

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
 Data File : VV032118.D
 Acq On : 15 Sep 2023 13:53
 Operator : SY/MD
 Sample : 04359-06 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 JLAD4

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: VV032118.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	68	74	88	rVB	122193	126445	15.30%	1.903%
2	1.532	146	153	165	rVB	96009	111201	13.46%	1.673%
3	2.060	308	317	328	rBV	186624	270283	32.71%	4.067%
4	2.449	430	438	452	rVB2	13503	22866	2.77%	0.344%
5	2.709	517	519	522	rBV2	463	276	0.03%	0.004%
6	2.841	558	560	562	rBV3	274	118	0.01%	0.002%
7	2.892	574	576	578	rBV	222	139	0.02%	0.002%
8	2.921	582	585	587	rBV2	233	133	0.02%	0.002%
9	2.957	592	596	597	rBV2	252	176	0.02%	0.003%
10	3.105	636	642	646	rBV3	487	632	0.08%	0.010%
11	3.182	664	666	670	rVB2	420	200	0.02%	0.003%
12	3.201	670	672	678	rBV	423	341	0.04%	0.005%
13	3.269	691	693	697	rVV2	321	143	0.02%	0.002%
14	3.429	740	743	747	rVB	156	117	0.01%	0.002%
15	3.490	760	762	766	rBV2	284	154	0.02%	0.002%
16	3.510	766	768	771	rBV	301	159	0.02%	0.002%
17	3.632	804	806	808	rVB2	180	91	0.01%	0.001%
