

Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031220\
 Data File : VV014867.D
 Acq On : 12 Mar 2020 14:52
 Operator : SY/MD
 Sample : PB127467TB
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB01

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % 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_V\METHOD\SOMVLM030620WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.315	63	70	83	rVB	178804	193234	8.35%	1.069%
2	1.579	144	152	166	rVB	136114	167657	7.25%	0.928%
3	2.119	311	320	337	rVB	289240	415371	17.95%	2.298%
4	2.528	440	447	459	rVB2	9681	15800	0.68%	0.087%
5	2.630	475	479	480	rBV4	997	716	0.03%	0.004%
6	2.730	509	510	512	rBV4	346	127	0.01%	0.001%
7	2.743	512	514	515	rBV	234	104	0.00%	0.001%
8	2.759	517	519	520	rBV	642	219	0.01%	0.001%
9	2.833	539	542	546	rVB3	723	461	0.02%	0.003%
10	2.859	549	550	553	rVB2	381	116	0.01%	0.001%
11	2.875	553	555	557	rBV2	703	285	0.01%	0.002%
12	2.888	557	559	561	rVB3	552	301	0.01%	0.002%
13	2.981	582	588	592	rBV2	682	875	0.04%	0.005%
14	3.036	602	605	607	rBV2	544	328	0.01%	0.002%
15	3.045	607	608	610	rVB2	510	130	0.01%	0.001%
16	3.139	633	637	638	rBV2	347	227	0.01%	0.001%
17	3.167	643	646	649	rVB2	452	295	0.01%	0.002%
18	3.180	649	650	651	rBV2	207	44	0.00%	0.000%
19	3.187	651	652	654	rBV2	494	242	0.01%	0.001%
20	3.229	663	665	669	rVB3	617	367	0.02%	0.002%
21	3.261	674	675	678	rBV2	209	100	0.00%	0.001%
