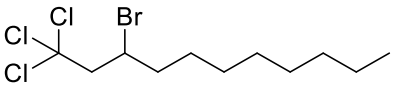
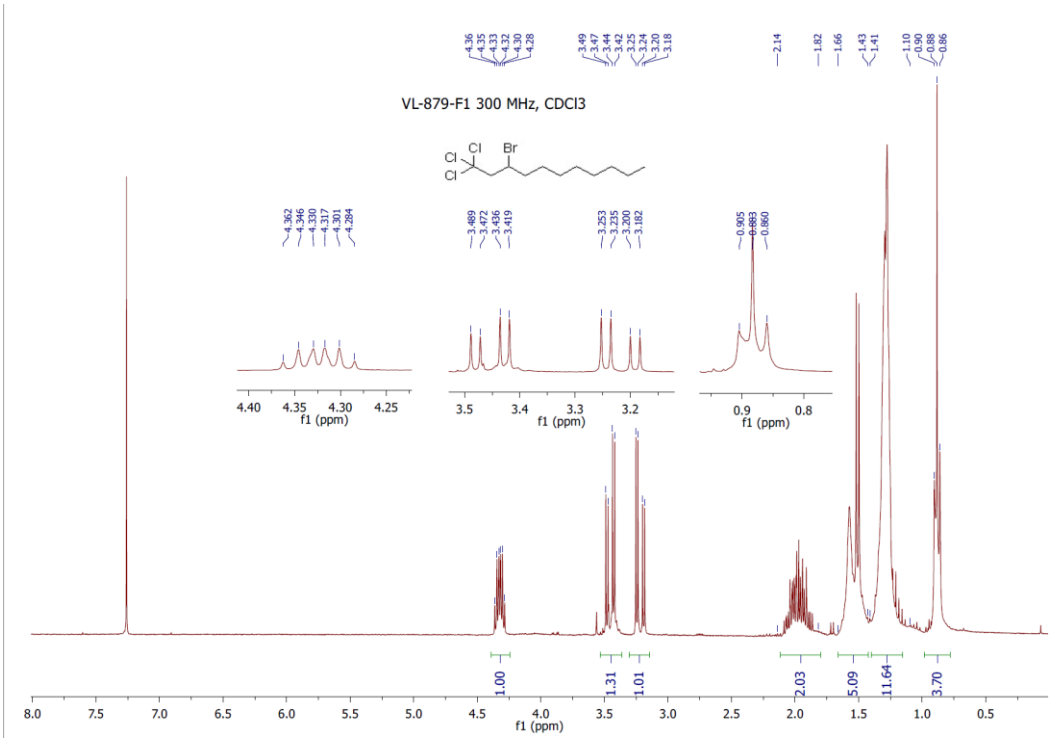
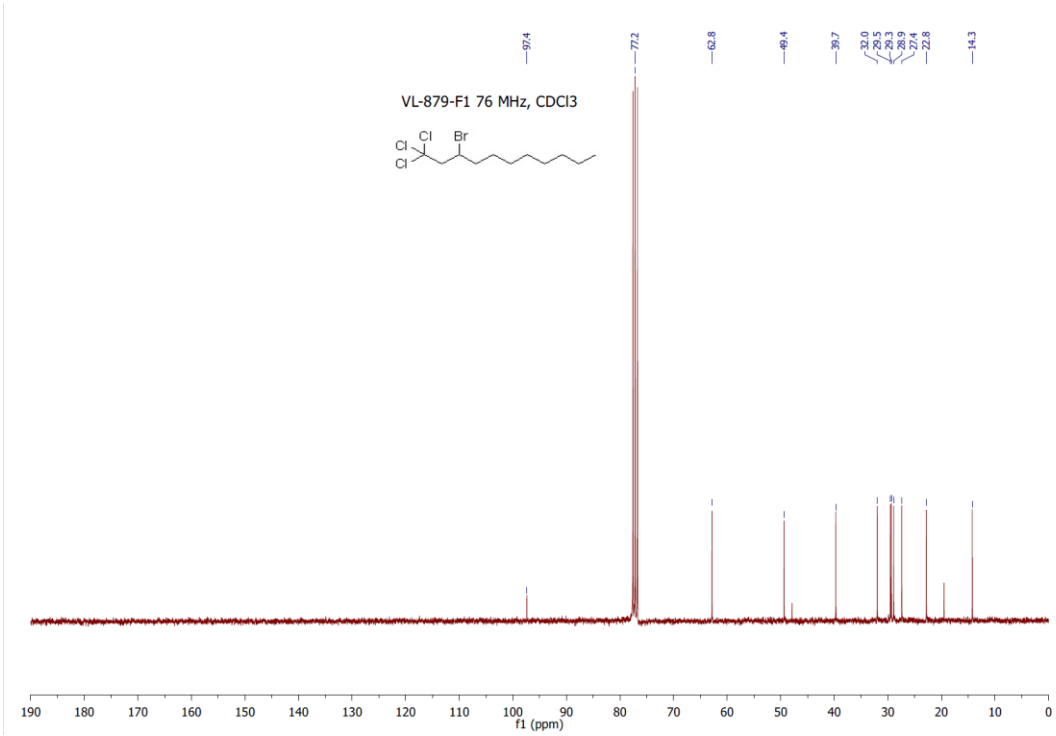
Electronic Supplementary Material (ESI) for ChemComm.

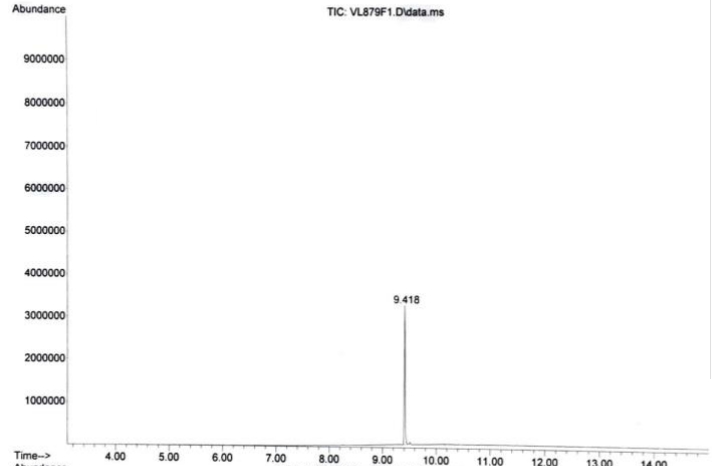


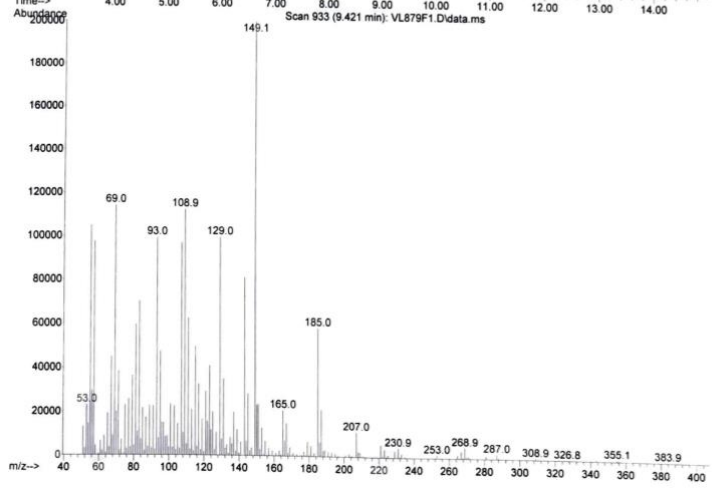
Chemical Formula: $C_{11}H_{20}BrCl_3$
Molecular Weight: 338,54





File :D:\DataMS\2017\08-2017\25082017\VL879F1.D
Operator : VL
Acquired : 25 Aug 2017 14:36 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL879F1
Misc Info :
Vial Number: 12





Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL879F1.D
Acq On : 25 Aug 2017 14:36
Operator : VL
Sample : VL879F1
Misc :
ALS Vial : 12 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

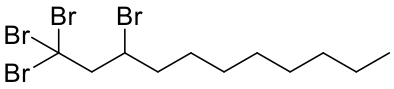
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL879F1.D\data.ms

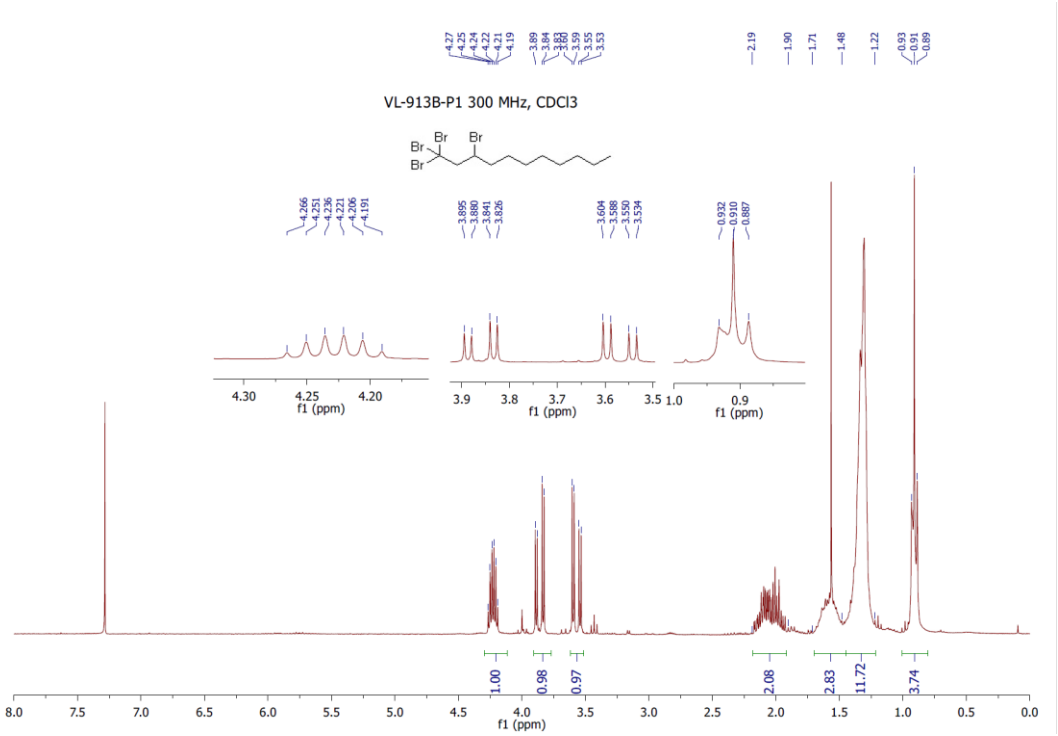
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.415	928	932	940	M	3263206	37874422	100.00%	98.492%
2	9.511	945	946	949	M2	53772	579768	1.53%	1.508%

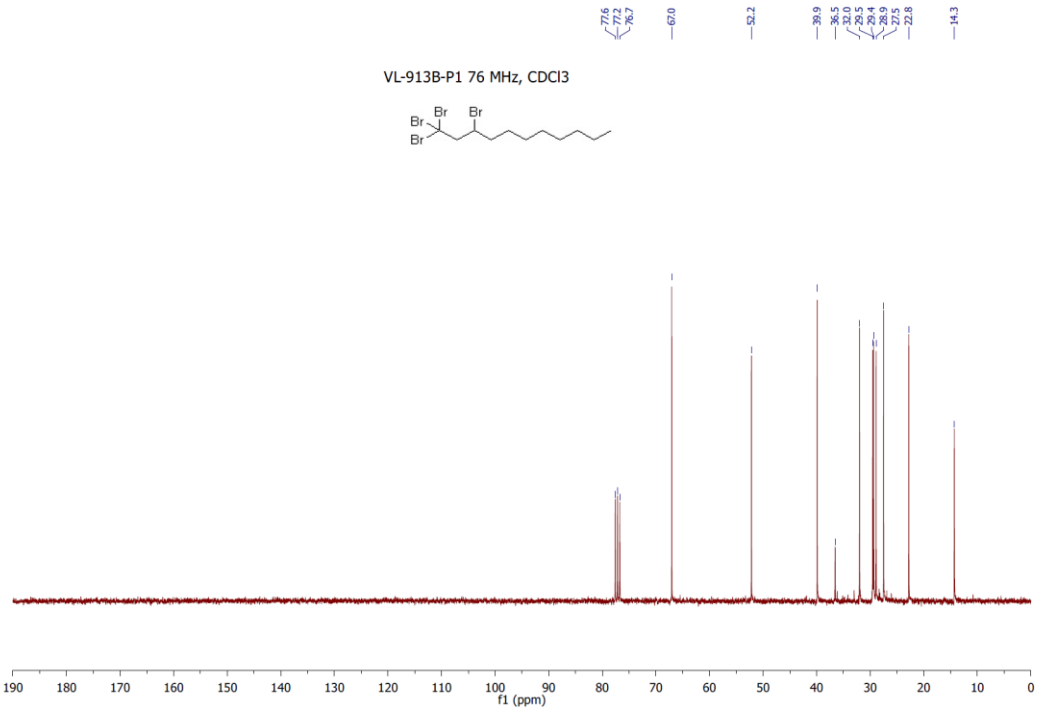
Sum of corrected areas: 38454190

hexadecenal.M Mon Oct 12 17:23:26 2020

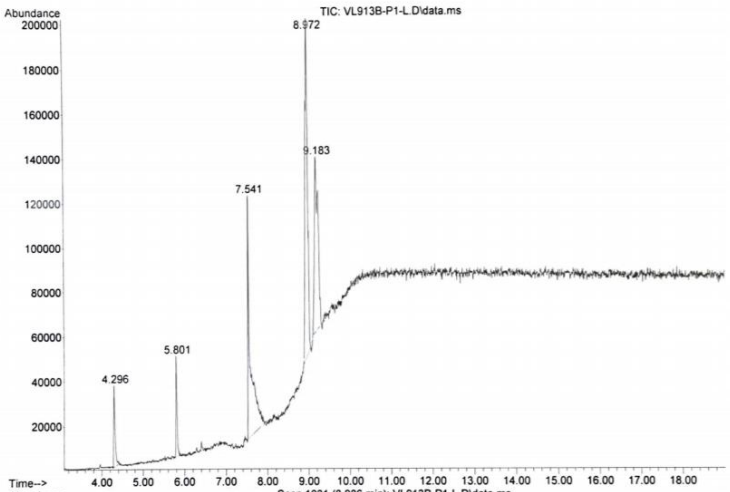


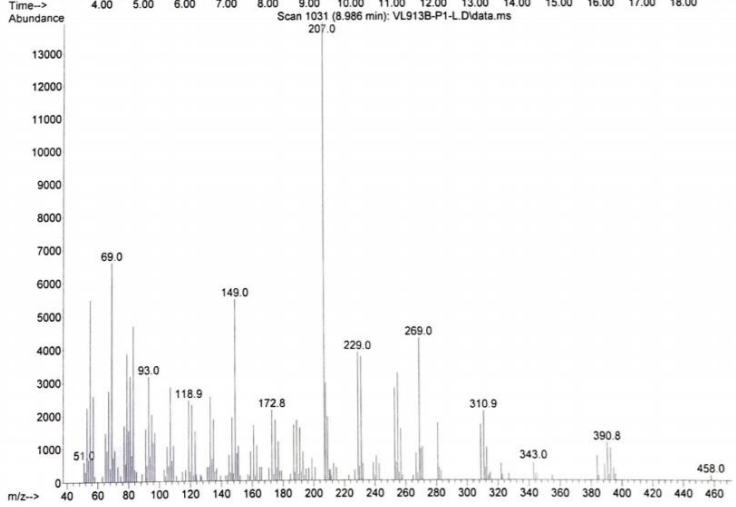
Chemical Formula: $C_{11}H_{20}Br_4$
Molecular Weight: 471,90





File :D:\DataMS\2017\07-2017\20-07-2017\VL913B-P1-L.D
Operator : VL
Acquired : 21 Jul 2017 4:26 using AcqMethod PDTLOURD.M
Instrument : 7890 5975
Sample Name: VL913B-P1
Misc Info :
Vial Number: 25





Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL913B-P1-L.D
Acq On : 21 Jul 2017 4:26
Operator : VL
Sample : VL913B-P1
Misc :
ALS Vial : 25 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

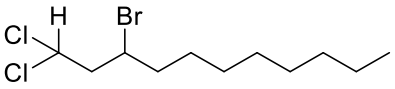
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL913B-P1-L.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.296	206	211	233	M	37285	814321	12.88%	4.664%
2	5.801	467	474	497	M	45706	788388	12.47%	4.516%
3	7.541	771	778	850	M3	114109	4721303	74.69%	27.042%
4	8.972	1014	1028	1042	M4	153591	6320921	100.00%	36.203%
5	9.183	1051	1065	1102	M8	79145	4814505	76.17%	27.575%

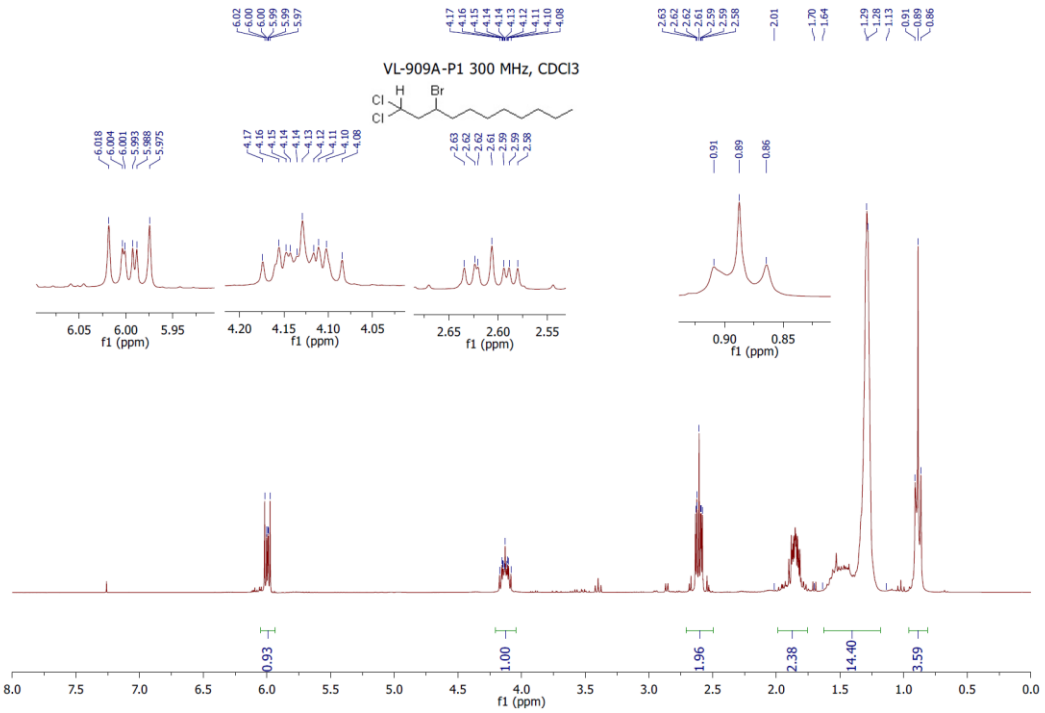
Sum of corrected areas: 17459439

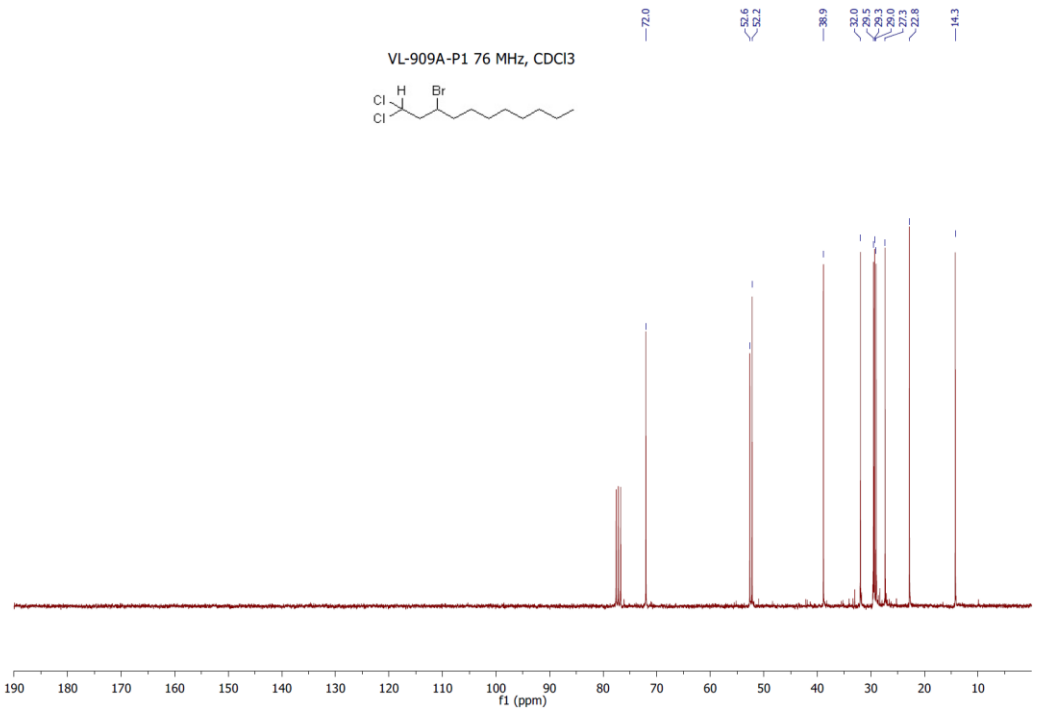
hexadecenal.M Mon Oct 12 17:19:55 2020



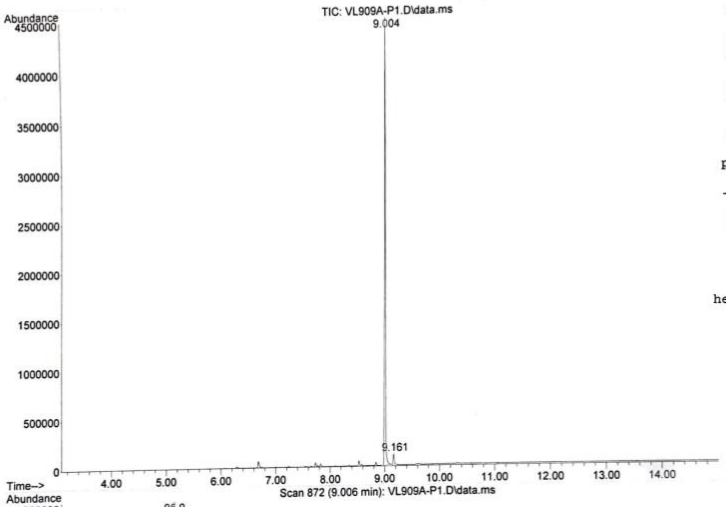
Chemical Formula: $C_{11}H_{21}BrCl_2$

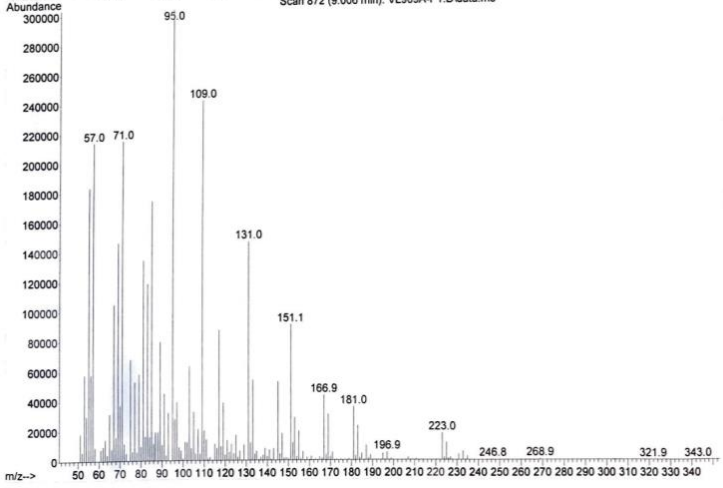
Molecular Weight: 304,09





File :D:\DataMS\2017\07-2017\20-07-2017\VL909A-P1.D
Operator : VL
Acquired : 20 Jul 2017 17:49 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL909A-P1
Misc Info :
Vial Number: 11





Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL909A-P1.D
Acq On : 20 Jul 2017 17:49
Operator : VL
Sample : VL909A-P1
Misc :
ALS Vial : 11 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL909A-P1.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.004	863	872	890	BB	4408175	53399979	100.00%	97.415%
2	9.161	891	895	901	M	109359	1416754	2.65%	2.585%

Sum of corrected areas: 54816733

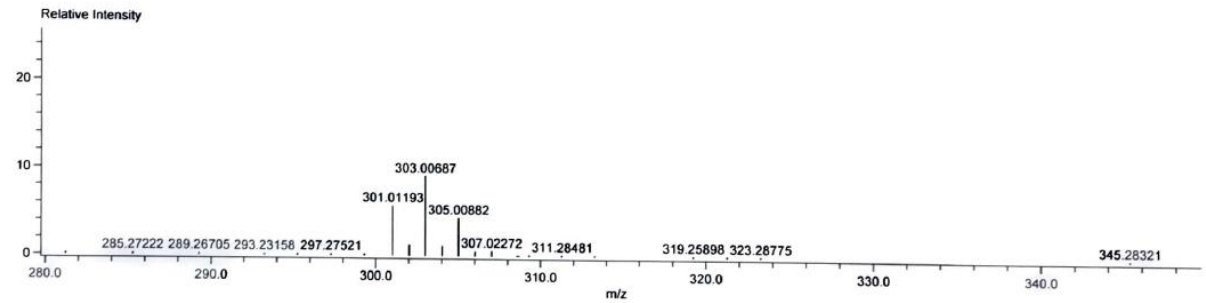
hexadecenal.M Tue Oct 13 11:11:27 2020

Data:CI-210720-VL909AP frais 3
Sample Name:
Description:
Ionization Mode:CI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Smooth[21]];Correct Base[];Average(MS[1] 9.84..9.85)

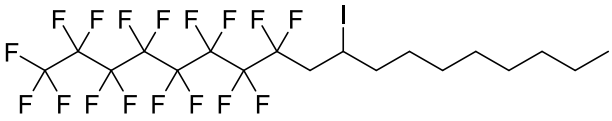
Charge number:1 Tolerance:50.00(ppm)
Element:^{12}C:0 .. 50, ^{1}H:0 .. 100, ^{10}B:0 .. 0, ^{79}Br:1 .. 1, ^{35}Cl:2 .. 2, ^{16}O:0 .. 0

Acquired:12:00:00 AM
Operator:AccuTof
Mass Calibration data:CAL-291118-CAL-EI-class4
Created:7/21/2020 5:47:57 PM
Created by:AccuTof

Unsaturation Number:-1000.0 .. 2000.0 (Fraction:Both)

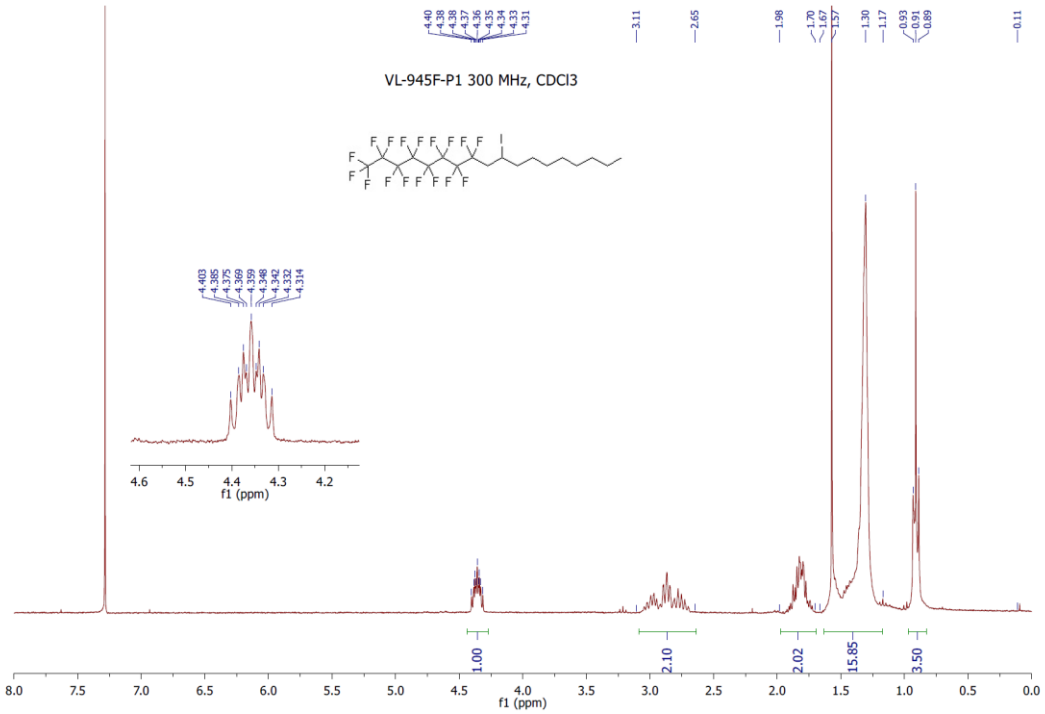


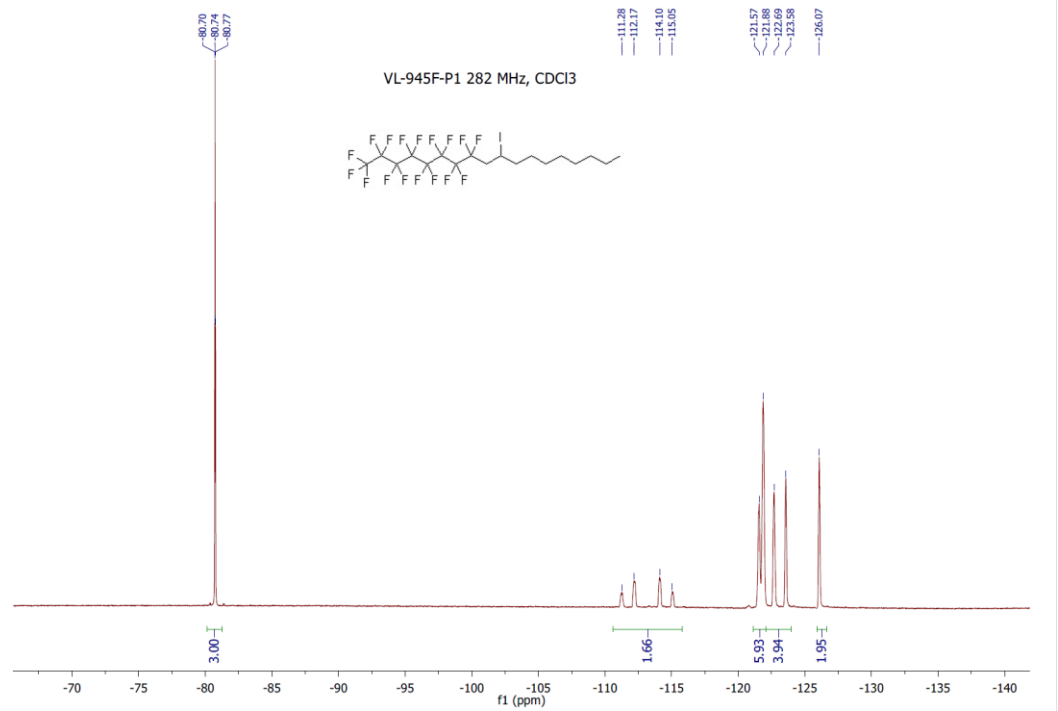
Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	Unsaturation Number
301.01193	22574.81	301.01254	-2.03	$^{12}C_{11}{}^{1}H_{26}{}^{79}Br_{1}{}^{35}Cl_{2}$	0.5

