

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
 Data File : VV032120.D
 Acq On : 15 Sep 2023 14:38
 Operator : SY/MD
 Sample : 04359-05 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 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: VV032120.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	90	rVB	116924	121843	15.06%	1.871%
2	1.532	146	153	168	rVB	94428	111274	13.75%	1.709%
3	2.060	308	317	329	rBV	179748	258639	31.96%	3.972%
4	2.449	430	438	454	rVB	13295	23362	2.89%	0.359%
5	2.703	512	517	520	rBV2	404	430	0.05%	0.007%
6	2.986	602	605	608	rBV	463	322	0.04%	0.005%
7	3.060	625	628	630	rBV	283	183	0.02%	0.003%
8	3.098	636	640	642	rBV4	249	202	0.02%	0.003%
9	3.114	642	645	650	rVV4	446	469	0.06%	0.007%
10	3.214	672	676	680	rVB2	261	251	0.03%	0.004%
11	3.291	697	700	702	rBV	182	147	0.02%	0.002%
12	3.320	707	709	714	rBV3	262	163	0.02%	0.003%
13	3.381	724	728	730	rBV	202	139	0.02%	0.002%
14	3.516	767	770	775	rBV2	121	129	0.02%	0.002%
15	3.574	784	788	791	rBV2	363	271	0.03%	0.004%
16	3.638	805	808	812	rBV2	383	210	0.03%	0.003%
17	3.725	833	835	838	rVB2	212	123	0.02%	0.002%
18	3.744	838	841	844	rVB2	200	121	0.01%	0.002%
19	3.790	844	855	892	rBV	64475	189540	23.42%	2.911%
20	4.253	983	999	1023	rBV2	119844	309268	38.21%	4.749%
