

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
 Data File : VU034744.D
 Acq On : 23 Sep 2019 19:45
 Operator : JC/SP
 Sample : PB123280TB
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB02

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\SOMULM091919WMA.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	1.177	24	27	33	rVB2	7288	5641	0.14%	0.021%
2	1.392	87	94	106	rBV	328924	345722	8.80%	1.270%
3	1.672	174	181	194	rVB	255809	325957	8.30%	1.198%
4	2.257	354	363	374	rVB	477866	720653	18.35%	2.648%
5	2.611	466	473	482	rBV5	4405	7074	0.18%	0.026%
6	2.685	482	496	509	rVB2	18786	37013	0.94%	0.136%
7	2.826	528	540	549	rBV2	12753	27954	0.71%	0.103%
8	2.955	576	580	584	rVB5	1474	1197	0.03%	0.004%
9	3.000	590	594	597	rVB5	1187	990	0.03%	0.004%
10	3.051	606	610	615	rBV4	1039	1071	0.03%	0.004%
11	3.151	639	641	644	rBV3	1276	755	0.02%	0.003%
12	3.177	646	649	657	rVB9	3172	3823	0.10%	0.014%
13	3.228	661	665	667	rBV3	983	709	0.02%	0.003%
14	3.341	697	700	704	rBV5	1150	940	0.02%	0.003%
15	3.386	709	714	718	rVV7	1348	1146	0.03%	0.004%
16	3.424	723	726	731	rVB5	1272	906	0.02%	0.003%
17	3.717	815	817	820	rVB4	1526	769	0.02%	0.003%
18	3.772	828	834	836	rBV5	1283	1302	0.03%	0.005%
19	3.823	846	850	856	rBV7	1764	2047	0.05%	0.008%
20	3.852	856	859	866	rVB6	1383	1258	0.03%	0.005%
21	3.913	876	878	884	rVB6	1456	1153	0.03%	0.004%
22	3.945	884	888	890	rBV4	1576	1317	0.03%	0.005%
23	3.984	897	900	904	rVB4	1040	838	0.02%	0.003%
24	4.003	904	906	910	rBV5	1281	876	0.02%	0.003%
25	4.026	910	913	917	rVB3	1484	1046	0.03%	0.004%
26	4.051	917	921	925	rBV2	1673	1546	0.04%	0.006%
27	4.151	940	952	979	rBV2	238759	657530	16.74%	2.416%
28	4.453	1041	1046	1048	rBV5	2348	1628	0.04%	0.006%
29	4.485	1054	1056	1061	rVB3	1165	732	0.02%	0.003%
30	4.514	1061	1065	1067	rVB4	1240	952	0.02%	0.003%
31	4.543	1070	1074	1081	rVB8	1874	2372	0.06%	0.009%
32	4.624	1081	1099	1125	rBV	373965	905192	23.04%	3.326%
33	5.054	1225	1233	1236	rBV10	1849	2061	0.05%	0.008%
34	5.103	1245	1248	1251	rBV5	1389	979	0.02%	0.004%

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 Title : VOC Analysis

35	5.315	1289	1314	1339	rBV2	777203	2318961	59.04%	8.522%
36	5.527	1370	1380	1402	rBV2	99297	214088	5.45%	0.787%
37	5.730	1438	1443	1444	rBV2	1768	1495	0.04%	0.005%
38	5.781	1455	1459	1461	rBV4	1673	1502	0.04%	0.006%
39	5.865	1467	1485	1504	rBV	660482	1521496	38.73%	5.591%
40	6.308	1610	1623	1643	rVB	544505	1089394	27.73%	4.003%
41	6.685	1727	1740	1770	rBV	2167324	3928086	100.00%	14.435%
42	7.070	1857	1860	1863	rBV4	2249	1938	0.05%	0.007%
43	7.206	1890	1902	1921	rVV	326019	593750	15.12%	2.182%
44	7.398	1951	1962	1992	rBV	267384	484371	12.33%	1.780%
45	7.543	1994	2007	2029	rBV	1076475	1931596	49.17%	7.098%
46	7.826	2083	2095	2116	rBV3	300698	553040	14.08%	2.032%
47	8.135	2173	2191	2207	rBV	520443	866629	22.06%	3.185%
48	8.212	2209	2215	2217	rBV2	22799	25904	0.66%	0.095%
49	8.289	2230	2239	2262	rVV	906500	1565246	39.85%	5.752%
50	8.395	2262	2272	2290	rVB	771533	1209927	30.80%	4.446%
51	8.508	2301	2307	2320	rVB2	42965	69675	1.77%	0.256%
52	8.717	2370	2372	2375	rBV3	1211	742	0.02%	0.003%
53	8.762	2382	2386	2389	rBV5	2547	1872	0.05%	0.007%
54	8.884	2411	2424	2448	rBV	1089894	1744328	44.41%	6.410%
55	9.067	2465	2481	2511	rVB	921396	1588736	40.45%	5.838%
56	9.276	2544	2546	2551	rBV6	1677	1573	0.04%	0.006%
57	9.312	2552	2557	2558	rBV5	3142	2167	0.06%	0.008%
58	9.427	2590	2593	2596	rVB4	2217	1276	0.03%	0.005%
59	9.495	2611	2614	2617	rBV4	1346	1109	0.03%	0.004%
60	9.585	2634	2642	2662	rVV4	22737	44482	1.13%	0.163%
61	9.746	2682	2692	2713	rBV2	124842	215384	5.48%	0.791%
62	9.913	2736	2744	2748	rBV5	4977	7211	0.18%	0.026%
63	9.932	2748	2750	2754	rVB3	2411	1444	0.04%	0.005%
64	9.961	2755	2759	2763	rBV6	2782	2968	0.08%	0.011%
65	10.061	2786	2790	2792	rBV4	1404	1112	0.03%	0.004%
66	10.138	2810	2814	2815	rBV4	1573	1144	0.03%	0.004%
67	10.408	2885	2898	2916	rBV	696682	1147803	29.22%	4.218%
68	10.524	2932	2934	2938	rBV5	1721	819	0.02%	0.003%
69	10.742	3000	3002	3003	rBV2	1997	798	0.02%	0.003%
70	10.881	3043	3045	3049	rVB3	1125	779	0.02%	0.003%
71	10.906	3049	3053	3057	rBV6	2035	1751	0.04%	0.006%

