

Data Path : Z:\voasrv\HPCHEM1\MSVOA U\Data\VU031519\
 Data File : VU030063.D
 Acq On : 14 Mar 2019 10:59
 Operator : JC/SP
 Sample : VLEB01
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 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_U\METHOD\SOMULM031319WMA.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	1.183	24	29	37	rBV2	11520	11665	0.43%	0.055%
2	1.399	89	96	108	rBV	223519	224769	8.32%	1.053%
3	1.682	175	184	204	rBV	173133	222009	8.22%	1.040%
4	2.273	357	368	379	rBV	376568	576997	21.36%	2.702%
5	2.428	412	416	420	rBV5	594	706	0.03%	0.003%
6	2.540	445	451	454	rBV3	546	534	0.02%	0.003%
7	2.579	461	463	465	rBV	573	354	0.01%	0.002%
8	2.621	472	476	479	rBV2	1231	1045	0.04%	0.005%
9	2.704	492	502	512	rVB2	8995	15381	0.57%	0.072%
10	2.884	555	558	562	rVB2	719	469	0.02%	0.002%
11	3.013	596	598	603	rVB2	689	470	0.02%	0.002%
12	3.039	603	606	611	rBV	407	351	0.01%	0.002%
13	3.186	647	652	655	rBV2	406	453	0.02%	0.002%
14	3.450	731	734	738	rVB3	816	685	0.03%	0.003%
15	3.514	750	754	758	rBV2	386	383	0.01%	0.002%
16	3.649	792	796	805	rBV3	603	594	0.02%	0.003%
17	3.704	810	813	824	rVB3	710	962	0.04%	0.005%
18	3.784	835	838	844	rVB	829	750	0.03%	0.004%
19	3.836	844	854	856	rBV	633	877	0.03%	0.004%
20	3.923	876	881	885	rVB2	505	535	0.02%	0.003%
21	3.984	896	900	902	rBV2	644	574	0.02%	0.003%
22	4.174	946	959	994	rBV	158179	424463	15.72%	1.988%
23	4.646	1088	1106	1132	rBV	278927	672320	24.89%	3.149%
24	4.936	1194	1196	1203	rVB4	628	488	0.02%	0.002%
25	4.987	1208	1212	1213	rBV2	465	372	0.01%	0.002%
26	5.058	1232	1234	1238	rVB2	539	351	0.01%	0.002%
27	5.112	1248	1251	1255	rBV3	500	440	0.02%	0.002%
28	5.141	1255	1260	1263	rBV4	515	461	0.02%	0.002%
29	5.337	1297	1321	1354	rBV2	589228	1729912	64.05%	8.102%
30	5.553	1378	1388	1405	rBV2	15190	32331	1.20%	0.151%
31	5.746	1443	1448	1451	rBV5	705	636	0.02%	0.003%
32	5.791	1459	1462	1466	rBV4	558	506	0.02%	0.002%
33	5.884	1473	1491	1513	rBV	528324	1112540	41.19%	5.211%
34	6.328	1615	1629	1650	rBV	375173	760192	28.14%	3.560%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
 Title : VOC Analysis

35	6.537	1686	1694	1699	rBV	5430	8402	0.31%	0.039%
36	6.579	1700	1707	1714	rBV2	11231	19743	0.73%	0.092%
37	6.701	1732	1745	1785	rBV	1500569	2701002	100.00%	12.651%
38	7.225	1896	1908	1931	rBV	222732	411264	15.23%	1.926%
39	7.418	1955	1968	1997	rBV	274478	485586	17.98%	2.274%
40	7.562	2000	2013	2033	rBV	841399	1487472	55.07%	6.967%
41	7.845	2091	2101	2119	rBV2	179767	319276	11.82%	1.495%
42	8.048	2162	2164	2167	rBV2	1065	566	0.02%	0.003%
43	8.074	2168	2172	2177	rBV3	1143	1065	0.04%	0.005%
44	8.154	2184	2197	2214	rBV2	178931	405957	15.03%	1.901%
45	8.260	2224	2230	2236	rBV	50165	65408	2.42%	0.306%
46	8.305	2236	2244	2266	rVB	618396	1046587	38.75%	4.902%
47	8.411	2266	2277	2303	rVB	1212187	1923492	71.21%	9.009%
48	8.521	2303	2311	2336	rVB	81969	142840	5.29%	0.669%
49	8.675	2355	2359	2360	rBV2	548	449	0.02%	0.002%
50	8.746	2379	2381	2389	rVB5	719	800	0.03%	0.004%
51	8.787	2389	2394	2398	rBV5	785	835	0.03%	0.004%
52	8.900	2417	2429	2458	rBV	914708	1431352	52.99%	6.704%
53	9.086	2470	2487	2523	rVB	800557	1354725	50.16%	6.345%
54	9.257	2534	2540	2544	rBV3	1462	1477	0.05%	0.007%
55	9.373	2571	2576	2577	rBV5	1248	988	0.04%	0.005%
56	9.440	2595	2597	2603	rBV3	573	462	0.02%	0.002%
57	9.469	2603	2606	2610	rVV4	555	427	0.02%	0.002%
58	9.501	2613	2616	2619	rVB2	707	464	0.02%	0.002%
59	9.604	2640	2648	2661	rBV	10335	17052	0.63%	0.080%
60	9.765	2687	2698	2718	rBV	50393	88295	3.27%	0.414%
61	9.919	2741	2746	2751	rBV4	376	496	0.02%	0.002%
62	9.980	2762	2765	2768	rBV5	605	482	0.02%	0.002%
63	10.061	2787	2790	2794	rBV3	458	397	0.01%	0.002%
64	10.128	2808	2811	2813	rBV3	497	366	0.01%	0.002%
65	10.141	2813	2815	2818	rVV	673	384	0.01%	0.002%
66	10.170	2818	2824	2830	rVB3	1220	1840	0.07%	0.009%
67	10.215	2833	2838	2840	rBV	670	535	0.02%	0.003%
68	10.305	2864	2866	2875	rBV3	437	469	0.02%	0.002%
69	10.427	2892	2904	2929	rVB	592200	942091	34.88%	4.412%
70	10.607	2945	2960	2974	rBV2	20109	35213	1.30%	0.165%
71	10.768	3003	3010	3020	rVV2	13395	19263	0.71%	0.090%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

