

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV112919\
 Data File : VV013841.D
 Acq On : 29 Nov 2019 11:49
 Operator : SY/MD
 Sample : K6060-01
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 B0AF1

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\SOMVLM110619WMA.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	1.206	30	36	55	rBV	168158	252628	7.71%	0.947%
2	1.319	65	71	88	rVB	351389	348377	10.63%	1.306%
3	1.582	146	153	165	rVB	301890	335266	10.23%	1.257%
4	2.129	315	323	334	rVB	588781	805135	24.56%	3.019%
5	2.431	413	417	419	rBV4	2711	2170	0.07%	0.008%
6	2.534	442	449	461	rVB2	25232	40481	1.24%	0.152%
7	2.579	461	463	466	rVB3	1433	467	0.01%	0.002%
8	2.643	478	483	486	rBV5	3873	4204	0.13%	0.016%
9	2.737	511	512	514	rBV2	1005	438	0.01%	0.002%
10	2.749	514	516	518	rVV3	1178	578	0.02%	0.002%
11	2.827	538	540	542	rVB3	1412	393	0.01%	0.001%
12	2.930	569	572	573	rBV3	934	397	0.01%	0.001%
13	2.952	578	579	580	rBV	621	203	0.01%	0.001%
14	2.981	586	588	591	rBV4	967	640	0.02%	0.002%
15	3.003	593	595	596	rBV2	1092	288	0.01%	0.001%
16	3.032	602	604	606	rBV3	1691	609	0.02%	0.002%
17	3.061	610	613	615	rBV3	2003	1083	0.03%	0.004%
18	3.087	619	621	624	rVB3	1680	965	0.03%	0.004%
19	3.113	624	629	630	rBV4	1080	904	0.03%	0.003%
20	3.158	637	643	649	rBV10	2114	2392	0.07%	0.009%
21	3.187	649	652	657	rBV4	1383	1243	0.04%	0.005%
22	3.216	657	661	663	rBV3	1730	1462	0.04%	0.005%
23	3.270	676	678	681	rVB3	1020	524	0.02%	0.002%
24	3.293	683	685	687	rBV3	1134	732	0.02%	0.003%
25	3.335	695	698	701	rBV4	1106	932	0.03%	0.003%
26	3.415	720	723	729	rVB7	1470	1775	0.05%	0.007%
27	3.444	729	732	734	rBV2	1335	846	0.03%	0.003%
28	3.505	749	751	755	rBV4	1163	874	0.03%	0.003%
29	3.531	756	759	761	rVV4	1838	955	0.03%	0.004%
30	3.627	787	789	792	rBV4	1281	811	0.02%	0.003%
31	3.679	803	805	806	rBV2	910	361	0.01%	0.001%
32	3.688	806	808	811	rVB3	1393	472	0.01%	0.002%
33	3.711	813	815	817	rBV3	1260	544	0.02%	0.002%
34	3.782	835	837	841	rBV4	734	413	0.01%	0.002%

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 Title : VOC Analysis

35	3.920	867	880	907	rBV	192095	509641	15.55%	1.911%
36	4.267	986	988	990	rBV3	2187	1099	0.03%	0.004%
37	4.399	1012	1029	1052	rBV	420211	1013997	30.94%	3.802%
38	4.682	1115	1117	1118	rBV	1070	369	0.01%	0.001%
39	4.772	1142	1145	1149	rVB6	2085	1350	0.04%	0.005%
40	4.859	1170	1172	1175	rBV4	1375	884	0.03%	0.003%
41	4.884	1178	1180	1181	rBV	1164	551	0.02%	0.002%
42	4.991	1210	1213	1215	rBV4	1587	884	0.03%	0.003%
43	5.090	1223	1244	1273	rBV2	985803	2503761	76.39%	9.387%
44	5.322	1307	1316	1340	rVB2	78268	162509	4.96%	0.609%
45	5.659	1407	1421	1441	rBV	740931	1468396	44.80%	5.505%
46	6.113	1551	1562	1588	rVB	566057	1125213	34.33%	4.219%
47	6.498	1671	1682	1712	rBV	1850756	3277735	100.00%	12.289%
48	7.026	1835	1846	1862	rBV	320391	561855	17.14%	2.107%
49	7.222	1898	1907	1919	rBV	220932	365088	11.14%	1.369%
50	7.357	1937	1949	1988	rVB	1234094	2160246	65.91%	8.099%
51	7.659	2033	2043	2060	rVB2	282150	484572	14.78%	1.817%
52	7.961	2126	2137	2153	rBV	390643	654893	19.98%	2.455%
53	8.125	2178	2188	2209	rBV2	767525	1350278	41.20%	5.063%
54	8.225	2211	2219	2240	rVB	735742	1151804	35.14%	4.318%
55	8.717	2361	2372	2396	rBV	877295	1410274	43.03%	5.287%
56	8.891	2415	2426	2440	rBV	1189346	1864892	56.90%	6.992%
57	9.244	2532	2536	2541	rBV8	2208	2620	0.08%	0.010%
58	9.585	2631	2642	2660	rBV	88738	157594	4.81%	0.591%
59	9.756	2687	2695	2699	rBV7	4121	6311	0.19%	0.024%
60	10.055	2787	2788	2789	rBV	896	340	0.01%	0.001%
61	10.257	2833	2851	2869	rBV	771259	1233336	37.63%	4.624%
62	10.476	2916	2919	2922	rVB5	1450	978	0.03%	0.004%
63	10.524	2932	2934	2937	rBV3	1717	1157	0.04%	0.004%
64	10.984	3075	3077	3079	rVB3	1739	693	0.02%	0.003%
65	10.997	3079	3081	3082	rBV2	761	346	0.01%	0.001%
66	11.084	3106	3108	3110	rBV2	770	402	0.01%	0.002%
67	11.125	3118	3121	3123	rBV4	1810	1305	0.04%	0.005%
68	11.157	3129	3131	3132	rBV2	1257	572	0.02%	0.002%
69	11.199	3142	3144	3146	rBV3	1859	889	0.03%	0.003%
70	11.289	3159	3172	3192	rBV	1030835	1592145	48.57%	5.969%
71	11.601	3267	3269	3274	rVB5	1373	1109	0.03%	0.004%

