

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061819\
 Data File : VU032829.D
 Acq On : 18 Jun 2019 17:07
 Operator : JC/SP
 Sample : K3363-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JP6

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_U\METHOD\SOMULM061719WMA.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	1.180	24	28	35	rBV	4611	3740	0.26%	0.034%
2	1.396	88	95	107	rVB	126459	123982	8.71%	1.139%
3	1.675	174	182	198	rVB	97762	118719	8.34%	1.091%
4	2.267	355	366	377	rBV	205887	304610	21.40%	2.798%
5	2.428	413	416	418	rBV3	511	306	0.02%	0.003%
6	2.553	452	455	462	rVB3	728	516	0.04%	0.005%
7	2.617	465	475	483	rBV3	2590	4511	0.32%	0.041%
8	2.695	491	499	510	rVB2	7937	13205	0.93%	0.121%
9	2.740	510	513	517	rBV4	383	310	0.02%	0.003%
10	2.817	533	537	539	rBV2	533	499	0.04%	0.005%
11	3.077	615	618	626	rVB4	382	493	0.03%	0.005%
12	3.174	643	648	652	rBV2	386	334	0.02%	0.003%
13	3.212	658	660	667	rVB2	500	354	0.02%	0.003%
14	3.251	667	672	677	rBV2	425	399	0.03%	0.004%
15	3.370	704	709	713	rBV2	420	378	0.03%	0.003%
16	3.421	722	725	728	rBV3	365	269	0.02%	0.002%
17	3.627	784	789	792	rBV2	296	273	0.02%	0.003%
18	3.891	866	871	876	rBV4	387	503	0.04%	0.005%
19	4.003	900	906	909	rBV3	422	384	0.03%	0.004%
20	4.170	945	958	982	rBV	86904	224782	15.79%	2.065%
21	4.640	1085	1104	1125	rBV	154124	362722	25.49%	3.332%
22	4.743	1133	1136	1140	rBV2	515	354	0.02%	0.003%
23	4.878	1172	1178	1183	rBV3	544	743	0.05%	0.007%
