

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
 Data File : VV032115.D
 Acq On : 15 Sep 2023 12:45
 Operator : SY/MD
 Sample : 04359-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 JYCA2

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: VV032115.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	89	rVB	134272	140187	15.43%	1.980%
2	1.532	146	153	165	rVB	106093	123035	13.54%	1.738%
3	2.060	308	317	328	rBV	205069	296100	32.60%	4.182%
4	2.449	432	438	452	rVB	8404	14048	1.55%	0.198%
5	2.510	453	457	463	rBV4	600	613	0.07%	0.009%
6	2.551	466	470	471	rBV3	542	402	0.04%	0.006%
7	2.600	483	485	487	rBV2	332	176	0.02%	0.002%
8	2.667	503	506	508	rBV2	200	136	0.01%	0.002%
9	2.706	515	518	522	rBV3	399	367	0.04%	0.005%
10	2.796	543	546	547	rBV	247	149	0.02%	0.002%
11	2.831	554	557	561	rVB	242	136	0.01%	0.002%
12	2.857	562	565	569	rBV2	430	312	0.03%	0.004%
13	2.953	592	595	596	rVV	198	105	0.01%	0.001%
14	3.095	636	639	640	rBV2	243	151	0.02%	0.002%
15	3.127	645	649	652	rBV3	335	326	0.04%	0.005%
16	3.182	664	666	668	rBV	252	139	0.02%	0.002%
17	3.265	689	692	695	rVB2	204	125	0.01%	0.002%
18	3.317	706	708	709	rBV2	251	87	0.01%	0.001%
19	3.362	719	722	726	rVB	398	265	0.03%	0.004%
20	3.381	726	728	730	rBV	200	89	0.01%	0.001%
21	3.394	730	732	735	rVV2	365	225	0.02%	0.003%
22	3.436	742	745	746	rBV	282	131	0.01%	0.002%
23	3.500	761	765	767	rBV2	228	139	0.02%	0.002%
24	3.523	770	772	778	rVB2	210	147	0.02%	0.002%
25	3.577	787	789	793	rVB2	351	180	0.02%	0.003%
26	3.619	798	802	803	rBV	267	147	0.02%	0.002%
27	3.658	811	814	816	rBV2	179	118	0.01%	0.002%
28	3.706	826	829	833	rBV2	297	190	0.02%	0.003%
29	3.789	845	855	887	rBV	68389	196829	21.67%	2.780%
30	4.252	983	999	1026	rBV	134908	347316	38.24%	4.905%
31	4.500	1074	1076	1082	rBV3	276	224	0.02%	0.003%
32	4.567	1094	1097	1100	rBV3	355	277	0.03%	0.004%
33	4.587	1100	1103	1105	rVB2	421	224	0.02%	0.003%
34	4.661	1122	1126	1128	rBV3	359	296	0.03%	0.004%
35	4.709	1137	1141	1142	rBV	177	117	0.01%	0.002%
36	4.748	1150	1153	1155	rBV3	199	116	0.01%	0.002%