22	3.293	684	685	688	rVB	396	143	0.01%	0.001%
23	3.309	688	690	691	rBV2	304	127	0.01%	0.001%
24	3.364	704	707	708	rBV2	444	199	0.01%	0.001%
25	3.405	718	720	721	rBV	247	103	0.00%	0.001%
26	3.434	728	729	736	rVB3	721	448	0.02%	0.002%
27	3.463	736	738	742	rBV2	479	352	0.02%	0.002%
28	3.479	742	743	744	rBV	317	82	0.00%	0.000%
29	3.511	750	753	754	rBV	349	162	0.01%	0.001%
30	3.521	754	756	759	rVV3	777	405	0.02%	0.002%
31	3.537	759	761	762	rVV	222	116	0.01%	0.001%
32	3.550	763	765	767	rVB	724	321	0.01%	0.002%
33	3.566	767	770	771	rVB	241	120	0.01%	0.001%
34	3.589	771	777	782	rBV3	607	706	0.03%	0.004%

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 Title : VOC Analysis

35	3.618	784	786	787	rVB	585	167	0.01%	0.001%
36	3.679	802	805	806	rBV	603	309	0.01%	0.002%
37	3.737	821	823	826	rBV2	492	257	0.01%	0.001%
38	3.794	838	841	843	rBV3	395	267	0.01%	0.001%
39	3.846	852	857	858	rBV3	734	481	0.02%	0.003%
40	3.923	869	881	936	rBV2	68208	318325	13.76%	1.761%
41	4.293	992	996	997	rBV3	677	435	0.02%	0.002%
42	4.376	1004	1022	1044	rBV	231013	568500	24.57%	3.146%
43	4.650	1105	1107	1109	rBV	295	151	0.01%	0.001%
44	4.669	1112	1113	1116	rBV	627	328	0.01%	0.002%
45	4.701	1122	1123	1127	rBV2	458	267	0.01%	0.001%
46	4.785	1147	1149	1156	rVB6	671	591	0.03%	0.003%
47	4.814	1156	1158	1160	rVV2	349	194	0.01%	0.001%
48	4.836	1164	1165	1168	rVB	536	198	0.01%	0.001%