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72	11.054	3096	3099	3100	rBV2	1509	923	0.02%	0.003%
73	11.122	3117	3120	3123	rBV3	1589	1166	0.03%	0.004%
74	11.238	3153	3156	3159	rBV3	1001	785	0.02%	0.003%
75	11.376	3195	3199	3200	rBV3	1280	938	0.02%	0.003%
76	11.392	3202	3204	3213	rVB8	2887	3888	0.10%	0.014%
77	11.459	3213	3225	3248	rBV	854989	1400141	35.64%	5.145%
78	11.836	3327	3342	3367	rBV	926656	1565539	39.86%	5.753%
79	12.228	3462	3464	3468	rBV4	1536	1305	0.03%	0.005%
80	12.537	3556	3560	3563	rBV3	2550	1740	0.04%	0.006%
81	12.578	3571	3573	3578	rBV5	1384	1089	0.03%	0.004%
82	12.668	3599	3601	3604	rBV3	1462	840	0.02%	0.003%
83	12.765	3629	3631	3633	rBV3	1354	727	0.02%	0.003%
84	12.797	3639	3641	3644	rBV4	1169	843	0.02%	0.003%
85	12.932	3680	3683	3686	rBV4	1317	997	0.03%	0.004%
86	12.951	3686	3689	3693	rVB4	1723	1230	0.03%	0.005%
87	13.196	3763	3765	3768	rBV3	1075	849	0.02%	0.003%
88	13.353	3811	3814	3816	rBV4	1329	823	0.02%	0.003%
89	13.401	3825	3829	3830	rBV3	1578	940	0.02%	0.003%
90	13.434	3836	3839	3842	rBV5	1330	776	0.02%	0.003%
91	13.453	3842	3845	3847	rBV3	1299	735	0.02%	0.003%
92	13.726	3925	3930	3936	rBV10	2781	2576	0.07%	0.009%
93	13.765	3940	3942	3947	rBV5	1785	1546	0.04%	0.006%
94	13.819	3957	3959	3964	rVB4	1877	1461	0.04%	0.005%
95	14.028	4022	4024	4027	rBV4	1727	875	0.02%	0.003%
96	14.250	4090	4093	4094	rBV2	1989	1134	0.03%	0.004%
97	14.469	4157	4161	4168	rVB8	2512	3146	0.08%	0.012%
98	14.610	4202	4205	4210	rBV7	2299	2464	0.06%	0.009%
99	14.781	4256	4258	4260	rBV2	1993	907	0.02%	0.003%
100	15.382	4443	4445	4450	rBV5	2964	2047	0.05%	0.008%