21	4.507	1076	1078	1085	rVB2	451	403	0.05%	0.006%
22	4.597	1104	1106	1110	rVB2	333	155	0.02%	0.002%
23	4.622	1110	1114	1118	rBV3	246	295	0.04%	0.005%
24	4.680	1130	1132	1134	rVB	263	111	0.01%	0.002%
25	4.786	1161	1165	1169	rVB2	320	224	0.03%	0.003%
26	4.854	1184	1186	1189	rBV	241	136	0.02%	0.002%
27	4.960	1203	1219	1246	rBV2	305041	809303	100.00%	12.428%
28	5.539	1387	1399	1426	rBV	220371	461434	57.02%	7.086%
29	5.831	1479	1490	1508	rVB3	8666	18846	2.33%	0.289%
30	5.896	1508	1510	1514	rVB2	412	195	0.02%	0.003%
31	5.924	1514	1519	1520	rBV3	424	304	0.04%	0.005%
32	5.992	1527	1540	1577	rBV	174517	374859	46.32%	5.757%
33	6.310	1624	1639	1642	rBV7	2078	4402	0.54%	0.068%
34	6.400	1658	1667	1709	rBV	66416	138341	17.09%	2.124%
35	6.918	1817	1828	1855	rBV	94740	185671	22.94%	2.851%
36	7.124	1882	1892	1902	rBV2	16856	29813	3.68%	0.458%

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

37	7.246	1919	1930	1955	rBV	359959	646010	79.82%	9.921%
38	7.558	2016	2027	2058	rBV2	78003	151731	18.75%	2.330%
39	7.867	2114	2123	2143	rVB2	22350	38696	4.78%	0.594%
40	7.979	2149	2158	2163	rBV3	4523	6720	0.83%	0.103%
41	8.027	2164	2173	2199	rVV	186646	357112	44.13%	5.484%
42	8.252	2238	2243	2259	rVB	12442	20256	2.50%	0.311%