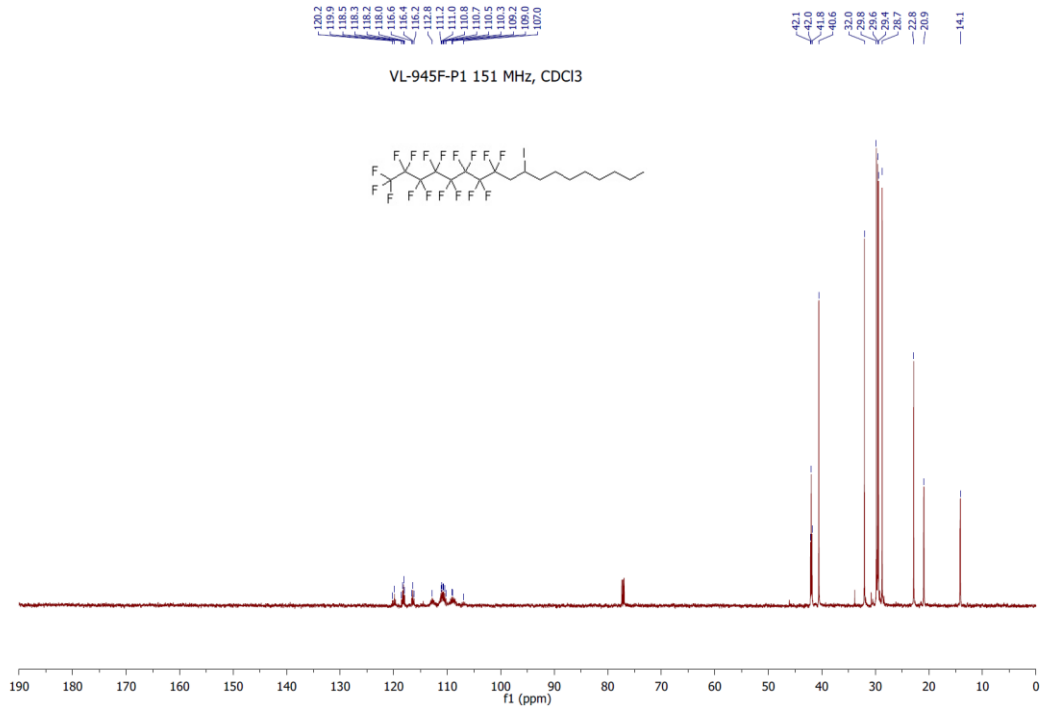


Chemical Formula: $C_{18}H_{20}F_{17}I$

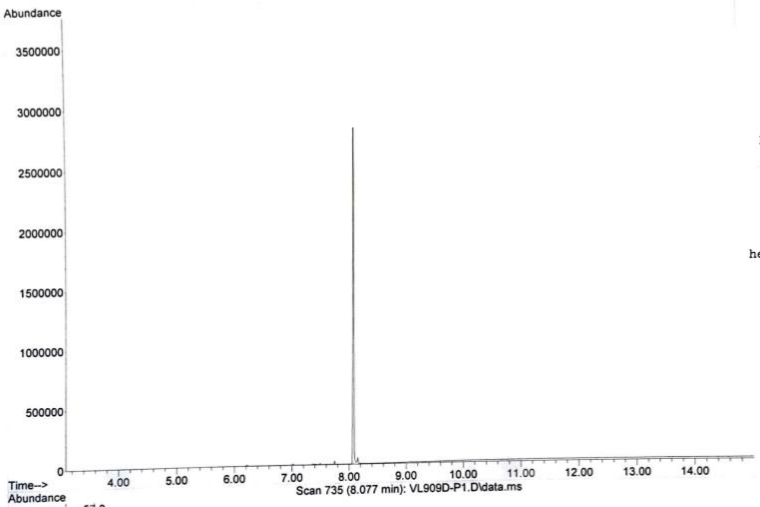
Molecular Weight: 686,24

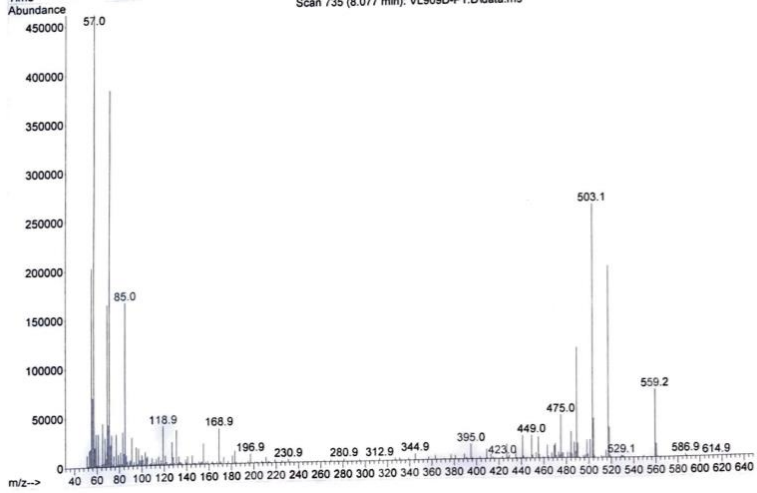





120.2
119.9
118.5
118.3
118.2
118.0
116.6
116.4
116.2
112.8
111.2
111.0
110.8
110.7
110.5
110.3
109.2
109.0
107.0
42.1
41.0
41.8
40.6
32.0
29.8
29.6
29.4
28.7
22.8
20.9
14.1
VL-945F-P1 151 MHz, CDCl3
F F F F F F F F I
F
F
F F F F F F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

File :D:\DataMS\2017\07-2017\20-07-2017\VL909D-P1.D
Operator : VL
Acquired : 20 Jul 2017 22:42 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL909D-P1
Misc Info :
Vial Number: 27





Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL909D-P1.D
Acq On : 20 Jul 2017 22:42
Operator : VL
Sample : VL909D-P1
Misc :
ALS Vial : 27 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

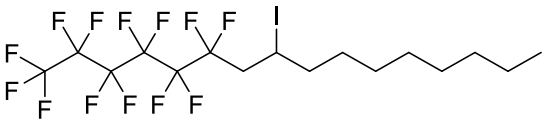
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL909D-P1.D\data.ms

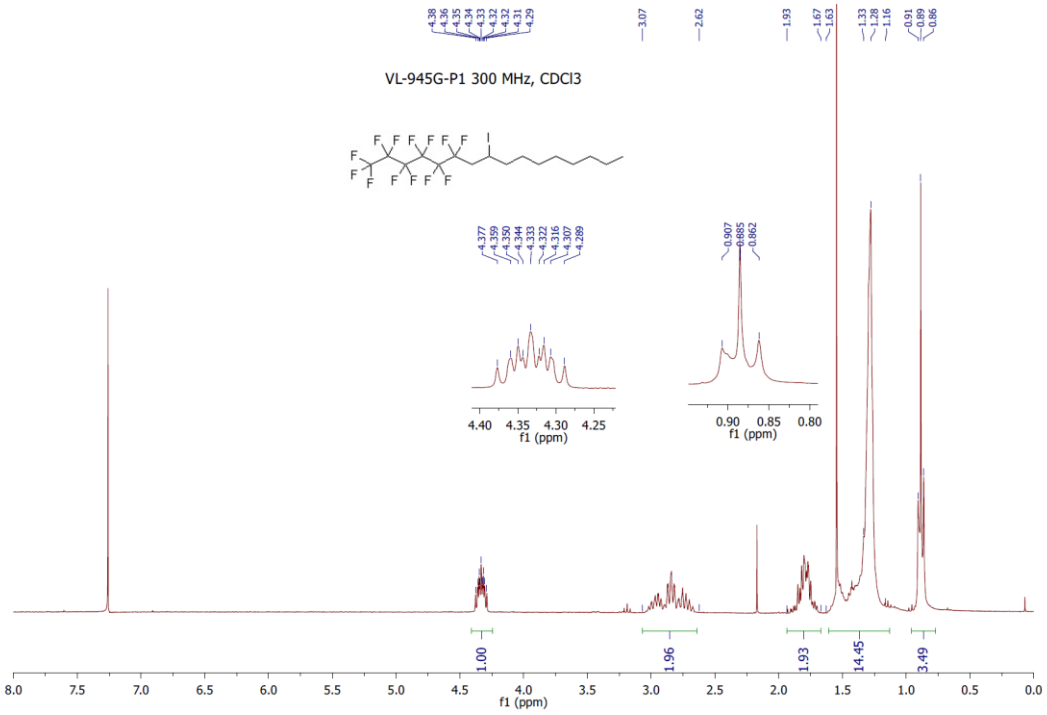
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.074	731	735	743	M	3927605	39640188	100.00%	100.000%

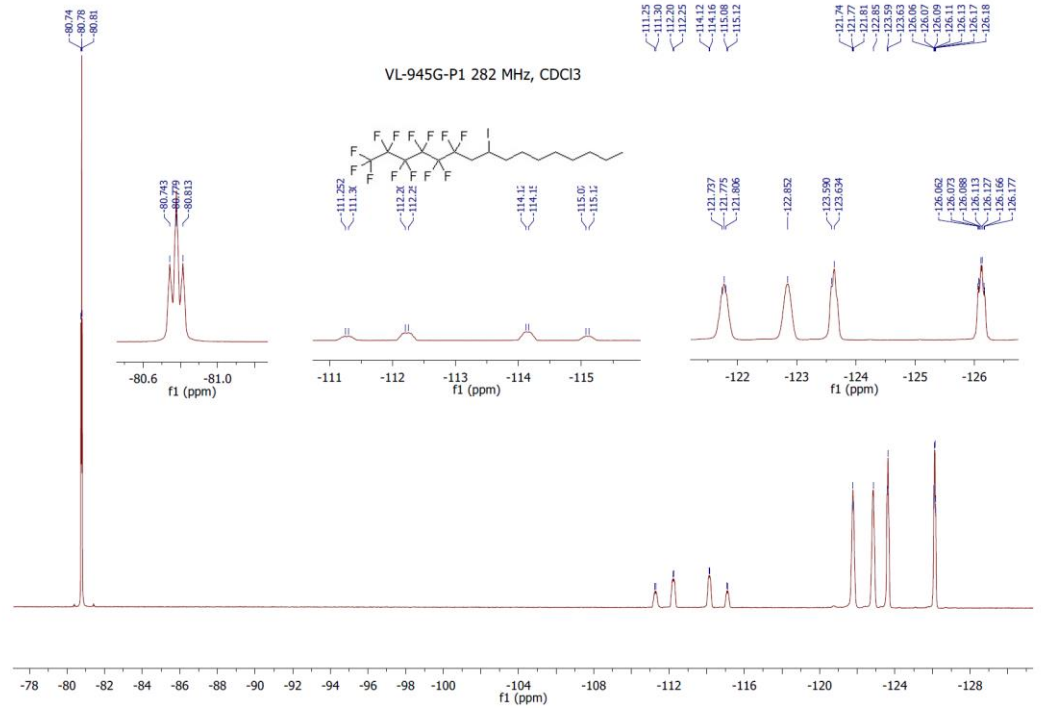
Sum of corrected areas: 39640188

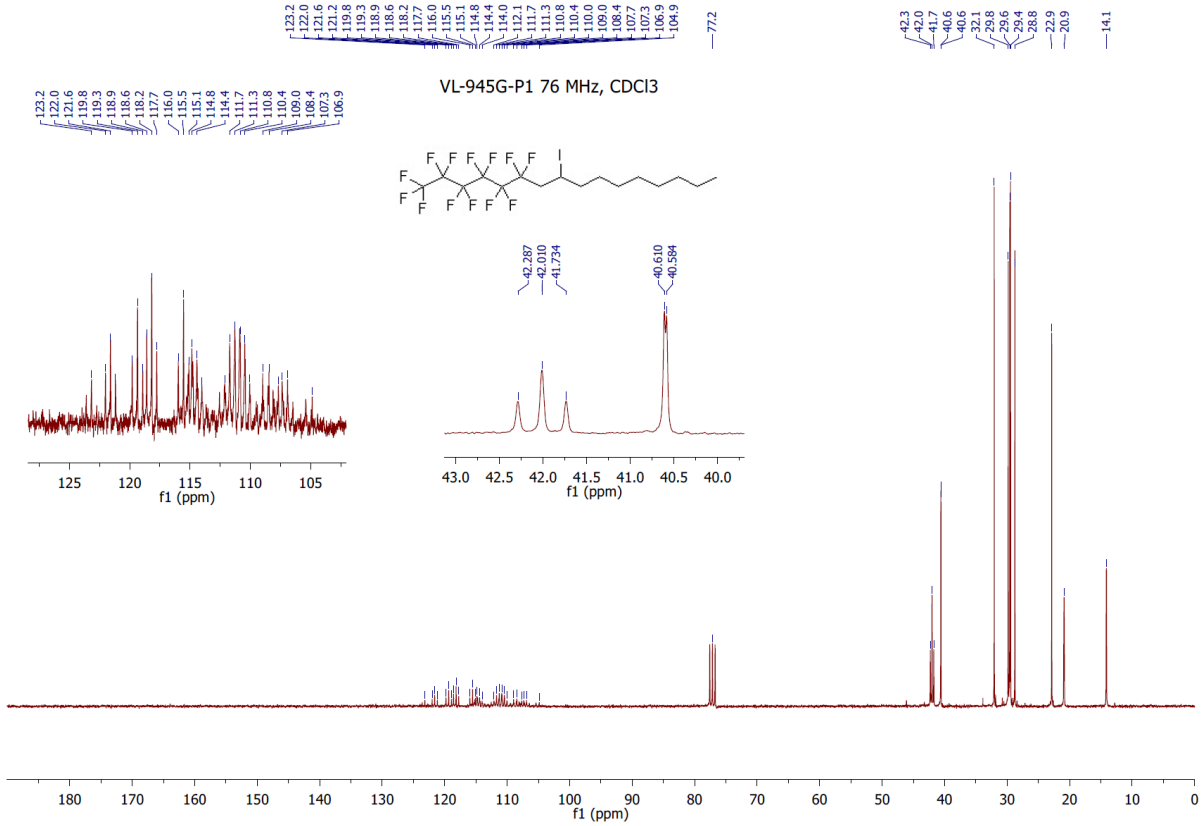
hexadecenal.M Tue Oct 13 11:12:36 2020



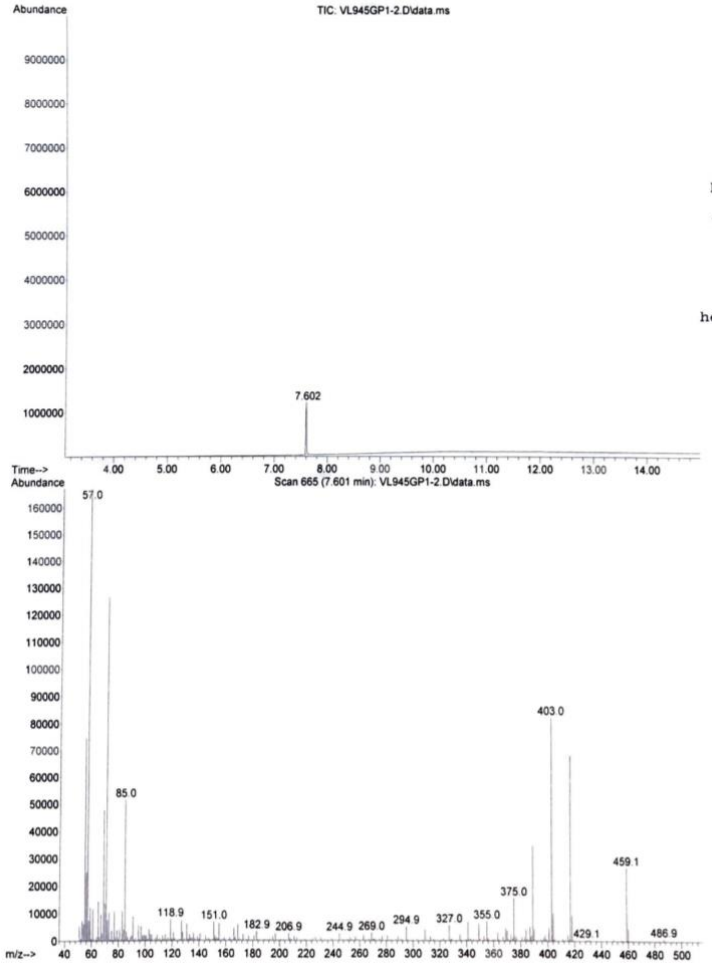
Chemical Formula: $C_{16}H_{20}F_{13}I$
Molecular Weight: 586,22






VL-945G-P1 76 MHz, CDCl3
f1 (ppm)

File :D:\DataMS\2017\08-2017\25082017\VL945GP1-2.D
Operator : VL
Acquired : 25 Aug 2017 14:17 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL945GP1
Misc Info :
Vial Number: 11



Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL945GP1-2.D
Acq On : 25 Aug 2017 14:17
Operator : VL
Sample : VL945GP1
Misc :
ALS Vial : 11 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

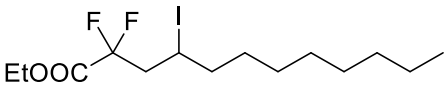
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL945GP1-2.D\data.ms

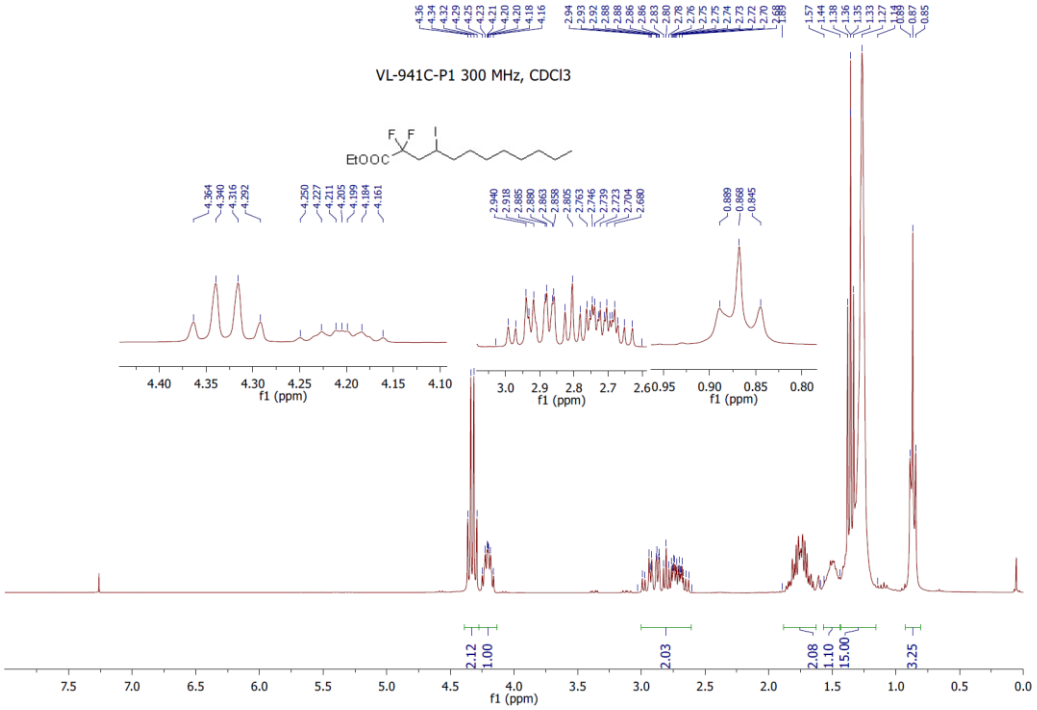
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.599	661	665	674	M2	1240777	12816362	100.00%	100.000%

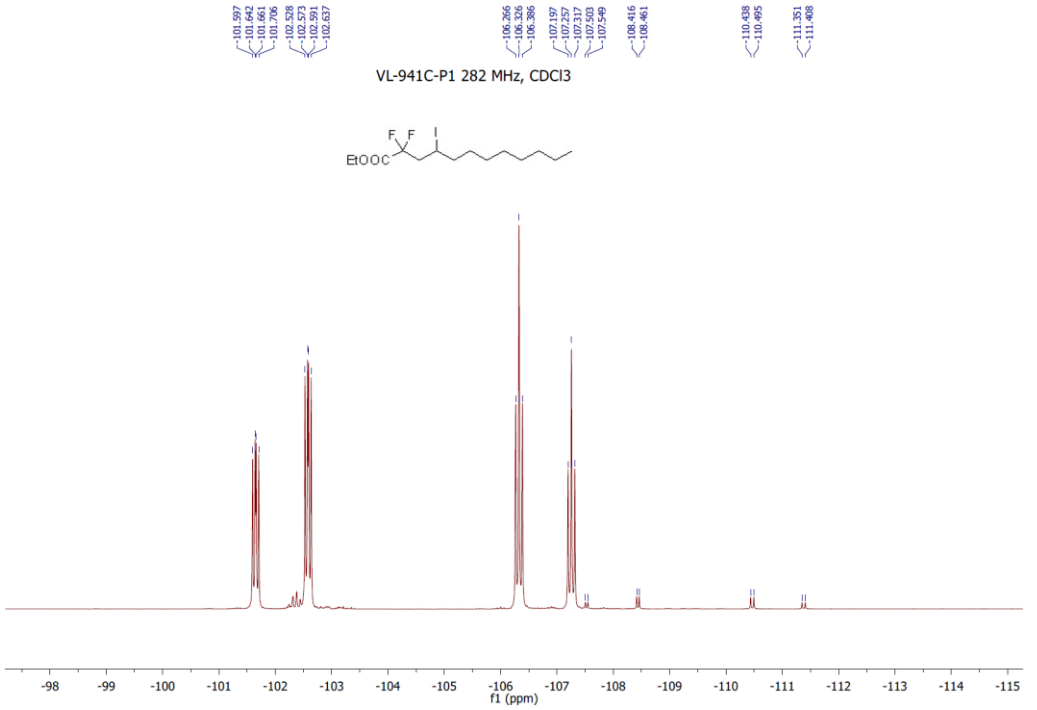
Sum of corrected areas: 12816362

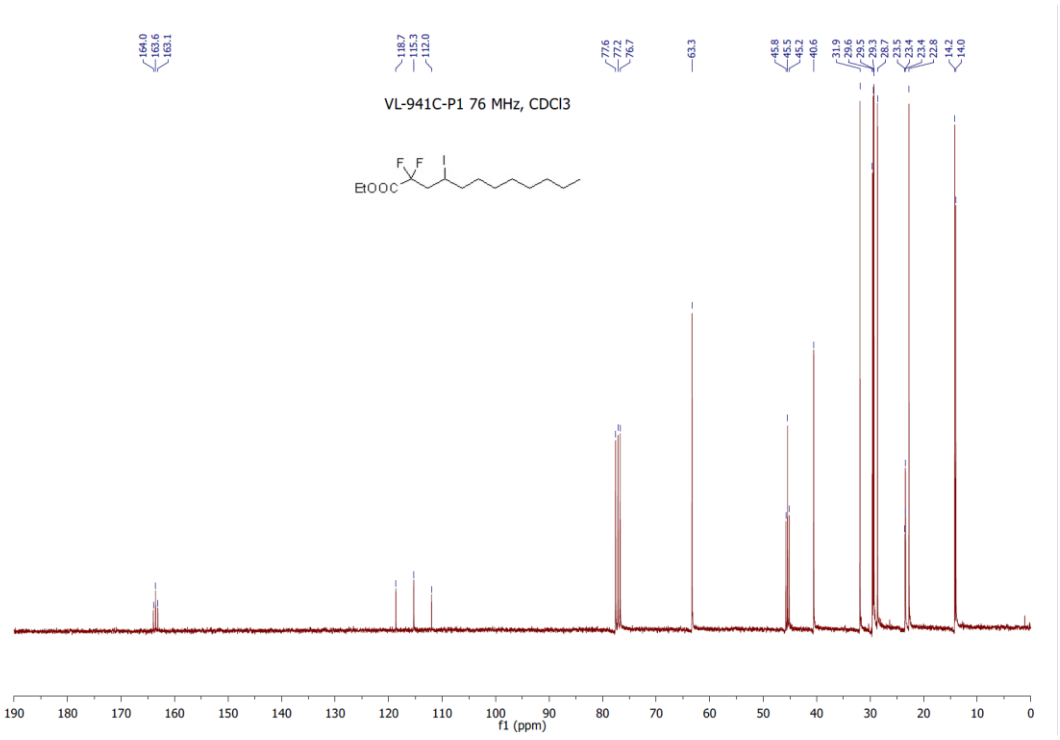
hexadecenal.M Mon Oct 12 17:04:16 2020



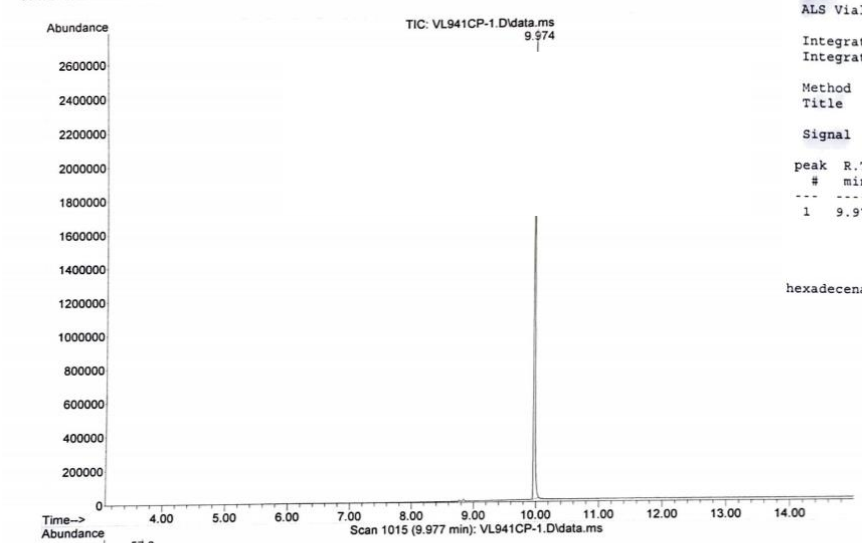
Chemical Formula: $C_{14}H_{25}F_2IO_2$
Molecular Weight: 390,25

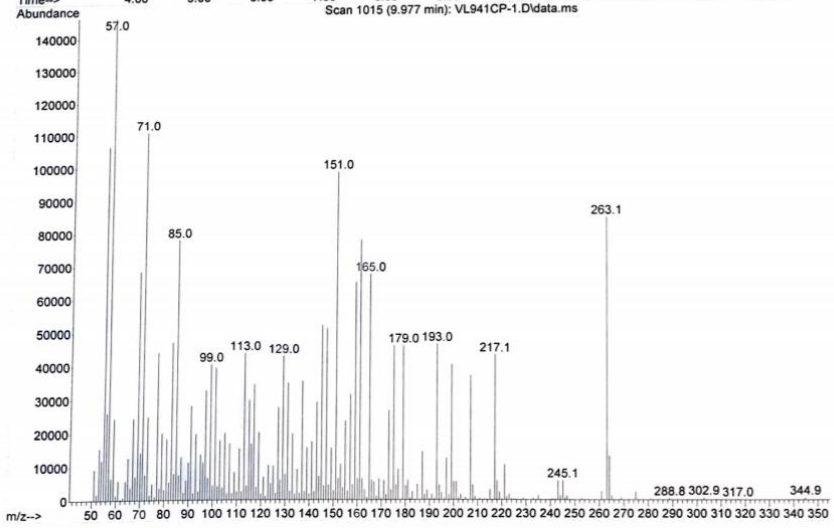





164.0
163.6
163.1
118.7
115.3
112.0
77.6
77.2
76.7
63.3
45.8
45.5
45.2
40.6
31.9
29.6
29.5
29.3
28.7
23.5
23.4
23.4
22.8
14.2
14.0
VL-941C-P1 76 MHz, CDCl3
F
F
I
EtOOC
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

```
File       :D:\DataMS\2017\07-2017\20-07-2017\VL941CP-1.D
Operator   : VL
Acquired   : 20 Jul 2017  20:52     using AcqMethod NORMAL.M
Instrument :    7890 5975
Sample Name: VL941CP-1
Misc Info  :
Vial Number: 21
```



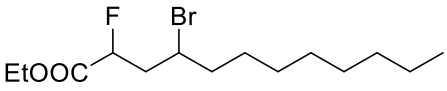


Area Percent Report

```
Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL941CP-1.D
Acq On    : 20 Jul 2017  20:52
Operator  : VL
Sample    : VL941CP-1
Misc      :
ALS Vial  : 21   Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method    : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title     :

Signal    : TIC: VL941CP-1.D\data.ms
```