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37	4.892	1194	1198	1199	rBV2	165	119	0.01%	0.002%
38	4.960	1203	1219	1244	rBV2	343539	908357	100.00%	12.829%
39	5.539	1387	1399	1422	rBV	241002	500901	55.14%	7.074%
40	5.831	1480	1490	1509	rVB3	8897	20344	2.24%	0.287%
41	5.928	1517	1520	1523	rBV2	290	209	0.02%	0.003%
42	5.992	1527	1540	1573	rBV	197379	422338	46.49%	5.965%
43	6.294	1628	1634	1635	rBV3	1813	1590	0.18%	0.022%
44	6.400	1659	1667	1691	rBV2	54075	113588	12.50%	1.604%
45	6.915	1814	1827	1858	rBV	108100	210093	23.13%	2.967%
46	7.127	1884	1893	1904	rBV2	17158	30614	3.37%	0.432%
47	7.246	1919	1930	1966	rBV	411385	733628	80.76%	10.361%
48	7.513	2011	2013	2017	rVB3	418	308	0.03%	0.004%
49	7.558	2017	2027	2055	rBV2	78224	150861	16.61%	2.131%
50	7.764	2087	2091	2094	rBV3	593	478	0.05%	0.007%
51	7.796	2099	2101	2103	rBV2	319	167	0.02%	0.002%
52	7.866	2112	2123	2139	rBV	22607	39964	4.40%	0.564%
53	7.979	2150	2158	2163	rBV3	3825	6136	0.68%	0.087%
54	8.027	2164	2173	2200	rVV	201095	384513	42.33%	5.431%
55	8.583	2343	2346	2347	rBV2	241	154	0.02%	0.002%
56	8.625	2349	2359	2378	rVV	45284	75664	8.33%	1.069%
57	8.786	2398	2409	2447	rBV	375468	632621	69.64%	8.935%
58	9.040	2485	2488	2490	rBV	374	227	0.02%	0.003%
59	9.072	2494	2498	2499	rBV2	341	213	0.02%	0.003%
60	9.226	2543	2546	2548	rBV	178	99	0.01%	0.001%
61	9.339	2578	2581	2582	rBV	282	157	0.02%	0.002%
62	9.423	2604	2607	2610	rBV2	256	157	0.02%	0.002%
63	9.471	2619	2622	2623	rVB	265	116	0.01%	0.002%
64	9.500	2624	2631	2632	rBV4	859	835	0.09%	0.012%
65	9.603	2660	2663	2673	rVB3	374	455	0.05%	0.006%
66	9.644	2673	2676	2677	rBV	185	99	0.01%	0.001%
67	9.706	2693	2695	2697	rVB	225	98	0.01%	0.001%
68	9.725	2698	2701	2703	rBV2	263	179	0.02%	0.003%
69	9.770	2713	2715	2720	rVV2	221	157	0.02%	0.002%
70	9.818	2728	2730	2731	rBV	414	159	0.02%	0.002%
71	9.876	2744	2748	2751	rBV3	207	213	0.02%	0.003%
72	9.892	2751	2753	2755	rVB	324	144	0.02%	0.002%
73	10.011	2786	2790	2793	rBV2	298	272	0.03%	0.004%
74	10.034	2794	2797	2801	rVV2	229	172	0.02%	0.002%
75	10.088	2811	2814	2817	rBV2	143	117	0.01%	0.002%
76	10.156	2822	2835	2858	rBV	255381	408673	44.99%	5.772%

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77	10.329	2883	2889	2896	rVB4	1031	1376	0.15%	0.019%
78	10.406	2908	2913	2917	rBV3	224	239	0.03%	0.003%
79	10.712	3006	3008	3012	rBV2	198	152	0.02%	0.002%
80	10.860	3051	3054	3055	rBV2	490	287	0.03%	0.004%
81	10.953	3081	3083	3087	rVB	227	117	0.01%	0.002%
82	10.992	3091	3095	3097	rBV	276	167	0.02%	0.002%
83	11.130	3134	3138	3145	rBV3	496	545	0.06%	0.008%
84	11.188	3145	3156	3178	rBV	417229	648394	71.38%	9.157%
85	11.474	3238	3245	3251	rVB2	1205	1719	0.19%	0.024%
86	11.564	3261	3273	3295	rBV	411310	648390	71.38%	9.157%
87	11.850	3360	3362	3363	rBV2	163	86	0.01%	0.001%
88	11.889	3372	3374	3376	rVB2	281	94	0.01%	0.001%
89	12.001	3407	3409	3412	rBV2	211	127	0.01%	0.002%
90	12.053	3420	3425	3428	rBV3	352	348	0.04%	0.005%
91	12.085	3431	3435	3436	rBV	242	149	0.02%	0.002%
92	12.197	3461	3470	3479	rBV	1558	2441	0.27%	0.034%
93	12.361	3518	3521	3523	rBV2	252	192	0.02%	0.003%
94	12.799	3654	3657	3659	rBV2	410	229	0.03%	0.003%
95	13.159	3767	3769	3773	rBV	251	121	0.01%	0.002%
96	13.207	3780	3784	3792	rBV3	801	877	0.10%	0.012%
97	13.345	3824	3827	3828	rBV2	214	133	0.01%	0.002%
98	13.451	3854	3860	3870	rVB3	3038	4023	0.44%	0.057%
99	13.689	3929	3934	3941	rBV4	1201	1420	0.16%	0.020%
100	13.911	4001	4003	4008	rVB3	331	134	0.01%	0.002%

