

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
 Data File : VU038645.D
 Acq On : 07 Jun 2020 03:16
 Operator : SY/MD
 Sample : L2911-08
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9D33

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.369	3	9	20	rVB	39073	39461	2.43%	0.290%
2	1.613	75	85	92	rBV	146824	171430	10.56%	1.261%
3	1.932	176	184	194	rVB	117216	148873	9.17%	1.095%
4	2.594	377	390	402	rBV	244906	402832	24.82%	2.962%
5	2.671	402	414	438	rVB	43946	110175	6.79%	0.810%
6	2.861	445	473	478	rBV2	17417	59146	3.64%	0.435%
7	4.671	1019	1036	1063	rBV	221570	633546	39.03%	4.658%
8	4.845	1077	1090	1113	rVB	60758	138591	8.54%	1.019%
9	5.102	1154	1170	1191	rBV	222773	480649	29.61%	3.534%
10	5.420	1257	1269	1288	rVB5	18708	41571	2.56%	0.306%
11	5.761	1351	1375	1393	rBV2	449553	1169336	72.05%	8.598%
12	6.279	1519	1536	1560	rBV	399406	770954	47.50%	5.669%
13	6.597	1623	1635	1647	rVB4	22035	42996	2.65%	0.316%
14	6.719	1657	1673	1693	rBV	274139	540750	33.32%	3.976%
15	7.590	1931	1944	1960	rBV	140655	248478	15.31%	1.827%
16	7.922	2032	2047	2066	rBV	522073	938805	57.84%	6.903%
17	8.201	2122	2134	2150	rBV	91269	153546	9.46%	1.129%
18	8.439	2198	2208	2218	rBV4	11231	18128	1.12%	0.133%
19	8.655	2256	2275	2308	rBV	888772	1623037	100.00%	11.934%