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72	11.666	3274	3289	3309	rBV	1108243	1765449	53.86%	6.619%
73	12.000	3391	3393	3394	rBV2	825	371	0.01%	0.001%
74	12.045	3405	3407	3410	rBV3	1218	934	0.03%	0.004%
75	12.093	3420	3422	3424	rBV3	1222	555	0.02%	0.002%
76	12.125	3431	3432	3434	rBV2	619	313	0.01%	0.001%
77	12.135	3434	3435	3438	rVB3	1230	486	0.01%	0.002%
78	12.151	3438	3440	3442	rBV3	1427	674	0.02%	0.003%
79	12.190	3450	3452	3454	rBV3	1286	750	0.02%	0.003%
80	12.344	3498	3500	3504	rBV3	1196	813	0.02%	0.003%
81	12.569	3568	3570	3574	rBV4	1323	889	0.03%	0.003%
82	12.685	3603	3606	3607	rBV3	2712	1329	0.04%	0.005%
83	12.887	3665	3669	3677	rBV9	1608	1788	0.05%	0.007%
84	12.919	3677	3679	3682	rBV2	1430	878	0.03%	0.003%
85	12.952	3687	3689	3691	rBV3	1159	726	0.02%	0.003%
86	13.006	3700	3706	3707	rBV3	991	1015	0.03%	0.004%
87	13.064	3721	3724	3727	rBV4	1575	784	0.02%	0.003%
88	13.418	3833	3834	3836	rBV2	684	181	0.01%	0.001%
89	13.434	3836	3839	3847	rBV7	2121	2714	0.08%	0.010%
90	13.537	3869	3871	3873	rBV3	1440	753	0.02%	0.003%
91	13.646	3903	3905	3908	rBV2	964	524	0.02%	0.002%
92	13.794	3945	3951	3955	rBV8	2857	3169	0.10%	0.012%
93	13.890	3978	3981	3985	rBV4	1884	1584	0.05%	0.006%
94	13.945	3995	3998	4001	rBV5	2045	1408	0.04%	0.005%
95	14.061	4032	4034	4037	rBV4	2009	1221	0.04%	0.005%
96	14.595	4198	4200	4201	rBV3	1582	665	0.02%	0.002%
97	14.823	4269	4271	4275	rBV4	1550	1057	0.03%	0.004%
98	14.842	4275	4277	4280	rBV2	2009	1244	0.04%	0.005%

