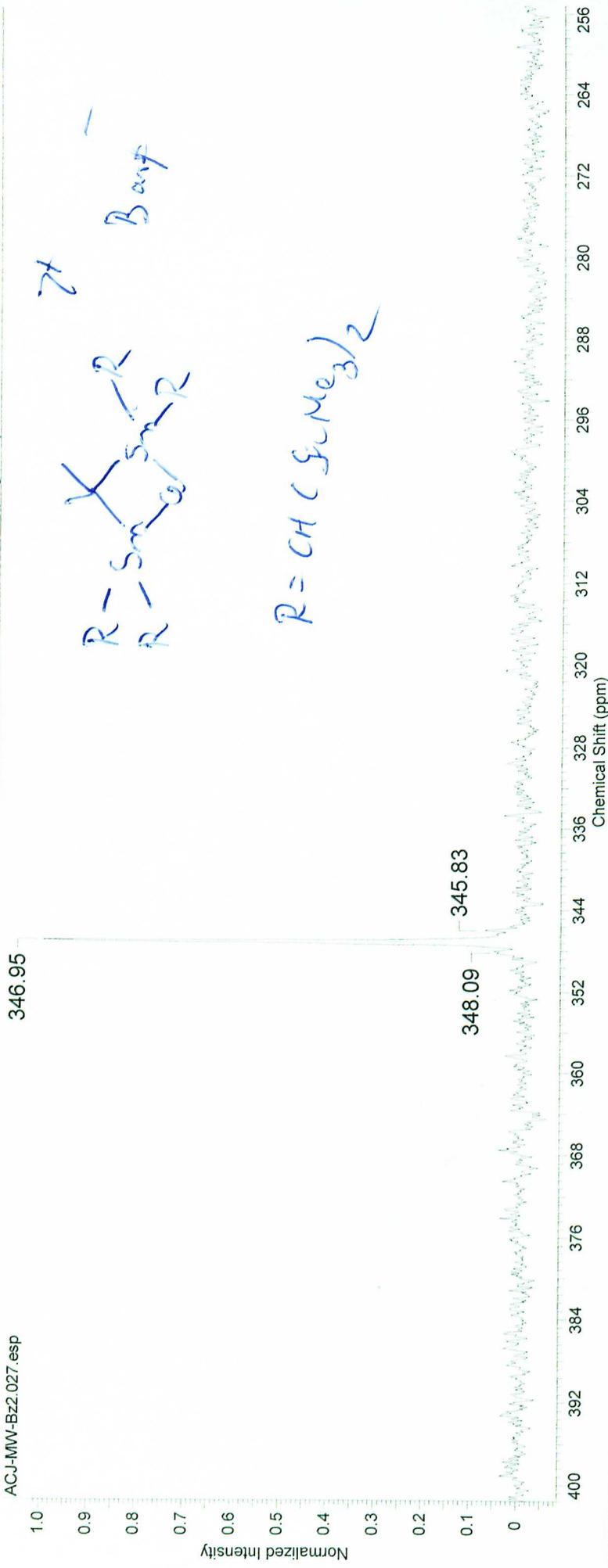
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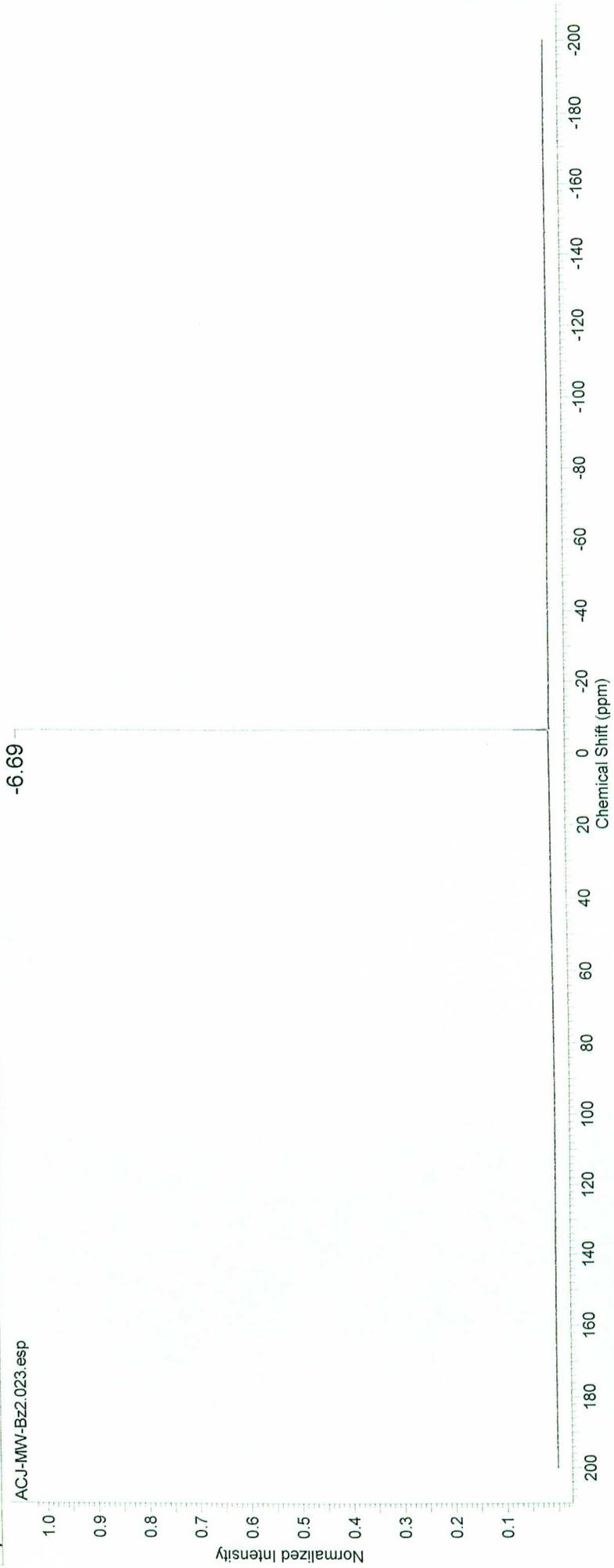
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2	346.95	38831.0	1.0000
3	348.09	38958.0	0.0460

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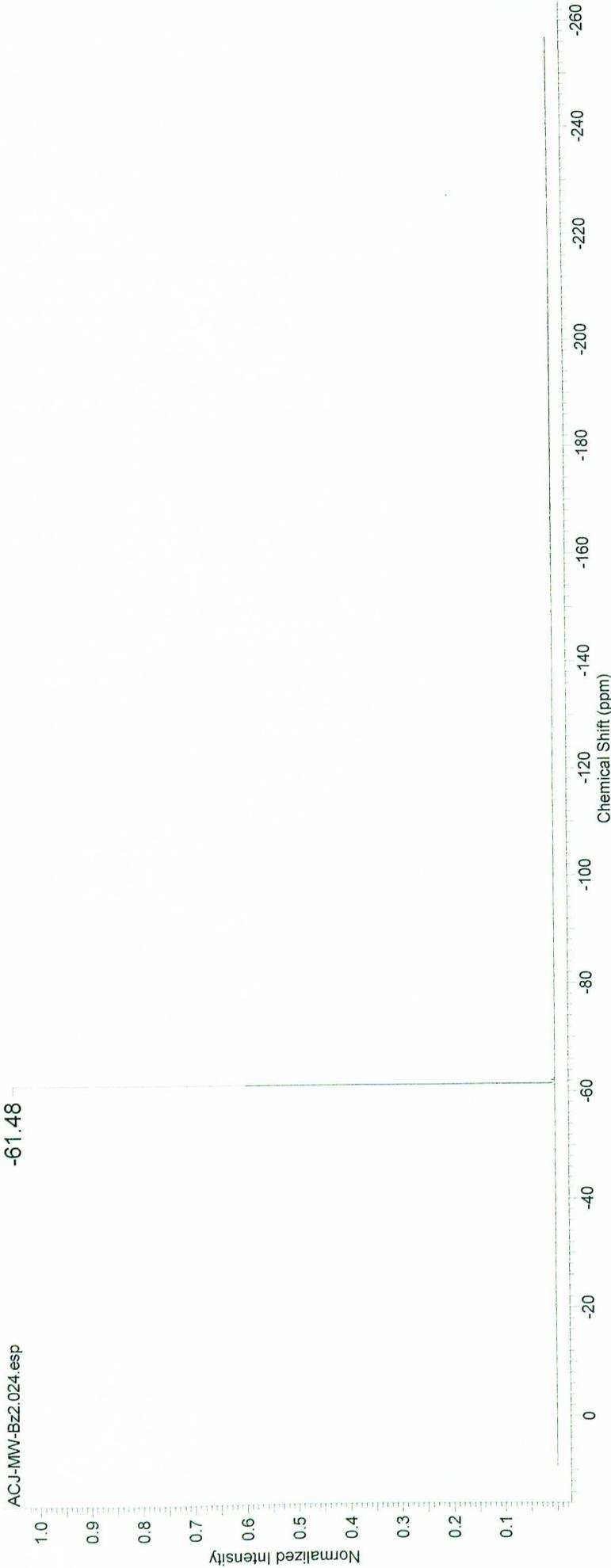
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				Temperature (degree C)	21.160
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				Solvent	CHLOROFORM-d



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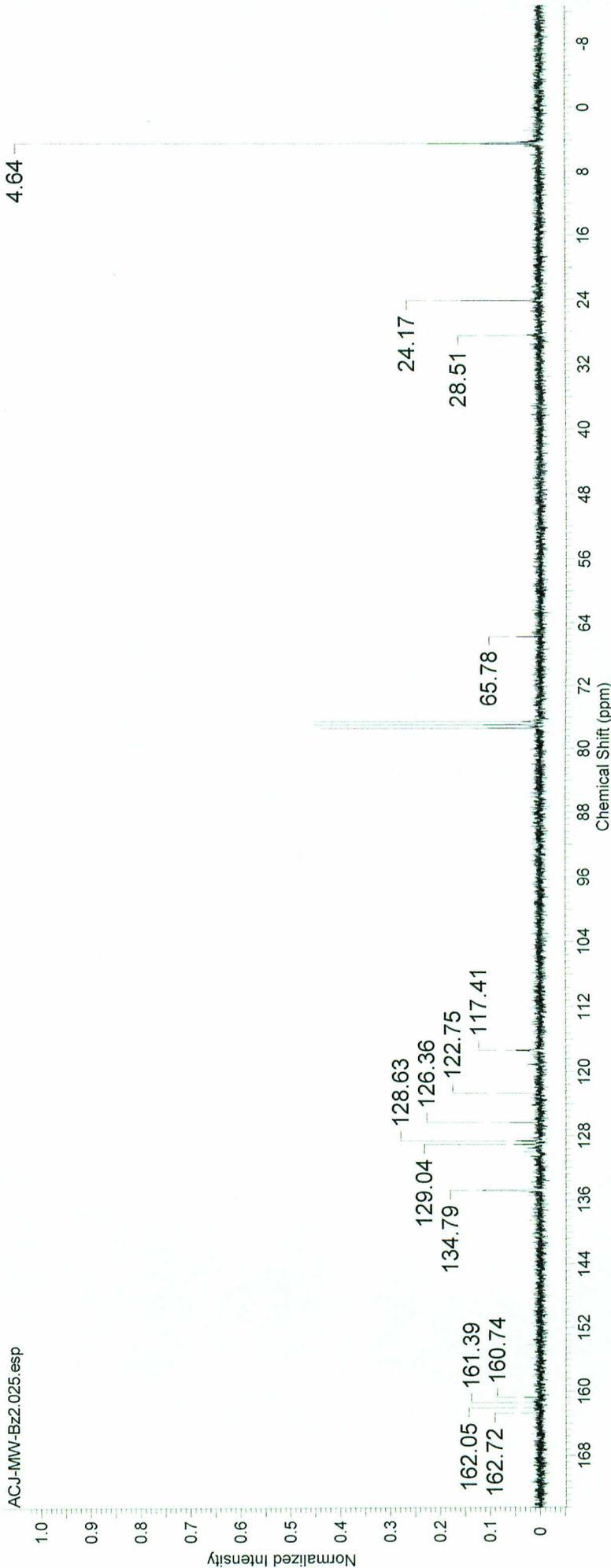
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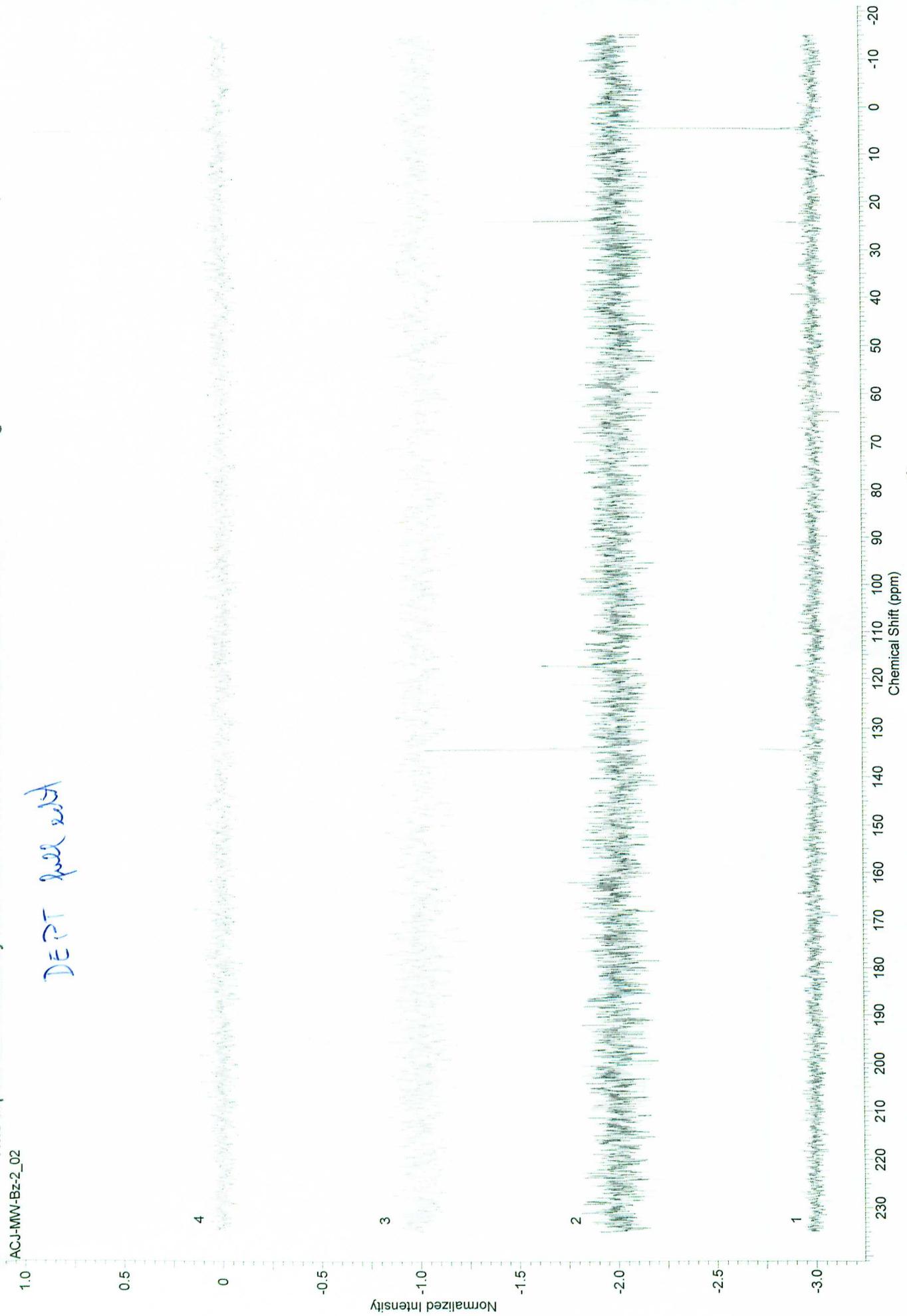
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Spectrum Offset (Hz)	9401.5547	Spectrum Type	STANDARD	Temperature (degree C)	21.160