20	8.951	2353	2367	2383	rVB3	12297	26841	1.65%	0.197%
21	9.436	2504	2518	2541	rBV	579826	977600	60.23%	7.188%
22	9.844	2634	2645	2667	rBV2	79497	140524	8.66%	1.033%
23	10.378	2799	2811	2821	rBV6	13888	25064	1.54%	0.184%
24	10.439	2821	2830	2840	rVB2	24873	41487	2.56%	0.305%
25	10.770	2915	2933	2939	rBV	237728	391546	24.12%	2.879%
26	10.947	2977	2988	3008	rVB3	146928	319468	19.68%	2.349%
27	11.336	3098	3109	3118	rBV3	36891	59175	3.65%	0.435%
28	11.404	3118	3130	3150	rVB7	95132	246129	15.16%	1.810%
29	11.645	3191	3205	3221	rBV9	43407	106209	6.54%	0.781%
30	11.732	3222	3232	3235	rVV9	13030	26688	1.64%	0.196%
31	11.767	3237	3243	3249	rVV5	23397	38470	2.37%	0.283%
32	11.825	3249	3261	3274	rVB	645407	1033486	63.68%	7.599%
33	12.028	3312	3324	3331	rBV6	34813	63904	3.94%	0.470%
34	12.082	3331	3341	3357	rVV5	72836	159551	9.83%	1.173%

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 Title : TRACE VOA SOM01.0

35	12.204	3357	3379	3398	rVB	622456	1175830	72.45%	8.646%
36	12.394	3428	3438	3442	rVV	22532	44806	2.76%	0.329%
37	12.430	3443	3449	3457	rVV4	41376	75795	4.67%	0.557%
38	12.475	3457	3463	3479	rVB8	27025	58821	3.62%	0.433%
39	12.635	3500	3513	3515	rBV10	10274	18290	1.13%	0.134%
40	12.687	3518	3529	3531	rBV6	15586	27990	1.72%	0.206%