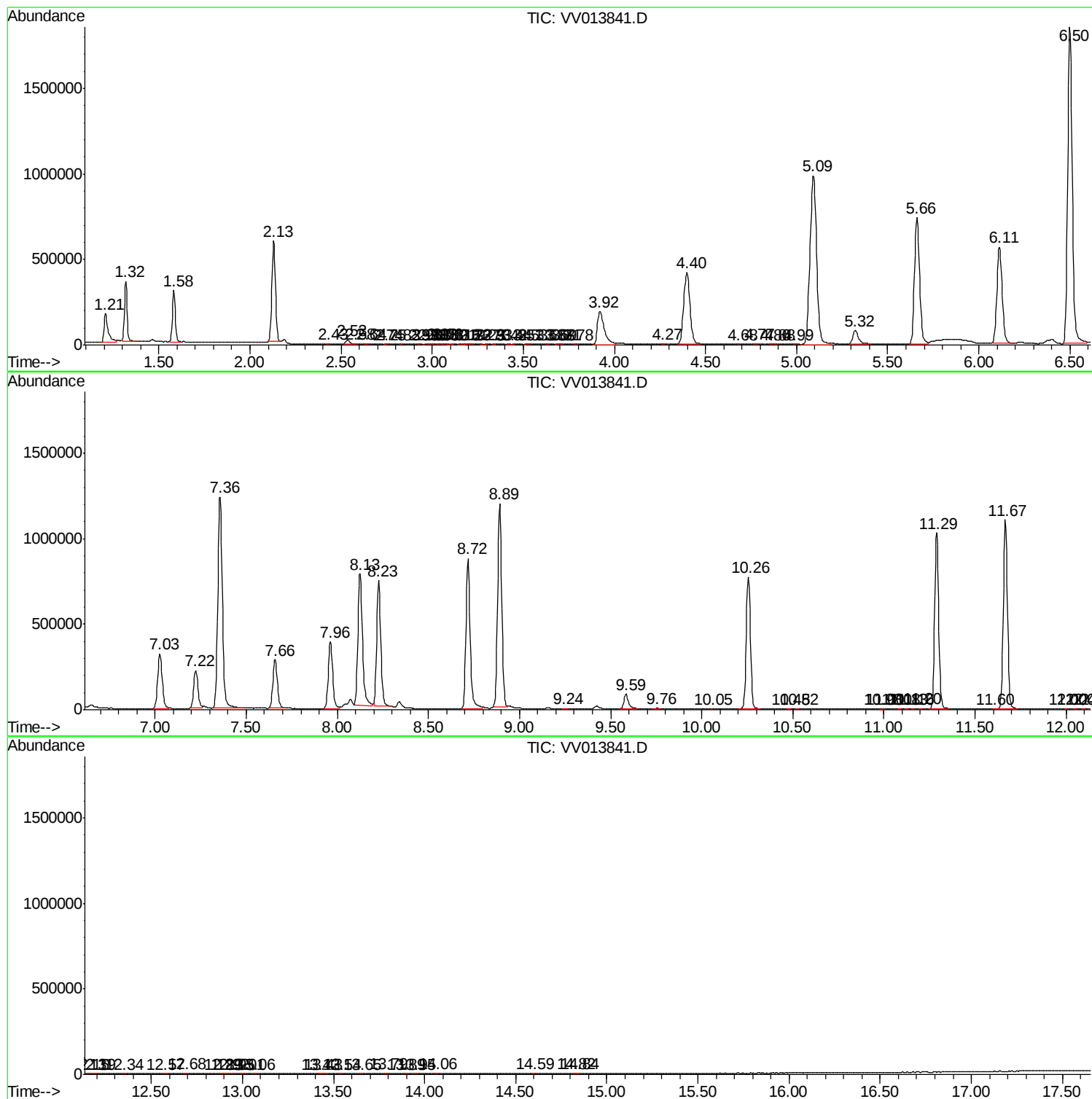
Sum of corrected areas: 26671924

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TIC Library : C:\DATABASE\NIST11.L
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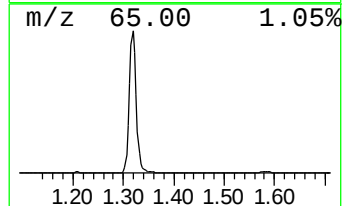
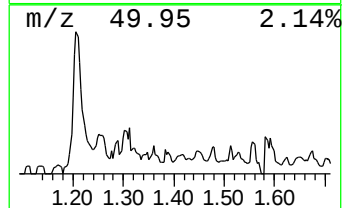
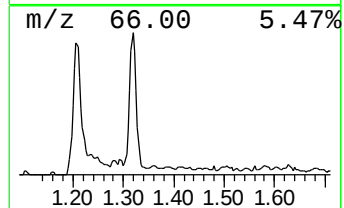
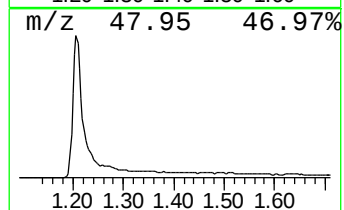
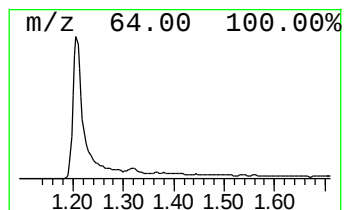
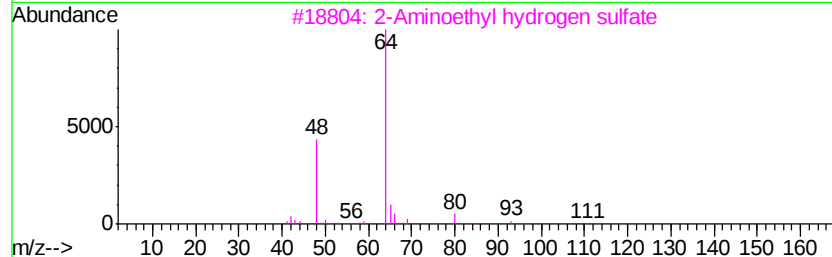
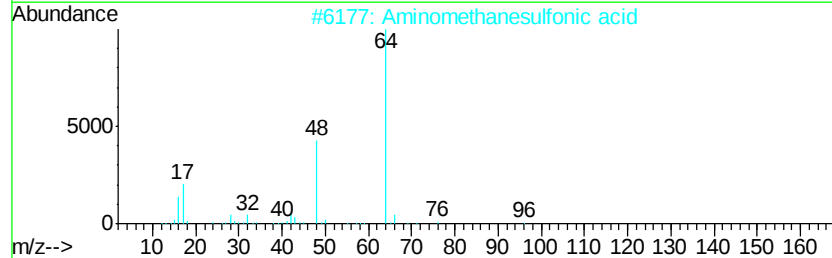
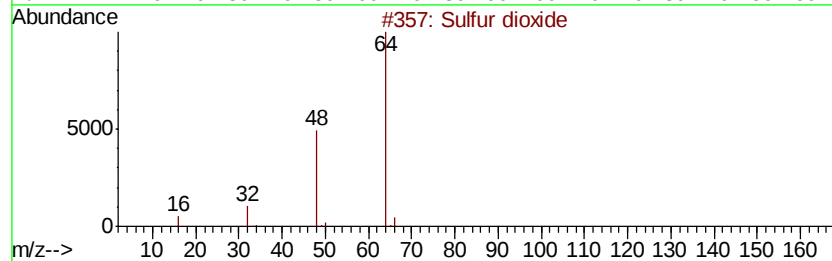
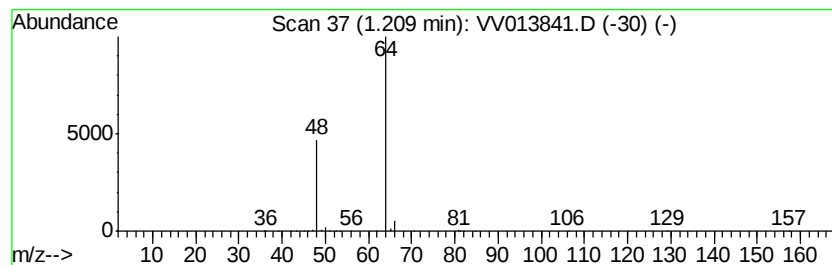
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM110619WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.21	8.60 ug/L	252628	1,4-Difluorobenzene	5.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Sulfur dioxide	64 02S	007446-09-5 83
2		Aminomethanesulfonic acid	111 CH5N03S	013881-91-9 74
3		2-Aminoethyl hydrogen sulfate	141 C2H7N04S	000926-39-6 74
4		L-Alanine, 3-sulfo-	169 C3H7N05S	000498-40-8 9
5		Sulfur dioxide	64 02S	007446-09-5 5