43	8.571	2338	2342	2345	rVB4	390	278	0.03%	0.004%
44	8.625	2349	2359	2379	rVV	54661	90418	11.17%	1.389%
45	8.789	2398	2410	2444	rBV	342652	582330	71.95%	8.943%
46	8.969	2463	2466	2473	rVB5	883	899	0.11%	0.014%
47	9.002	2473	2476	2481	rBV2	191	143	0.02%	0.002%
48	9.027	2481	2484	2488	rVB3	466	294	0.04%	0.005%
49	9.053	2488	2492	2493	rBV2	273	173	0.02%	0.003%
50	9.137	2517	2518	2522	rBV2	251	146	0.02%	0.002%
51	9.223	2543	2545	2550	rBV2	268	172	0.02%	0.003%
52	9.284	2561	2564	2565	rBV	207	103	0.01%	0.002%
53	9.349	2577	2584	2585	rBV3	763	716	0.09%	0.011%
54	9.458	2616	2618	2621	rVB2	256	120	0.01%	0.002%
55	9.500	2624	2631	2636	rBV5	1556	2154	0.27%	0.033%
56	9.657	2677	2680	2684	rVB	387	235	0.03%	0.004%
57	9.709	2693	2696	2699	rBV4	407	254	0.03%	0.004%
58	9.744	2704	2707	2713	rVB3	343	267	0.03%	0.004%
59	9.776	2713	2717	2721	rBV2	266	283	0.03%	0.004%
60	9.837	2730	2736	2739	rBV3	255	280	0.03%	0.004%
61	9.876	2745	2748	2751	rVB2	505	270	0.03%	0.004%
62	9.895	2751	2754	2756	rBV3	255	142	0.02%	0.002%
63	10.037	2795	2798	2800	rBV	222	132	0.02%	0.002%
64	10.156	2822	2835	2864	rBV	232400	375234	46.37%	5.762%
65	10.255	2864	2866	2869	rVB	319	167	0.02%	0.003%
66	10.304	2876	2881	2882	rBV3	287	188	0.02%	0.003%