72	10.877	3036	3044	3048	rBV3	1618	2304	0.09%	0.011%
73	10.897	3048	3050	3053	rVB3	1261	642	0.02%	0.003%
74	10.916	3053	3056	3060	rBV3	640	446	0.02%	0.002%
75	10.971	3066	3073	3076	rBV4	707	767	0.03%	0.004%
76	11.292	3171	3173	3179	rVB2	538	443	0.02%	0.002%
77	11.366	3191	3196	3197	rBV2	525	456	0.02%	0.002%
78	11.418	3208	3212	3219	rVB5	1307	1743	0.06%	0.008%
79	11.479	3219	3231	3254	rBV	787714	1272479	47.11%	5.960%
80	11.858	3335	3349	3367	rBV	816294	1331496	49.30%	6.236%
81	12.157	3439	3442	3448	rBV6	846	766	0.03%	0.004%
82	12.479	3532	3542	3554	rVB2	7962	13683	0.51%	0.064%
83	12.652	3593	3596	3599	rVB3	707	484	0.02%	0.002%
84	12.688	3600	3607	3610	rBV3	634	756	0.03%	0.004%
85	12.713	3611	3615	3618	rBV2	612	409	0.02%	0.002%
86	12.742	3620	3624	3627	rBV3	454	421	0.02%	0.002%
87	12.897	3666	3672	3675	rBV4	960	1000	0.04%	0.005%
88	13.215	3767	3771	3776	rVB3	587	513	0.02%	0.002%
89	13.244	3776	3780	3784	rBV2	549	607	0.02%	0.003%
90	13.327	3803	3806	3810	rVB3	475	338	0.01%	0.002%
91	13.408	3828	3831	3836	rBV2	709	671	0.02%	0.003%
92	13.520	3863	3866	3869	rBV2	729	486	0.02%	0.002%
93	13.649	3903	3906	3910	rBV3	480	360	0.01%	0.002%
94	13.893	3979	3982	3985	rBV2	516	352	0.01%	0.002%
95	13.999	4011	4015	4016	rBV2	843	597	0.02%	0.003%
96	14.276	4096	4101	4110	rVB2	2552	3724	0.14%	0.017%
97	14.379	4129	4133	4134	rBV	620	433	0.02%	0.002%
98	14.488	4164	4167	4170	rBV3	682	454	0.02%	0.002%
99	14.999	4322	4326	4327	rBV2	517	442	0.02%	0.002%
100	15.282	4412	4414	4416	rBV2	738	400	0.01%	0.002%

