

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
 Data File : VV032117.D
 Acq On : 15 Sep 2023 13:30
 Operator : SY/MD
 Sample : 04359-05 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 JLAD3

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M

Title : VOC Analysis

Signal : TIC: VV032117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	91	rBV	161236	168447	15.33%	2.066%
2	1.532	146	153	170	rVB	129627	152821	13.91%	1.874%
3	2.060	308	317	329	rBV	250180	358946	32.67%	4.402%
4	2.362	408	411	413	rBV2	593	394	0.04%	0.005%
5	2.449	430	438	451	rVB	13102	21653	1.97%	0.266%
6	2.551	464	470	471	rBV3	688	687	0.06%	0.008%
7	2.715	519	521	523	rBV2	318	149	0.01%	0.002%
8	2.780	540	541	544	rBV	198	123	0.01%	0.002%
9	2.850	560	563	564	rBV	170	78	0.01%	0.001%
10	2.870	567	569	570	rVB	307	85	0.01%	0.001%
11	3.011	611	613	614	rBV	188	62	0.01%	0.001%
12	3.117	637	646	650	rBV5	833	1256	0.11%	0.015%
13	3.217	675	677	679	rBV3	281	161	0.01%	0.002%
14	3.285	695	698	701	rBV2	241	182	0.02%	0.002%
15	3.371	723	725	728	rVB	197	110	0.01%	0.001%
16	3.442	742	747	748	rVB	326	164	0.01%	0.002%
17	3.458	748	752	754	rBV	236	180	0.02%	0.002%
18	3.568	784	786	791	rVB2	164	78	0.01%	0.001%
19	3.606	796	798	801	rVB	306	124	0.01%	0.002%
20	3.625	801	804	805	rBV2	196	81	0.01%	0.001%
21	3.635	805	807	810	rVB2	251	134	0.01%	0.002%
22	3.651	810	812	814	rBV	209	99	0.01%	0.001%