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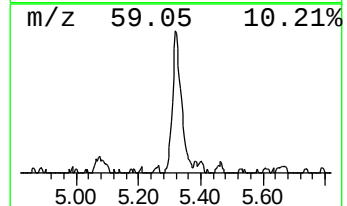
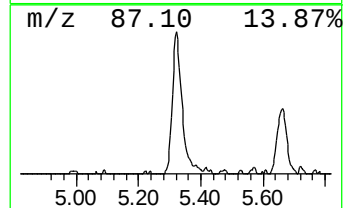
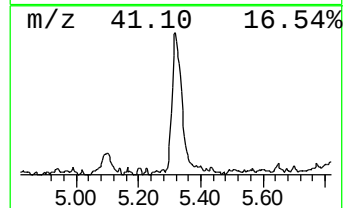
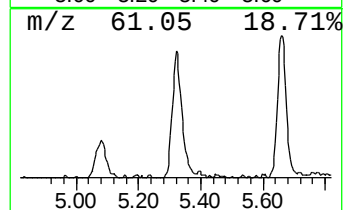
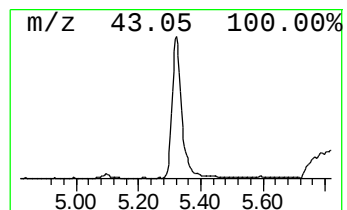
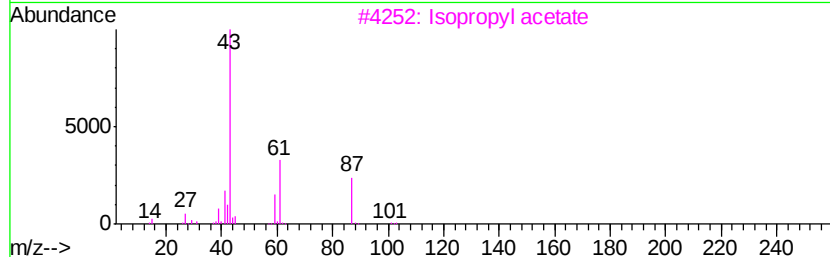
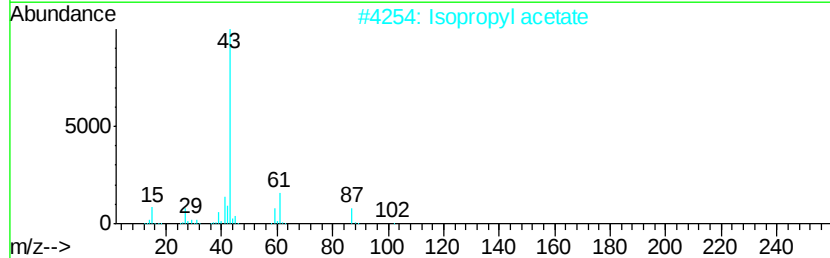
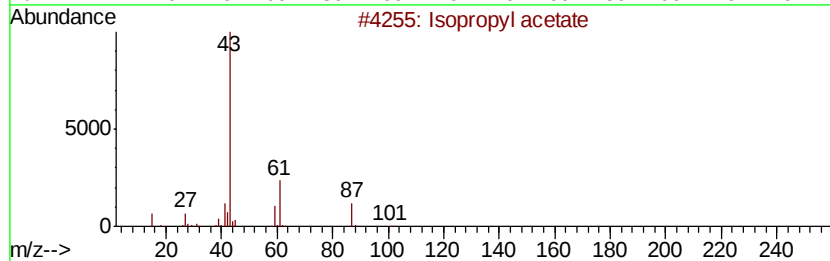
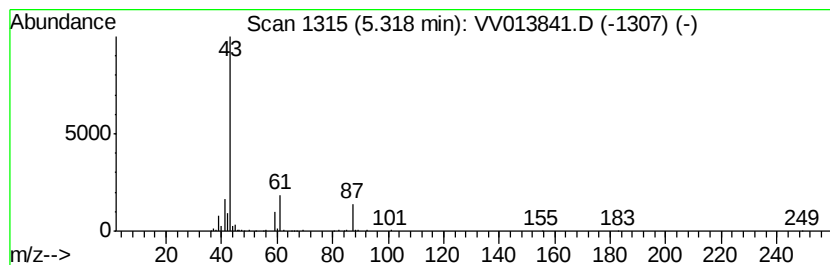
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	5.53 ug/L	162509	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	72
2		Isopropyl acetate	102	C5H10O2	000108-21-4	64
3		Isopropyl acetate	102	C5H10O2	000108-21-4	59
4		Isopropyl acetate	102	C5H10O2	000108-21-4	28
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28



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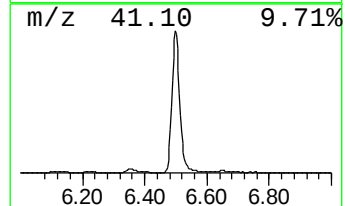
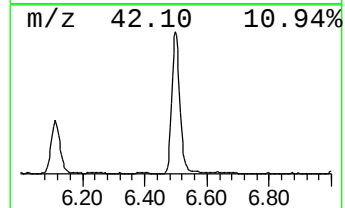
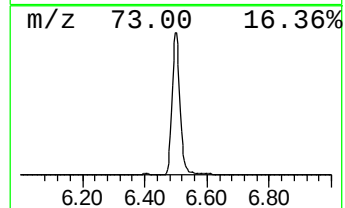
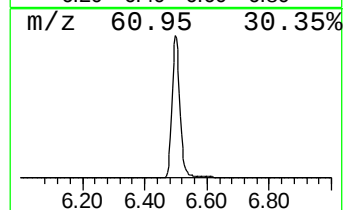
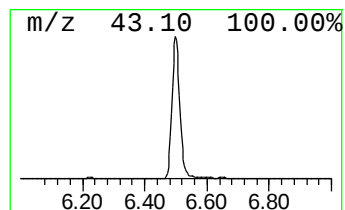
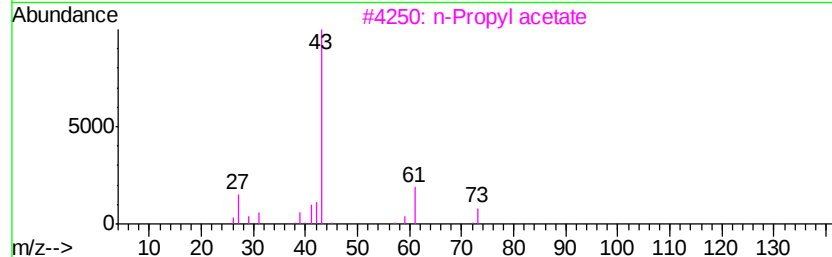
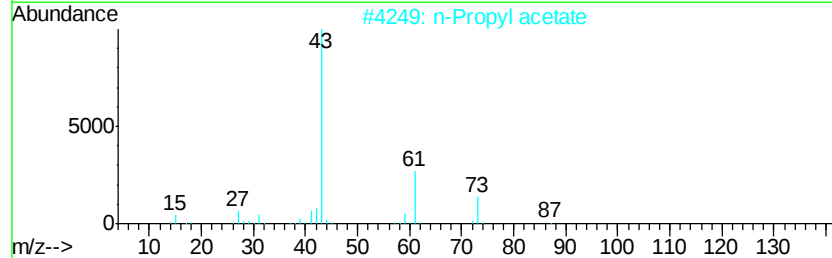
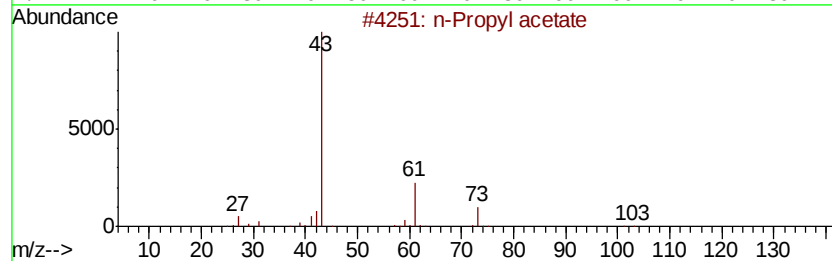
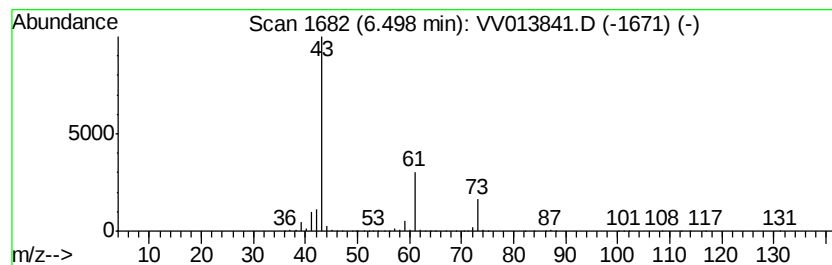
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Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	111.61 ug/L	3277740	1,4-Difluorobenzene	5.66