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	4.64	349.8	1.0000	4	28.51	2151.8	0.1109	7	122.75	9263.9	0.0896
2	4.65	351.3	0.8511	5	65.78	4984.5	0.0504	8	126.36	9536.3	0.0984
3	24.17	1824.1	0.2144	6	117.41	8860.6	0.0704	9	128.63	9707.1	0.0631
								10	129.04	9738.3	0.0543
								11	134.79	10172.1	0.1269
								12	160.74	12130.3	0.0338
								13	161.39	12179.7	0.0317
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ACJ-MW-Bz-2\_02

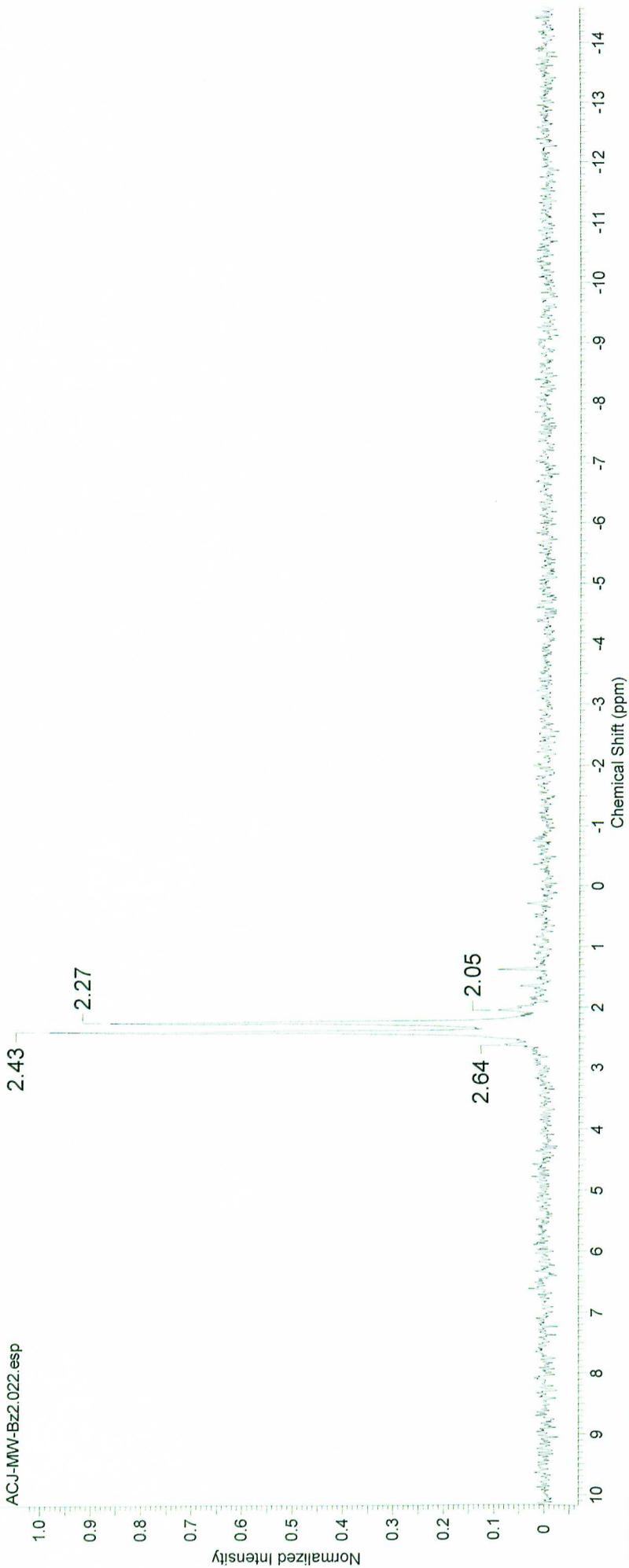
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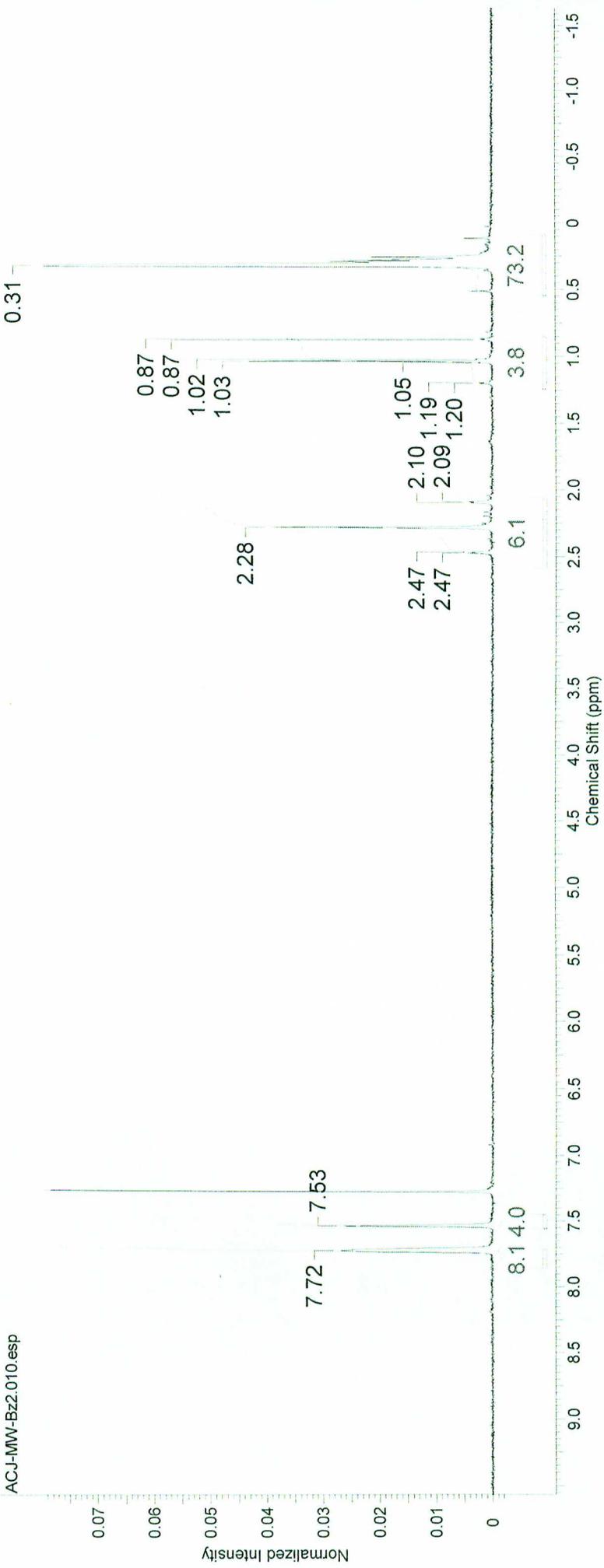
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3	2.43	145.1	1.0000
4	2.64	157.4	0.0763

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Solvent	CHLOROFORM-d	Temperature (degree C)	21.160	Sweep Width (Hz)			5994.84



No.	(ppm)	Value	Absolute Value	Non-Negative Value
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2	3.468 .. 1.243	8.4071493	1.28334056e+8	3.84071493
3	5.19 .. 2.586	1.4210081	2.05232800e+8	6.14210081
4	5.114 .. 7.623	9.9878693	1.33615888e+8	3.99878693
5	5.114 .. 7.798	1.3018703	2.71662944e+8	8.13018703

# Elementaranalysenauftrag

MICHAEL WAGNER

Auftraggeber

382013837

Telefon

13.4.15

Datum

MW-B22

Probenbezeichnung  
(max. 7 Stellen)

Die Substanz enthält:

CH<sub>2</sub>CF<sub>3</sub>Si

Smp.:

auf Abruf?

Sdp.:

Luftempfindlich:

Bemerkungen:

hygroskopisch:

Einwaage:

theor.

a

prakt.

b

a) 1.361

% C: 41.67

% H: 5.22

% N: ✓

41.7

5.3

✓

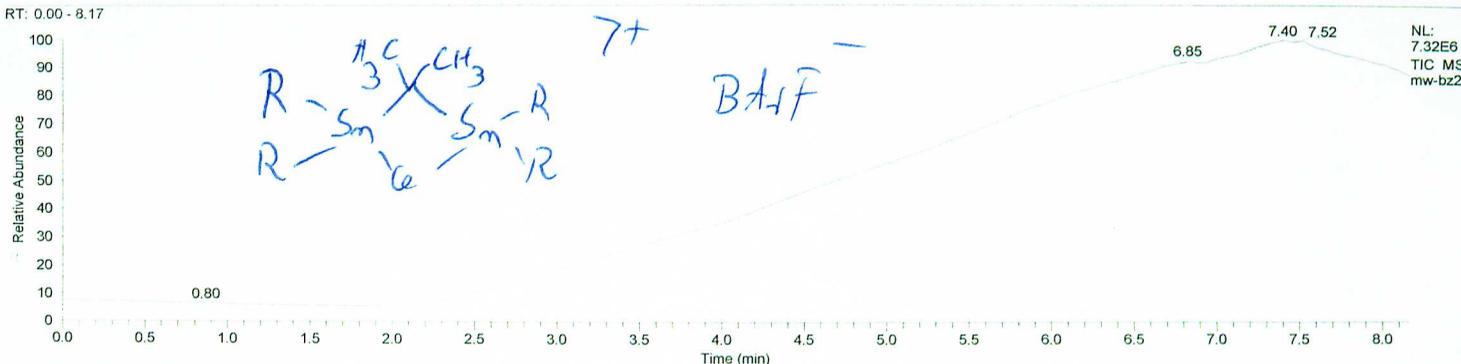
41.9

5.4

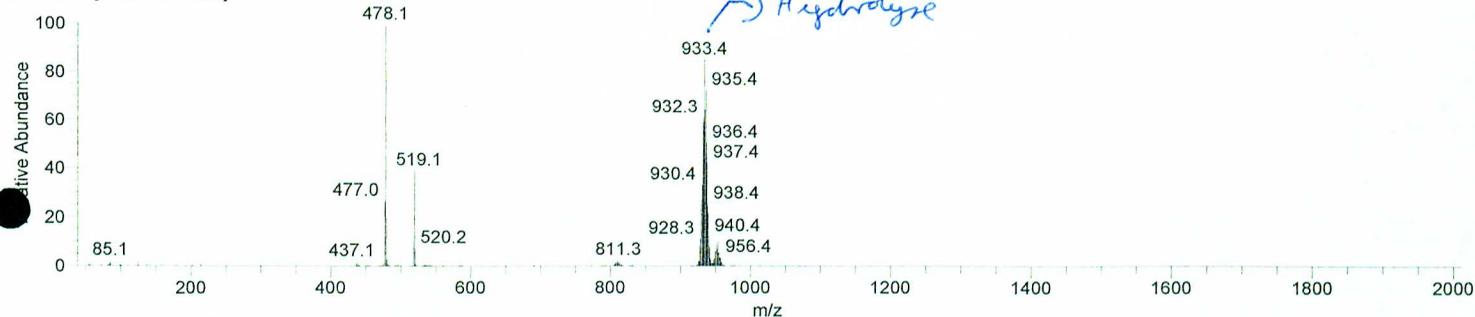
✓

Arbeitskreisleiter

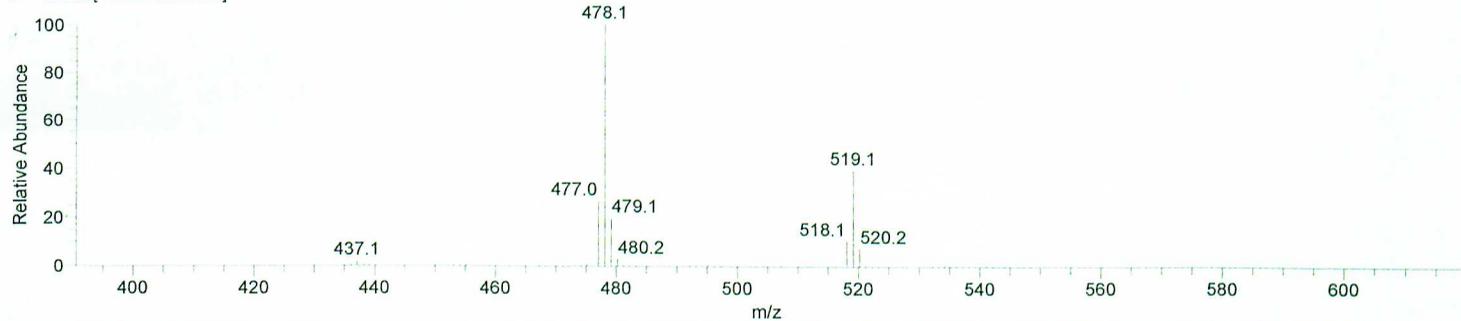
15.4.15 M. K. [Signature]  
Datum der Ausführung



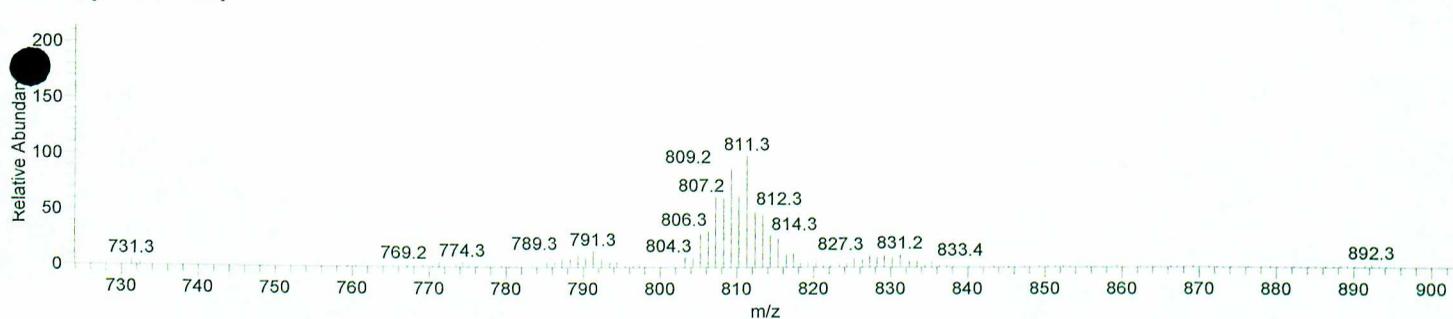
mw-bz2#258-273 RT: 7.71-8.17 AV: 16 SB: 70 0.06-2.11 NL: 6.61E5  
T: + c ESI [ 49.99-1999.99]