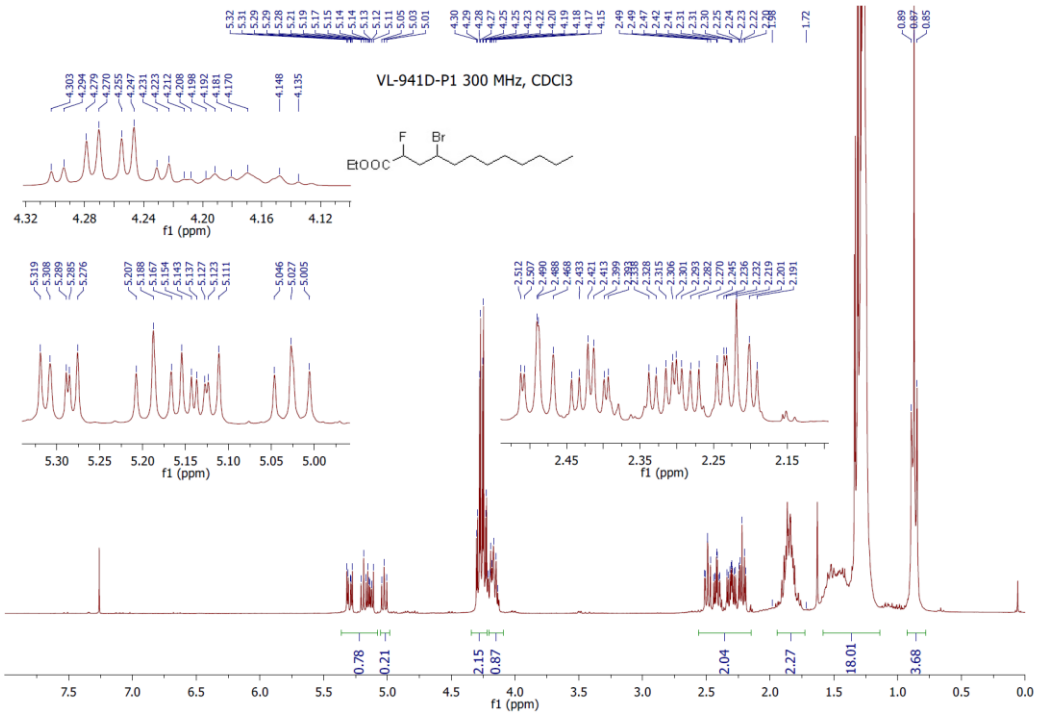
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.974	1010	1015	1028	M	2894124	39411859	100.00%	100.000%

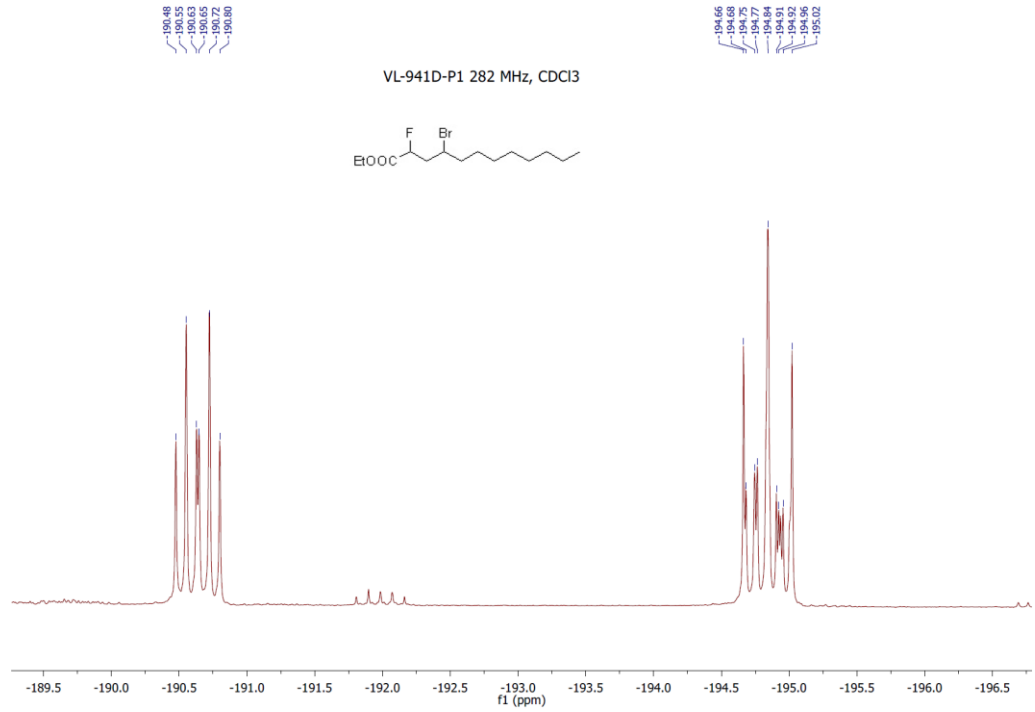
```
Sum of corrected areas:    39411859

hexadecenal.M Mon Oct 12 17:21:16 2020
```

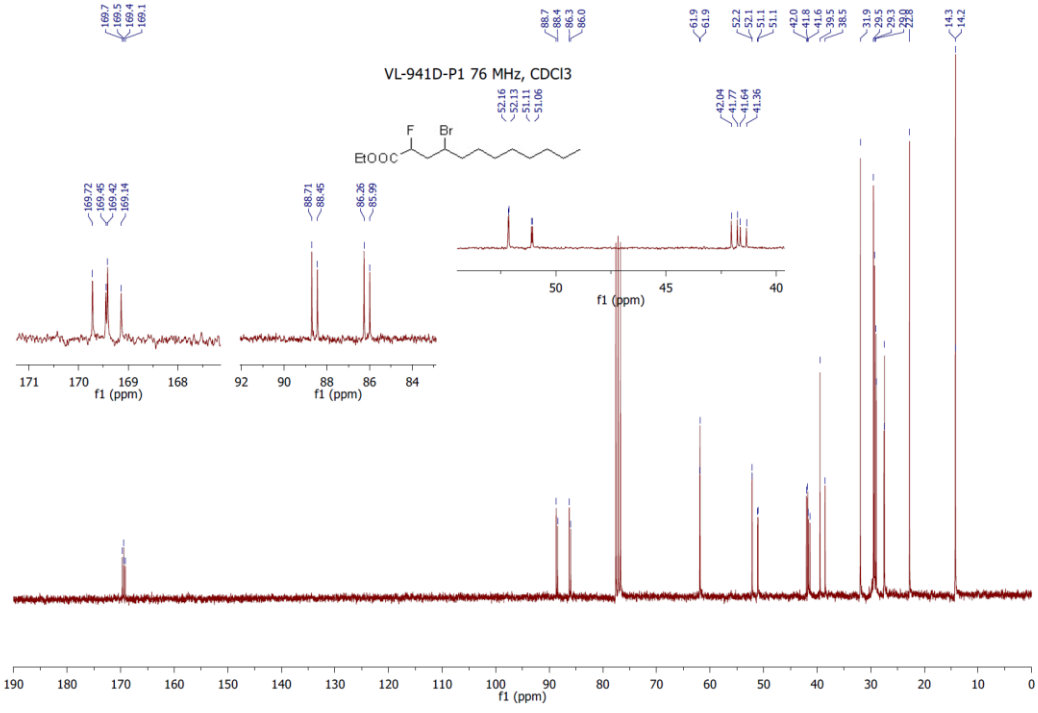


Chemical Formula: $C_{14}H_{26}BrFO_2$

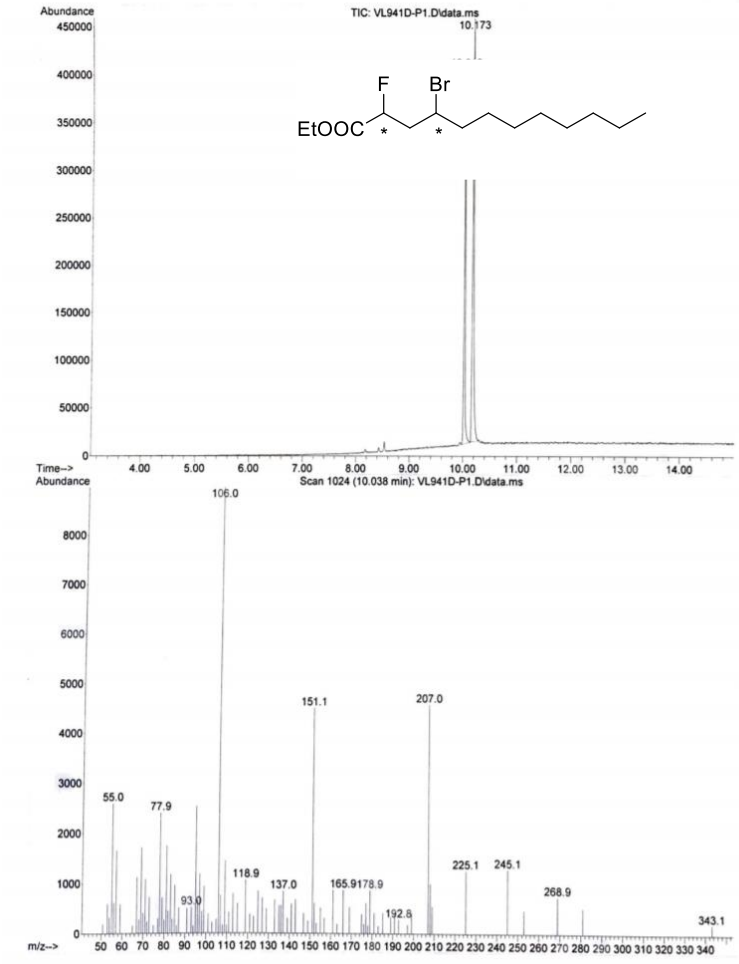
Molecular Weight: 325,26




-190.48
-190.55
-190.63
-190.65
-190.72
-190.80
-194.66
-194.68
-194.75
-194.77
-194.84
-194.91
-194.92
-194.96
-195.02
VL-941D-P1 282 MHz, CDCl3
F
Br
EtOOC
-189.5
-190.0
-190.5
-191.0
-191.5
-192.0
-192.5
-193.0
-193.5
-194.0
-194.5
-195.0
-195.5
-196.0
-196.5
f1 (ppm)


169.7
169.5
169.4
169.1
88.7
88.4
86.3
86.0
61.9
61.9
52.2
52.1
51.1
51.1
42.0
41.8
41.6
39.5
38.5
31.9
29.5
29.3
25.8
14.3
14.2
VL-941D-P1 76 MHz, CDCl3
52.16
52.13
51.11
51.06
42.04
41.77
41.64
41.36
F
Br
EtOOC
169.72
169.45
169.42
169.14
88.71
88.45
86.26
85.99
50
45
40
f1 (ppm)
171
170
169
168
f1 (ppm)
92
90
88
86
84
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

File :D:\DataMS\2017\07-2017\20-07-2017\VL941D-P1.D
Operator : VL
Acquired : 20 Jul 2017 19:57 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL941D-P1
Misc Info :
Vial Number: 18



Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL941D-P1.D
Acq On : 20 Jul 2017 19:57
Operator : VL
Sample : VL941D-P1
Misc :
ALS Vial : 18 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

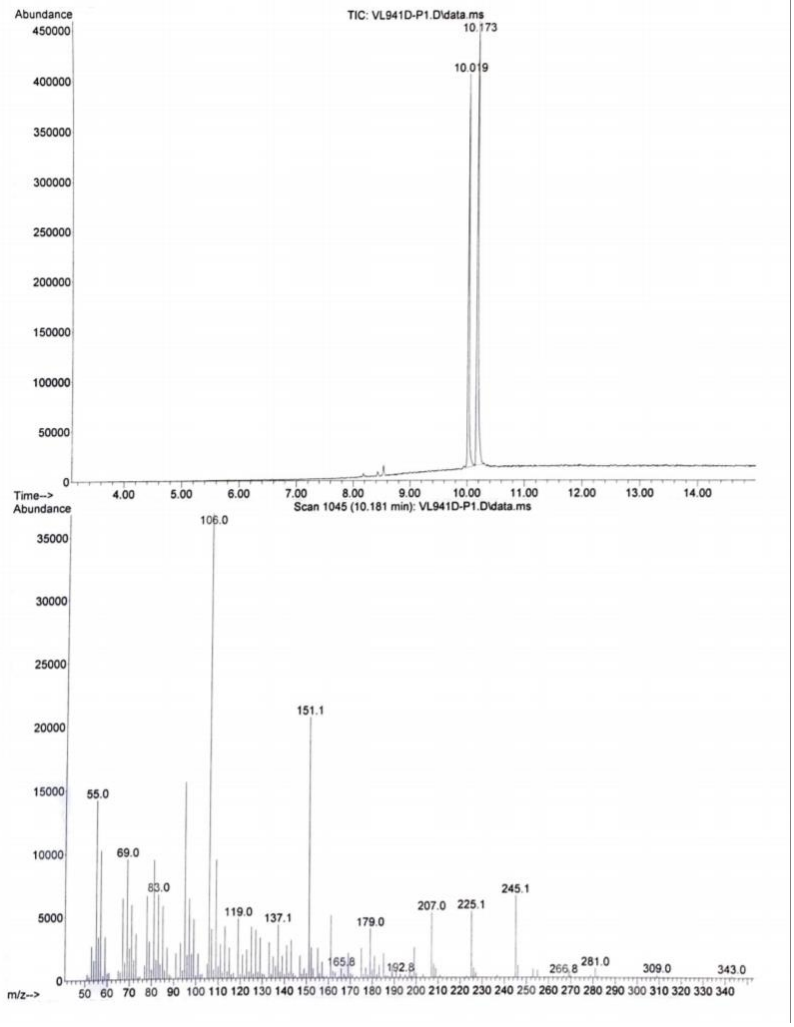
Signal : TIC: VL941D-P1.D\data.ms

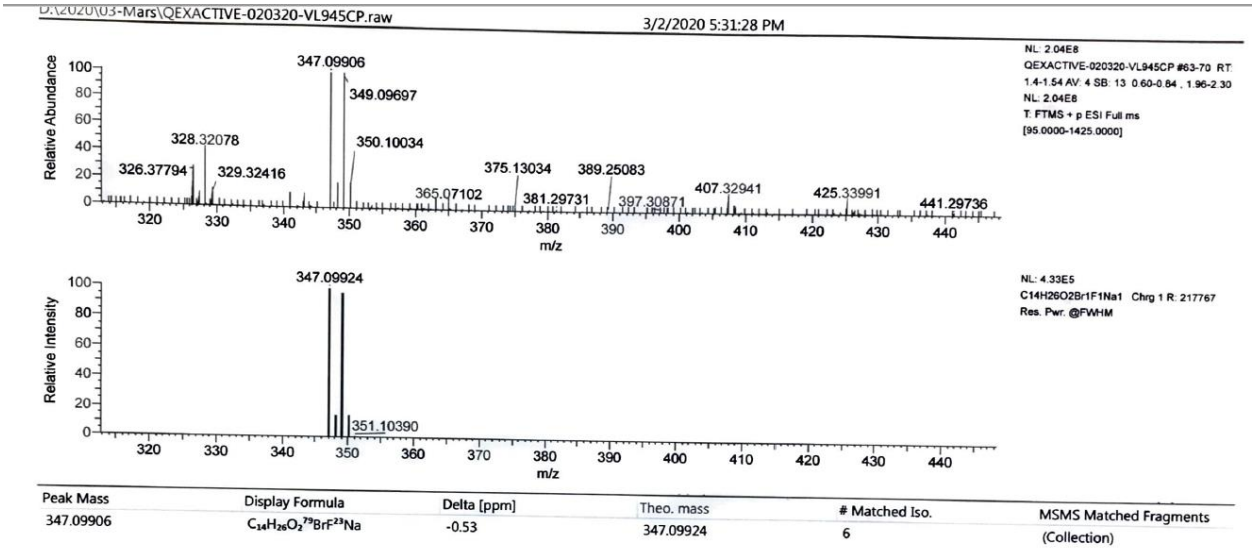
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.019	1013	1021	1029	M	394684	5392494	68.82%	40.766%
2	10.173	1036	1044	1061	M	446647	7835502	100.00%	59.234%

Sum of corrected areas: 13227996

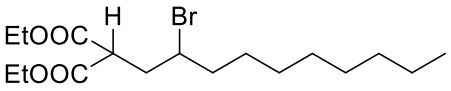
hexadecenal.M Mon Oct 12 20:01:36 2020

```
File       :D:\DataMS\2017\07-2017\20-07-2017\VL941D-P1.D
Operator   : VL
Acquired   : 20 Jul 2017  19:57     using AcqMethod NORMAL.M
Instrument :    7890 5975
Sample Name: VL941D-P1
Misc Info  :
Vial Number: 18
```



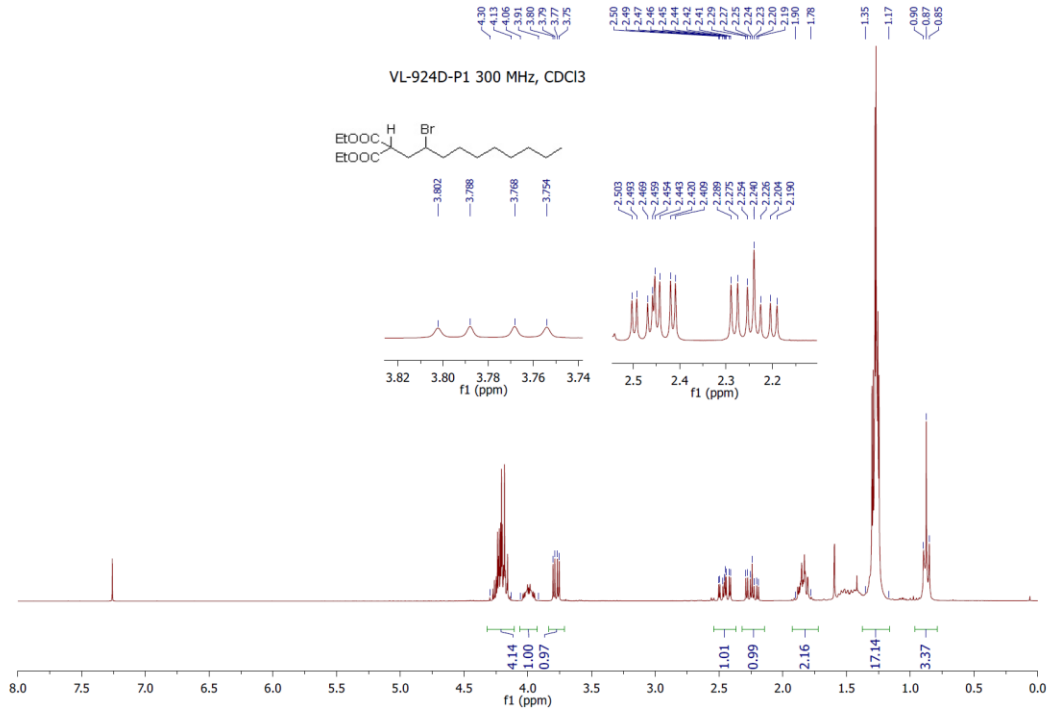


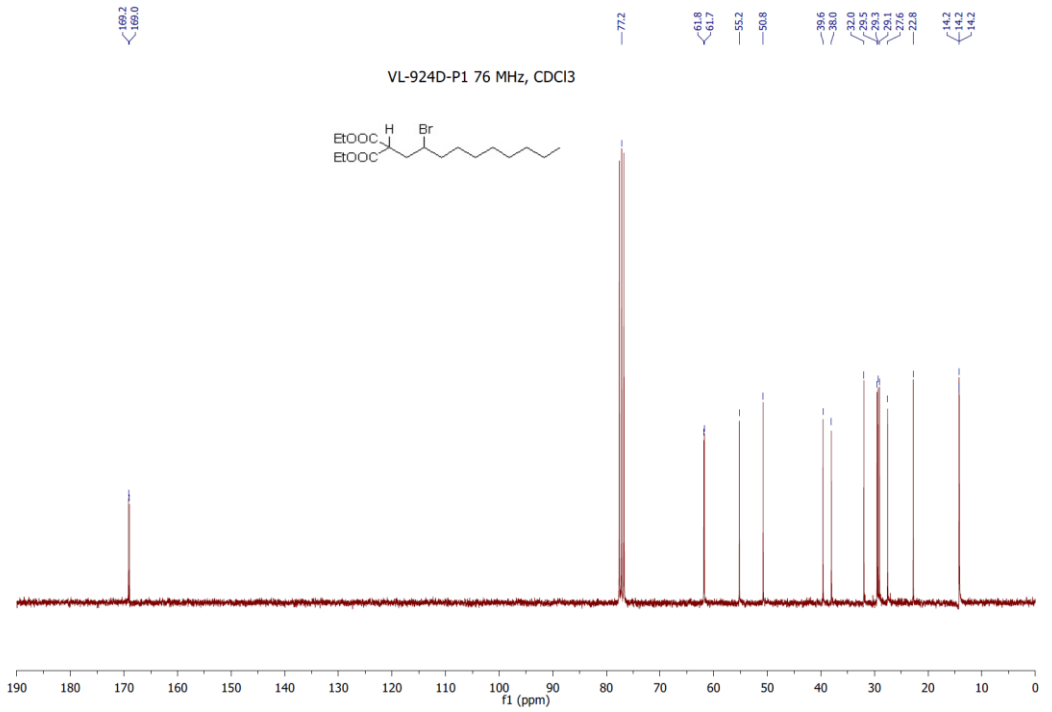
Peak Mass	Display Formula	Delta [ppm]	Theo. mass	# Matched Iso.	MSMS Matched Fragments
347.09906	$C_{14}H_{26}O_2{}^{79}BrF^{23}Na$	-0.53	347.09924	6	(Collection)



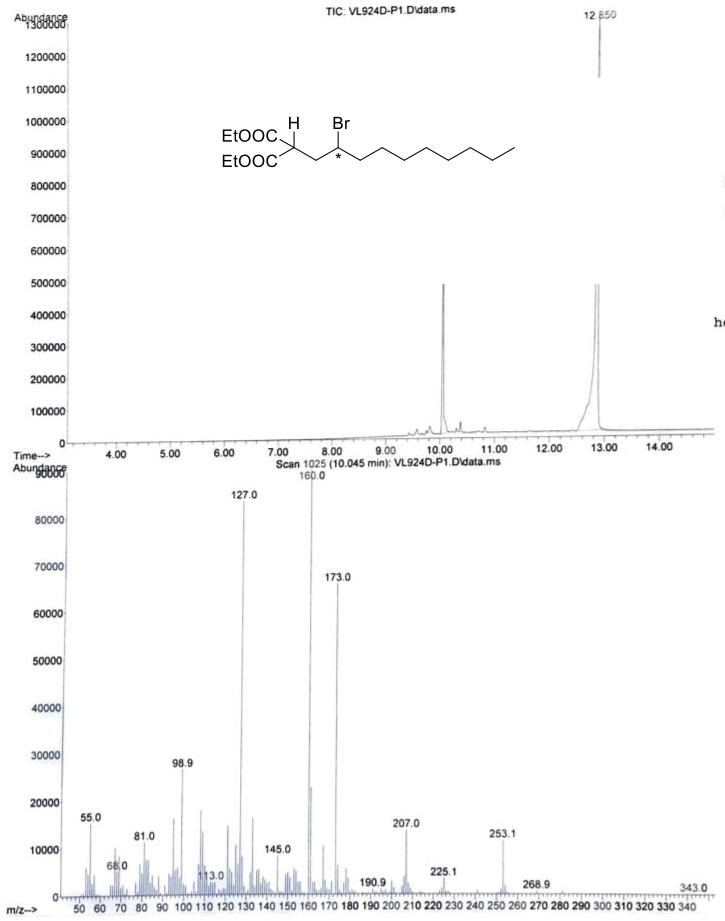
Chemical Formula: $C_{17}H_{31}BrO_4$

Molecular Weight: 379,34





```
File        :D:\DataMS\2017\07-2017\20-07-2017\VL924D-P1.D
Operator    : VL
Acquired    : 20 Jul 2017  21:29     using AcqMethod NORMAL.M
Instrument :
    7890 5975
Sample Name: VL924D-P1
Misc Info   :
Vial Number: 23
```



Area Percent Report

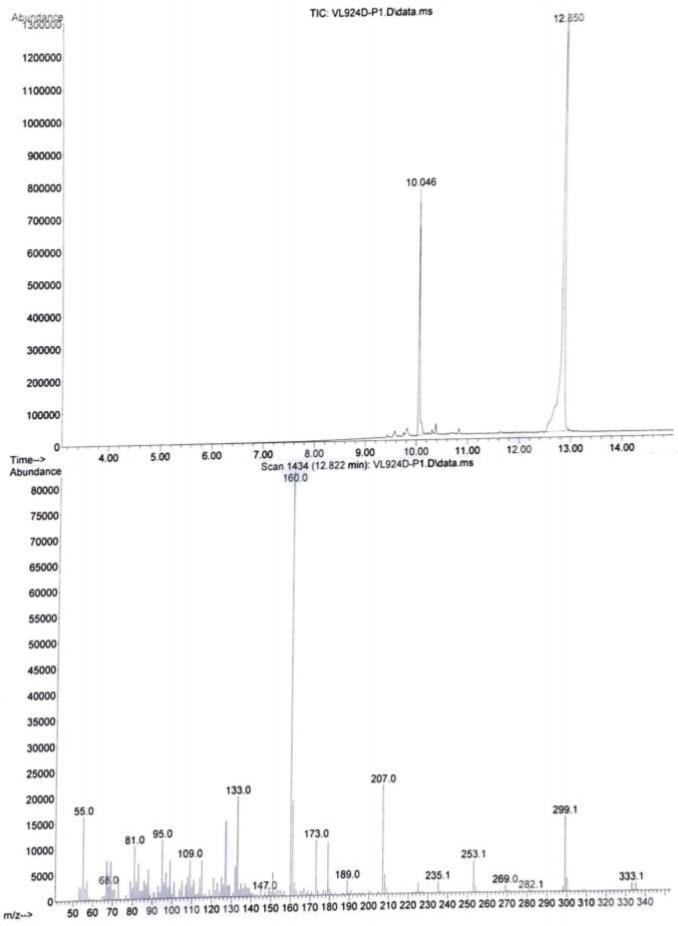
```
Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL924D-P1.D
Acq On    : 20 Jul 2017  21:29
Operator  : VL
Sample    : VL924D-P1
Misc      :
ALS Vial  : 23   Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method    : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title     :

Signal    : TIC: VL924D-P1.D\data.ms
```

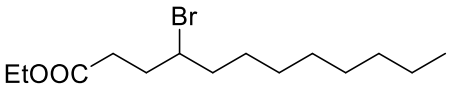
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.046	1020	1025	1043	M	767628	11464620	24.18%	19.471%
2	12.850	1387	1438	1459	M	1286094	47417206	100.00%	80.529%

Sum of corrected areas: 58881826

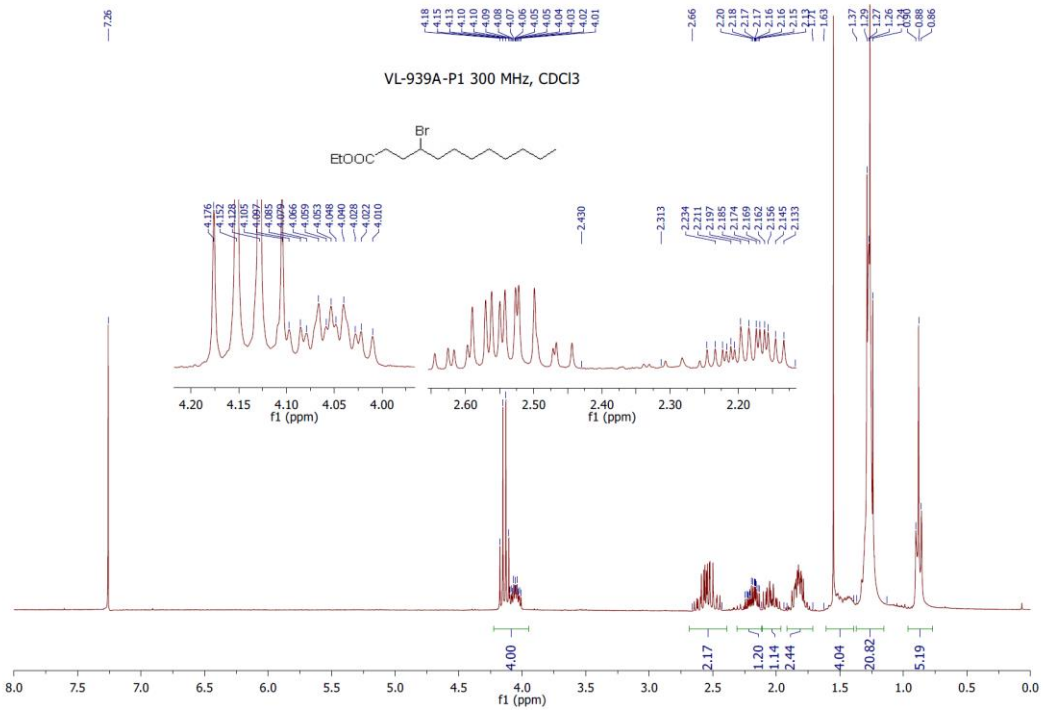
hexadecenal.M Tue Oct 13 10:59:45 2020

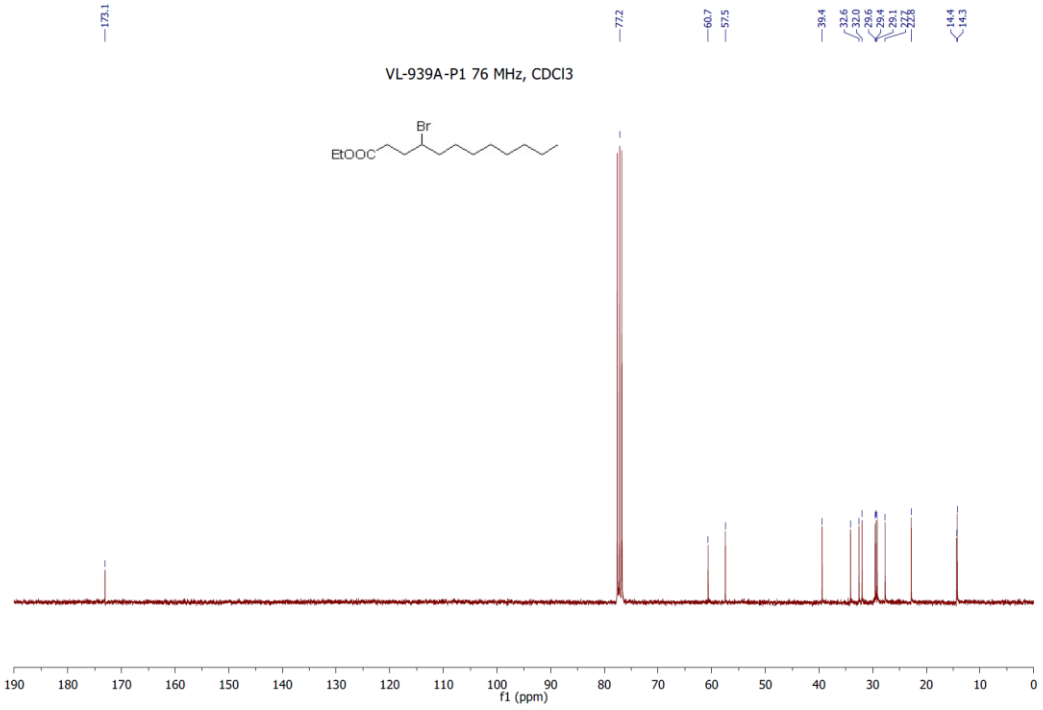
File :D:\DataMS\2017\07-2017\20-07-2017\VL924D-P1.D
Operator : VL
Acquired : 20 Jul 2017 21:29 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL924D-P1
Misc Info :
Vial Number: 23



