

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102619\
 Data File : VU035522.D
 Acq On : 26 Oct 2019 16:44
 Operator : JC/SP
 Sample : K5536-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEK32

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\SOMULM102619WMA.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	1.372	4	10	18	rBV2	46250	55421	1.37%	0.193%
2	1.613	78	85	99	rBV	340623	377954	9.33%	1.314%
3	1.932	176	184	198	rVB	263397	346146	8.55%	1.204%
4	2.594	378	390	406	rBV	479805	790655	19.52%	2.750%
5	2.671	407	414	427	rVB2	15003	25752	0.64%	0.090%
6	2.826	453	462	480	rVB4	5481	13637	0.34%	0.047%
7	2.999	508	516	526	rVB2	3952	7779	0.19%	0.027%
8	3.086	531	543	562	rVB	40442	79288	1.96%	0.276%
9	3.231	579	588	603	rVB2	7247	16631	0.41%	0.058%
10	3.321	613	616	620	rBV2	513	434	0.01%	0.002%
11	3.395	632	639	645	rVV6	1551	2775	0.07%	0.010%
12	3.427	648	649	654	rVV2	1064	802	0.02%	0.003%
13	3.449	654	656	664	rVV3	793	760	0.02%	0.003%
14	3.485	664	667	672	rVB3	644	461	0.01%	0.002%
15	3.517	672	677	682	rBV4	707	769	0.02%	0.003%
16	3.629	704	712	714	rBV4	821	909	0.02%	0.003%
17	3.716	734	739	741	rBV3	949	849	0.02%	0.003%
18	3.848	776	780	781	rBV2	963	726	0.02%	0.003%
19	3.919	800	802	810	rVB5	435	400	0.01%	0.001%
20	3.951	810	812	818	rVB2	704	441	0.01%	0.002%
21	4.022	829	834	835	rBV2	599	430	0.01%	0.001%
22	4.038	835	839	843	rBV3	1168	1043	0.03%	0.004%
23	4.137	862	870	871	rBV3	2546	3106	0.08%	0.011%
24	4.266	907	910	914	rBV2	522	398	0.01%	0.001%
25	4.301	917	921	925	rBV3	559	556	0.01%	0.002%
26	4.356	936	938	942	rVB3	457	344	0.01%	0.001%
27	4.391	942	949	953	rBV3	725	766	0.02%	0.003%
28	4.411	953	955	958	rBV2	575	335	0.01%	0.001%
29	4.504	978	984	987	rVB4	514	557	0.01%	0.002%
30	4.543	993	996	999	rBV3	727	424	0.01%	0.001%
31	4.694	1027	1043	1067	rBV	239542	580510	14.33%	2.019%
32	5.002	1137	1139	1144	rVB3	548	364	0.01%	0.001%
33	5.031	1146	1148	1154	rVB3	580	537	0.01%	0.002%
34	5.115	1156	1174	1194	rBV	414594	908557	22.43%	3.160%

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 Title : VOC Analysis

35	5.330	1235	1241	1243	rBV4	1915	2017	0.05%	0.007%
36	5.433	1257	1273	1284	rBV8	3709	8107	0.20%	0.028%
37	5.488	1287	1290	1296	rVB4	560	587	0.01%	0.002%
38	5.771	1355	1378	1411	rBV2	915018	2379728	58.75%	8.276%
39	5.970	1428	1440	1460	rBV	113256	224718	5.55%	0.781%
40	6.198	1468	1511	1514	rBV3	161552	799165	19.73%	2.779%
41	6.292	1532	1540	1598	rVB	958534	2426732	59.91%	8.439%
42	6.735	1663	1678	1696	rBV	544106	1073108	26.49%	3.732%
43	7.089	1775	1788	1823	rBV	2250915	4050478	100.00%	14.086%
44	7.604	1936	1948	1973	rBV	302865	546571	13.49%	1.901%
45	7.784	1993	2004	2016	rBV	269450	450183	11.11%	1.566%
46	7.935	2037	2051	2067	rBV	1093817	1940236	47.90%	6.747%
47	8.211	2124	2137	2167	rBV2	260046	510459	12.60%	1.775%
48	8.507	2216	2229	2245	rBV	418285	703755	17.37%	2.447%
49	8.613	2249	2262	2271	rVV3	58534	129633	3.20%	0.451%
50	8.677	2271	2282	2300	rVV2	717417	1379428	34.06%	4.797%
51	8.767	2301	2310	2332	rVB	799172	1317106	32.52%	4.580%
52	9.099	2409	2413	2417	rBV4	1181	1301	0.03%	0.005%
53	9.250	2447	2460	2495	rBV	868147	1457715	35.99%	5.069%
54	9.449	2500	2522	2558	rVB	1096044	1951731	48.19%	6.787%
55	9.597	2564	2568	2579	rVB	4066	5661	0.14%	0.020%
56	9.681	2588	2594	2599	rBV5	3346	4733	0.12%	0.016%
57	9.719	2600	2606	2619	rVB2	11471	18801	0.46%	0.065%
58	9.954	2671	2679	2697	rVB	20494	35600	0.88%	0.124%
59	10.108	2715	2727	2749	rBV	85926	164172	4.05%	0.571%
60	10.275	2771	2779	2786	rBV4	3941	6630	0.16%	0.023%
61	10.427	2823	2826	2829	rBV	609	403	0.01%	0.001%
62	10.513	2845	2853	2858	rBV5	1853	2584	0.06%	0.009%
63	10.658	2893	2898	2901	rBV5	591	532	0.01%	0.002%
64	10.787	2925	2938	2957	rBV	682450	1141491	28.18%	3.970%
65	10.854	2957	2959	2964	rVB2	942	652	0.02%	0.002%
66	10.925	2978	2981	2989	rVB4	1047	1214	0.03%	0.004%
67	11.015	3004	3009	3012	rBV5	1127	1123	0.03%	0.004%
68	11.115	3033	3040	3049	rVB5	3231	4484	0.11%	0.016%
69	11.198	3064	3066	3069	rBV	596	382	0.01%	0.001%
70	11.369	3115	3119	3122	rBV3	685	538	0.01%	0.002%
71	11.433	3136	3139	3145	rVB3	1127	749	0.02%	0.003%