49	4.865	1168	1174	1181	rBV5	1038	1474	0.06%	0.008%
50	4.897	1181	1184	1187	rVB2	646	393	0.02%	0.002%
51	4.926	1188	1193	1194	rBV2	504	364	0.02%	0.002%
52	4.936	1194	1196	1199	rVV2	582	327	0.01%	0.002%
53	4.965	1203	1205	1207	rBV2	329	182	0.01%	0.001%
54	4.990	1212	1213	1217	rBV2	507	257	0.01%	0.001%
55	5.007	1217	1218	1220	rVB2	365	96	0.00%	0.001%
56	5.074	1220	1239	1262	rBV2	569548	1440048	62.24%	7.968%
57	5.309	1302	1312	1329	rVB	52971	111913	4.84%	0.619%
58	5.643	1385	1416	1435	rBV	564342	1745317	75.43%	9.658%
59	6.097	1548	1557	1582	rVB	317677	633004	27.36%	3.503%
60	6.486	1666	1678	1710	rBV	1182246	2313693	100.00%	12.803%
61	7.010	1830	1841	1858	rBV	187139	326521	14.11%	1.807%
62	7.209	1892	1903	1930	rBV	169965	316595	13.68%	1.752%
63	7.338	1932	1943	1982	rVB	719064	1285471	55.56%	7.113%
64	7.640	2027	2037	2059	rVB2	177151	315395	13.63%	1.745%
65	7.945	2121	2132	2150	rBV	344674	585847	25.32%	3.242%
66	8.113	2174	2184	2204	rVB2	438139	864656	37.37%	4.785%
67	8.212	2206	2215	2236	rVB	553277	888993	38.42%	4.919%
68	8.701	2356	2367	2392	rBV	773643	1237277	53.48%	6.846%
69	8.875	2408	2421	2436	rBV	700802	1142150	49.36%	6.320%
70	9.373	2570	2576	2578	rBV4	1264	1192	0.05%	0.007%
71	9.405	2578	2586	2600	rVV3	18923	31972	1.38%	0.177%

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72	9.566	2625	2636	2656	rBV	112036	180307	7.79%	0.998%