24	4.984	1205	1211	1214	rBV4	469	463	0.03%	0.004%
25	5.103	1243	1248	1252	rBV2	293	245	0.02%	0.002%
26	5.331	1294	1319	1345	rBV2	310852	915515	64.33%	8.410%
27	5.547	1377	1386	1398	rVV	5459	11531	0.81%	0.106%
28	5.653	1415	1419	1422	rBV3	395	322	0.02%	0.003%
29	5.675	1422	1426	1430	rVV2	403	297	0.02%	0.003%
30	5.807	1463	1467	1473	rBV3	427	499	0.04%	0.005%
31	5.881	1476	1490	1516	rBV	282744	548870	38.57%	5.042%
32	6.048	1535	1542	1545	rBV7	769	932	0.07%	0.009%
33	6.167	1576	1579	1580	rBV2	746	391	0.03%	0.004%
34	6.225	1595	1597	1600	rVB2	431	267	0.02%	0.002%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
 Title : VOC Analysis

35	6.325	1613	1628	1647	rBV	210648	417101	29.31%	3.831%
36	6.421	1650	1658	1667	rBV	6203	10914	0.77%	0.100%
37	6.530	1685	1692	1696	rBV2	2600	3861	0.27%	0.035%
38	6.572	1700	1705	1712	rBV	4522	6817	0.48%	0.063%
39	6.698	1731	1744	1780	rBV	804260	1423211	100.00%	13.074%
40	6.977	1830	1831	1837	rVB4	701	484	0.03%	0.004%
41	7.016	1837	1843	1849	rVB3	394	461	0.03%	0.004%
42	7.064	1854	1858	1861	rBV	344	284	0.02%	0.003%
43	7.106	1866	1871	1877	rVB2	651	762	0.05%	0.007%
44	7.222	1895	1907	1930	rBV	108773	192464	13.52%	1.768%
45	7.415	1951	1967	1990	rBV	143675	250192	17.58%	2.298%
46	7.559	1998	2012	2029	rBV	432901	753237	52.93%	6.919%
47	7.701	2050	2056	2065	rVB5	1949	3321	0.23%	0.031%
48	7.842	2089	2100	2122	rBV2	90751	157815	11.09%	1.450%