18	3.728	833	836	842	rVB2	272	221	0.03%	0.003%
19	3.793	846	856	882	rBV	62396	174244	21.09%	2.622%
20	4.252	983	999	1024	rBV	121764	317542	38.43%	4.779%
21	4.825	1175	1177	1180	rBV	187	87	0.01%	0.001%
22	4.847	1180	1184	1186	rVV	207	172	0.02%	0.003%
23	4.873	1190	1192	1197	rVB3	329	190	0.02%	0.003%
24	4.960	1203	1219	1246	rBV2	312357	826346	100.00%	12.436%
25	5.539	1387	1399	1420	rBV	232637	481827	58.31%	7.251%
26	5.831	1482	1490	1502	rBV5	8091	15715	1.90%	0.236%
27	5.992	1527	1540	1576	rBV	178636	383991	46.47%	5.779%
28	6.304	1629	1637	1641	rBV2	1710	2890	0.35%	0.043%
29	6.400	1658	1667	1699	rBV	67046	139553	16.89%	2.100%
30	6.854	1805	1808	1816	rVB3	344	342	0.04%	0.005%
31	6.918	1816	1828	1864	rBV	97348	191022	23.12%	2.875%
32	7.127	1884	1893	1903	rBV2	17490	30178	3.65%	0.454%
33	7.246	1919	1930	1966	rBV	370393	668469	80.89%	10.060%
34	7.558	2015	2027	2058	rBV2	78342	151704	18.36%	2.283%
35	7.735	2080	2082	2086	rVB3	532	291	0.04%	0.004%
36	7.866	2111	2123	2144	rBV	23034	41841	5.06%	0.630%

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

