

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
 Data File : VV031979.D
 Acq On : 08 Sep 2023 12:42
 Operator : SY/MD
 Sample : 04280-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 JLAD0

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: VV031979.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	90	rVB	135094	146585	13.77%	1.593%
2	1.529	145	152	168	rVB	109789	133875	12.58%	1.455%
3	2.060	307	317	328	rBV	221811	321948	30.25%	3.498%
4	2.314	394	396	401	rVB4	552	386	0.04%	0.004%
5	2.449	427	438	451	rBV	14793	25084	2.36%	0.273%
6	2.552	463	470	474	rBV5	2297	3225	0.30%	0.035%
7	2.690	510	513	517	rBV2	451	344	0.03%	0.004%
8	2.757	531	534	538	rBV4	330	324	0.03%	0.004%
9	2.880	566	572	573	rBV3	802	824	0.08%	0.009%
10	2.973	596	601	610	rVB6	707	1176	0.11%	0.013%
11	3.224	675	679	685	rVB4	882	791	0.07%	0.009%
12	3.253	685	688	691	rBV3	490	385	0.04%	0.004%
13	3.481	755	759	762	rVB4	562	460	0.04%	0.005%
14	3.629	803	805	812	rVB4	336	315	0.03%	0.003%
15	3.690	818	824	829	rBV3	427	511	0.05%	0.006%
16	3.712	829	831	837	rVB4	483	390	0.04%	0.004%
17	3.741	837	840	844	rBV3	711	586	0.06%	0.006%
18	3.789	844	855	888	rBV2	95701	280560	26.36%	3.048%
19	4.253	982	999	1029	rBV	157540	405203	38.07%	4.403%
20	4.886	1191	1196	1199	rBV3	631	441	0.04%	0.005%