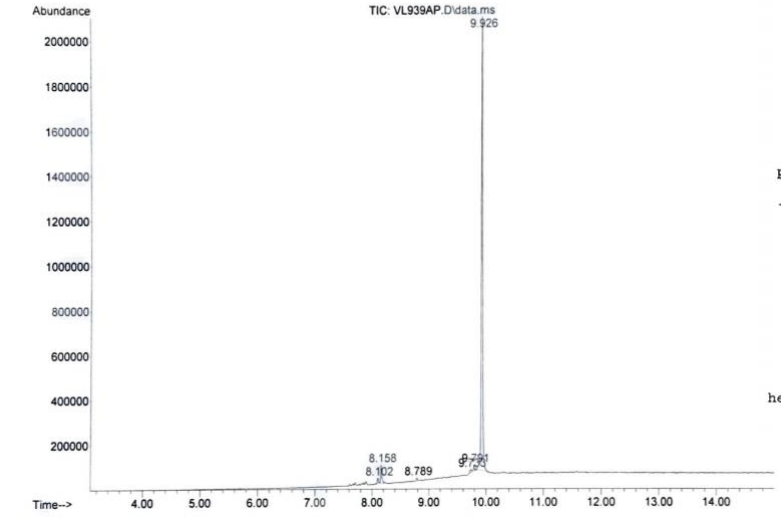


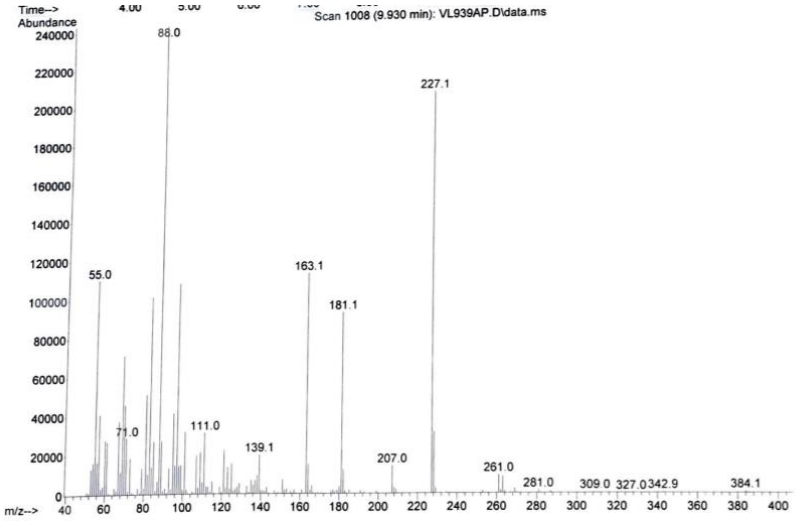
Chemical Formula: $C_{14}H_{27}BrO_2$
Molecular Weight: 307,27





File :D:\DataMS\2017\08-2017\25082017\VL939AP.D
Operator : VL
Acquired : 25 Aug 2017 16:26 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL939AP
Misc Info :
Vial Number: 18





Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL939AP.D
Acq On : 25 Aug 2017 16:26
Operator : VL
Sample : VL939AP
Misc :
ALS Vial : 18 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

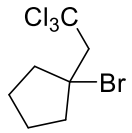
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL939AP.D\data.ms

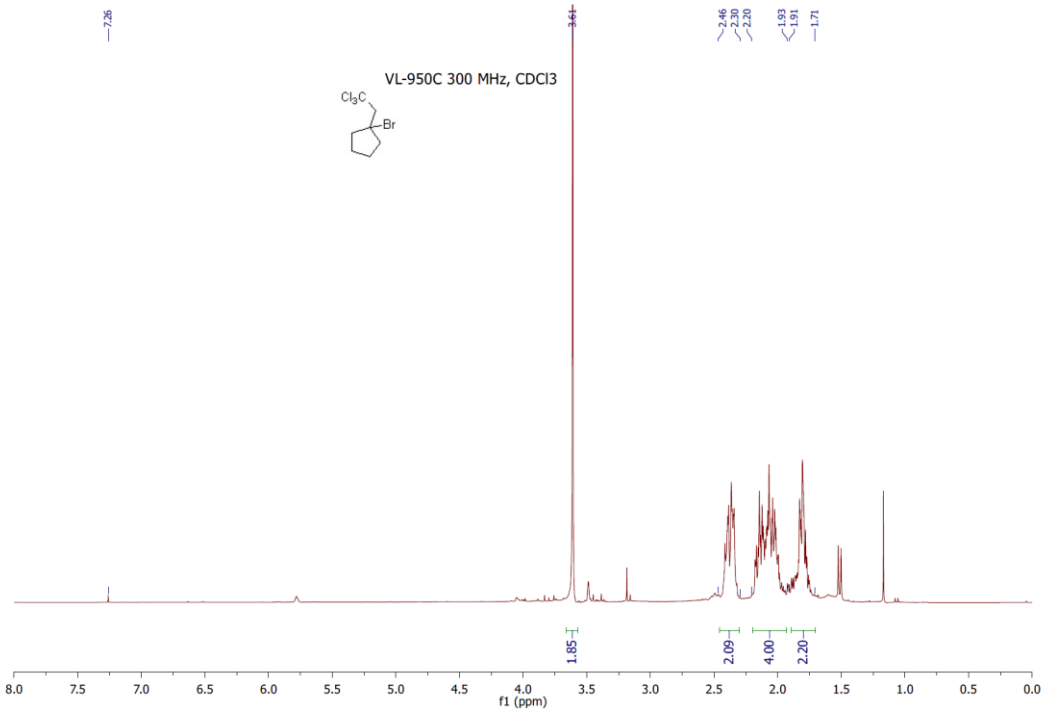
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.102	735	739	743	M4	22813	303467	0.98%	0.920%
2	8.158	744	747	757	M	81954	1204845	3.91%	3.651%
3	8.789	838	840	844	M3	13514	142818	0.46%	0.433%
4	9.733	973	979	983	M2	11988	256709	0.83%	0.778%
5	9.791	983	988	990	M	25607	245963	0.80%	0.745%
6	9.926	993	1007	1021	M	2126644	30848201	100.00%	93.474%

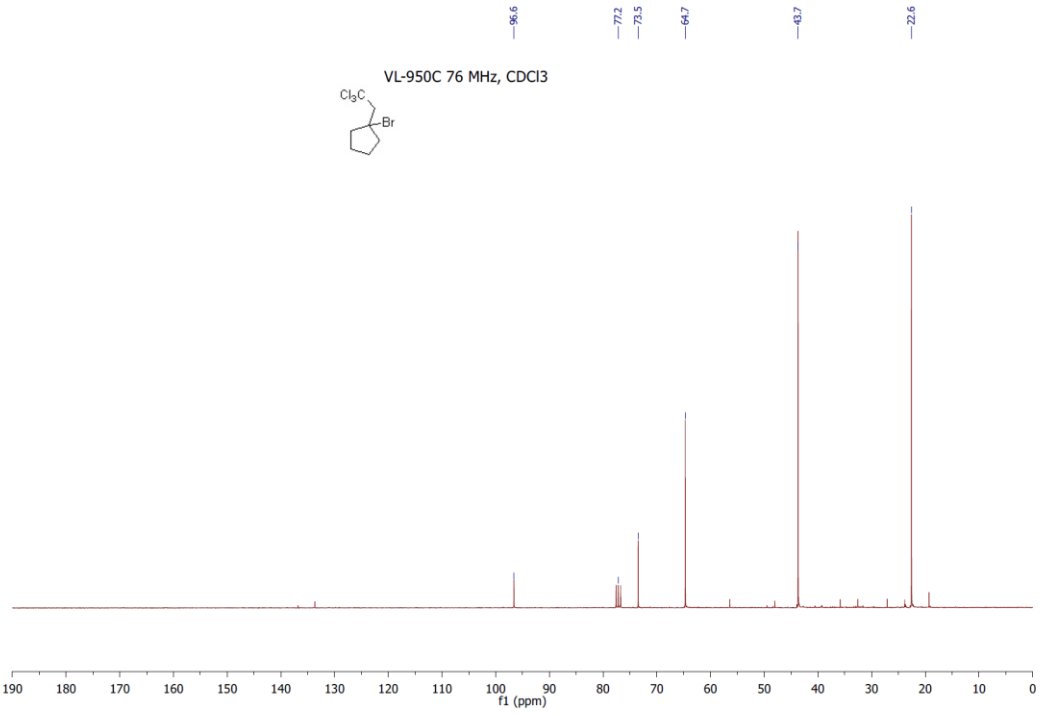
Sum of corrected areas: 33002004

hexadecenal.M Mon Oct 12 17:01:22 2020

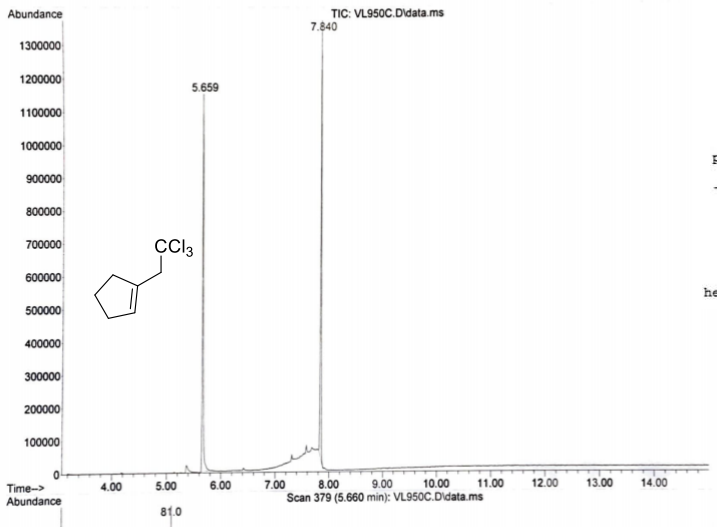


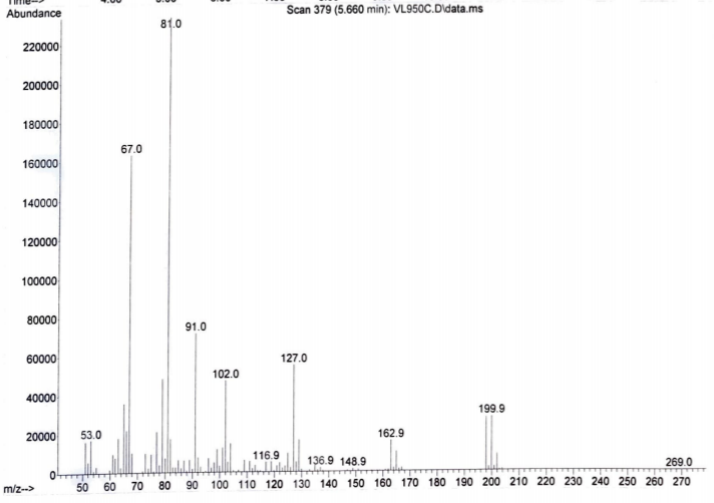
Chemical Formula: $C_7H_{10}BrCl_3$
Molecular Weight: 280,4110





File :D:\DataMS\2017\07-2017\20-07-2017\VL950C.D
Operator : VL
Acquired : 20 Jul 2017 19:02 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL950C
Misc Info :
Vial Number: 15





Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL950C.D
Acq On : 20 Jul 2017 19:02
Operator : VL
Sample : VL950C
Misc :
ALS Vial : 15 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

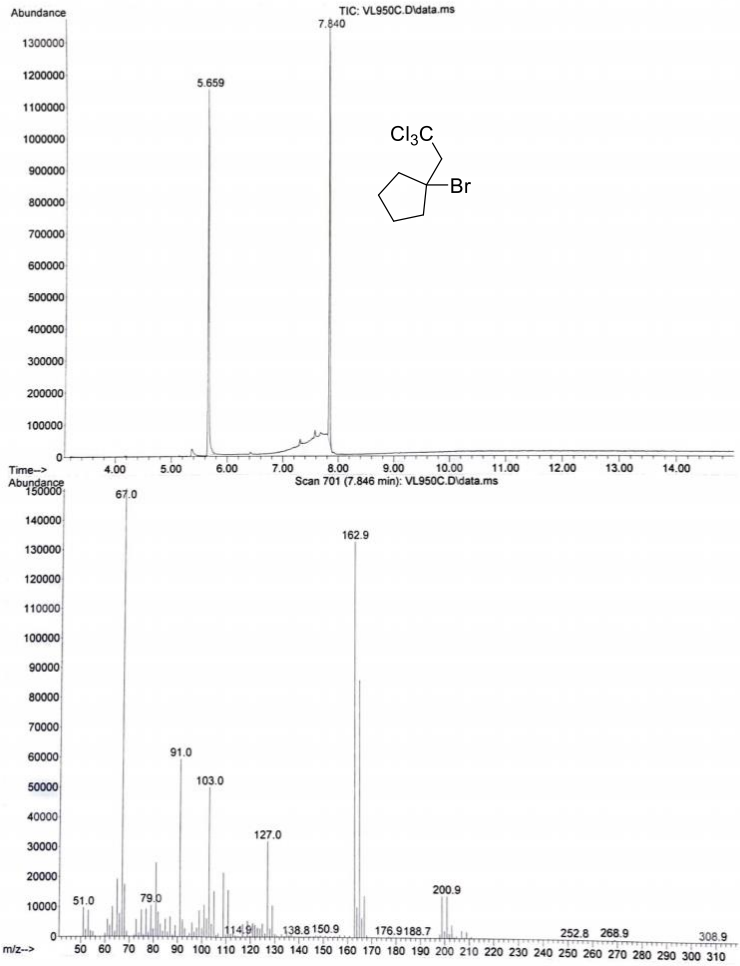
Signal : TIC: VL950C.D\data.ms

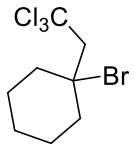
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.659	374	379	400	M	1163213	14710638	100.00%	50.845%
2	7.840	695	700	707	M	1332377	14221945	96.68%	49.155%

Sum of corrected areas: 28932583

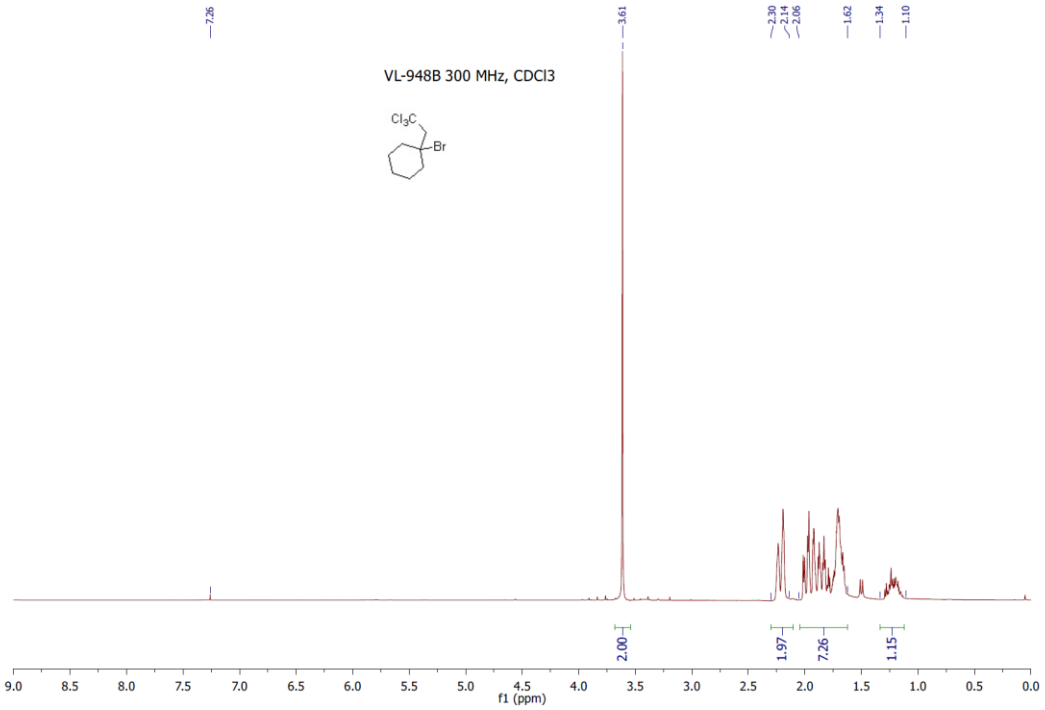
hexadecenal.M Tue Oct 13 11:15:26 2020

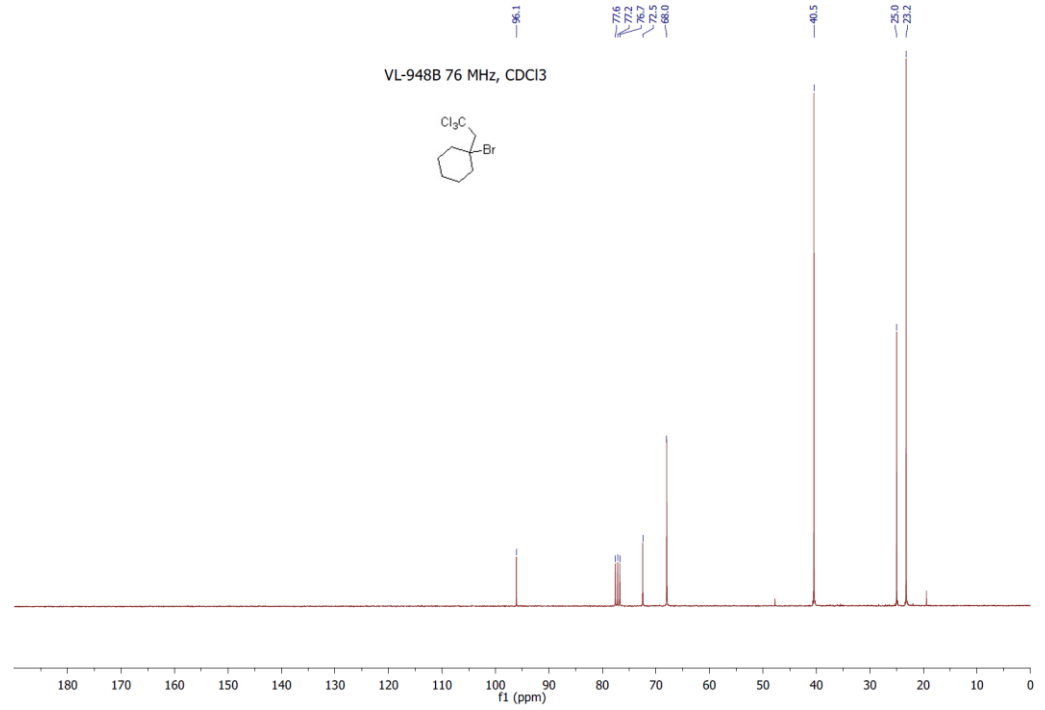
File :D:\DataMS\2017\07-2017\20-07-2017\VL950C.D
Operator : VL
Acquired : 20 Jul 2017 19:02 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL950C
Misc Info :
Vial Number: 15



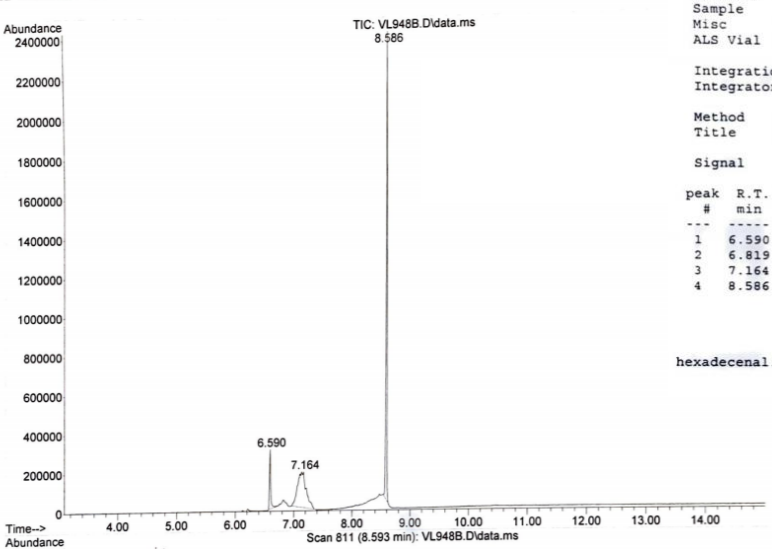


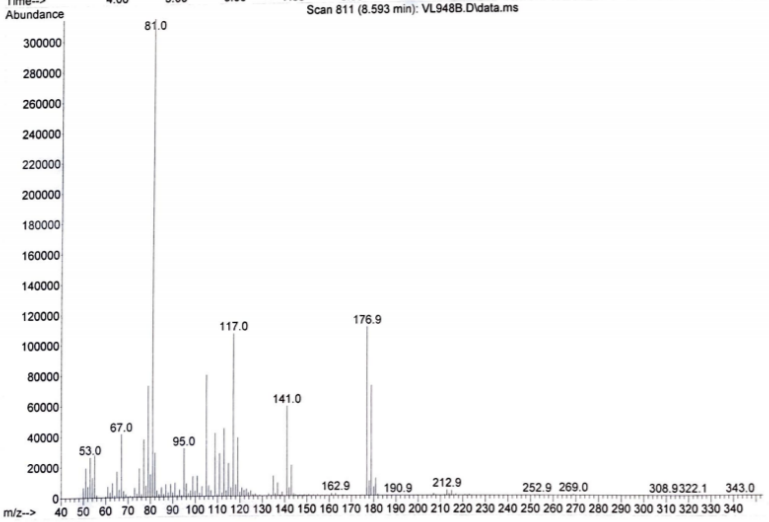
Chemical Formula: $C_8H_{12}BrCl_3$
Molecular Weight: 294,44





```
File       :D:\DataMS\2017\07-2017\20-07-2017\VL948B.D
Operator   : VL
Acquired   : 20 Jul 2017  18:44     using AcqMethod NORMAL.M
Instrument :    7890 5975
Sample Name: VL948B
Misc Info  :
Vial Number: 14
```





Area Percent Report

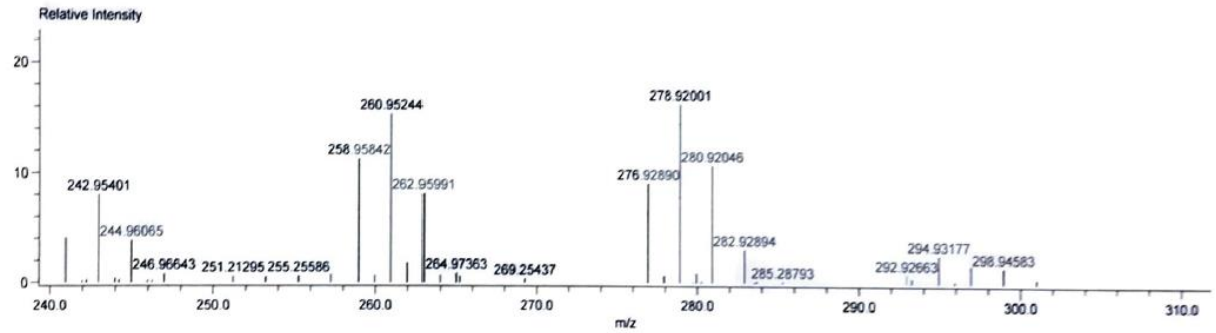
```
Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL948B.D
Acq On    : 20 Jul 2017  18:44
Operator  : VL
Sample    : VL948B
Misc      :
ALS Vial  : 14   Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method    : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title     :

Signal    : TIC: VL948B.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.590	512	516	530	M	307576	4332772	16.97%	8.592%
2	6.819	539	550	569	M3	30517	1527652	5.98%	3.029%
3	7.164	570	601	632	M2	187456	19039938	74.58%	37.755%
4	8.586	805	810	818	M	2384472	25530281	100.00%	50.625%

```
Sum of corrected areas:    50430643

hexadecenal.M Mon Oct 12 17:11:34 2020
```

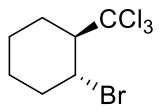
```
Data CI-200720-VL948B
Sample Name:
Description:
Ionization Mode: CI+
History: Determine m/z[Peak Detect[Centroid,30,Area],Smooth[25]],Correct Base[],Average(MS[1] 9.58 .9.59)

Charge number:1                                   Tolerance:50.00(ppm)
Element:12C:0 .. 50, 1H:0 .. 100, 79Br:1 .. 1, 35Cl:3 .. 3, 19F:0 .. 0, 14N:0 .. 0, 16O:0 .. 2
```

```
Acquired:7/20/2020 10:30:15 AM
Operator:AccuTof
Mass Calibration data:CAL-291118-CAL-EI-class4
Created:7/20/2020 3:24:36 PM
Created by:AccuTof