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72	11.491	3150	3157	3169	rVB4	5509	9098	0.22%	0.032%
73	11.594	3185	3189	3192	rBV3	516	373	0.01%	0.001%
74	11.632	3199	3201	3204	rVB2	659	366	0.01%	0.001%
75	11.722	3222	3229	3231	rBV5	590	550	0.01%	0.002%
76	11.771	3238	3244	3252	rVB5	2807	3799	0.09%	0.013%
77	11.838	3252	3265	3282	rBV	820612	1407112	34.74%	4.893%
78	12.053	3329	3332	3334	rBV	510	357	0.01%	0.001%
79	12.082	3338	3341	3342	rBV3	1385	772	0.02%	0.003%
80	12.115	3348	3351	3356	rVB4	768	695	0.02%	0.002%
81	12.140	3356	3359	3363	rVB4	740	478	0.01%	0.002%
82	12.217	3370	3383	3402	rBV	791543	1351928	33.38%	4.701%
83	12.481	3461	3465	3469	rBV3	767	679	0.02%	0.002%
84	12.504	3469	3472	3476	rVB2	658	517	0.01%	0.002%
85	12.584	3493	3497	3499	rBV2	753	547	0.01%	0.002%
86	12.632	3509	3512	3513	rBV	644	394	0.01%	0.001%
87	12.664	3518	3522	3526	rBV4	804	938	0.02%	0.003%
88	12.870	3583	3586	3589	rBV3	556	476	0.01%	0.002%
89	12.912	3595	3599	3605	rBV6	939	1042	0.03%	0.004%
90	13.076	3647	3650	3653	rBV2	678	468	0.01%	0.002%
91	13.240	3697	3701	3711	rVB5	2300	3221	0.08%	0.011%
92	13.372	3738	3742	3746	rVB4	781	742	0.02%	0.003%
93	13.394	3746	3749	3752	rBV2	742	603	0.01%	0.002%
94	13.446	3763	3765	3769	rVB2	795	625	0.02%	0.002%
95	13.471	3771	3773	3780	rVB4	558	564	0.01%	0.002%
96	13.536	3789	3793	3798	rBV4	656	759	0.02%	0.003%
97	13.642	3824	3826	3829	rBV2	889	555	0.01%	0.002%
98	13.706	3843	3846	3849	rBV2	907	803	0.02%	0.003%
99	14.108	3968	3971	3980	rVB5	2888	3321	0.08%	0.012%
100	14.439	4070	4074	4078	rBV3	1416	1435	0.04%	0.005%