41	12.822	3560	3571	3589	rVB6	23394	62839	3.87%	0.462%
42	13.166	3670	3678	3689	rBV7	36406	61067	3.76%	0.449%
43	13.246	3695	3703	3713	rVB4	19652	30221	1.86%	0.222%
44	14.278	4016	4024	4032	rBV4	10483	19379	1.19%	0.142%
45	14.468	4071	4083	4091	rBV9	14177	28302	1.74%	0.208%
46	14.516	4093	4098	4108	rVB9	11733	18236	1.12%	0.134%
47	15.072	4260	4271	4283	rVB5	36318	62545	3.85%	0.460%
48	15.175	4291	4303	4310	rBV10	9130	17669	1.09%	0.130%
49	15.352	4349	4358	4372	rVV6	39351	76251	4.70%	0.561%
50	15.433	4375	4383	4391	rVV7	18535	35079	2.16%	0.258%
51	15.481	4391	4398	4411	rVB5	27811	49532	3.05%	0.364%
52	15.603	4424	4436	4450	rBV3	28774	55135	3.40%	0.405%
53	16.031	4559	4569	4581	rBV3	18532	37352	2.30%	0.275%
54	16.140	4594	4603	4615	rBV3	8491	19621	1.21%	0.144%
55	16.452	4690	4700	4712	rBV3	13052	22251	1.37%	0.164%
56	17.384	4979	4990	5005	rVB	113724	214331	13.21%	1.576%

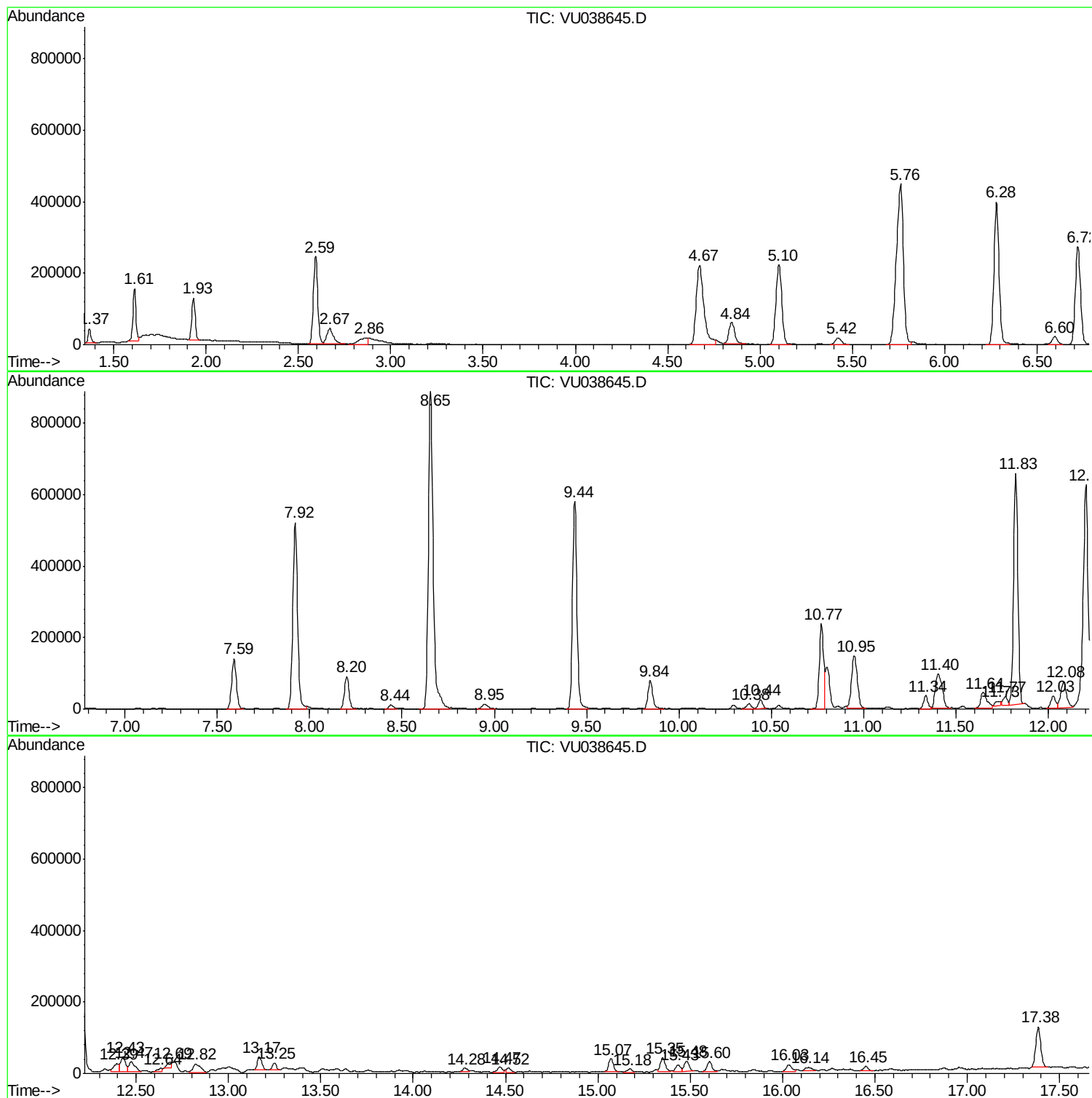
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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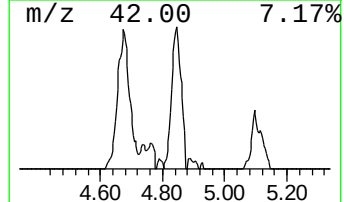
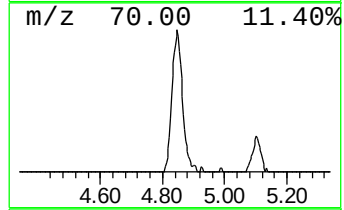
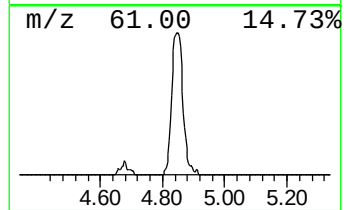
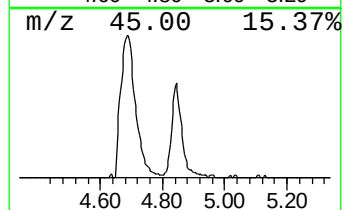
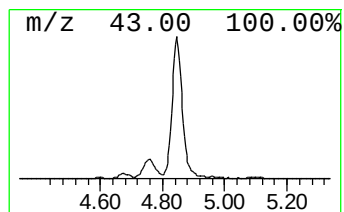
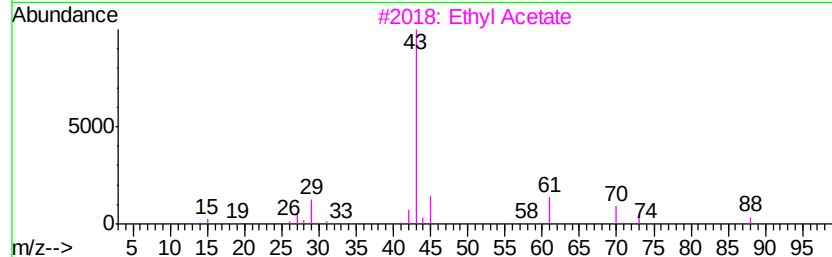
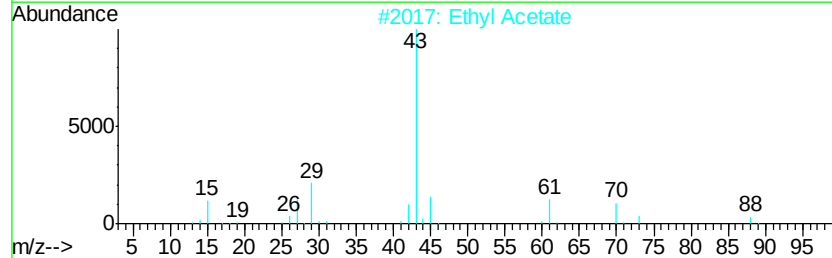