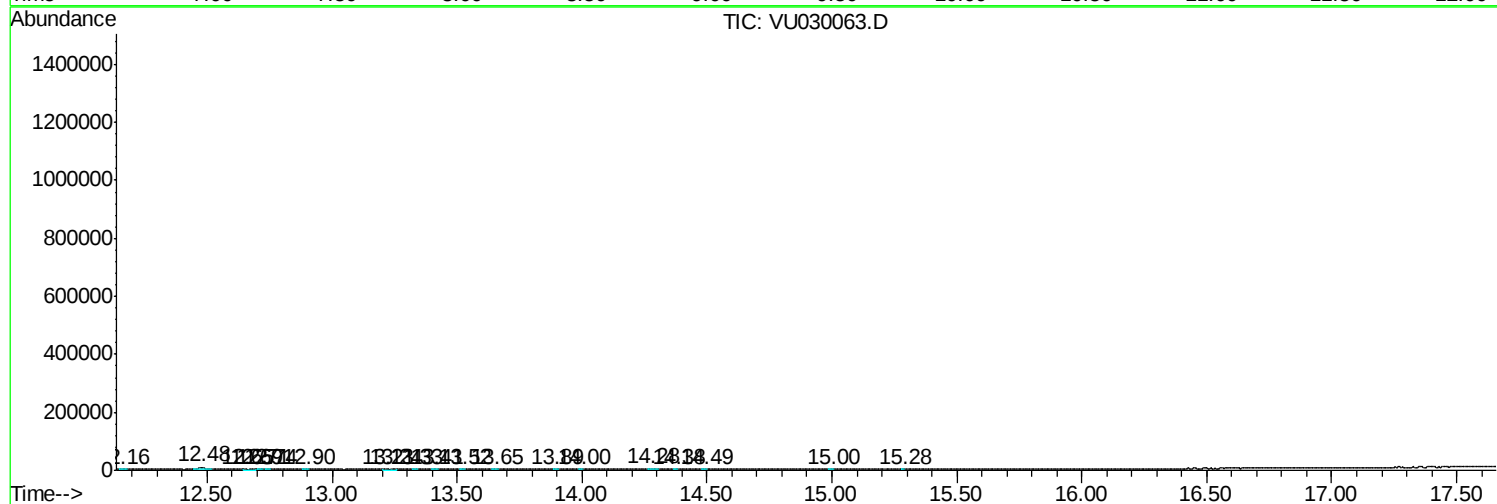
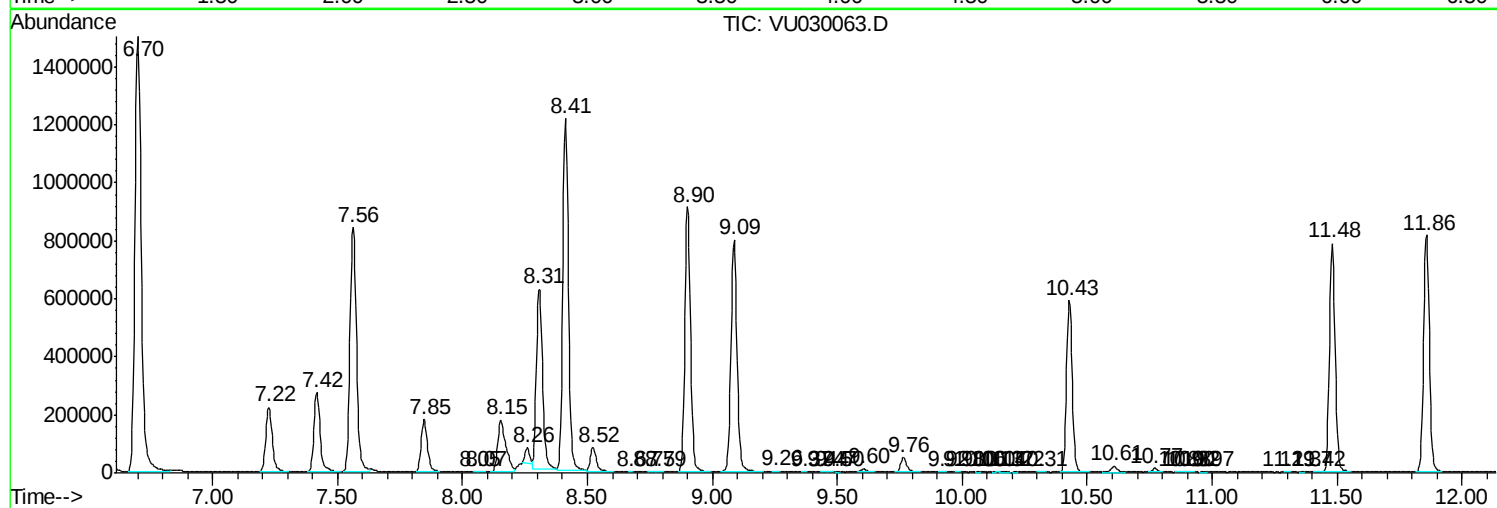
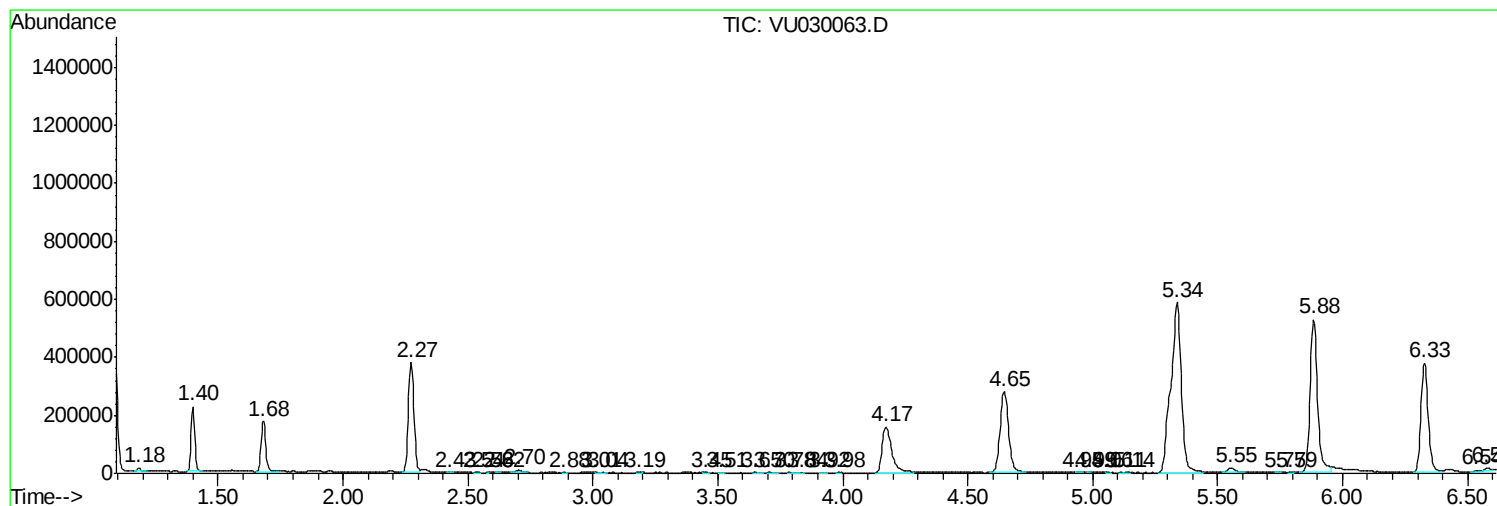
Sum of corrected areas: 21350769

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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