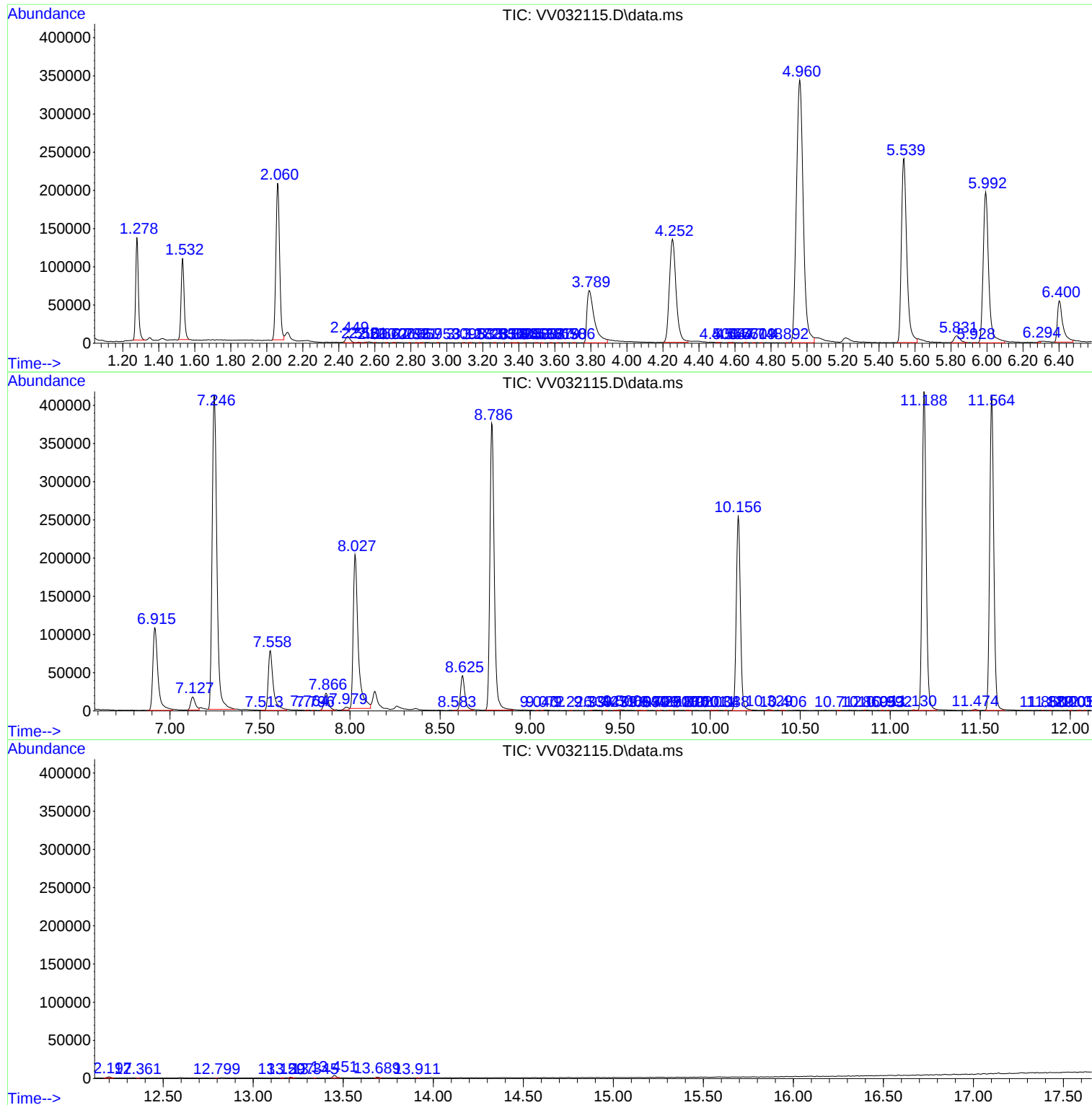
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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