37	8.027	2165	2173	2199	rBV	185465	342493	41.45%	5.154%
38	8.252	2237	2243	2261	rVB	12930	22557	2.73%	0.339%
39	8.413	2291	2293	2297	rBV4	512	359	0.04%	0.005%
40	8.474	2310	2312	2315	rBV2	536	302	0.04%	0.005%
41	8.625	2348	2359	2378	rBV	55155	93880	11.36%	1.413%
42	8.789	2398	2410	2436	rBV	363288	609455	73.75%	9.172%
43	9.063	2492	2495	2498	rBV3	429	399	0.05%	0.006%
44	9.210	2535	2541	2545	rBV2	523	486	0.06%	0.007%
45	9.249	2551	2553	2557	rBV3	309	219	0.03%	0.003%
46	9.275	2558	2561	2563	rBV	240	178	0.02%	0.003%
47	9.436	2610	2611	2615	rBV2	191	88	0.01%	0.001%
48	9.503	2622	2632	2636	rBV6	1804	3005	0.36%	0.045%
49	9.551	2645	2647	2651	rVB3	492	361	0.04%	0.005%
50	9.603	2657	2663	2665	rVB2	316	291	0.04%	0.004%
51	9.683	2686	2688	2695	rVB2	390	366	0.04%	0.006%
52	9.718	2695	2699	2701	rBV2	270	172	0.02%	0.003%
53	9.751	2701	2709	2711	rBV2	384	408	0.05%	0.006%
54	9.815	2724	2729	2733	rBV3	318	358	0.04%	0.005%
55	9.834	2733	2735	2738	rBV2	204	131	0.02%	0.002%
56	9.873	2744	2747	2749	rBV2	371	237	0.03%	0.004%
57	9.924	2760	2763	2767	rBV	330	199	0.02%	0.003%
58	10.030	2793	2796	2801	rBV	270	158	0.02%	0.002%