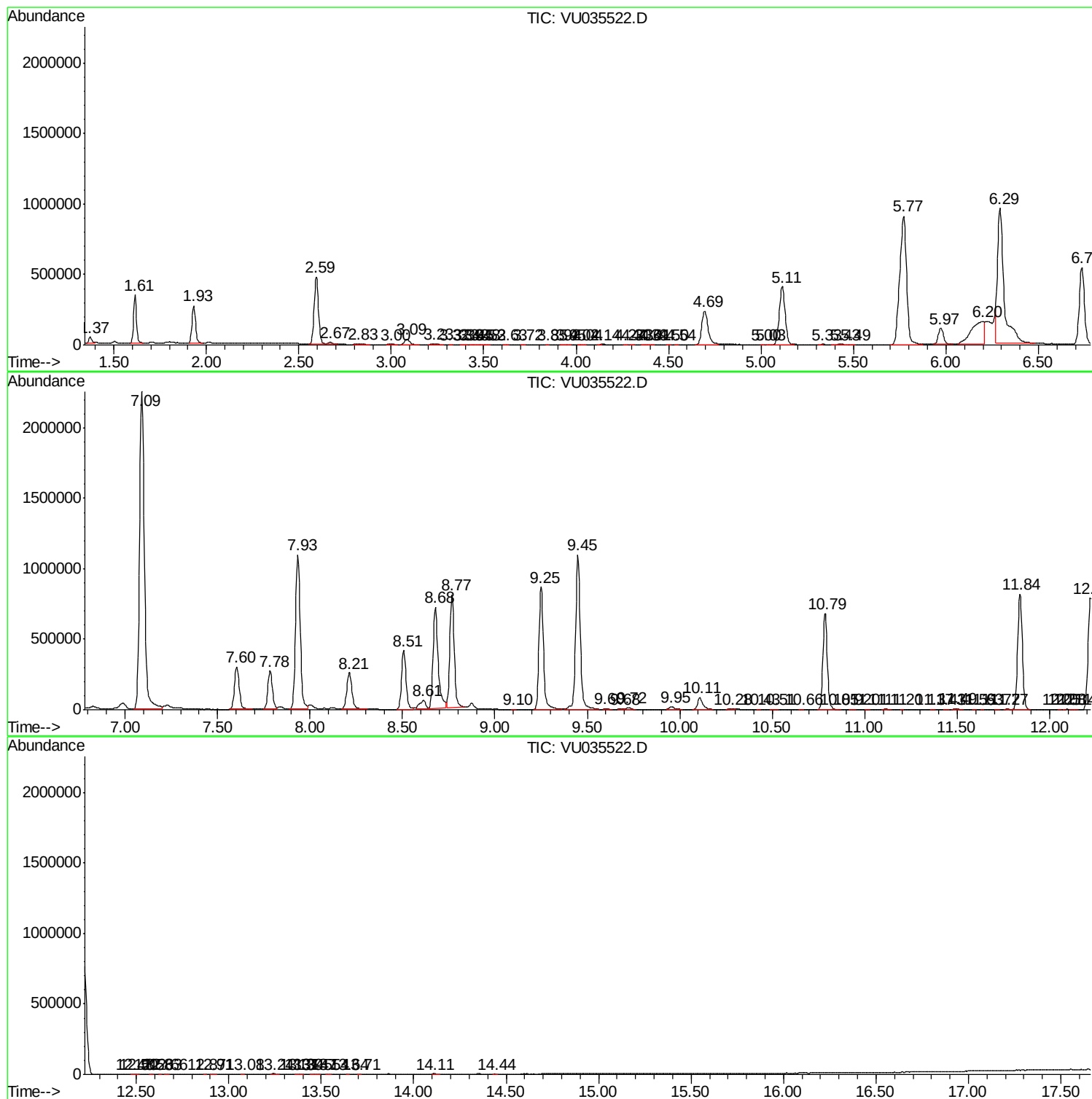
Sum of corrected areas: 28756240

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

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



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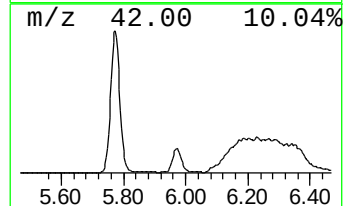
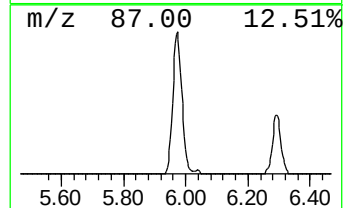
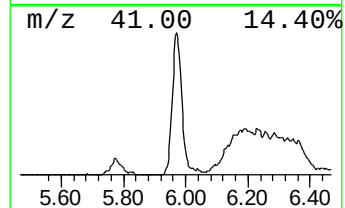
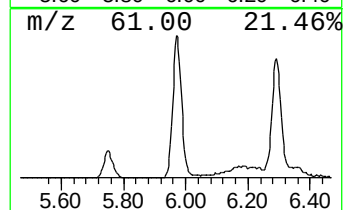
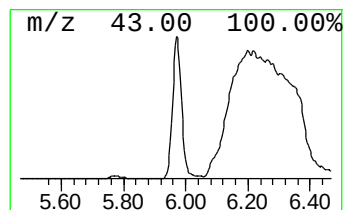
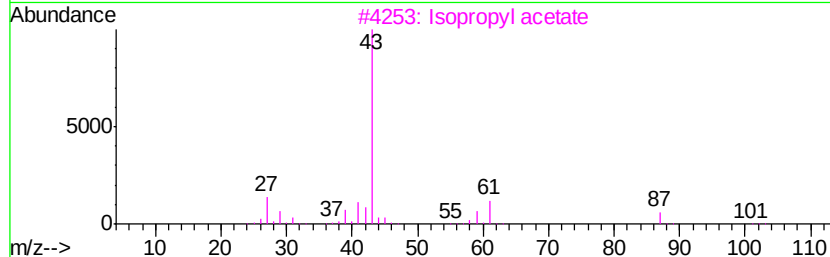
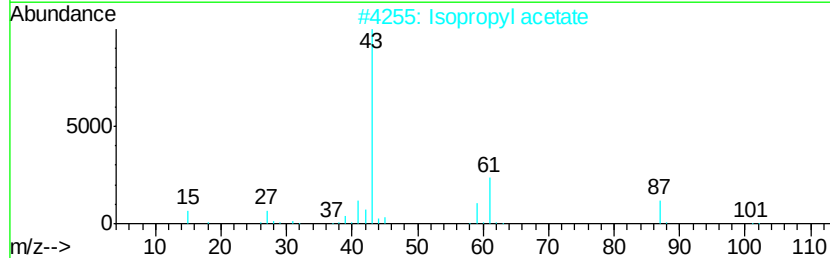
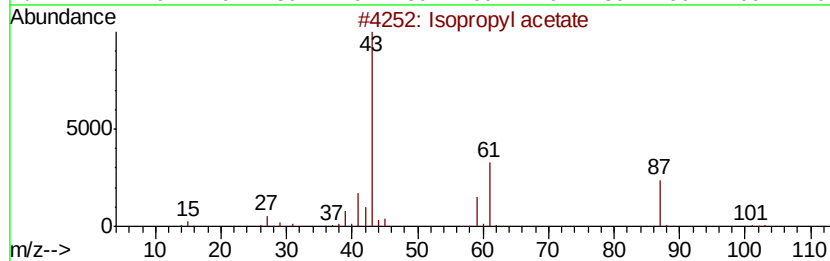
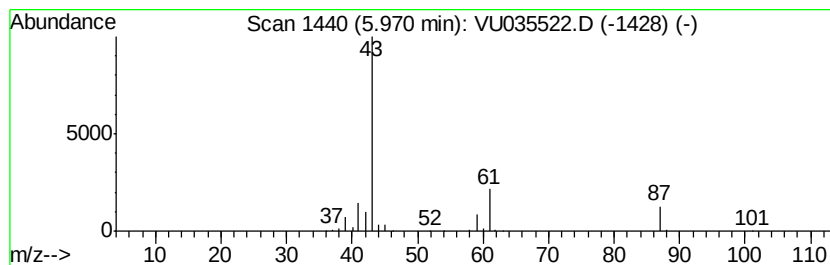
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102619WMA.M
Quant Title : VOC Analysis

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.
5.97	4.63 ug/L	224718	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	83
2		Isopropyl acetate	102	C5H10O2	000108-21-4	78
3		Isopropyl acetate	102	C5H10O2	000108-21-4	72
4		Isopropyl acetate	102	C5H10O2	000108-21-4	56
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28



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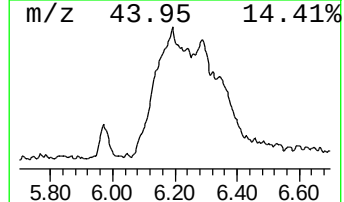
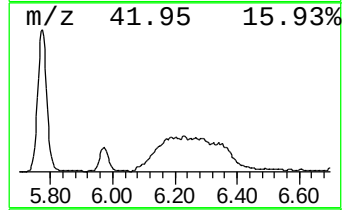
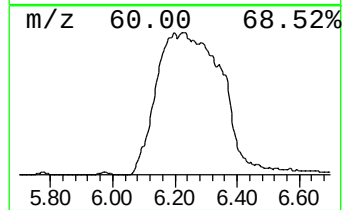
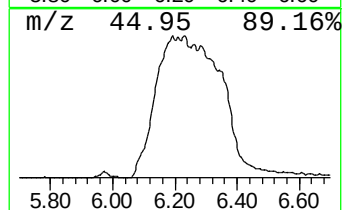
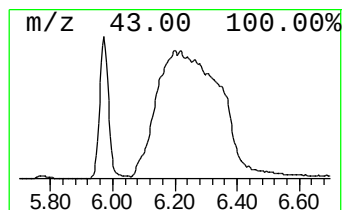
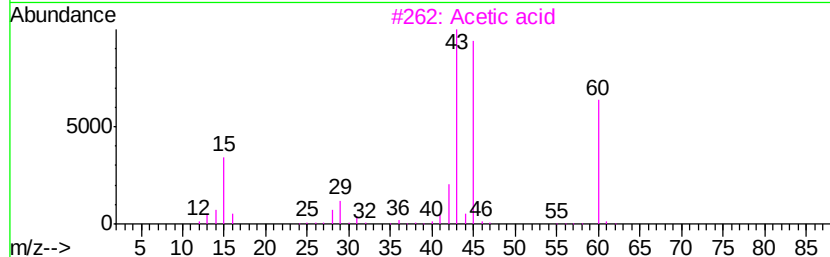
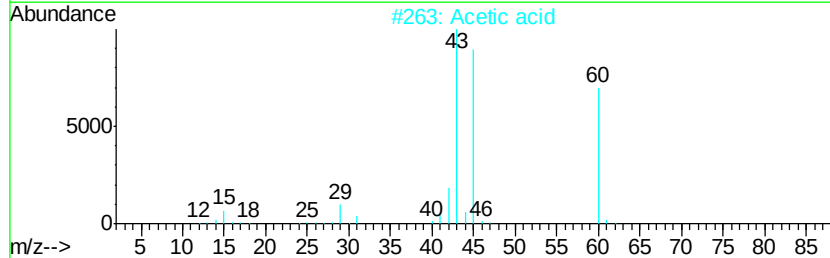
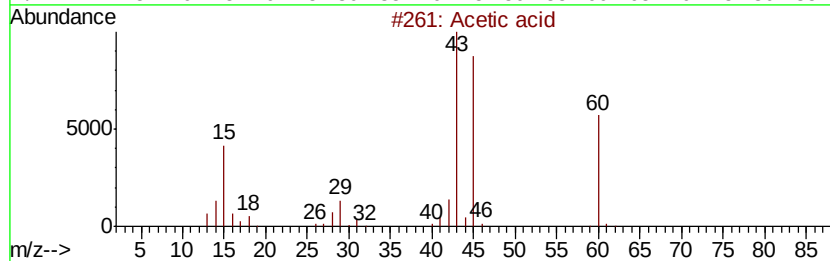
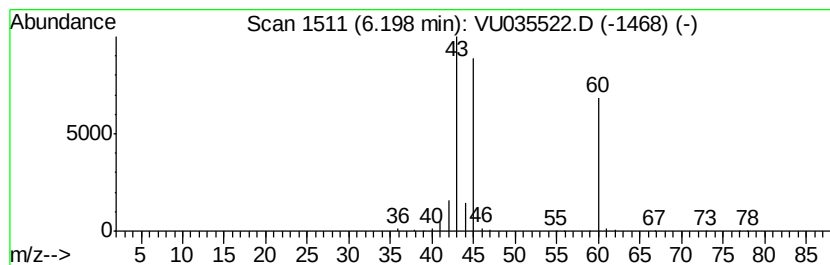
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Quant Title : VOC Analysis