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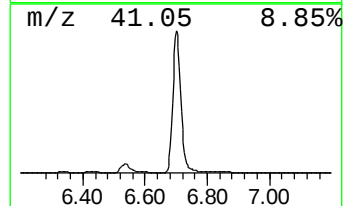
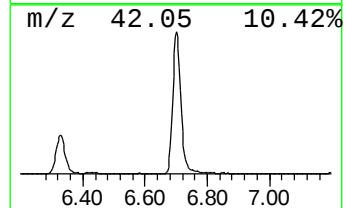
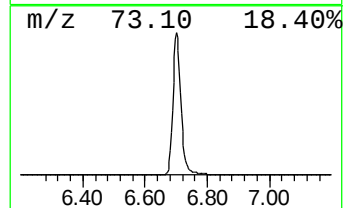
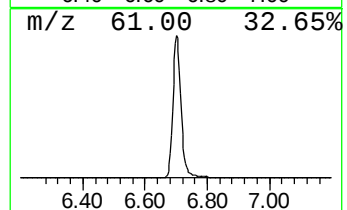
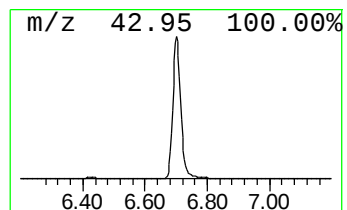
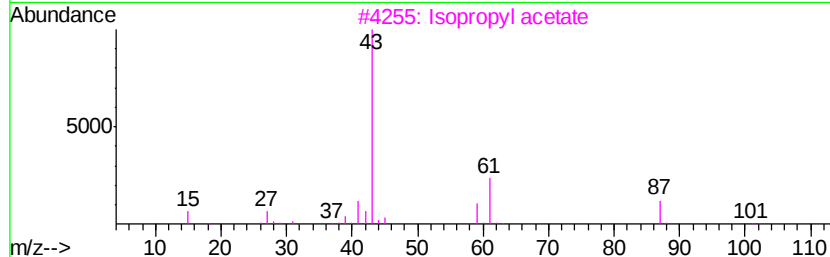
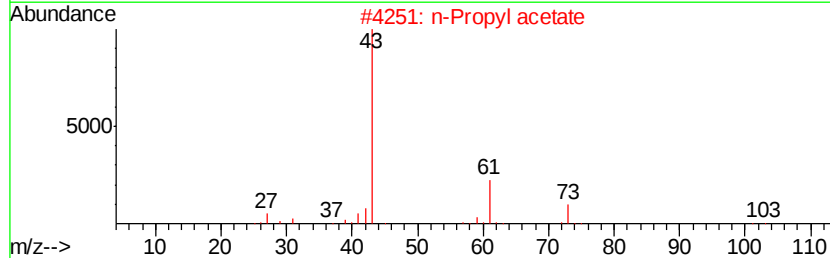
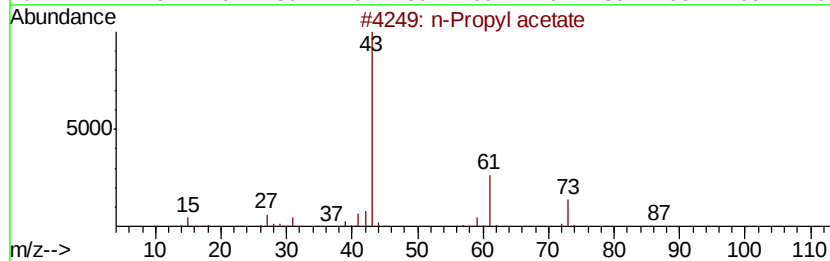
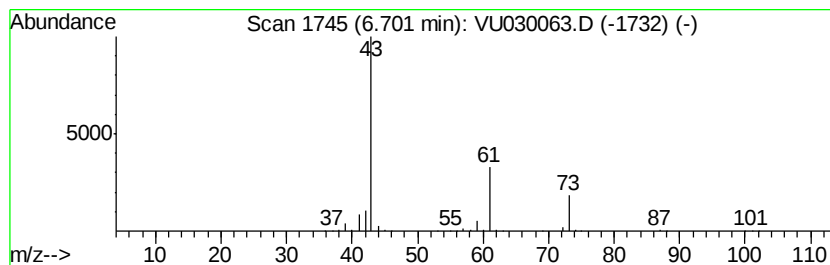
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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	121.39 ug/L	2701000	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	83
3		Isopropyl acetate	102	C5H10O2	000108-21-4	36
4		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
5		n-Propyl acetate	102	C5H10O2	000109-60-4	9



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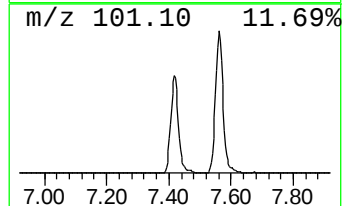
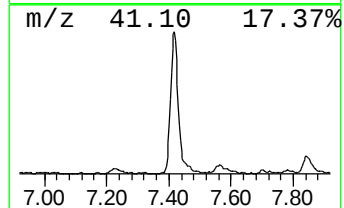
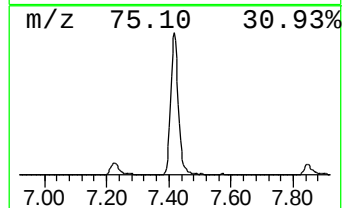
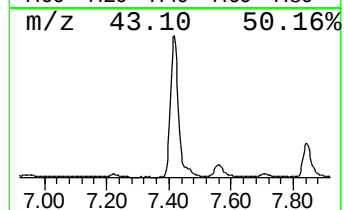
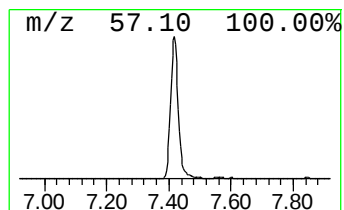
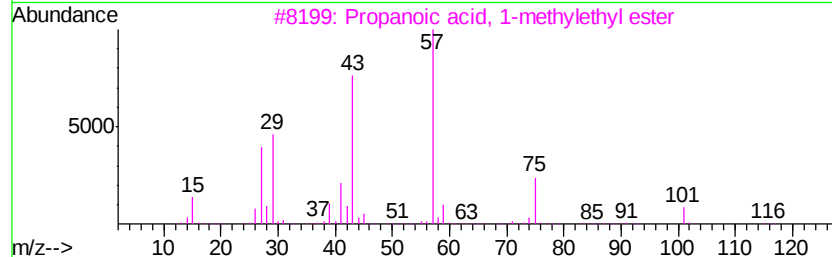
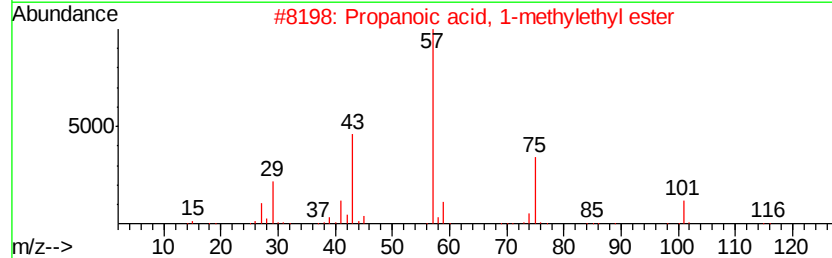
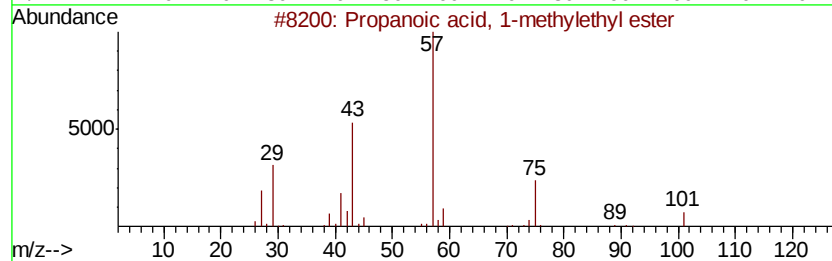
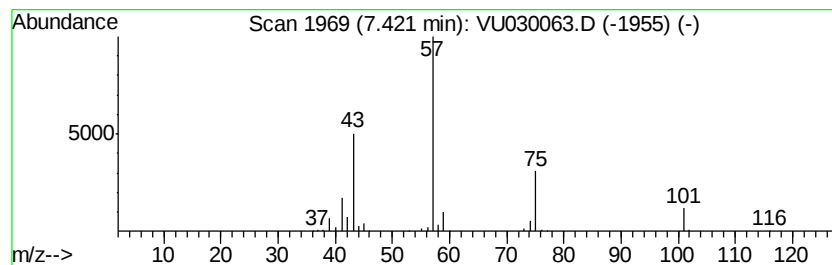
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Quant Title : VOC Analysis