21	4.960	1202	1219	1245	rBV2	408271	1064403	100.00%	11.565%
22	5.217	1288	1299	1315	rBV2	8078	20745	1.95%	0.225%
23	5.433	1363	1366	1370	rVB4	560	386	0.04%	0.004%
24	5.539	1386	1399	1420	rBV	335455	688384	64.67%	7.480%
25	5.786	1471	1476	1477	rBV4	587	505	0.05%	0.005%
26	5.831	1478	1490	1506	rVV2	10278	21861	2.05%	0.238%
27	5.915	1513	1516	1518	rBV2	649	381	0.04%	0.004%
28	5.992	1526	1540	1578	rBV	231776	498764	46.86%	5.419%
29	6.256	1620	1622	1624	rBV2	595	321	0.03%	0.003%
30	6.294	1626	1634	1637	rBV4	2696	3843	0.36%	0.042%
31	6.400	1658	1667	1700	rBV	109123	218838	20.56%	2.378%
32	6.918	1817	1828	1858	rBV	139271	264490	24.85%	2.874%
33	7.127	1883	1893	1904	rBV	26020	44566	4.19%	0.484%
34	7.246	1919	1930	1965	rBV	487698	873937	82.11%	9.496%
35	7.558	2017	2027	2056	rVV2	117852	224359	21.08%	2.438%
36	7.867	2109	2123	2138	rBV	34425	61284	5.76%	0.666%

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

37	7.979	2148	2158	2164	rBV4	6789	11389	1.07%	0.124%
38	8.027	2164	2173	2199	rVV	278101	533324	50.11%	5.795%
39	8.137	2200	2207	2233	rVV	52561	96371	9.05%	1.047%
40	8.252	2235	2243	2266	rVB2	25534	48147	4.52%	0.523%
41	8.365	2273	2278	2299	rVB5	6454	12757	1.20%	0.139%
42	8.442	2299	2302	2306	rBV4	771	704	0.07%	0.008%
43	8.625	2348	2359	2375	rBV	95177	153004	14.37%	1.662%