Unsaturation Number:-1000.0 .. 2000.0 (Fraction:Both)
```



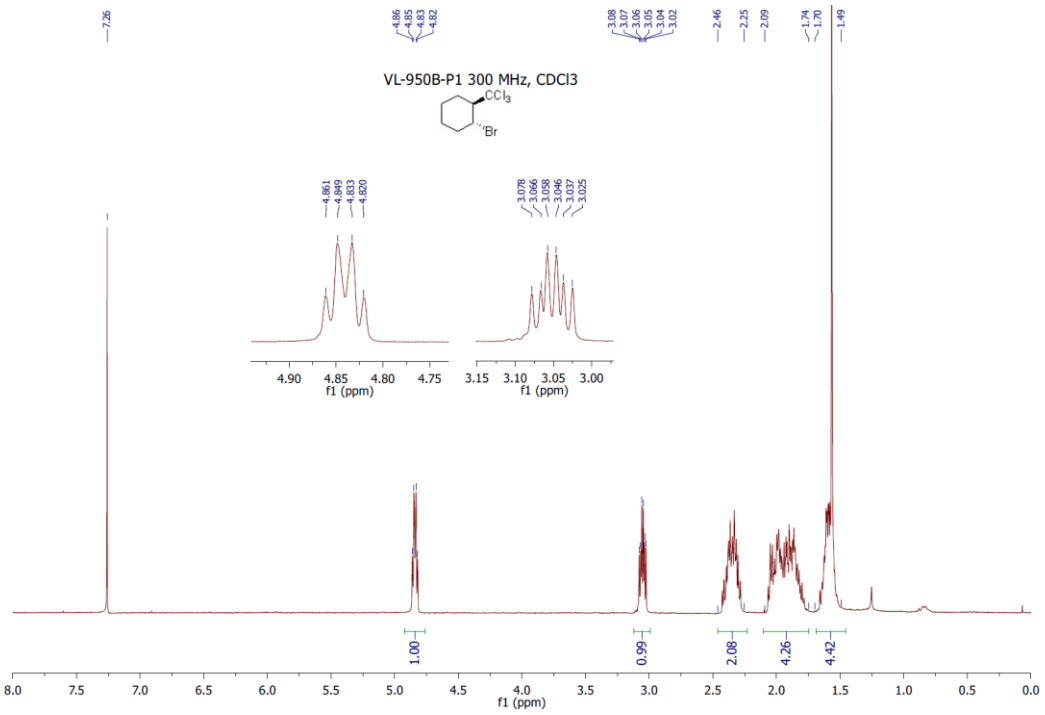
Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	Unsaturation Number
292.92663	570.67	292.92662	0.02	$^{12}C_8{}^1H_{13}{}^{79}Br_1{}^{35}Cl_3$	0.5

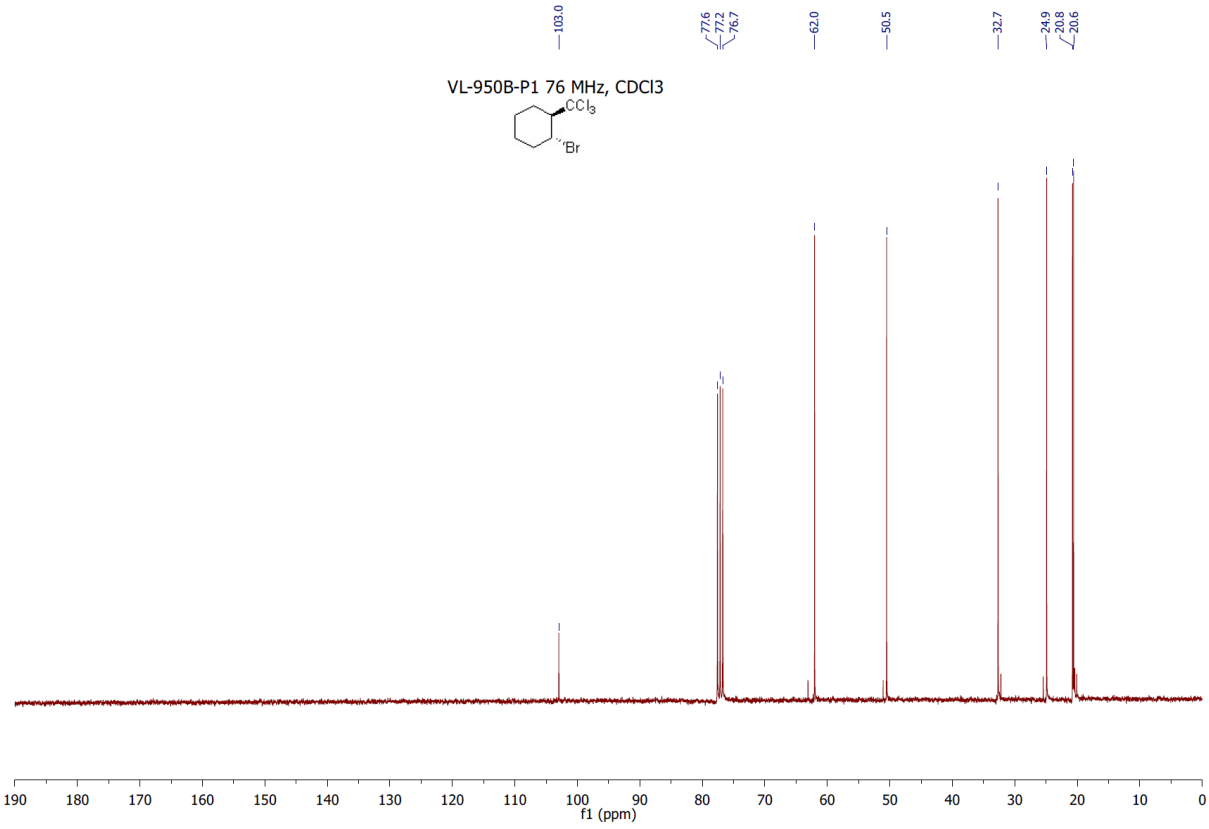
CCl3



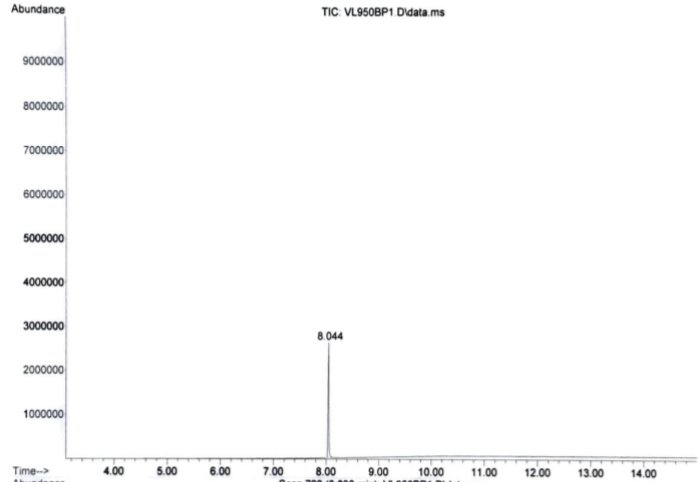
Chemical Formula: $C_7H_{10}BrCl_3$

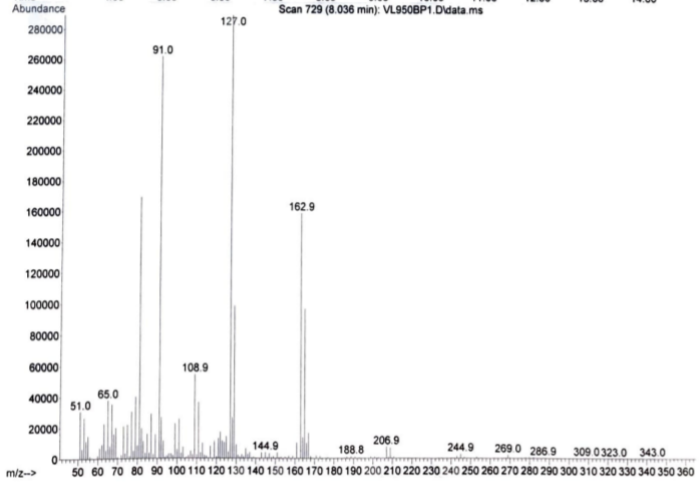
Molecular Weight: 280,41




103.0
77.6
77.2
76.7
62.0
50.5
32.7
24.9
20.8
20.6
VL-950B-P1 76 MHz, CDCl3
CCl3
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

File :D:\DataMS\2017\08-2017\25082017\VL950BP1.D
Operator : VL
Acquired : 25 Aug 2017 15:12 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL950BP1
Misc Info :
Vial Number: 14





Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL950BP1.D
Acq On : 25 Aug 2017 15:12
Operator : VL
Sample : VL950BP1
Misc :
ALS Vial : 14 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

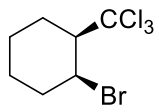
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL950BP1.D\data.ms

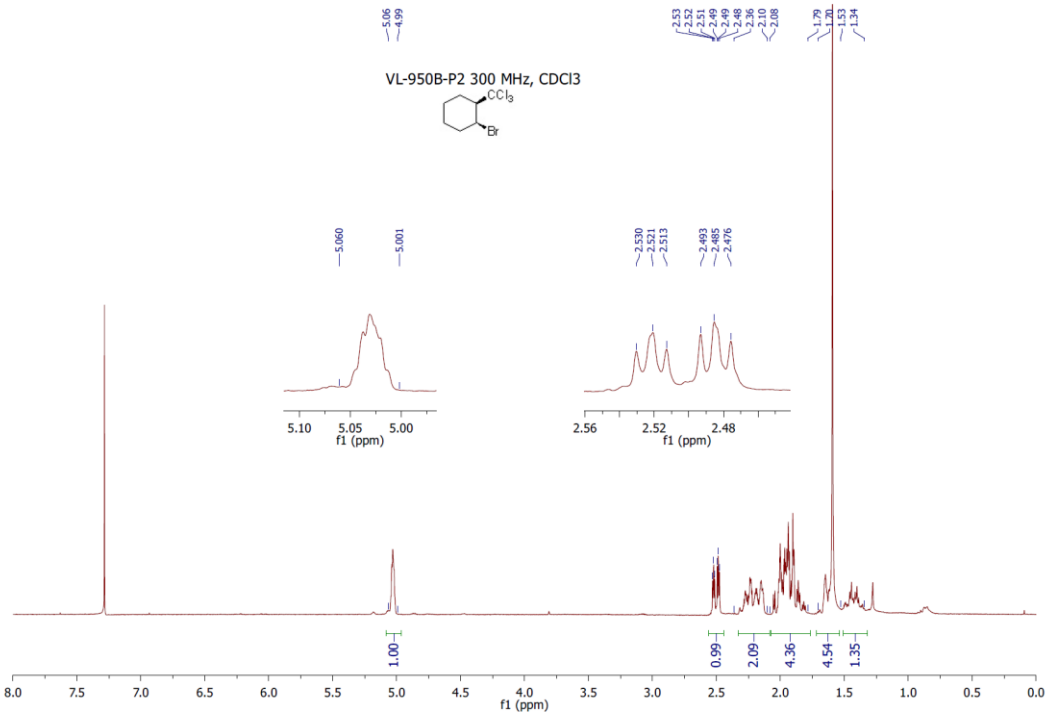
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.281	613	618	624	M5	8014	140883	0.45%	0.450%
2	8.041	725	730	756	M	2663143	31144299	100.00%	99.550%

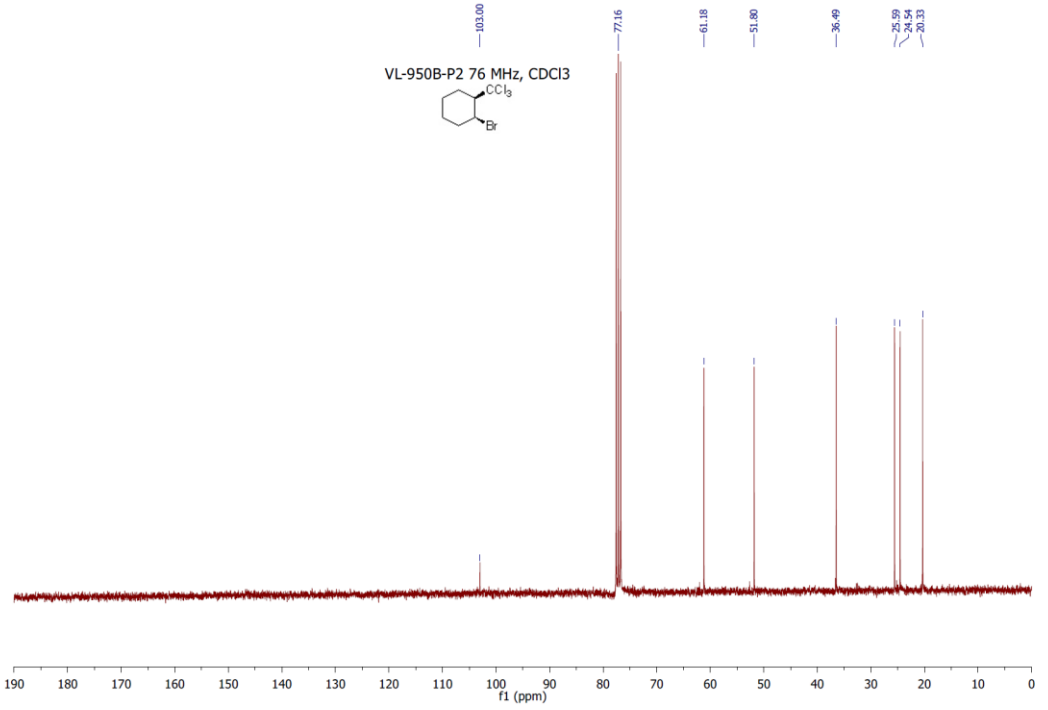
Sum of corrected areas: 31285183

hexadecenal.M Mon Oct 12 17:00:19 2020

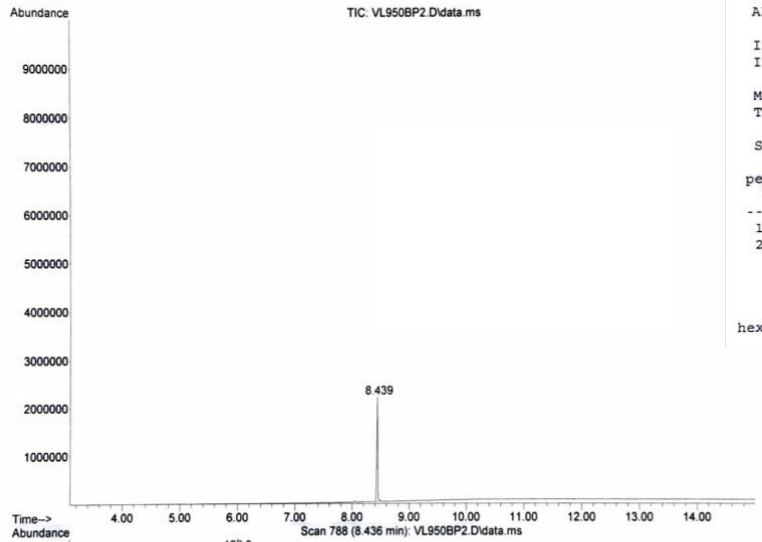


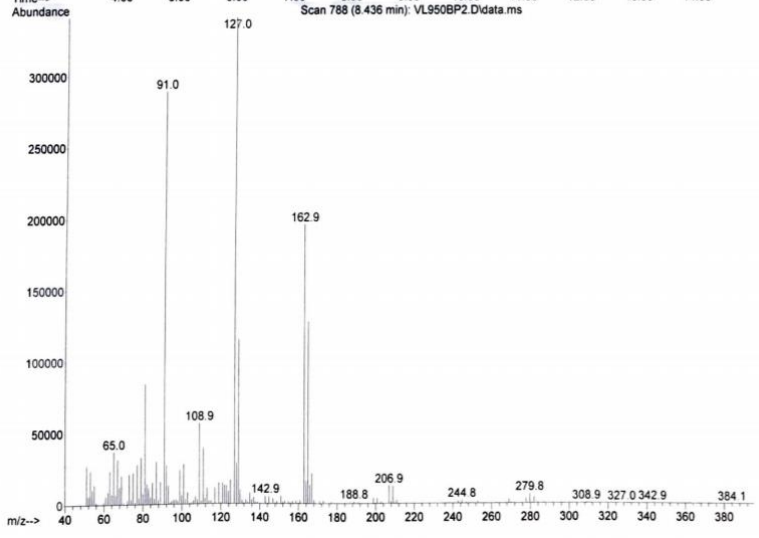
Chemical Formula: $C_7H_{10}BrCl_3$
Molecular Weight: 280,41





File :D:\DataMS\2017\08-2017\25082017\VL950BP2.D
Operator : VL
Acquired : 25 Aug 2017 14:54 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL950BP2
Misc Info :
Vial Number: 13





Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL950BP2.D
Acq On : 25 Aug 2017 14:54
Operator : VL
Sample : VL950BP2
Misc :
ALS Vial : 13 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

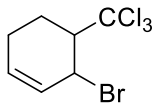
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL950BP2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.049	728	731	735	M	31593	389598	1.55%	1.522%
2	8.436	784	788	802	M	2184454	25204725	100.00%	98.478%

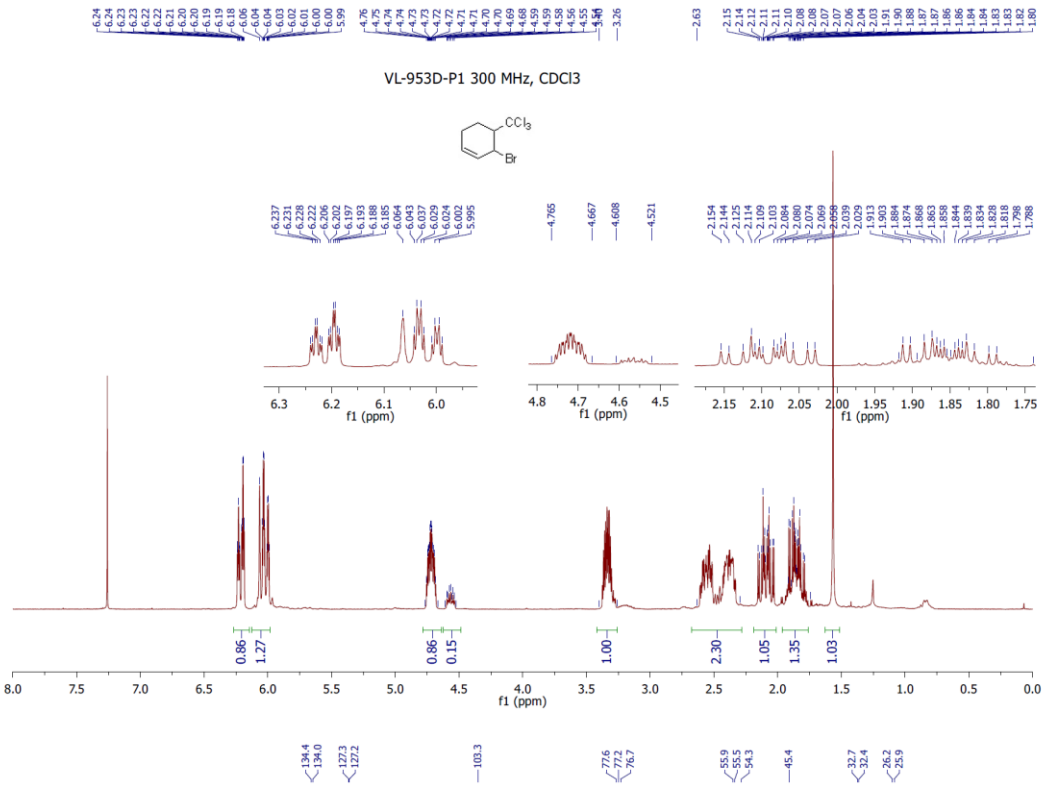
Sum of corrected areas: 25594323

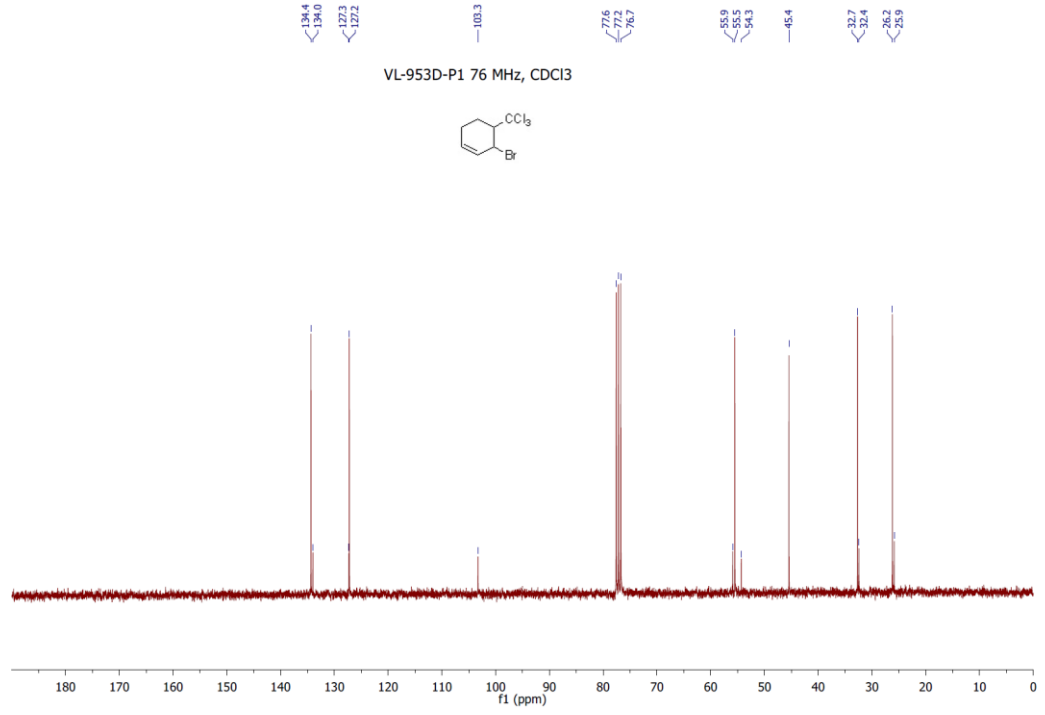
hexadecenal.M Mon Oct 12 16:59:44 2020



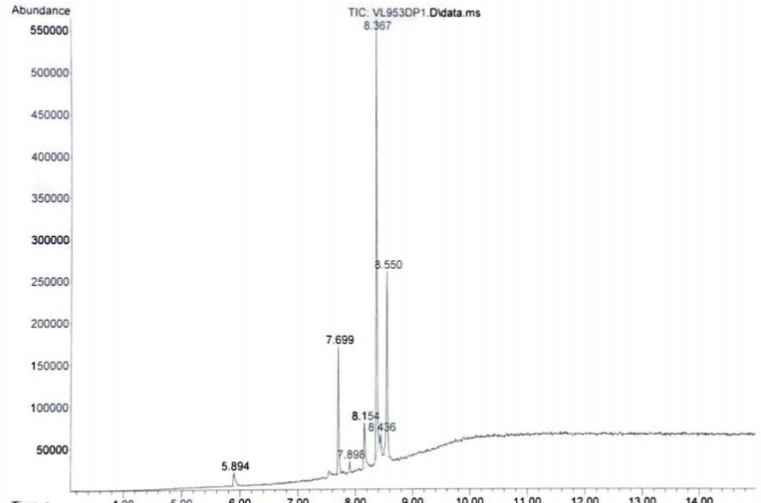
Chemical Formula: $C_7H_8BrCl_3$

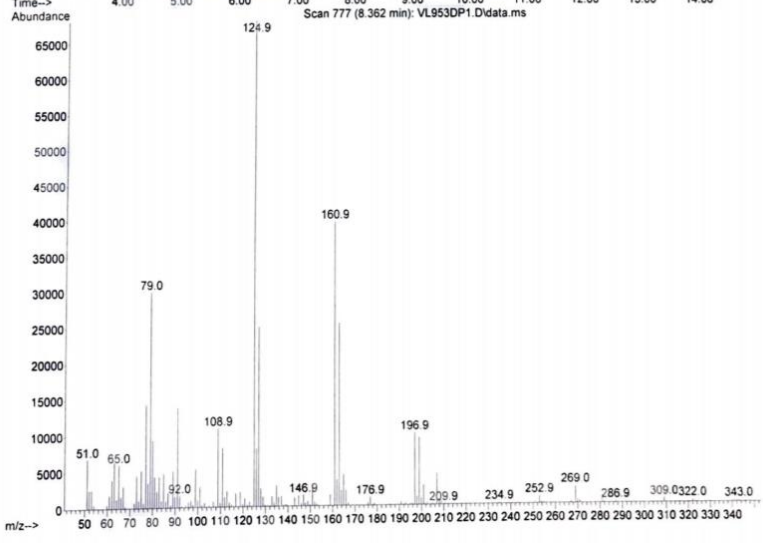
Molecular Weight: 278,40





File :D:\DataMS\2017\08-2017\25082017\VL953DP1.D
Operator : VL
Acquired : 25 Aug 2017 17:21 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL953DP1
Misc Info :
Vial Number: 21





Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL953DP1.D
Acq On : 25 Aug 2017 17:21
Operator : VL
Sample : VL953DP1
Misc :
ALS Vial : 21 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

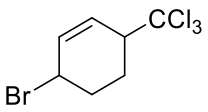
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL953DP1.D\data.ms

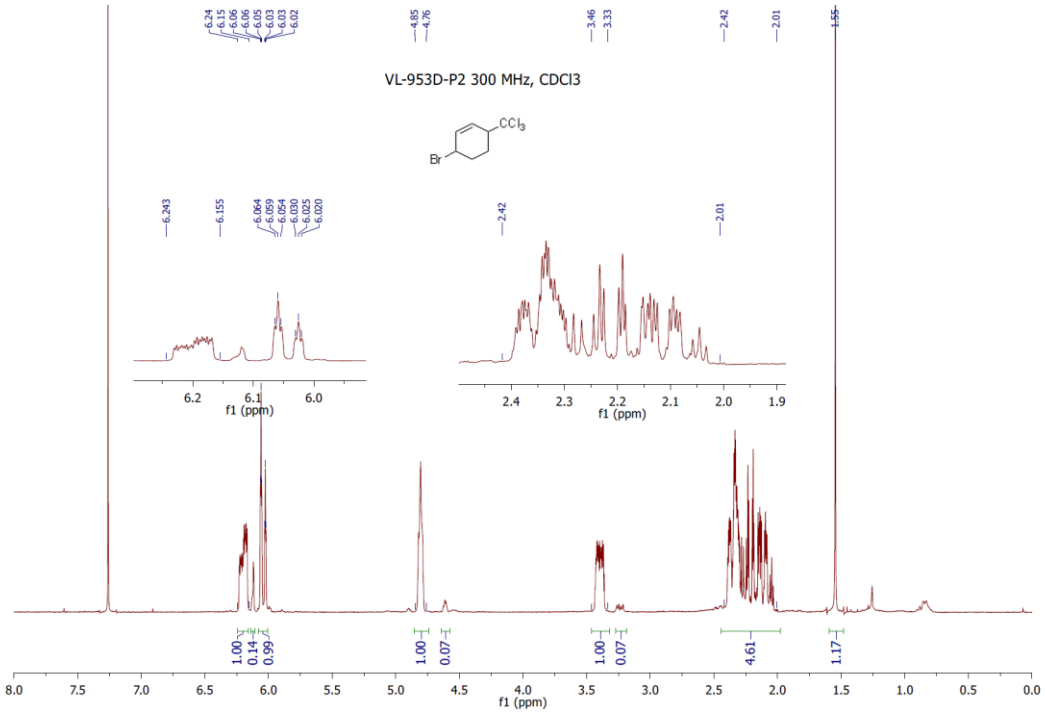
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.894	410	414	430	M	15620	392649	6.29%	2.955%
2	7.699	676	679	688	M	158023	1954009	31.32%	14.707%
3	7.898	705	709	714	M2	12979	148611	2.38%	1.119%
4	8.154	742	746	760	M2	56103	1084410	17.38%	8.162%
5	8.367	773	778	785	M	527437	6238759	100.00%	46.955%
6	8.436	786	788	794	M4	13710	125477	2.01%	0.944%
7	8.550	796	805	816	M	227107	3342657	53.58%	25.158%