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.
7.42	21.82 ug/L	485586	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	83
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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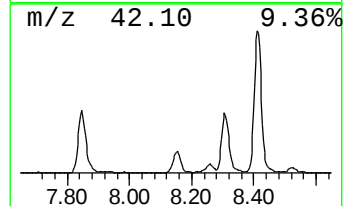
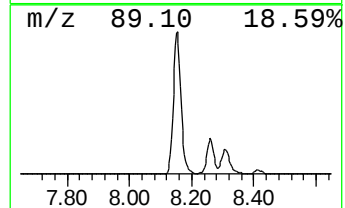
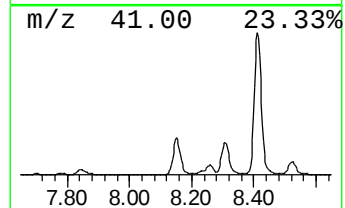
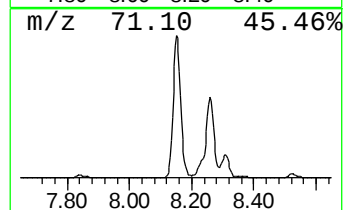
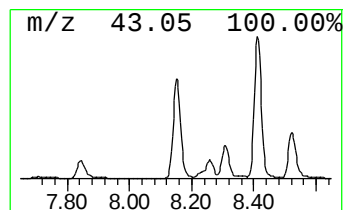
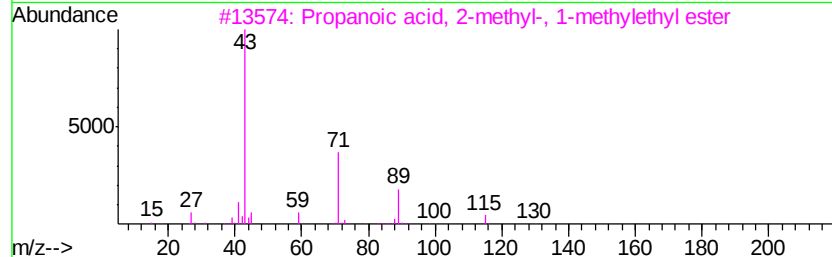
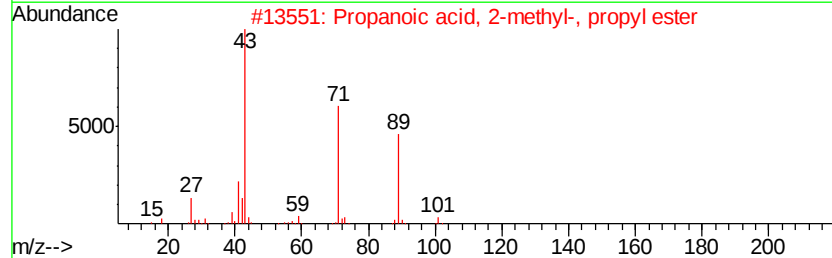
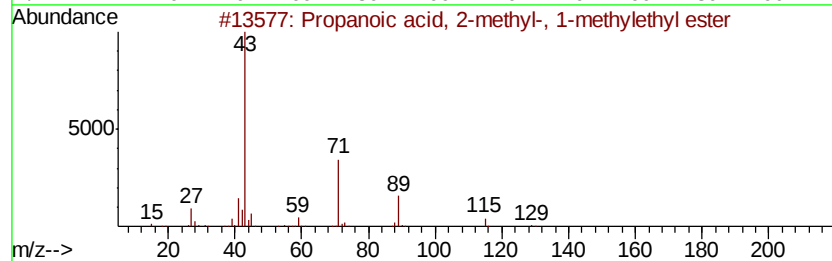
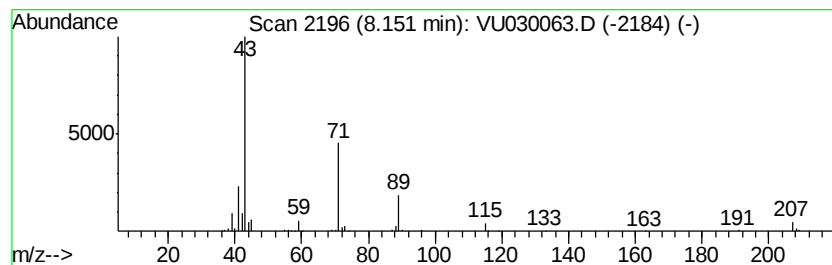
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
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	14.98 ug/L	405957	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72	
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64	
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64	
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	50	
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	50	



Data Path : Z:\voasrv\HPCHEM1\MSVOA U\Data\VU031519\
Data File : VU030063.D
Acq On : 14 Mar 2019 10:59
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