67	10.329	2882	2889	2893	rVV3	1193	1318	0.16%	0.020%
68	10.381	2900	2905	2908	rBV3	412	308	0.04%	0.005%
69	10.410	2911	2914	2916	rBV	277	157	0.02%	0.002%
70	10.468	2929	2932	2934	rVV2	201	108	0.01%	0.002%
71	10.551	2956	2958	2961	rBV	214	127	0.02%	0.002%
72	10.680	2995	2998	3001	rBV2	390	257	0.03%	0.004%
73	10.738	3010	3016	3018	rBV2	160	161	0.02%	0.002%
74	10.789	3028	3032	3034	rBV	284	200	0.02%	0.003%
75	10.825	3038	3043	3046	rBV3	312	281	0.03%	0.004%
76	10.963	3082	3086	3087	rVB2	200	106	0.01%	0.002%

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 Title : VOC Analysis

77	11.063	3113	3117	3120	rBV2	141	114	0.01%	0.002%
78	11.188	3143	3156	3177	rBV	388078	602536	74.45%	9.253%
79	11.419	3226	3228	3233	rVB3	383	236	0.03%	0.004%
80	11.564	3261	3273	3298	rBV	365988	580515	71.73%	8.915%
81	11.786	3336	3342	3344	rBV	233	240	0.03%	0.004%
82	11.863	3364	3366	3371	rVB2	349	234	0.03%	0.004%
83	11.892	3371	3375	3377	rBV2	358	221	0.03%	0.003%
84	11.998	3404	3408	3412	rBV2	212	233	0.03%	0.004%
85	12.021	3413	3415	3418	rVV2	295	157	0.02%	0.002%
86	12.069	3428	3430	3432	rBV	312	142	0.02%	0.002%
87	12.198	3463	3470	3479	rBV3	1887	2865	0.35%	0.044%
88	12.278	3493	3495	3496	rBV3	232	106	0.01%	0.002%
89	12.342	3512	3515	3519	rVB	378	255	0.03%	0.004%