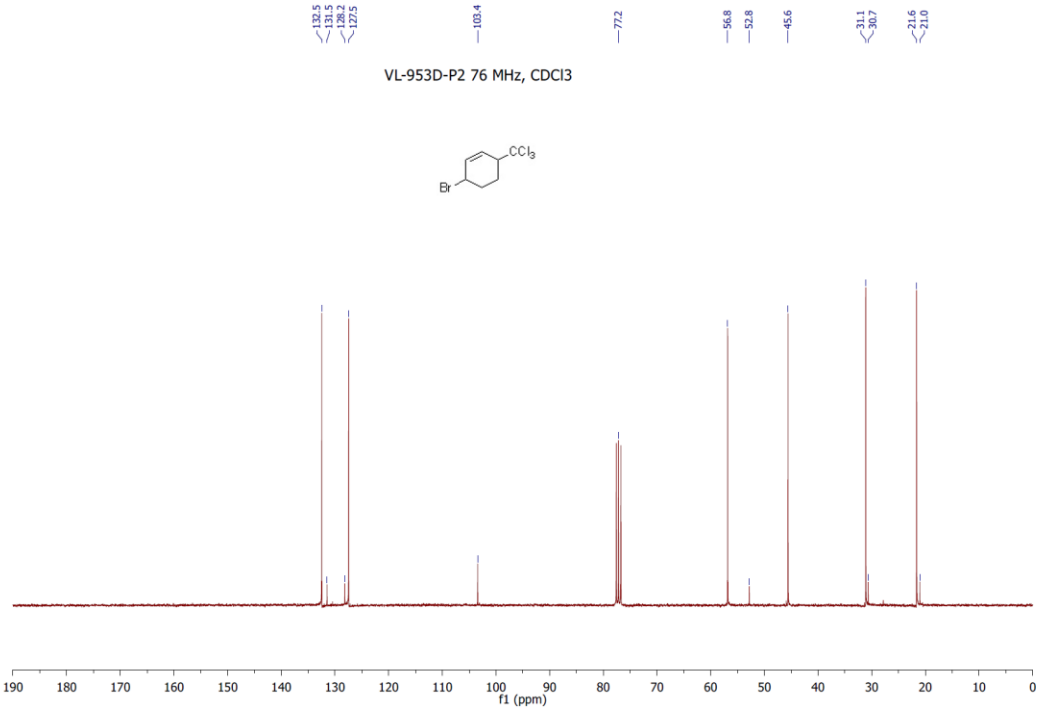
Sum of corrected areas: 13286572

hexadecenal.M Mon Oct 12 16:58:07 2020

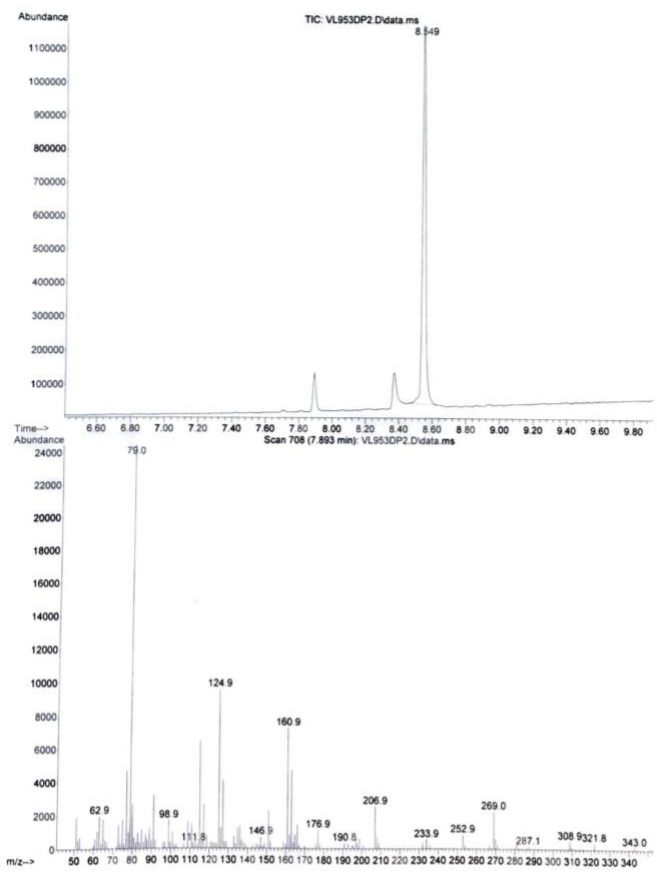


Chemical Formula: $C_7H_8BrCl_3$
Molecular Weight: 278,40





File :D:\DataMS\2017\08-2017\25082017\VL953DP2.D
Operator : VL
Acquired : 25 Aug 2017 17:03 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL953DP2
Misc Info :
Vial Number: 20



Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL953DP2.D
Acq On : 25 Aug 2017 17:03
Operator : VL
Sample : VL953DP2
Misc :
ALS Vial : 20 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

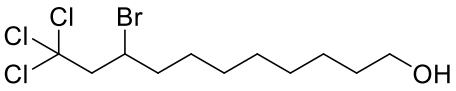
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL953DP2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.893	704	708	713	M	116687	1389076	9.16%	7.553%
2	8.373	775	779	791	M	105268	1838245	12.12%	9.995%
3	8.546	800	804	815	M	1262993	15163731	100.00%	82.452%

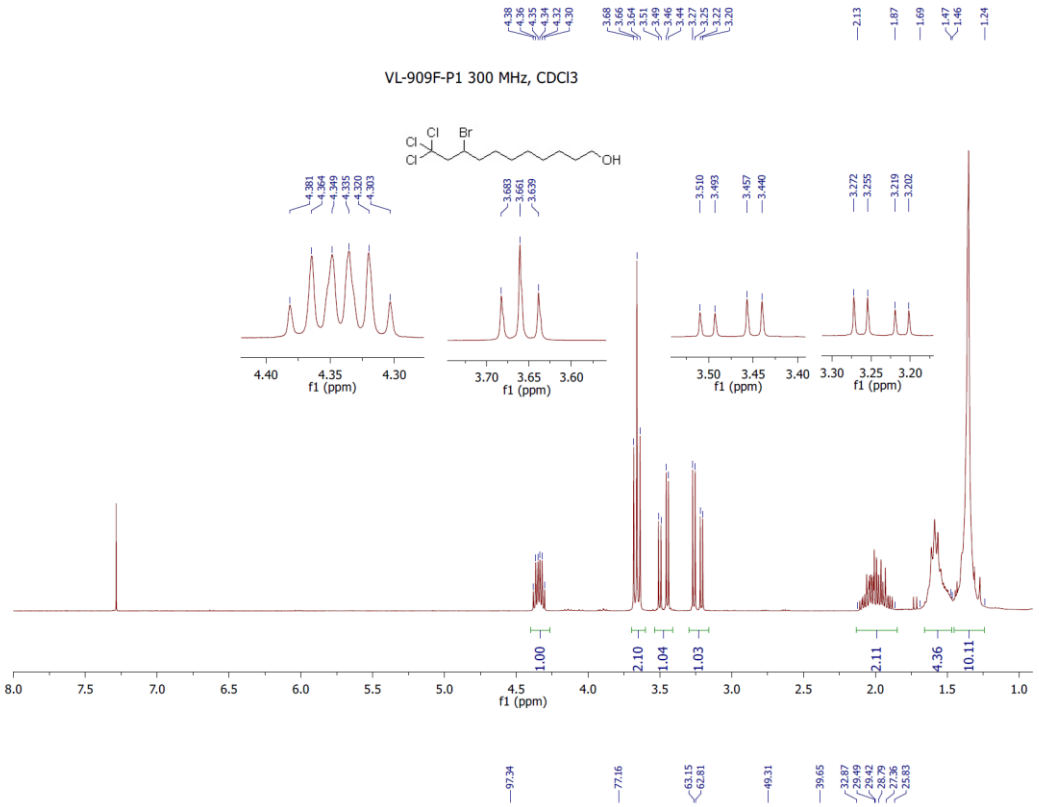
Sum of corrected areas: 18391053

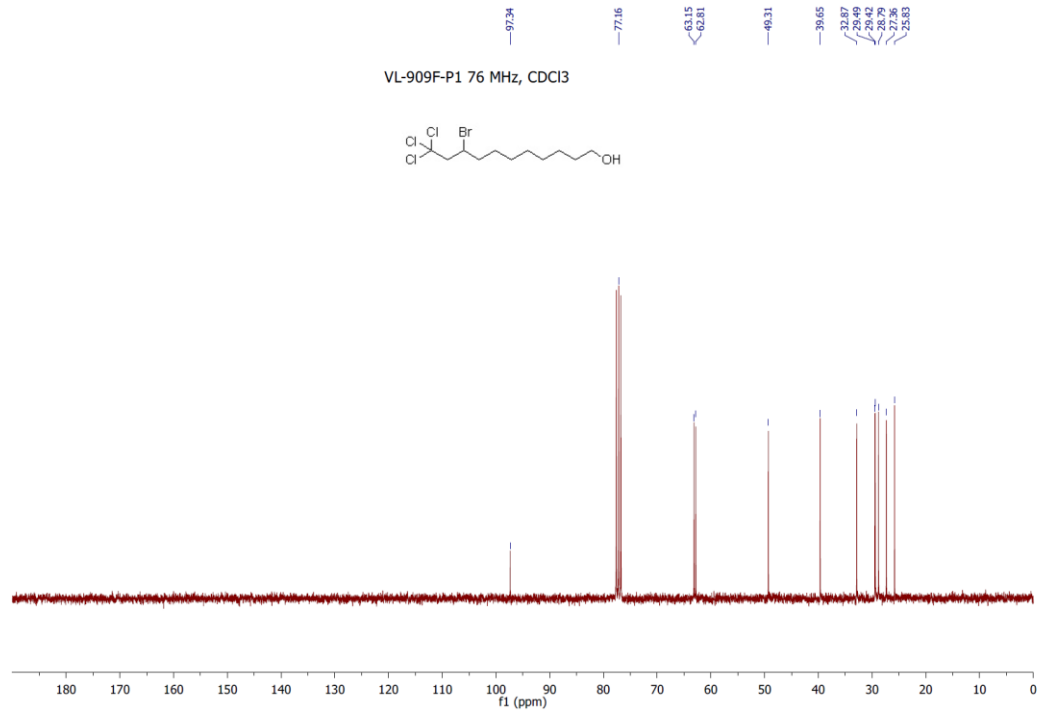
hexadecenal.M Mon Oct 12 16:57:09 2020



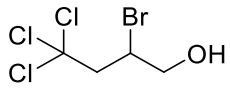
Chemical Formula: $C_{11}H_{20}BrCl_3O$

Molecular Weight: 354,53

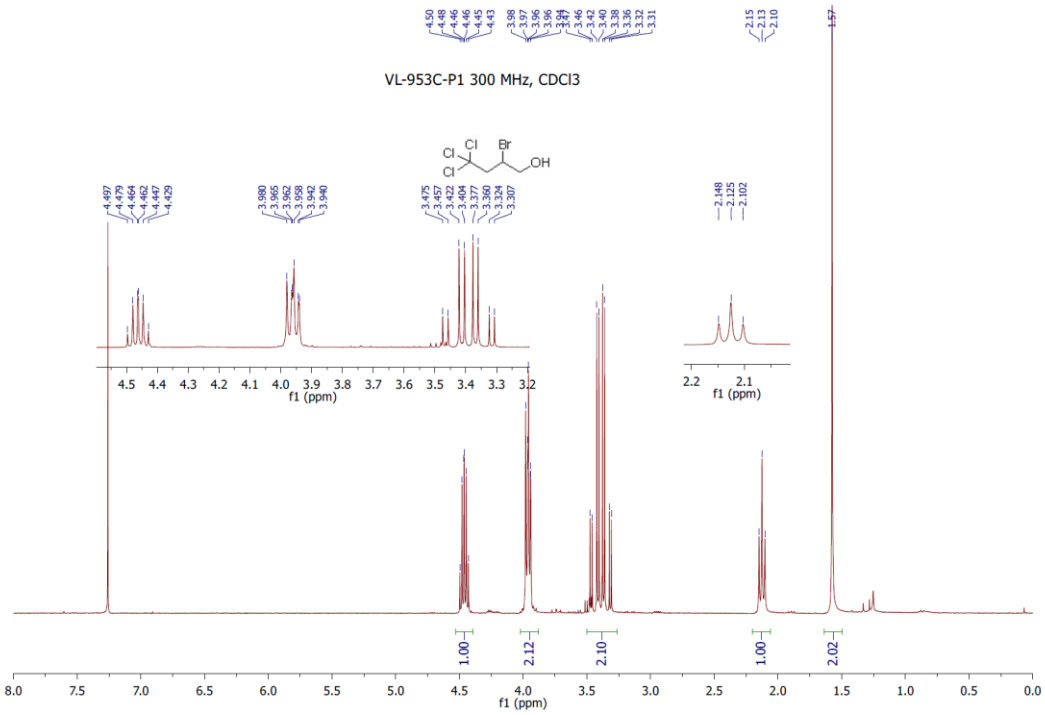


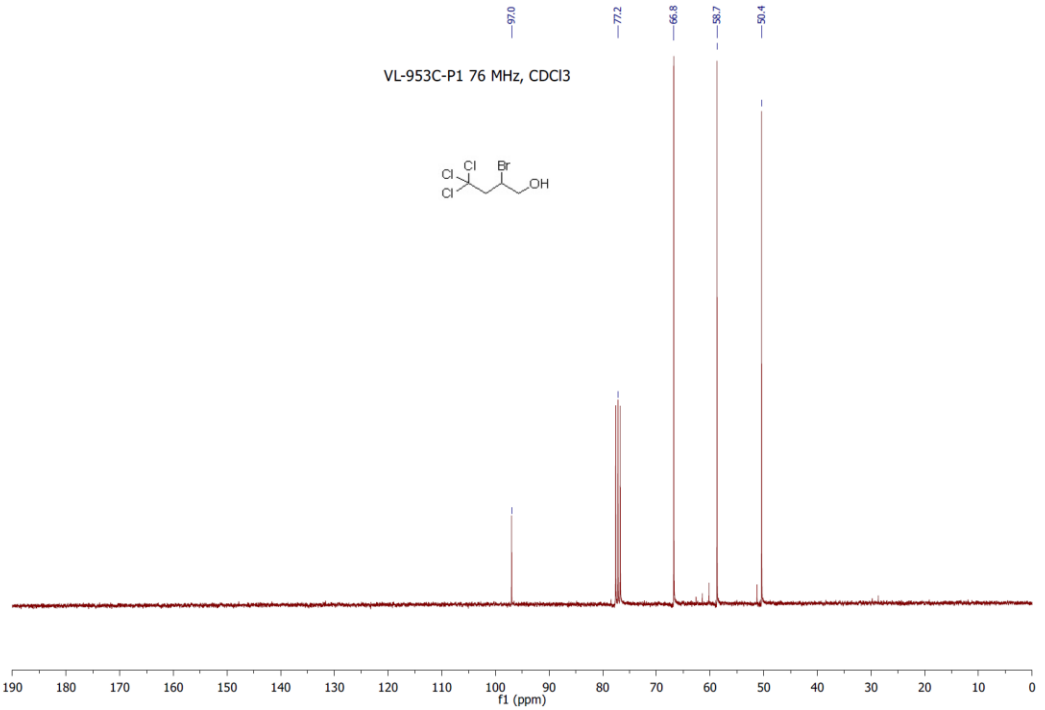


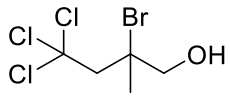
HRMS



Chemical Formula: $C_4H_6BrCl_3O$
Molecular Weight: 256,35

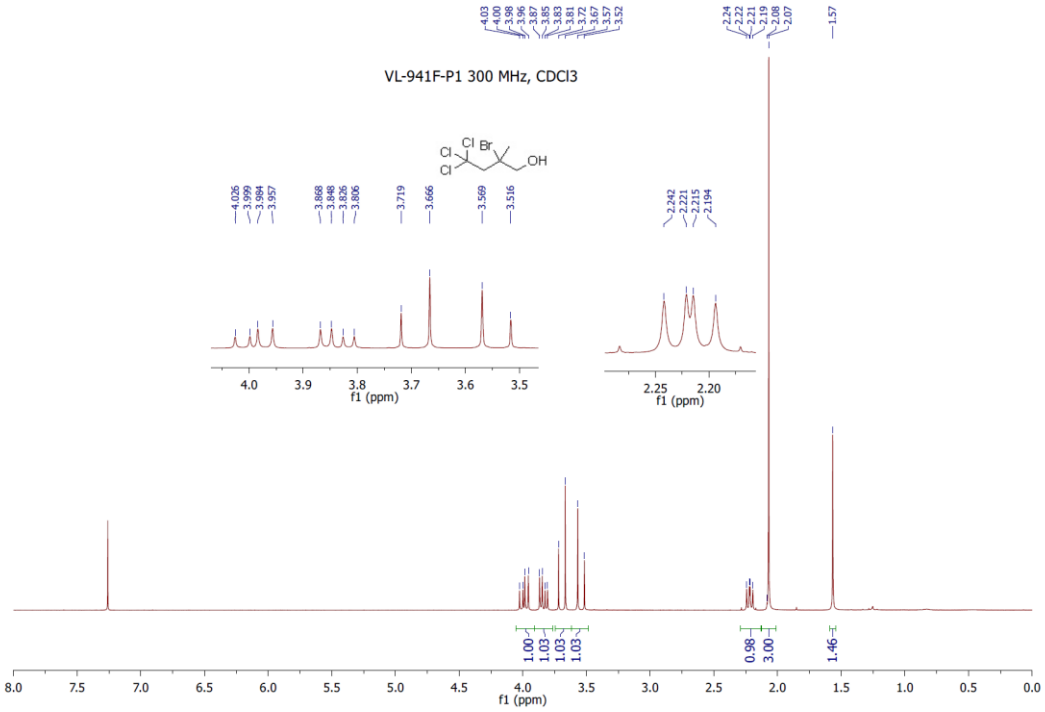


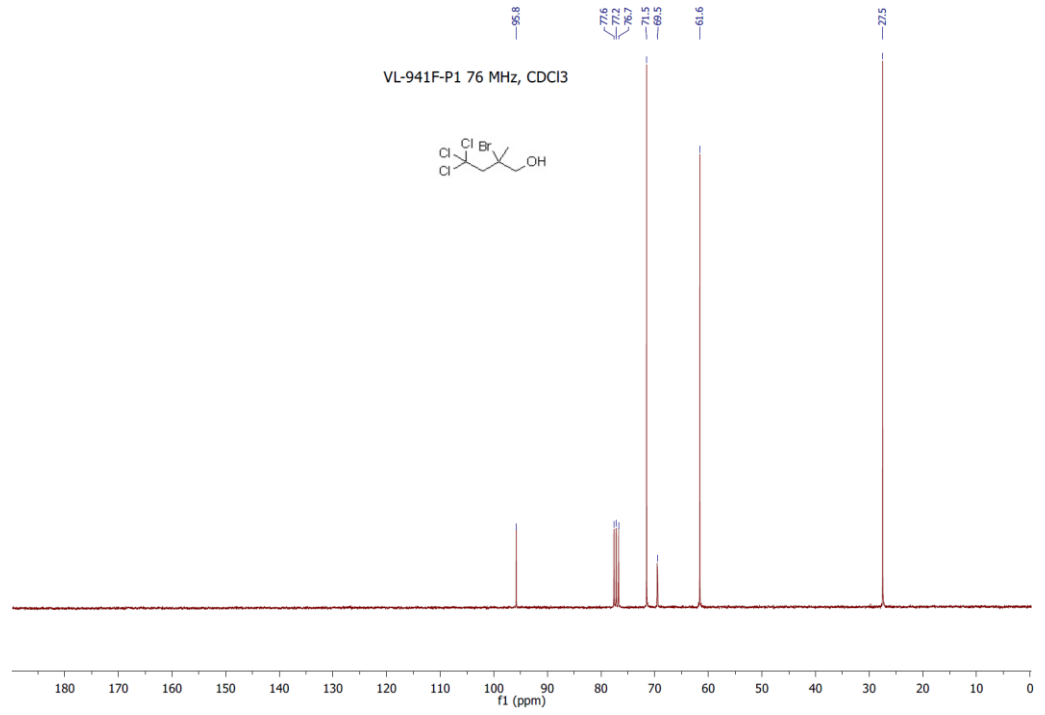




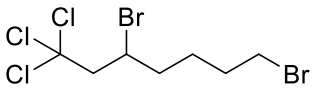
Chemical Formula: $C_5H_8BrCl_3O$

Molecular Weight: 270,37



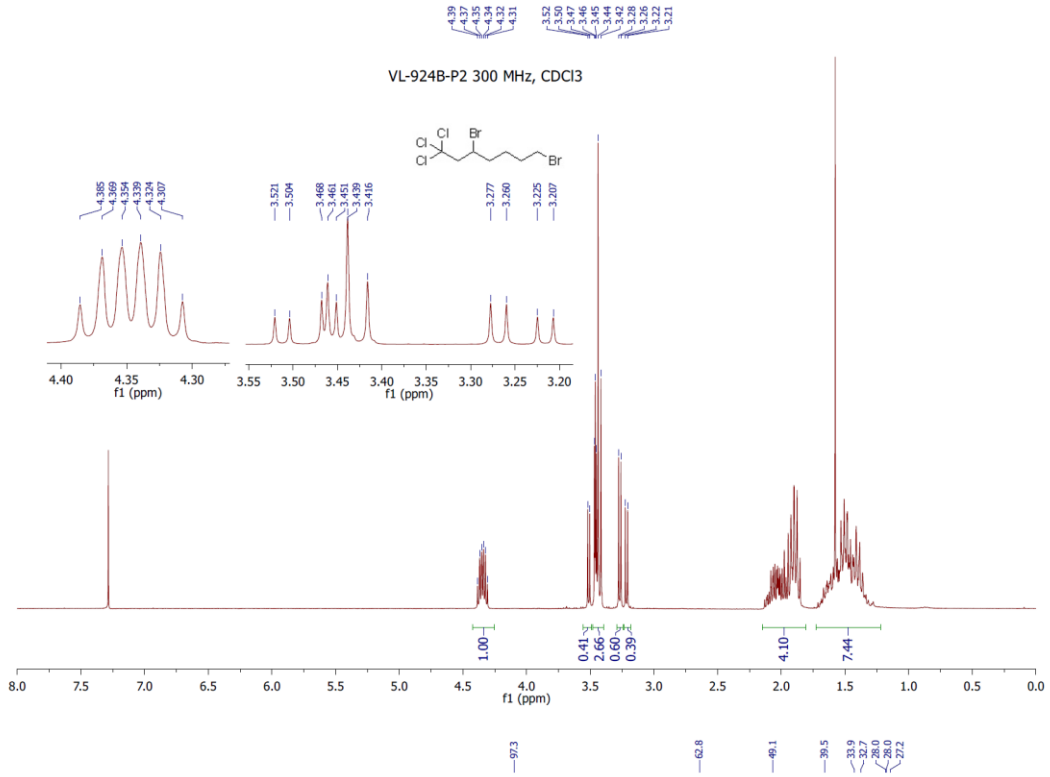


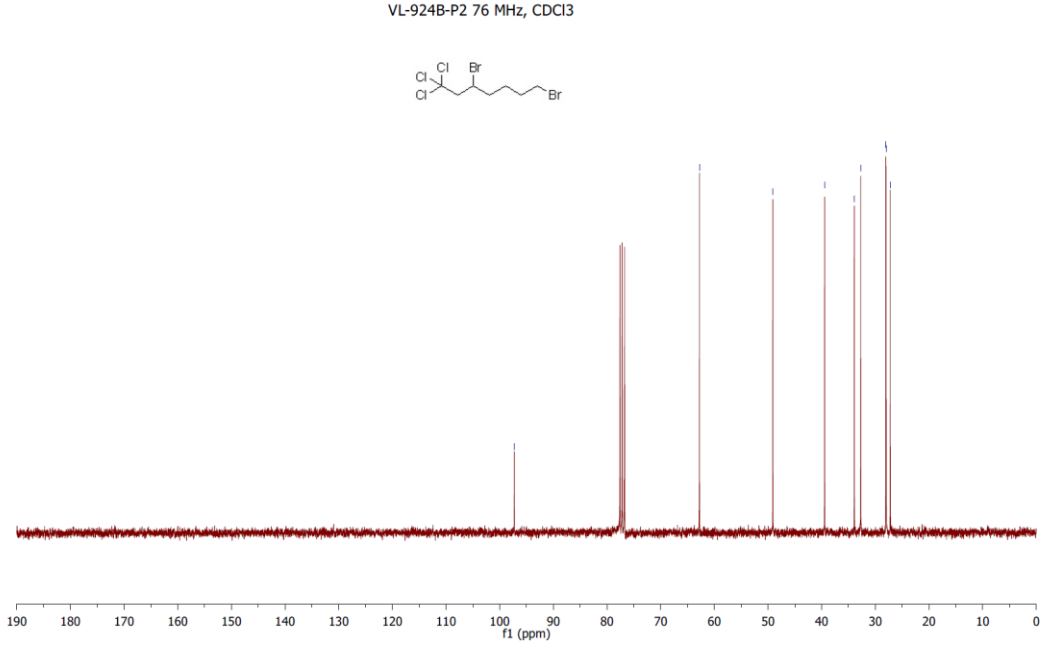
HRMS

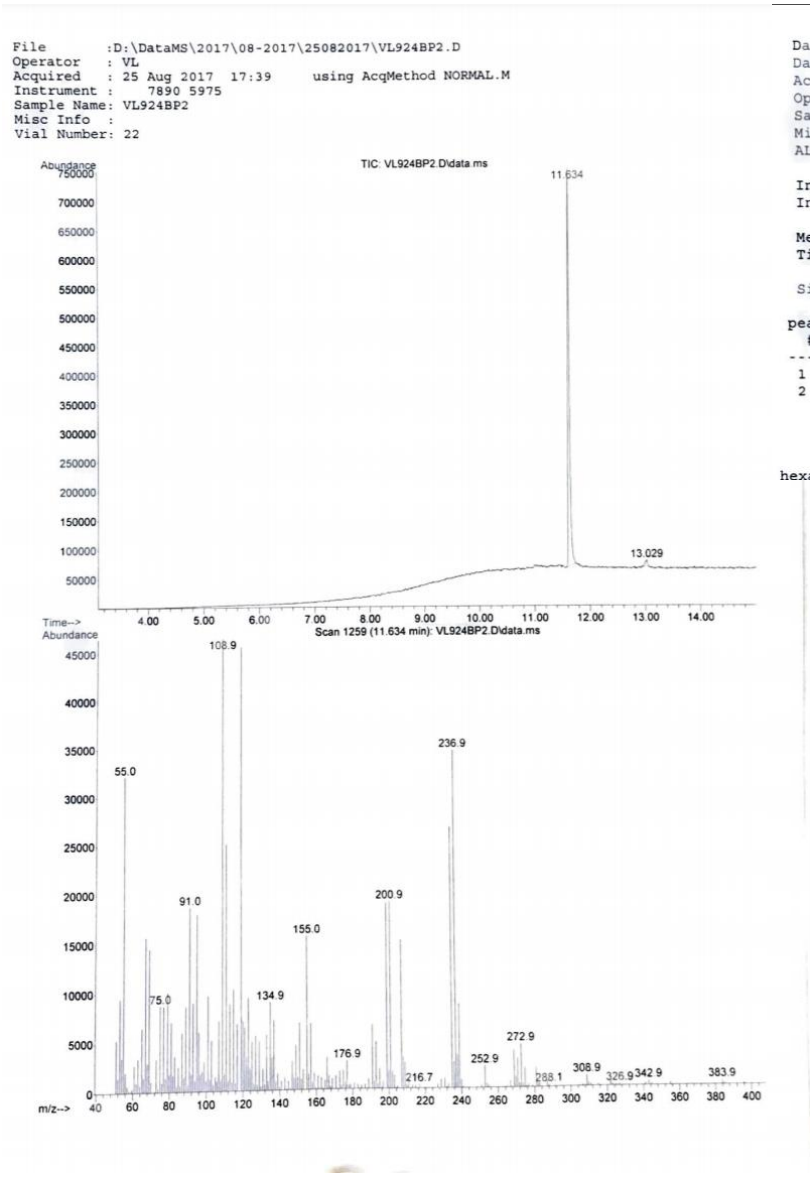


Chemical Formula: $C_7H_{11}Br_2Cl_3$

Molecular Weight: 361,32







Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL924BP2.D
Acq On : 25 Aug 2017 17:39
Operator : VL
Sample : VL924BP2
Misc :
ALS Vial : 22 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

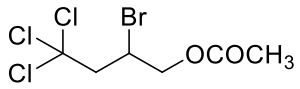
Signal : TIC: VL924BP2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	11.634	1252	1259	1279	M	685219	14476579	100.00%	97.743%
2	13.029	1453	1465	1469	M	11846	334290	2.31%	2.257%

Sum of corrected areas: 14810869

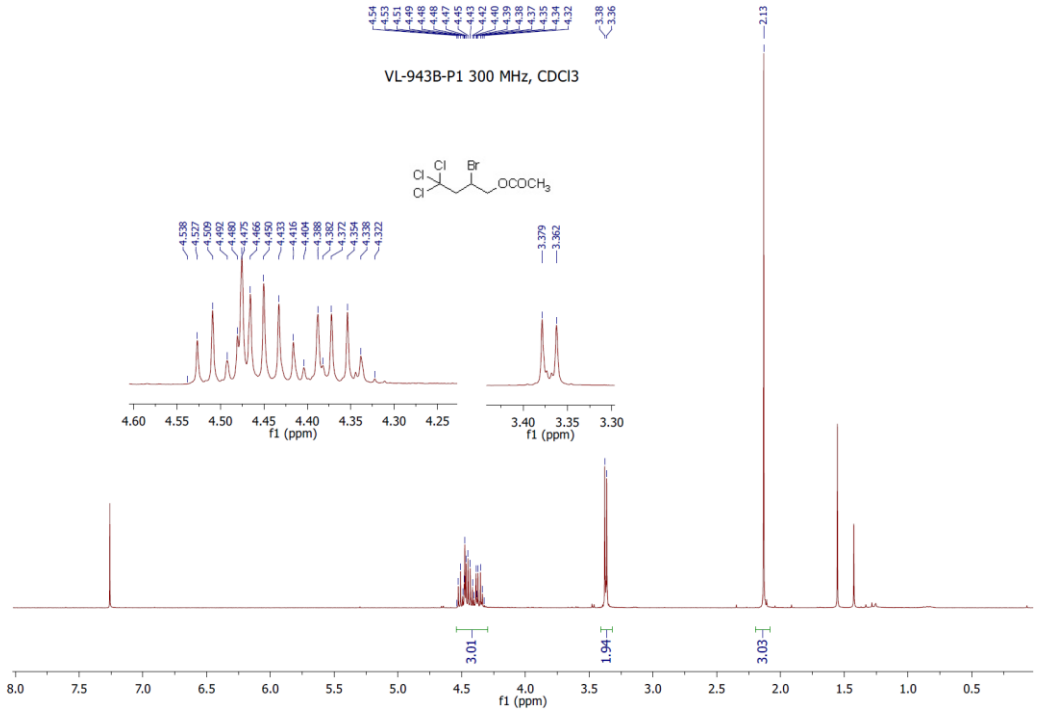
hexadecenal.M Mon Oct 12 16:54:26 2020

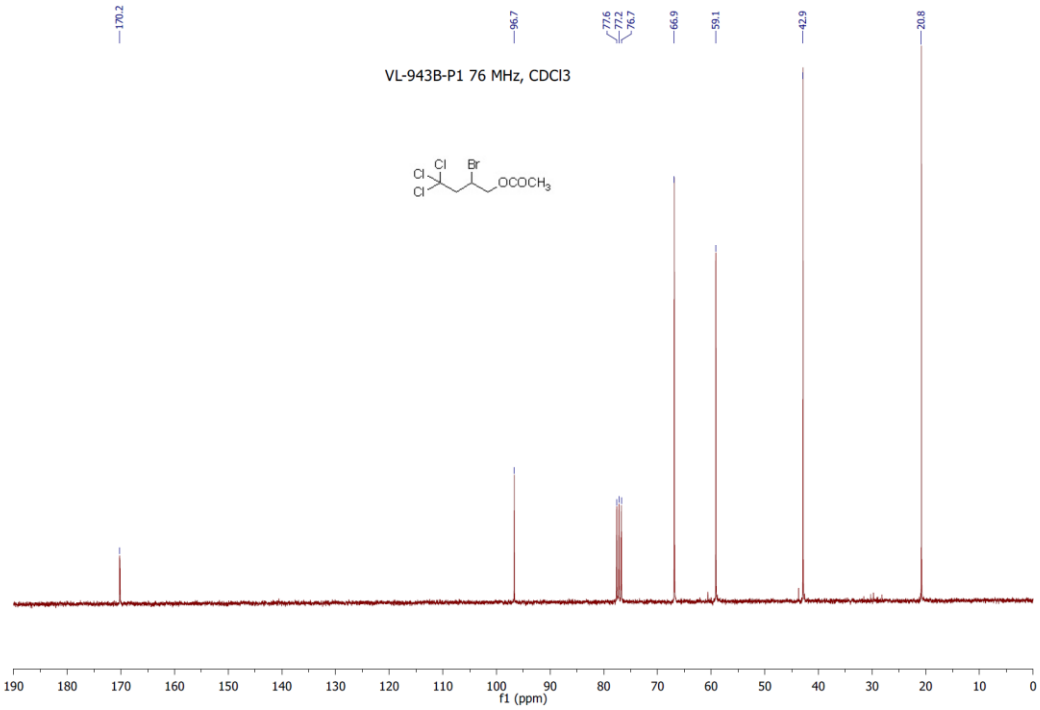
HRMS



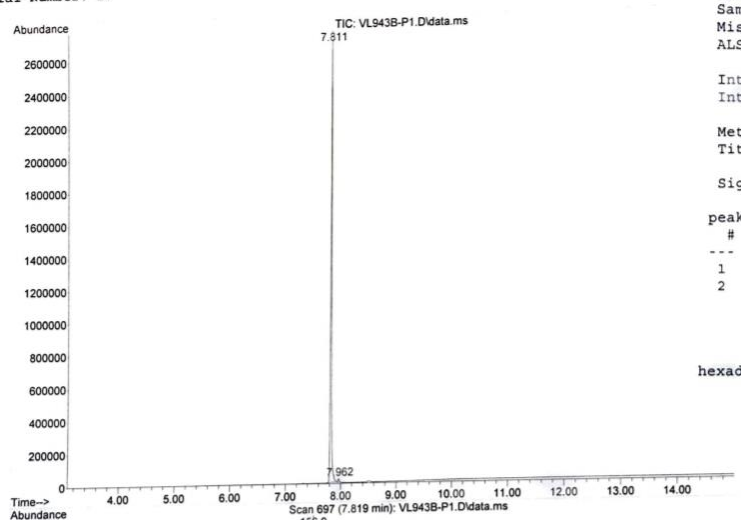
Chemical Formula: $C_6H_8BrCl_3O_2$

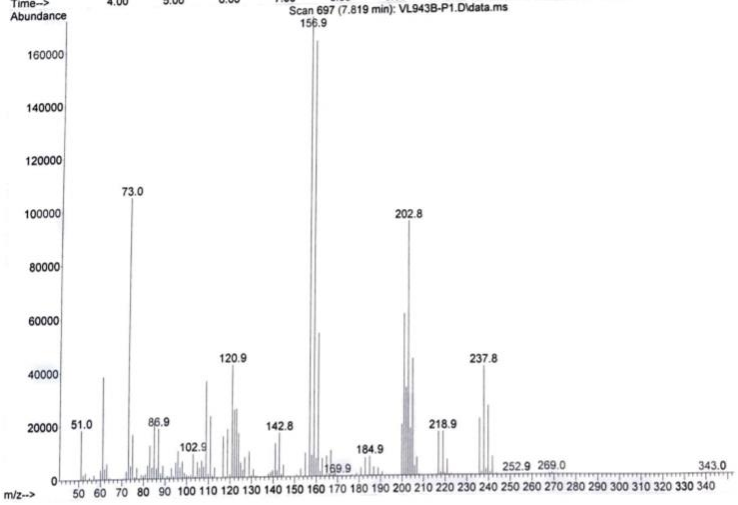
Molecular Weight: 298,38





File :D:\DataMS\2017\07-2017\20-07-2017\VL943B-P1.D
Operator : VL
Acquired : 20 Jul 2017 19:39 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL943B-P1
Misc Info :
Vial Number: 17





Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL943B-P1.D
Acq On : 20 Jul 2017 19:39
Operator : VL
Sample : VL943B-P1
Misc :
ALS Vial : 17 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

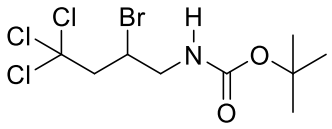
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL943B-P1.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.811	691	696	711	M	2783608	34494690	100.00%	99.295%
2	7.962	715	718	721	M2	20191	244945	0.71%	0.705%

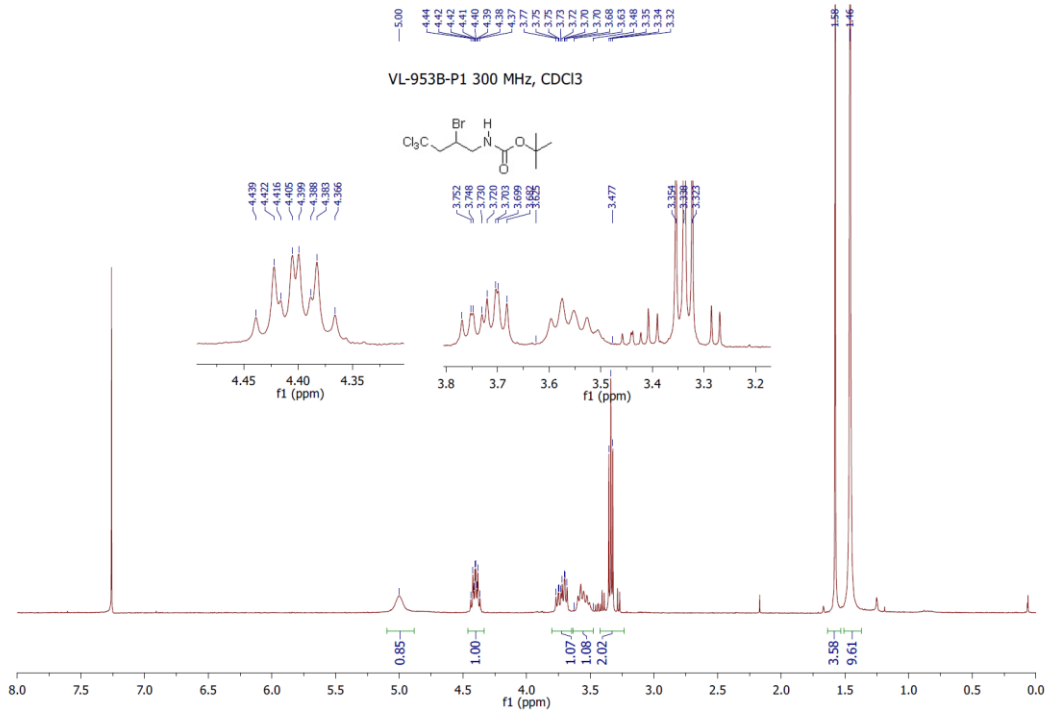
Sum of corrected areas: 34739635

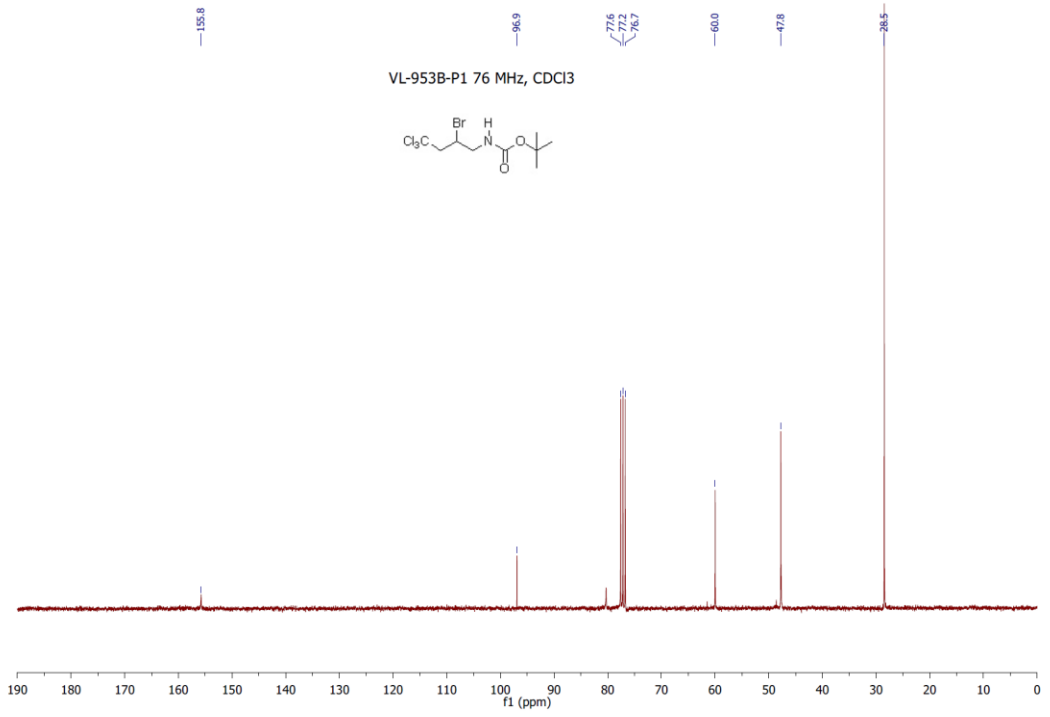
hexadecenal.M Mon Oct 12 17:09:49 2020



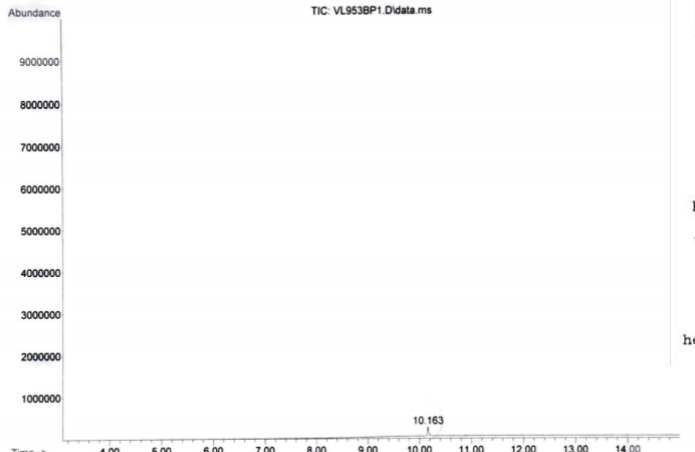
Chemical Formula: $C_9H_{15}BrCl_3NO_2$

Molecular Weight: 355,48