73	10.238	2833	2845	2862	rBV	462997	722592	31.23%	3.998%
74	10.559	2939	2945	2953	rVB4	8220	12035	0.52%	0.067%
75	10.836	3029	3031	3032	rBV	451	208	0.01%	0.001%
76	10.875	3040	3043	3047	rBV2	889	779	0.03%	0.004%
77	11.270	3154	3166	3186	rBV	700746	1082688	46.79%	5.991%
78	11.553	3249	3254	3259	rBV5	1869	2290	0.10%	0.013%
79	11.646	3270	3283	3301	rBV	722070	1131445	48.90%	6.261%
80	11.936	3370	3373	3379	rBV5	1001	896	0.04%	0.005%
81	12.067	3411	3414	3416	rBV3	634	438	0.02%	0.002%
82	12.186	3449	3451	3454	rBV2	691	419	0.02%	0.002%
83	12.518	3551	3554	3556	rBV2	445	238	0.01%	0.001%
84	12.900	3671	3673	3676	rVB3	1071	470	0.02%	0.003%
85	13.228	3772	3775	3776	rBV2	711	376	0.02%	0.002%
86	13.286	3790	3793	3797	rBV4	923	683	0.03%	0.004%
87	13.781	3942	3947	3950	rBV6	1559	1713	0.07%	0.009%
88	14.299	4105	4108	4109	rBV	706	384	0.02%	0.002%

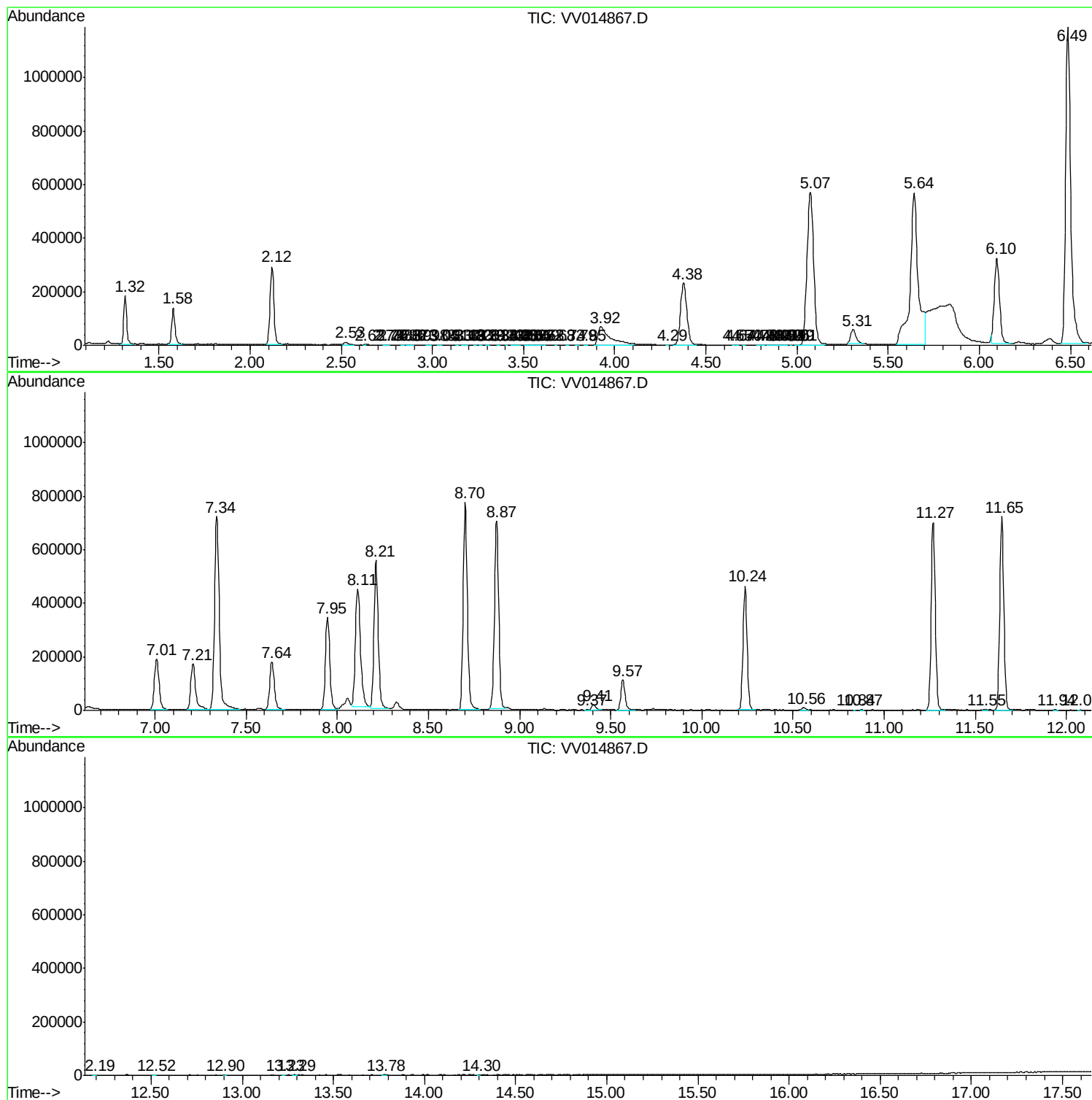
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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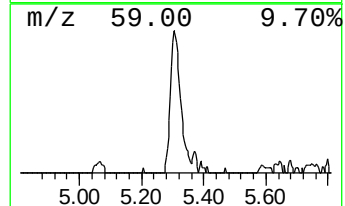
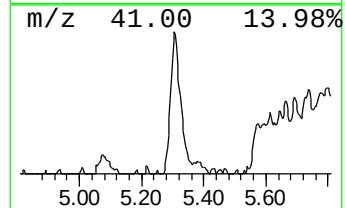
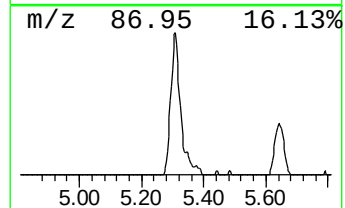
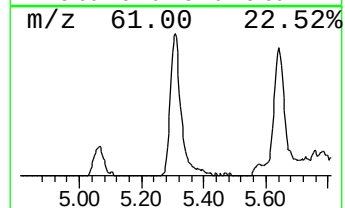
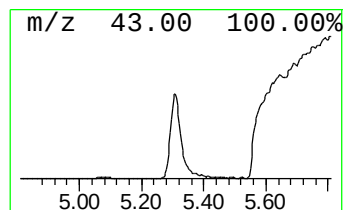
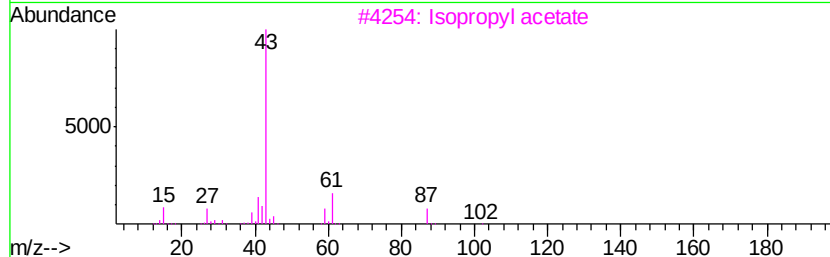
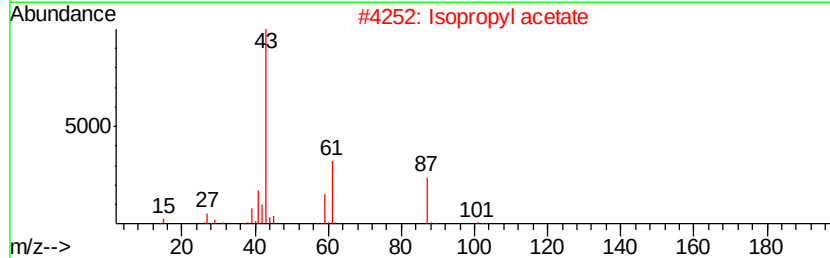
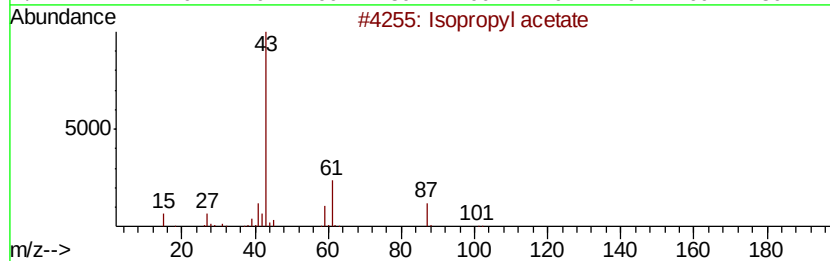
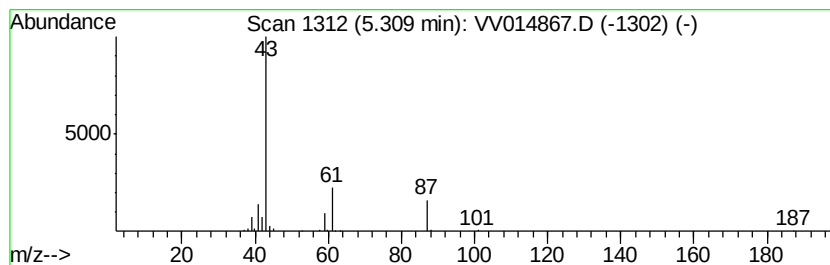