90	12.548	3576	3579	3580	rBV2	205	107	0.01%	0.002%
91	12.593	3590	3593	3597	rVB3	393	340	0.04%	0.005%
92	12.693	3620	3624	3630	rVB3	350	310	0.04%	0.005%
93	12.863	3676	3677	3681	rVB	368	197	0.02%	0.003%
94	12.998	3716	3719	3725	rBV2	285	253	0.03%	0.004%
95	13.111	3752	3754	3756	rVB	392	157	0.02%	0.002%
96	13.204	3781	3783	3788	rVB2	446	349	0.04%	0.005%
97	13.632	3913	3916	3919	rVB	304	168	0.02%	0.003%
98	13.837	3978	3980	3981	rBV	282	110	0.01%	0.002%
99	13.976	4014	4023	4026	rBV3	735	1148	0.14%	0.018%
100	14.509	4185	4189	4192	rBV2	327	352	0.04%	0.005%

Sum of corrected areas: 6511869

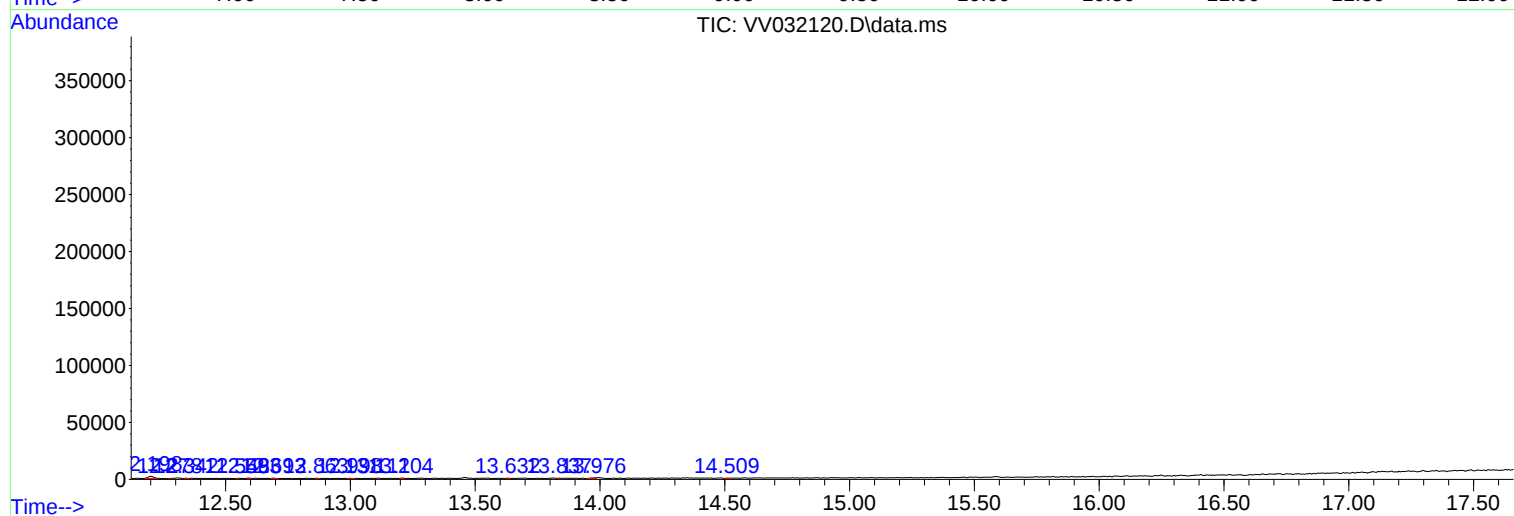
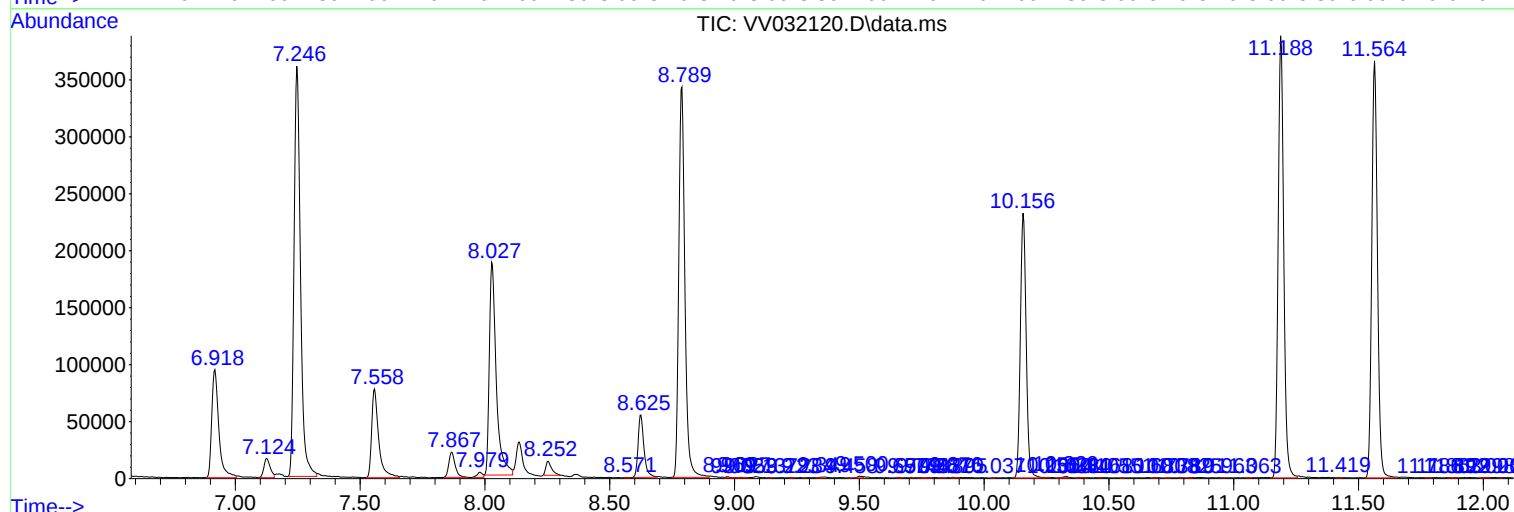
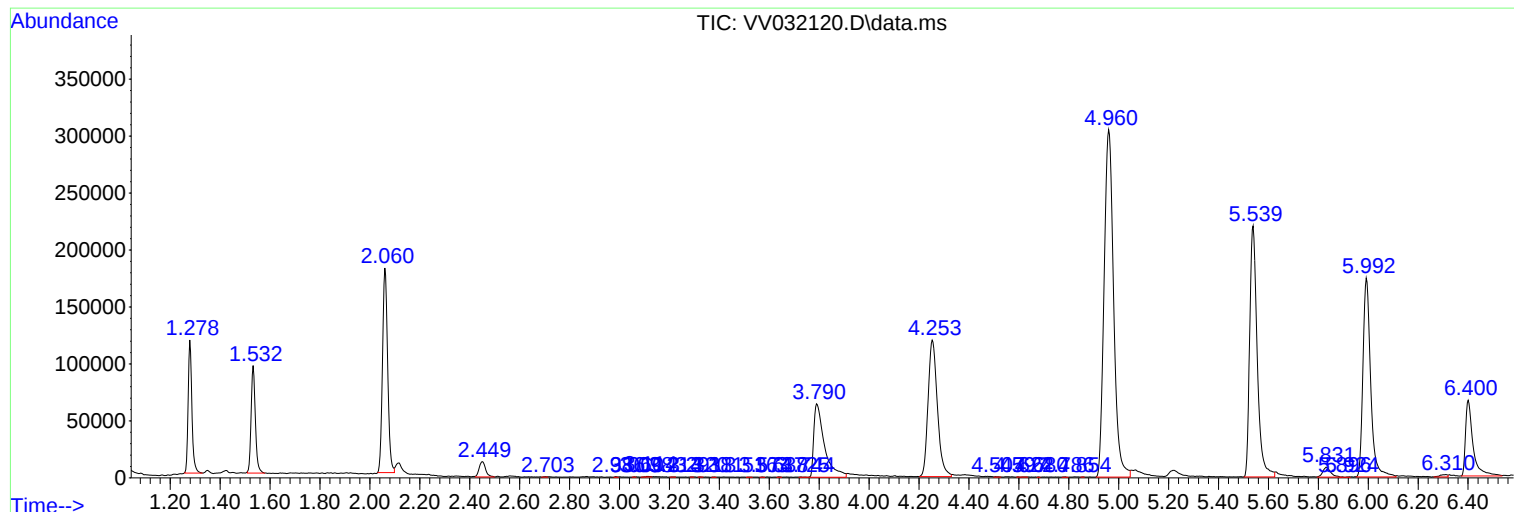
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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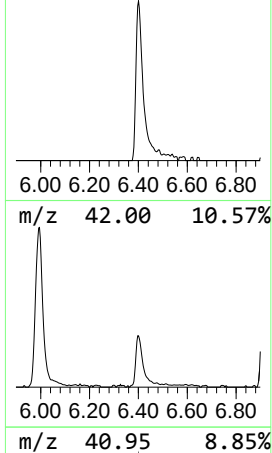
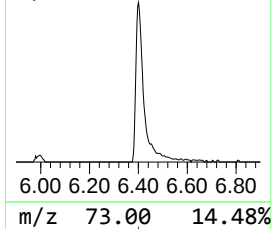
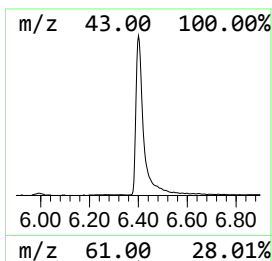
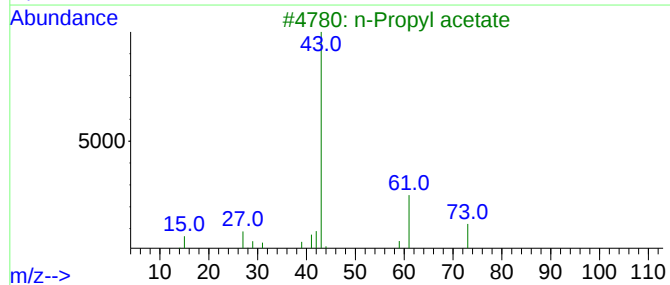
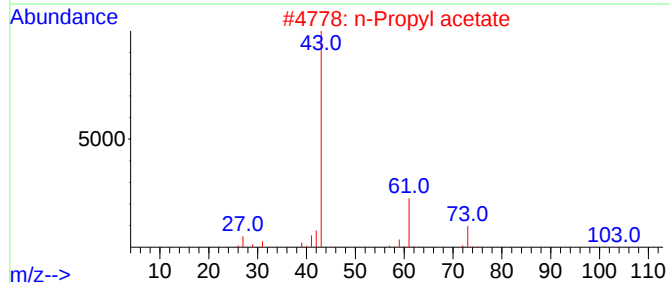
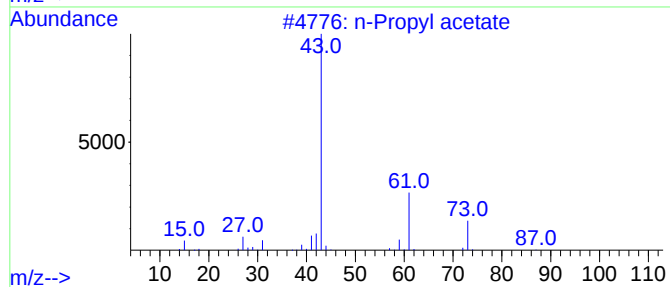
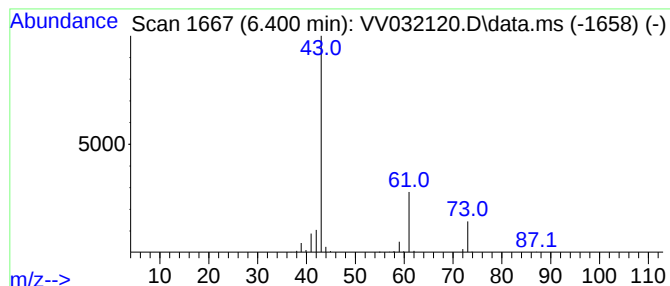
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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.