59	10.056	2801	2804	2807	rVB2	186	130	0.02%	0.002%
60	10.111	2818	2821	2823	rBV	282	184	0.02%	0.003%
61	10.156	2823	2835	2860	rVV	237155	372679	45.10%	5.608%
62	10.252	2864	2865	2871	rVB	336	233	0.03%	0.004%
63	10.281	2871	2874	2877	rBV3	423	297	0.04%	0.004%
64	10.333	2881	2890	2898	rVB5	1784	2674	0.32%	0.040%
65	10.368	2899	2901	2904	rVB2	165	80	0.01%	0.001%
66	10.397	2908	2910	2913	rVV	187	81	0.01%	0.001%
67	10.416	2914	2916	2919	rVB	215	103	0.01%	0.002%
68	10.477	2933	2935	2936	rBV	327	172	0.02%	0.003%
69	10.580	2962	2967	2969	rBV2	202	202	0.02%	0.003%
70	10.619	2975	2979	2983	rBV2	349	282	0.03%	0.004%
71	10.638	2983	2985	2988	rVV	206	119	0.01%	0.002%
72	10.654	2988	2990	2993	rVB	180	76	0.01%	0.001%
73	10.686	2997	3000	3001	rBV2	189	102	0.01%	0.002%
74	10.773	3025	3027	3028	rBV	213	89	0.01%	0.001%
75	10.870	3051	3057	3063	rBV3	585	635	0.08%	0.010%
76	10.899	3063	3066	3070	rVB3	327	235	0.03%	0.004%

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Title : VOC Analysis

77	10.934	3074	3077	3079	rBV	221	145	0.02%	0.002%
78	10.976	3087	3090	3096	rVB2	318	331	0.04%	0.005%