```
File       :D:\DataMS\2017\08-2017\25082017\VL953BP1.D
Operator   : VL
Acquired   : 25 Aug 2017  17:58     using AcqMethod NORMAL.M
Instrument :
    7890 5975
Sample Name: VL953BP1
Misc Info  :
Vial Number: 23
```



Area Percent Report

```
Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL953BP1.D
Acq On    : 25 Aug 2017  17:58
Operator  : VL
Sample    : VL953BP1
Misc      :
ALS Vial  : 23   Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method    : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title     :

Signal    : TIC: VL953BP1.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.160	1036	1042	1055	M	223039	3692113	100.00%	100.000%

Sum of corrected areas: 3692113

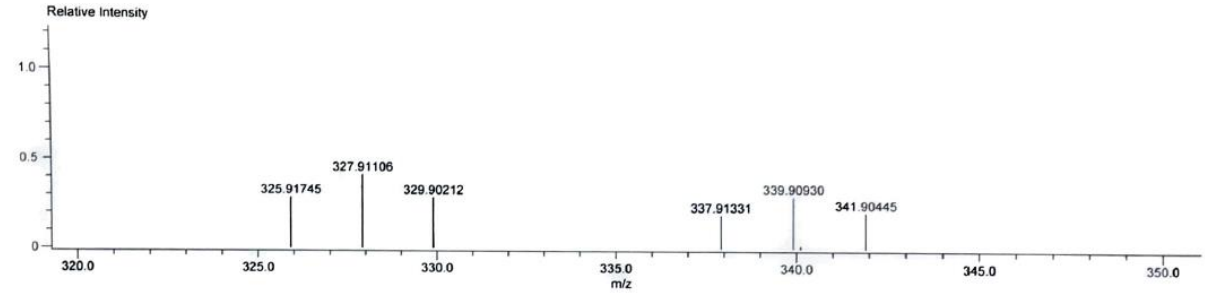
hexadecenal.M Mon Oct 12 17:12:28 2020

Data:CI-240620-VL953BP
Sample Name:
Description:
Ionization Mode:CI+
History:Determine m/z[Peak Detect[Centroid,30,Area]];Correct Base[];Average(MS[1] 10.62..10.66)

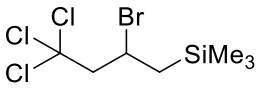
Acquired:6/24/2020 2:05:32 PM
Operator:AccuTof
Mass Calibration data:CAL-291118-CAL-EI-class4
Created:6/24/2020 5:43:27 PM
Created by:AccuTof

Charge number:1
Element:^{12}C:0 .. 50, ^{1}H:0 .. 100, ^{81}Br:1 .. 1, ^{35}Cl:3 .. 3, ^{14}N:1 .. 1, ^{16}O:0 .. 2
Tolerance:50.00(ppm)

Unsaturation Number:-1000.0 .. 2000.0 (Fraction:Both)

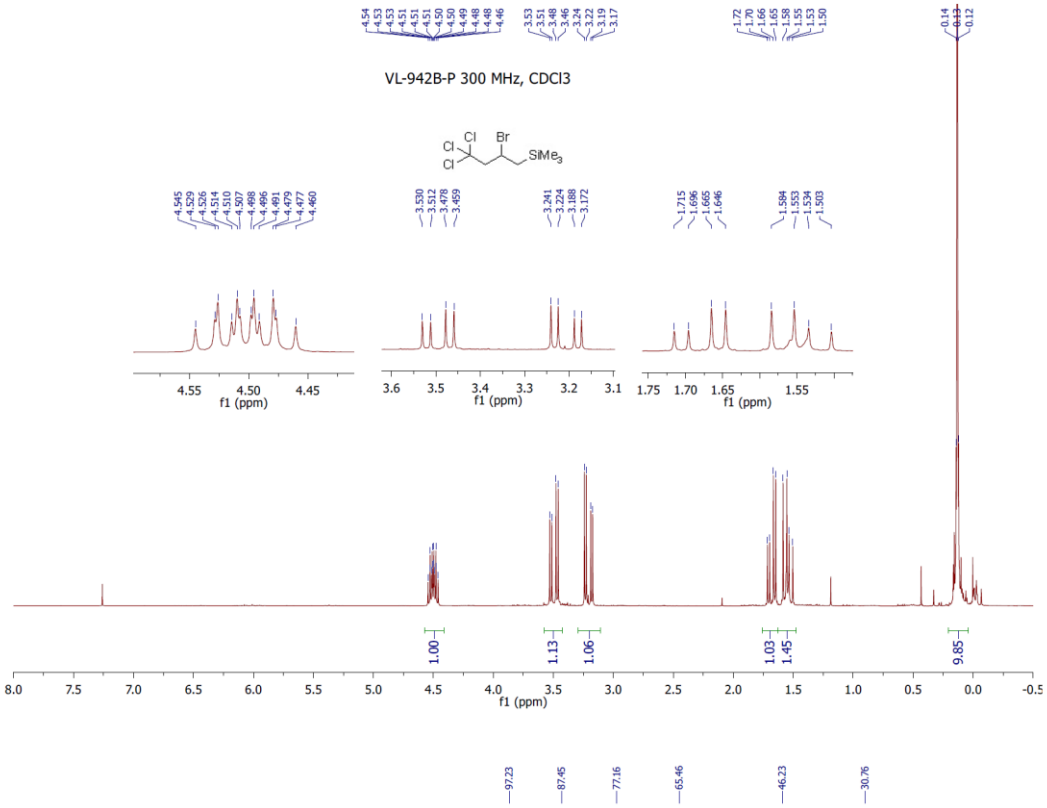


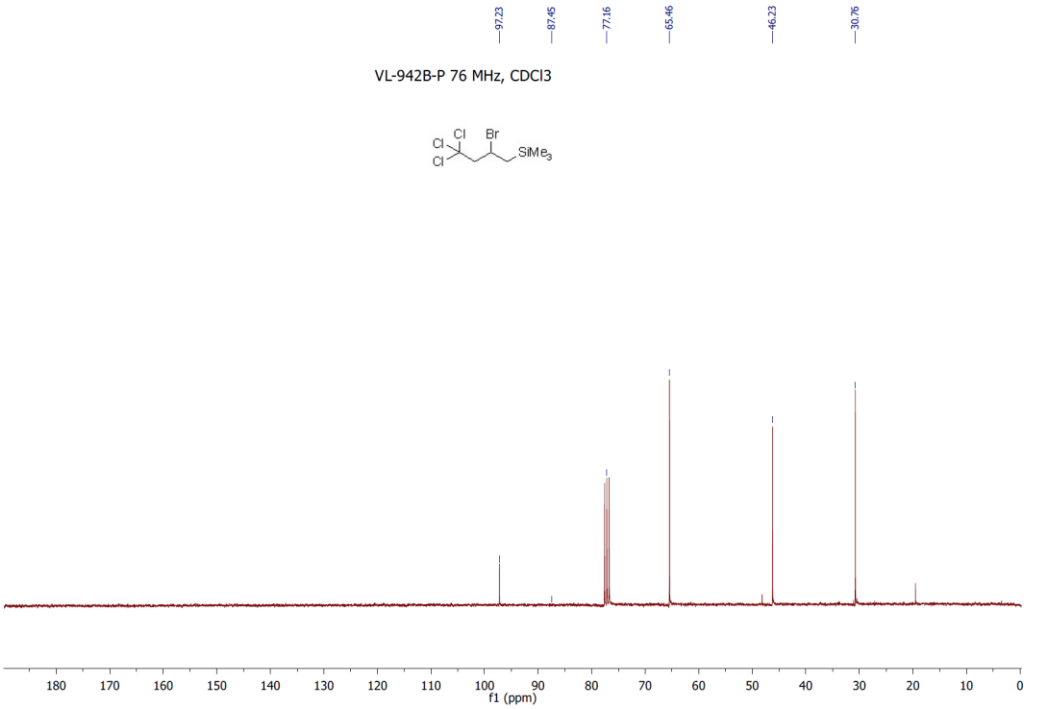
Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	Unsaturation Number
339.90930	666.56	339.90965	-1.03	$^{12}C_8{}^{1}H_{12}{}^{81}Br_1{}^{35}Cl_3{}^{14}N_1{}^{16}O_2$	1.5

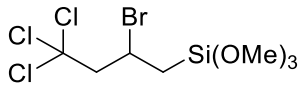


Chemical Formula: $C_7H_{14}BrCl_3Si$

Molecular Weight: 312,53

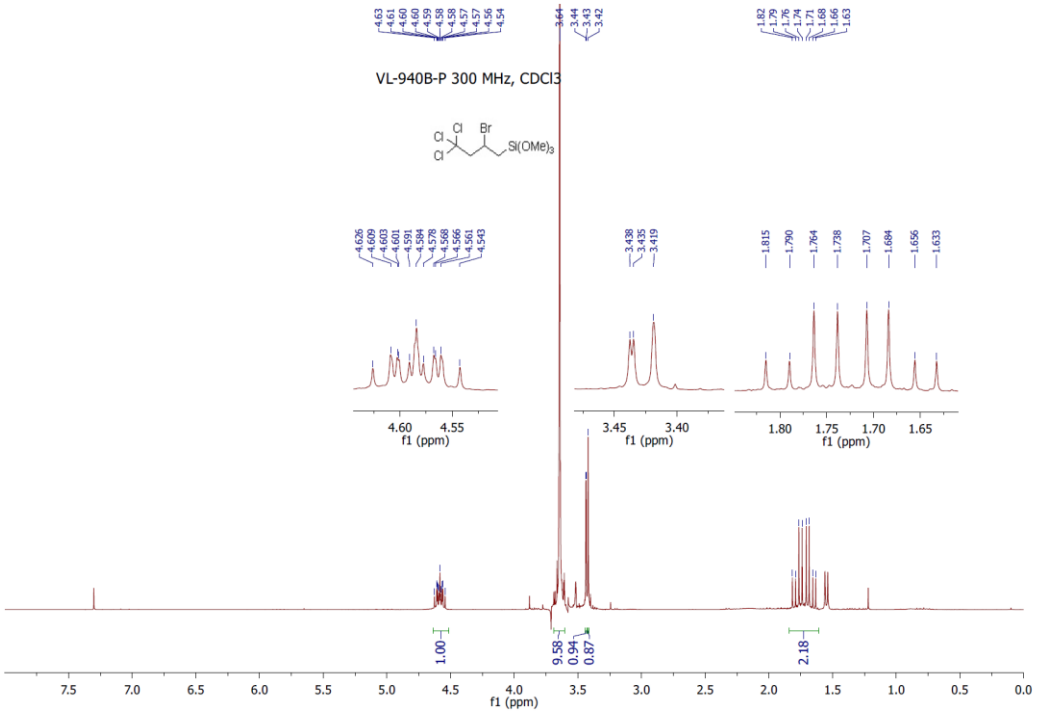


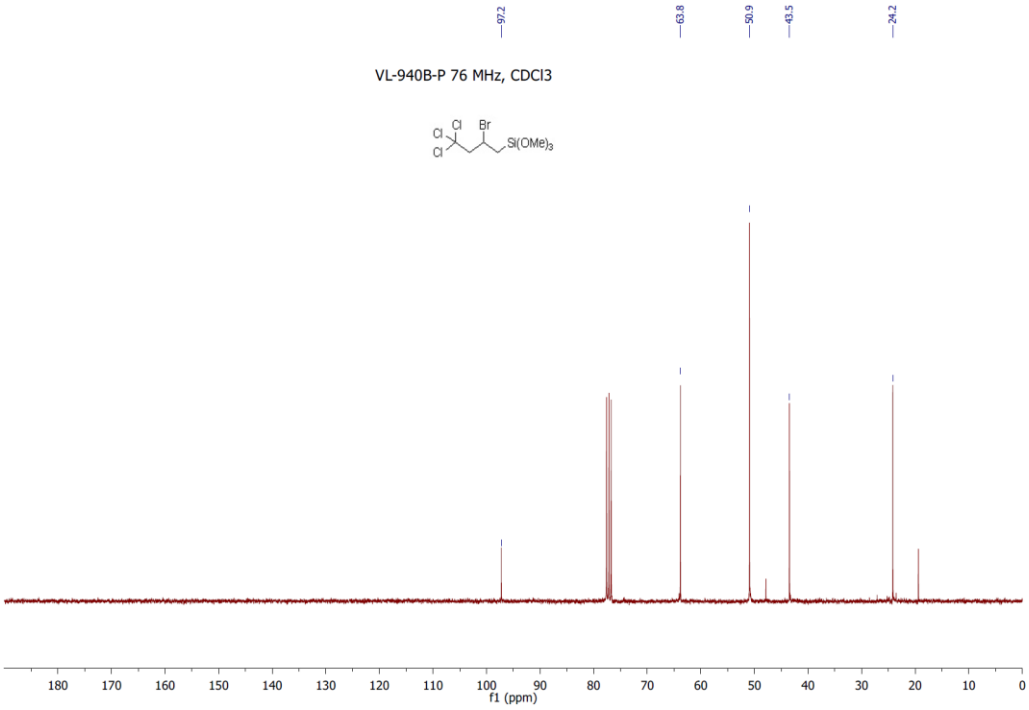




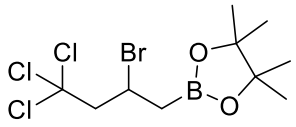
Chemical Formula: $C_7H_{14}BrCl_3O_3Si$

Molecular Weight: 360,53



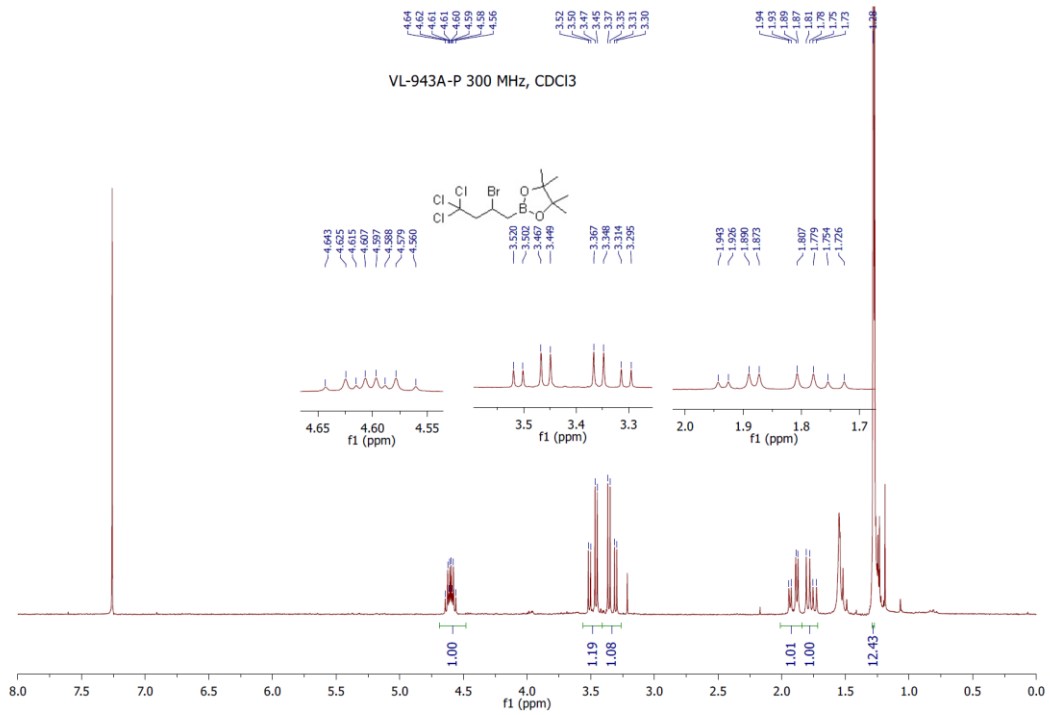


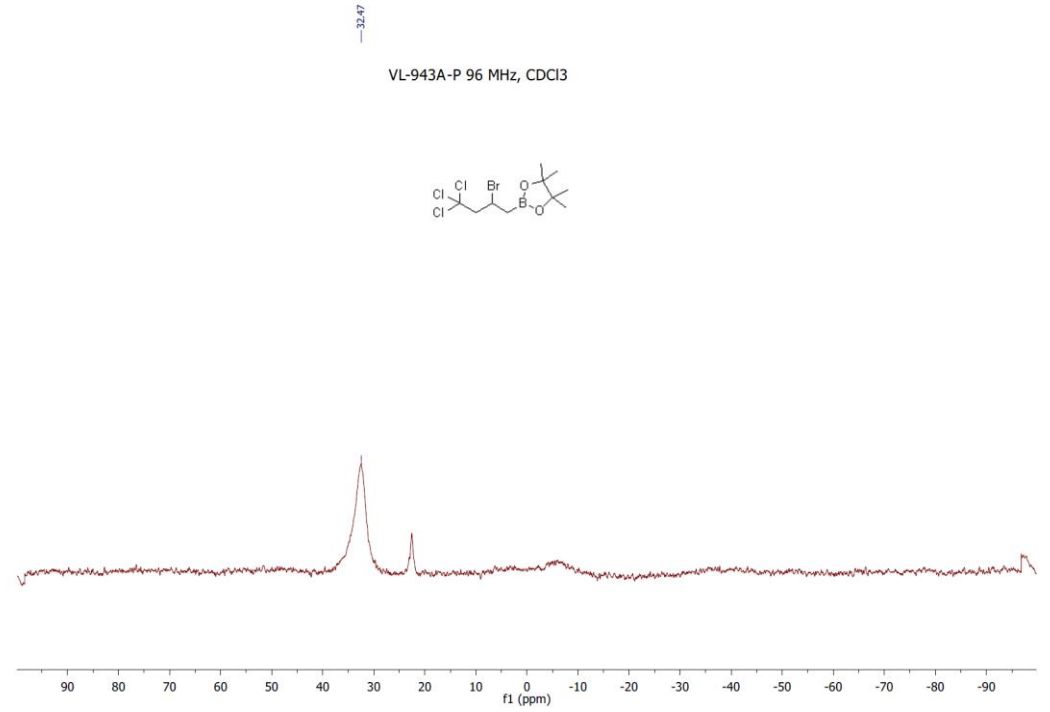
HRMS

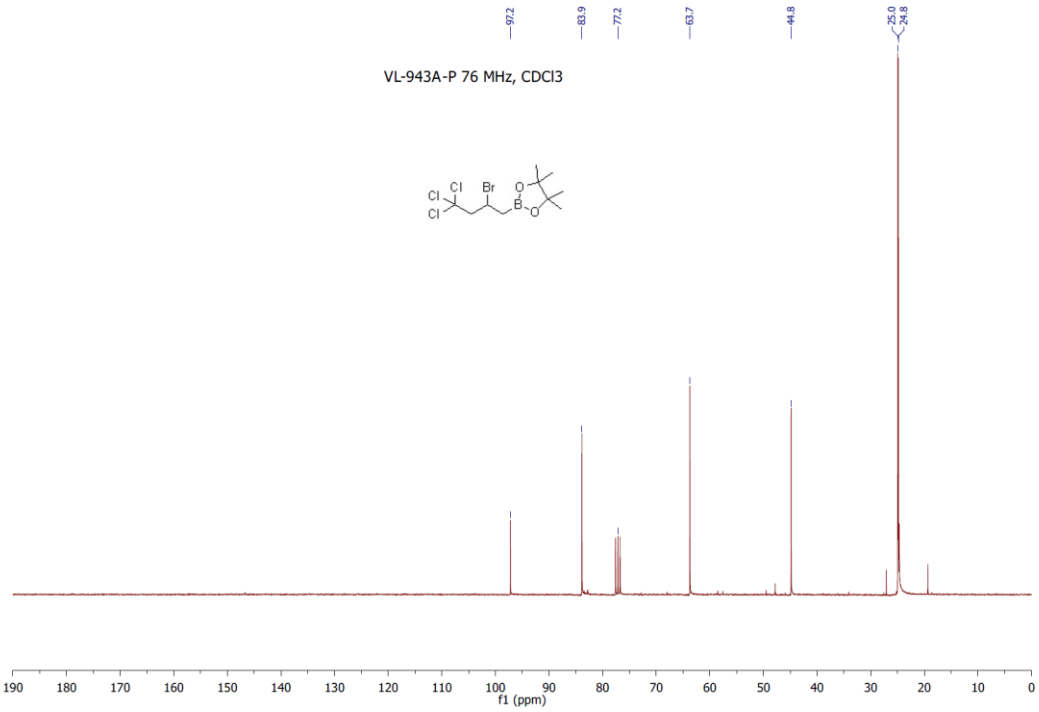


Chemical Formula: $C_{10}H_{17}BBrCl_3O_2$

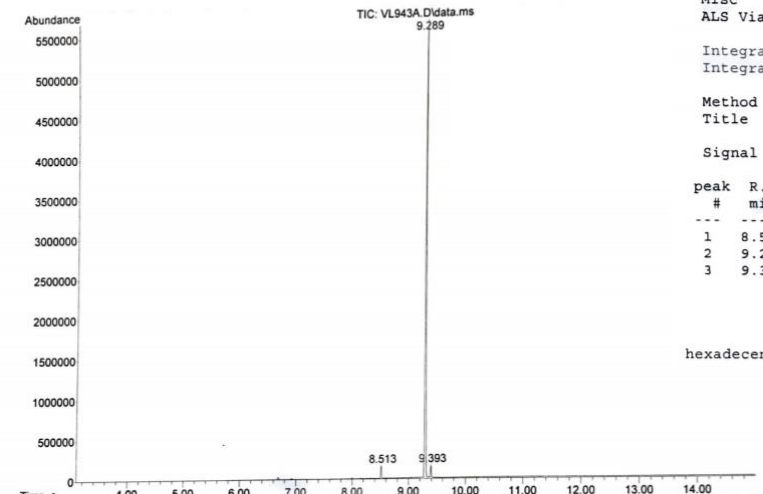
Molecular Weight: 366,31

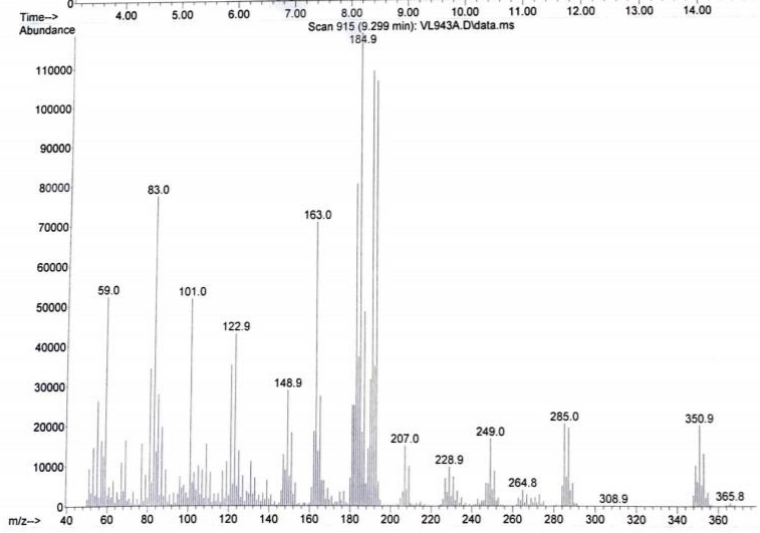





97.2
83.9
77.2
63.7
44.8
25.0
24.8
VL-943A-P 76 MHz, CDCl3
Cl
Cl
Cl
Br
O
B
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

```
File       :D:\DataMS\2017\07-2017\20-07-2017\VL943A.D
Operator   : VL
Acquired   : 20 Jul 2017  21:10     using AcqMethod NORMAL.M
Instrument :    7890 5975
Sample Name: VL943A
Misc Info  :
Vial Number: 22
```