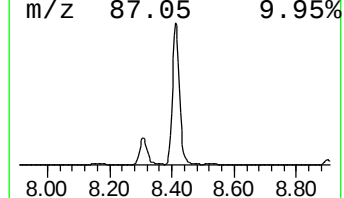
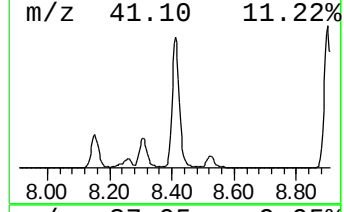
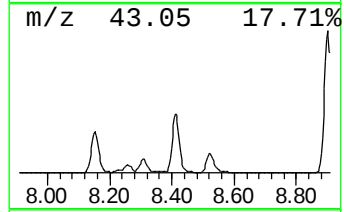
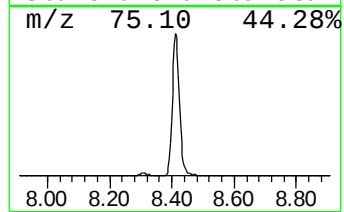
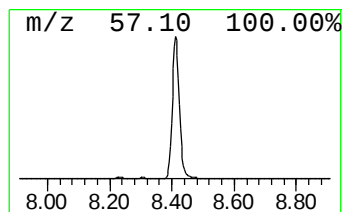
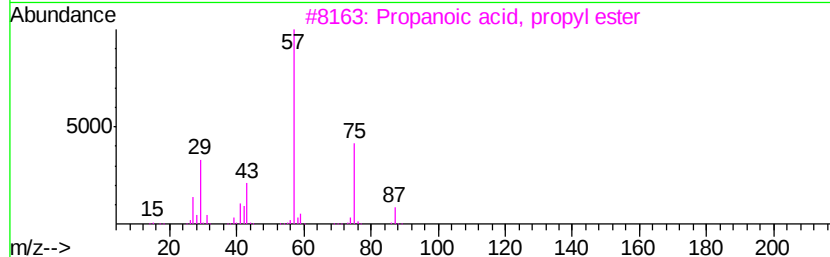
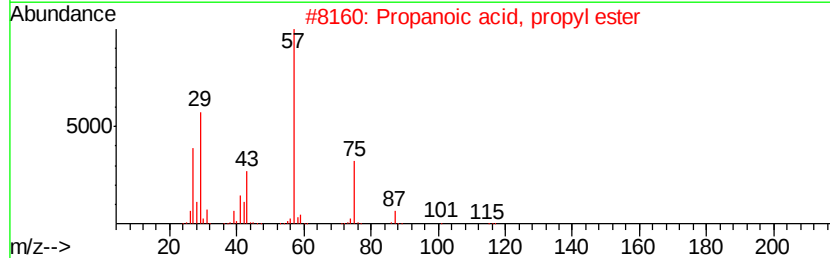
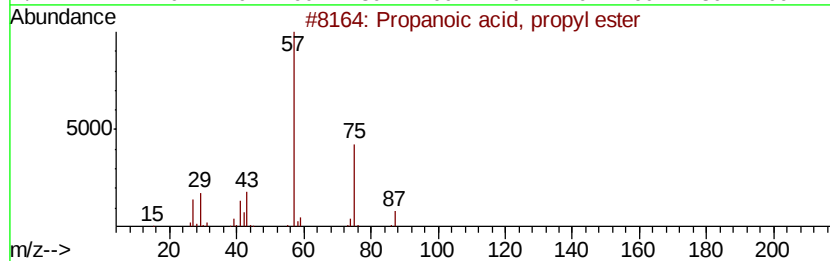
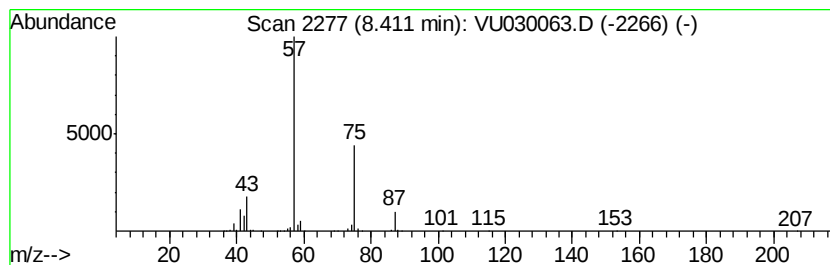
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Quant Title : VOC Analysis

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	70.99 ug/L	1923490	Chlorobenzene-d5	9.09

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	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA U\Data\VU031519\
Data File : VU030063.D
Acq On : 14 Mar 2019 10:59
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

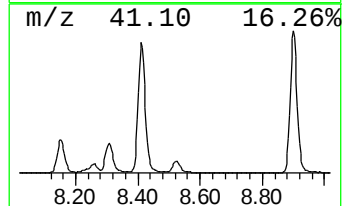
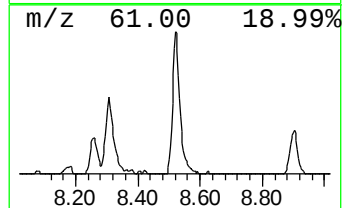
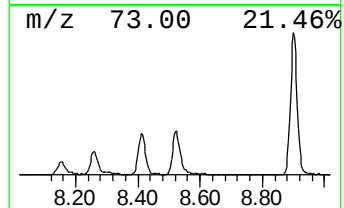
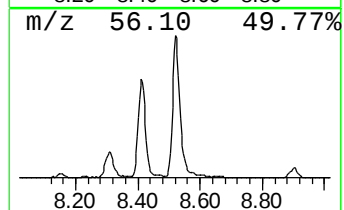
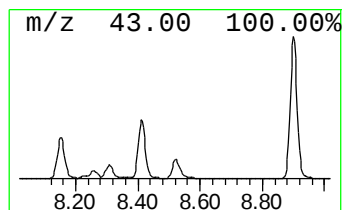
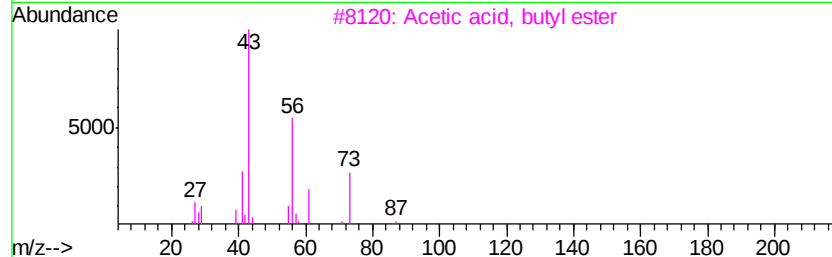
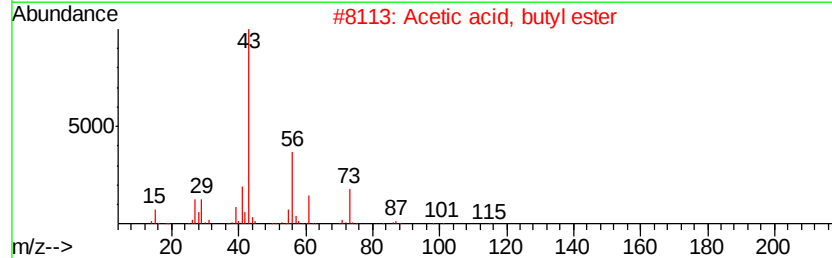
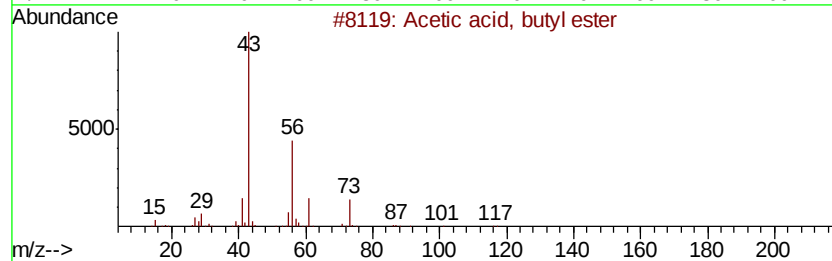
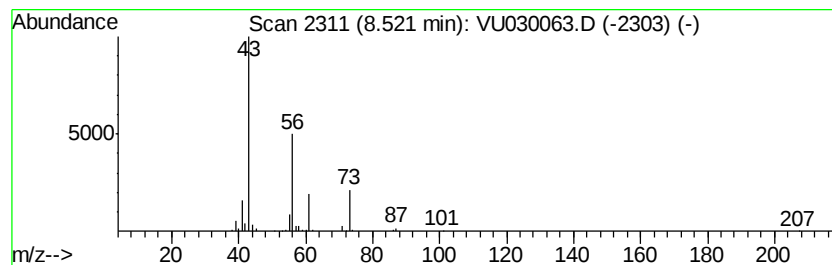
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Quant Title : VOC Analysis