79	11.188	3145	3156	3178	rBV	405712	629051	76.12%	9.467%
80	11.365	3210	3211	3214	rVB2	280	110	0.01%	0.002%
81	11.387	3216	3218	3221	rBV	291	181	0.02%	0.003%
82	11.564	3261	3273	3300	rBV	374383	593336	71.80%	8.929%
83	11.757	3329	3333	3336	rBV	307	165	0.02%	0.002%
84	11.786	3339	3342	3345	rBV	253	214	0.03%	0.003%
85	11.818	3349	3352	3354	rBV	292	183	0.02%	0.003%
86	12.030	3412	3418	3421	rBV3	313	261	0.03%	0.004%
87	12.117	3442	3445	3448	rBV	161	110	0.01%	0.002%
88	12.194	3464	3469	3470	rBV	1304	993	0.12%	0.015%
89	12.326	3508	3510	3511	rBV	293	118	0.01%	0.002%
90	12.381	3525	3527	3529	rBV	307	140	0.02%	0.002%
91	12.821	3662	3664	3669	rBV2	260	167	0.02%	0.003%
92	12.876	3675	3681	3684	rBV2	437	498	0.06%	0.007%
93	13.066	3737	3740	3743	rBV	367	218	0.03%	0.003%
94	13.217	3780	3787	3791	rVB4	740	778	0.09%	0.012%
95	13.455	3853	3861	3869	rBV3	1534	2334	0.28%	0.035%
96	13.615	3908	3911	3913	rBV	441	211	0.03%	0.003%
97	13.921	4003	4006	4007	rBV	302	154	0.02%	0.002%
98	13.966	4018	4020	4021	rBV	294	143	0.02%	0.002%
99	14.098	4059	4061	4066	rBV2	356	269	0.03%	0.004%