23	3.667	814	817	820	rVB2	295	164	0.01%	0.002%
24	3.690	820	824	828	rBV	128	160	0.01%	0.002%
25	3.706	828	829	830	rBV	126	40	0.00%	0.000%
26	3.738	836	839	840	rBV	200	86	0.01%	0.001%
27	3.754	840	844	845	rBV	284	206	0.02%	0.003%
28	3.789	845	855	892	rBV	84599	239714	21.82%	2.940%
29	4.252	982	999	1023	rBV	164739	420239	38.25%	5.153%
30	4.612	1107	1111	1115	rVB2	366	289	0.03%	0.004%
31	4.638	1115	1119	1120	rBV	266	161	0.01%	0.002%
32	4.667	1125	1128	1131	rBV	184	124	0.01%	0.002%
33	4.757	1153	1156	1157	rBV	270	131	0.01%	0.002%
34	4.834	1178	1180	1184	rBV3	210	125	0.01%	0.002%
35	4.902	1196	1201	1202	rBV2	248	199	0.02%	0.002%
36	4.960	1202	1219	1247	rBV2	418408	1098792	100.00%	13.474%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
 Title : VOC Analysis

37	5.214	1290	1298	1313	rBV3	5403	13474	1.23%	0.165%
38	5.474	1377	1379	1381	rBV3	252	145	0.01%	0.002%
39	5.538	1387	1399	1420	rBV	220608	460084	41.87%	5.642%
40	5.831	1479	1490	1507	rBV2	11082	24441	2.22%	0.300%
41	5.992	1527	1540	1571	rBV	240046	507290	46.17%	6.221%
42	6.220	1609	1611	1615	rBV3	456	295	0.03%	0.004%
43	6.397	1658	1666	1692	rBV	78666	160151	14.58%	1.964%
44	6.783	1782	1786	1789	rVB2	358	246	0.02%	0.003%
45	6.799	1789	1791	1797	rVB2	390	350	0.03%	0.004%
46	6.831	1799	1801	1806	rBV2	270	183	0.02%	0.002%
47	6.915	1817	1827	1857	rBV	133753	251904	22.93%	3.089%