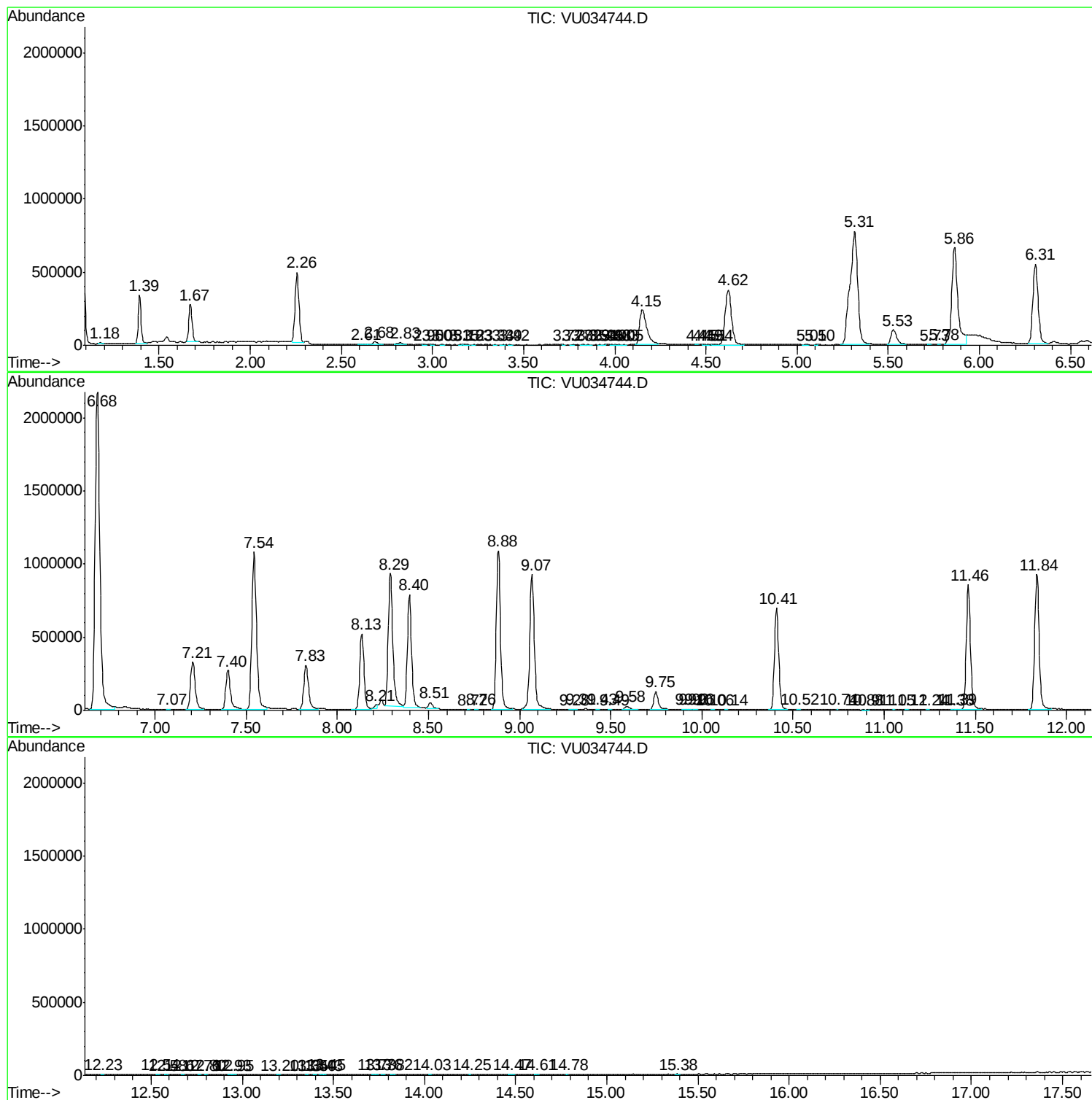
Sum of corrected areas: 27212175

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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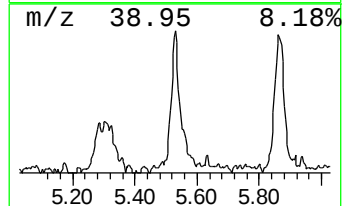
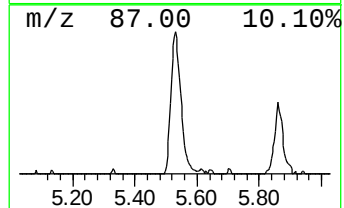
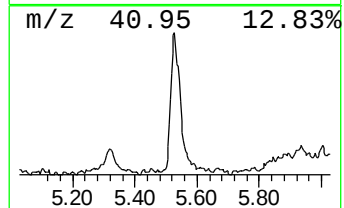
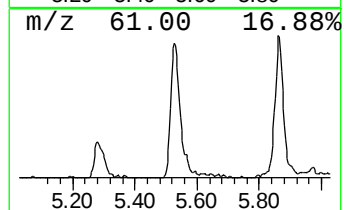
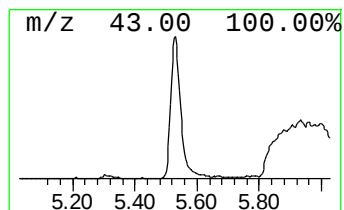
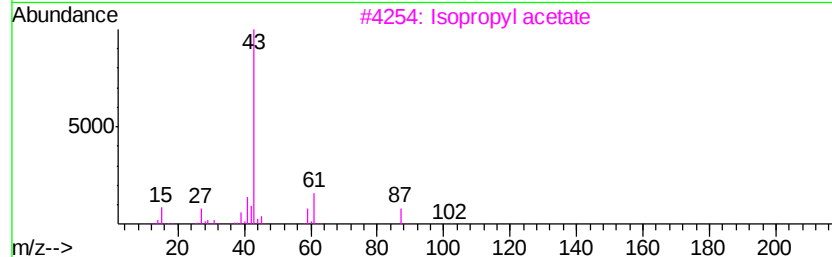
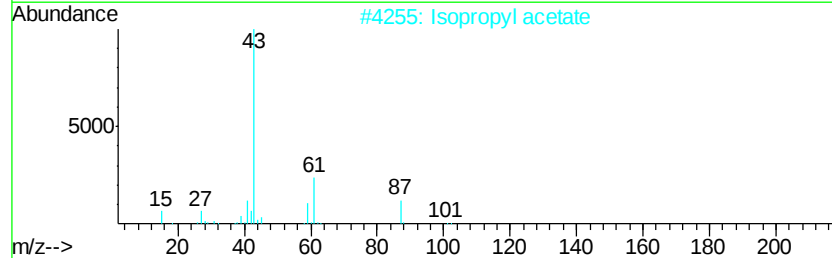
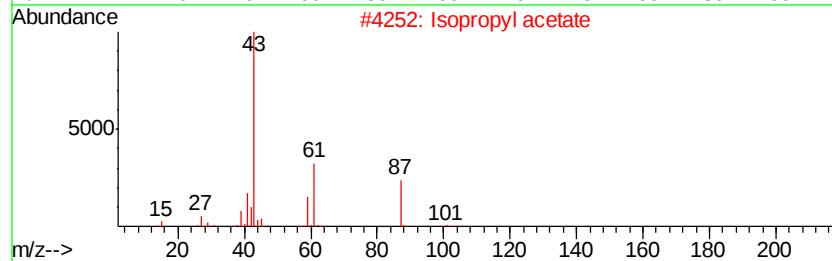
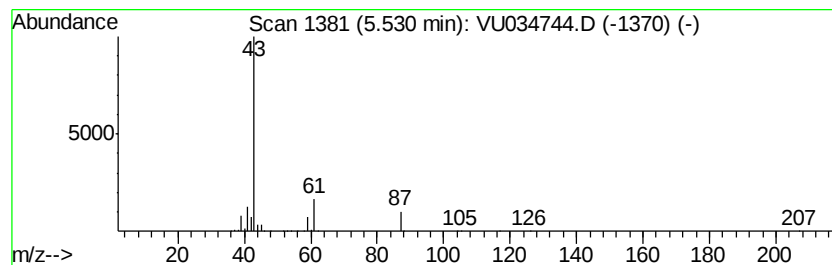
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	7.04 ug/L	214088	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	78
2		Isopropyl acetate	102	C5H10O2	000108-21-4	74
3		Isopropyl acetate	102	C5H10O2	000108-21-4	72
4		Isopropyl acetate	102	C5H10O2	000108-21-4	56
5		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9