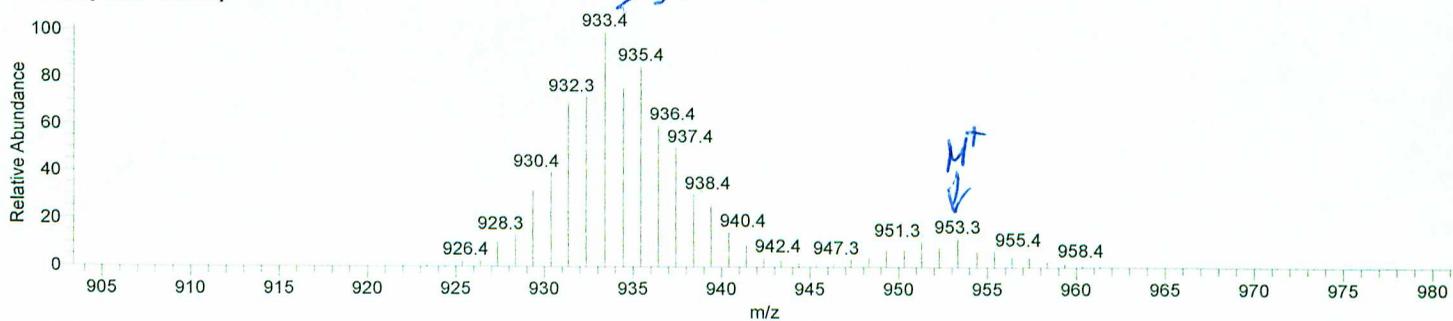
mw-bz2#258-273 RT: 7.71-8.17 AV: 16 SB: 70 0.06-2.11 NL: 6.61E5  
T: + c ESI [ 49.99-1999.99]



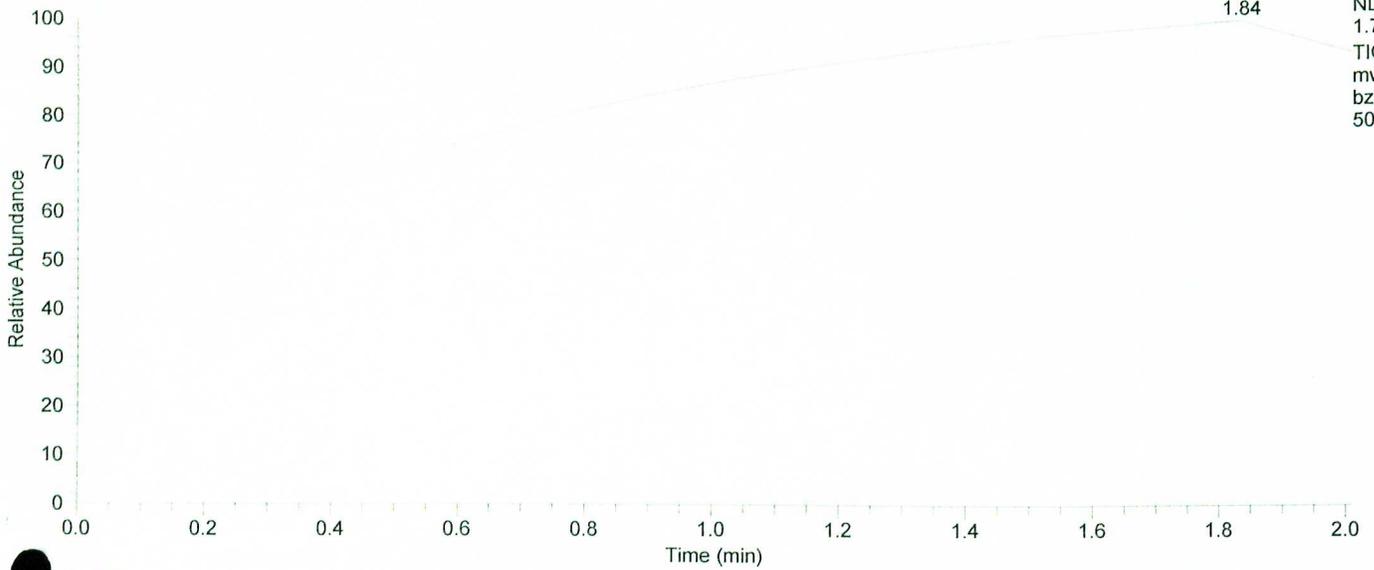
mw-bz2#258-273 RT: 7.71-8.17 AV: 16 SB: 70 0.06-2.11 NL: 1.71E4  
T: + c ESI [ 49.99-1999.99]



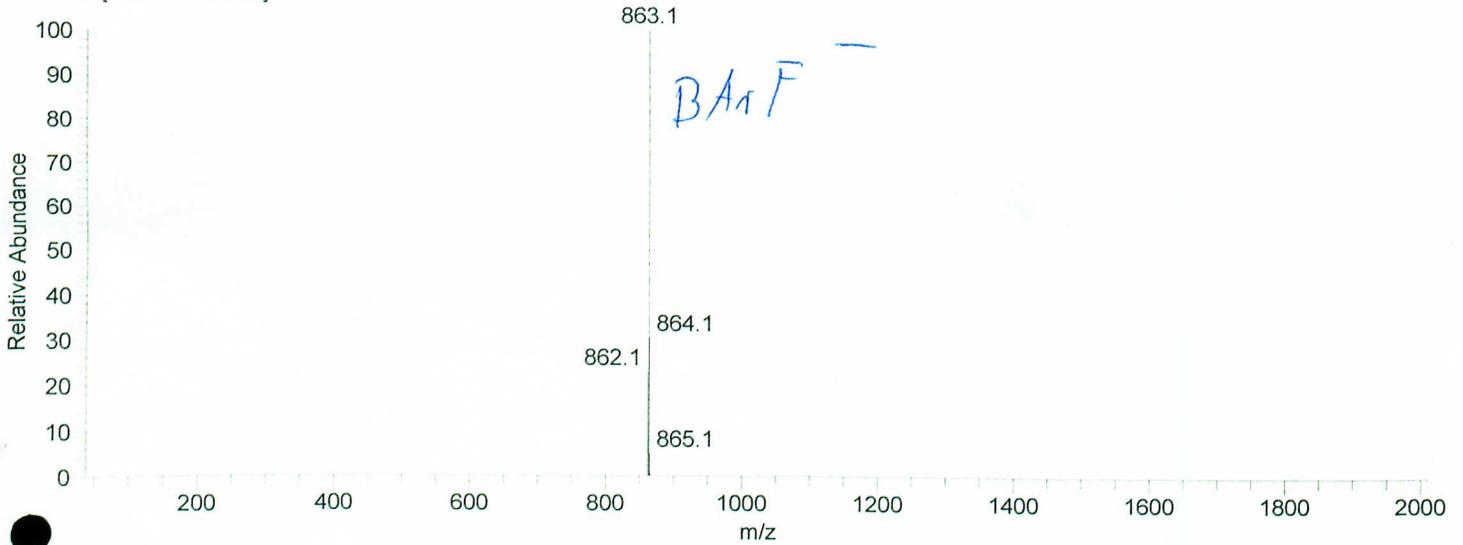
mw-bz2#258-273 RT: 7.71-8.17 AV: 16 SB: 70 0.06-2.11 NL: 5.68E5  
T: + c ESI [ 49.99-1999.99]



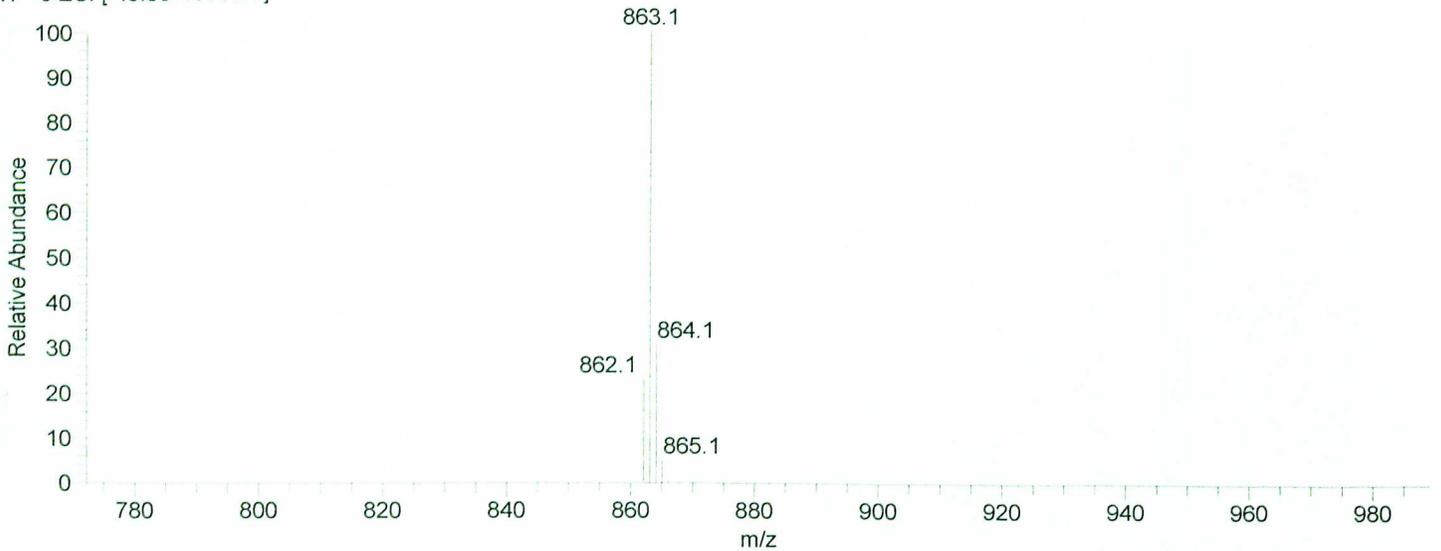
FIT: 0.00 - 2.01



mw-bz2\_150415050213#71-75 RT: 1.76-1.86 AV: 5 NL: 1.11E7  
T: - c ESI [ 49.99-1999.99]



mw-bz2\_150415050213#71-75 RT: 1.76-1.86 AV: 5 NL: 1.11E7  
T: - c ESI [ 49.99-1999.99]





SEMQuant Ergebnis. Ausgegeben um 09:41:23 am 17.04.15  
 Bearbeiter: meuris  
 Klient: none  
 Job: Uni intern  
 Spektrumname: AC Jurkschat MW-BZ2-1

System Auflösung = 73 eV

Quantitative Methode: ZAF ( 4 Iterationen ).  
 Analysiert mit allen Elementen und normalisiertem Ergebnis.

Elmt	Spekt. Typ	Gewichts %	Atom %		Absolutinh
C K	ED	50.47	68.47	47,5	C 41,7
F K	ED	28.10	24.10	26,5	
Si K	ED	9.15	5.31	8,6	
Cl K	ED	1.33	0.61	1,25	Cl 1,95
Sn L	ED	10.94	1.50	10,30	
Total		100.00	100.00		F 25,1
Elmt	Spekt. Typ	Gewichts %	Atom %		
F K	ED	49.23	70.12	25,8	Si 12,4
Si K	ED	22.52	21.70	11,8	
Cl K	ED	3.25	2.48	1,7	
Sn L	ED	25.00	5.70	13,1	Sm 13,1
Total		100.00	100.00		

SEMQuant Ergebnis. Ausgegeben um 09:43:17 am 17.04.15  
 Bearbeiter: meuris  
 Klient: none  
 Job: Uni intern  
 Spektrumname: AC Jurkschat MW-BZ2-2

Hitachi REM 54500  
 Oxford Link 150  
 20 kV

Elmt	Spekt. Typ	Gewichts %	Atom %	
F K	ED	47.87	69.19	4 25,1
Si K	ED	22.67	22.17	11,9
Cl K	ED	3.36	2.60	1,8
Sn L	ED	26.11	6.04	13,7
Total		100.00	100.00	

Elmt	Spekt. Typ	Gewichts %	Atom %	
C K	ED	48.34	67.01	45,5
F K	ED	28.30	24.80	26,6
Si K	ED	9.80	5.81	9,3
Cl K	ED	1.46	0.69	1,37
Sn L	ED	12.10	1.70	11,4
Total		100.00	100.00	

# Elementaranalysenauftrag

MW-Be 3  
Probenbezeichnung  
(max. 7 Stellen)

16.4.15  
Datum

MICHAEL WAGNER / 3820/3837  
Auftraggeber  
Telefon

CHOBFSnSi

Die Substanz enthält:  
Smp.: \_\_\_\_\_  
Sdp.: \_\_\_\_\_  
Bemerkungen: \_\_\_\_\_

\_\_\_\_\_ auf Abruf? \_\_\_\_\_

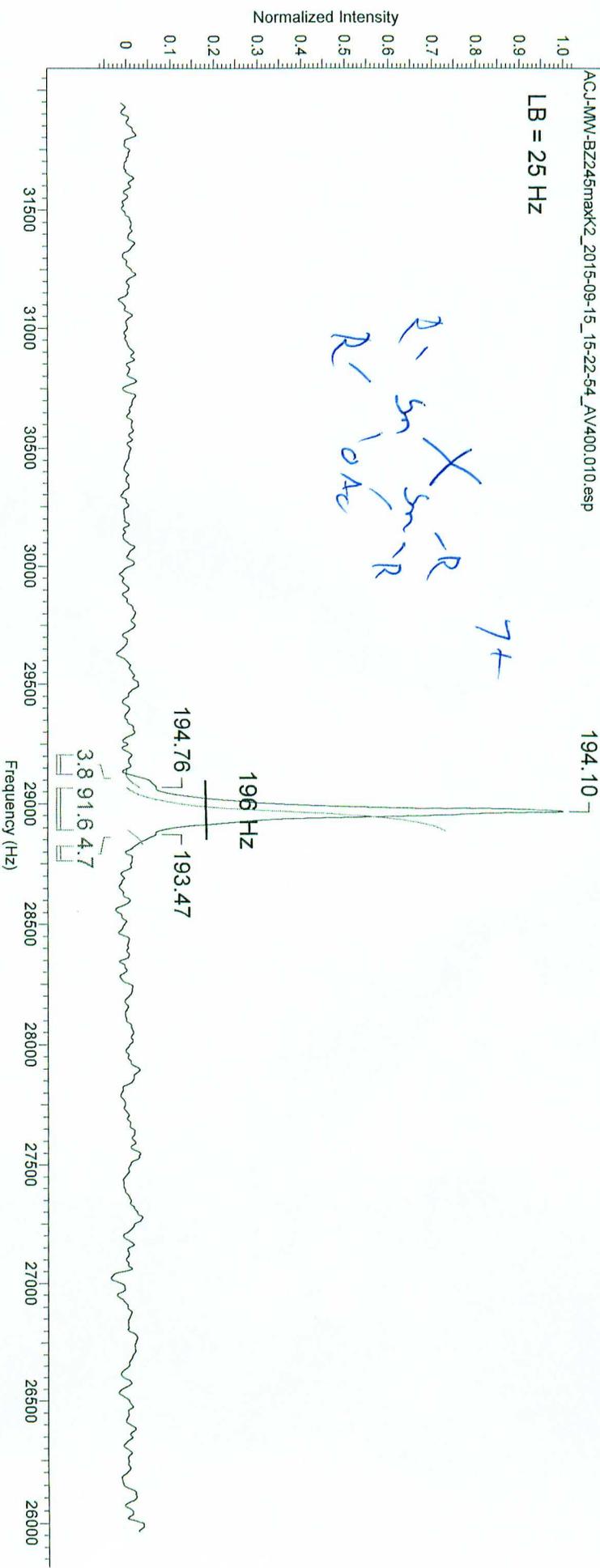
luftempfindlich:   
hygroskopisch:

Einwaage:	theor.		prakt.	
	a	b	a	b
a) 1,306	% C: 42,44		42,1	42,1
b) 1,545	% H: 5,32		5,6	5,6
	% N: /		/	/

29.4.15 M. Wagner  
Datum der Ausführung

\_\_\_\_\_  
Arbeitskreisleiter

Acquisition Time (sec)	0.4999	Date	16 Sep 2015 08:43:12	Date Stamp	16 Sep 2015 08:43:12	
File Name	C:\Users\mwl\Desktop\ACU-MW-BZ245maxK2_2015-09-15_15-22-54_AV400\10\fid				Frequency (MHz)	149.26
Nucleus	119Sn	Number of Transients	6144	Origin	spect	
Owner	guest	Points Count	32768	Pulse Sequence	zqlg45	
SW/cyclical (Hz)	5980.86	Solvent	CHLOROFORM-D	Receiver Gain	196.87	
Spectrum Type	STANDARD	Sweep Width (Hz)	5980.68	Temperature (degree C)	25.148	
				Spectrum Offset (Hz)	28955.6133	



No.	(ppm)	Value	Absolute Value	Non-Negative Value	No.	(ppm)	(Hz)	Height
1	1648 .. 193.4	66379929	1.296724566e+8	4.66379929	1	193.47	28875.9	0.0667
2	5711 .. 194.1	58193207	2.54438400e+9	91.58193207	2	194.10	28970.3	1.0000
3	7449 .. 195.3	75426936	1.04303360e+8	3.75426936	3	194.76	29068.3	0.0678

This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

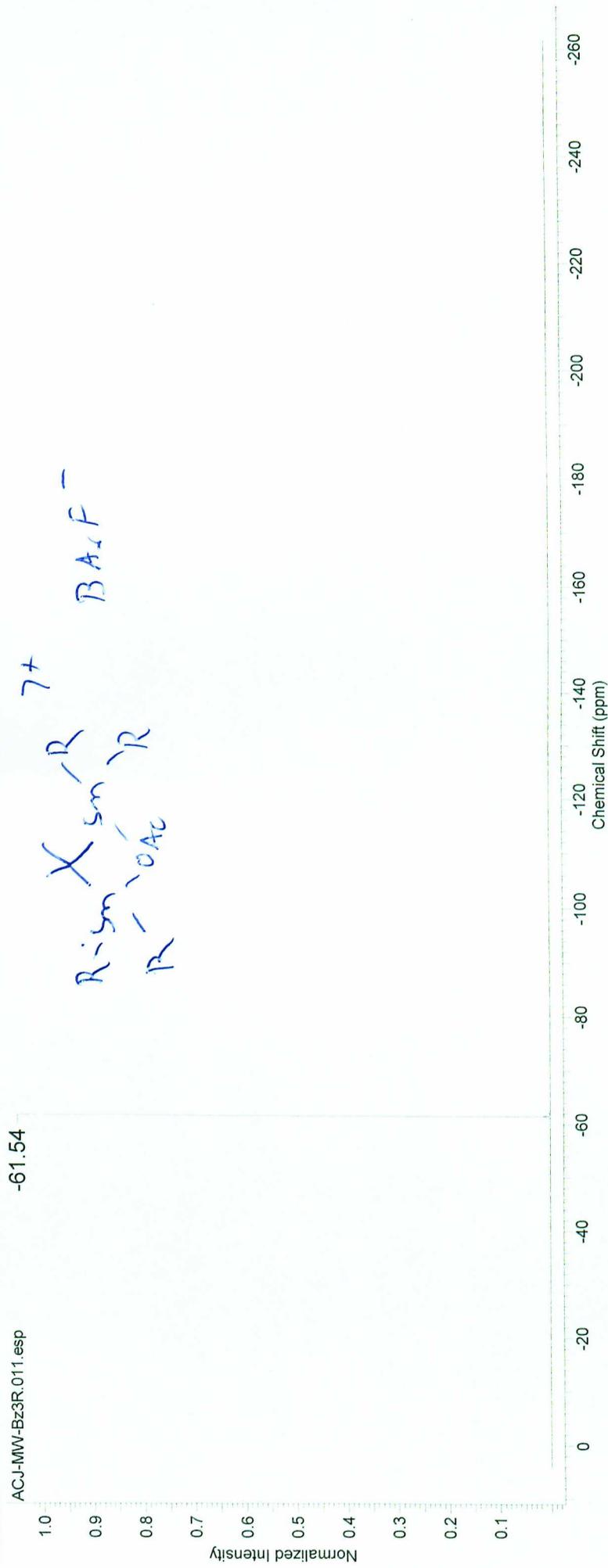
Acquisition Time (sec)	0.8503	Comment	z_B11lg CDCI3 u guest 38	Date	17 Apr 2015 18:21:04
Date Stamp	17 Apr 2015 18:21:04	File Name	C:\Users\mmw\Desktop\MMW-Bz-kation\ACJ-MW-Bz3R\10\fid	Origin	spect
Frequency (MHz)	96.29	Nucleus	11B	Number of Transients	256
Owner	guest	Points Count	32768	Pulse Sequence	zgig
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-9.7496	Receiver Gain	812.70
Temperature (degree C)	22.160	Spectrum Type	STANDARD	SW(cyclical) (Hz)	38535.64
				Sweep Width (Hz)	38534.47



No.	(ppm)	(Hz)	Height
1	-6.70	-645.4	1.0000

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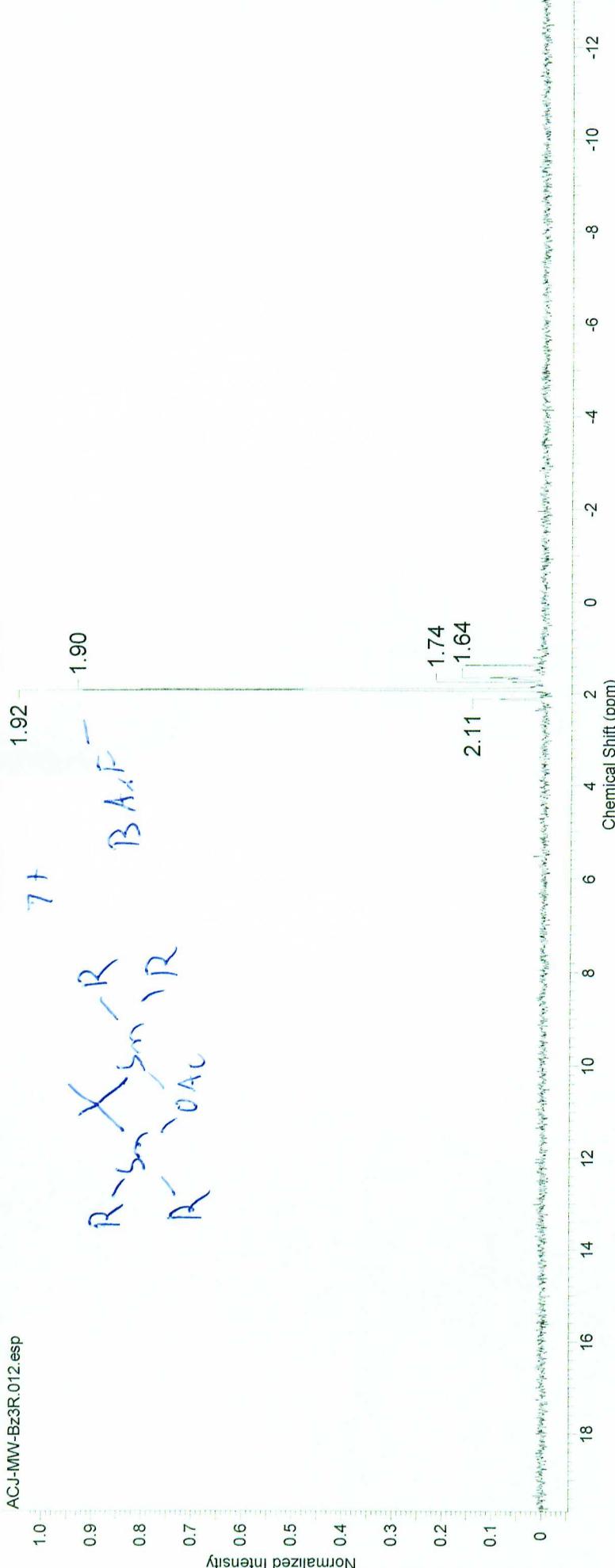
Acquisition Time (sec)	0.4358	Comment	z_F19 CDCI3 u guest 38	Date	17 Apr 2015 18:31:44
Date Stamp	17 Apr 2015 18:31:44	File Name	C:\Users\mw\Desktop\MW-Bz-kation\ACJ-MW-Bz3R11\Fid	Frequency (MHz)	282.40
Nucleus	19F	Number of Transients	128	Original Points Count	32768
Points Count	32768	Pulse Sequence	zg30	Receiver Gain	1024.00
Solvent	CHLOROFORM-d	Temperature (degree C)	22.160	SW(cyclical) (Hz)	75187.97
				Spectrum Type	STANDARD
				Sweep Width (Hz)	75185.67



No.	(ppm)	(Hz)	Height
1	-61.54	-17378.8	1.0000

This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

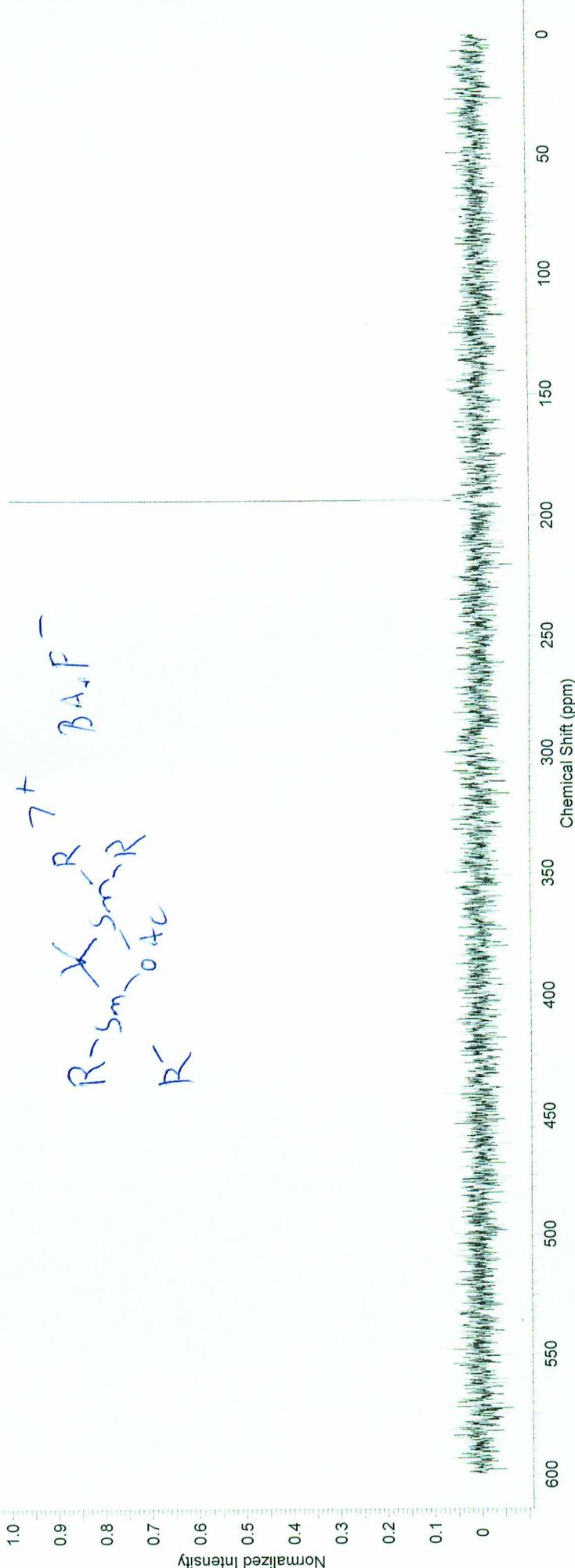
Acquisition Time (sec) 1.1010    Comment z\_S129\_INEPT1r CDC13 u guest 38    Date 17 Apr 2015 19:01:36  
 Date Stamp 17 Apr 2015 19:01:36    File Name C:\Users\mw\Desktop\MW-Bz-kation\ACJ-MW-Bz3R\12\fid    Origin spect  
 Frequency (MHz) 59.63    Nucleus 29Si    Number of Transients 512    Pulse Sequence ineptrd  
 Original Points Count 32768    Owner guest    Points Count 65536    Solvent CHLOROFORM-d  
 Receiver Gain 4597.60    SW(cyclical) (Hz) 29761.90    Temperature (degree C) 22.160



No.	(ppm)	(Hz)	Height
1	1.64	97.9	0.1138
2	1.74	103.8	0.0679
3	1.90	113.3	0.8813
4	1.92	114.7	1.0000
5	2.11	126.0	0.0926