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.31	3.21 ug/L	111913	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	78
2		Isopropyl acetate	102	C5H10O2	000108-21-4	59
3		Isopropyl acetate	102	C5H10O2	000108-21-4	39
4		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28



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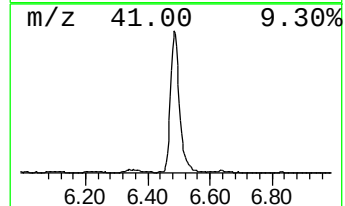
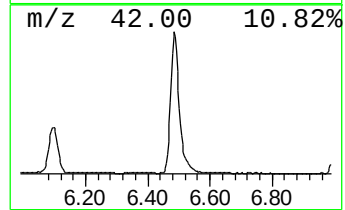
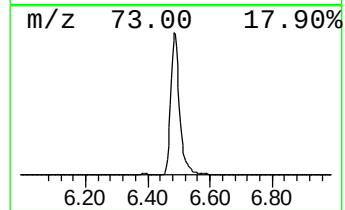
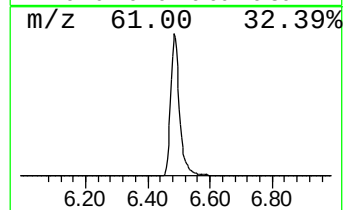
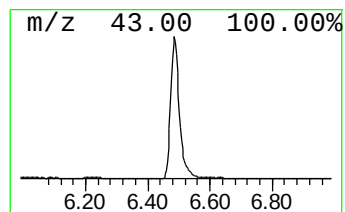
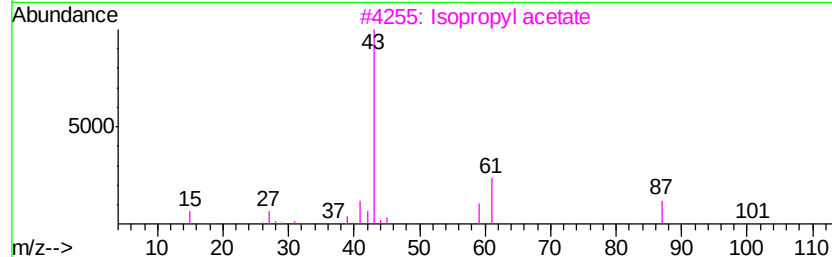
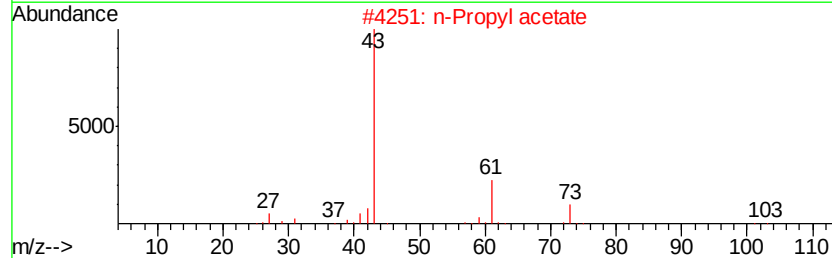
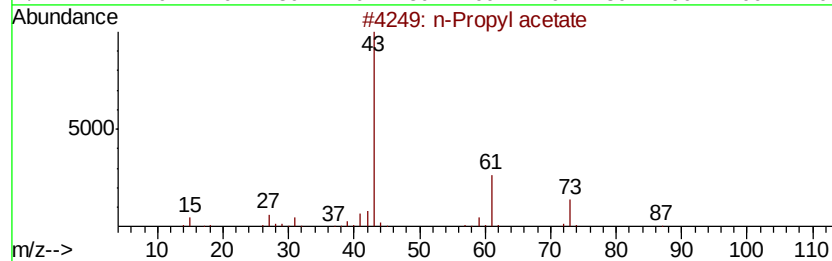
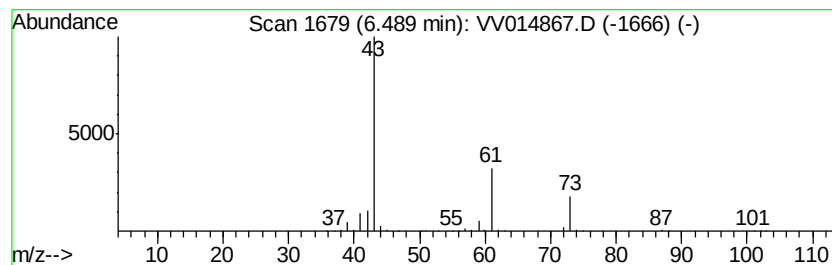
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	66.28 ug/L	2313690	1,4-Difluorobenzene	5.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Propyl acetate	102 C5H10O2	000109-60-4	83
2	n-Propyl acetate	102 C5H10O2	000109-60-4	83
3	Isopropyl acetate	102 C5H10O2	000108-21-4	36
4	1-Butanamine	73 C4H11N	000109-73-9	9
5	Propanal, 2,3-dihydroxy-, (S)-	90 C3H6O3	000497-09-6	9



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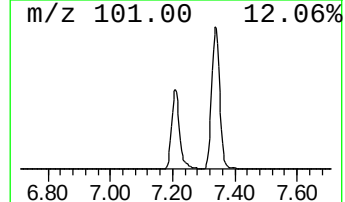
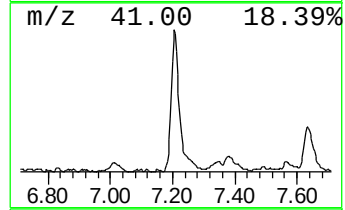
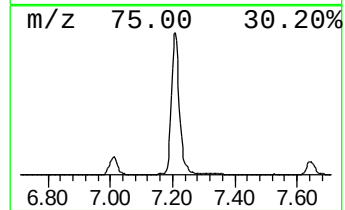
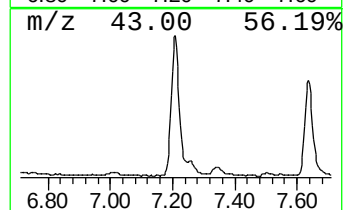
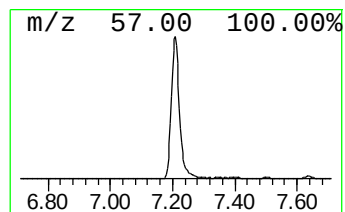