48	7.127	1884	1893	1905	rBV	20218	35827	3.26%	0.439%
49	7.246	1919	1930	1965	rBV	504953	890564	81.05%	10.921%
50	7.554	2016	2026	2048	rBV2	103506	194307	17.68%	2.383%
51	7.866	2111	2123	2146	rBV	26790	49715	4.52%	0.610%
52	8.027	2164	2173	2199	rBV	253355	470317	42.80%	5.767%
53	8.249	2236	2242	2263	rVB2	16270	31092	2.83%	0.381%
54	8.548	2333	2335	2336	rBV	363	174	0.02%	0.002%
55	8.622	2348	2358	2385	rBV	69998	116963	10.64%	1.434%
56	8.789	2398	2410	2431	rBV	344994	582120	52.98%	7.138%
57	9.156	2521	2524	2526	rVB	230	114	0.01%	0.001%
58	9.169	2526	2528	2529	rBV	211	87	0.01%	0.001%
59	9.278	2558	2562	2563	rBV3	246	200	0.02%	0.002%
60	9.435	2609	2611	2612	rBV	296	116	0.01%	0.001%
61	9.503	2626	2632	2638	rBV5	1867	2648	0.24%	0.032%
62	9.619	2666	2668	2669	rBV	342	113	0.01%	0.001%
63	9.648	2674	2677	2678	rBV	115	72	0.01%	0.001%
64	9.670	2681	2684	2685	rBV2	199	114	0.01%	0.001%
65	9.699	2688	2693	2694	rBV	205	181	0.02%	0.002%
66	9.770	2713	2715	2717	rBV	259	145	0.01%	0.002%
67	9.866	2743	2745	2747	rVB	336	133	0.01%	0.002%
68	9.879	2747	2749	2753	rVB2	395	249	0.02%	0.003%
69	9.902	2753	2756	2758	rVB3	338	151	0.01%	0.002%
70	9.927	2762	2764	2767	rBV3	298	148	0.01%	0.002%
71	10.037	2794	2798	2799	rBV	289	156	0.01%	0.002%
72	10.107	2817	2820	2822	rVB2	292	140	0.01%	0.002%
73	10.156	2822	2835	2859	rBV	307596	493672	44.93%	6.054%