100	14.561	4202	4205	4207	rBV2	455	319	0.04%	0.005%

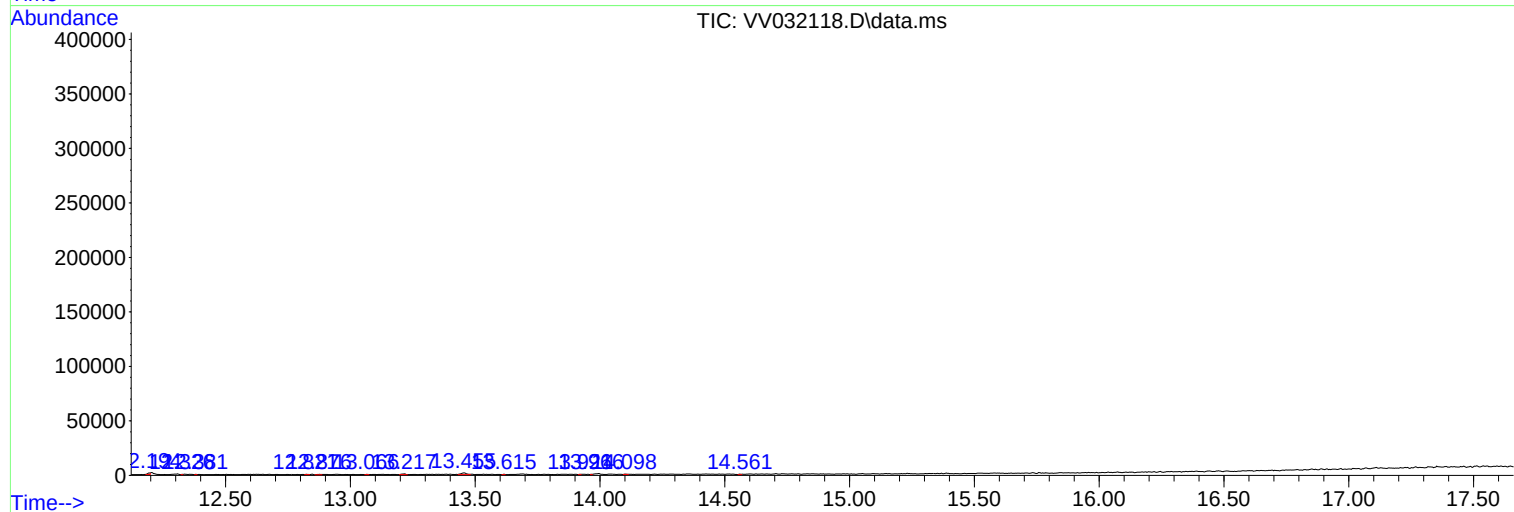
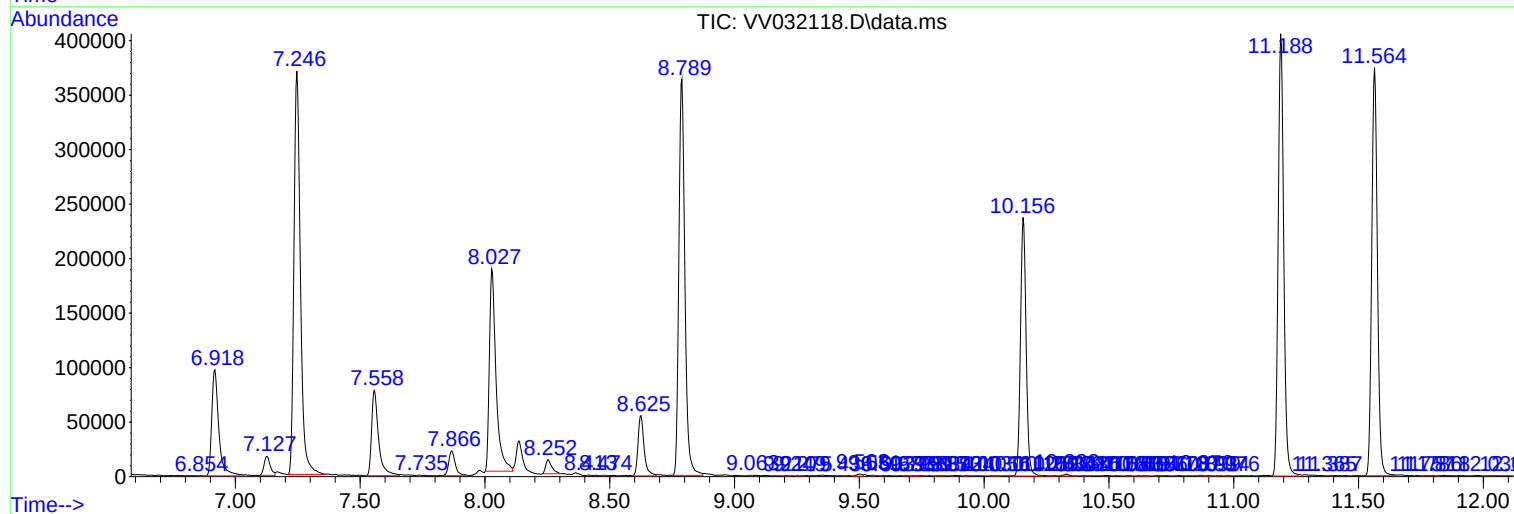
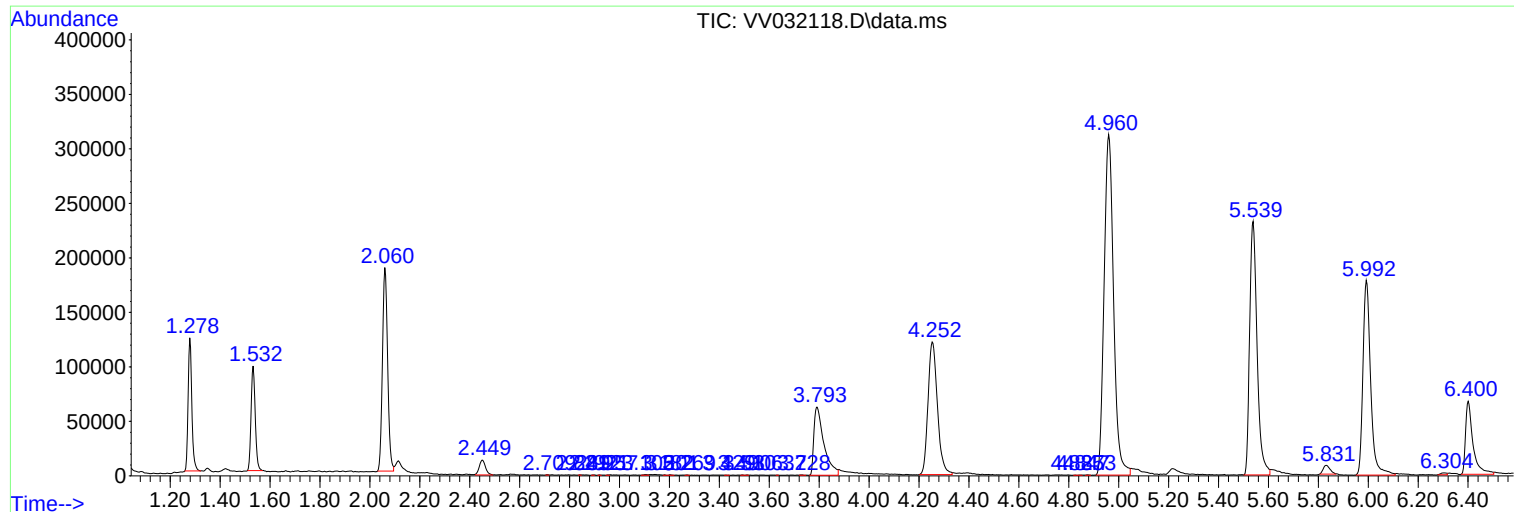
Sum of corrected areas: 6645003

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MSVOA_V
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JLAD4

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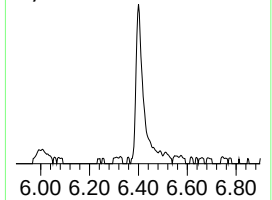
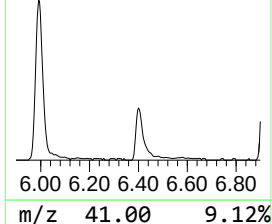
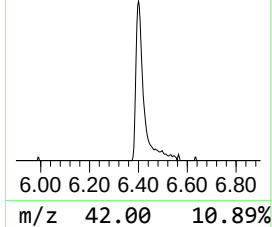
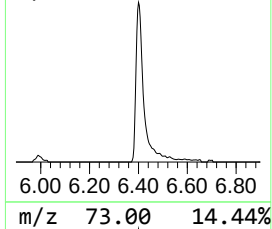
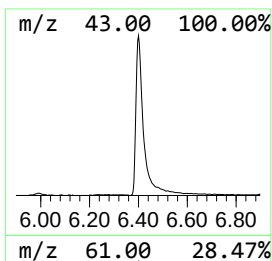
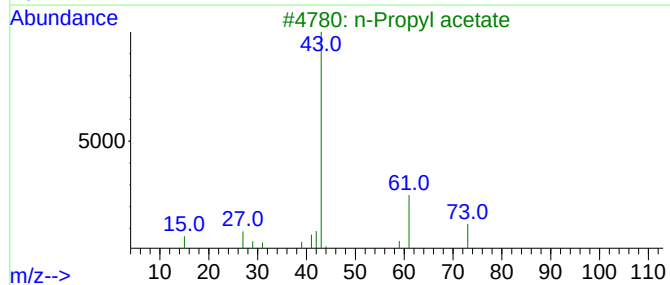
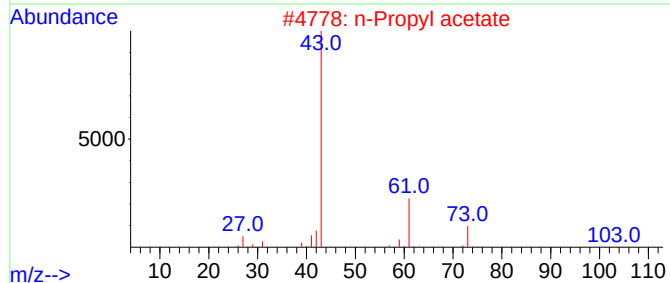
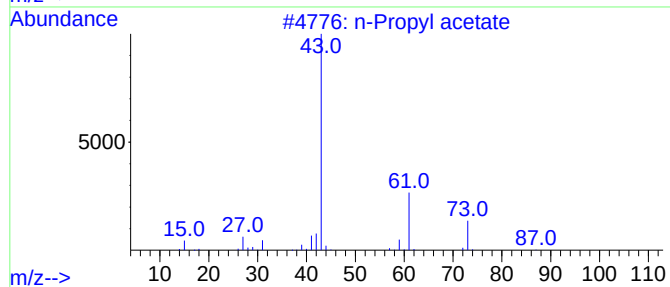
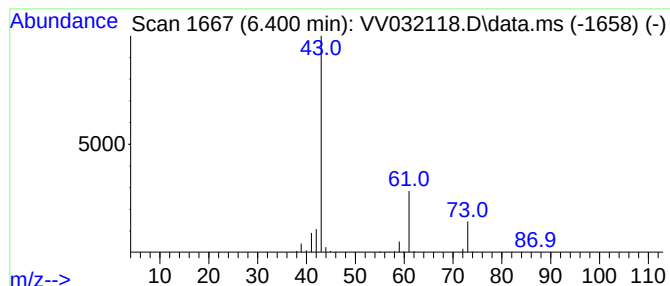
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.400	14.48 ug/L	139553	1,4-Difluorobenzene	5.539

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	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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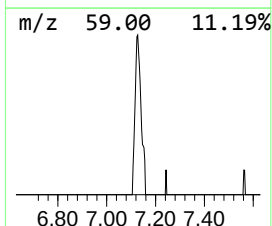
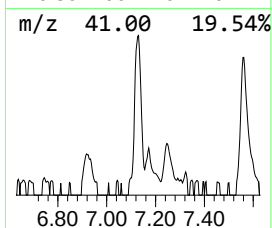
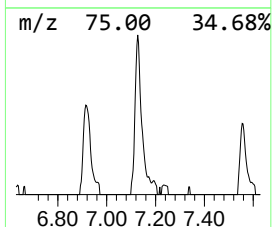