49	8.006	2147	2151	2154	rVB3	349	269	0.02%	0.002%
50	8.148	2183	2195	2211	rVV	79780	132490	9.31%	1.217%
51	8.225	2211	2219	2221	rVV2	9314	11232	0.79%	0.103%
52	8.257	2223	2229	2235	rVV	34210	53133	3.73%	0.488%
53	8.305	2235	2244	2265	rVV	301274	521405	36.64%	4.790%
54	8.408	2266	2276	2302	rVV	594353	945281	66.42%	8.683%
55	8.521	2303	2311	2332	rVB	41215	70373	4.94%	0.646%
56	8.691	2361	2364	2368	rBV	537	389	0.03%	0.004%
57	8.720	2371	2373	2379	rBV3	399	394	0.03%	0.004%
58	8.897	2416	2428	2447	rBV	401934	627085	44.06%	5.760%
59	9.083	2470	2486	2514	rBV	426678	709525	49.85%	6.518%
60	9.373	2572	2576	2584	rVB3	675	874	0.06%	0.008%
61	9.421	2588	2591	2593	rBV3	348	261	0.02%	0.002%
62	9.556	2630	2633	2636	rVV2	453	276	0.02%	0.003%
63	9.601	2636	2647	2658	rVV3	5704	9982	0.70%	0.092%
64	9.762	2685	2697	2718	rBV	24087	38703	2.72%	0.356%
65	9.903	2739	2741	2744	rBV2	413	247	0.02%	0.002%
66	9.987	2764	2767	2776	rVB4	389	492	0.03%	0.005%
67	10.106	2796	2804	2809	rBV3	578	897	0.06%	0.008%
68	10.279	2851	2858	2862	rBV3	470	672	0.05%	0.006%
69	10.312	2864	2868	2870	rBV2	318	262	0.02%	0.002%
70	10.427	2891	2904	2929	rVB	297280	481682	33.84%	4.425%
71	10.534	2934	2937	2939	rBV	372	257	0.02%	0.002%

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72	10.617	2961	2963	2969	rVB4	373	270	0.02%	0.002%
73	10.672	2976	2980	2991	rBV3	482	666	0.05%	0.006%
74	10.765	3003	3009	3010	rBV2	375	292	0.02%	0.003%
75	10.807	3019	3022	3029	rVB3	270	296	0.02%	0.003%