6.400	14.99 ug/L	138341	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	64
5	Isopropyl acetate			102	C5H10O2	000108-21-4	38



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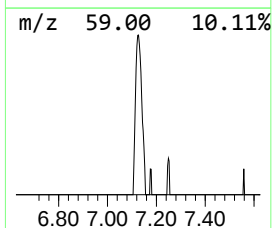
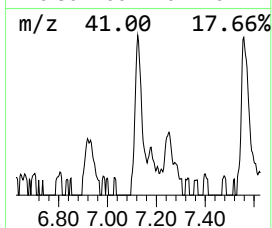
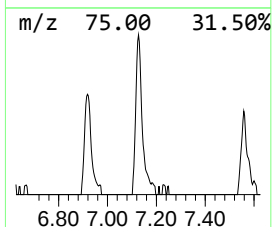
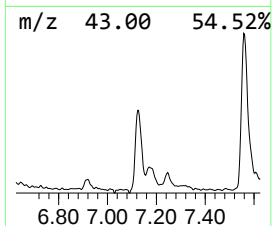
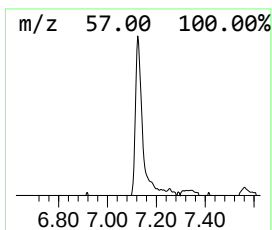
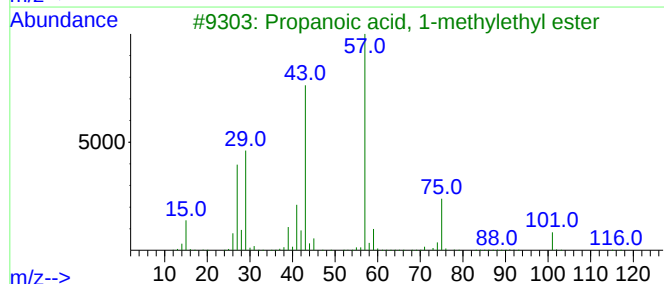
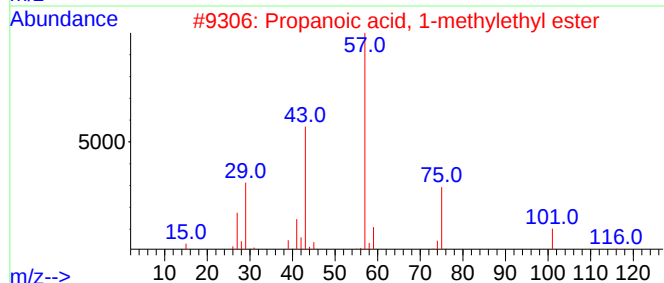
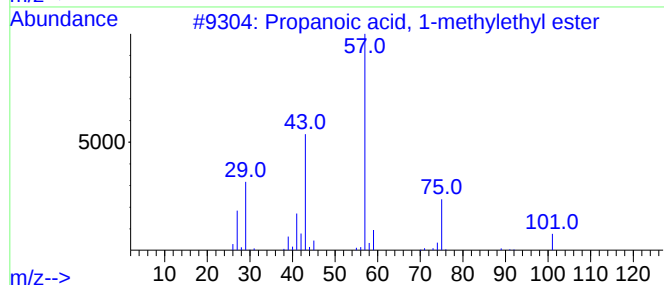
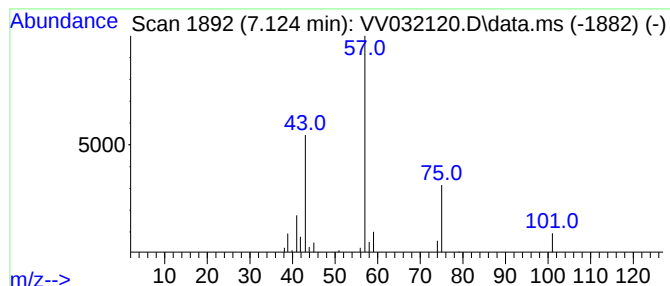
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.124	3.23 ug/L	29813	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	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59



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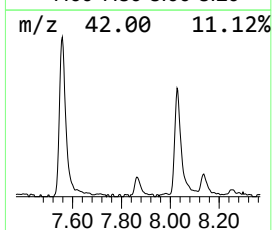