74	10.516	2945	2947	2949	rBV2	282	135	0.01%	0.002%
75	10.632	2978	2983	2984	rBV	386	271	0.02%	0.003%
76	10.657	2988	2991	2992	rBV	77	45	0.00%	0.001%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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 Title : VOC Analysis

77	10.705	3004	3006	3009	rVB	192	77	0.01%	0.001%
78	10.731	3011	3014	3017	rVB3	420	282	0.03%	0.003%
79	10.760	3017	3023	3026	rBV3	219	275	0.03%	0.003%
80	10.914	3069	3071	3073	rVB	241	76	0.01%	0.001%
81	10.976	3087	3090	3091	rBV	126	64	0.01%	0.001%
82	11.059	3111	3116	3121	rBV2	517	463	0.04%	0.006%
83	11.085	3122	3124	3125	rBV	184	60	0.01%	0.001%
84	11.188	3145	3156	3177	rBV	395463	606679	55.21%	7.440%
85	11.477	3245	3246	3248	rBV	242	113	0.01%	0.001%
86	11.487	3248	3249	3252	rVV2	240	126	0.01%	0.002%
87	11.564	3261	3273	3299	rBV	501759	784622	71.41%	9.622%
88	11.824	3352	3354	3355	rBV	224	100	0.01%	0.001%
89	12.001	3407	3409	3412	rBV2	170	74	0.01%	0.001%
90	12.037	3418	3420	3422	rBV2	174	82	0.01%	0.001%
91	12.197	3465	3470	3479	rVB4	1617	2461	0.22%	0.030%
92	12.593	3589	3593	3599	rBV5	625	802	0.07%	0.010%
93	12.696	3623	3625	3631	rVB2	265	185	0.02%	0.002%
94	12.834	3666	3668	3669	rBV2	204	94	0.01%	0.001%
95	13.066	3738	3740	3743	rBV	207	128	0.01%	0.002%
96	13.271	3802	3804	3807	rVB	275	78	0.01%	0.001%
97	13.326	3819	3821	3826	rVB2	328	206	0.02%	0.003%
98	13.458	3853	3862	3874	rBV3	1523	2691	0.24%	0.033%