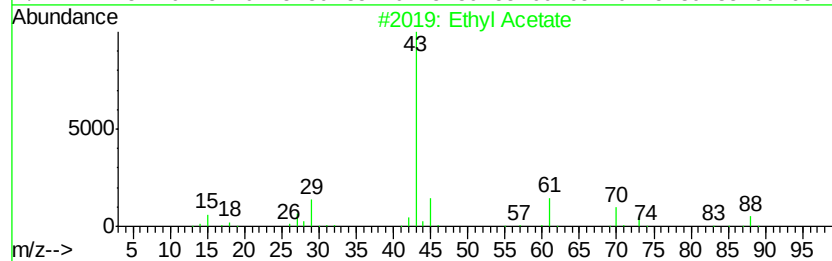
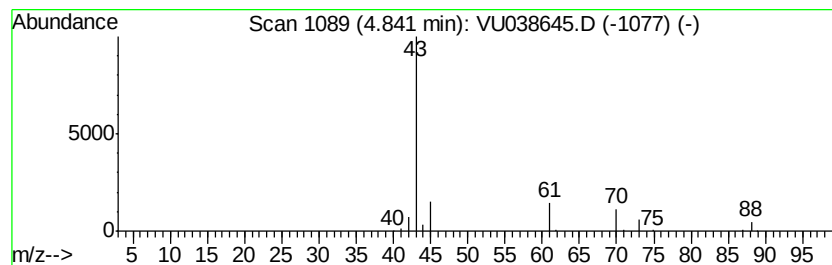
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 Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 1 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.90 ug/L	138591	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	64
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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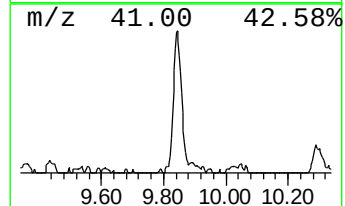
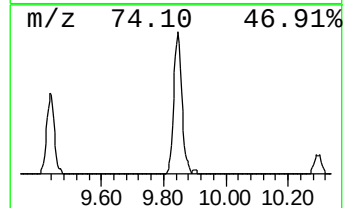
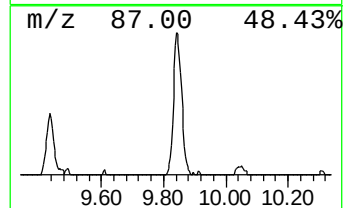
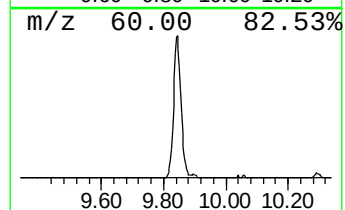
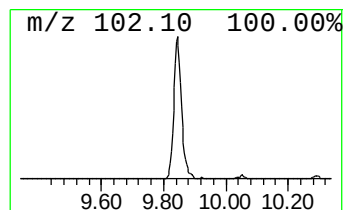
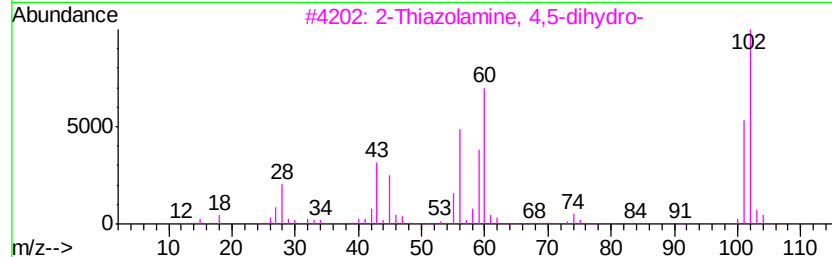
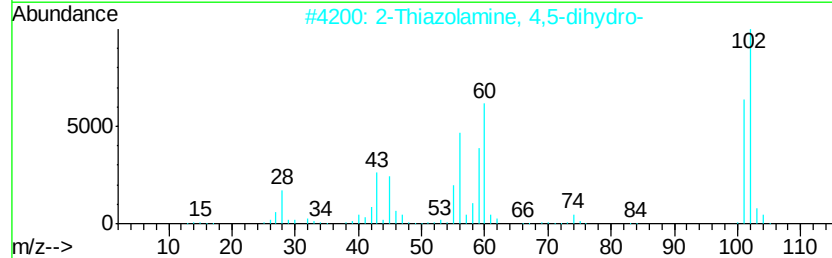
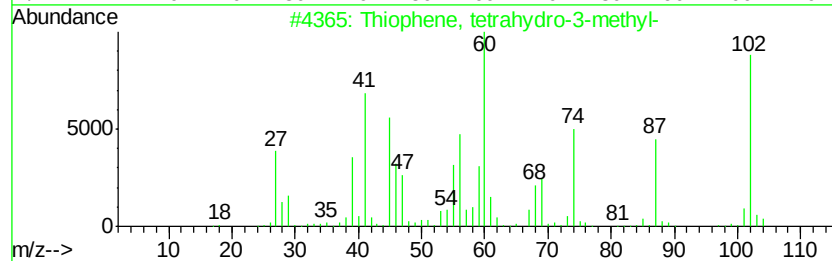
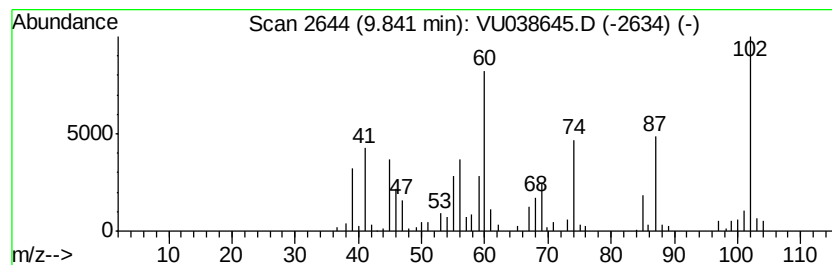
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	0.72 ug/L	140524	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	94
2		2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	38
3		2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	35
4		2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	35
5		Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	22



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ALS Vial : 1 Sample Multiplier: 1