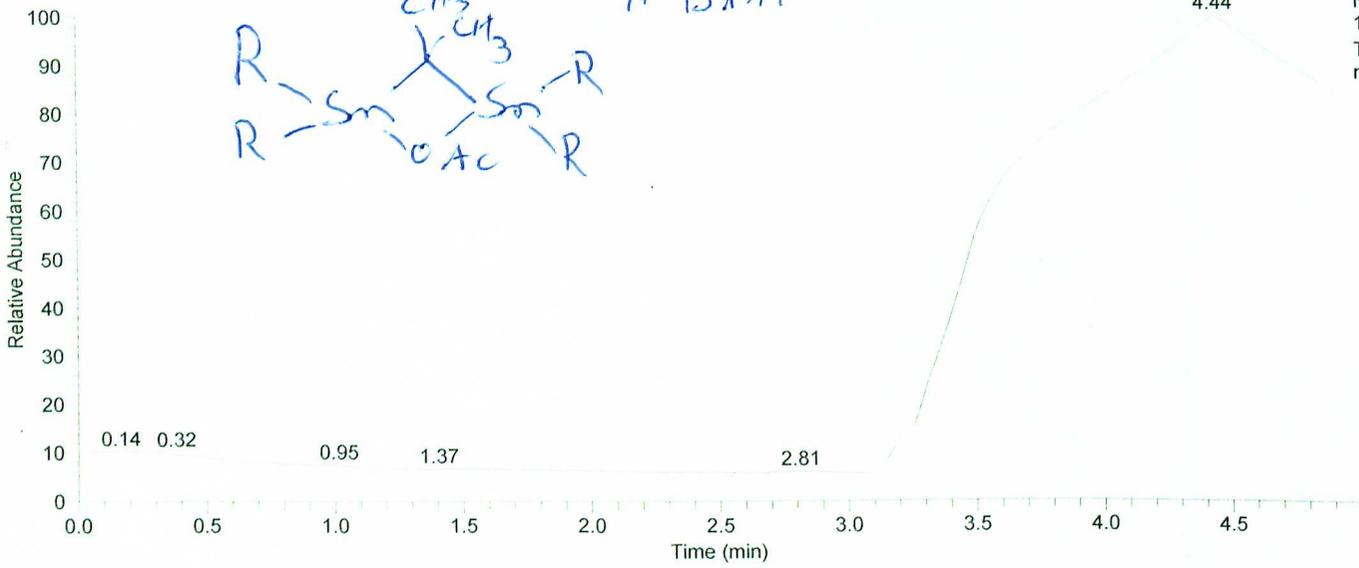
Acquisition Time (sec)	0.4882	Comment	z_Sn119_IG CDC13 u guest 38	Date	17 Apr 2015 19:42:08
Date Stamp	17 Apr 2015 19:42:08	File Name	C:\Users\mw\Desktop\MW-Bz-kation\ACJ-MW-Bz3R\13\fid	Origin	spect
Frequency (MHz)	111.92	Nucleus	119Sn	Number of Transients	1024
Original Points Count	32768	Owner	guest	Points Count	65536
Receiver Gain	13004.00	SW(cyclical) (Hz)	67114.09	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	33532.0156	Spectrum Type	STANDARD	Sweep Width (Hz)	67113.07
				Temperature (degree C)	22.160

ACJ-MW-Bz3R.013.esp



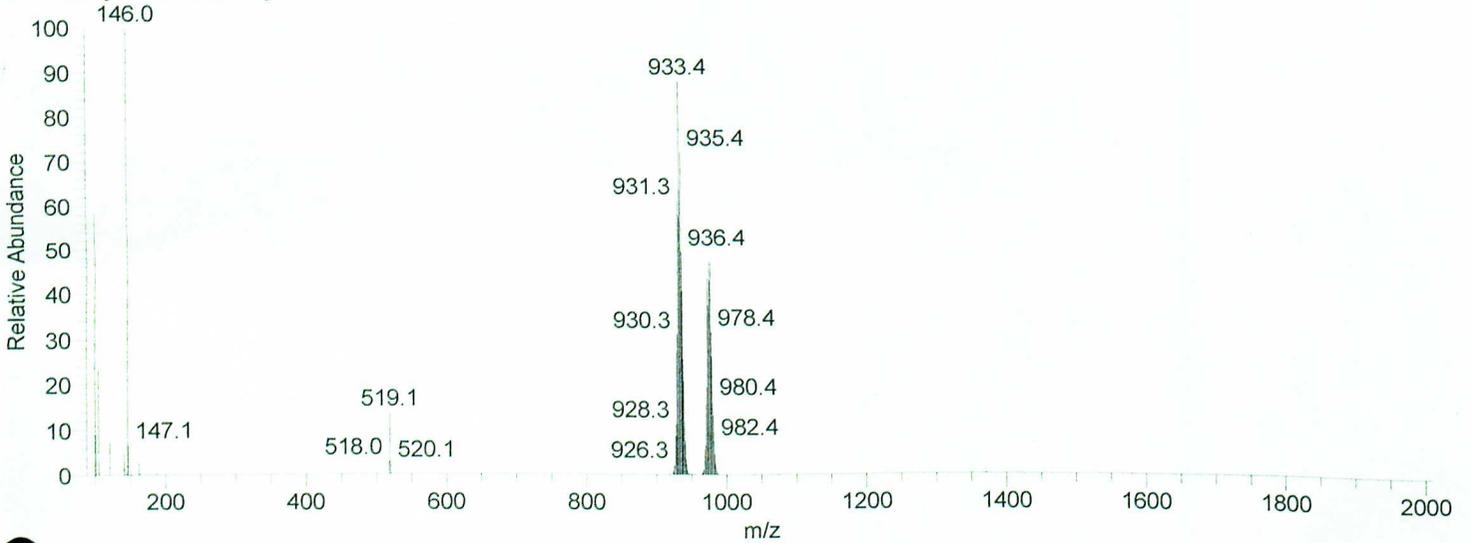
No.	(ppm)	(Hz)	Height
1	193.40	21645.0	1.0000

RT: 0.00 - 4.99

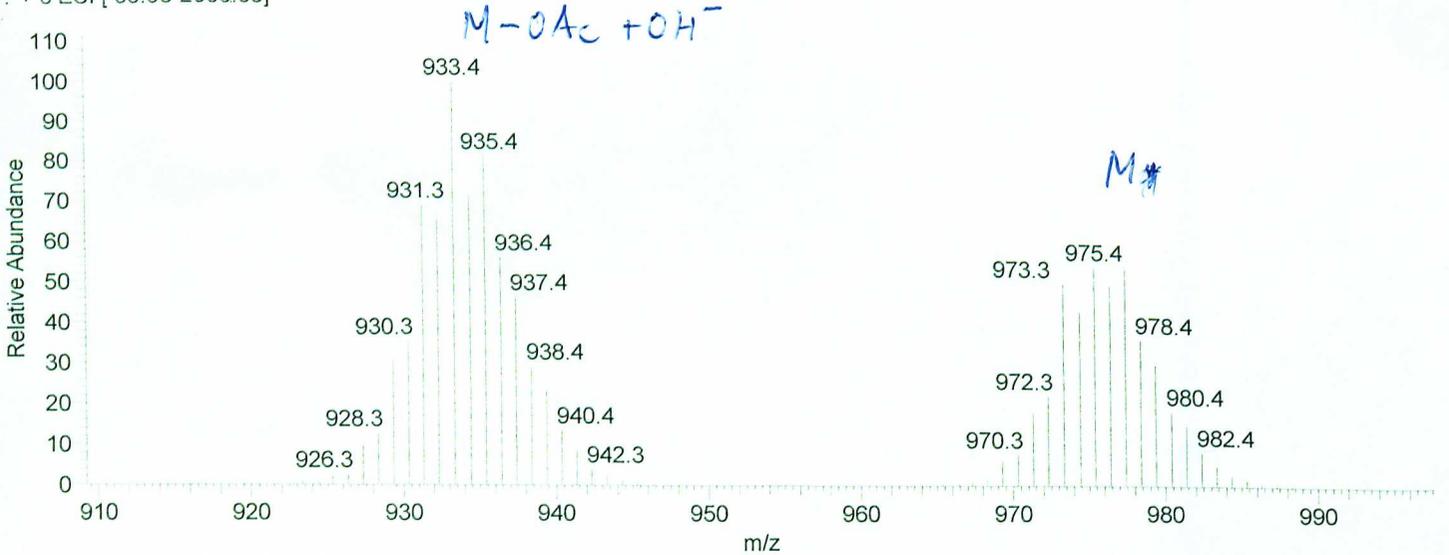


NL: 1.49E6  
TIC MS  
mw-bz-3

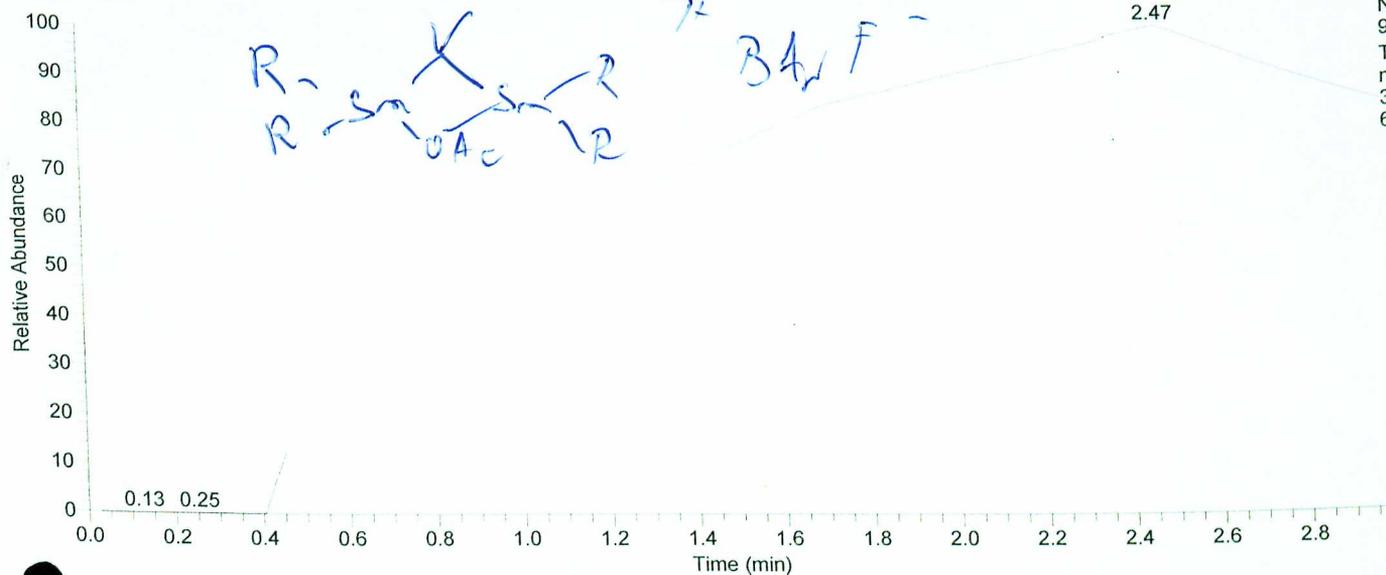
mw-bz-3#166-175 RT: 4.30-4.55 AV: 10 SB: 13 0.09-0.40 NL: 1.13E5  
T: + c ESI [ 99.98-2000.03]



mw-bz-3#166-175 RT: 4.30-4.55 AV: 10 SB: 13 0.09-0.40 NL: 9.89E4  
T: + c ESI [ 99.98-2000.03]

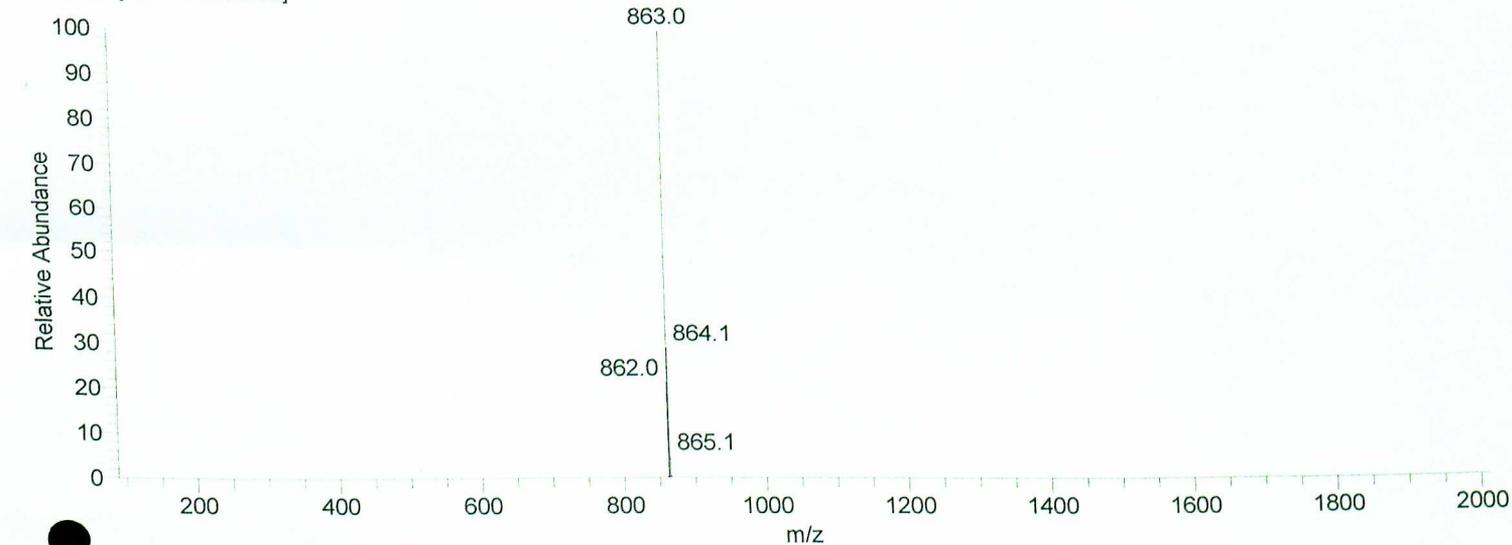


RT: 0.00 - 2.98

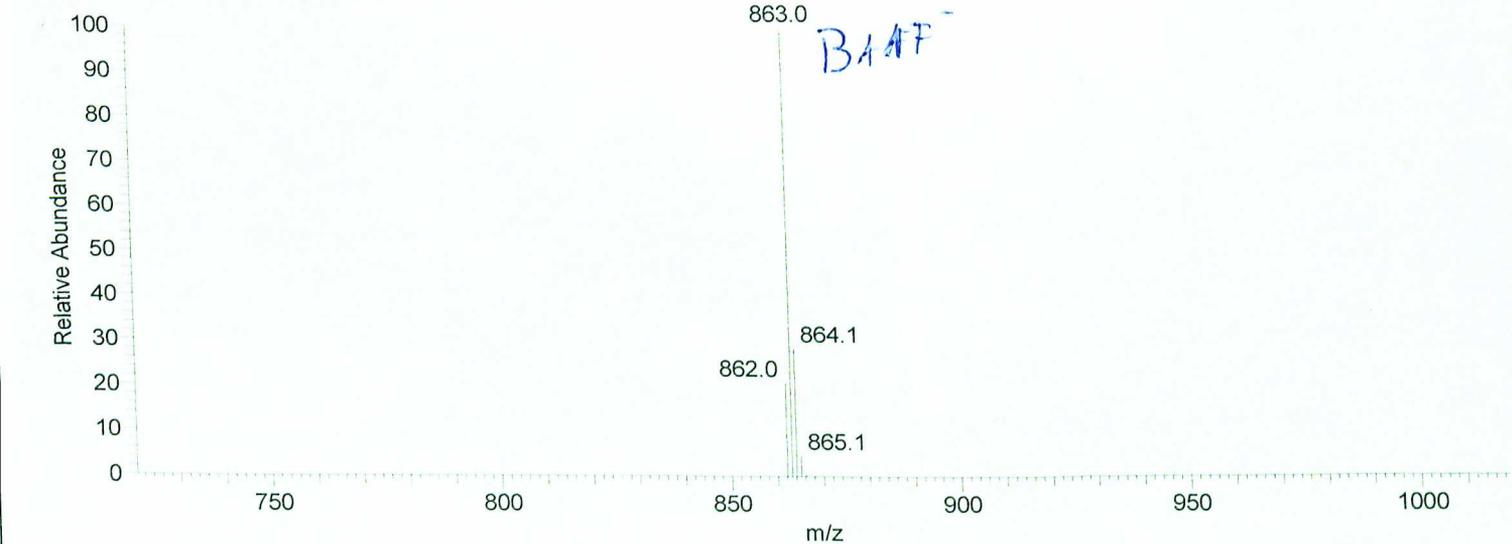


NL: 9.02E6  
TIC MS  
mw-bz-3\_150427063813

mw-bz-3\_150427063813#94-102 RT: 2.37-2.58 AV: 9 NL: 5.74E6  
T: - c ESI [ 99.98-2000.03]