99	13.754	3953	3954	3956	rBV3	222	111	0.01%	0.001%

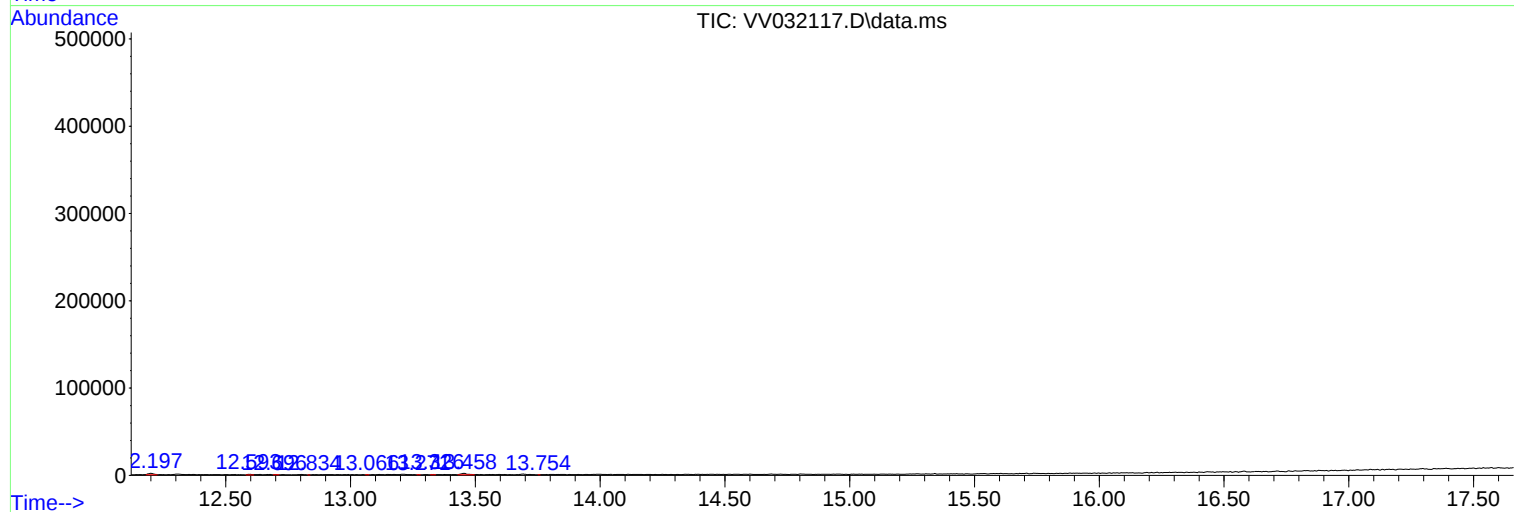
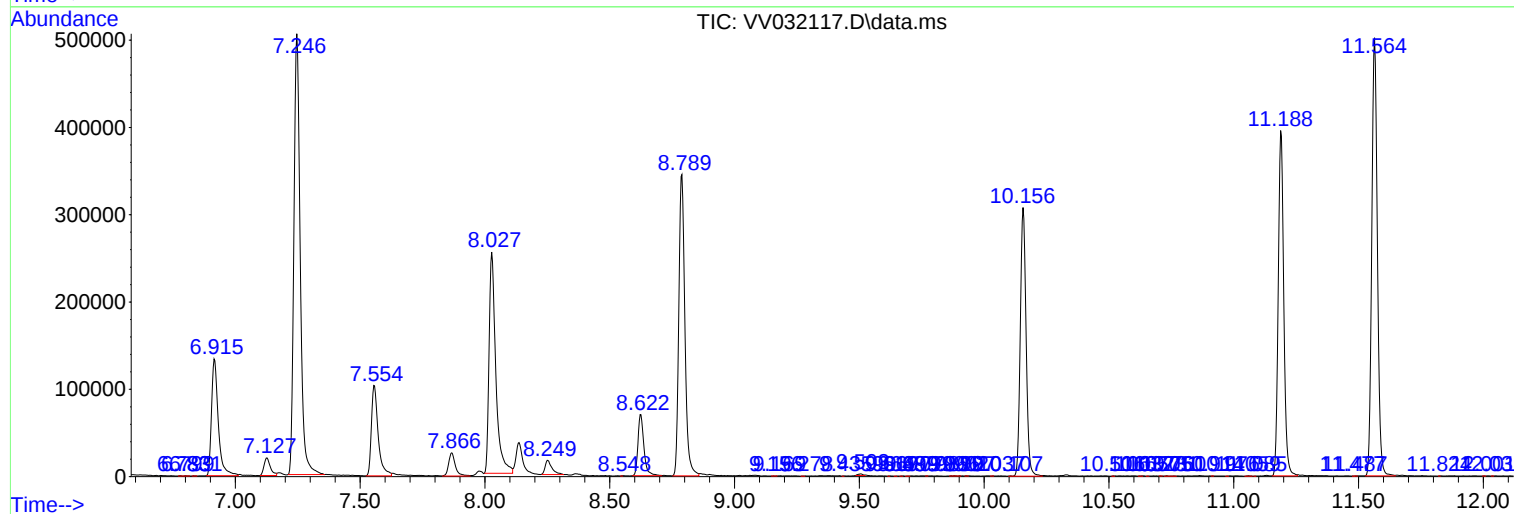
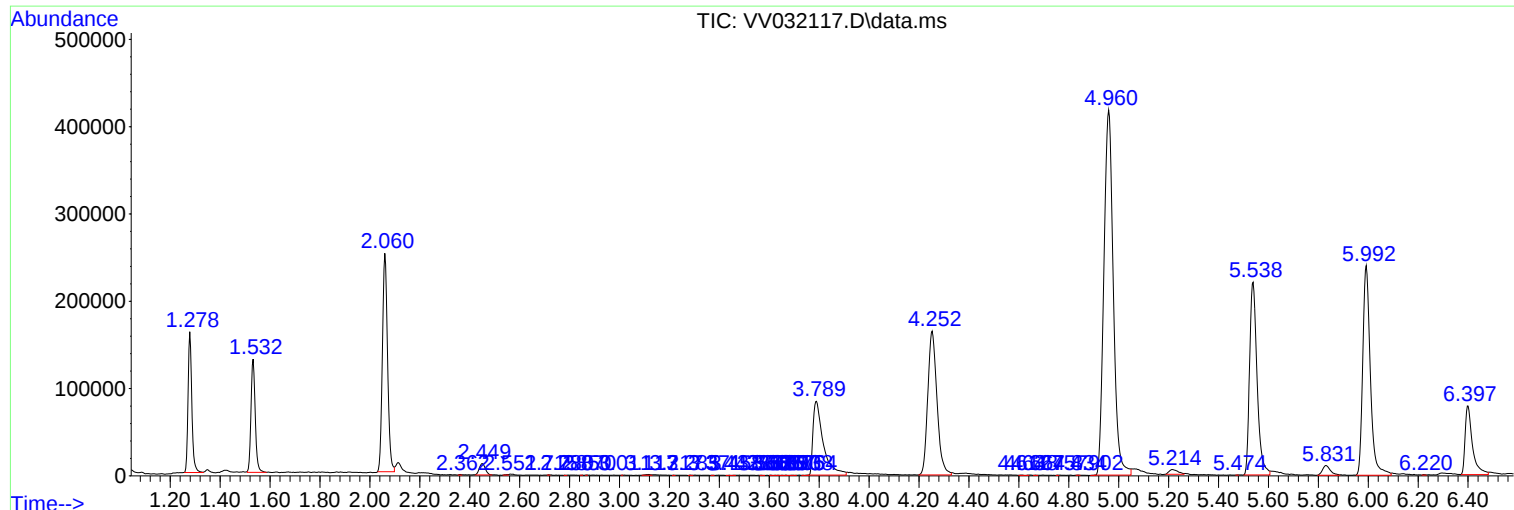
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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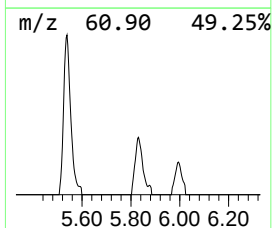
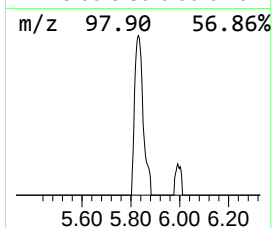
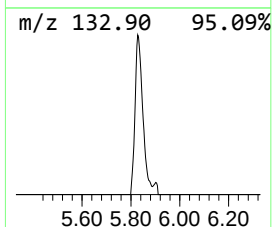
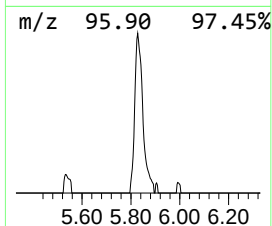
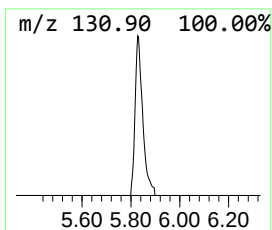
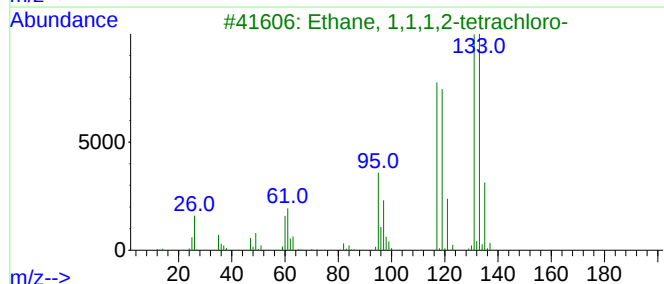
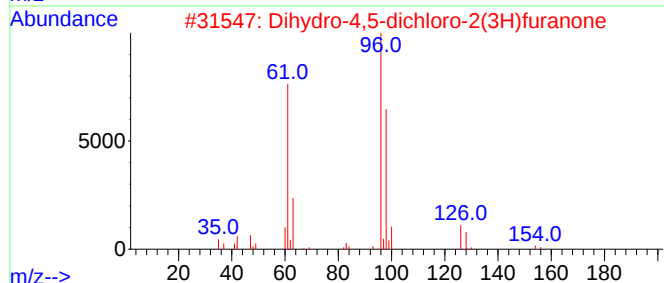
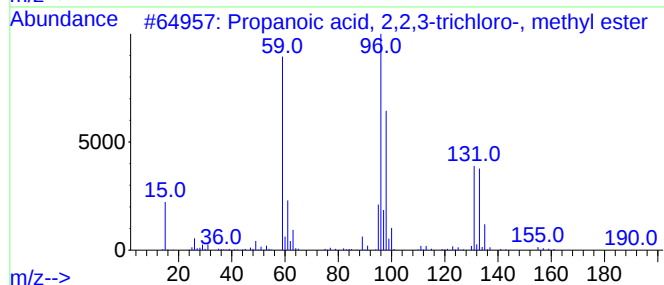
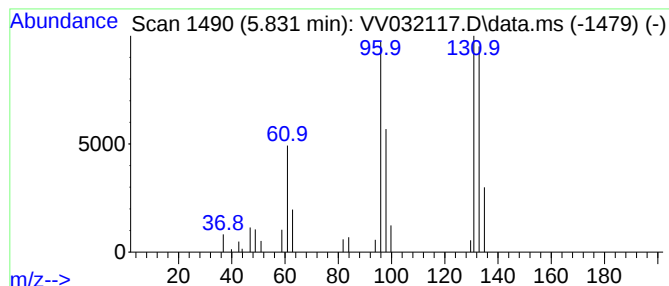
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.831	2.66 ug/L	24441	1,4-Difluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	40
2			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23



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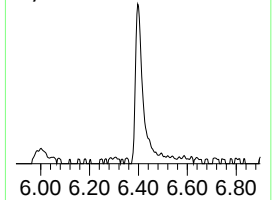
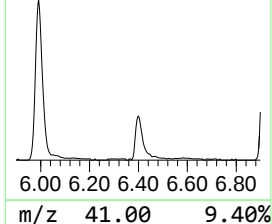
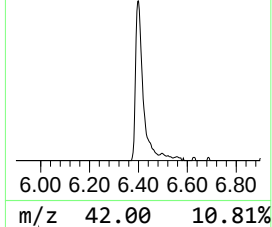
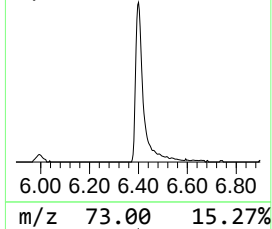
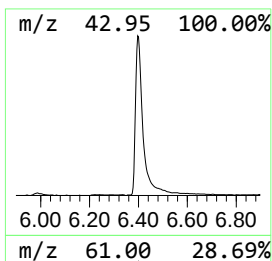
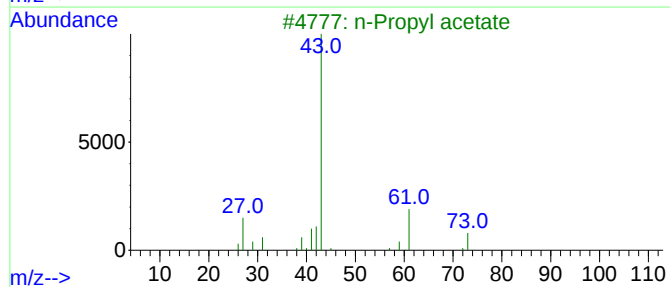
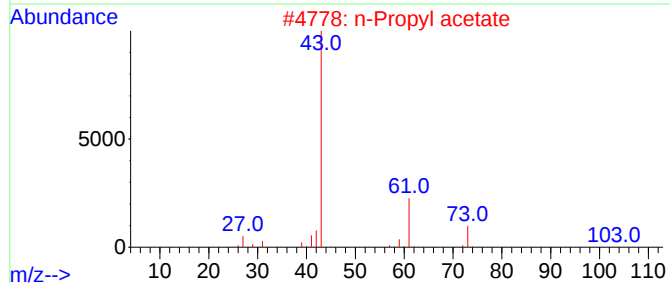
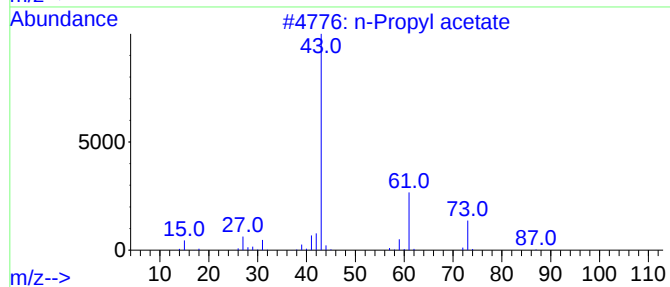
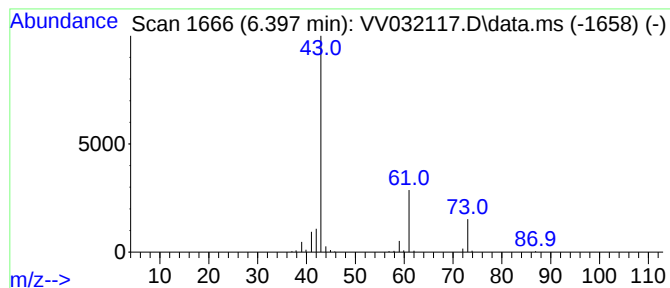