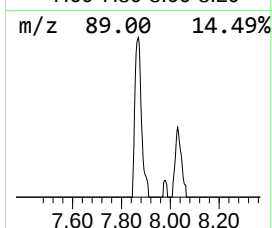
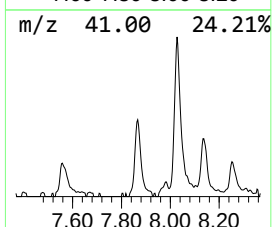
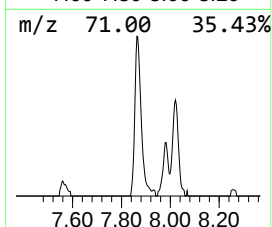
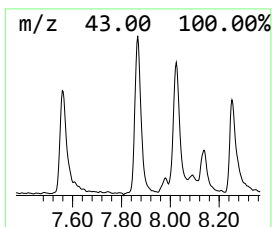
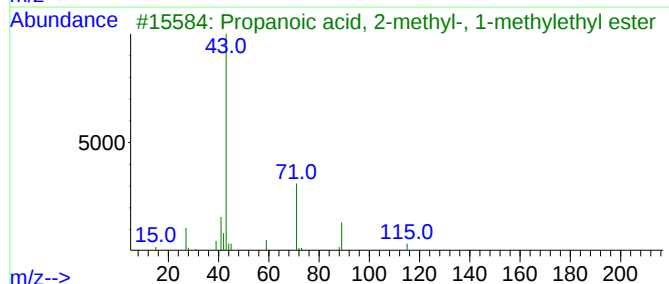
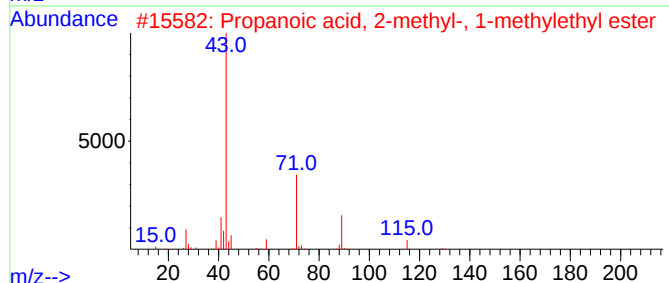
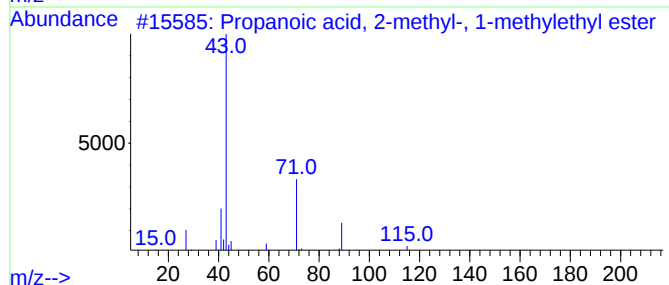
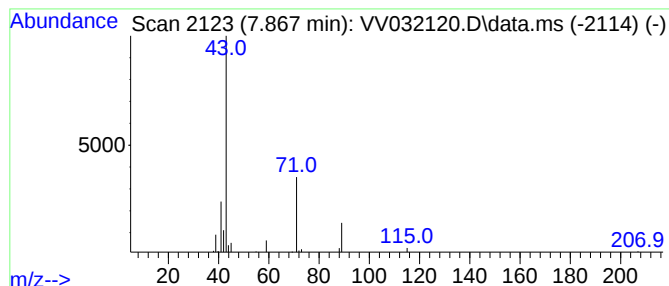
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.867	3.32 ug/L	38696	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	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032120.D
Acq On : 15 Sep 2023 14:38
Operator : SY/MD
Sample : 04359-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD3

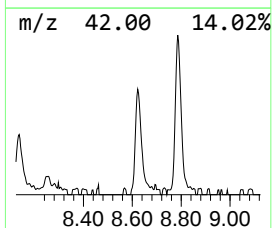
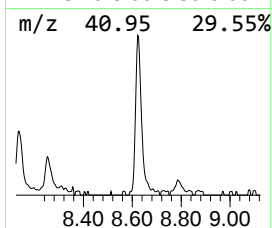
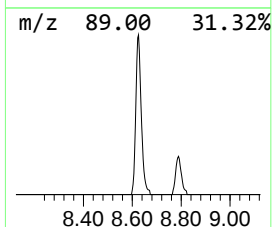
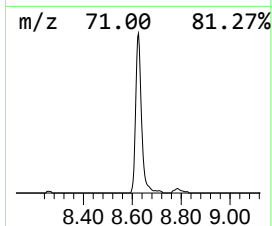
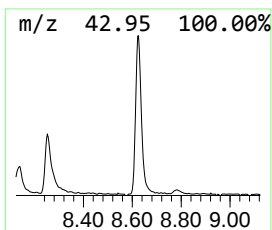