44	8.789	2398	2410	2439	rBV	516330	852825	80.12%	9.266%
45	9.072	2494	2498	2502	rBV6	734	709	0.07%	0.008%
46	9.156	2518	2524	2526	rBV3	585	549	0.05%	0.006%
47	9.207	2535	2540	2545	rBV3	617	679	0.06%	0.007%
48	9.355	2576	2586	2587	rBV5	1344	1841	0.17%	0.020%
49	9.497	2619	2630	2639	rBV8	4975	9445	0.89%	0.103%
50	9.960	2770	2774	2781	rBV4	419	565	0.05%	0.006%
51	10.005	2784	2788	2792	rBV5	616	552	0.05%	0.006%
52	10.053	2800	2803	2808	rVB3	433	316	0.03%	0.003%
53	10.085	2808	2813	2817	rBV5	768	642	0.06%	0.007%
54	10.117	2817	2823	2824	rBV3	670	573	0.05%	0.006%
55	10.159	2824	2836	2855	rVV	301874	484799	45.55%	5.268%
56	10.329	2885	2889	2893	rBV4	770	660	0.06%	0.007%
57	10.397	2904	2910	2913	rBV4	726	859	0.08%	0.009%
58	10.593	2968	2971	2973	rBV2	475	311	0.03%	0.003%
59	10.625	2976	2981	2983	rBV5	508	382	0.04%	0.004%
60	10.638	2983	2985	2990	rVB2	529	384	0.04%	0.004%
61	10.725	3010	3012	3018	rBV6	733	663	0.06%	0.007%
62	10.841	3042	3048	3052	rVB4	487	535	0.05%	0.006%
63	10.860	3052	3054	3057	rBV	642	420	0.04%	0.005%
64	10.963	3084	3086	3091	rBV2	623	398	0.04%	0.004%
65	11.108	3129	3131	3133	rBV2	474	346	0.03%	0.004%
66	11.188	3145	3156	3179	rBV	573650	888469	83.47%	9.654%
67	11.416	3224	3227	3229	rBV2	495	333	0.03%	0.004%
68	11.519	3254	3259	3261	rBV4	1253	1067	0.10%	0.012%