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	17.40 ug/L	160151	1,4-Difluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	78
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	56



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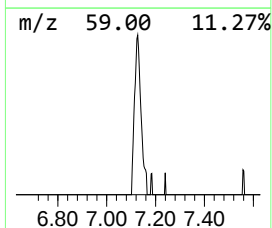
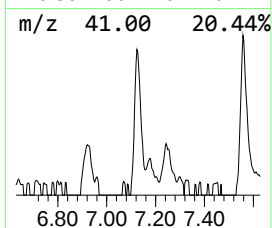
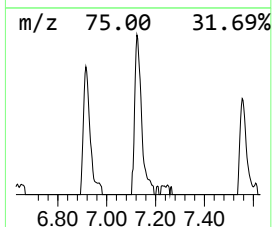
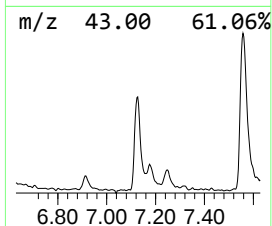
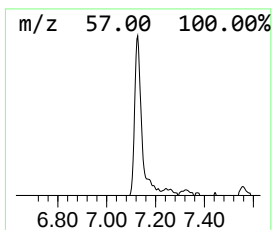
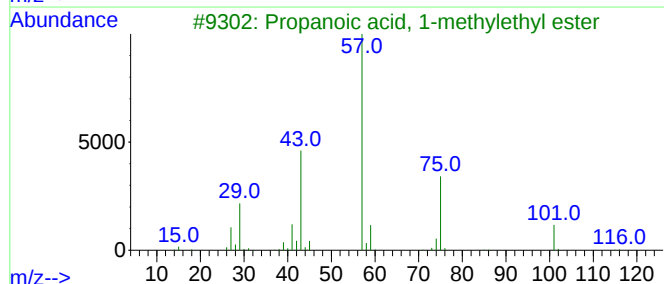
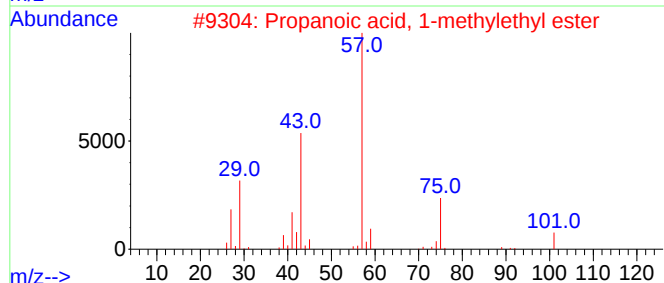
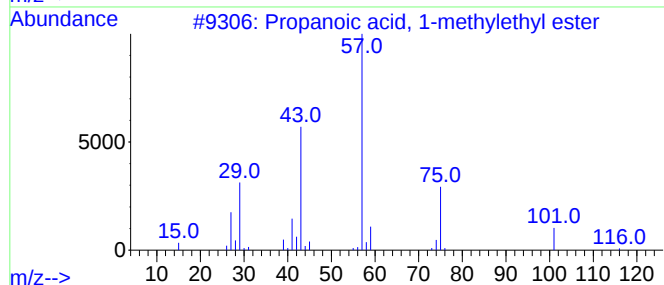
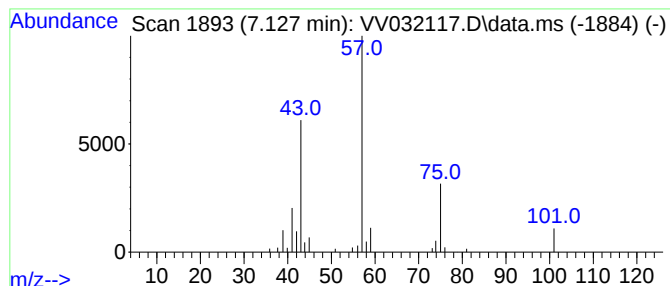
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.89 ug/L	35827	1,4-Difluorobenzene	5.538

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	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032117.D
Acq On : 15 Sep 2023 13:30
Operator : SY/MD
Sample : 04359-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD3

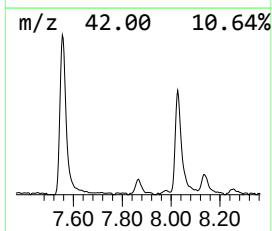
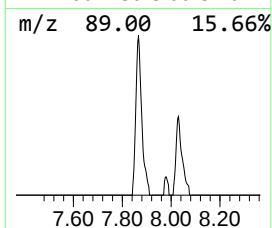
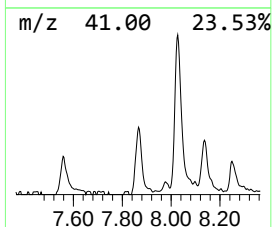
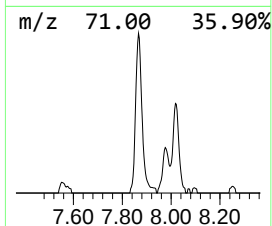
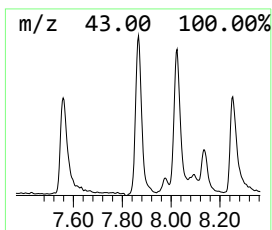
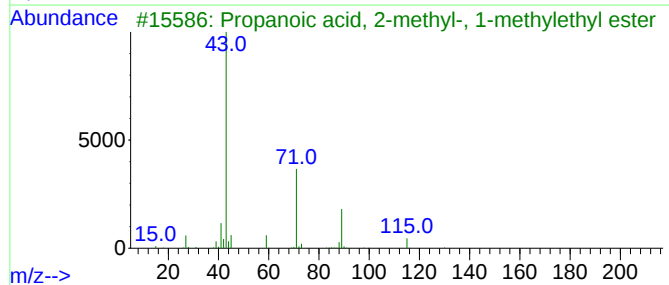
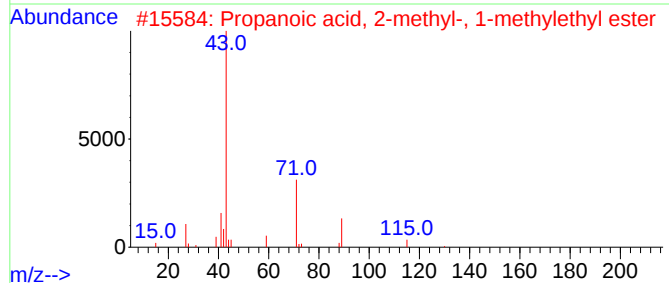
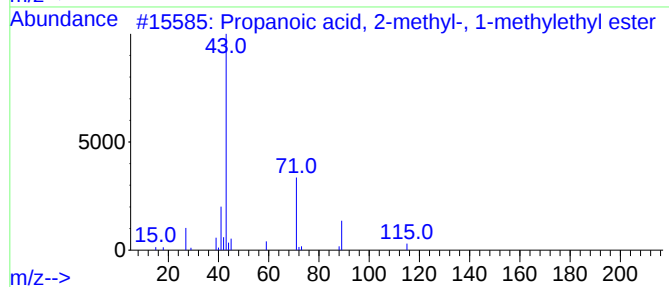
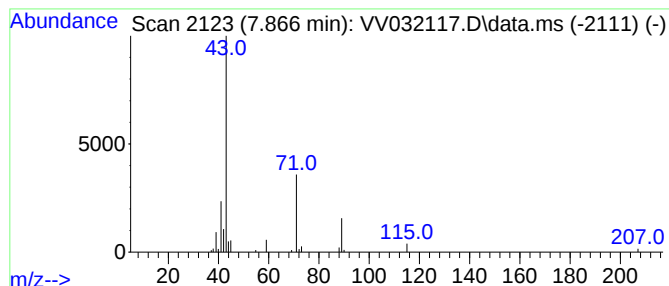
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.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.