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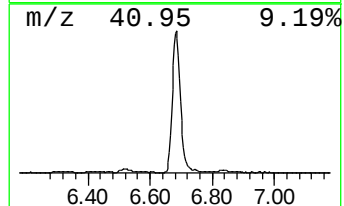
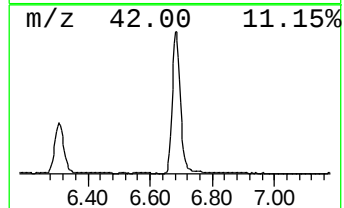
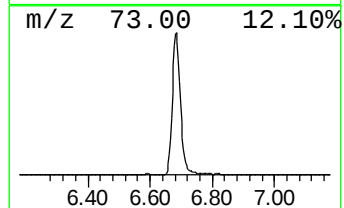
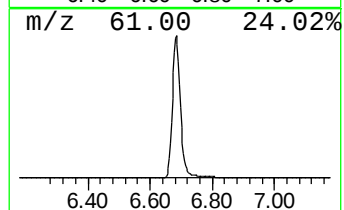
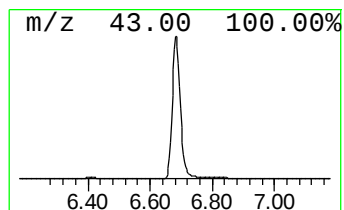
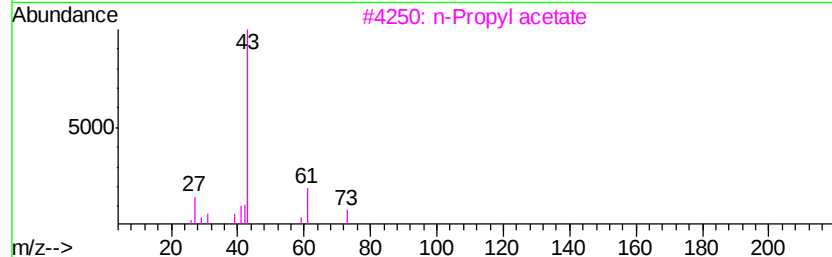
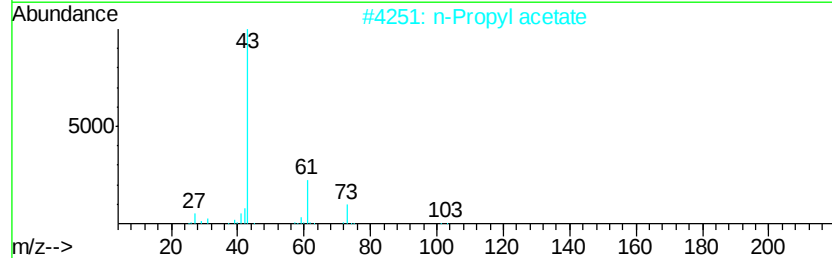
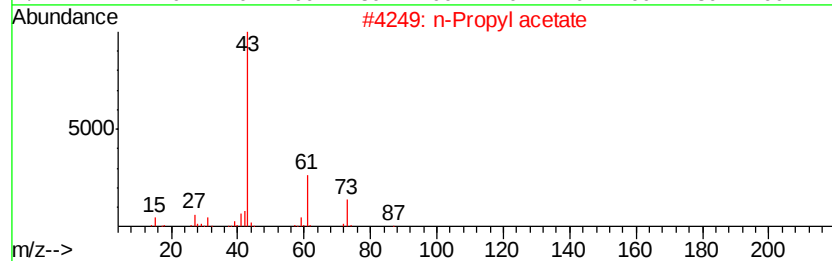
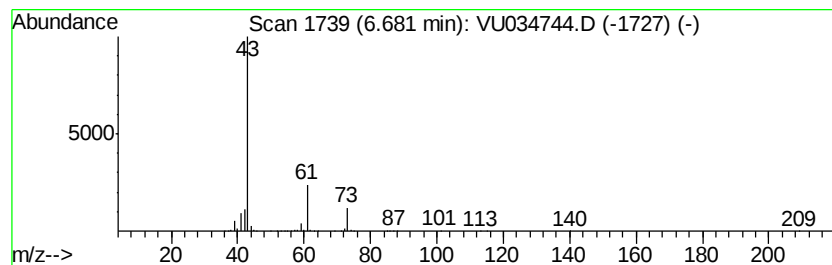
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Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	129.09 ug/L	3928090	1,4-Difluorobenzene	5.86
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	78
3	n-Propyl acetate	102 C5H10O2	000109-60-4	45
4	Isopropyl acetate	102 C5H10O2	000108-21-4	38
5	Isobutylamine	73 C4H11N	000078-81-9	7



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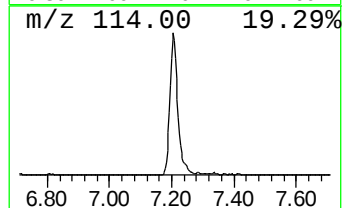
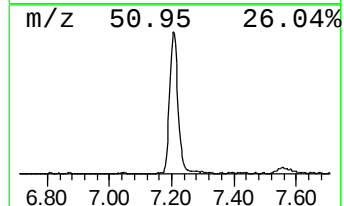
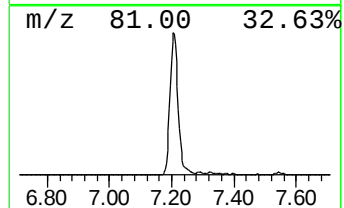
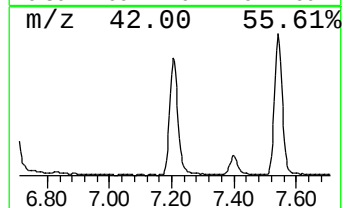
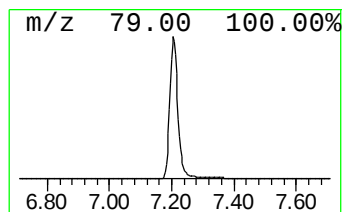
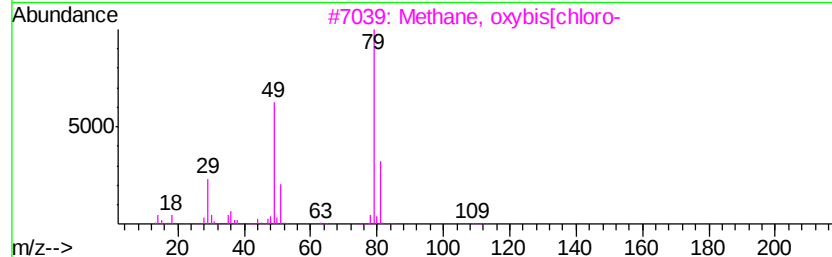
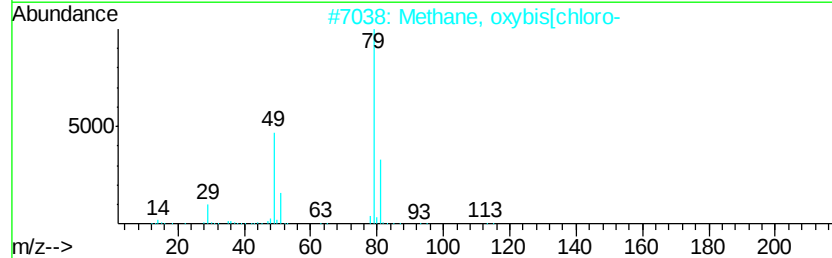
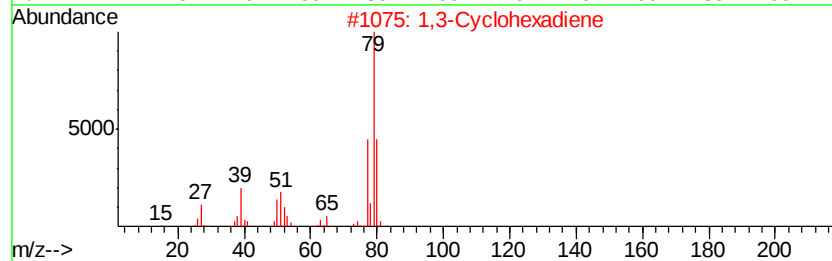
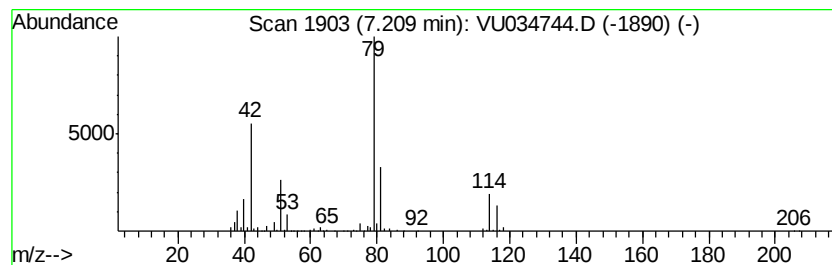
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	19.51 ug/L	593750	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclohexadiene	80	C6H8	000592-57-4	28
2		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	23
3		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	9
4		1,3,5-Hexatriene	80	C6H8	002235-12-3	9
5		1,4-Cyclohexadiene	80	C6H8	000628-41-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
Data File : VU034744.D
Acq On : 23 Sep 2019 19:45
Operator : JC/SP
Sample : PB123280TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