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	n-Propyl	acetate	102	C5H10O2	000109-60-4	78
4	Isopropyl	acetate	102	C5H10O2	000108-21-4	36
5	Isobutyl	acetate	116	C6H12O2	000110-19-0	9



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Operator : SY/MD
Sample : K6060-01
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
B0AF1

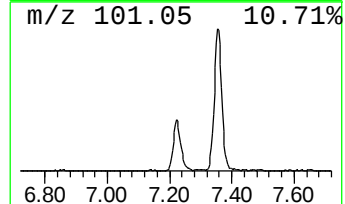
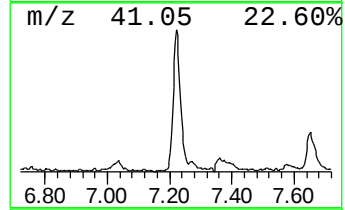
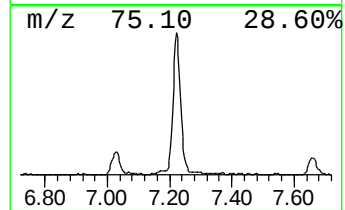
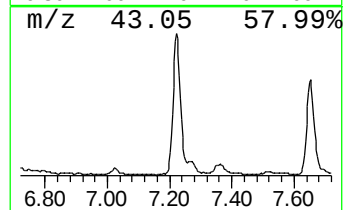
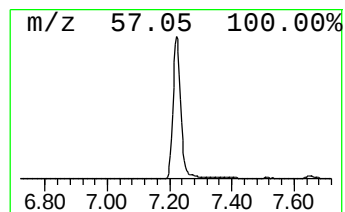
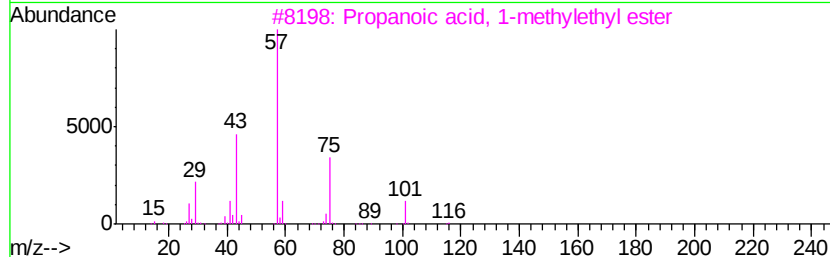
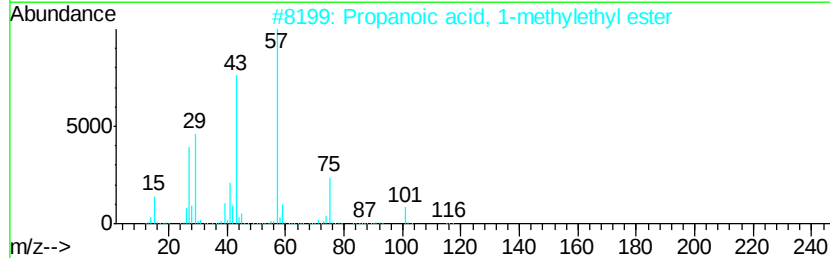
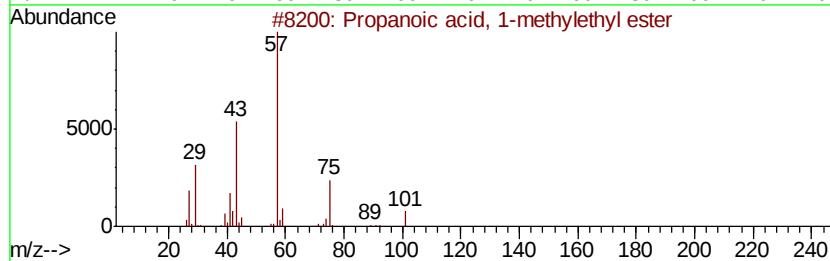
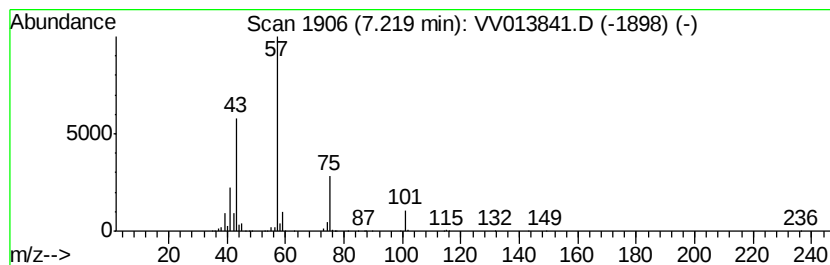
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	12.43 ug/L	365088	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV112919\
Data File : VV013841.D
Acq On : 29 Nov 2019 11:49
Operator : SY/MD
Sample : K6060-01
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
B0AF1