76	10.852	3033	3036	3041	rVB2	487	378	0.03%	0.003%
77	11.048	3090	3097	3101	rBV3	331	425	0.03%	0.004%
78	11.222	3147	3151	3154	rBV2	355	258	0.02%	0.002%
79	11.286	3164	3171	3173	rBV2	353	320	0.02%	0.003%
80	11.418	3207	3212	3219	rBV4	512	589	0.04%	0.005%
81	11.479	3219	3231	3253	rBV	441077	700504	49.22%	6.435%
82	11.710	3301	3303	3311	rVB3	683	543	0.04%	0.005%
83	11.768	3318	3321	3323	rBV3	524	327	0.02%	0.003%
84	11.855	3335	3348	3370	rBV	428276	706477	49.64%	6.490%
85	12.167	3444	3445	3448	rBV	417	263	0.02%	0.002%
86	12.431	3525	3527	3530	rVB2	489	270	0.02%	0.002%
87	12.472	3535	3540	3541	rBV2	458	362	0.03%	0.003%
88	12.749	3624	3626	3629	rBV2	472	262	0.02%	0.002%
89	12.771	3630	3633	3636	rVV3	420	280	0.02%	0.003%
90	12.791	3636	3639	3644	rVV3	495	360	0.03%	0.003%
91	12.868	3661	3663	3667	rVB2	428	265	0.02%	0.002%
92	13.305	3792	3799	3803	rBV	419	606	0.04%	0.006%
93	13.710	3923	3925	3929	rBV3	387	315	0.02%	0.003%
94	13.794	3948	3951	3955	rBV3	663	464	0.03%	0.004%
95	13.916	3987	3989	3993	rVB3	779	443	0.03%	0.004%
96	14.096	4043	4045	4050	rVB	491	349	0.02%	0.003%
97	14.148	4058	4061	4067	rBV3	310	318	0.02%	0.003%
98	14.630	4209	4211	4213	rBV3	574	300	0.02%	0.003%
99	14.649	4214	4217	4218	rBV3	804	428	0.03%	0.004%
100	14.942	4305	4308	4311	rBV4	863	680	0.05%	0.006%

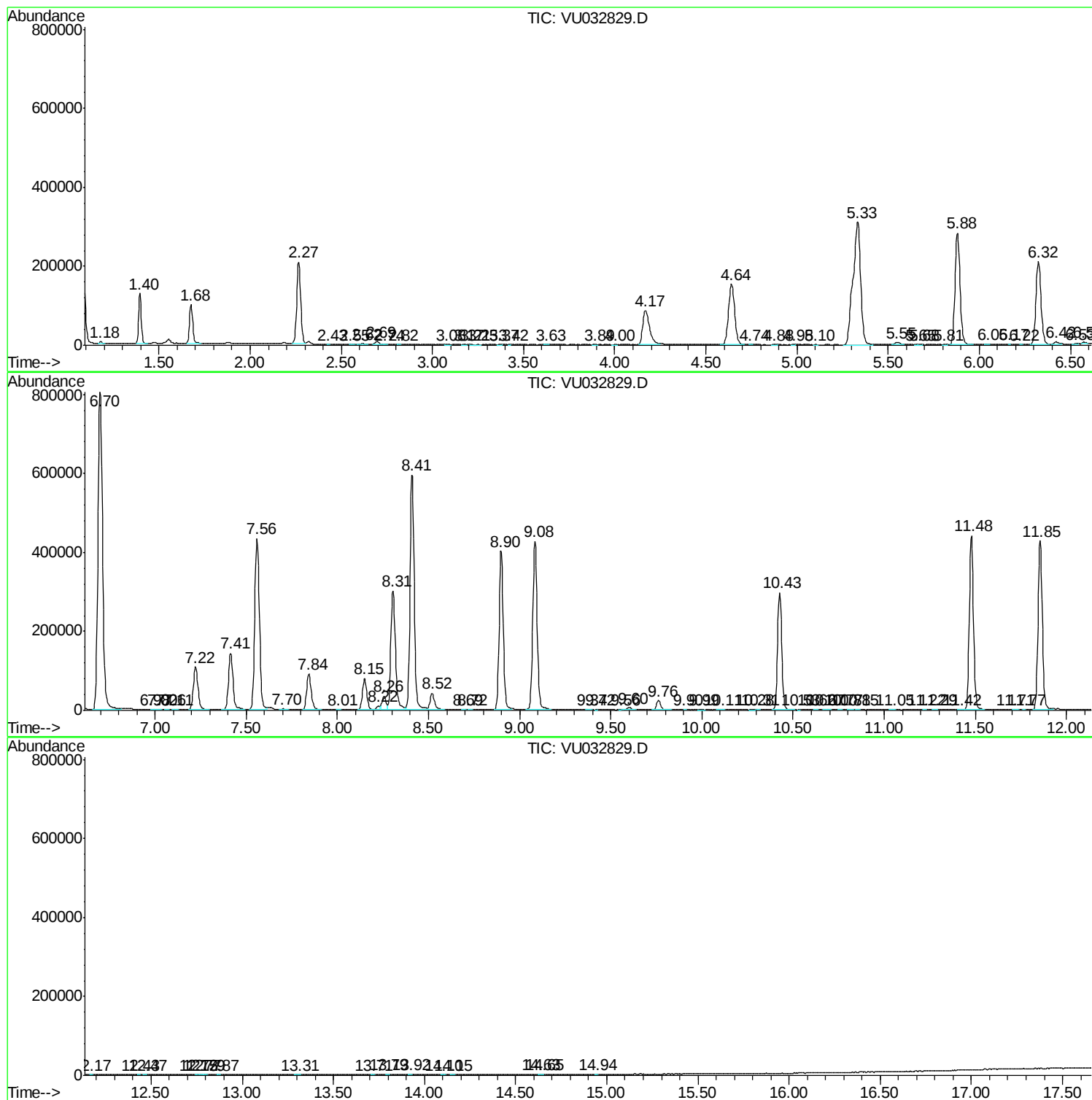
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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