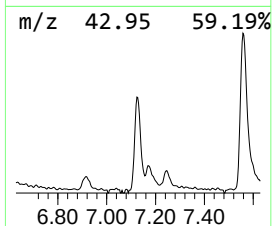
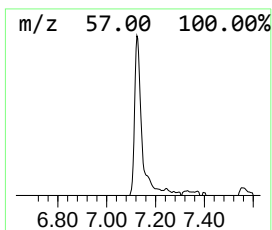
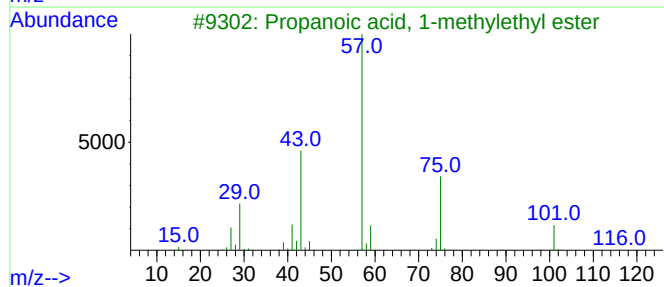
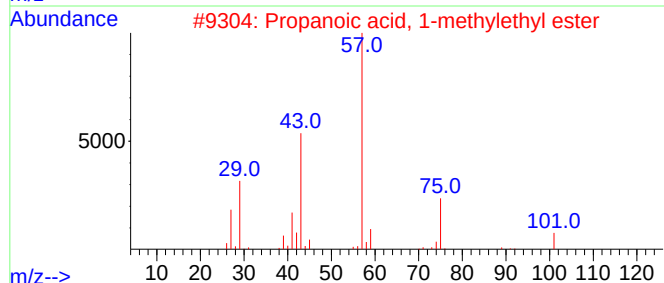
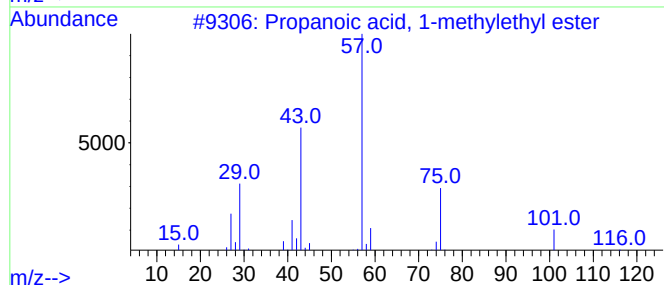
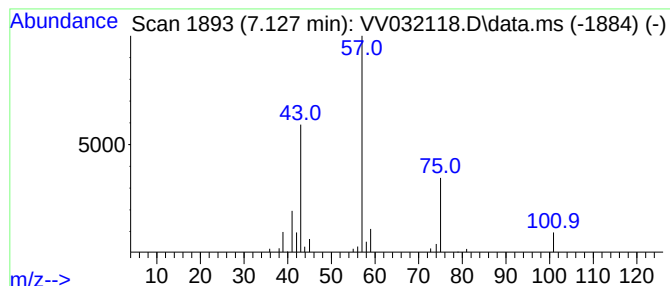
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.13 ug/L	30178	1,4-Difluorobenzene	5.539

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	72
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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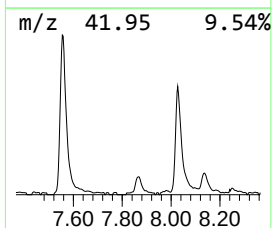
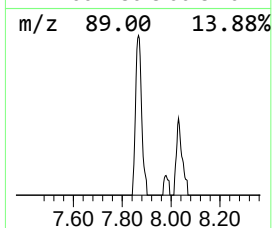
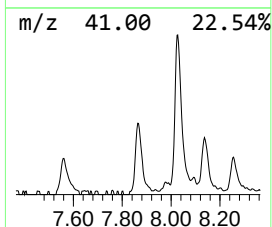
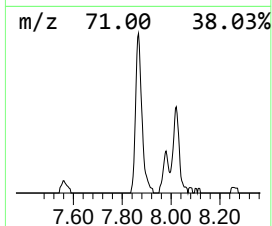
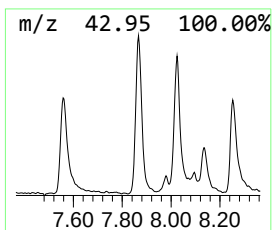
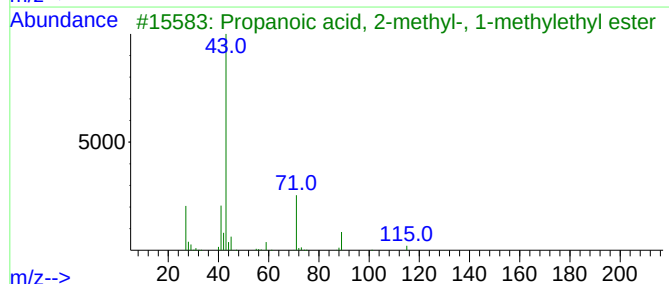
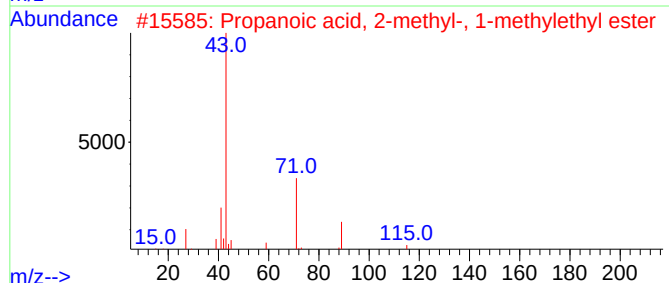
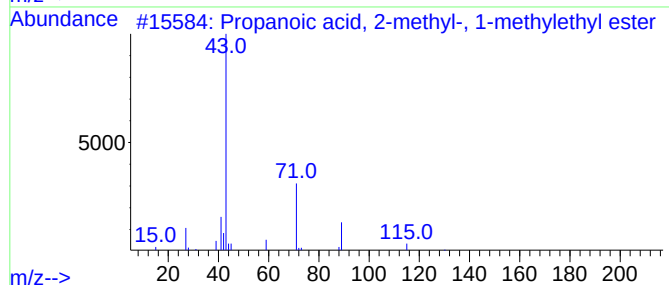
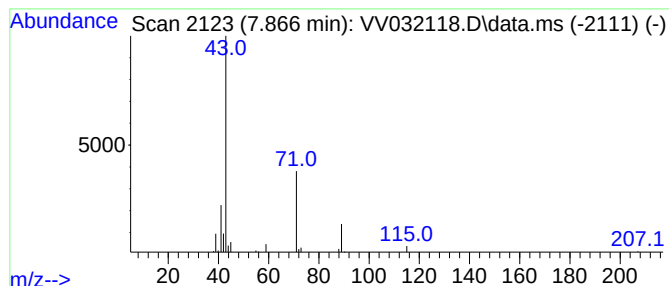
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	3.43 ug/L	41841	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	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032118.D
Acq On : 15 Sep 2023 13:53