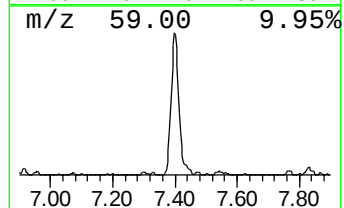
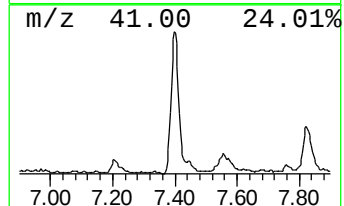
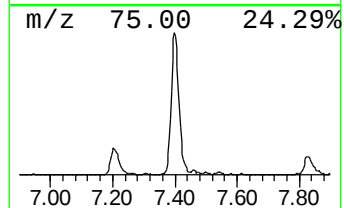
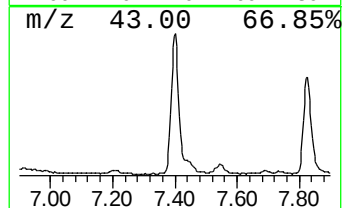
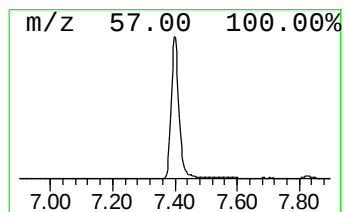
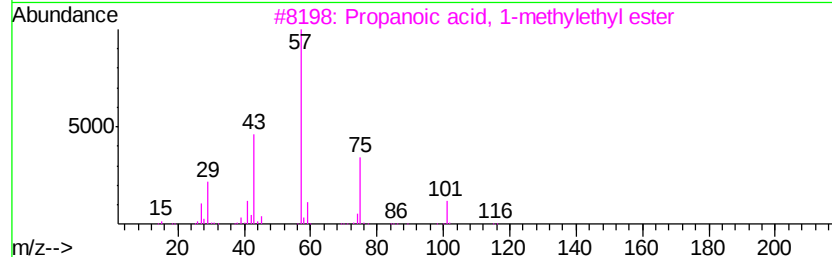
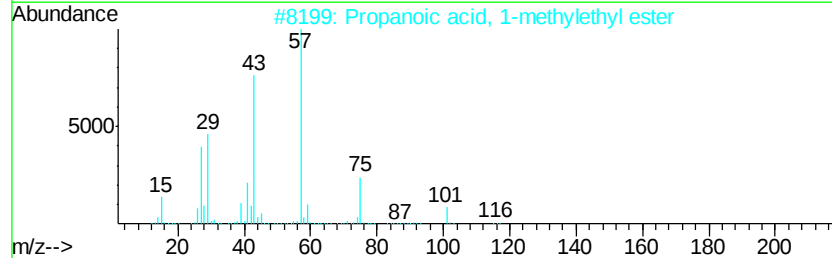
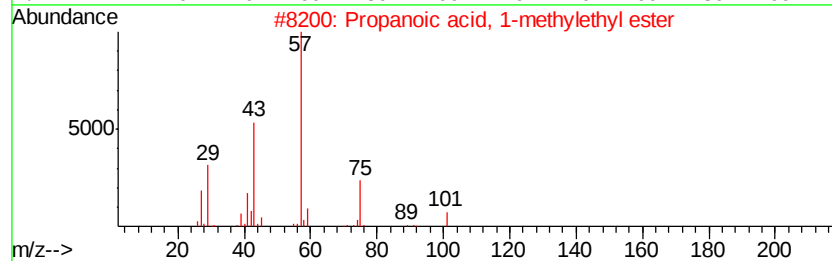
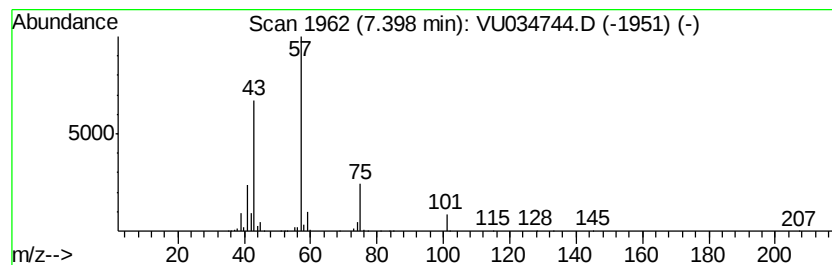
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	15.92 ug/L	484371	1,4-Difluorobenzene	5.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	72
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2		000637-78-5	56
5	Propanoic acid, propyl ester	116	C6H12O2		000106-36-5	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
Data File : VU034744.D
Acq On : 23 Sep 2019 19:45
Operator : JC/SP
Sample : PB123280TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