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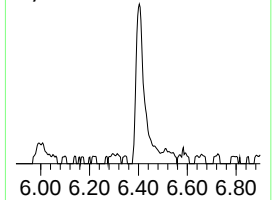
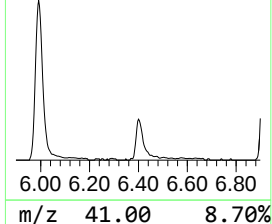
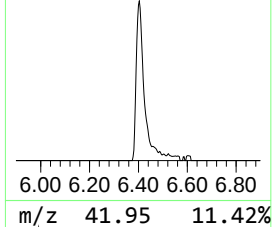
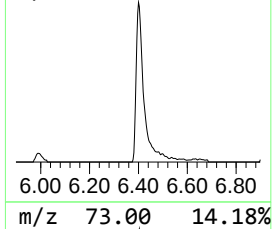
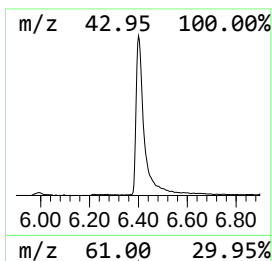
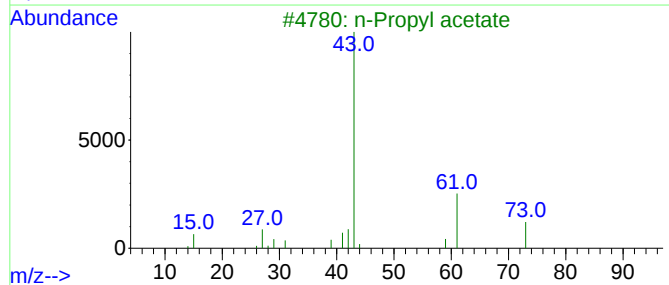
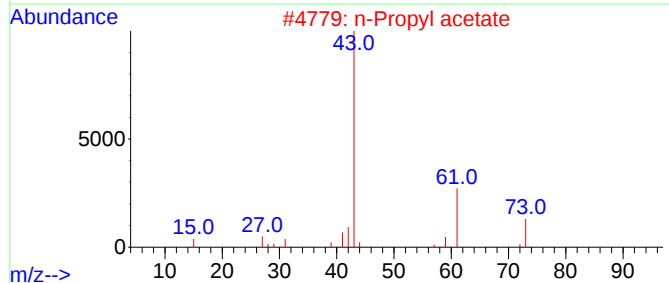
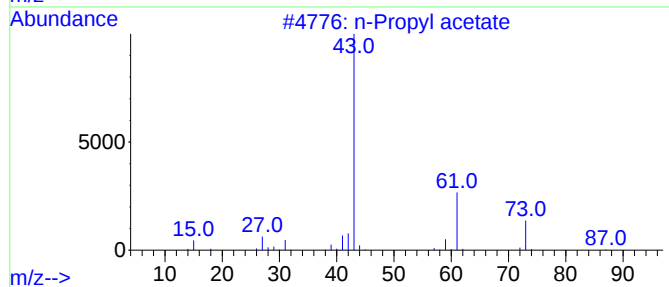
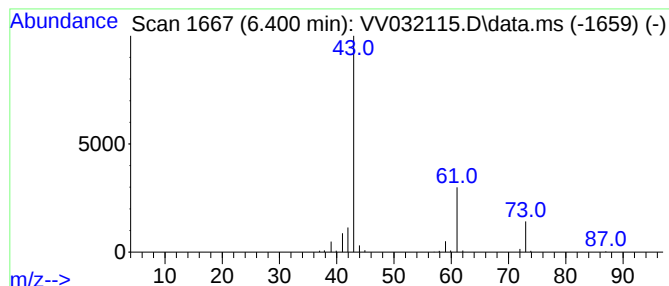
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.400	11.34 ug/L	113588	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	50