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

Peak Number 2 Acetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.20	16.47 ug/L	799165	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	90
2		Acetic acid	60	C2H4O2	000064-19-7	90
3		Acetic acid	60	C2H4O2	000064-19-7	90
4		Ammonium acetate	77	C2H7NO2	000631-61-8	64
5		Acetic acid	60	C2H4O2	000064-19-7	50



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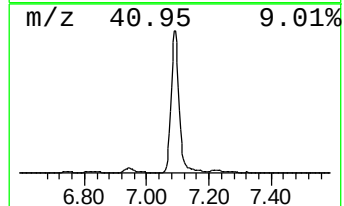
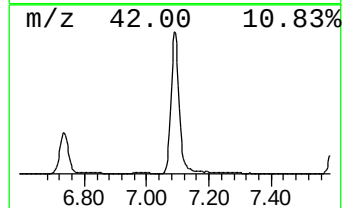
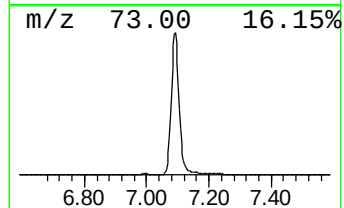
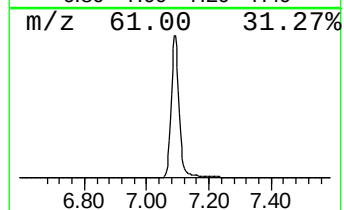
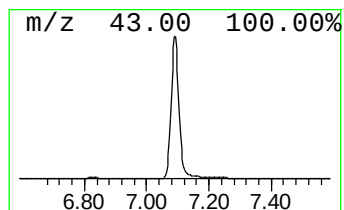
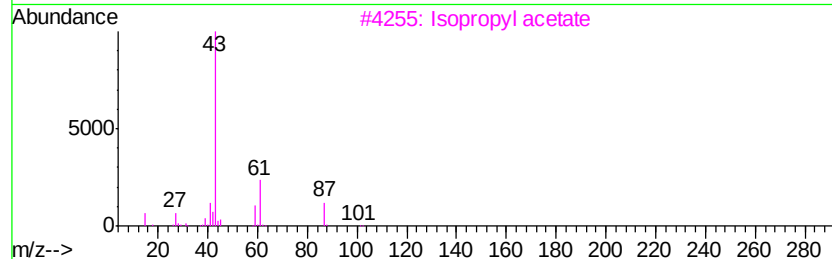
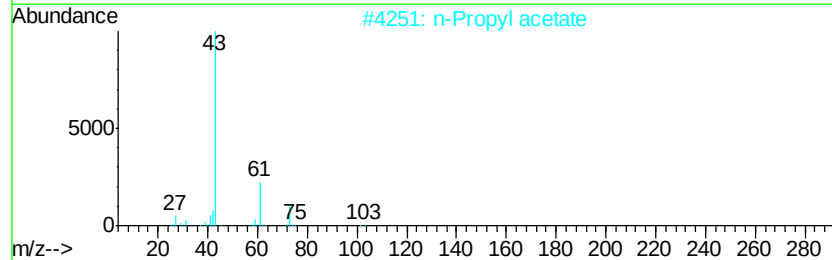
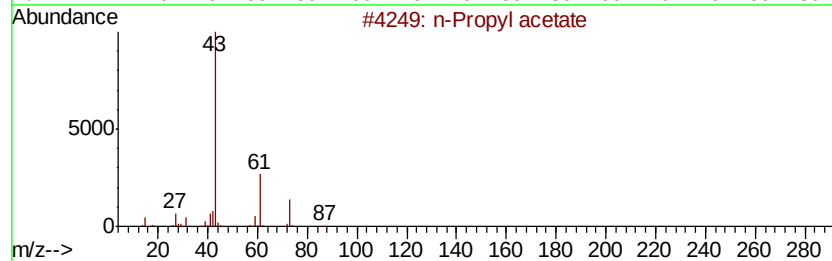
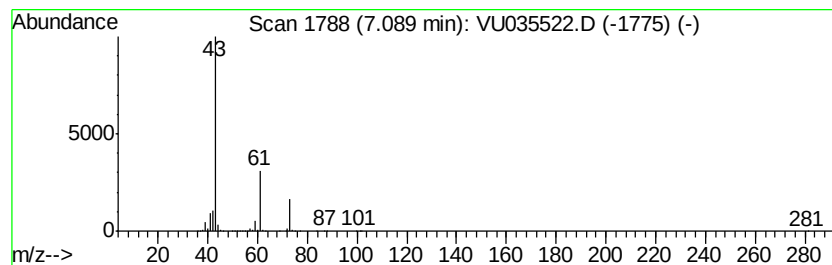
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Quant Title : VOC Analysis

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Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.09	83.46 ug/L	4050480	1,4-Difluorobenzene	6.29
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	n-Propyl acetate	102 C5H10O2	000109-60-4	9