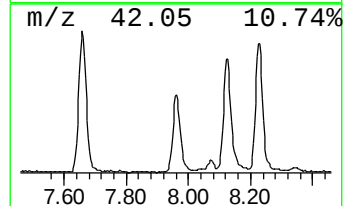
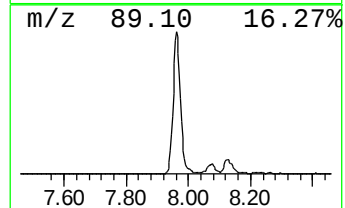
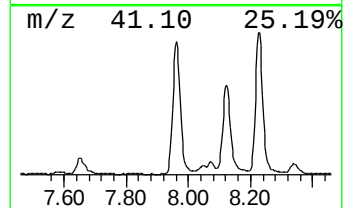
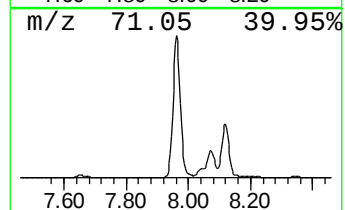
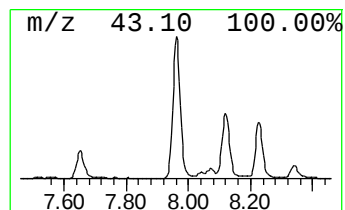
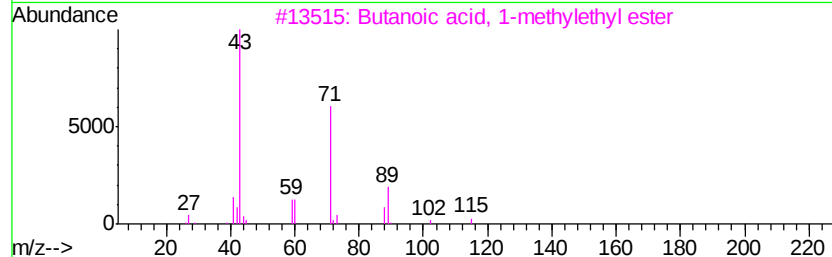
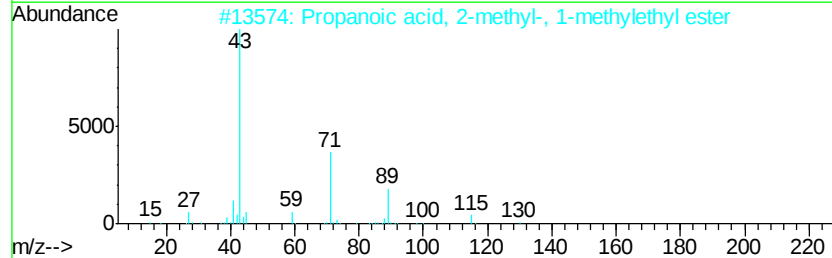
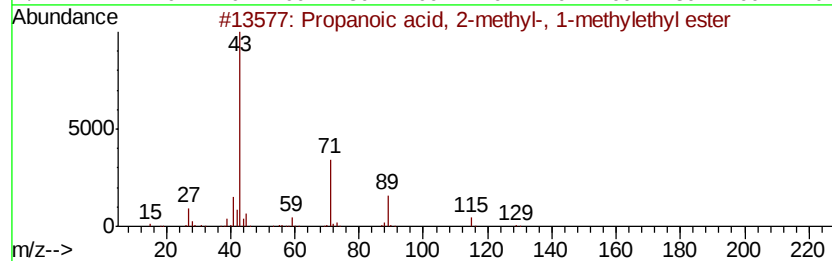
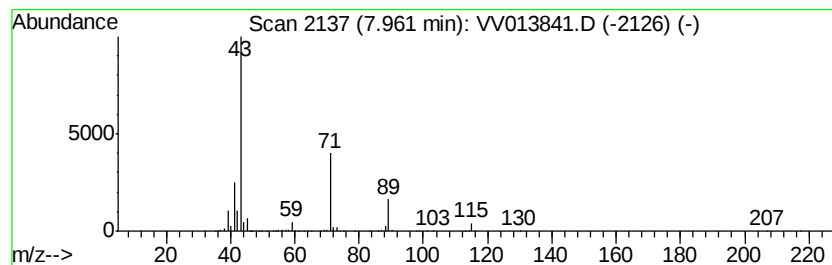
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	17.56 ug/L	654893	Chlorobenzene-d5	8.89