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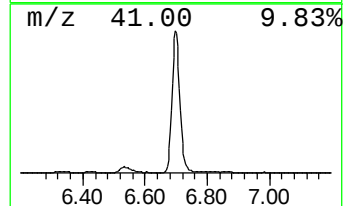
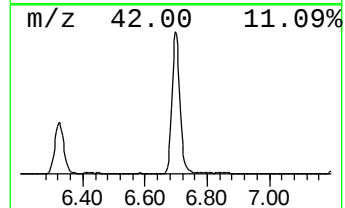
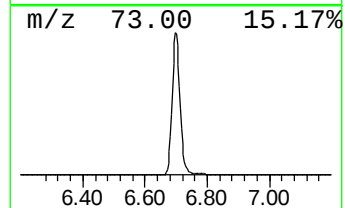
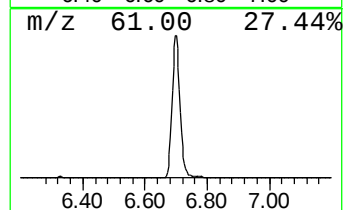
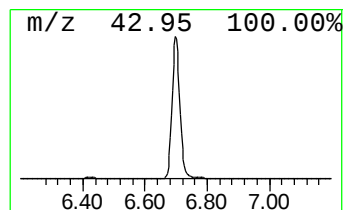
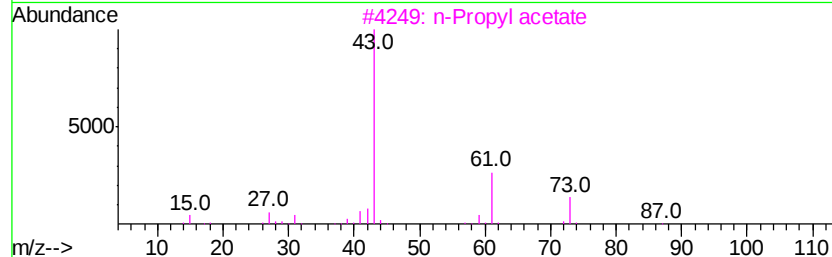
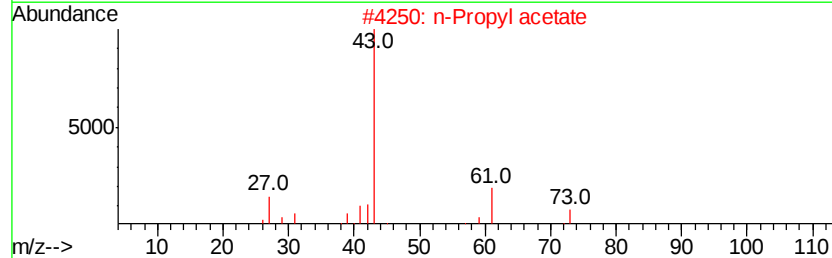
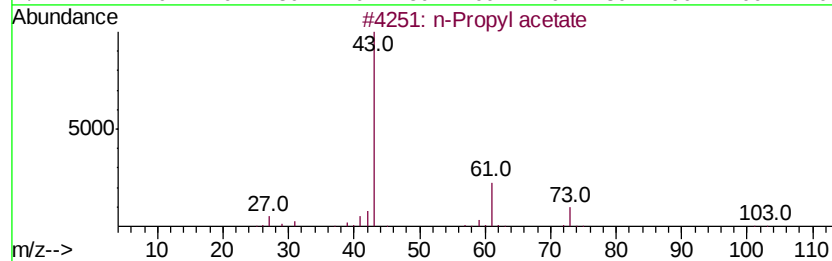
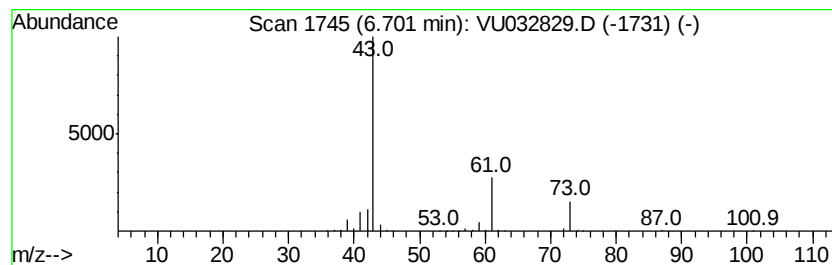
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	129.65 ug/L	1423210	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		n-Propyl acetate	102	C5H10O2	000109-60-4	78
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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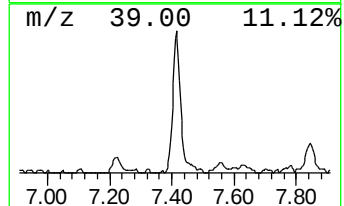
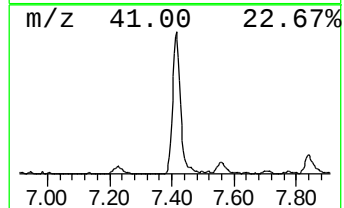
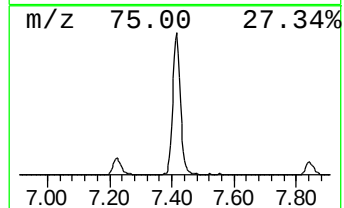
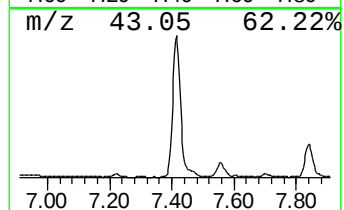
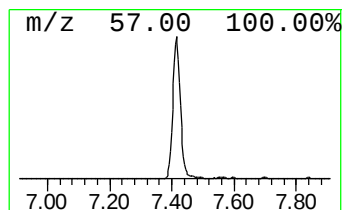
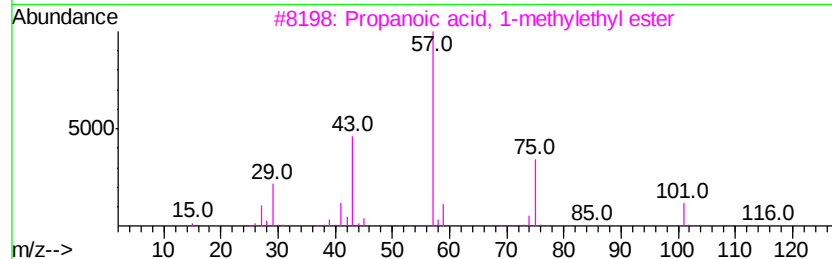
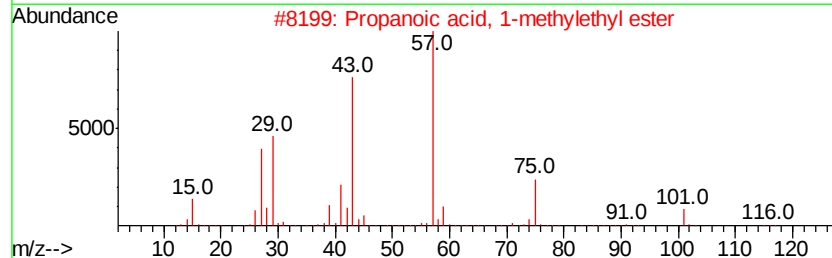
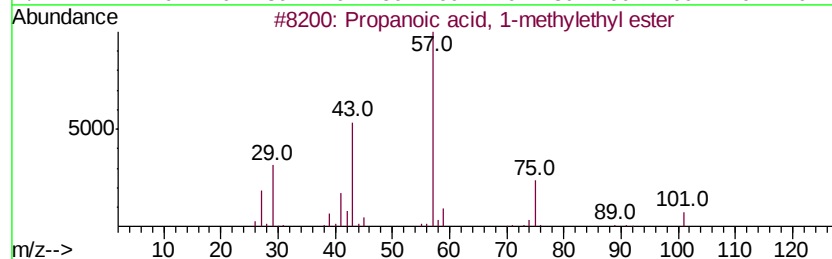
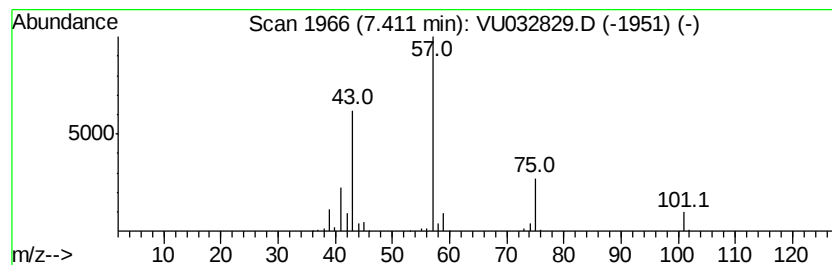
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	22.79 ug/L	250192	1,4-Difluorobenzene	5.88

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	83
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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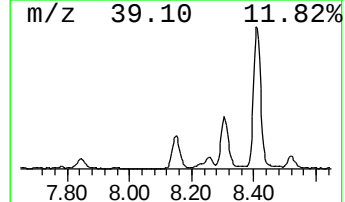
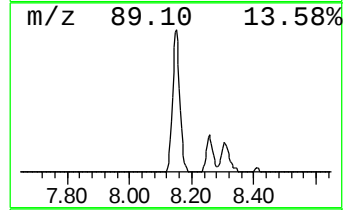