69	11.564	3261	3273	3292	rVV	492975	771545	72.49%	8.383%
70	11.706	3315	3317	3320	rVB	837	357	0.03%	0.004%
71	11.780	3336	3340	3342	rBV2	515	380	0.04%	0.004%
72	11.796	3342	3345	3349	rVB3	808	584	0.05%	0.006%
73	11.828	3352	3355	3358	rBV4	873	580	0.05%	0.006%
74	11.908	3378	3380	3383	rVV2	604	383	0.04%	0.004%
75	12.062	3426	3428	3430	rBV	541	361	0.03%	0.004%
76	12.098	3435	3439	3442	rBV3	506	365	0.03%	0.004%

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Title : VOC Analysis

77	12.127	3444	3448	3450	rBV3	461	448	0.04%	0.005%
78	12.172	3459	3462	3464	rBV3	499	364	0.03%	0.004%
79	12.194	3466	3469	3476	rVB4	904	1087	0.10%	0.012%
80	12.226	3476	3479	3483	rVB4	530	413	0.04%	0.004%
81	12.300	3497	3502	3503	rBV4	605	463	0.04%	0.005%
82	12.336	3510	3513	3518	rVB4	558	427	0.04%	0.005%
83	12.390	3528	3530	3535	rVB3	482	356	0.03%	0.004%
84	12.709	3625	3629	3632	rBV3	546	438	0.04%	0.005%
85	13.056	3732	3737	3739	rBV4	364	327	0.03%	0.004%
86	13.178	3772	3775	3778	rBV3	539	420	0.04%	0.005%
87	13.207	3781	3784	3790	rVB4	1314	1460	0.14%	0.016%
88	13.255	3795	3799	3802	rBV3	814	736	0.07%	0.008%
89	13.297	3808	3812	3816	rVB5	866	625	0.06%	0.007%
90	13.320	3816	3819	3821	rBV3	711	441	0.04%	0.005%
91	13.451	3853	3860	3865	rBV7	1583	1997	0.19%	0.022%
92	13.548	3886	3890	3893	rBV	652	625	0.06%	0.007%