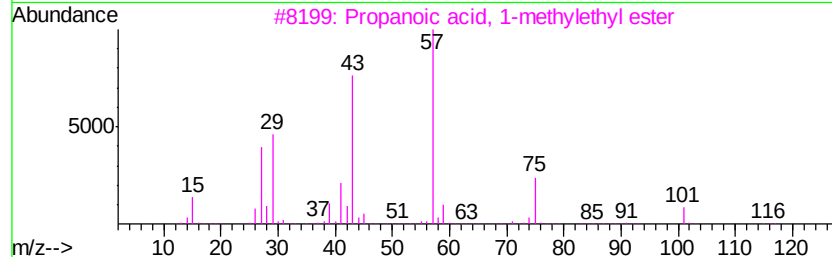
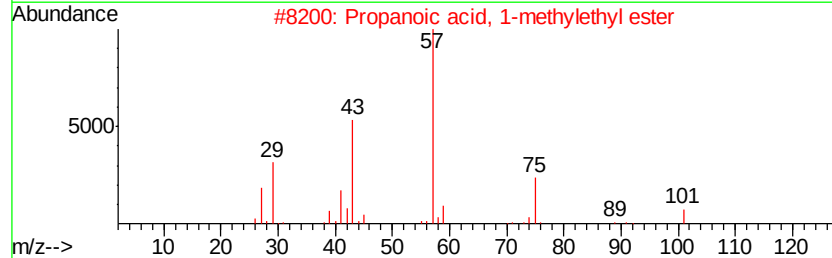
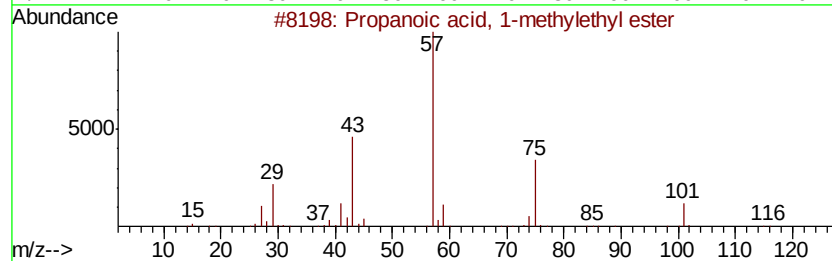
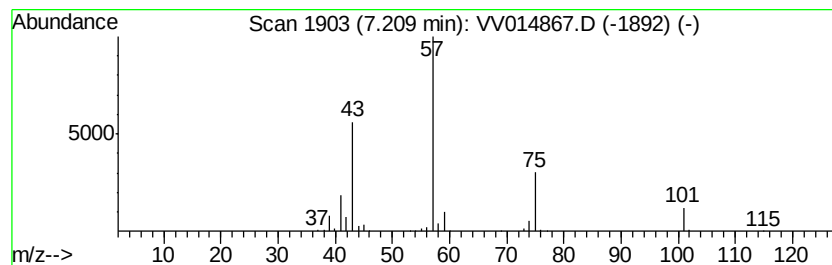
Instrument :
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ClientSampled :
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.21	9.07 ug/L	316595	1,4-Difluorobenzene	5.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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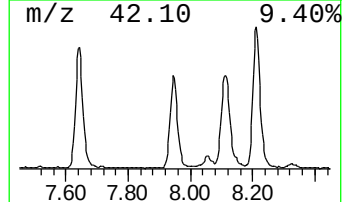
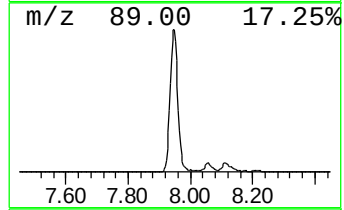
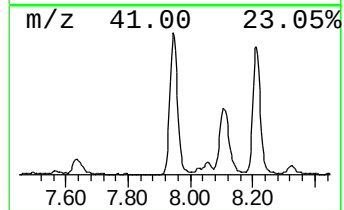
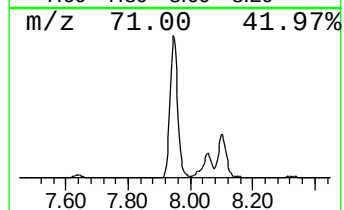
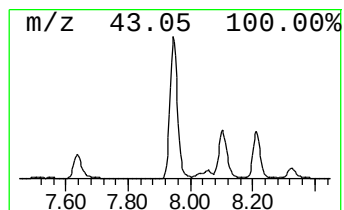
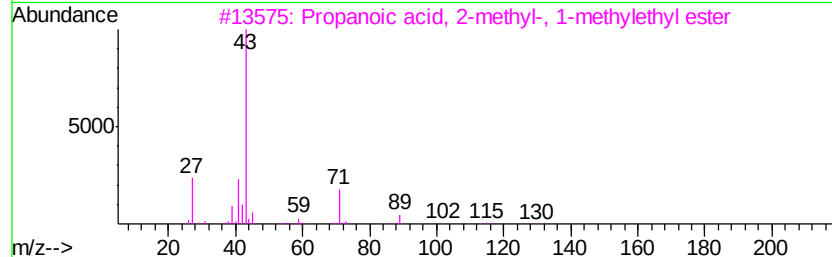
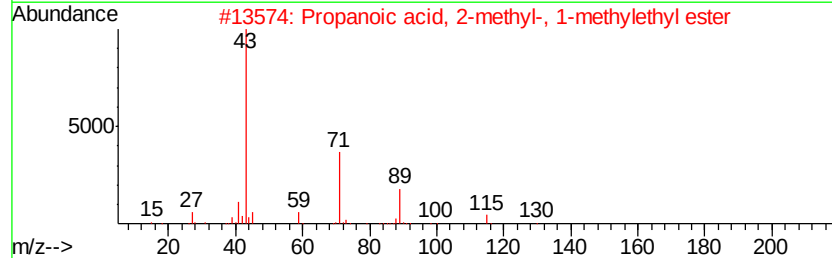
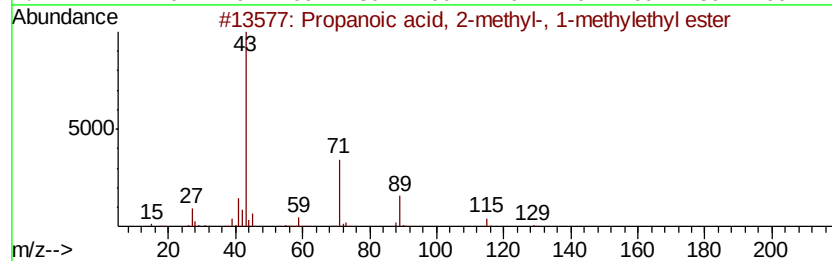
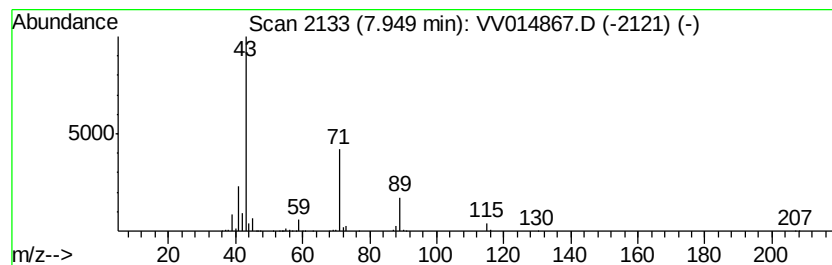
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.95	25.65 ug/L	585847	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83		
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78		
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78		
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64		
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56		



Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031220\
Data File : VV014867.D
Acq On : 12 Mar 2020 14:52
Operator : SY/MD
Sample : PB127467TB
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