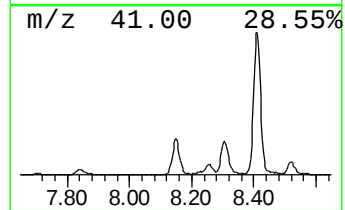
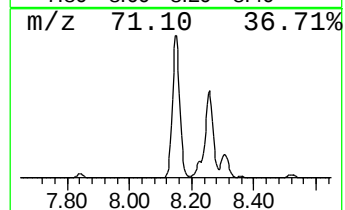
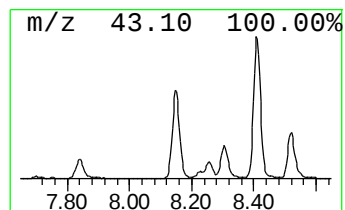
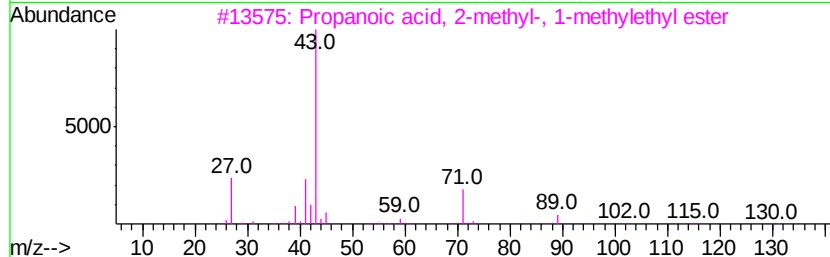
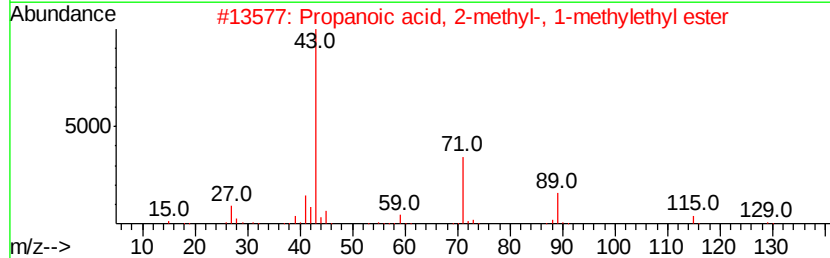
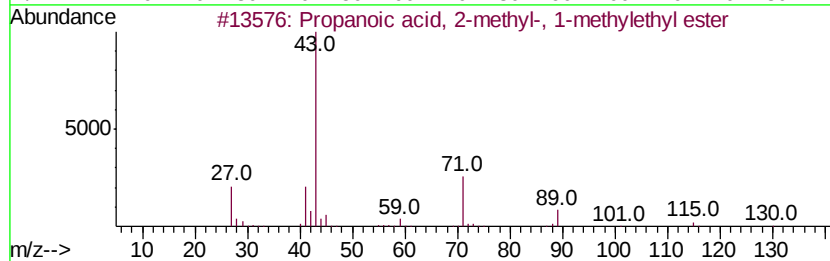
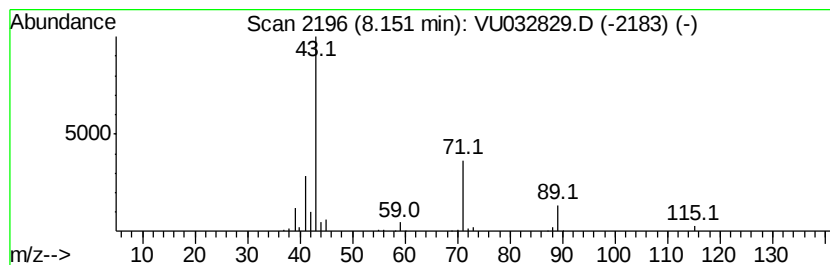
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.34 ug/L	132490	Chlorobenzene-d5	9.08

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	83		
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83		
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64		
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032829.D
Acq On : 18 Jun 2019 17:07
Operator : JC/SP
Sample : K3363-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JP6

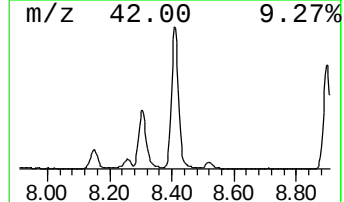
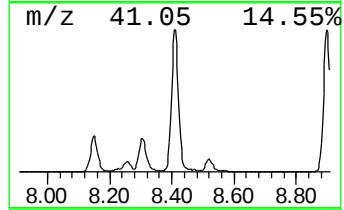
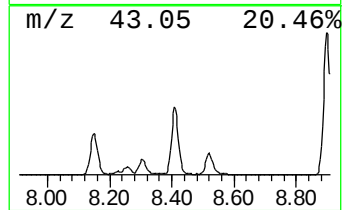
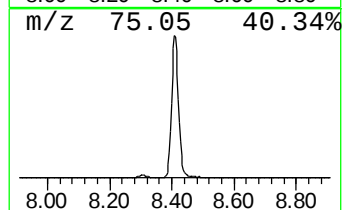
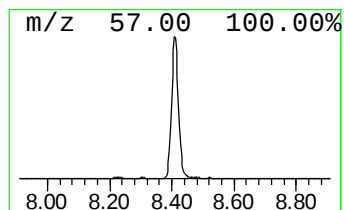
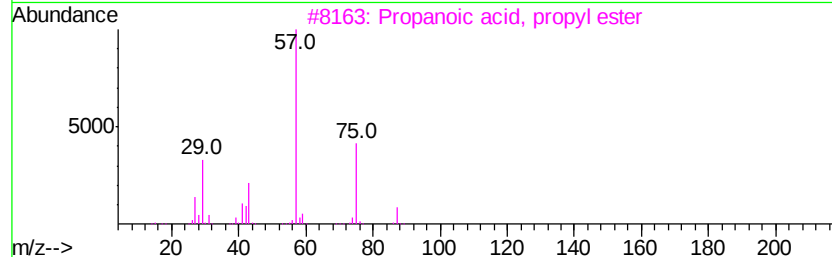
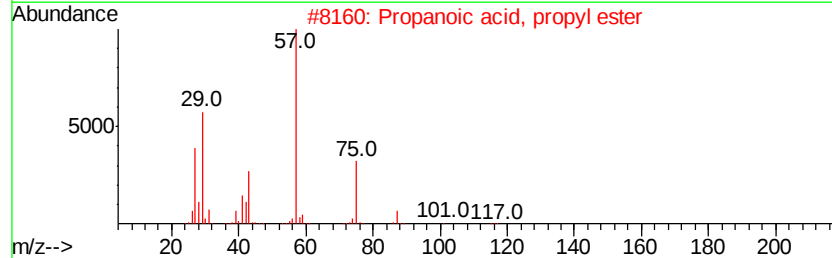
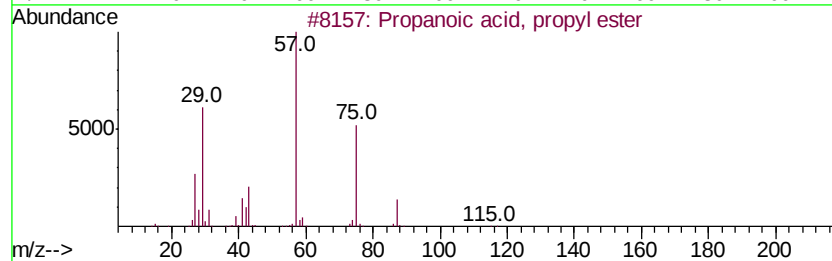
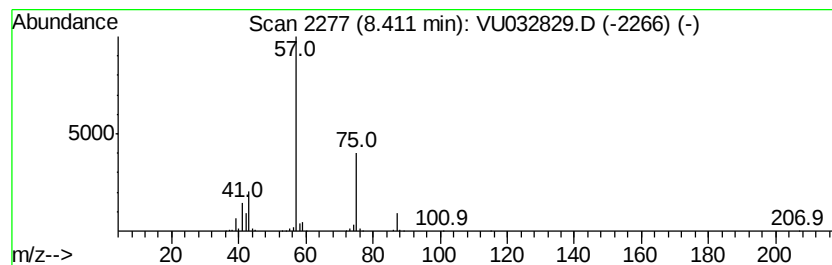
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	66.61 ug/L	945281	Chlorobenzene-d5	9.08

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	78
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032829.D
Acq On : 18 Jun 2019 17:07
Operator : JC/SP
Sample : K3363-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JP6