93	13.615	3908	3911	3914	rVB4	631	405	0.04%	0.004%
94	13.680	3929	3931	3936	rBV4	649	624	0.06%	0.007%
95	14.149	4074	4077	4081	rVB4	702	480	0.05%	0.005%
96	14.172	4081	4084	4085	rBV2	602	326	0.03%	0.004%
97	14.188	4085	4089	4094	rVV5	595	523	0.05%	0.006%
98	14.365	4141	4144	4146	rBV3	581	444	0.04%	0.005%
99	14.689	4243	4245	4248	rVB3	664	337	0.03%	0.004%
100	15.146	4384	4387	4389	rBV4	692	523	0.05%	0.006%

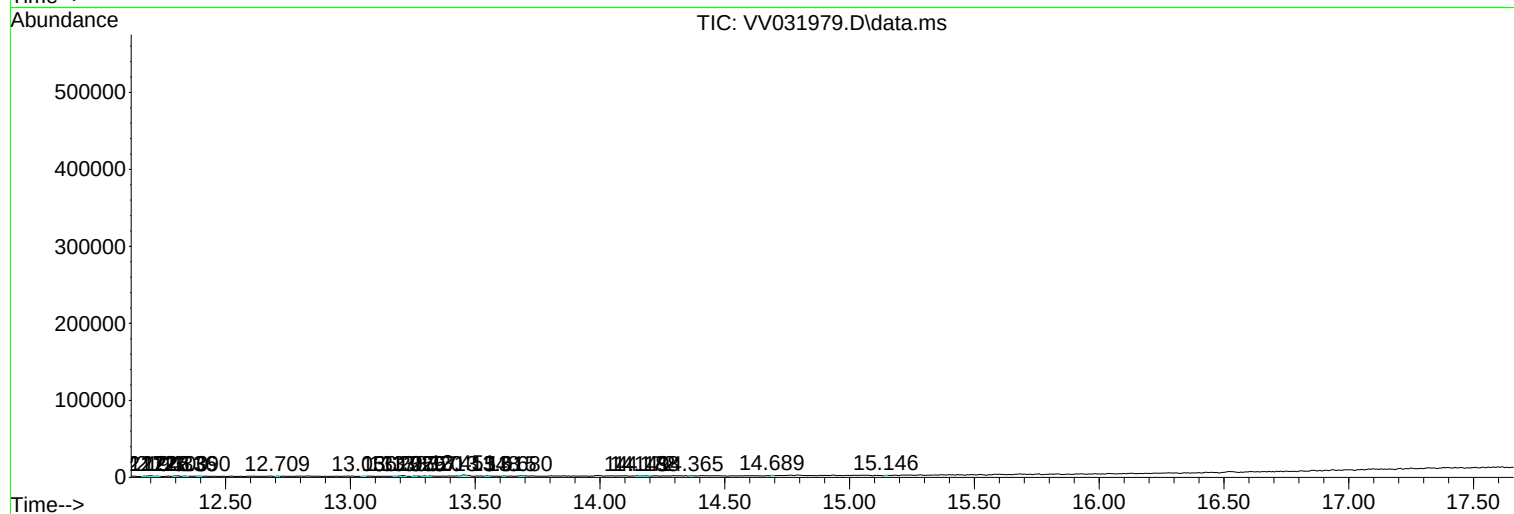
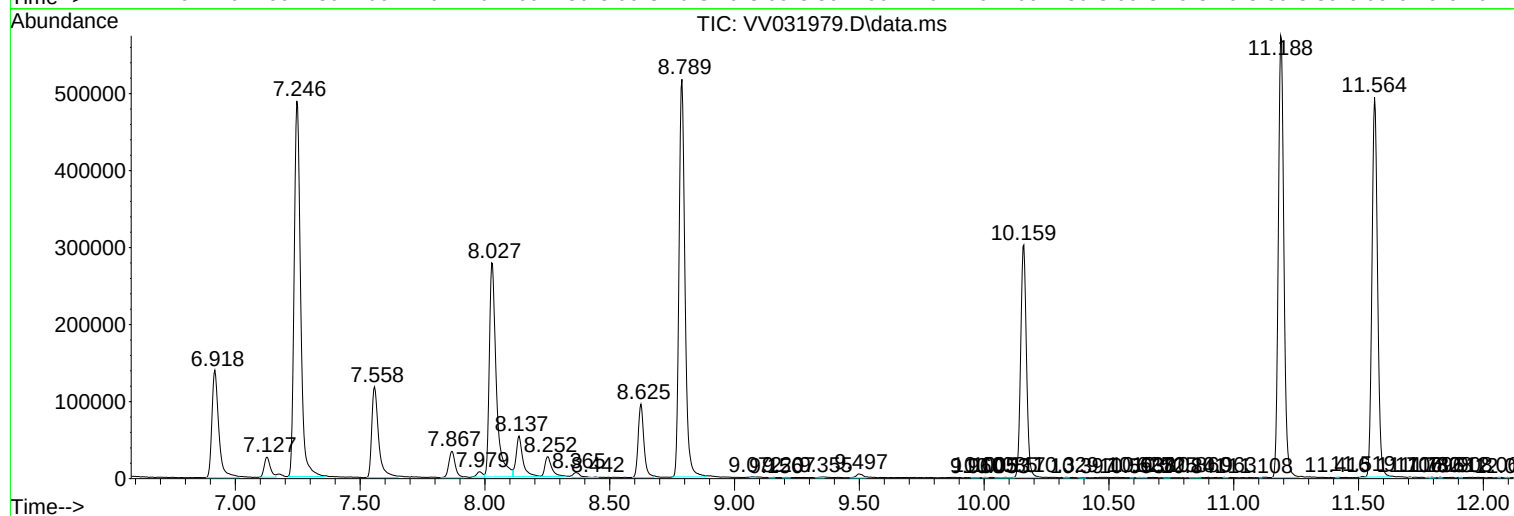
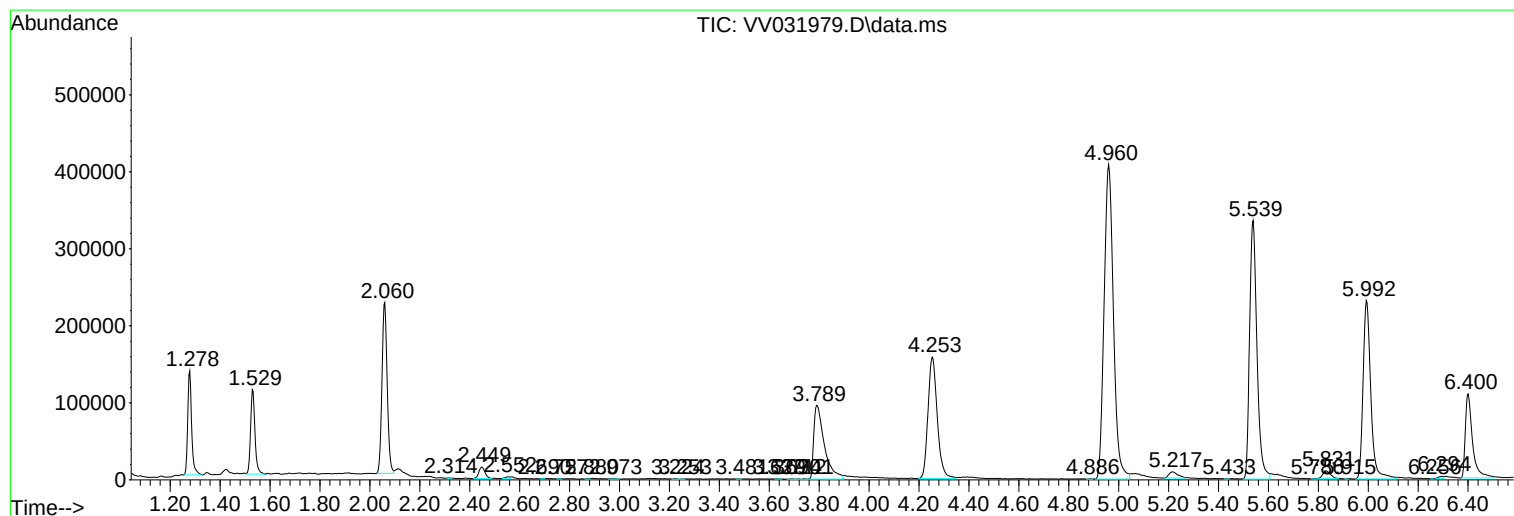
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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



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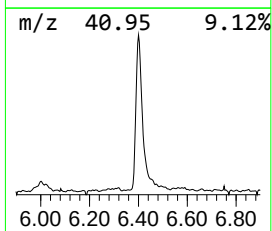
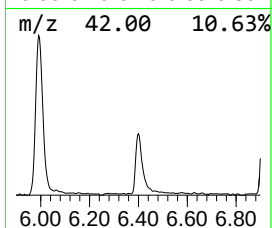
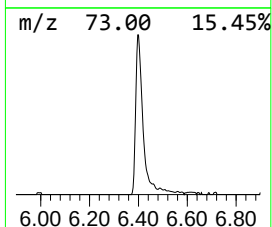
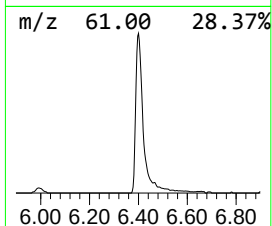
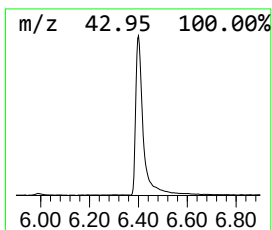
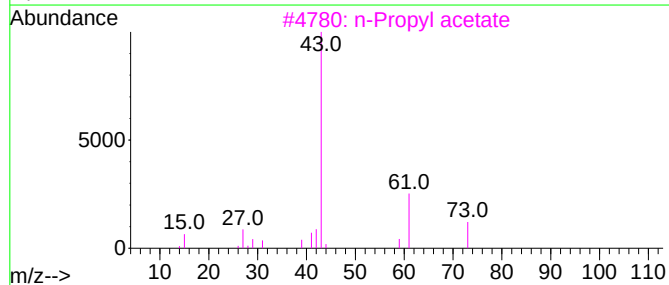
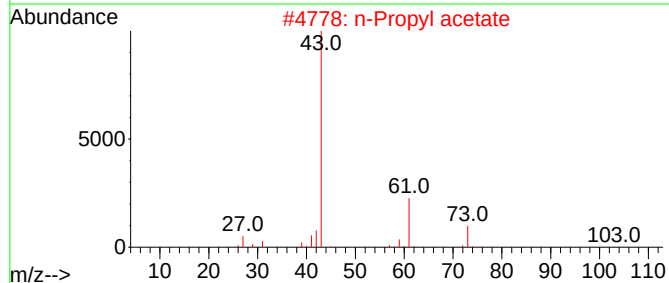
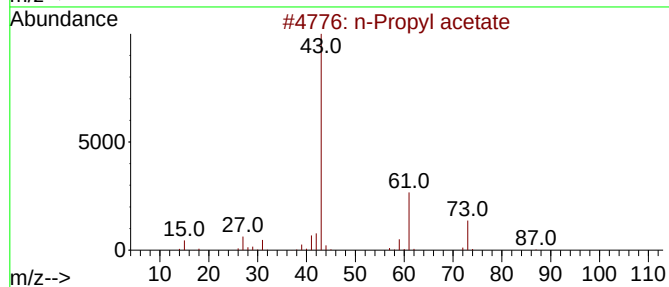
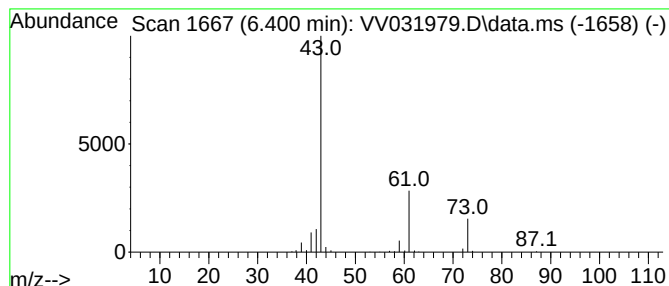
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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	15.90 ug/L	218838	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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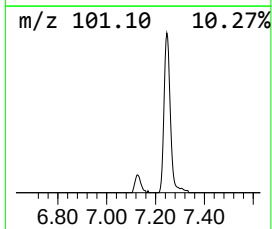