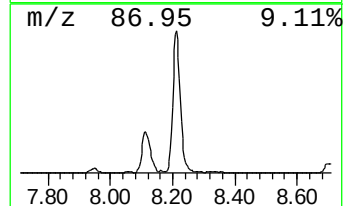
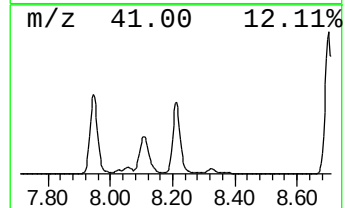
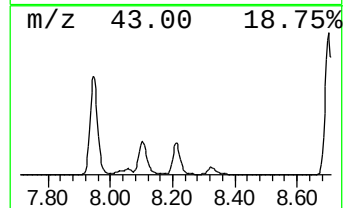
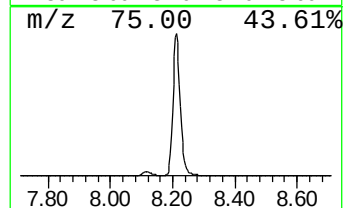
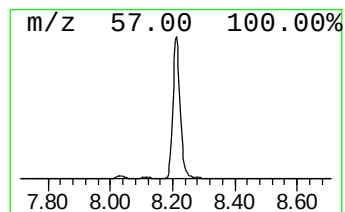
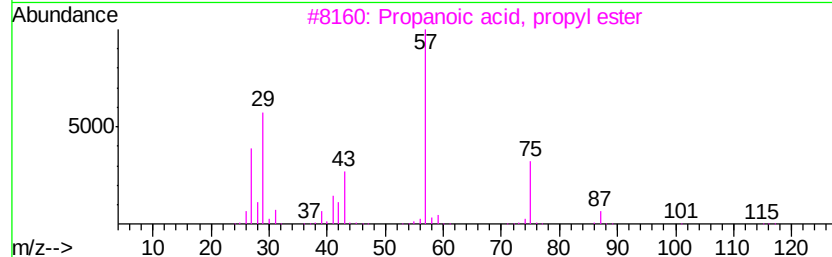
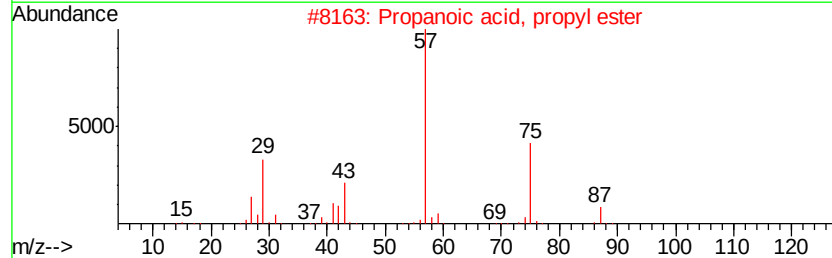
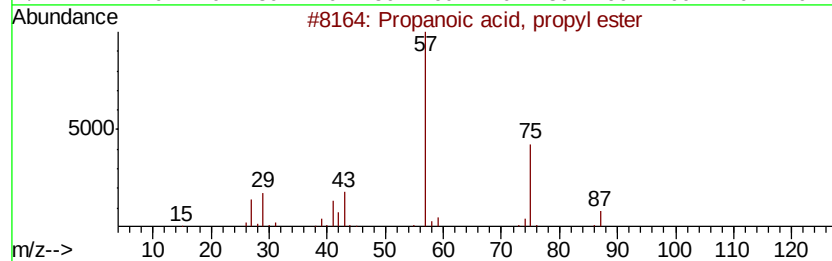
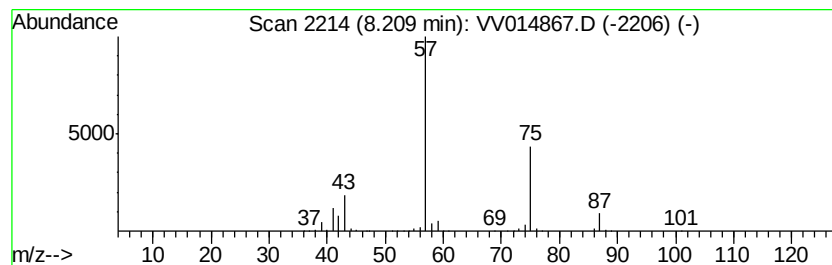
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.21	38.92 ug/L	888993	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031220\
Data File : VV014867.D
Acq On : 12 Mar 2020 14:52
Operator : SY/MD
Sample : PB127467TB
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

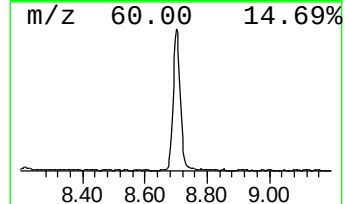
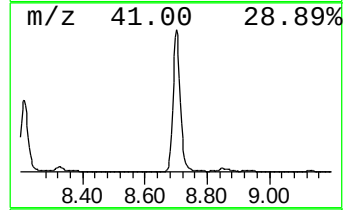
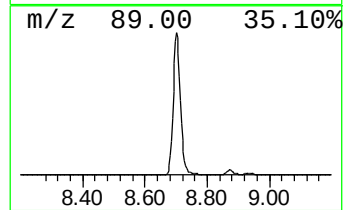
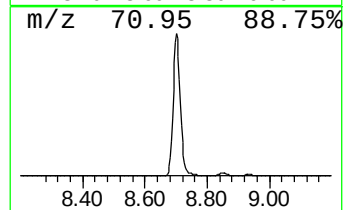
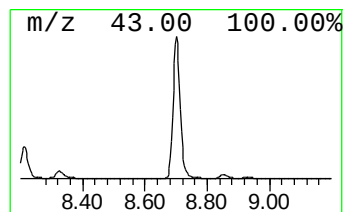
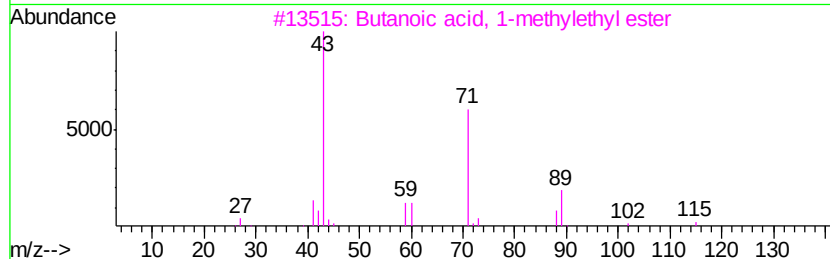
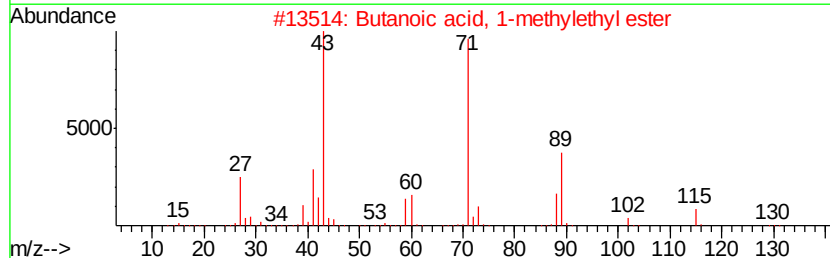
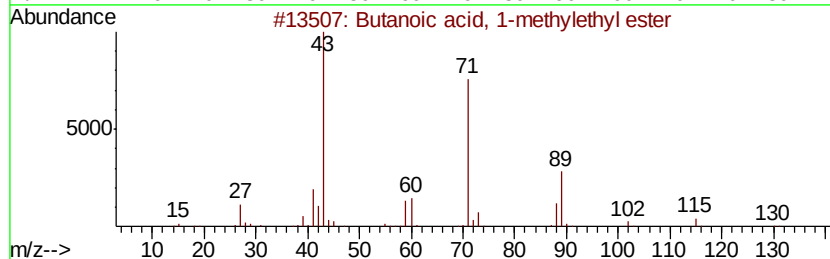
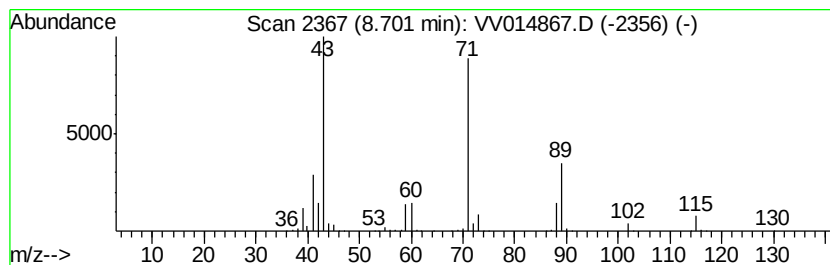
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Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	54.16 ug/L	1237280	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	97
2		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA V\Data\VV031220\
Data File : VV014867.D
Acq On : 12 Mar 2020 14:52
Operator : SY/MD
Sample : PB127467TB