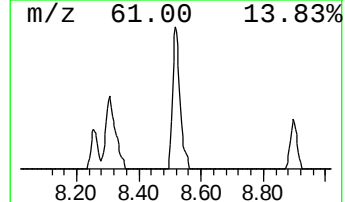
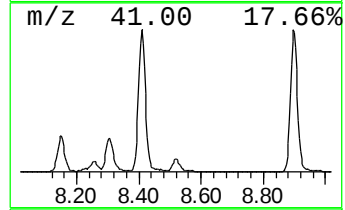
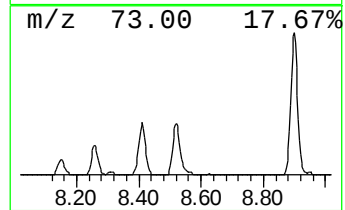
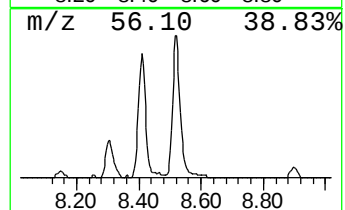
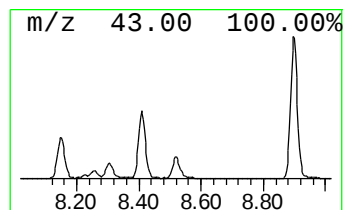
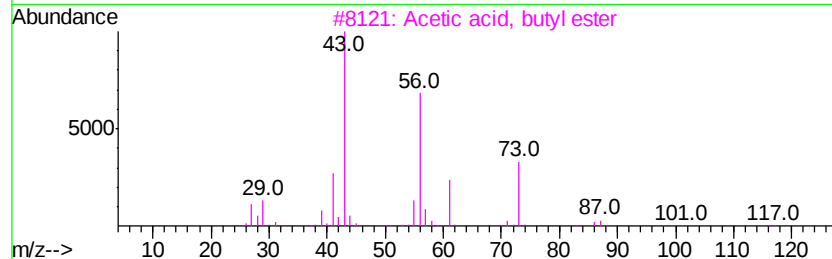
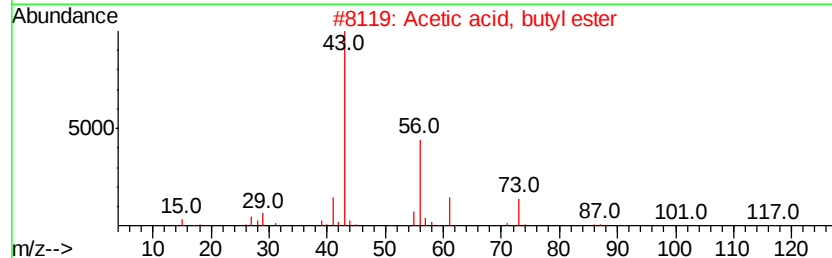
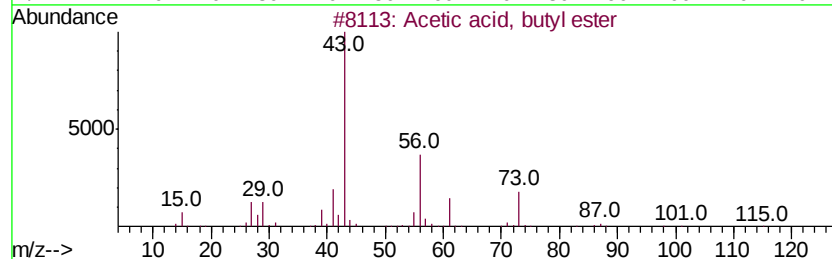
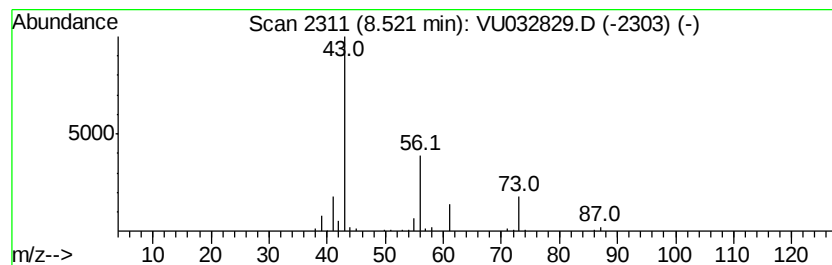
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	4.96 ug/L	70373	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
3		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
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Acq On : 18 Jun 2019 17:07
Operator : JC/SP
Sample : K3363-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JP6

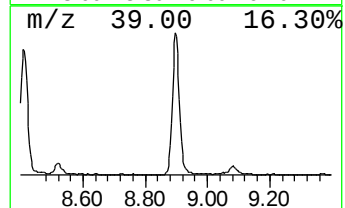
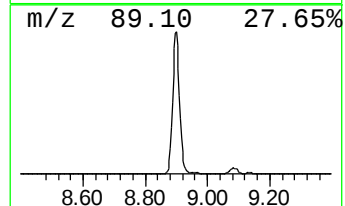
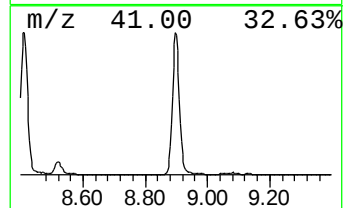
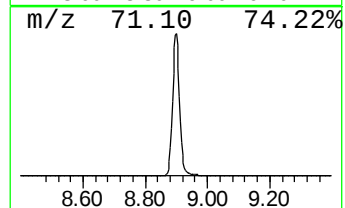
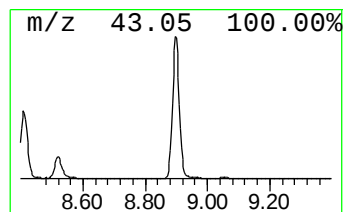
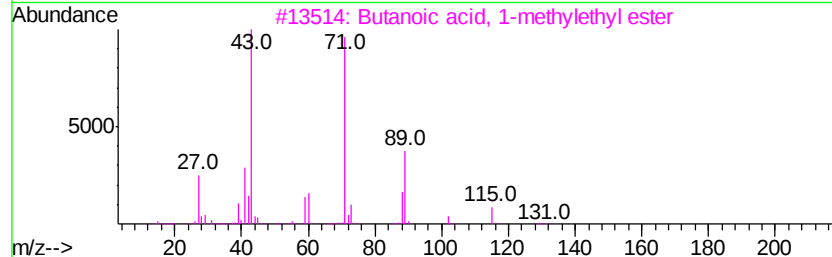
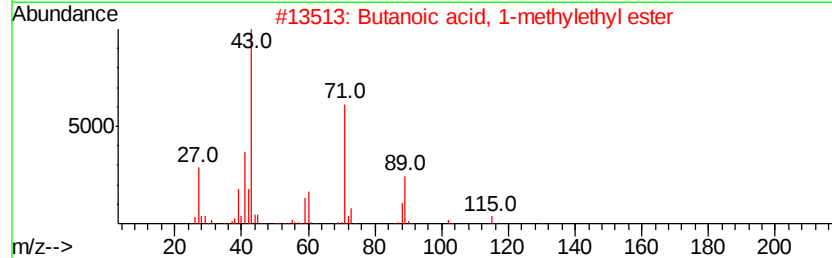
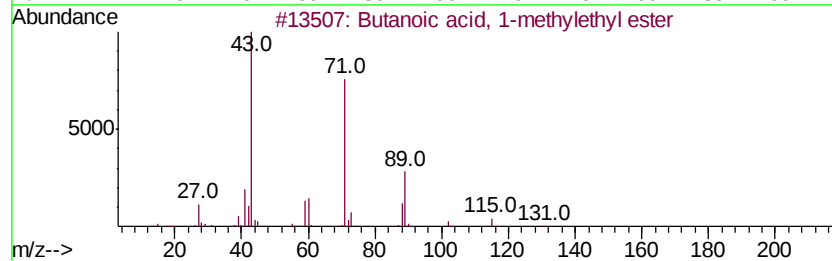
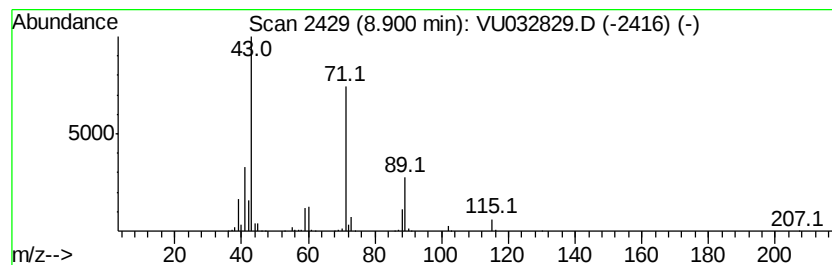
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Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	44.19 ug/L	627085	Chlorobenzene-d5	9.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
4		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061819\
Data File : VU032829.D
Acq On : 18 Jun 2019 17:07
Operator : JC/SP