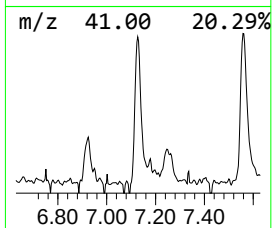
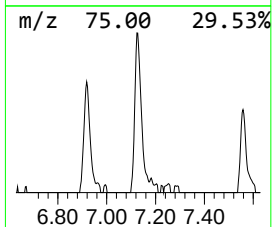
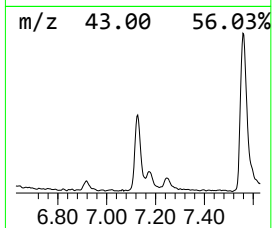
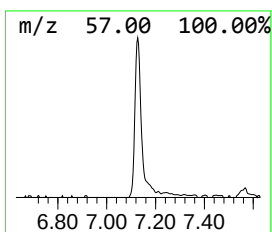
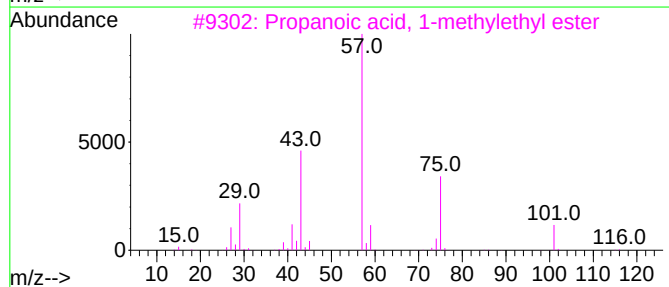
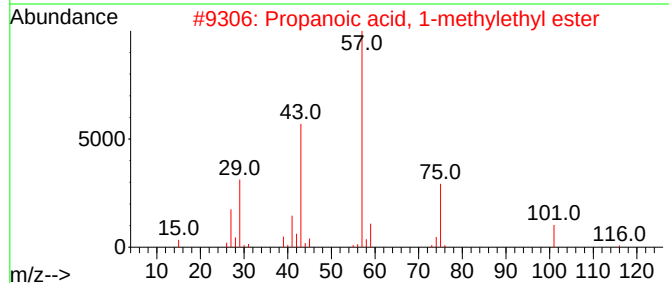
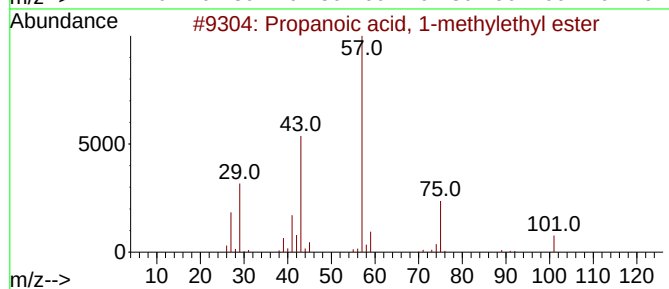
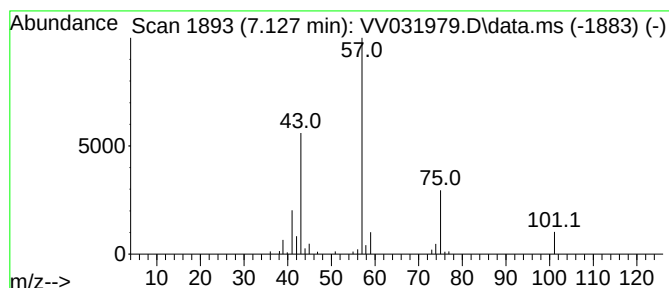
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.24 ug/L	44566	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	86
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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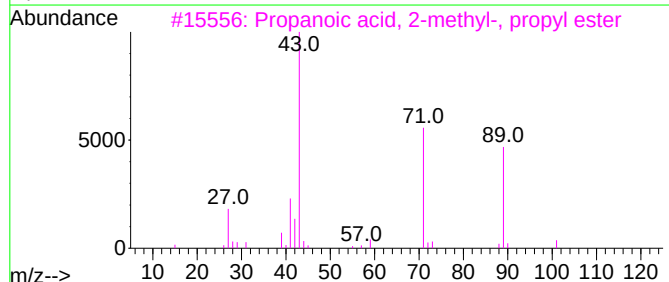
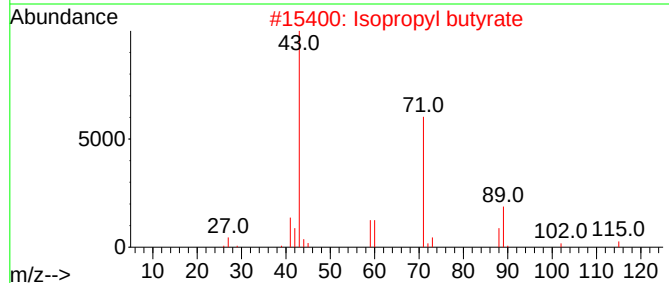
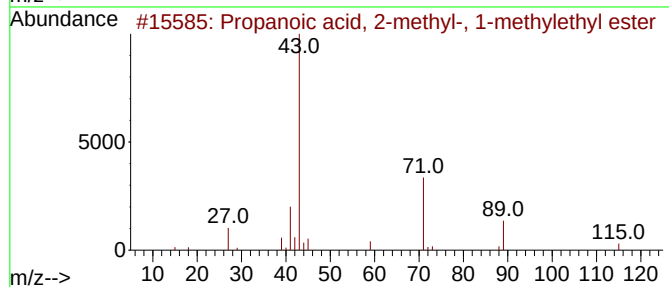
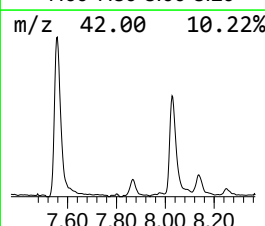
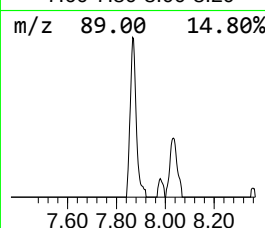
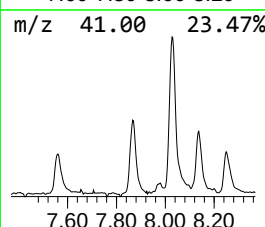
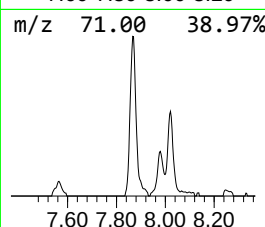
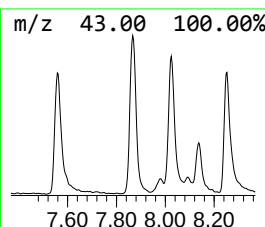
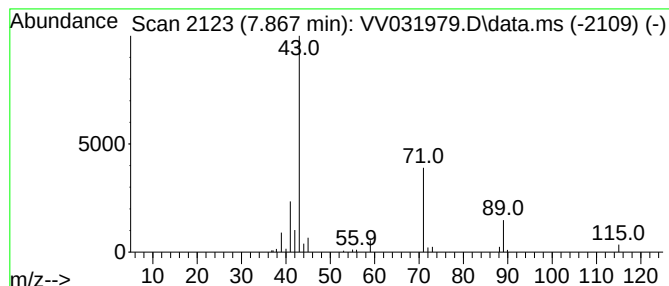
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.867	3.59 ug/L	61284	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	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\VV090823\
Data File : VV031979.D
Acq On : 08 Sep 2023 12:42
Operator : SY/MD
Sample : 04280-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD0