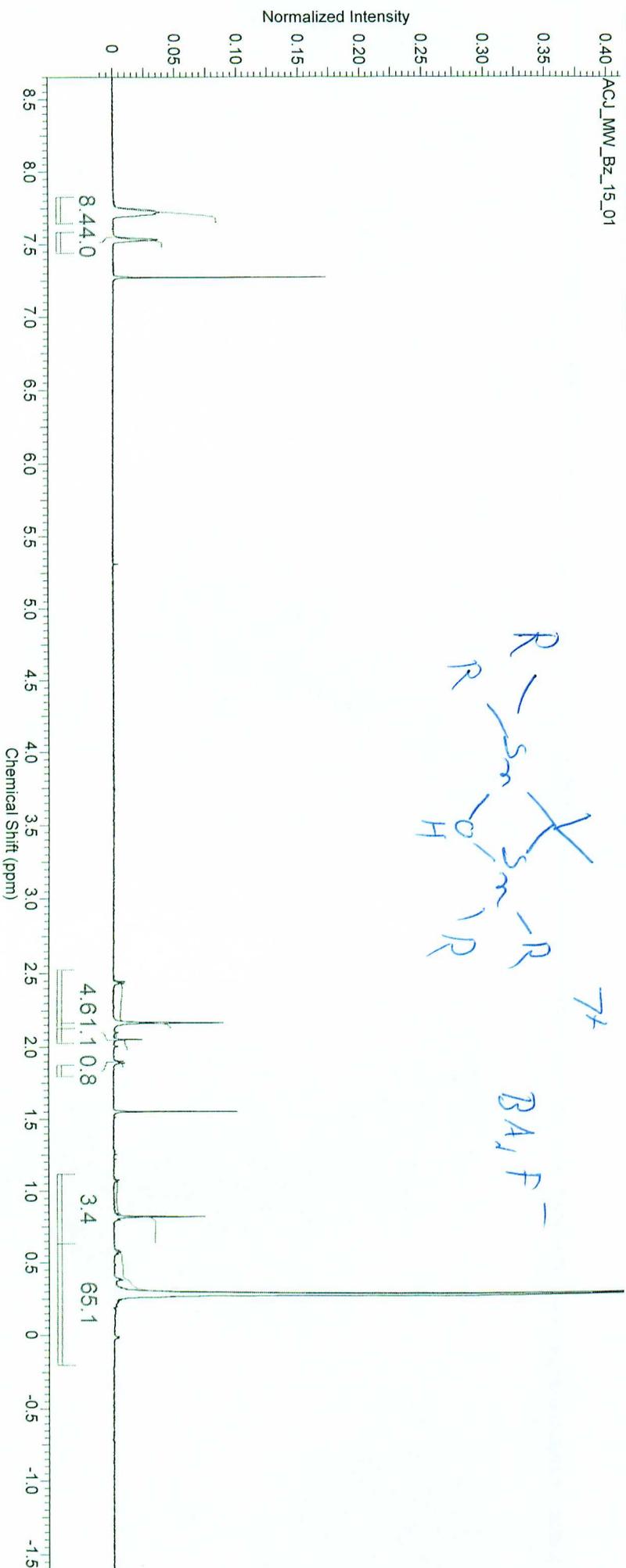


mw-bz-3\_150427063813#94-102 RT: 2.37-2.58 AV: 9 NL: 5.74E6  
T: - c ESI [ 99.98-2000.03]



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Acquisition Time (sec)	2.5585	Comment	ACJ_MW_Bz_15_in CDCl3 date: 17. Juni 2015	STANDARD 1H OBSERVE
Date	Jun 17 2015	Date Stamp	Jun 17 2015	
Frequency (MHz)	200.13	Nucleus	<sup>1</sup> H	File Name
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain
Spectrum Offset (Hz)	1600.9471	Spectrum Type	STANDARD	Number of Transients
				39.00
				Sweep Width (Hz)
				4003.20
				Temperature (degree C)
				AMBIENT TEMPERATURE



No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2020 ..	0.635,06887054	1.42101376e+9	65.06887054
2	5331 ..	1.116,35797739	7.33335600e+7	3.35797739
3	8583 ..	1.930,76438361	1.66930760e+7	0.76438361
4	9791 ..	2.111,09978235	2.40177180e+7	1.09978235
5	1275 ..	2.524,63792562	1.01285856e+8	4.63792562
6	4744 ..	7.613,99881840	8.73286400e+7	3.99881840
7	9453 ..	7.828,40270996	1.83503520e+8	8.40270996

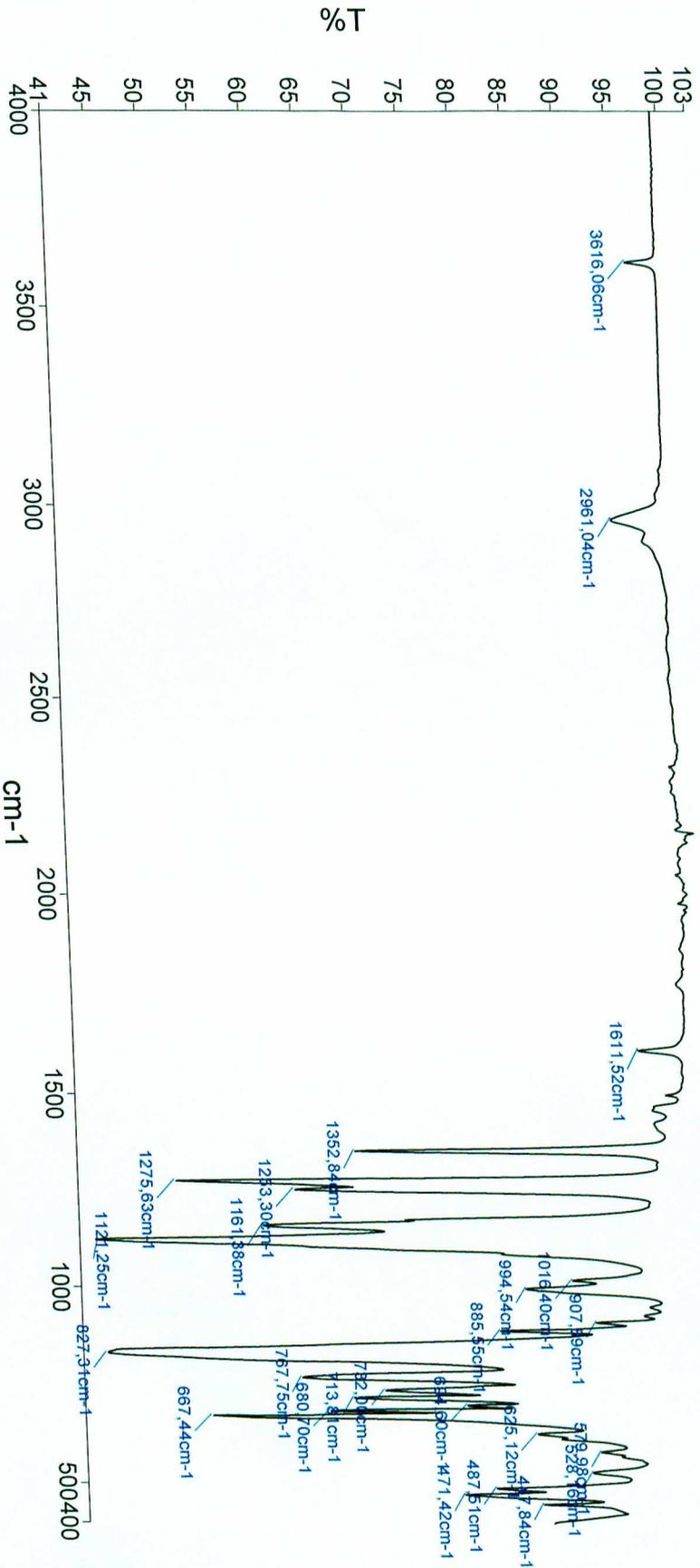
MW-Bz2 CDG / Toluol

Leist im Kildelaker

PerkinElmer Spectrum Version 10.03.08  
Montag, 18. Mai 2015 16:12

Anwender  
Datum/ Uhrzeit

Jurkschat  
Montag, 18. Mai 2015 16:12



# Elementaranalysenauftrag

MICHAEL WAGNER / 3820/3837 / 27.6.15  
Auftraggeber / Telefon / Datum

Die Substanz enthält:

CHOBESISm

MW-B2-15  
Probenbezeichnung  
(max. 7 Stellen)

Smp.: \_\_\_\_\_ auf Abruf? \_\_\_\_\_

Sdp.: \_\_\_\_\_

Luftempfindlich:

Bemerkungen: \_\_\_\_\_

hygroskopisch:

## Einwaage:

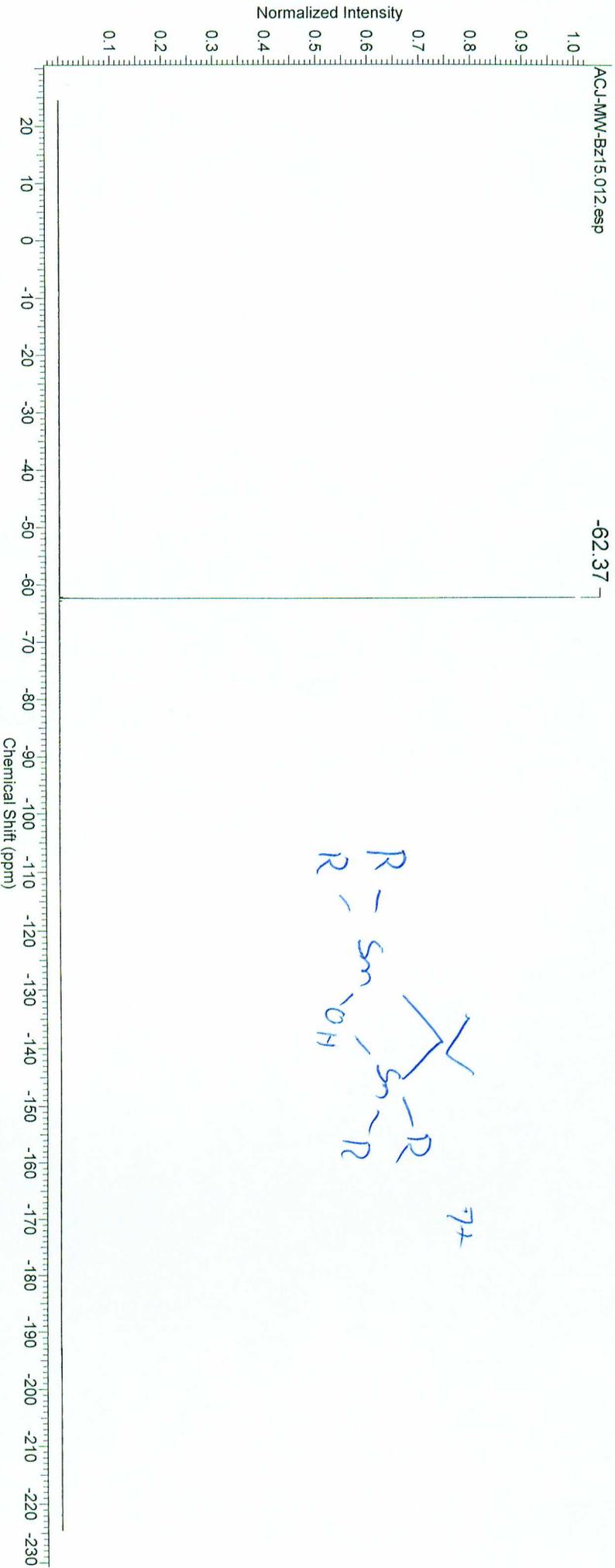
	theor.	a	b
a) <u>1.151</u>	% C: <u>42,10</u>	<u>40,7</u>	<u>41,3</u>
b) <u>1.058</u>	% H: <u>5,33</u>	<u>5,5</u>	<u>5,9</u>
	% N: _____		

Arbeitskreisleiter \_\_\_\_\_

24.6.15 N. K. Müller  
Datum der Ausführung

This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

Acquisition Time (sec)	0.6991	Date	18 Jun 2015 23:24:16	Date Stamp	18 Jun 2015 23:24:16	Nucleus	<sup>19</sup> F
File Name	C:\Users\mw\Desktop\MMW-Bz-kation\ACJ-MMW-Bz15\12\fid			Frequency (MHz)	376.61	Owner	quest
Number of Transients	64	Origin	spect	Original Points Count	65536	Points Count	65536
Pulse Sequence	zg30	Receiver Gain	196.87	SW(cyclical) (Hz)	93750.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	-37661.1289	Spectrum Type	STANDARD	Sweep Width (Hz)	93748.57	Temperature (degree C)	26.147