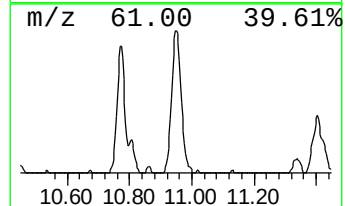
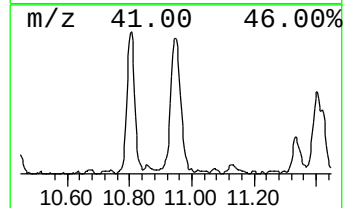
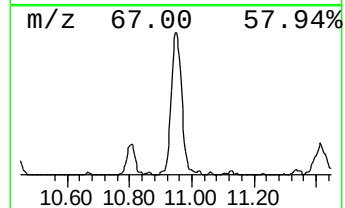
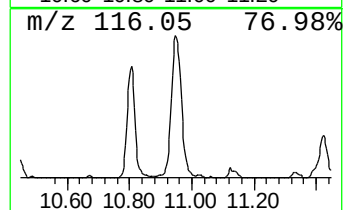
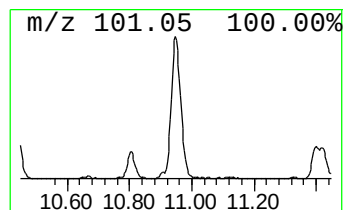
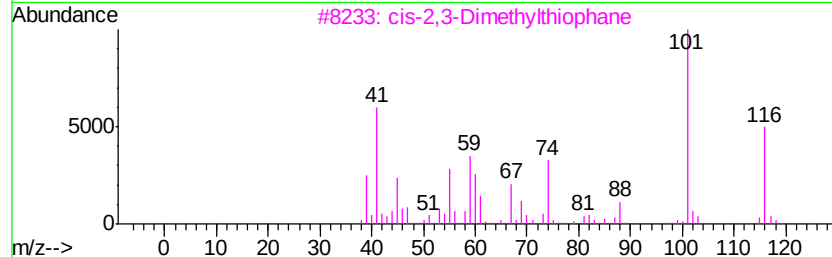
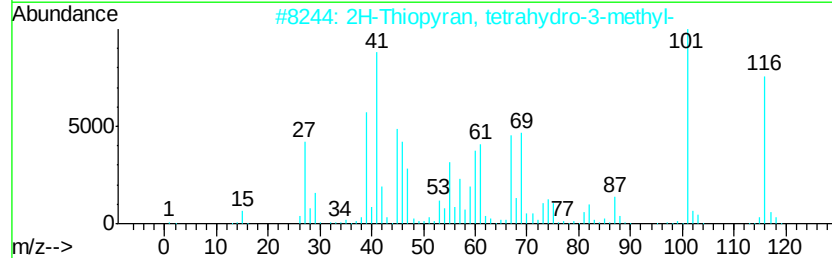
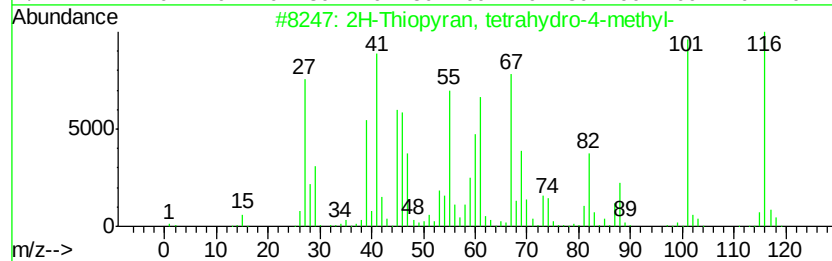
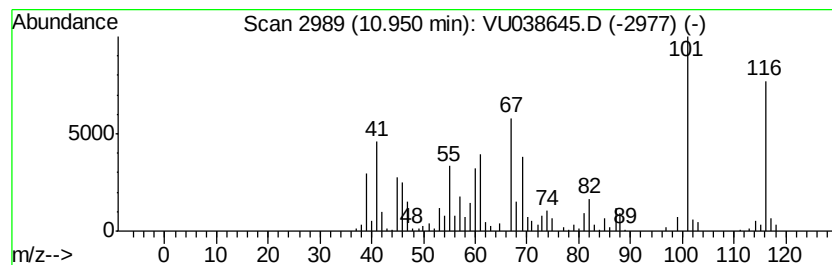
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2H-Thiopyran, tetrahydro-4-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.95	1.55 ug/L	319468	1,4-Dichlorobenzene-d4	11.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Thiopyran, tetrahydro-4-methyl-	116	C6H12S	005161-17-1	94
2	2H-Thiopyran, tetrahydro-3-methyl-	116	C6H12S	005258-50-4	91
3	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	53
4	Allylthiourea	116	C4H8N2S	000109-57-9	43
5	3-Ethylthiolane	116	C6H12S	062184-67-2	35



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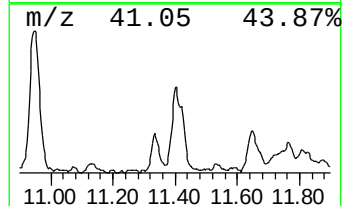
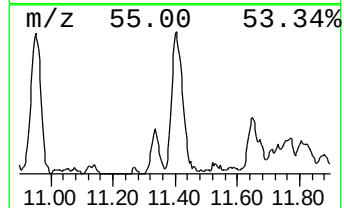
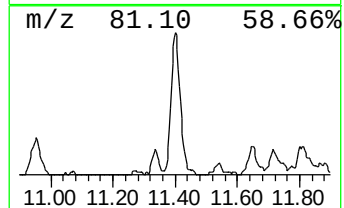
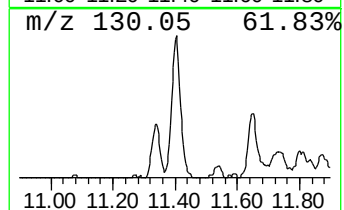
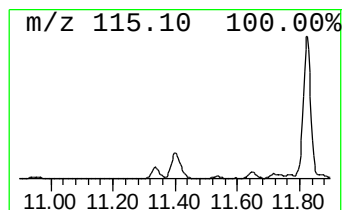
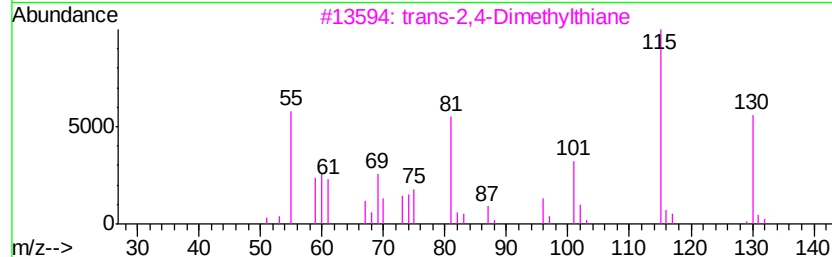
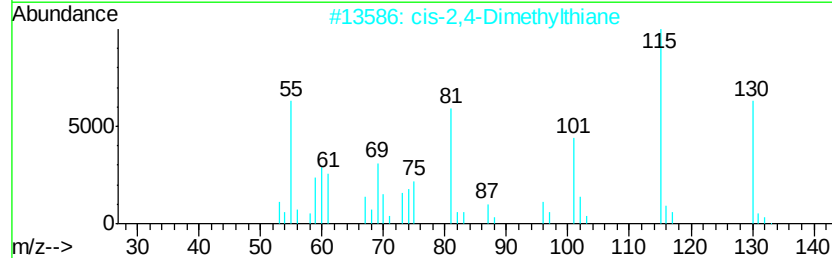
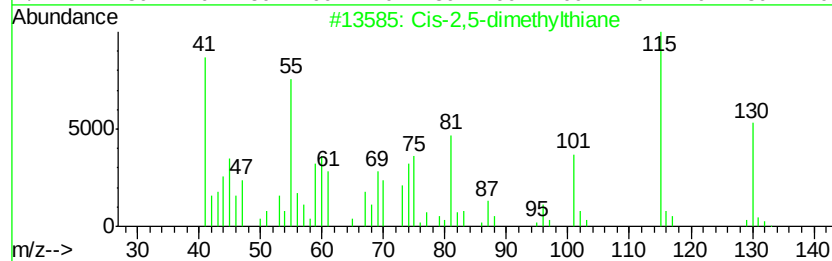