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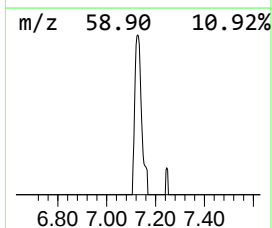
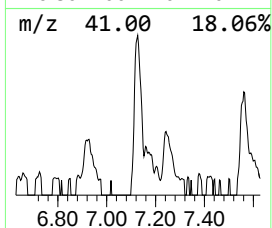
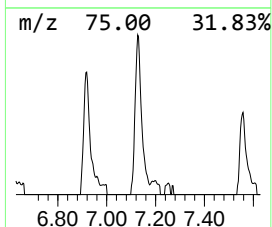
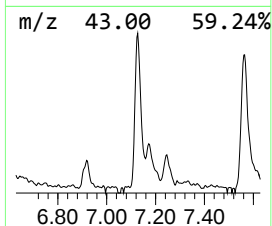
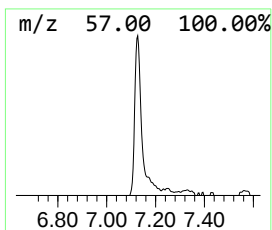
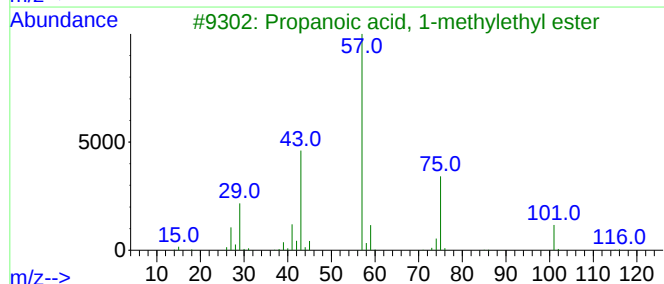
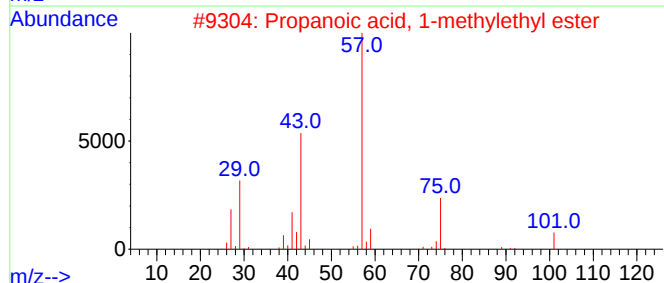
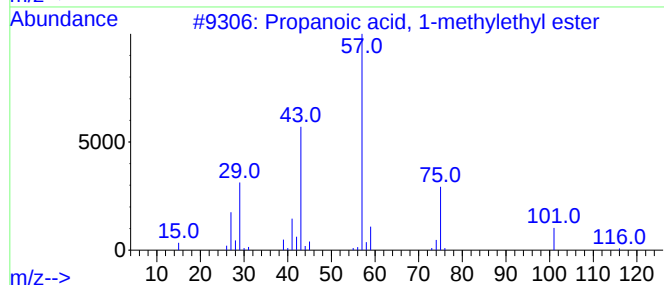
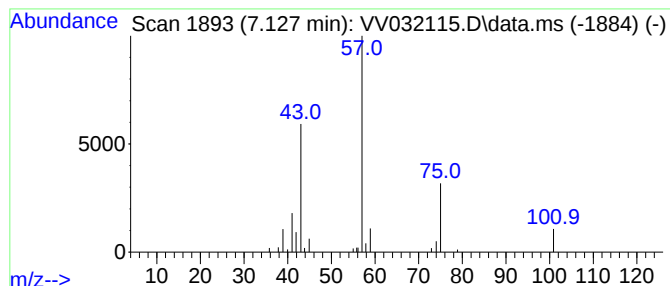
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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	3.06 ug/L	30614	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	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59