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ClientSampleId :
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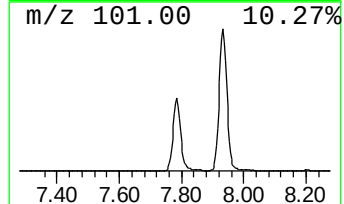
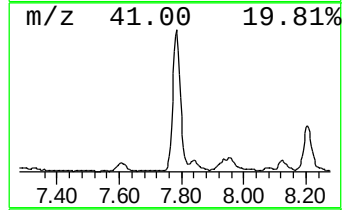
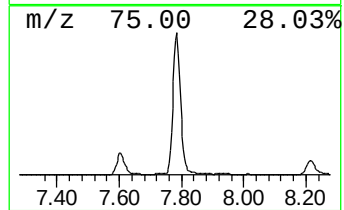
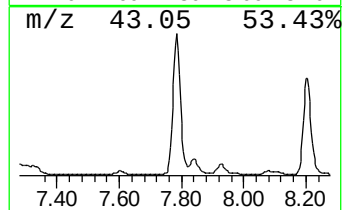
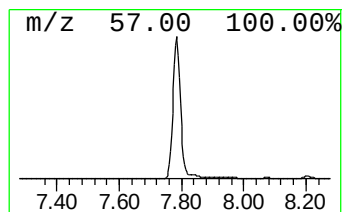
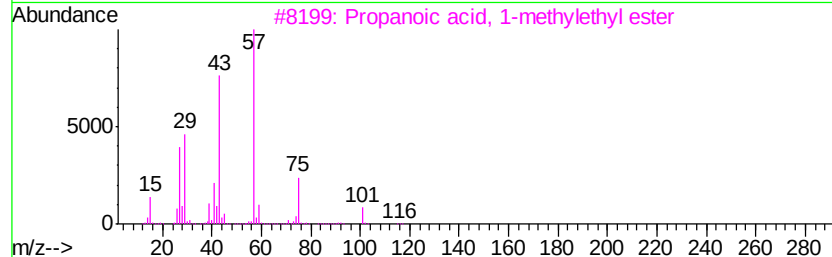
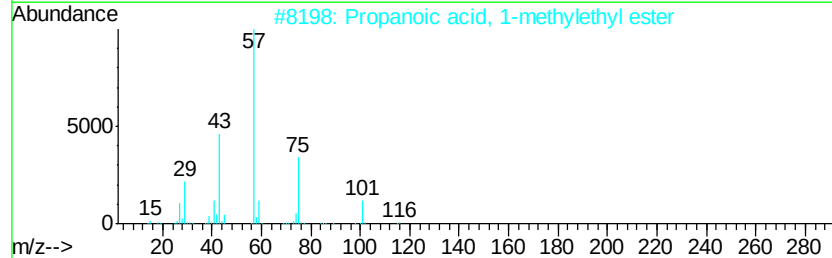
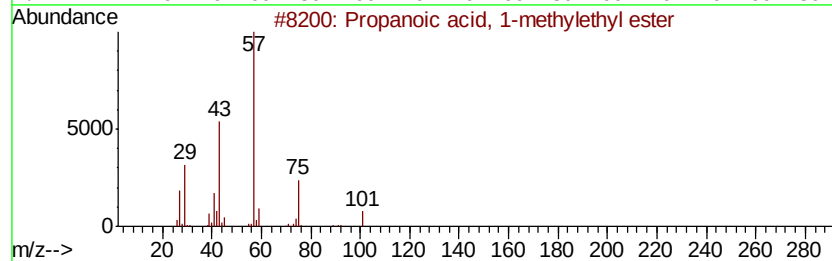
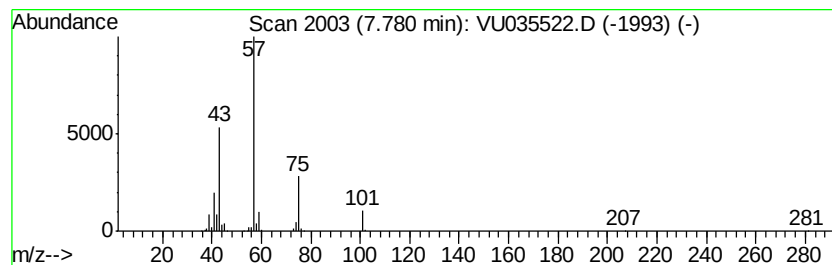
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	9.28 ug/L	450183	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	86
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, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035522.D
Acq On : 26 Oct 2019 16:44
Operator : JC/SP
Sample : K5536-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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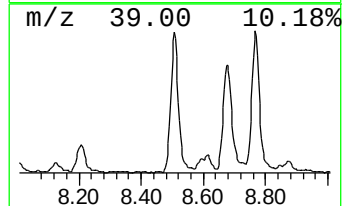
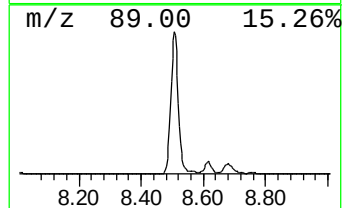
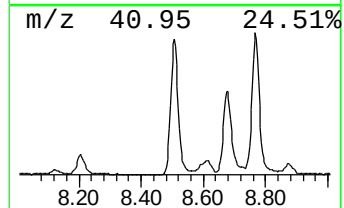
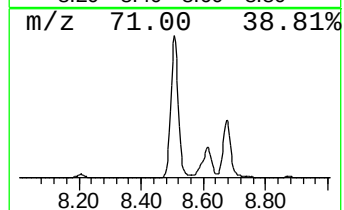
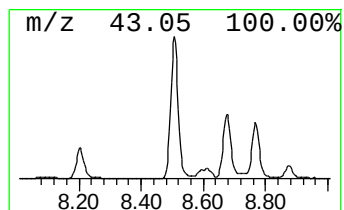
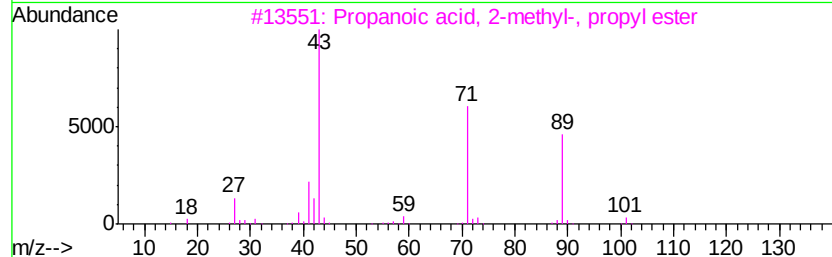
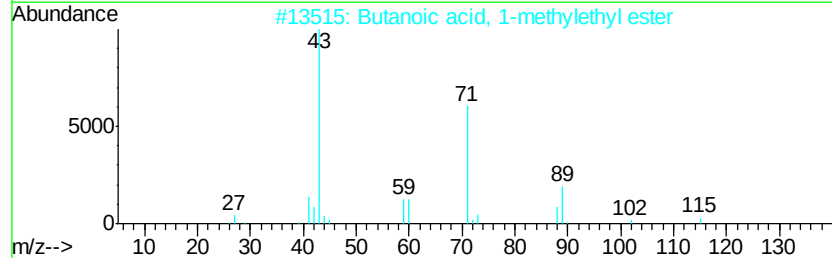
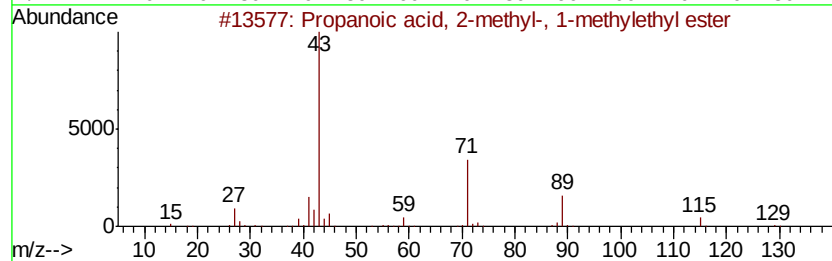
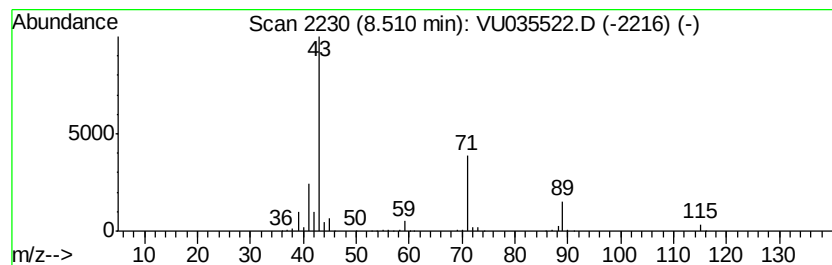
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	18.03 ug/L	703755	Chlorobenzene-d5	9.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
3		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035522.D
Acq On : 26 Oct 2019 16:44
Operator : JC/SP