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	5.27 ug/L	142840	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83	
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78	
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72	
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72	
5	Isobutyl acetate	116	C6H12O2	000110-19-0	33	



Data Path : Z:\voasrv\HPCHEM1\MSVOA U\Data\VU031519\
Data File : VU030063.D
Acq On : 14 Mar 2019 10:59
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

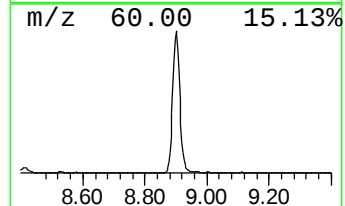
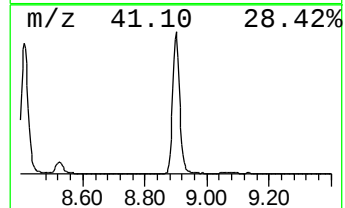
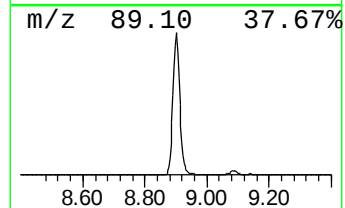
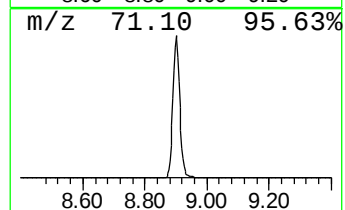
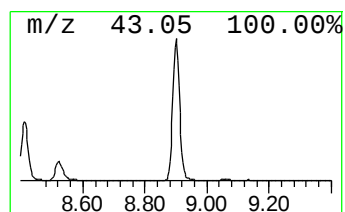
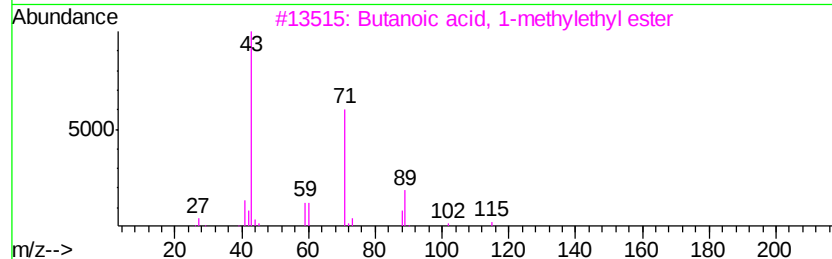
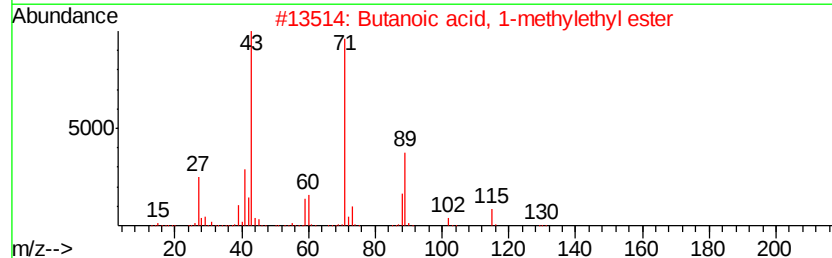
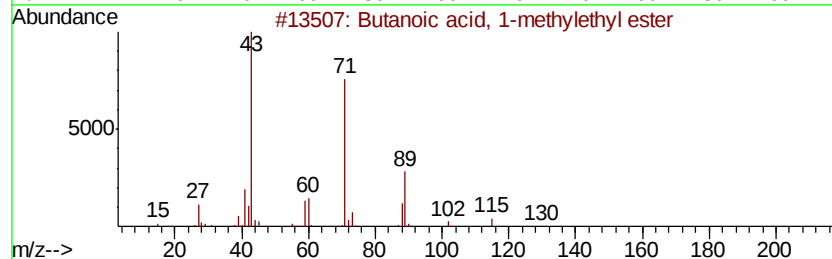
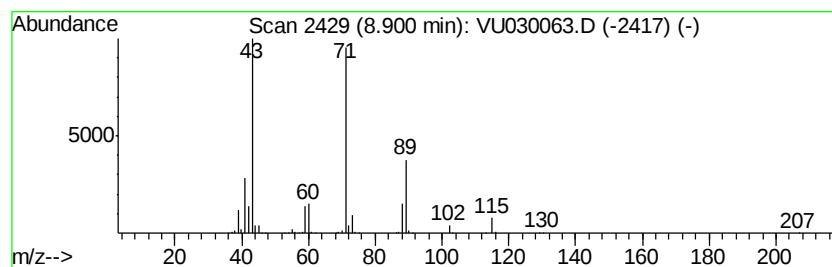
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	52.83 ug/L	1431350	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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, propyl ester	130	C7H14O2	000105-66-8	72	
5	Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64	