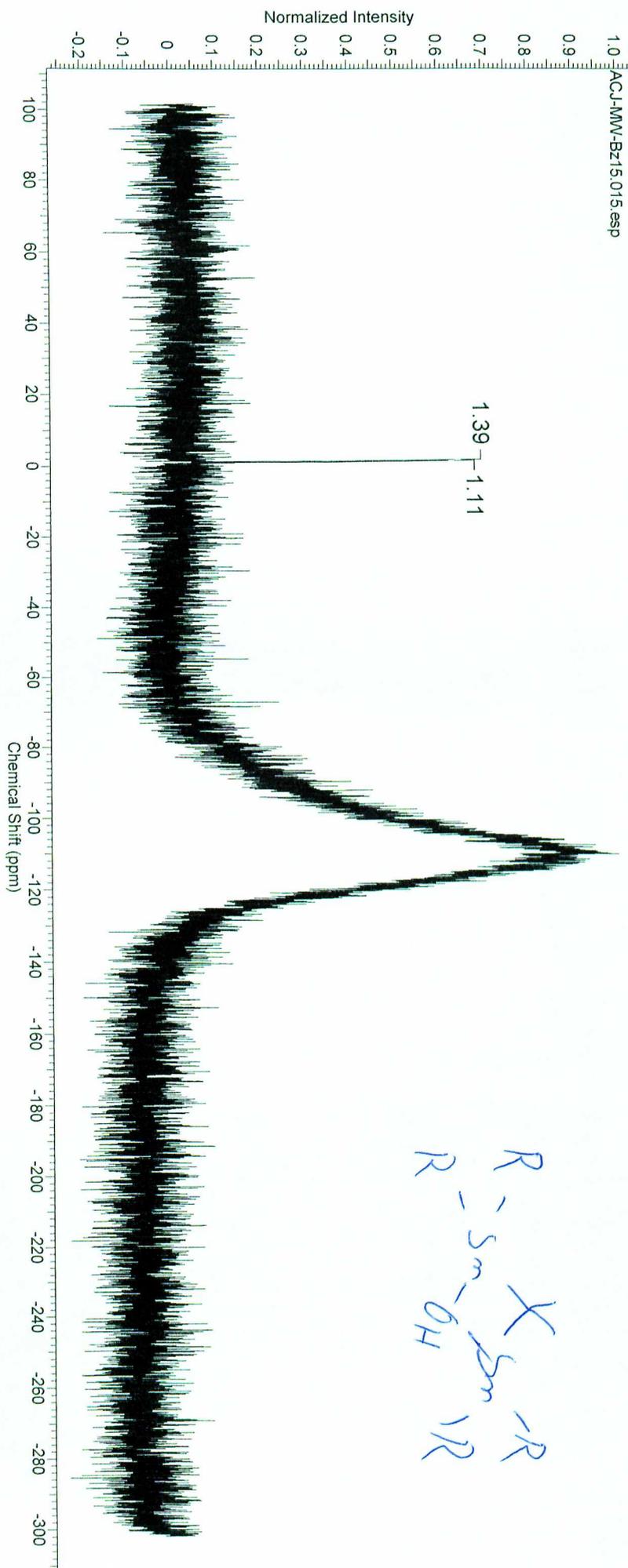


No.	(ppm)	(Hz)	Height
1	-62.37	-23488.3	1.0000



This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

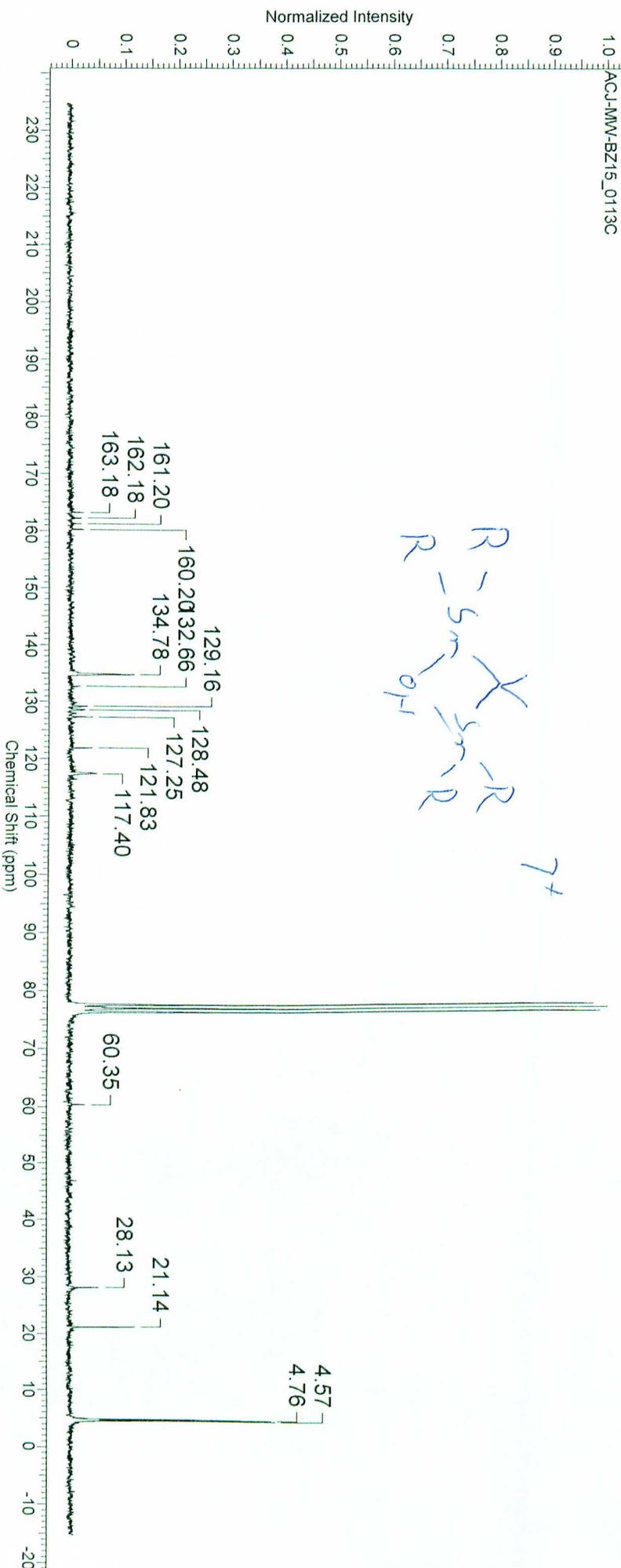
Acquisition Time (sec)	1.0224	Date	19 Jun 2015 02:04:16	Date Stamp	19 Jun 2015 02:04:16
File Name	C:\Users\mww\Desktop\MMW-Bz-kation\ACJ-MMW-Bz1515.fid	Origin	spect	Frequency (MHz)	79.52
Number of Transients	512	Receiver Gain	196.67	Owner	quest
Pulse Sequence	zgpg30	Spectrum Type	STANDARD	Original Points Count	32768
Spectrum Offset (Hz)	-7951.8418	SW/(cyclical) (Hz)	32051.28	Sweep Width (Hz)	32051.04
		Temperature (degree C)	26.148	Solvent	CHLOROFORM-D
				Nucleus	29Si
				Points Count	131072



No.	(ppm)	(Hz)	Height
1	1.11	88.5	0.6237
2	1.39	110.3	0.6386

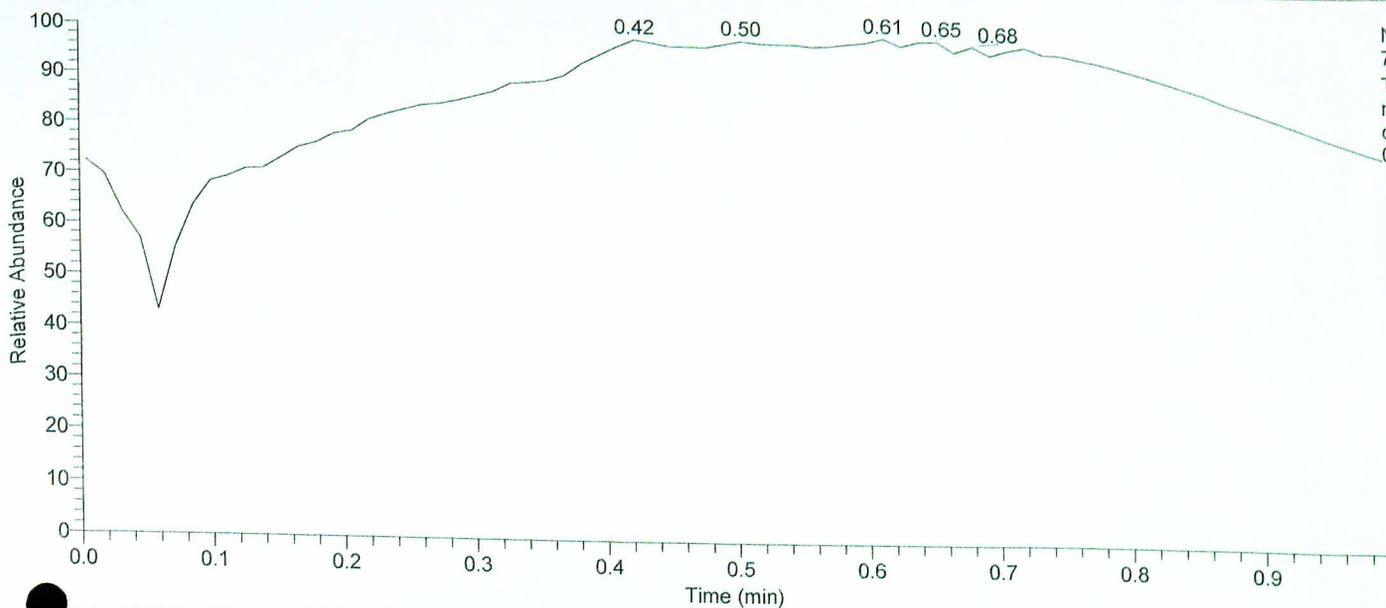
This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

Acquisition Time (sec)	1.4980	Comment	ACJ-MW-BZ15_in CDCI3 date: 19. Juni 2015 13C OBSERVE pad=2 run with findz0 before acquisition
Date	Jun 19 2015	Date Stamp	Jun 19 2015
Frequency (MHz)	50.33	Nucleus	13C
Points Count	65536	Pulse Sequence	s2pul
Spectrum Offset (Hz)	5522.9375	Spectrum Type	STANDARD
		Sweep Width (Hz)	12578.62
		Temperature (degree C)	AMBIENT TEMPERATURE



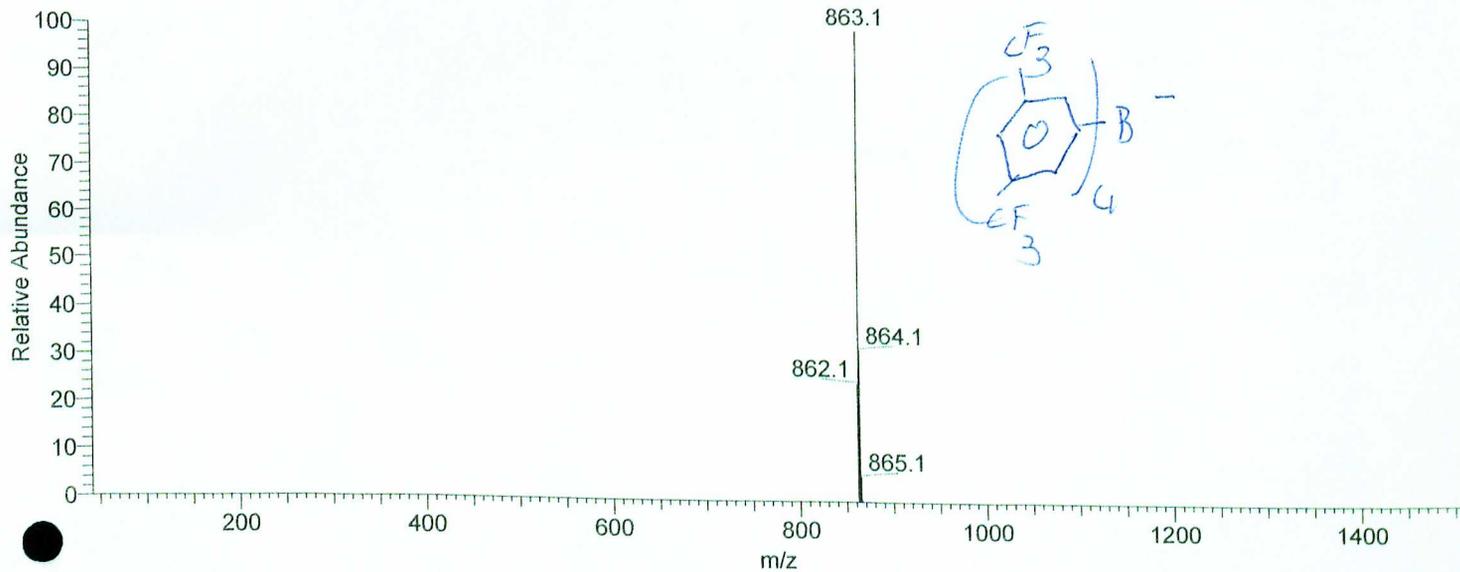
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	4.57	230.2	0.3824	5	60.35	3037.1	0.0293	9	128.48	6466.0	0.0217
2	4.76	239.8	0.3746	6	117.40	5908.4	0.0475	10	129.16	6500.4	0.0303
3	21.14	1064.1	0.1218	7	121.83	6131.5	0.0397	11	132.66	6676.6	0.0165
4	28.13	1416.0	0.0553	8	127.25	6404.0	0.0393	12	134.78	6783.3	0.1178
								13	160.20	8062.7	0.0224
								14	161.20	8112.8	0.0178
								15	162.18	8162.4	0.0178
								16	163.18	8212.5	0.0226