7.866	4.27 ug/L	49715	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
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	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032117.D
Acq On : 15 Sep 2023 13:30
Operator : SY/MD
Sample : 04359-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD3

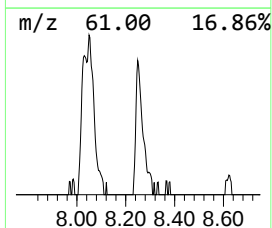
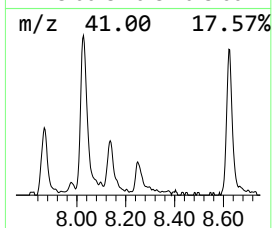
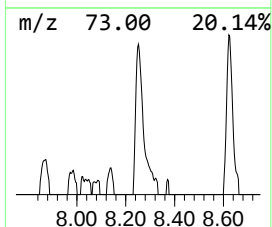
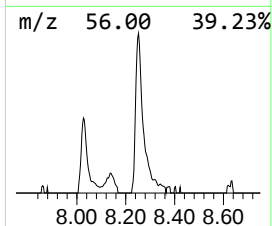
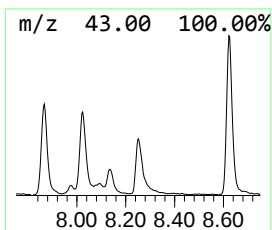
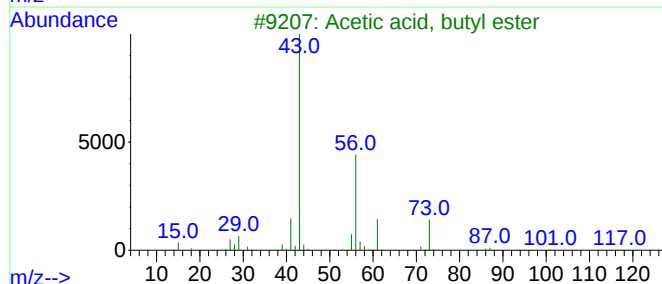
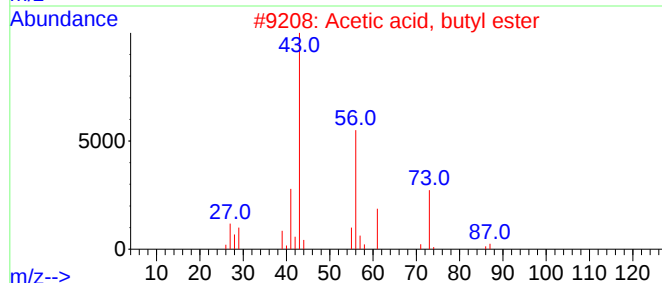
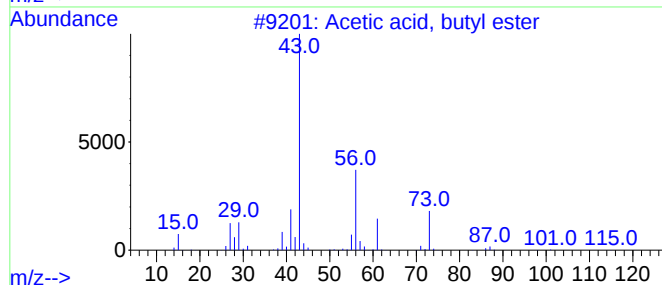
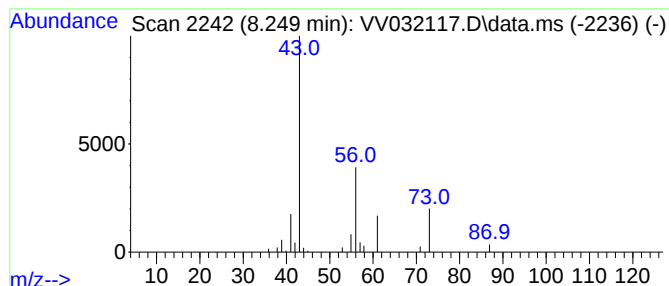
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	2.67 ug/L	31092	Chlorobenzene-d5	8.789

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	74		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56		
5	Isobutylamine	73	C4H11N	000078-81-9	9		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032117.D
Acq On : 15 Sep 2023 13:30
Operator : SY/MD