Data Path : Z:\voasrv\HPCHEM1\MSVOA U\Data\VU031519\
Data File : VU030063.D
Acq On : 14 Mar 2019 10:59
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

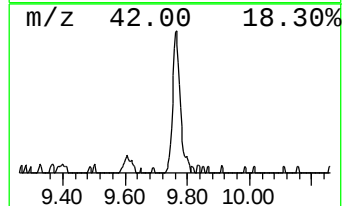
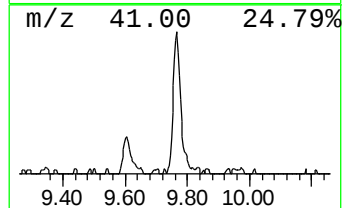
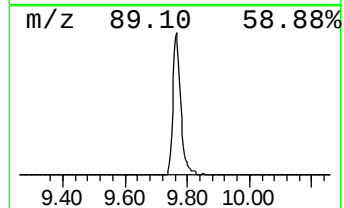
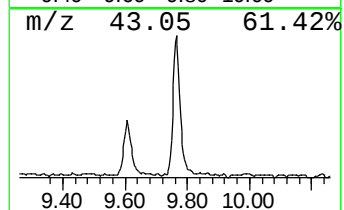
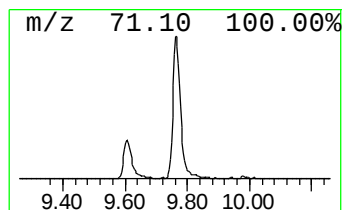
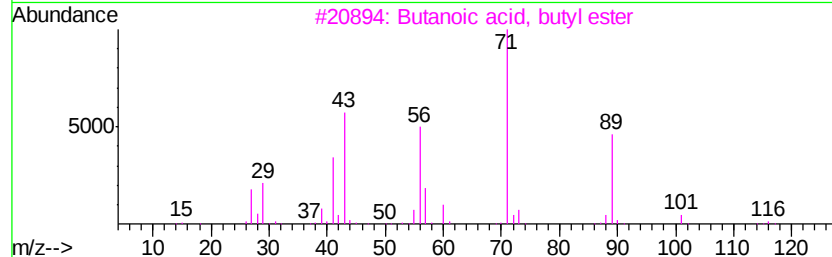
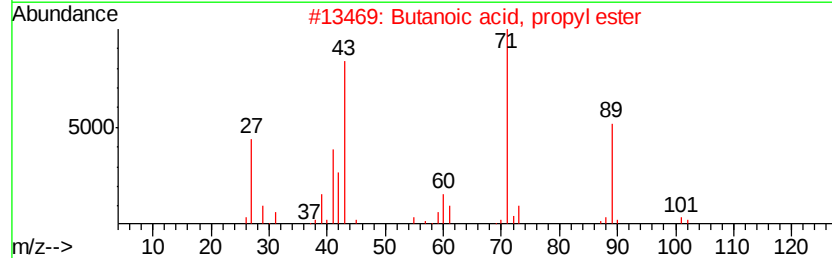
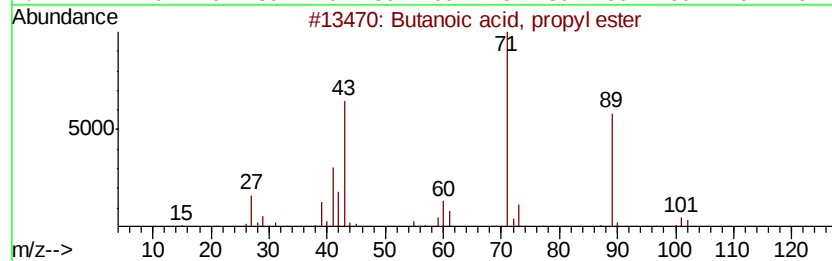
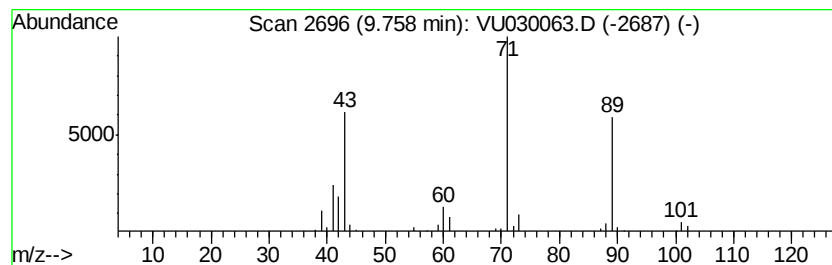
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Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.26 ug/L	88295	Chlorobenzene-d5	9.09

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	80
3		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	78
4		Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031519\
Data File : VU030063.D
Acq On : 14 Mar 2019 10:59
Operator : JC/SP
Sample : VLEB01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.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	121.4	ug/L	2701000	1	5.88	1112540	50.0
Propanoic acid, 1...	7.42	21.8	ug/L	485586	1	5.88	1112540	50.0
Propanoic acid, 2...	8.15	15.0	ug/L	405957	2	9.09	1354730	50.0
Propanoic acid, p...	8.41	71.0	ug/L	1923490	2	9.09	1354730	50.0
Acetic acid, buty...	8.52	5.3	ug/L	142840	2	9.09	1354730	50.0
Butanoic acid, 1-...	8.90	52.8	ug/L	1431350	2	9.09	1354730	50.0
Butanoic acid, pr...	9.76	3.3	ug/L	88295	2	9.09	1354730	50.0