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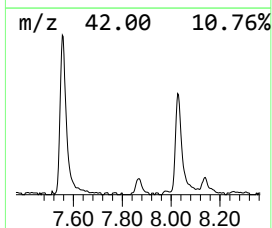
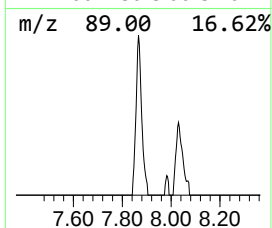
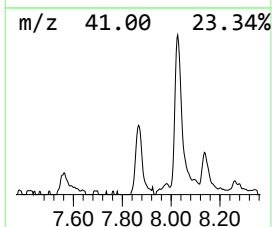
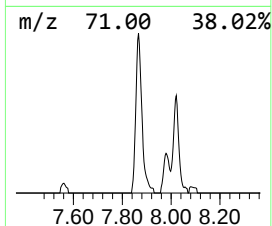
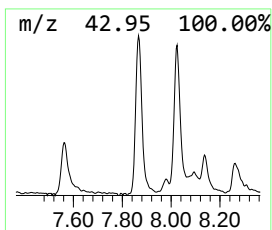
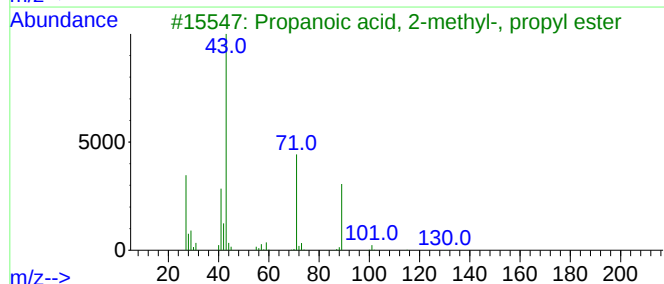
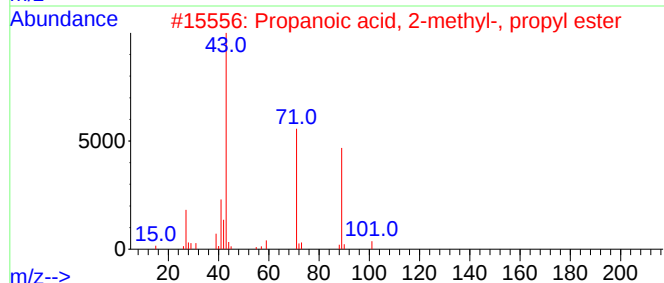
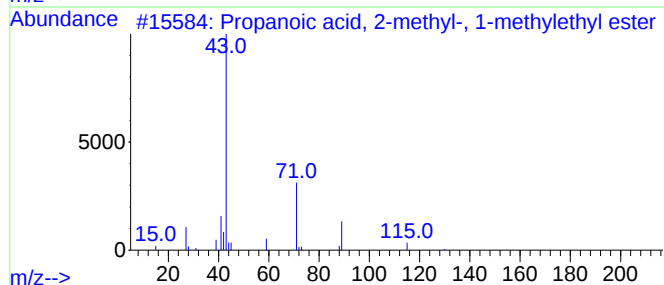
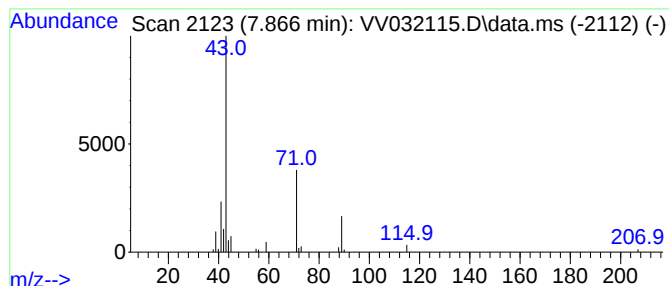
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	3.16 ug/L	39964	Chlorobenzene-d5	8.786

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-, propy...	130	C7H14O2	000644-49-5	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032115.D
Acq On : 15 Sep 2023 12:45
Operator : SY/MD
Sample : 04359-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA2