Sample : 04359-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD3

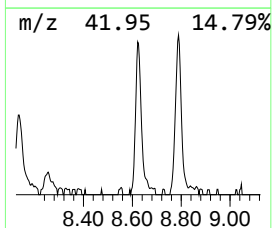
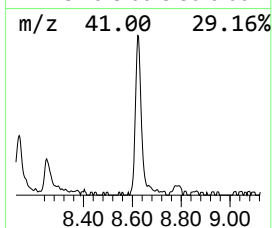
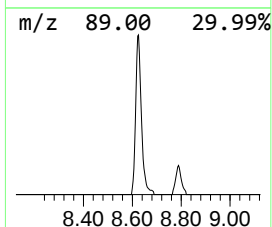
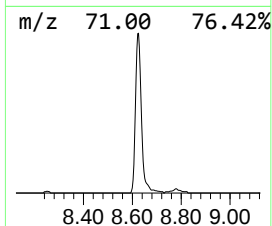
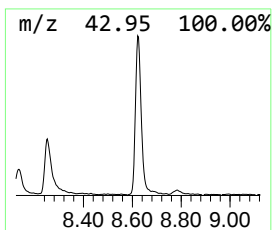
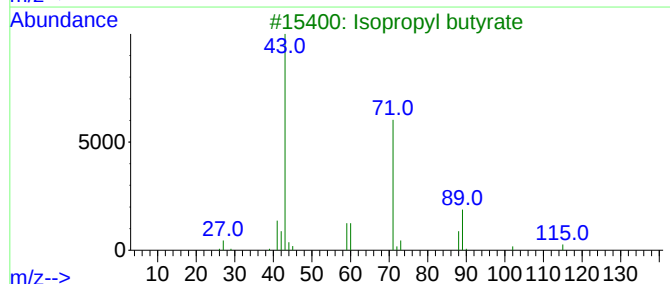
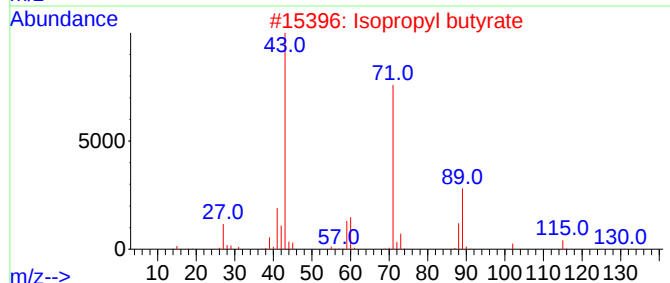
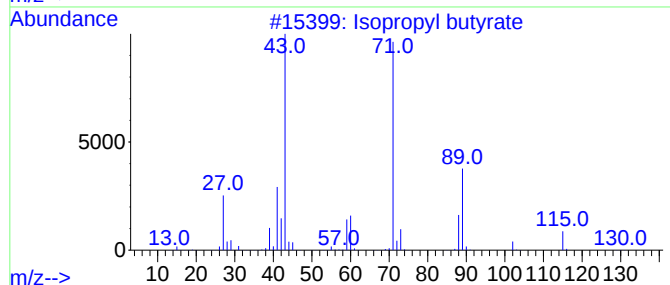
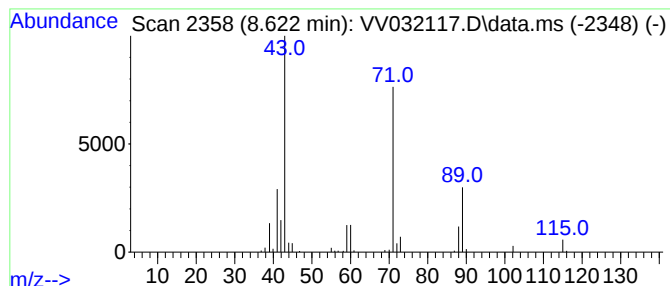
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	10.05 ug/L	116963	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	80
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032117.D
Acq On : 15 Sep 2023 13:30
Operator : SY/MD
Sample : 04359-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.831	2.7	ug/L	24441	1	5.538	460084	50.0
n-Propyl acetate	6.397	17.4	ug/L	160151	1	5.538	460084	50.0
Propanoic acid,...	7.127	3.9	ug/L	35827	1	5.538	460084	50.0
Propanoic acid,...	7.866	4.3	ug/L	49715	2	8.789	582120	50.0
Acetic acid, bu...	8.249	2.7	ug/L	31092	2	8.789	582120	50.0
Isopropyl butyrate	8.622	10.1	ug/L	116963	2	8.789	582120	50.0