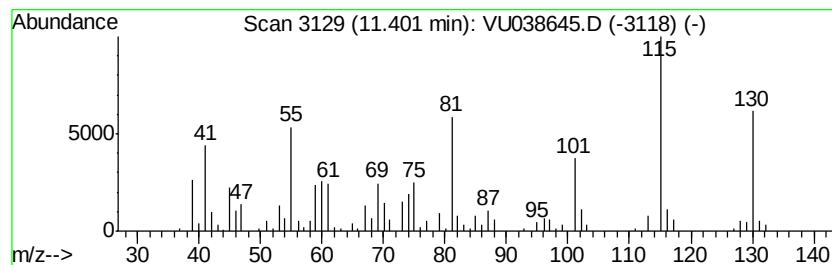
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cis-2,5-dimethylthiane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.40	1.19 ug/L	246129	1,4-Dichlorobenzene-d4	11.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cis-2,5-dimethylthiane	130	C7H14S	1000215-06-6	97
2	cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	96
3	trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	95
4	4-Ethylthiane	130	C7H14S	040324-31-0	53
5	Cis-2,3-dimethylthiane	130	C7H14S	1000215-06-5	50



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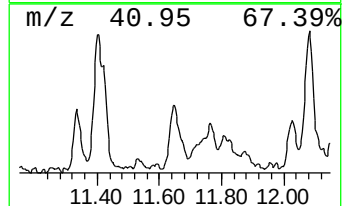
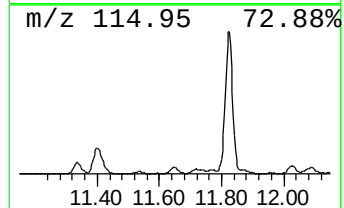
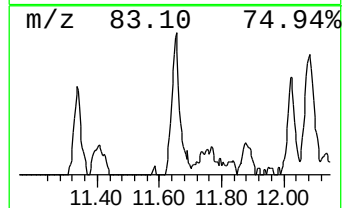
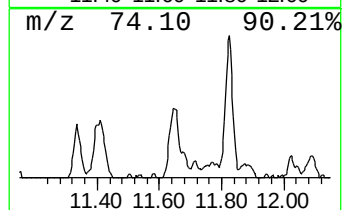
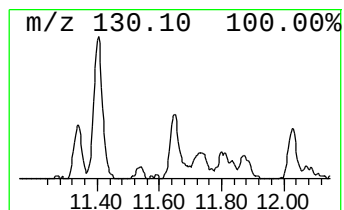
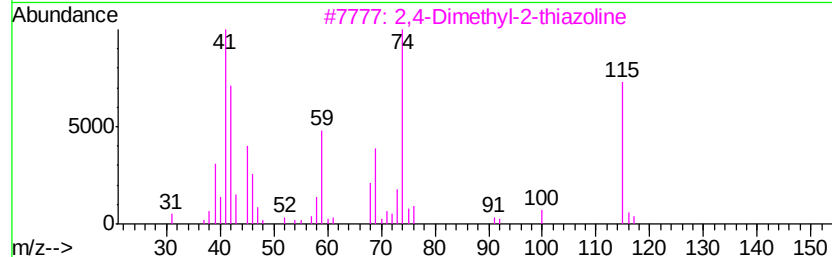
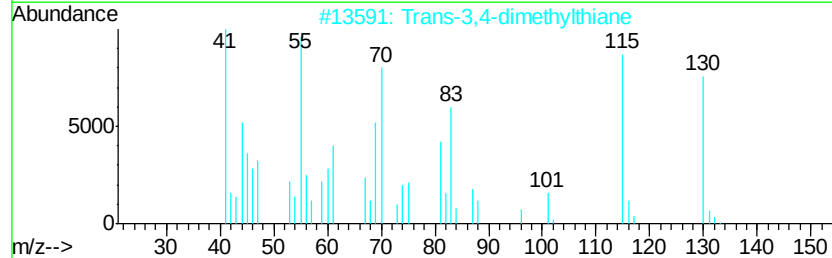
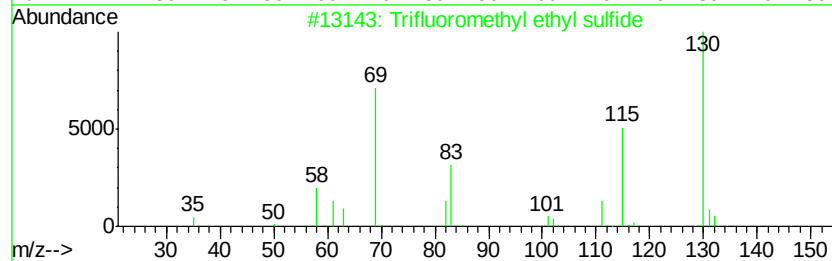
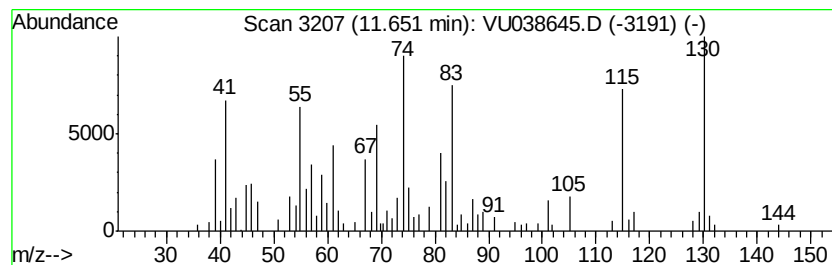
Instrument :
MSVOA_U
ClientSampled :
F9D33

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.65	0.51 ug/L	106209	1,4-Dichlorobenzene-d4	11.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoromethyl ethyl sulfide	130	C3H5F3S	013003-31-1	38
2	Trans-3,4-dimethylthiane	130	C7H14S	1000215-07-1	35
3	2,4-Dimethyl-2-thiazoline	115	C5H9NS	006114-40-5	30