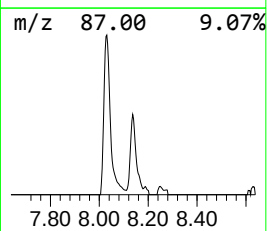
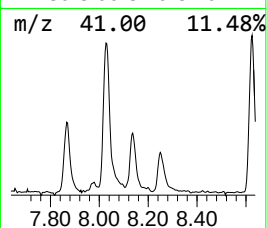
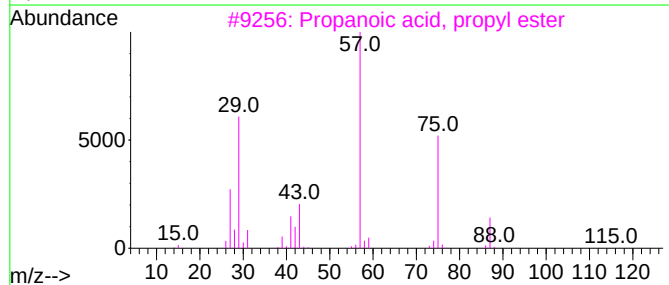
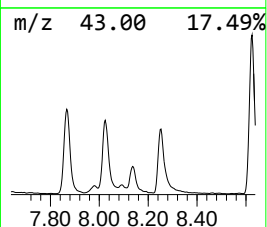
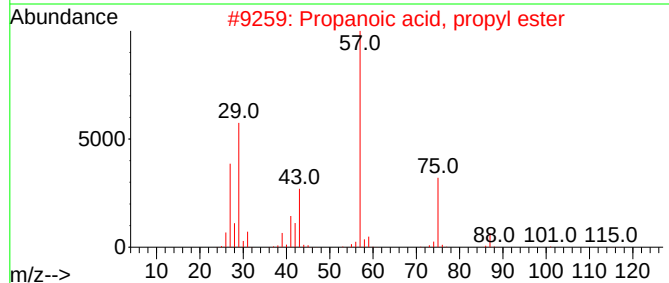
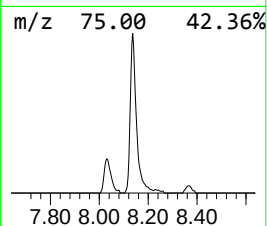
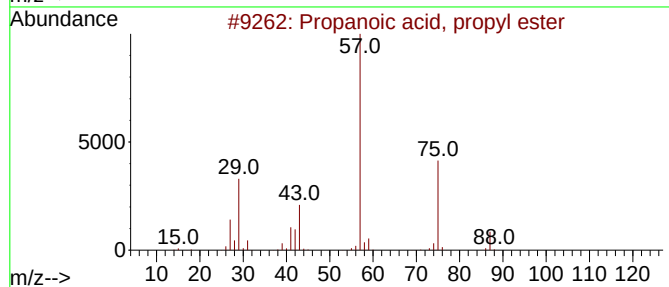
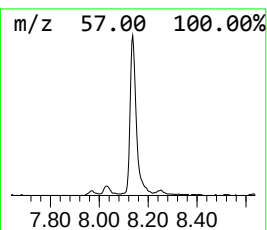
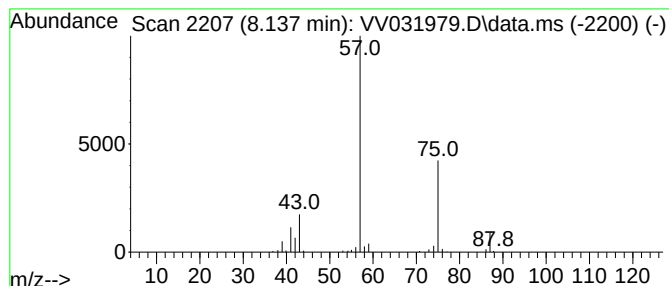
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.137	5.65 ug/L	96371	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031979.D
Acq On : 08 Sep 2023 12:42
Operator : SY/MD
Sample : 04280-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD0

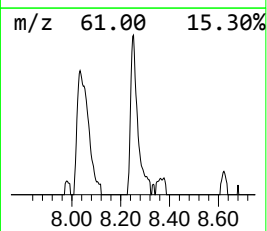
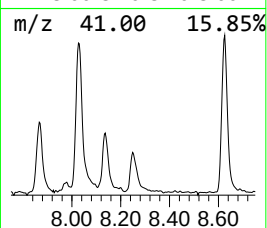
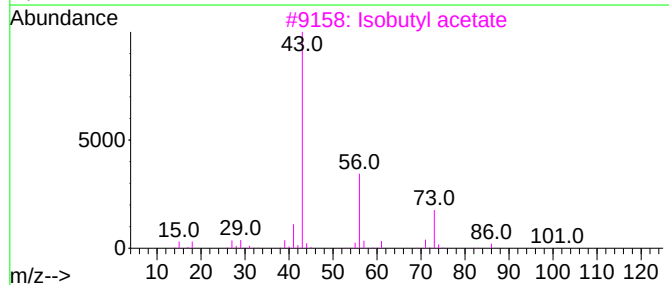
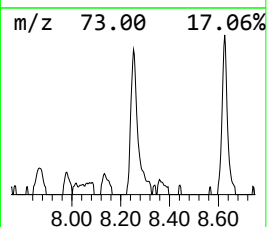
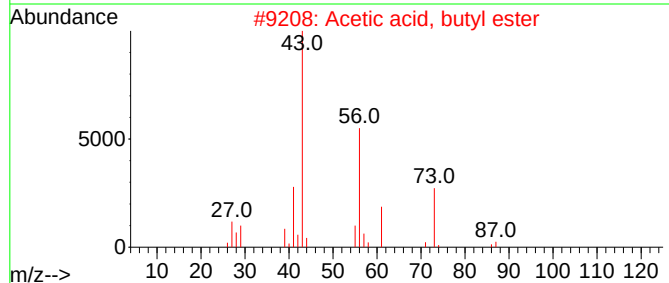
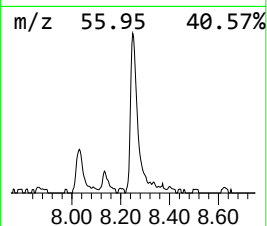
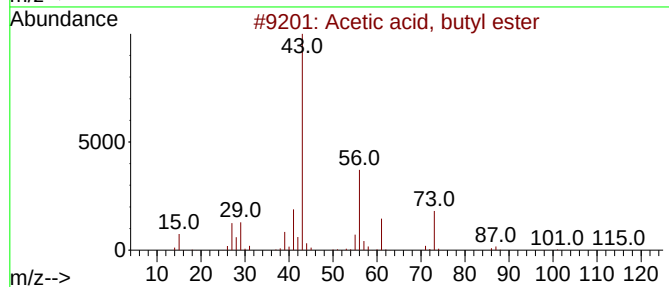
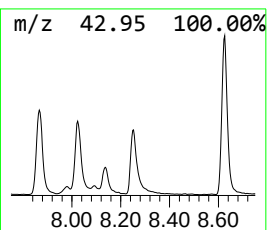
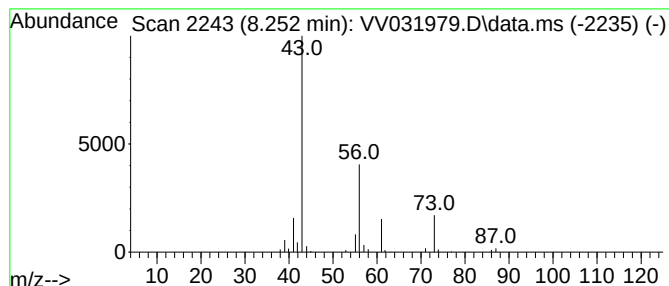
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.252	2.82 ug/L	48147	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3			Isobutyl acetate	116	C6H12O2	000110-19-0	39
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	37
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031979.D