Operator : SY/MD
Sample : 04359-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD4

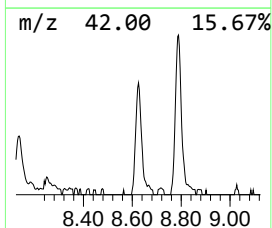
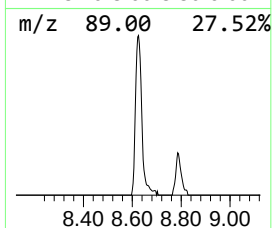
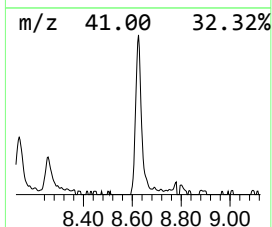
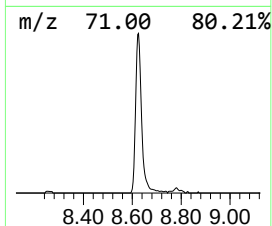
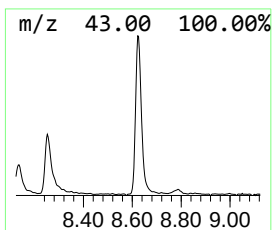
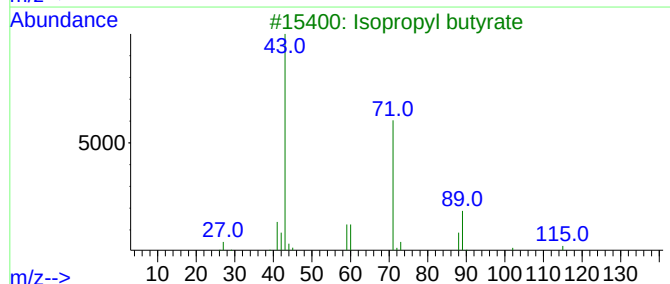
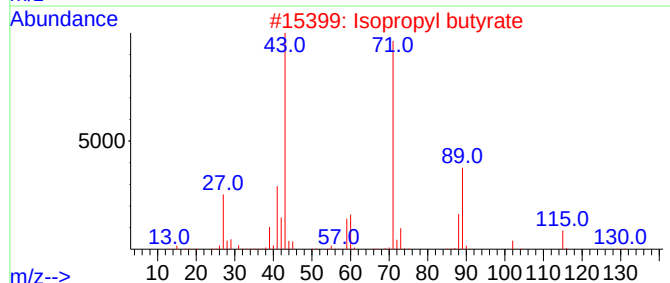
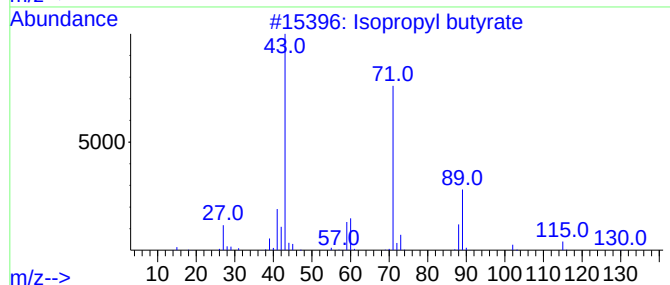
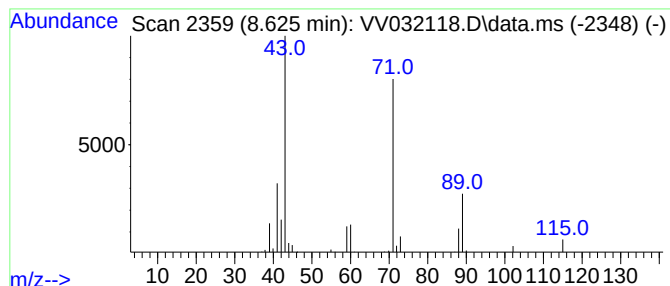
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Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.625	7.70 ug/L	93880	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	90
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032118.D
Acq On : 15 Sep 2023 13:53
Operator : SY/MD
Sample : 04359-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD4

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.400	14.5	ug/L	139553	1	5.539	481827	50.0
Propanoic acid,...	7.127	3.1	ug/L	30178	1	5.539	481827	50.0
Propanoic acid,...	7.866	3.4	ug/L	41841	2	8.789	609455	50.0
Isopropyl butyrate	8.625	7.7	ug/L	93880	2	8.789	609455	50.0