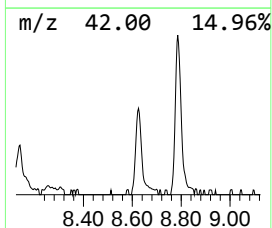
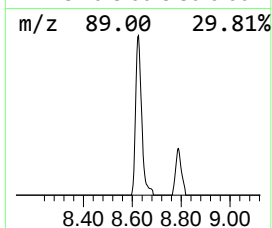
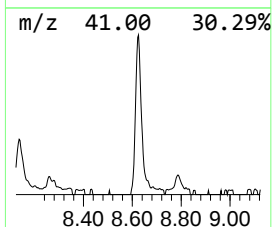
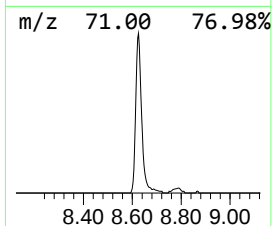
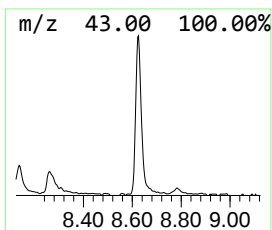
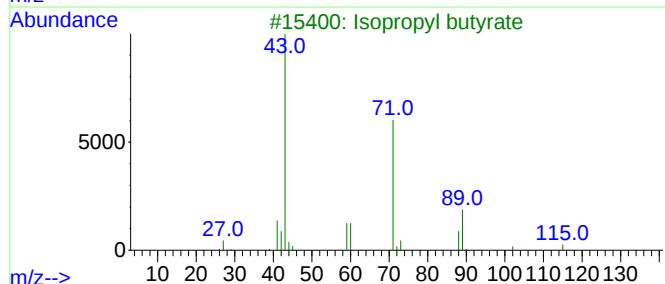
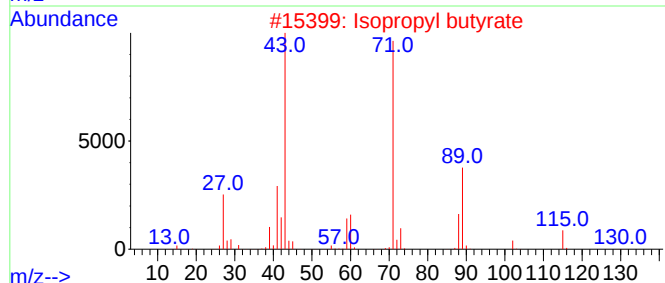
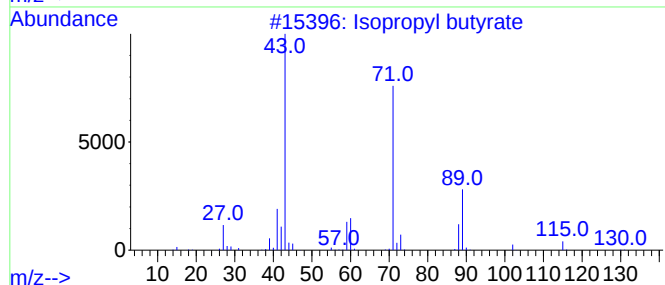
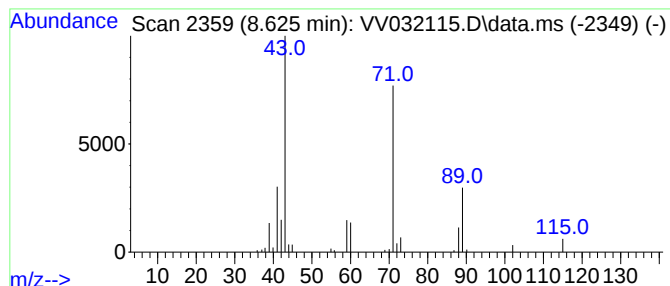
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Quant Title : VOC Analysis

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	5.98 ug/L	75664	Chlorobenzene-d5	8.786

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-, 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 : VV032115.D
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Sample : 04359-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA2

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	11.3	ug/L	113588	1	5.539	500901	50.0
Propanoic acid,...	7.127	3.1	ug/L	30614	1	5.539	500901	50.0
Propanoic acid,...	7.866	3.2	ug/L	39964	2	8.786	632621	50.0
Isopropyl butyrate	8.625	6.0	ug/L	75664	2	8.786	632621	50.0