Sample : K5536-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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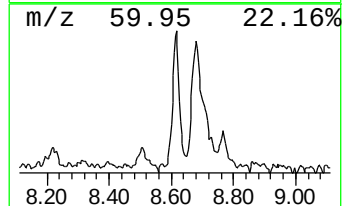
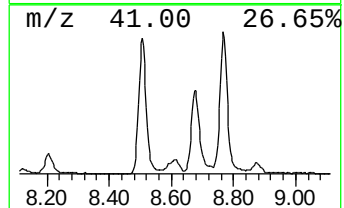
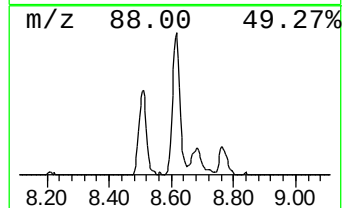
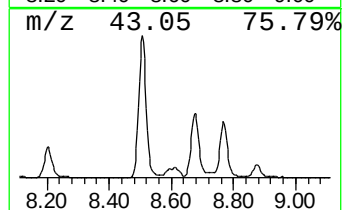
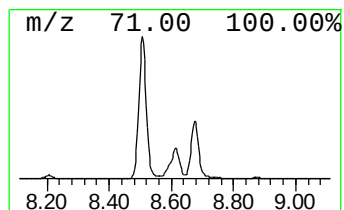
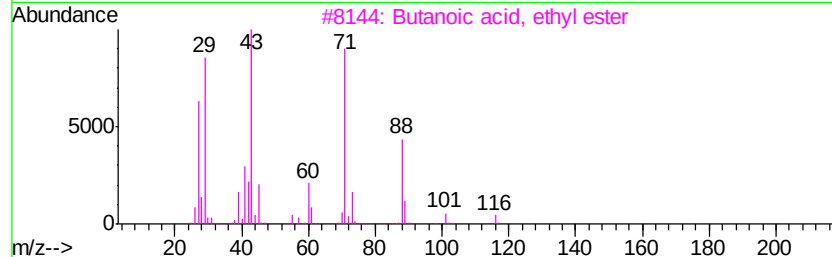
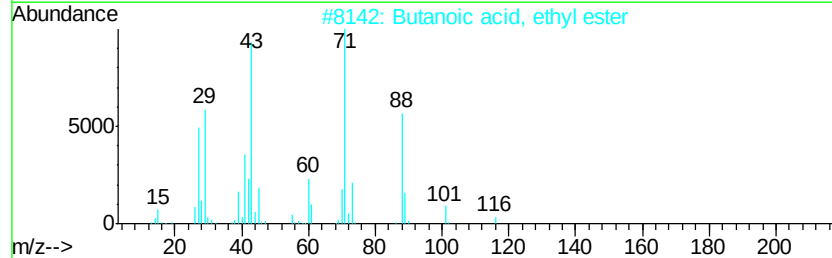
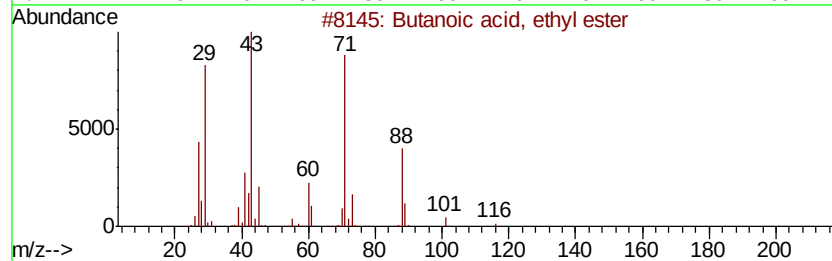
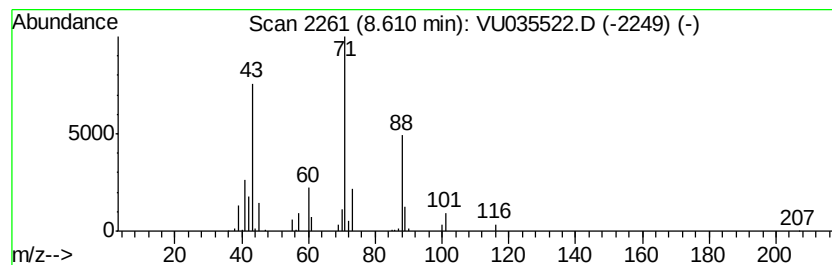
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Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.61	3.32 ug/L	129633	Chlorobenzene-d5	9.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
2		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	70
3		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	49
4		4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	47
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035522.D
Acq On : 26 Oct 2019 16:44
Operator : JC/SP
Sample : K5536-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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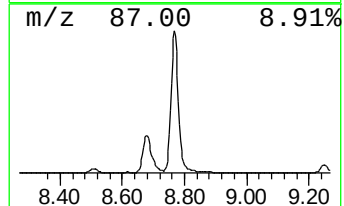
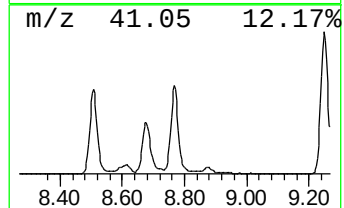
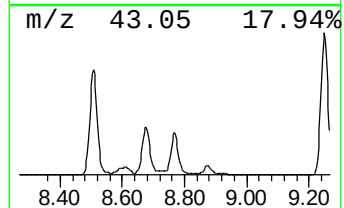
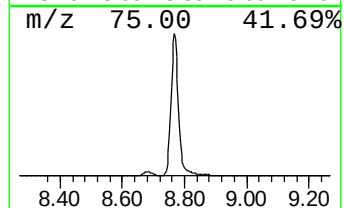
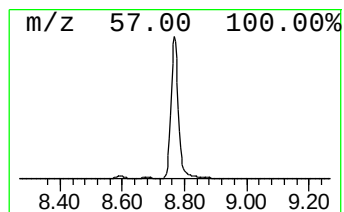
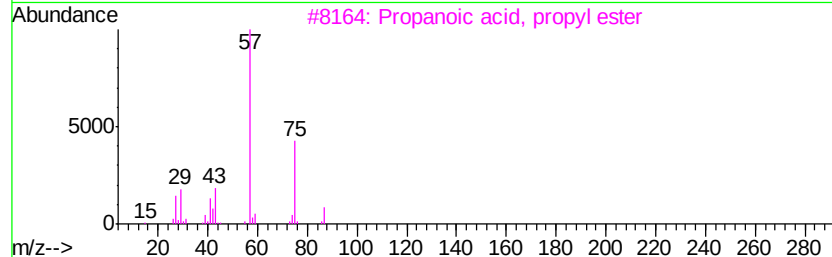
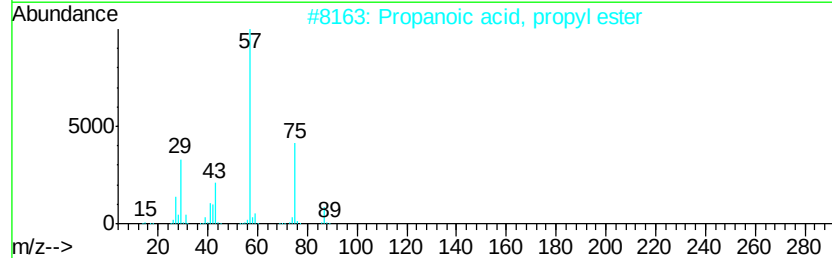
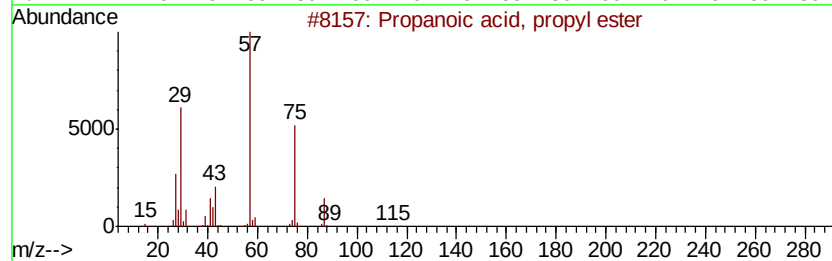
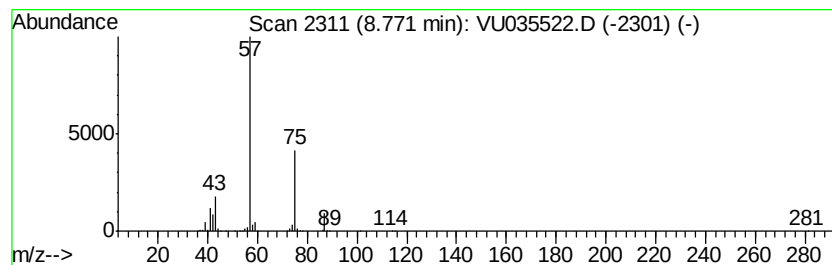
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Quant Title : VOC Analysis