Acq On : 08 Sep 2023 12:42
Operator : SY/MD
Sample : 04280-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD0

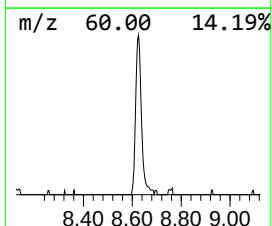
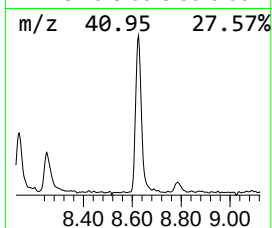
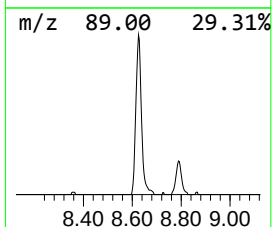
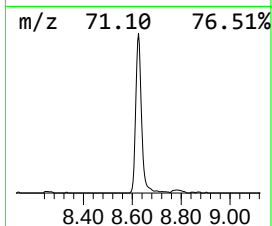
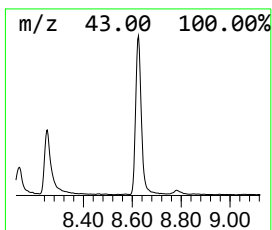
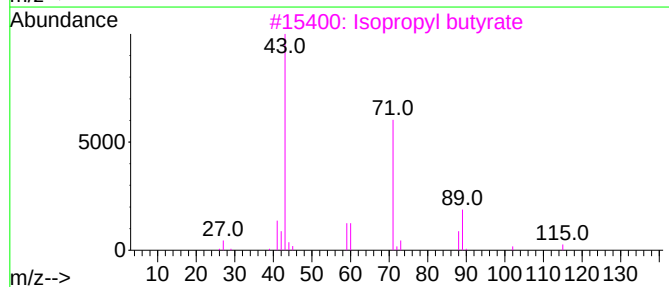
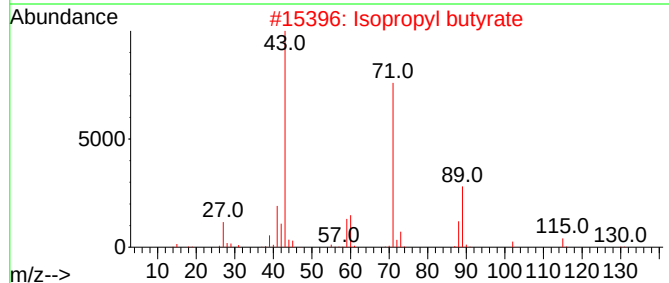
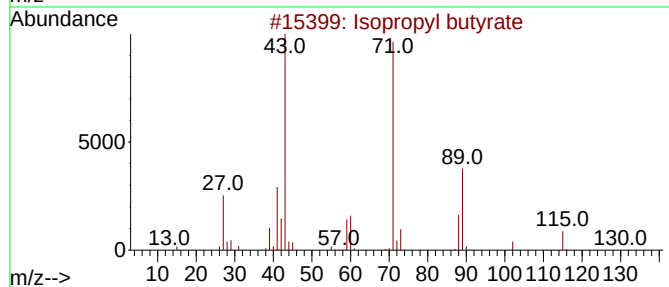
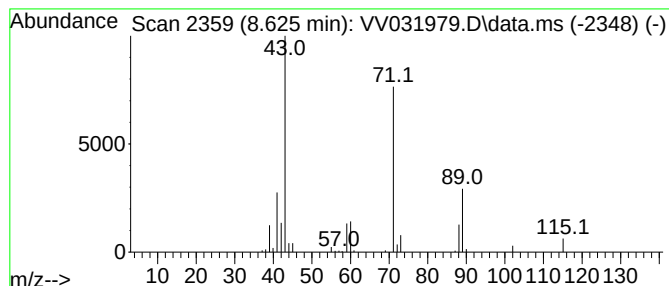
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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.
8.625	8.97 ug/L	153004	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-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031979.D
Acq On : 08 Sep 2023 12:42
Operator : SY/MD
Sample : 04280-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD0

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
n-Propyl acetate	6.400	15.9	ug/L	218838	1	5.539	688384	50.0
Propanoic acid,...	7.127	3.2	ug/L	44566	1	5.539	688384	50.0
Propanoic acid,...	7.867	3.6	ug/L	61284	2	8.789	852825	50.0
Propanoic acid,...	8.137	5.7	ug/L	96371	2	8.789	852825	50.0
Acetic acid, bu...	8.252	2.8	ug/L	48147	2	8.789	852825	50.0
Isopropyl butyrate	8.625	9.0	ug/L	153004	2	8.789	852825	50.0