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	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72	
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64	
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV112919\
Data File : VV013841.D
Acq On : 29 Nov 2019 11:49
Operator : SY/MD
Sample : K6060-01
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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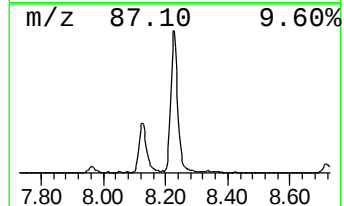
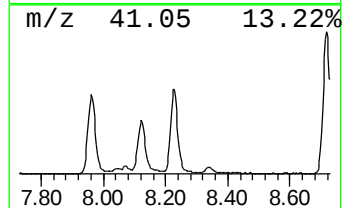
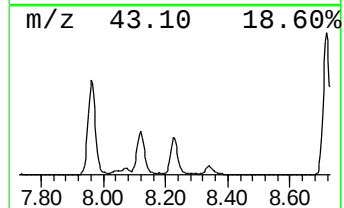
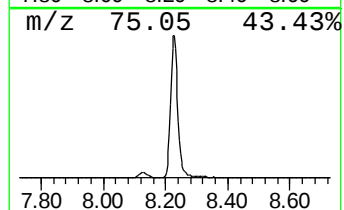
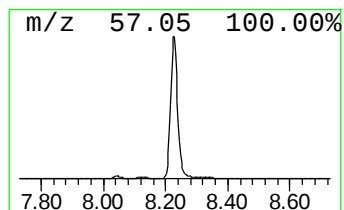
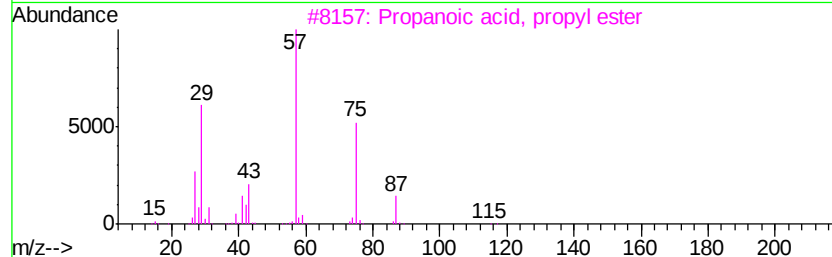
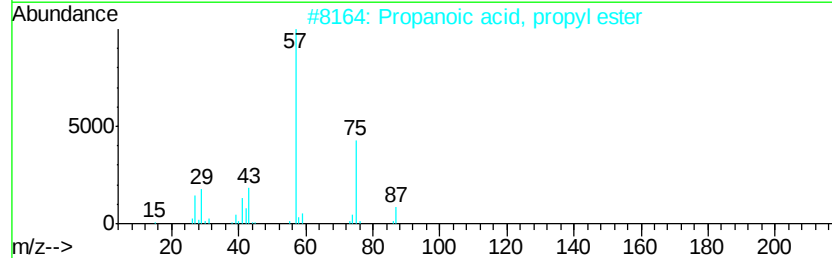
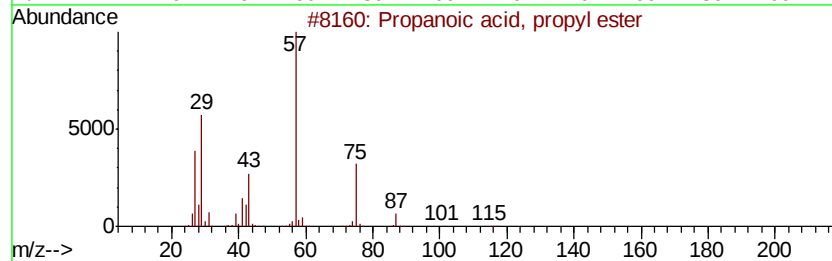
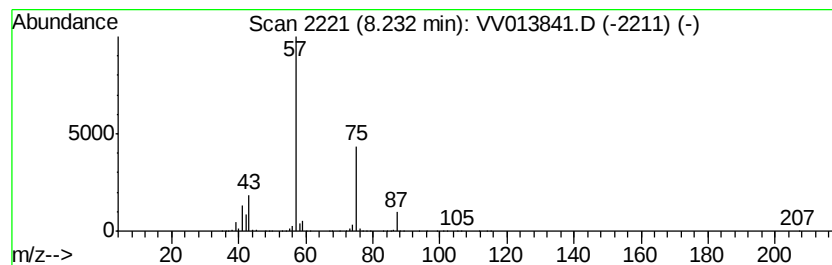
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Quant Title : VOC Analysis

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	30.88 ug/L	1151800	Chlorobenzene-d5	8.89

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	83
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV112919\
Data File : VV013841.D
Acq On : 29 Nov 2019 11:49
Operator : SY/MD
Sample : K6060-01
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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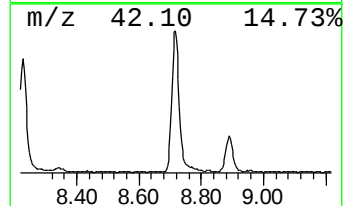
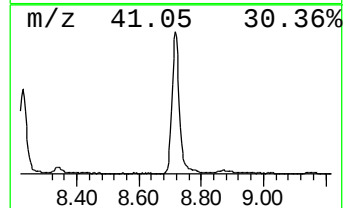
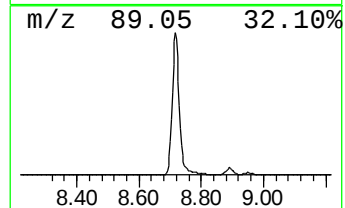
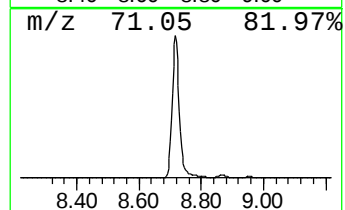
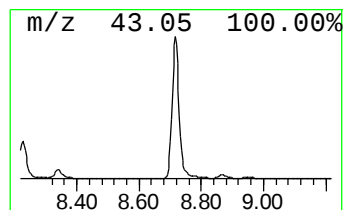
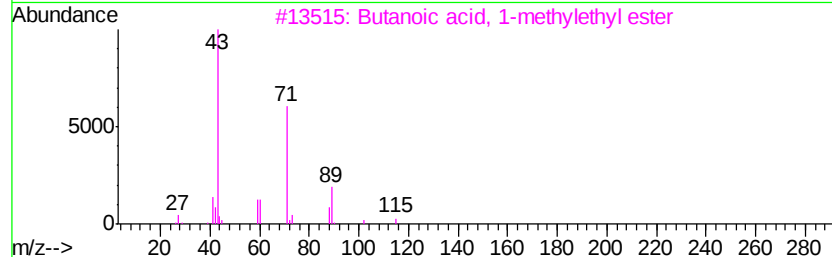
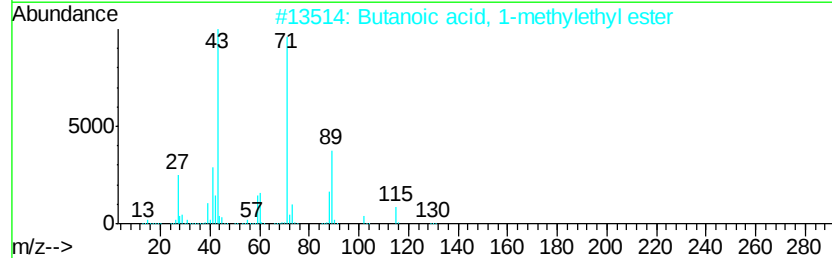
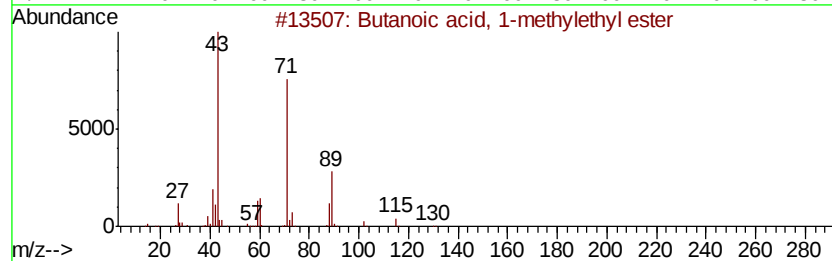
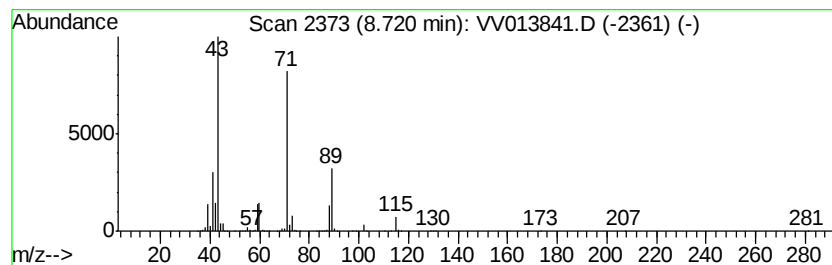
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Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	37.81 ug/L	1410270	Chlorobenzene-d5	8.89