RT: 0.00 - 0.99

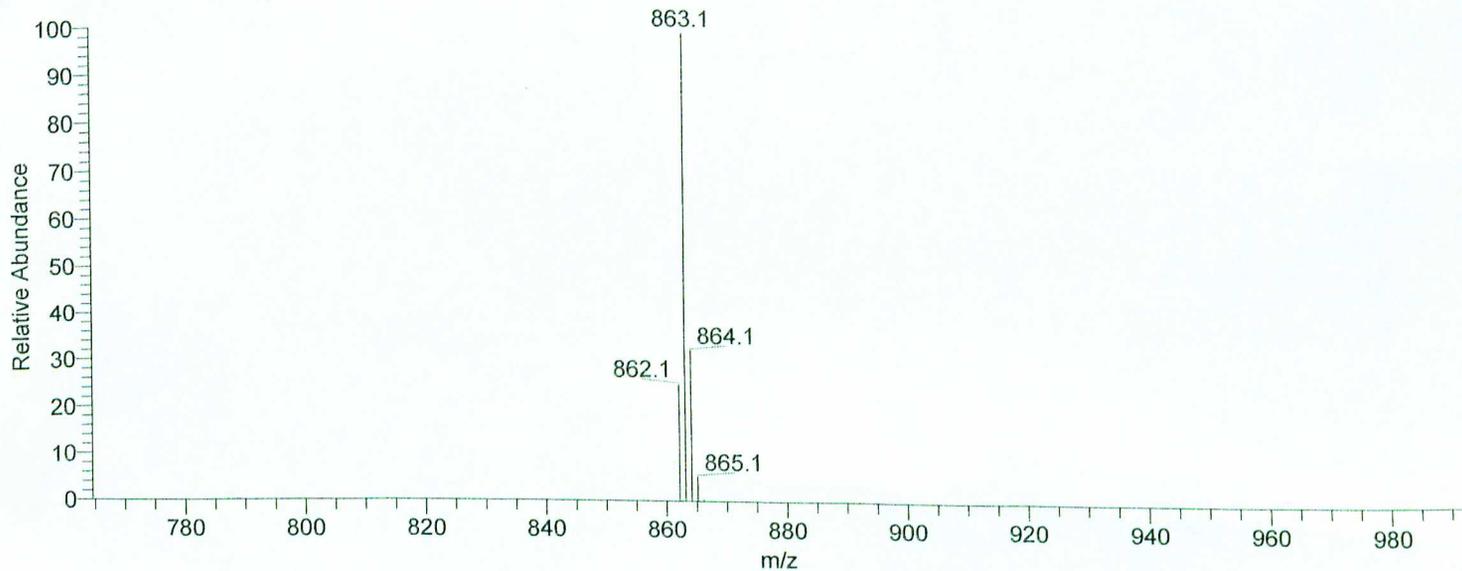


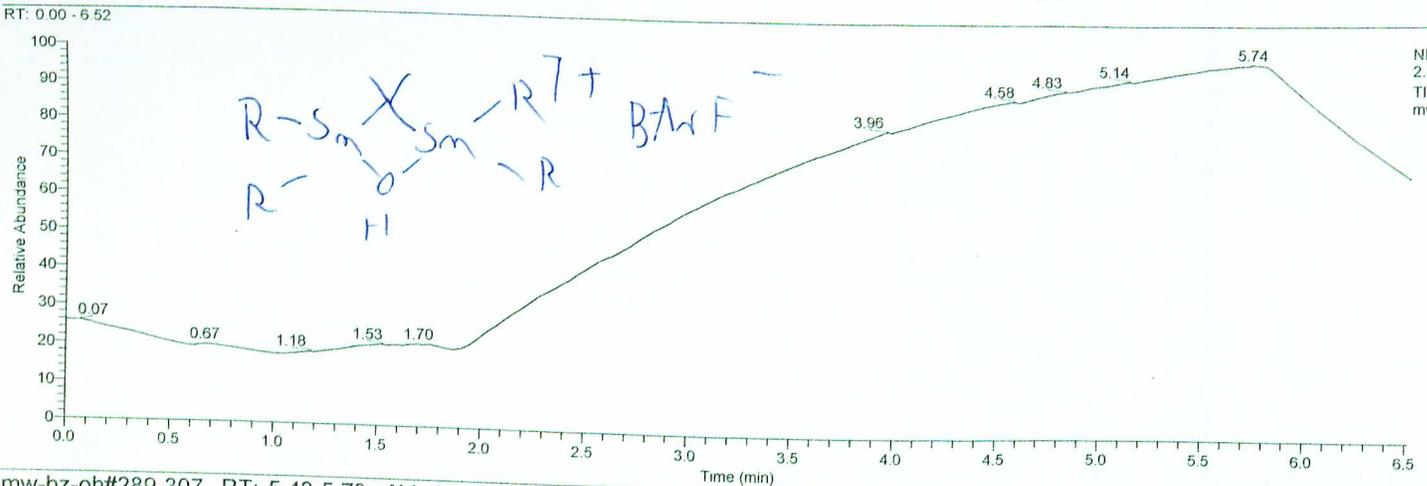
NL:  
7.73E6  
TIC MS  
mw-bz-  
oh\_150806  
030503

mw-bz-oh\_150806030503#38-56 RT: 0.50-0.75 AV: 19 NL: 4.69E6  
T: - c ESI [49.99-1500.02]

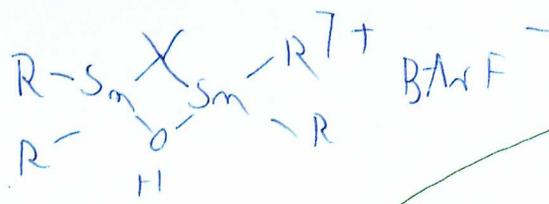


mw-bz-oh\_150806030503#38-56 RT: 0.50-0.75 AV: 19 NL: 4.69E6  
T: - c ESI [49.99-1500.02]

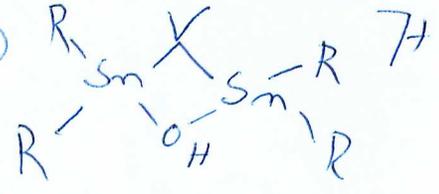
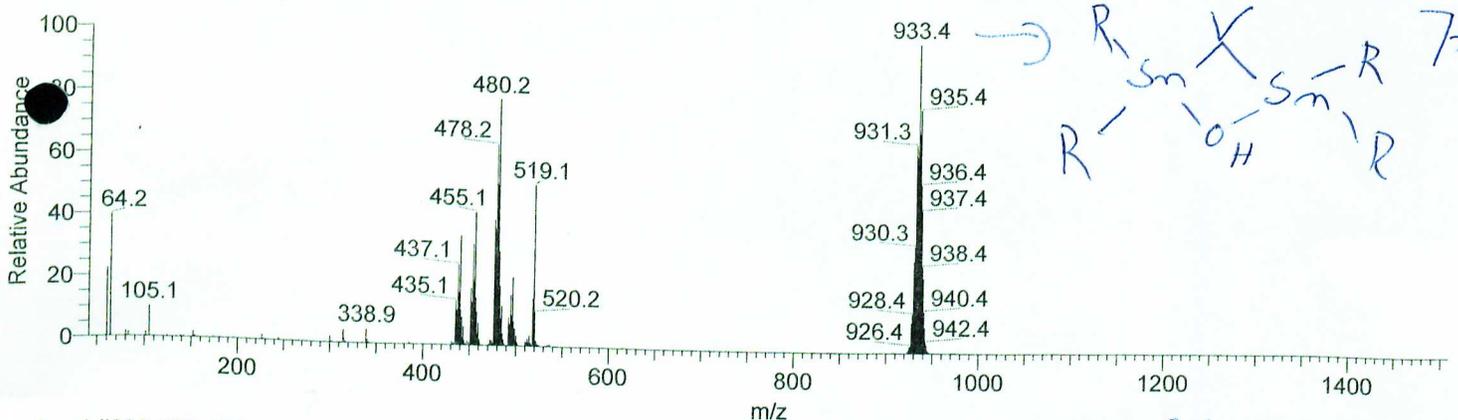




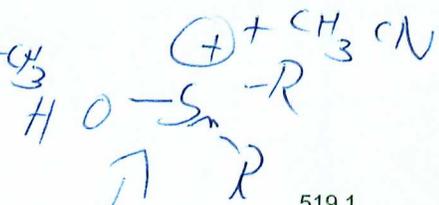
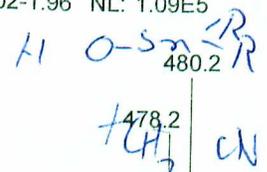
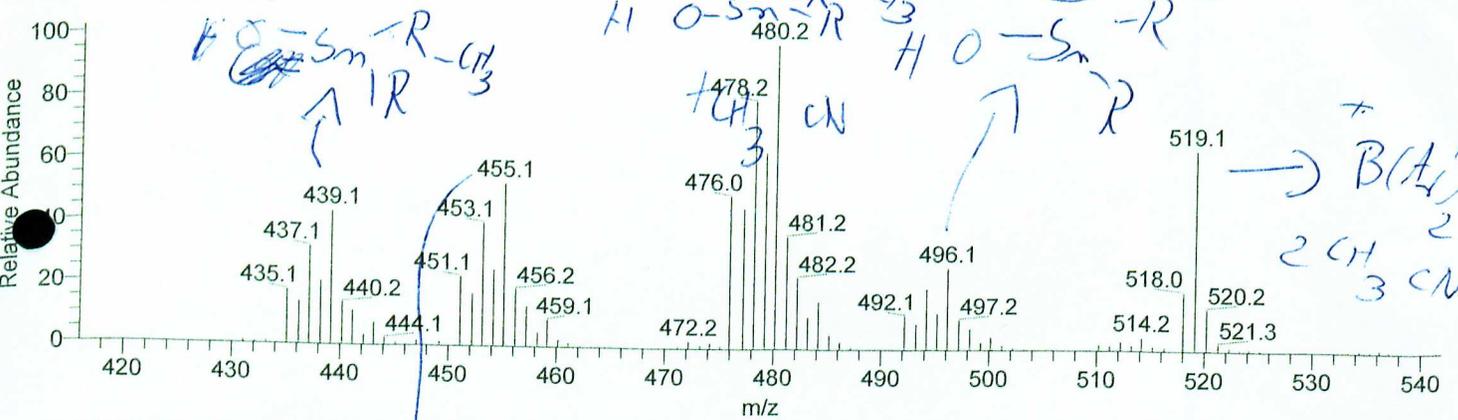
NL: 2.55E6  
TIC MS  
mw-bz-oh



mw-bz-oh#289-307 RT: 5.43-5.78 AV: 19 SB: 107 0.02-1.96 NL: 1.38E5  
T: + c ESI [ 49.99-1500.02]

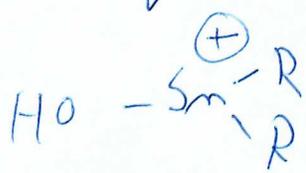
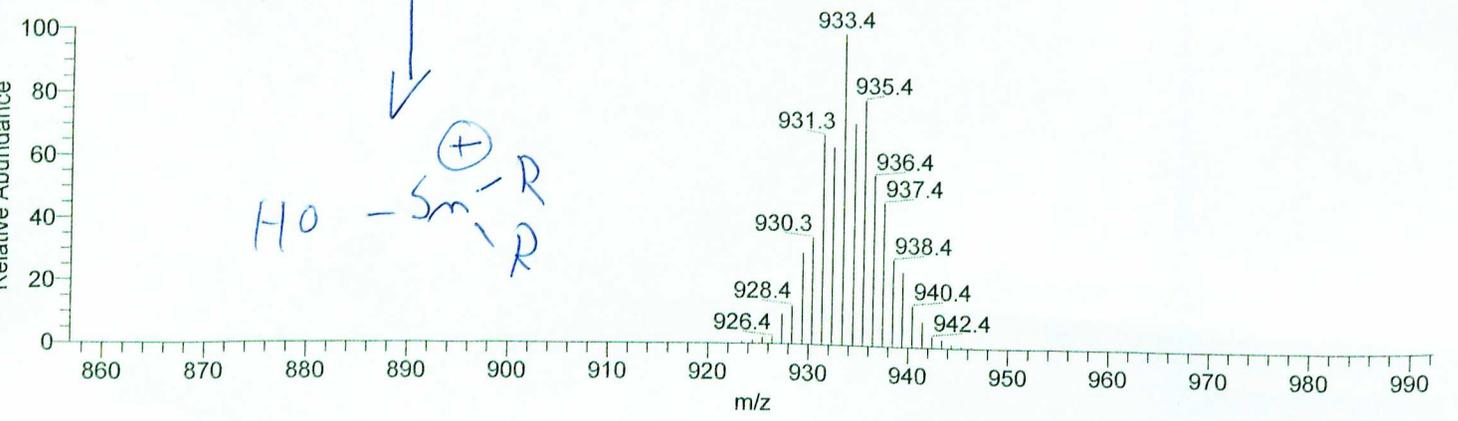


mw-bz-oh#289-307 RT: 5.43-5.78 AV: 19 SB: 107 0.02-1.96 NL: 1.09E5  
T: + c ESI [ 49.99-1500.02]



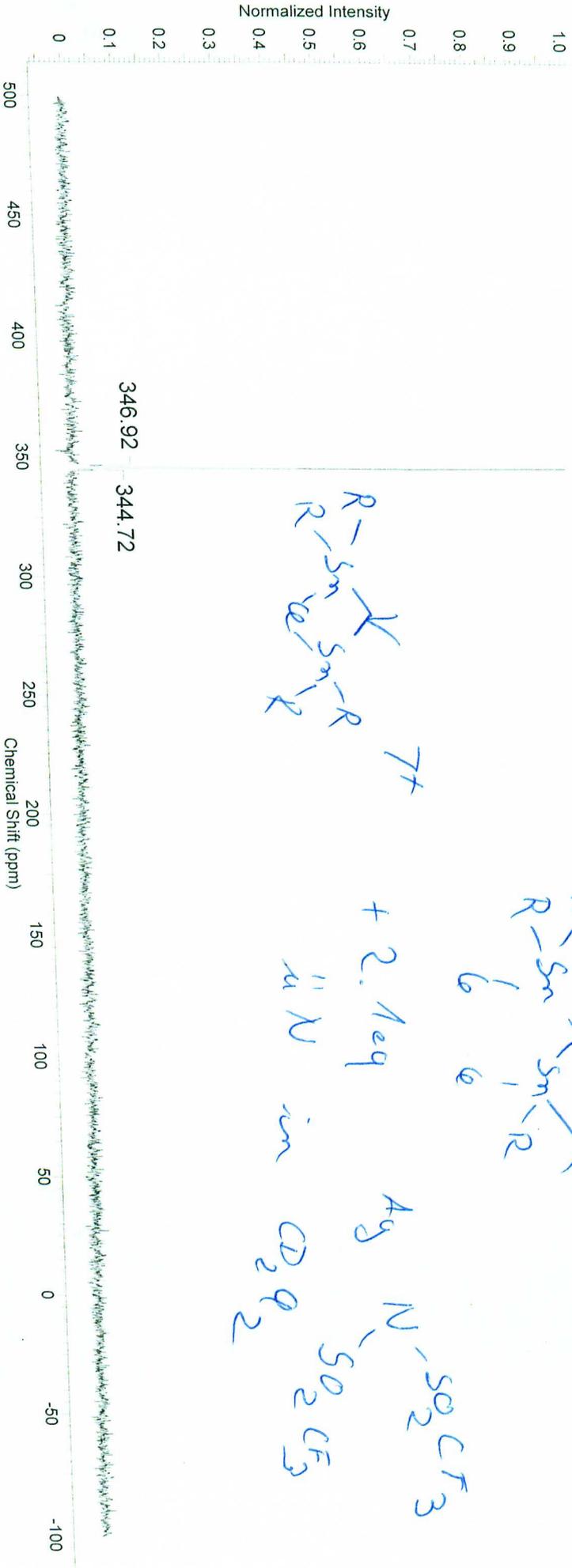
$B(ArF)$   
 $2CH_2$   
 $3CN$

mw-bz-oh#289-307 RT: 5.43-5.78 AV: 19 SB: 107 0.02-1.96 NL: 1.38E5  
T: + c ESI [ 49.99-1500.02]



**Acquisition Time (sec)** 0.3499      **Comment** z\_Sn19\_IG\_CD2Cl2\_u.guest.36  
**Date Stamp** 01 May 2015 10:21:04  
**Frequency (MHz)** 111.92      **Nucleus** 119Sn  
**Original Points Count** 23486      **Owner** guest  
**Receiver Gain** 13004.00      **SW(cyclical) (Hz)** 67114.09  
**Spectrum Offset (Hz)** 22339.9766      **Spectrum Type** STANDARD      **Sweep Width (Hz)** 67113.07  
**Temperature (degree C)** 21.160

ACJ-MW-Bz-11.011.esp      345.82



No.	(ppm)	(Hz)	Height
1	344.72	38561.4	0.0480
2	345.82	38704.3	1.0000
3	346.92	38827.1	0.0613