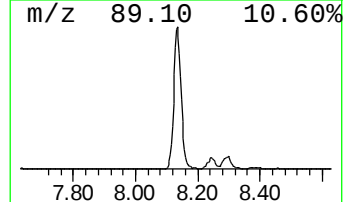
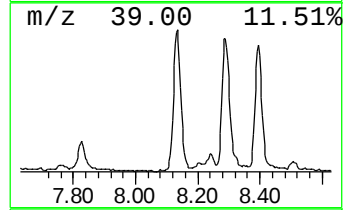
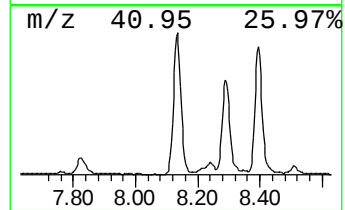
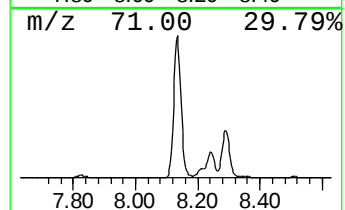
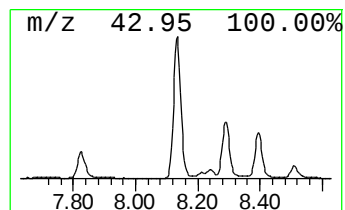
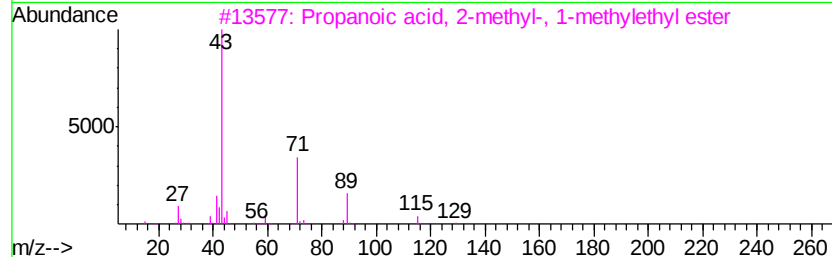
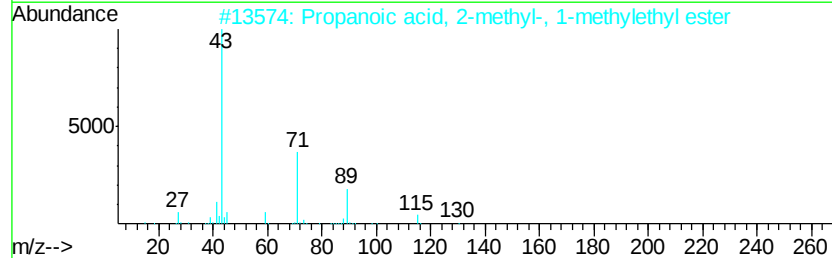
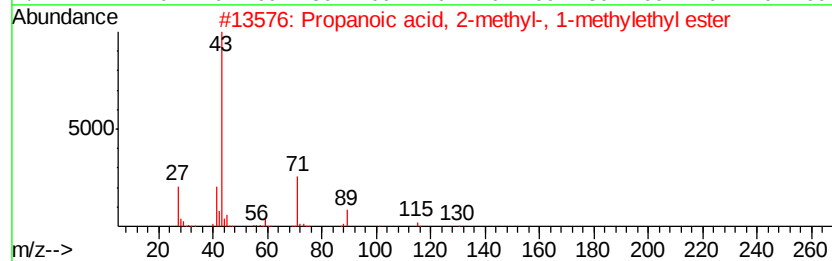
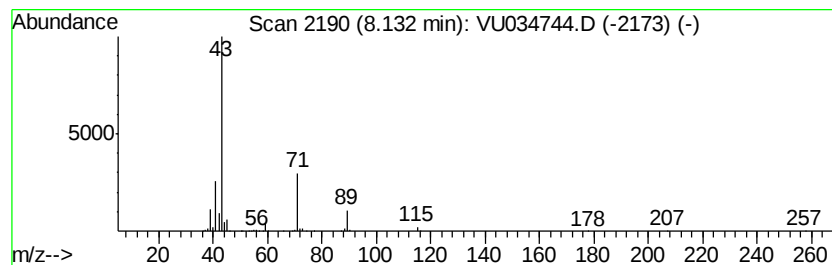
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	27.27 ug/L	866629	Chlorobenzene-d5	9.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83		
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78		
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53		
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53		
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	39		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
Data File : VU034744.D
Acq On : 23 Sep 2019 19:45
Operator : JC/SP
Sample : PB123280TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