4	Cis-2,3-dimethylthiane	130	C7H14S	1000215-06-5	27
5	Sulfide, butyl propenyl	130	C7H14S	024298-51-9	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038645.D
Acq On : 07 Jun 2020 03:16
Operator : SY/MD
Sample : L2911-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
F9D33

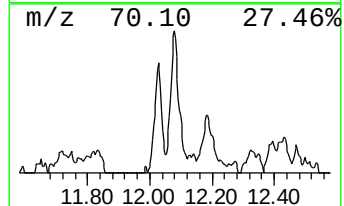
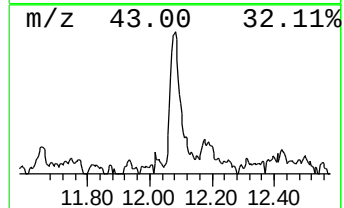
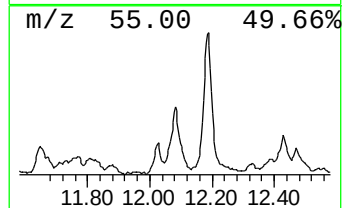
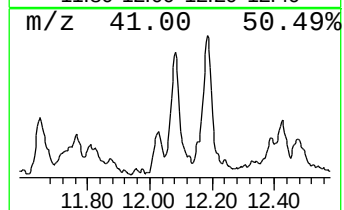
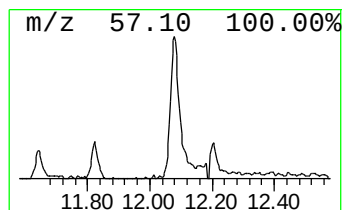
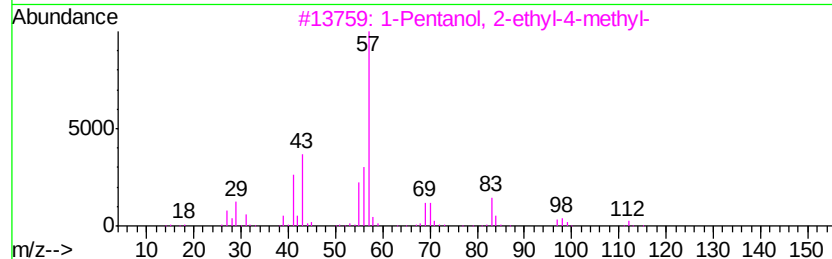
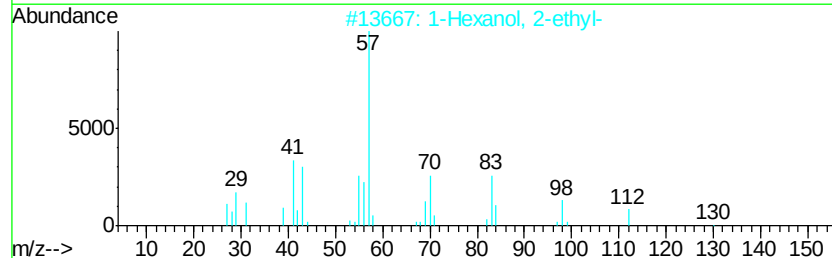
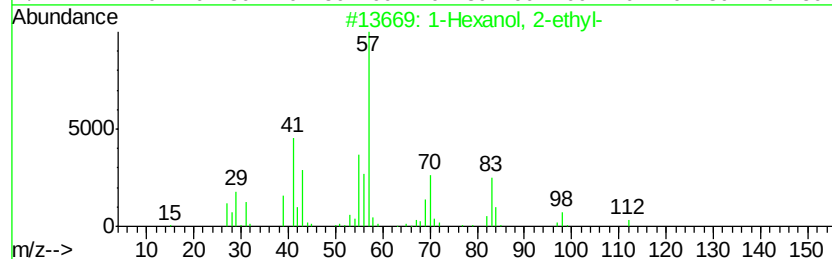
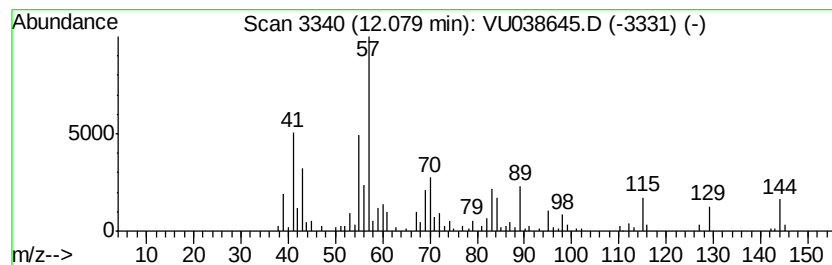
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	0.77 ug/L	159551	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	27
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	27
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	27
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	22
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038645.D
Acq On : 07 Jun 2020 03:16
Operator : SY/MD
Sample : L2911-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9D33

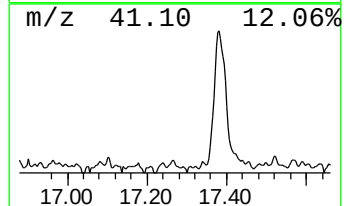
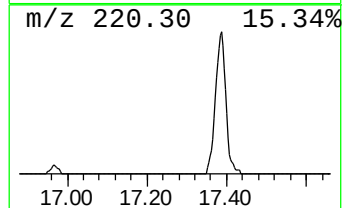
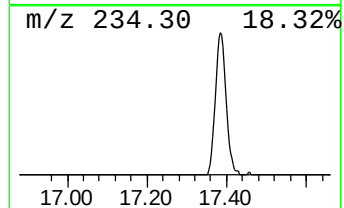