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

Peak Number 8 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	33.74 ug/L	1317110	Chlorobenzene-d5	9.45

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:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035522.D
Acq On : 26 Oct 2019 16:44
Operator : JC/SP
Sample : K5536-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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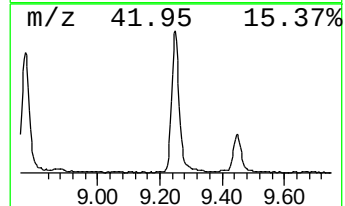
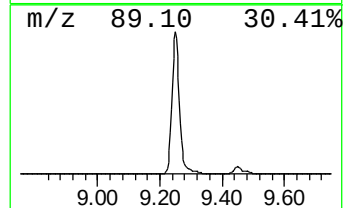
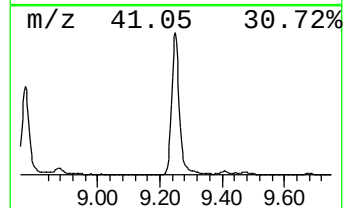
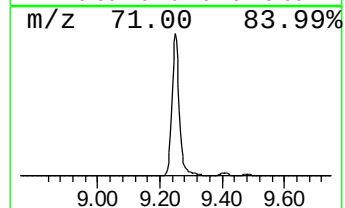
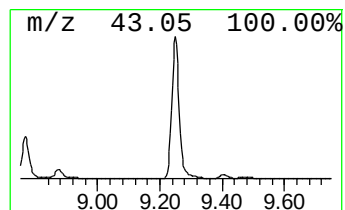
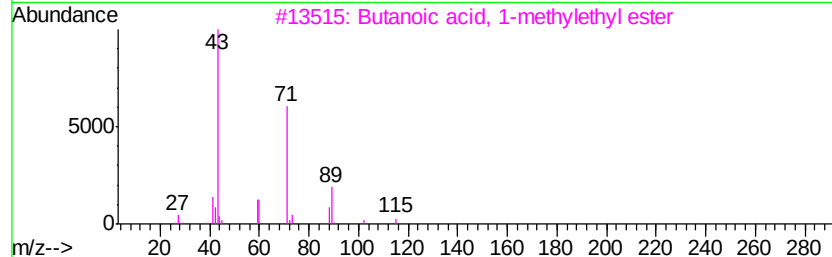
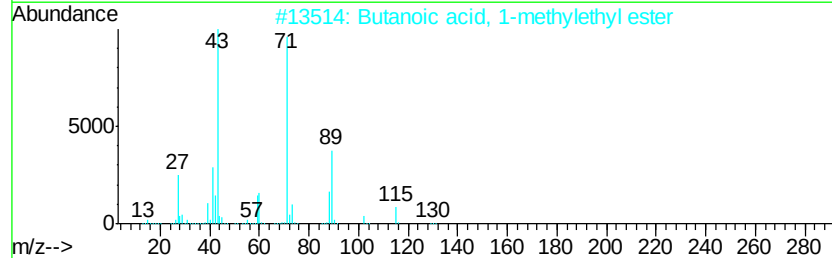
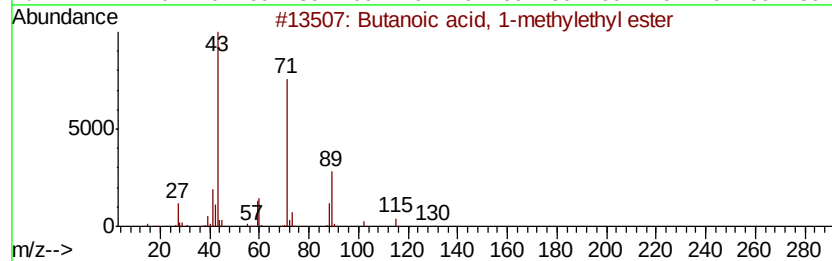
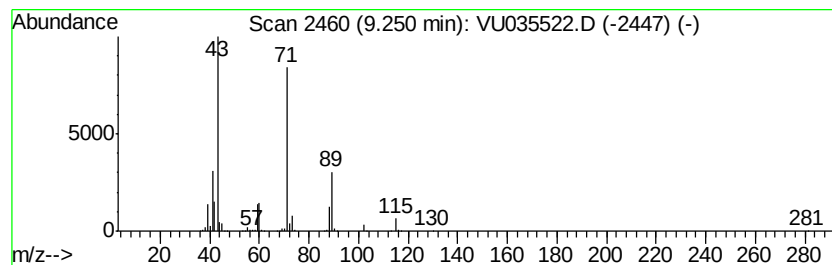
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Quant Title : VOC Analysis