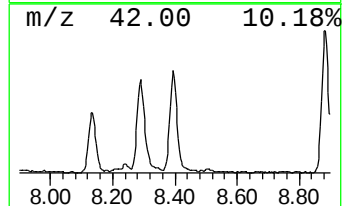
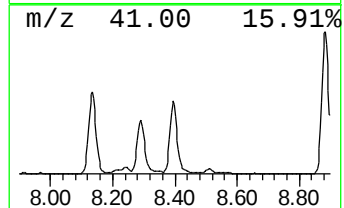
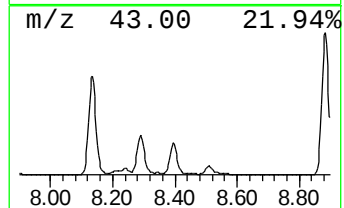
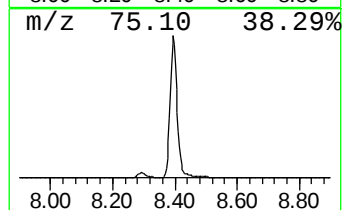
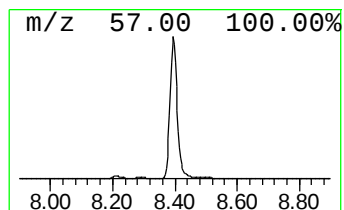
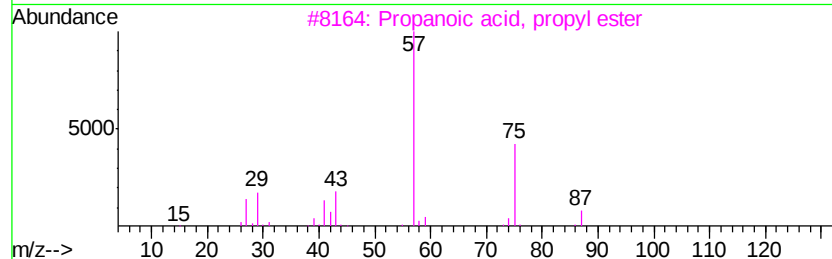
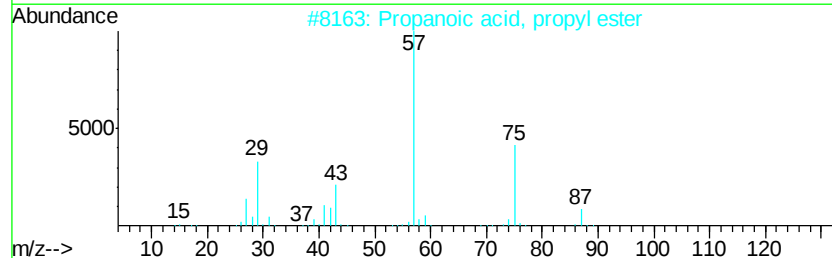
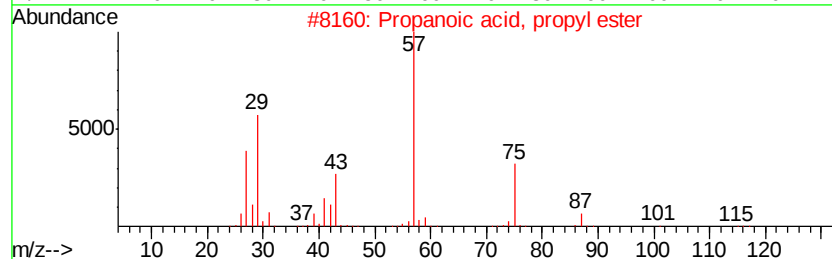
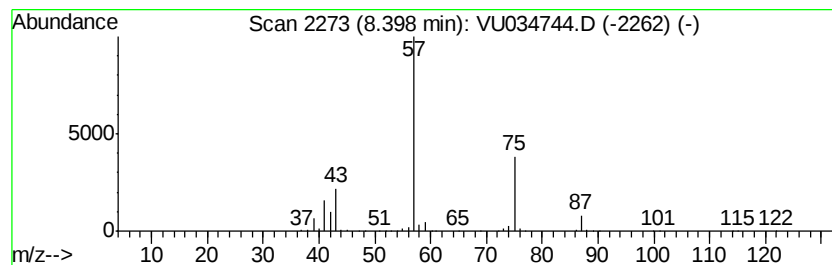
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	38.08 ug/L	1209930	Chlorobenzene-d5	9.07

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	78
4		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
Data File : VU034744.D
Acq On : 23 Sep 2019 19:45
Operator : JC/SP
Sample : PB123280TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

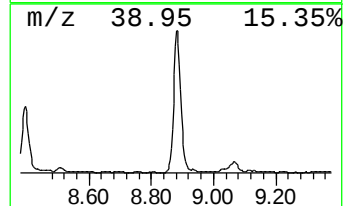
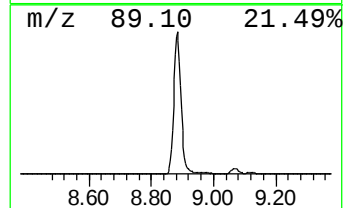
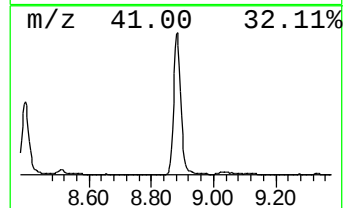
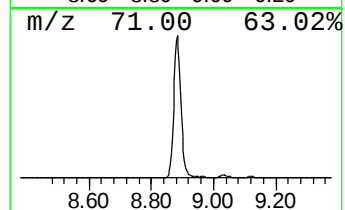
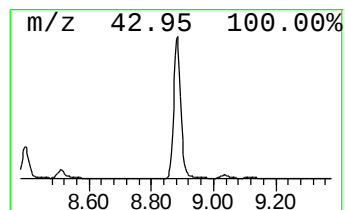
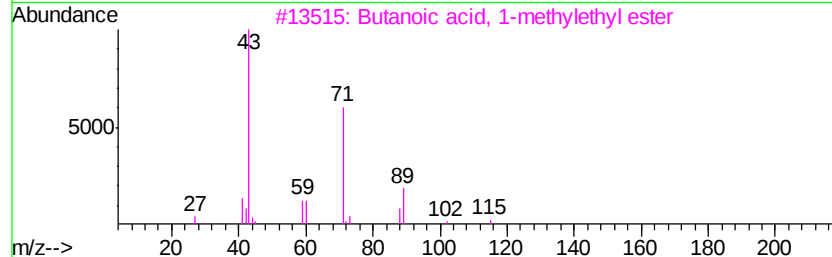
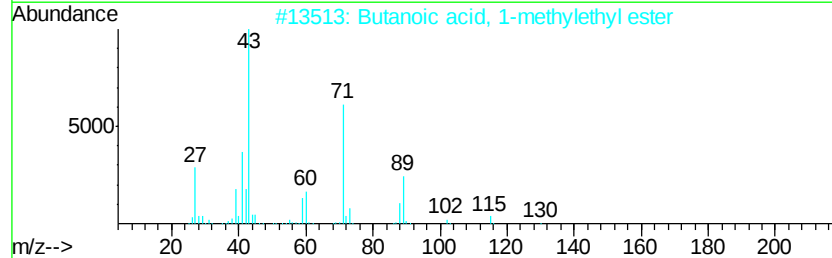
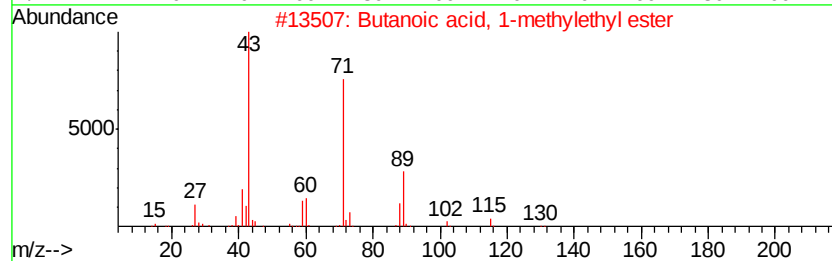
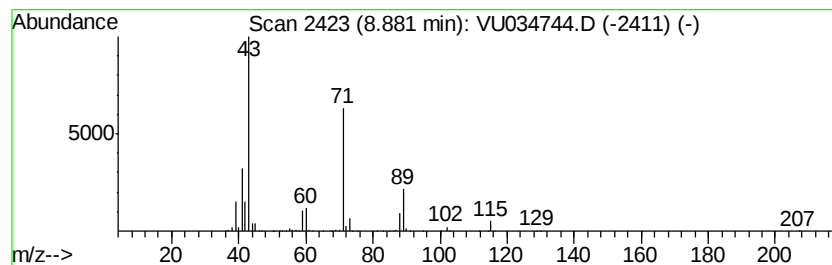
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	54.90 ug/L	1744330	Chlorobenzene-d5	9.07