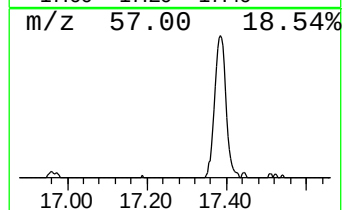
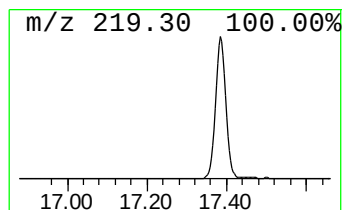
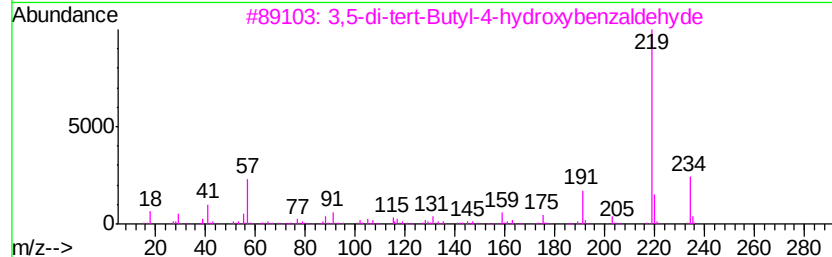
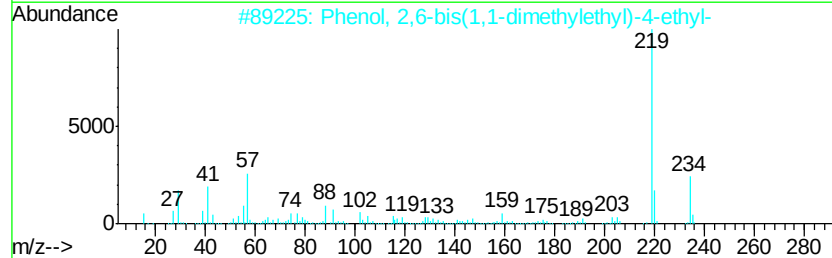
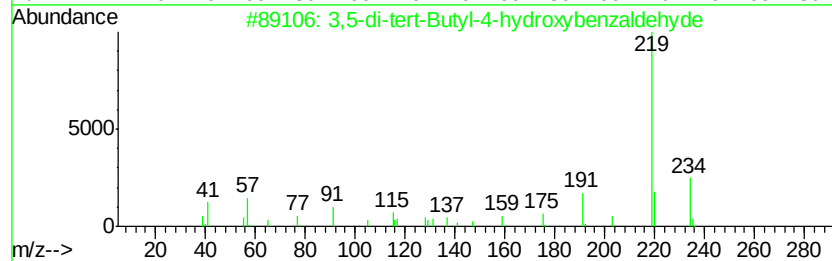
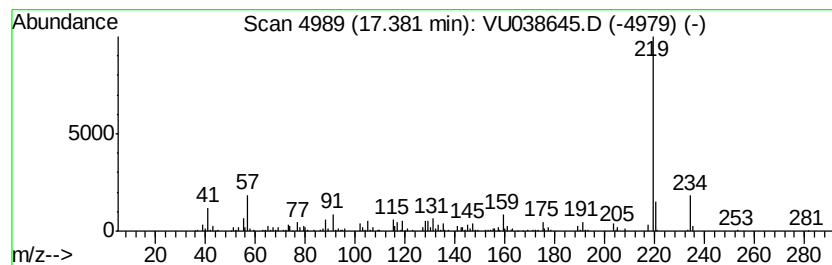
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	1.04 ug/L	214331	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	93
2		Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	90
3		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87
4		Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	86
5		3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	80



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038645.D
Acq On : 07 Jun 2020 03:16
Operator : SY/MD
Sample : L2911-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9D33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.84	0.9	ug/L	138591	1	6.28	770954	5.0
Thiophene, tetrahydro-	9.84	0.7	ug/L	140524	2	9.44	977600	5.0
2H-Thiopyran, tetrahydro-	10.95	1.6	ug/L	319468	3	11.82	1033490	5.0
Cis-2,5-dimethyltetrahydro-	11.40	1.2	ug/L	246129	3	11.82	1033490	5.0
unknown-01	11.65	0.5	ug/L	106209	3	11.82	1033490	5.0
unknown-02	12.08	0.8	ug/L	159551	3	11.82	1033490	5.0
3,5-di-tert-Butyl-4-methylphenol	17.38	1.0	ug/L	214331	3	11.82	1033490	5.0