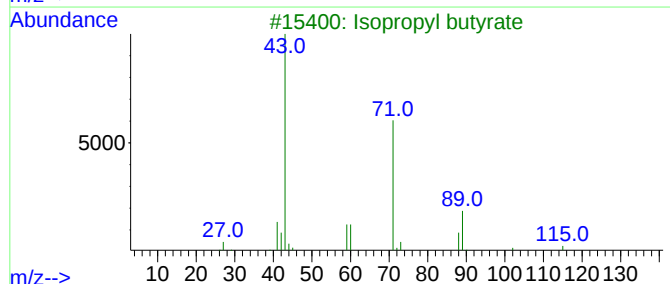
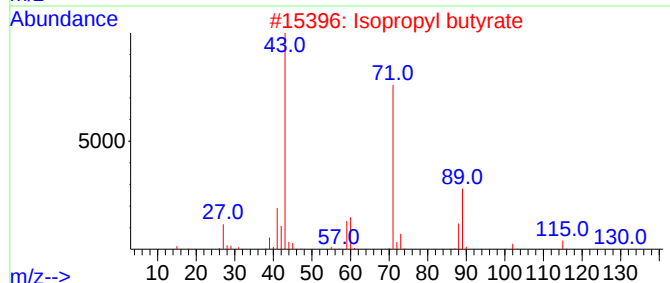
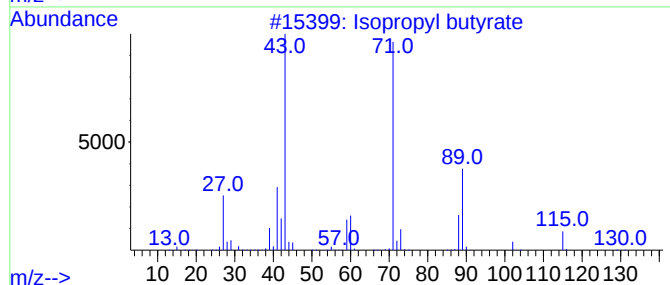
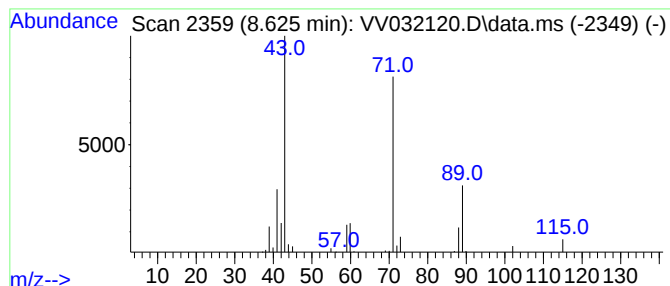
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Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.625	7.76 ug/L	90418	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
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	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032120.D
Acq On : 15 Sep 2023 14:38
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Sample : 04359-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.400	15.0	ug/L	138341	1	5.539	461434	50.0
Propanoic acid,...	7.124	3.2	ug/L	29813	1	5.539	461434	50.0
Propanoic acid,...	7.867	3.3	ug/L	38696	2	8.789	582330	50.0
Isopropyl butyrate	8.625	7.8	ug/L	90418	2	8.789	582330	50.0