Sample : K3363-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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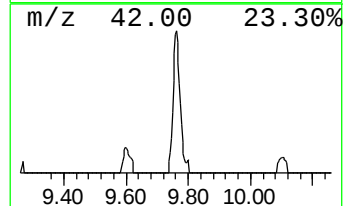
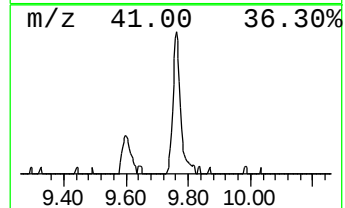
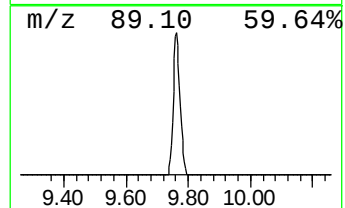
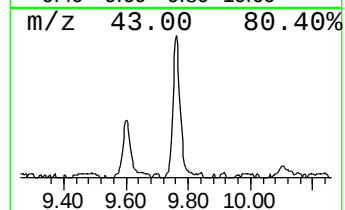
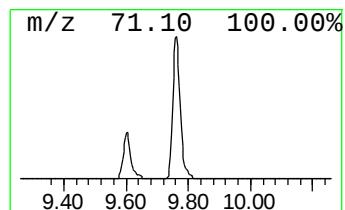
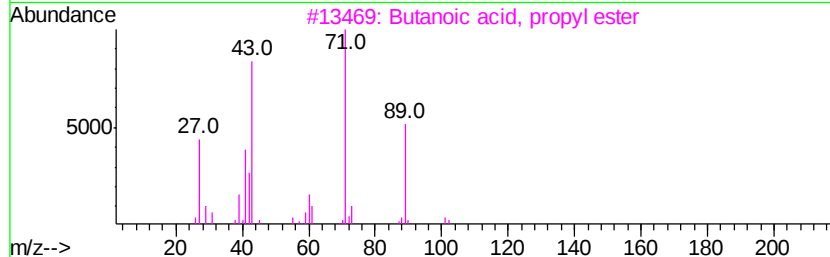
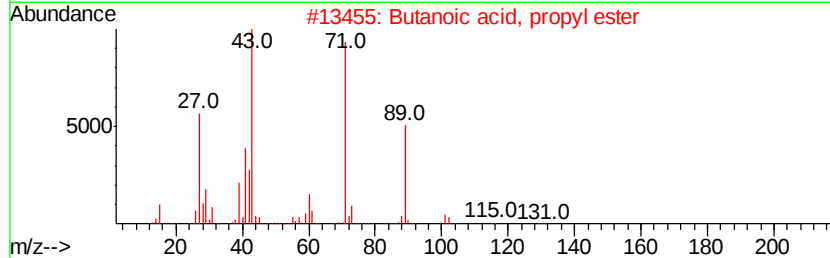
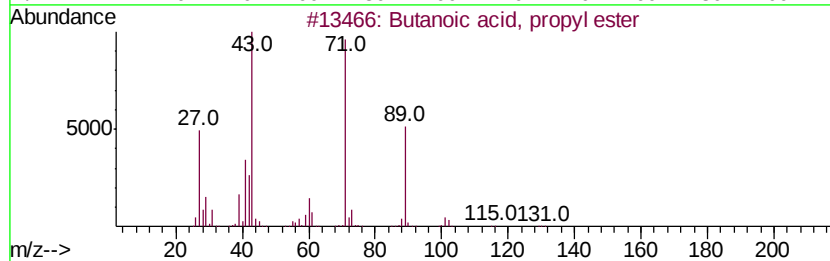
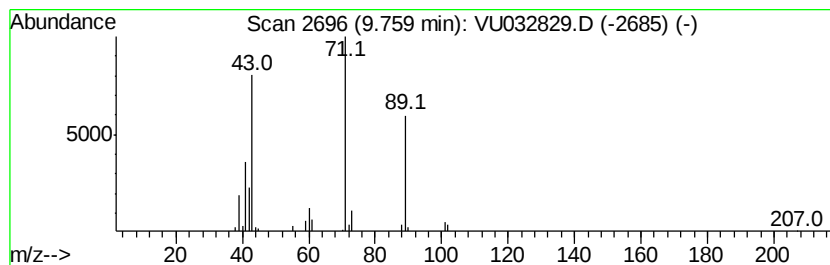
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Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.73 ug/L	38703	Chlorobenzene-d5	9.08

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	78
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061819\
Data File : VU032829.D
Acq On : 18 Jun 2019 17:07
Operator : JC/SP
Sample : K3363-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JP6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM061719WMA.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
n-Propyl acetate	6.70	129.7	ug/L	1423210	1	5.88	548870	50.0
Propanoic acid, 1...	7.41	22.8	ug/L	250192	1	5.88	548870	50.0
Propanoic acid, 2...	8.15	9.3	ug/L	132490	2	9.08	709525	50.0
Propanoic acid, p...	8.41	66.6	ug/L	945281	2	9.08	709525	50.0
Acetic acid, buty...	8.52	5.0	ug/L	70373	2	9.08	709525	50.0
Butanoic acid, 1-...	8.90	44.2	ug/L	627085	2	9.08	709525	50.0
Butanoic acid, pr...	9.76	2.7	ug/L	38703	2	9.08	709525	50.0