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

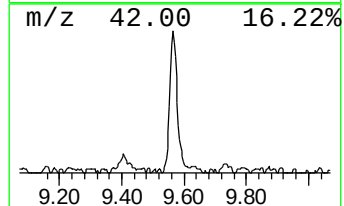
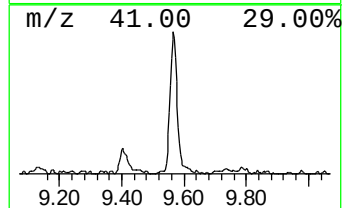
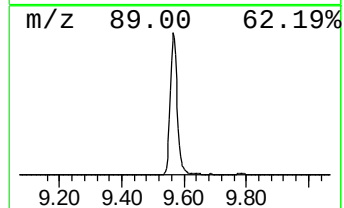
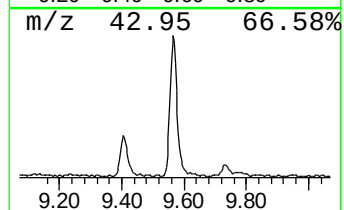
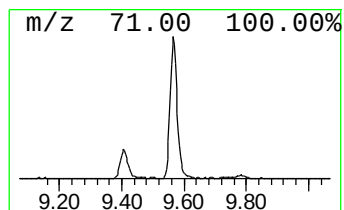
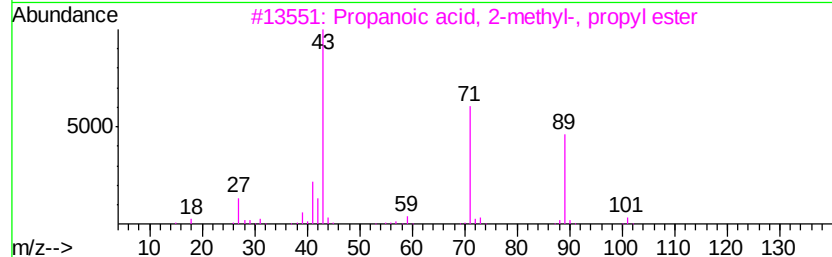
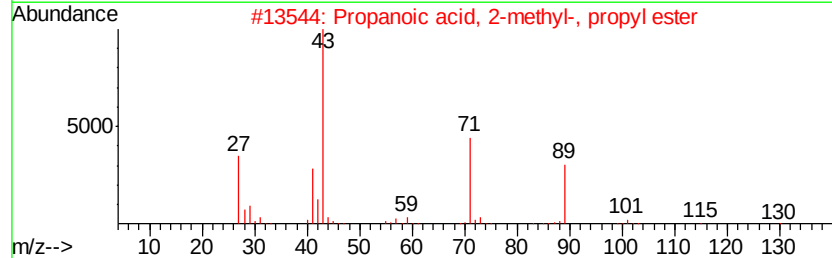
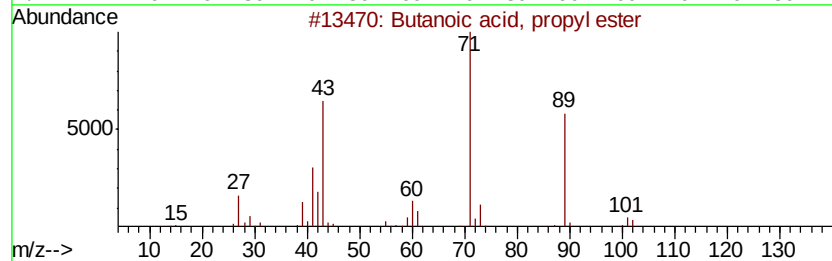
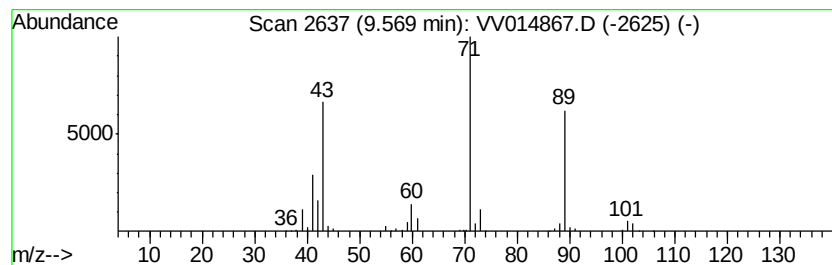
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Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	7.89 ug/L	180307	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
3		Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
4		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5		Malic Acid	134	C4H6O5	006915-15-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031220\
Data File : VV014867.D
Acq On : 12 Mar 2020 14:52
Operator : SY/MD
Sample : PB127467TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl acetate	5.31	3.2	ug/L	111913	1	5.64	1745320	50.0
n-Propyl acetate	6.49	66.3	ug/L	2313690	1	5.64	1745320	50.0
Propanoic acid, 1...	7.21	9.1	ug/L	316595	1	5.64	1745320	50.0
Propanoic acid, 2...	7.95	25.6	ug/L	585847	2	8.87	1142150	50.0
Propanoic acid, p...	8.21	38.9	ug/L	888993	2	8.87	1142150	50.0
Butanoic acid, 1-...	8.70	54.2	ug/L	1237280	2	8.87	1142150	50.0
Butanoic acid, pr...	9.57	7.9	ug/L	180307	2	8.87	1142150	50.0