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

Peak Number 9 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.25	37.34 ug/L	1457720	Chlorobenzene-d5	9.45

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	91
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102619\
Data File : VU035522.D
Acq On : 26 Oct 2019 16:44
Operator : JC/SP
Sample : K5536-02
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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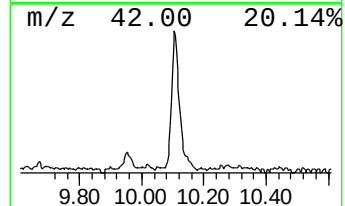
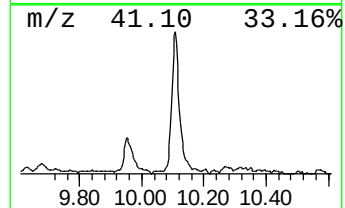
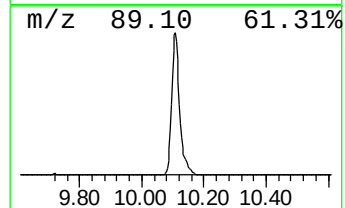
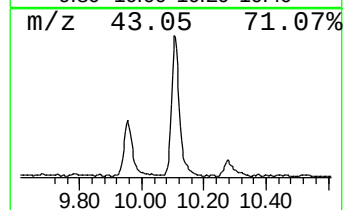
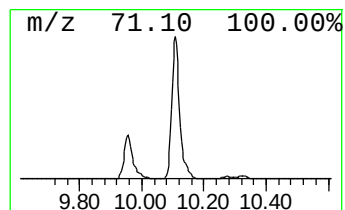
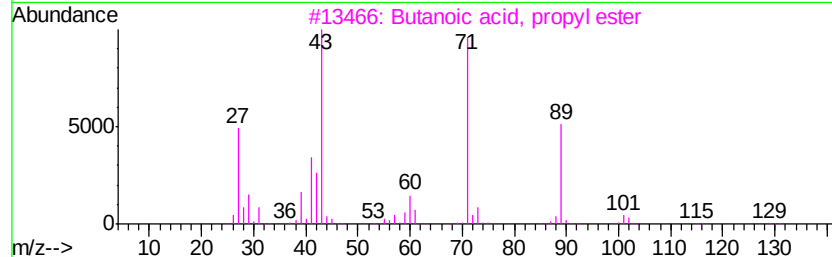
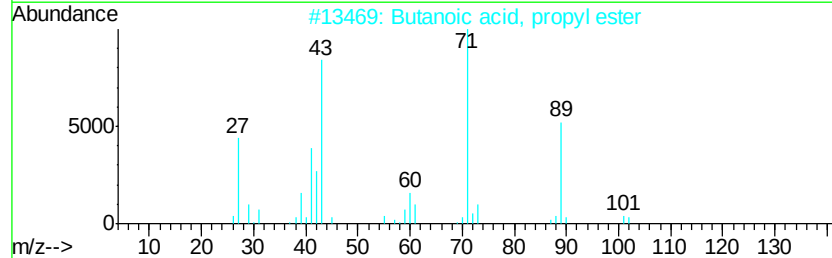
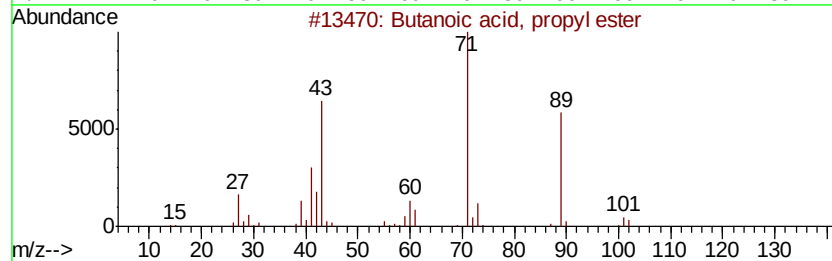
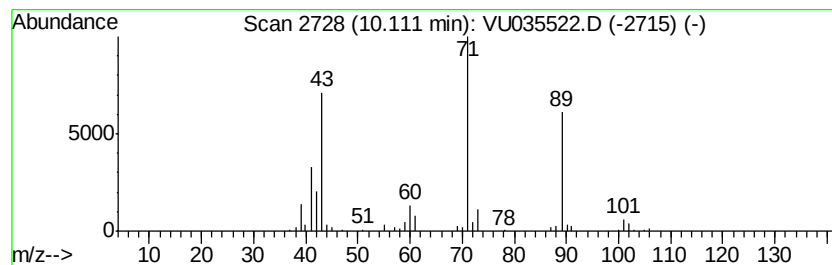
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Quant Title : VOC Analysis

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

Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.11	4.21 ug/L	164172	Chlorobenzene-d5	9.45

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:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU102619\
Data File : VU035522.D
Acq On : 26 Oct 2019 16:44
Operator : JC/SP
Sample : K5536-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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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
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Acetic acid	6.20	16.5	ug/L	799165	1	6.29	2426730	50.0
n-Propyl acetate	7.09	83.5	ug/L	4050480	1	6.29	2426730	50.0
Propanoic acid, 1...	7.78	9.3	ug/L	450183	1	6.29	2426730	50.0
Propanoic acid, 2...	8.51	18.0	ug/L	703755	2	9.45	1951730	50.0
Butanoic acid, et...	8.61	3.3	ug/L	129633	2	9.45	1951730	50.0
Propanoic acid, p...	8.77	33.7	ug/L	1317110	2	9.45	1951730	50.0
Butanoic acid, 1-...	9.25	37.3	ug/L	1457720	2	9.45	1951730	50.0
Butanoic acid, pr...	10.11	4.2	ug/L	164172	2	9.45	1951730	50.0