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	78
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV112919\
Data File : VV013841.D
Acq On : 29 Nov 2019 11:49
Operator : SY/MD
Sample : K6060-01
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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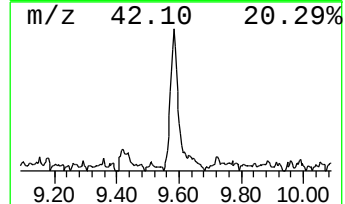
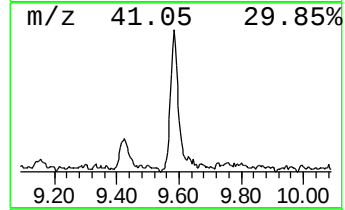
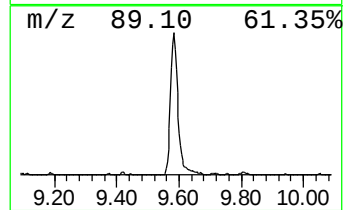
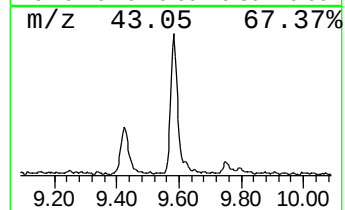
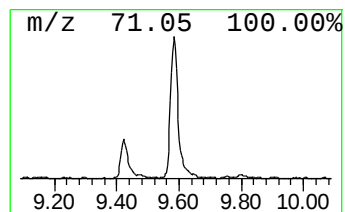
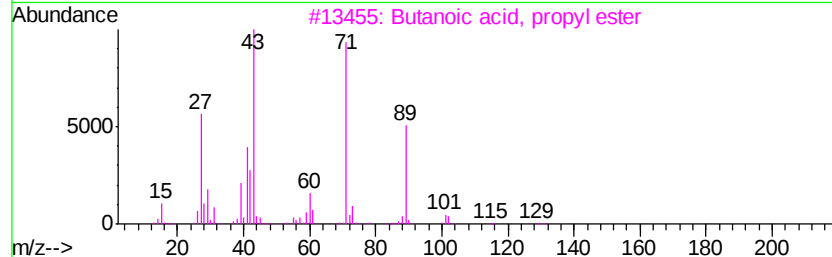
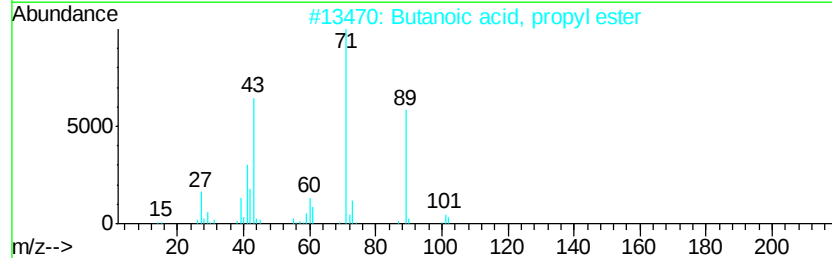
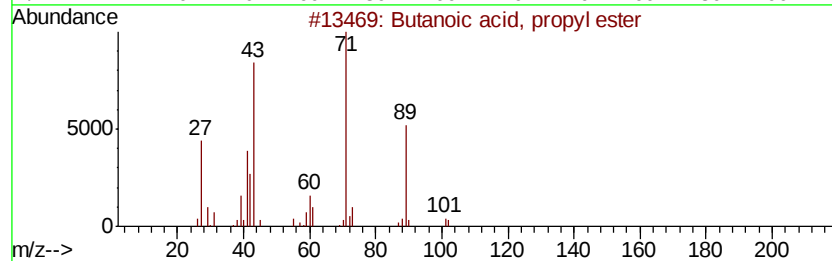
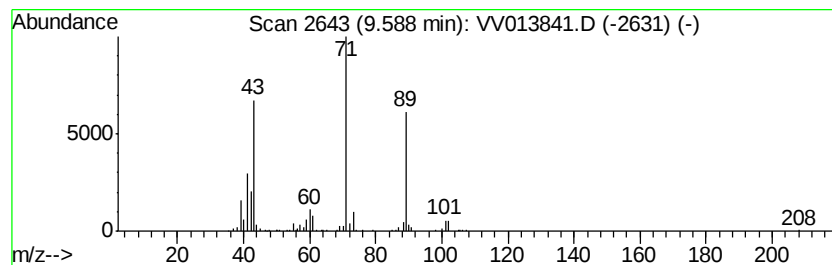
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Quant Title : VOC Analysis

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

Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	4.23 ug/L	157594	Chlorobenzene-d5	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
5		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV112919\
Data File : VV013841.D
Acq On : 29 Nov 2019 11:49
Operator : SY/MD
Sample : K6060-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
B0AF1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM110619WMA.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
Sulfur dioxide	1.21	8.6	ug/L	252628	1	5.66	1468400	50.0
Isopropyl acetate	5.32	5.5	ug/L	162509	1	5.66	1468400	50.0
n-Propyl acetate	6.50	111.6	ug/L	3277740	1	5.66	1468400	50.0
Propanoic acid, 1...	7.22	12.4	ug/L	365088	1	5.66	1468400	50.0
Propanoic acid, 2...	7.96	17.6	ug/L	654893	2	8.89	1864890	50.0
Propanoic acid, p...	8.23	30.9	ug/L	1151800	2	8.89	1864890	50.0
Butanoic acid, 1-...	8.72	37.8	ug/L	1410270	2	8.89	1864890	50.0
Butanoic acid, pr...	9.59	4.2	ug/L	157594	2	8.89	1864890	50.0