Area Percent Report

```
Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL943A.D
Acq On    : 20 Jul 2017  21:10
Operator  : VL
Sample    : VL943A
Misc      :
ALS Vial  : 22   Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method    : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title     :

Signal    : TIC: VL943A.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.513	797	799	803	M	160633	1457192	2.29%	2.183%
2	9.289	909	914	919	M	5985358	63679568	100.00%	95.387%
3	9.393	926	929	933	M	153844	1622065	2.55%	2.430%

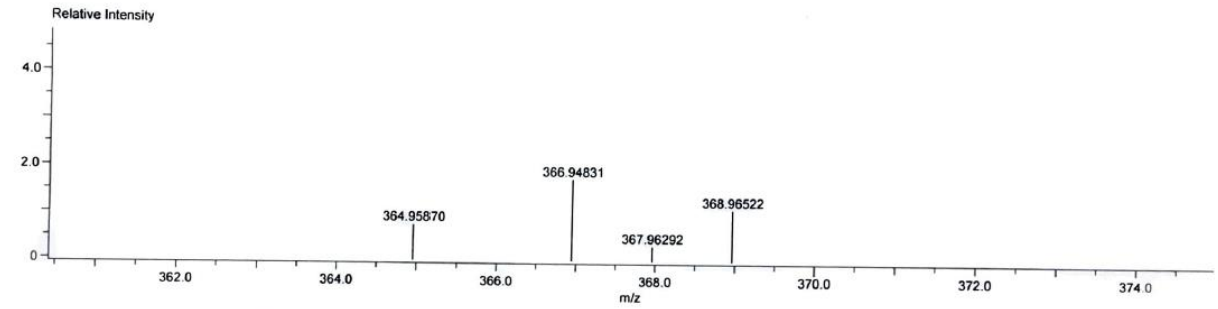
```
                    Sum of corrected areas:    66758825

hexadecenal.M Mon Oct 12 17:13:09 2020
```

Data:CI-210720-VL943A CONC
Sample Name:
Description:
Ionization Mode:CI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Smooth[5]];Correct Base[];Average(MS[1] 10.08..10.09)

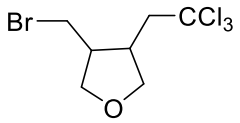
Charge number:1
Element:^{12}C:0 .. 50, ^{1}H:0 .. 100, ^{10}B:1 .. 1, ^{81}Br:1 .. 1, ^{35}Cl:3 .. 3, ^{14}N:0 .. 0, ^{16}O:2 .. 2
Tolerance:50.00(ppm)

Acquired:7/21/2020 11:08:39 AM
Operator:AccuTof
Mass Calibration data:CAL-291118-CAL-EI-class4
Created:7/21/2020 11:47:29 AM
Created by:AccuTof

Unsaturation Number:-1000.0 .. 2000.0 (Fraction:Both)

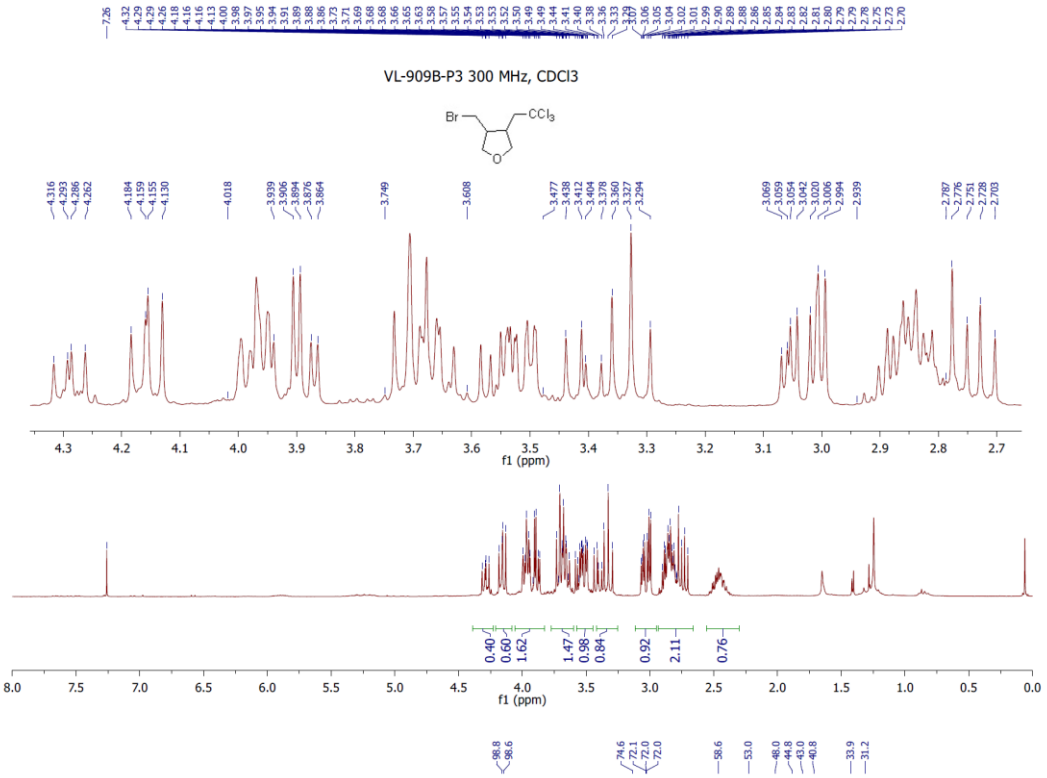


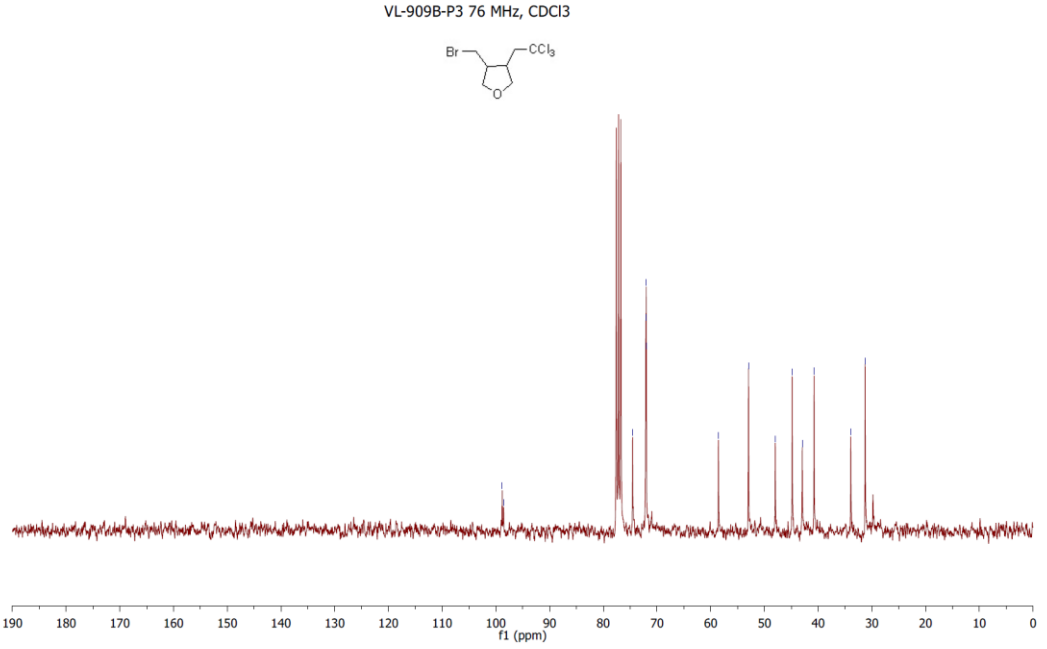
Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	Unsaturation Number
364.95870	351.33	364.95864	0.15	$^{12}C_{10}{}^{1}H_{17}{}^{10}B_{1}{}^{81}Br_{1}{}^{35}Cl_{3}{}^{16}O_{2}$	1.0



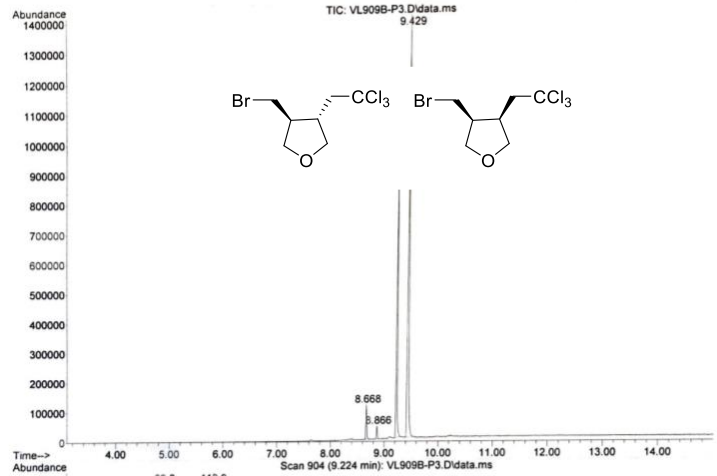
Chemical Formula: $C_7H_{10}BrCl_3O$

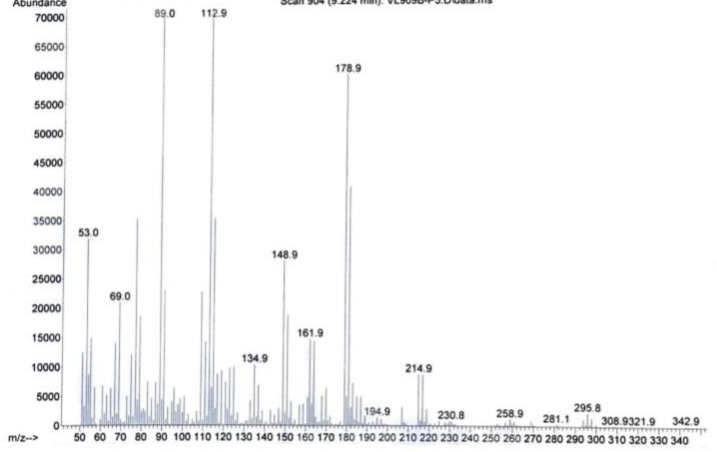
Molecular Weight: 296,41





File :D:\DataMS\2017\07-2017\20-07-2017\VL909B-P3.D
Operator : VL
Acquired : 20 Jul 2017 22:24 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL909B-P3
Misc Info :
Vial Number: 26





Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL909B-P3.D
Acq On : 20 Jul 2017 22:24
Operator : VL
Sample : VL909B-P3
Misc :
ALS Vial : 26 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

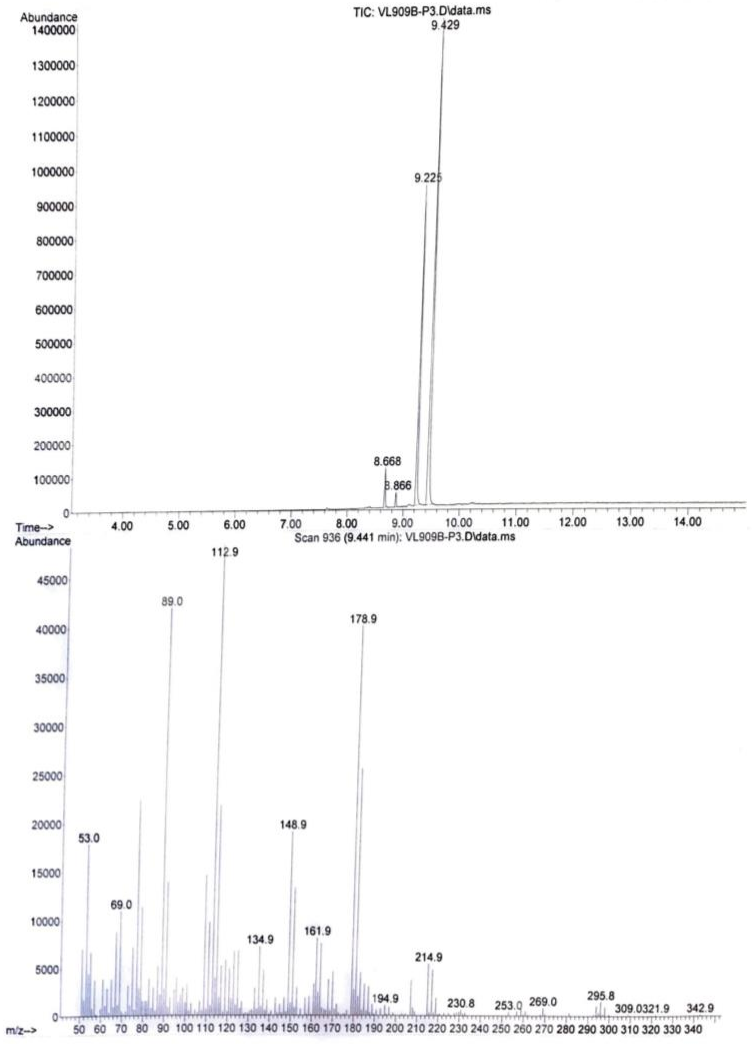
Signal : TIC: VL909B-P3.D\data.ms

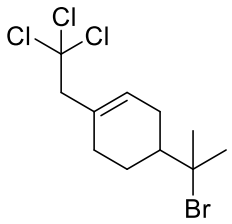
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.668	819	822	829	M	115902	1257455	6.28%	3.831%
2	8.866	848	851	855	M2	45511	500668	2.50%	1.525%
3	9.225	900	904	914	M	949932	11038741	55.13%	33.633%
4	9.429	930	934	949	M	1420660	20024082	100.00%	61.010%

Sum of corrected areas: 32820946

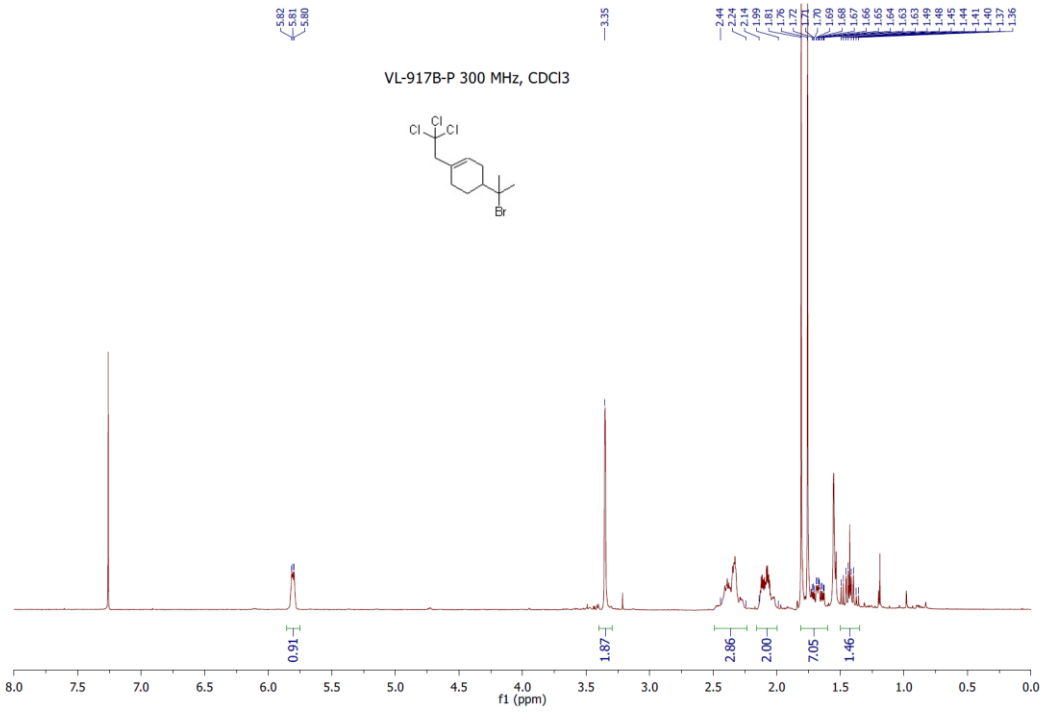
hexadecenal.M Mon Oct 12 17:09:04 2020

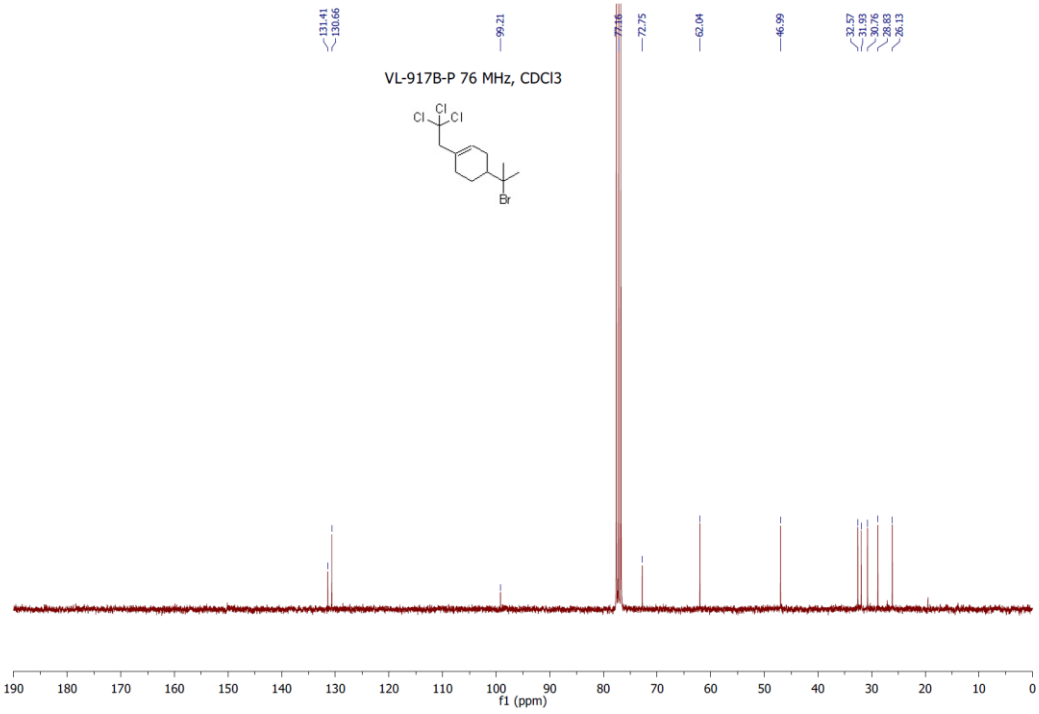
```
File       :D:\DataMS\2017\07-2017\20-07-2017\VL909B-P3.D
Operator   : VL
Acquired   : 20 Jul 2017  22:24     using AcqMethod NORMAL.M
Instrument :    7890 5975
Sample Name: VL909B-P3
Misc Info  :
Vial Number: 26
```



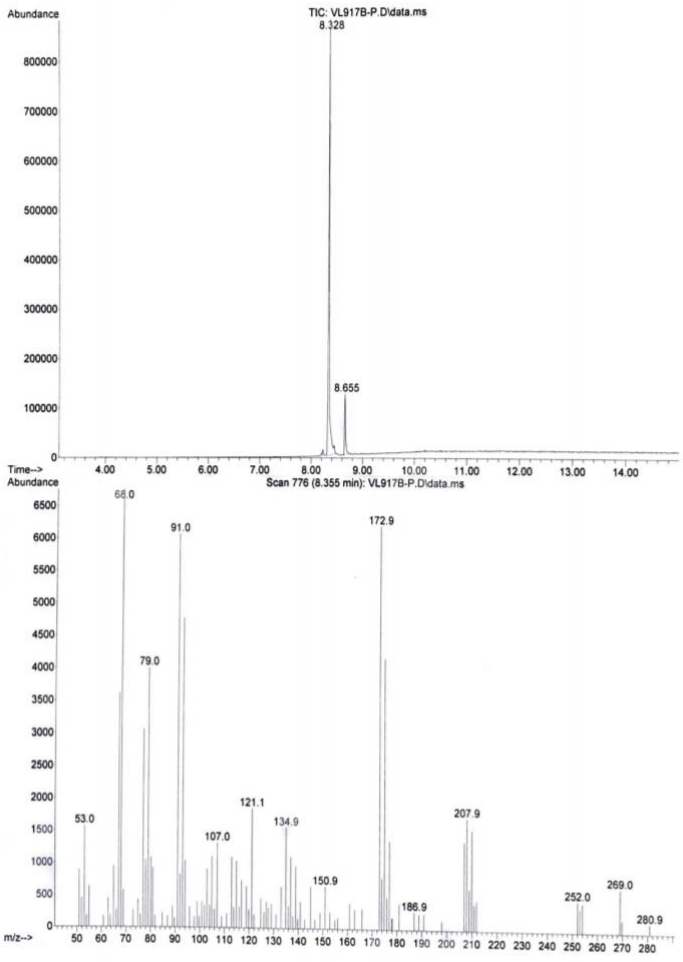


Chemical Formula: $C_{11}H_{16}BrCl_3$
Molecular Weight: 334,50




131.41
130.66
99.21
77.16
72.75
62.04
46.99
32.57
31.93
30.76
28.83
26.13
VL-917B-P 76 MHz, CDCl3
Cl
Cl
Cl
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

File :D:\DataMS\2017\07-2017\20-07-2017\VL917B-P.D
Operator : VL
Acquired : 20 Jul 2017 21:47 using AcqMethod NORMAL.M
Instrument : 7890 5975
Sample Name: VL917B-P
Misc Info :
Vial Number: 24



Area Percent Report

Data Path : D:\DataMS\2017\07-2017\20-07-2017\
Data File : VL917B-P.D
Acq On : 20 Jul 2017 21:47
Operator : VL
Sample : VL917B-P
Misc :
ALS Vial : 24 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

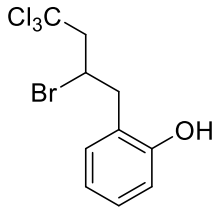
Method : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title :

Signal : TIC: VL917B-P.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.328	767	772	795	M	876441	12589634	100.00%	87.307%
2	8.655	816	820	834	M	123438	1830285	14.54%	12.693%

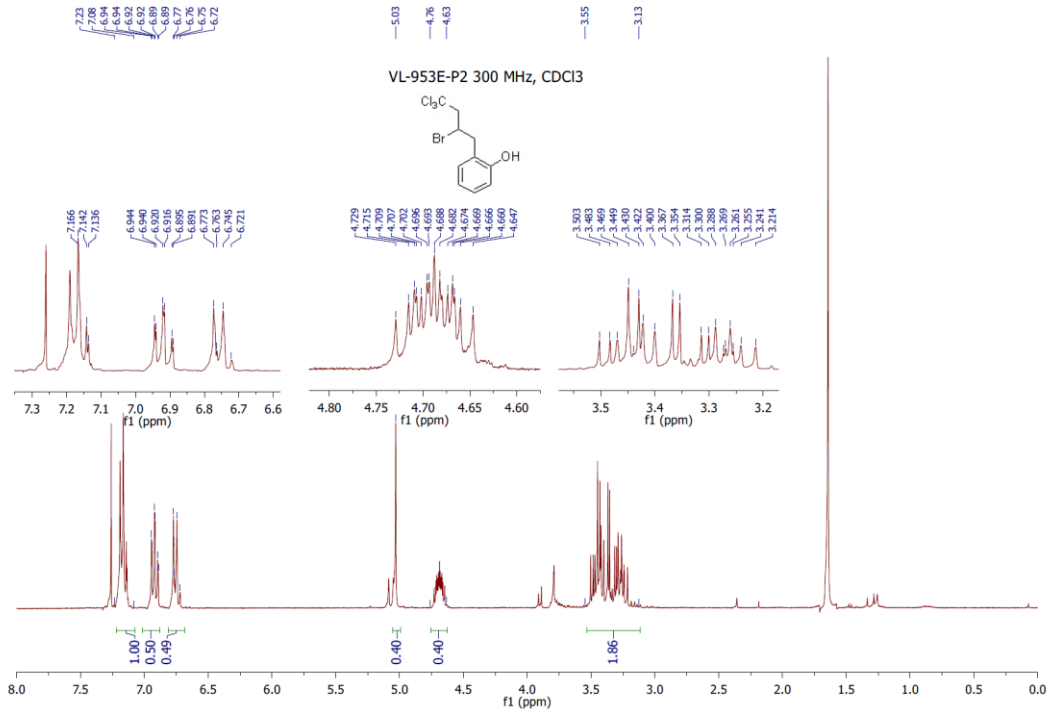
Sum of corrected areas: 14419919

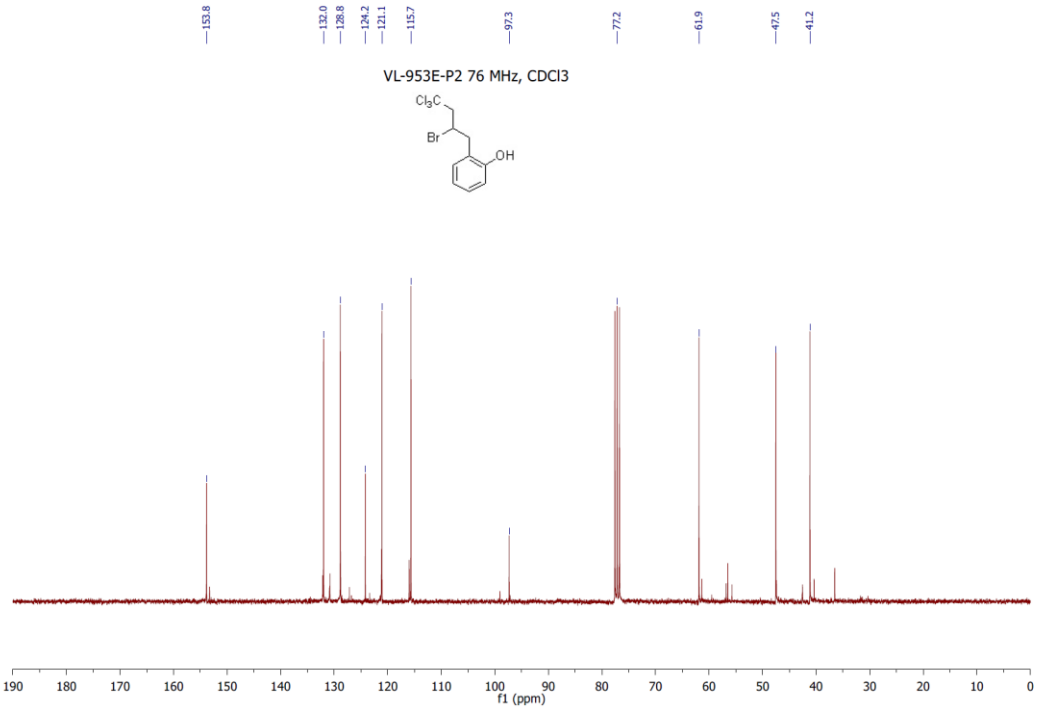
hexadecenal.M Mon Oct 12 17:07:37 2020



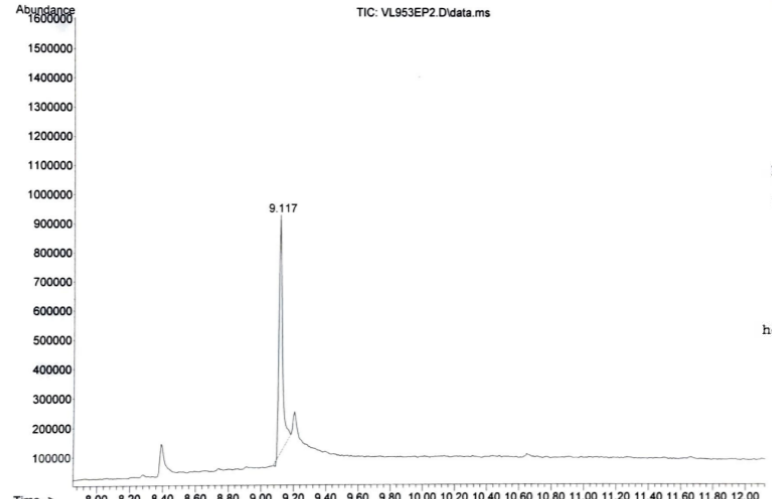
Chemical Formula: $C_{10}H_{10}BrCl_3O$

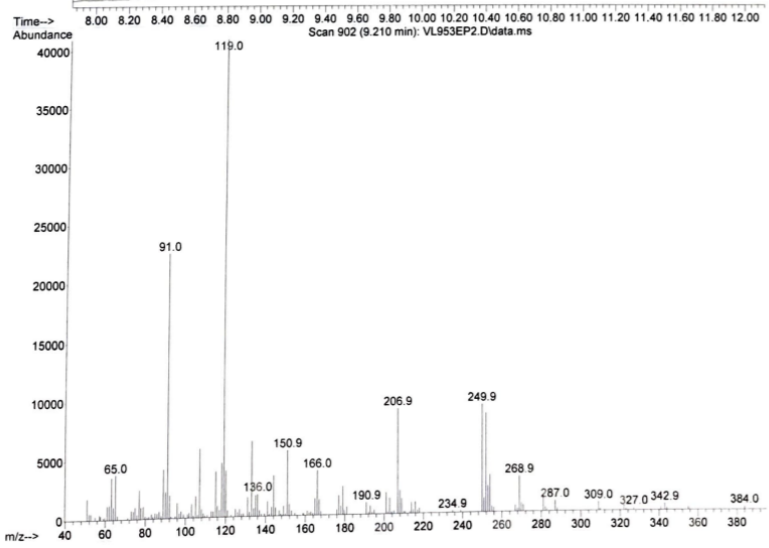
Molecular Weight: 332,44




153.8
132.0
128.8
124.2
121.1
115.7
97.3
77.2
61.9
47.5
41.2
VL-953E-P2 76 MHz, CDCl3
Cl3C
Br
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

```
File       :D:\DataMS\2017\08-2017\25082017\VL953EP2.D
Operator   : VL
Acquired   : 25 Aug 2017  15:49     using AcqMethod NORMAL.M
Instrument :    7890 5975
Sample Name: VL953EP2
Misc Info  :
Vial Number: 16
```





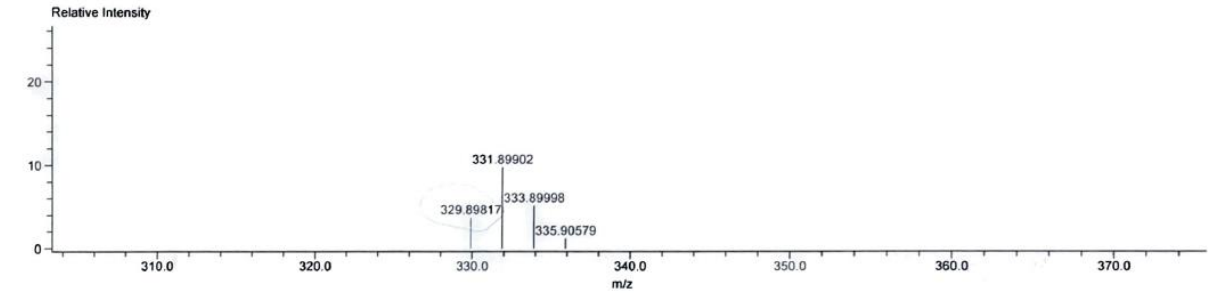

```
                                                    Area Percent Report

Data Path : D:\DataMS\2017\08-2017\25082017\
Data File : VL953EP2.D
Acq On    : 25 Aug 2017  15:49
Operator  : VL
Sample    : VL953EP2
Misc      :
ALS Vial  : 16   Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method    : C:\msdchem\1\methods\DBWAXconfig\hexadecenal.M
Title     :

Signal     : TIC: VL953EP2.D\data.ms

peak  R.T. first  max last  PK   peak      corr.    corr.    % of
  #   min  scan scan scan  TY  height      area     % max.   total
---  ----- ----- ---- ---- --- -------  -------  ------  -------
  1  8.391   777  781  794   M   112674  2140071  17.53%  13.776%
  2  9.114   884  888  898   M   832556 12207185 100.00%  78.578%
  3  9.203   898  901  911   M2   80908  1187935   9.73%   7.647%

                          Sum of corrected areas:    15535191

hexadecenal.M Mon Oct 12 17:22:37 2020
```

Data:EI-280220-VL953EP
Sample Name:
Description:
Ionization Mode:EI+
History:Determine m/z[Peak **Detect[Centroid,30,Area];Smooth[7];Correct Base[];Average(MS[1] 12.37..12.47)**

Acquired:2/28/2020 3:28:40 PM
Operator:AccuTof
Mass Calibration data:CAL-291**118-CAL-EI-class4**
Created:2/28/2020 4:21:19 PM
Created by:AccuTof

Charge number:1 Tolerance:50.00(ppm)
Element:^{12}C:0 .. 50, ^{1}H:0 .. 100, ^{79}Br:1 .. 1, ^{35}Cl:3 .. 3, ^{16}O:0 .. 1

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	Unsaturation Number
329.89817	816.08	329.89806	0.32	$^{12}C_{16}{}^{1}H_{30}{}^{79}Br_{1}{}^{35}Cl_{3}{}^{16}O_{1}$	4.0