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	86
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
Data File : VU034744.D
Acq On : 23 Sep 2019 19:45
Operator : JC/SP
Sample : PB123280TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

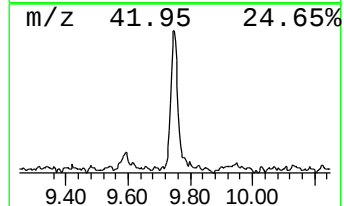
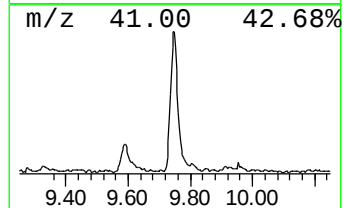
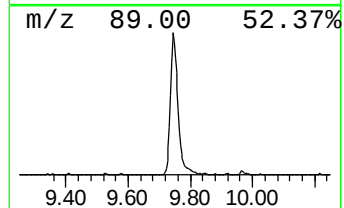
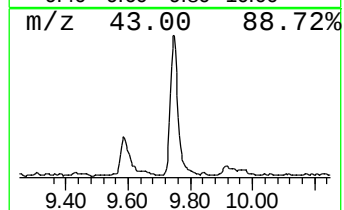
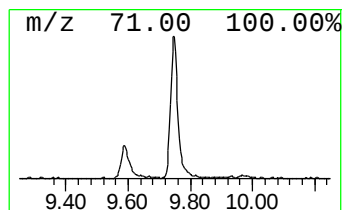
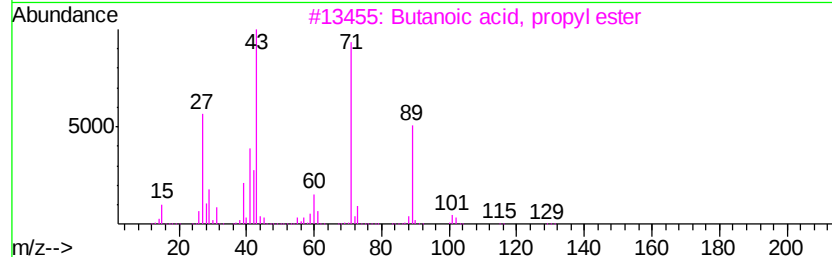
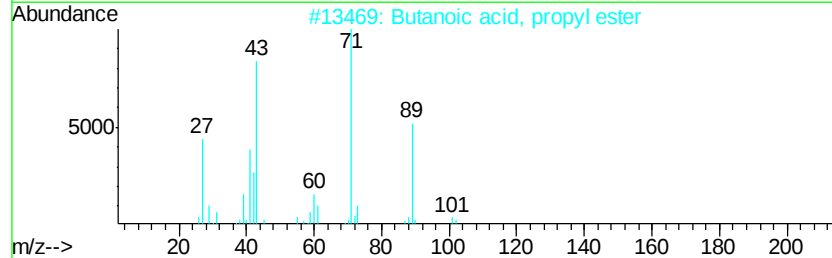
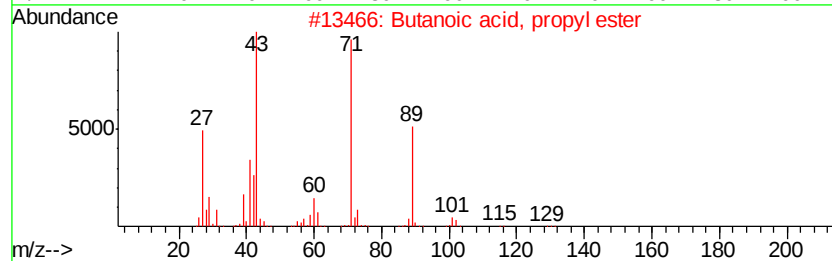
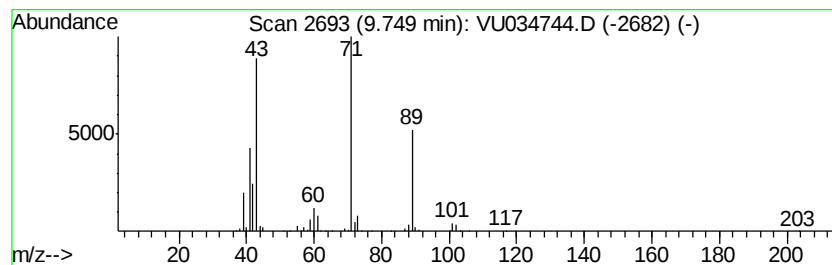
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Quant Title : VOC Analysis

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.
9.75	6.78 ug/L	215384	Chlorobenzene-d5	9.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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	83
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
5			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092319\
Data File : VU034744.D
Acq On : 23 Sep 2019 19:45
Operator : JC/SP
Sample : PB123280TB
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl acetate	5.53	7.0	ug/L	214088	1	5.86	1521500	50.0
n-Propyl acetate	6.68	129.1	ug/L	3928090	1	5.86	1521500	50.0
unknown-01	7.21	19.5	ug/L	593750	1	5.86	1521500	50.0
Propanoic acid, 1...	7.40	15.9	ug/L	484371	1	5.86	1521500	50.0
Propanoic acid, 2...	8.13	27.3	ug/L	866629	2	9.07	1588740	50.0
Propanoic acid, p...	8.40	38.1	ug/L	1209930	2	9.07	1588740	50.0
Butanoic acid, 1-...	8.88	54.9	ug/L	1744330	2	9.07	1588740	50.0
Butanoic acid, pr...	9.75	6.8	ug/L	215384	2	9.07	1588740	50.0