

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
 Data File : VV031981.D
 Acq On : 08 Sep 2023 13:29
 Operator : SY/MD
 Sample : 04280-03 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 JLAD2

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: VV031981.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	88	rBV	123109	134285	13.82%	1.571%
2	1.529	146	152	169	rVB	97779	121076	12.46%	1.416%
3	2.060	307	317	329	rBV	202977	293959	30.26%	3.438%
4	2.449	429	438	448	rBV	19052	31158	3.21%	0.364%
5	2.651	500	501	509	rVB3	416	357	0.04%	0.004%
6	2.699	509	516	520	rBV3	695	811	0.08%	0.009%
7	2.950	591	594	599	rBV5	387	323	0.03%	0.004%
8	3.021	612	616	618	rBV3	408	316	0.03%	0.004%
9	3.265	685	692	696	rVB4	395	396	0.04%	0.005%
10	3.371	720	725	727	rBV3	592	512	0.05%	0.006%
11	3.551	776	781	783	rVB4	429	404	0.04%	0.005%
12	3.574	783	788	792	rBV5	361	345	0.04%	0.004%
13	3.622	799	803	806	rBV3	577	523	0.05%	0.006%
14	3.661	812	815	817	rBV3	563	388	0.04%	0.005%
15	3.728	833	836	838	rBV2	483	336	0.03%	0.004%
16	3.793	843	856	895	rBV	84421	244202	25.14%	2.856%
17	4.156	965	969	973	rBV3	602	478	0.05%	0.006%
18	4.252	984	999	1028	rBV	142829	368200	37.90%	4.307%
19	4.522	1080	1083	1085	rBV3	703	466	0.05%	0.005%
20	4.584	1098	1102	1108	rVV4	622	740	0.08%	0.009%
21	4.719	1141	1144	1149	rBV4	515	501	0.05%	0.006%
22	4.960	1203	1219	1247	rBV2	368441	971533	100.00%	11.363%
23	5.214	1287	1298	1316	rBV2	8224	19735	2.03%	0.231%
24	5.487	1378	1383	1387	rBV4	547	580	0.06%	0.007%
25	5.539	1387	1399	1423	rBV	331288	681901	70.19%	7.976%
26	5.831	1479	1490	1514	rVB4	9455	21780	2.24%	0.255%
27	5.995	1524	1541	1573	rBV	211632	454082	46.74%	5.311%
28	6.301	1627	1636	1639	rBV2	2655	4121	0.42%	0.048%
29	6.400	1658	1667	1700	rBV	99053	196021	20.18%	2.293%
30	6.757	1774	1778	1783	rBV5	549	600	0.06%	0.007%
31	6.918	1815	1828	1860	rBV	126220	243720	25.09%	2.851%
32	7.127	1884	1893	1904	rBV	23533	41715	4.29%	0.488%
33	7.249	1919	1931	1959	rBV	437131	791954	81.52%	9.263%
34	7.558	2017	2027	2054	rBV	105093	199406	20.52%	2.332%
35	7.866	2111	2123	2142	rBV2	31497	56588	5.82%	0.662%
36	7.979	2146	2158	2164	rBV4	6961	11706	1.20%	0.137%

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 Title : VOC Analysis

37	8.030	2164	2174	2199	rVV	260929	492973	50.74%	5.766%
38	8.136	2200	2207	2227	rVB	42677	75779	7.80%	0.886%
39	8.252	2235	2243	2257	rBV2	19854	35493	3.65%	0.415%
40	8.362	2275	2277	2294	rVB6	4297	6861	0.71%	0.080%
41	8.564	2336	2340	2343	rBV6	637	438	0.05%	0.005%
42	8.625	2348	2359	2380	rBV	79163	132486	13.64%	1.550%
43	8.789	2398	2410	2433	rBV	499388	843279	86.80%	9.863%
44	9.056	2491	2493	2495	rBV2	784	530	0.05%	0.006%
45	9.210	2536	2541	2542	rBV2	479	367	0.04%	0.004%
46	9.236	2546	2549	2553	rVB3	377	336	0.03%	0.004%
47	9.310	2570	2572	2576	rVB2	580	361	0.04%	0.004%
48	9.342	2576	2582	2583	rBV4	950	875	0.09%	0.010%
49	9.500	2622	2631	2648	rBV6	2746	6282	0.65%	0.073%
50	9.792	2714	2722	2728	rBV6	661	990	0.10%	0.012%
51	9.873	2743	2747	2750	rBV4	587	535	0.06%	0.006%
52	9.966	2772	2776	2779	rVV4	484	375	0.04%	0.004%
53	10.008	2786	2789	2791	rVV2	559	331	0.03%	0.004%
54	10.030	2791	2796	2802	rVB5	443	536	0.06%	0.006%
55	10.159	2824	2836	2855	rBV	281959	448791	46.19%	5.249%
56	10.275	2870	2872	2877	rVB5	589	437	0.04%	0.005%
57	10.477	2931	2935	2939	rBV3	475	463	0.05%	0.005%
58	10.548	2953	2957	2961	rVB3	476	375	0.04%	0.004%
59	10.596	2967	2972	2975	rBV3	604	615	0.06%	0.007%
60	10.660	2990	2992	2996	rVB4	605	309	0.03%	0.004%
61	10.754	3018	3021	3024	rVB3	550	357	0.04%	0.004%
62	10.902	3062	3067	3069	rBV4	326	321	0.03%	0.004%
63	11.062	3111	3117	3119	rBV3	511	406	0.04%	0.005%
64	11.091	3123	3126	3129	rBV3	433	355	0.04%	0.004%
65	11.191	3145	3157	3178	rBV	558971	874832	90.05%	10.232%
66	11.522	3253	3260	3262	rBV5	986	1282	0.13%	0.015%
67	11.564	3262	3273	3293	rVV	444703	707047	72.78%	8.270%
68	11.824	3352	3354	3357	rVB2	515	325	0.03%	0.004%
69	11.918	3377	3383	3385	rBV4	510	535	0.06%	0.006%
70	11.947	3388	3392	3395	rBV5	374	349	0.04%	0.004%
71	12.049	3421	3424	3430	rVB4	778	537	0.06%	0.006%
72	12.197	3467	3470	3479	rVB6	1058	1528	0.16%	0.018%
73	12.236	3479	3482	3485	rVB3	509	341	0.04%	0.004%
74	12.268	3488	3492	3496	rVB4	440	424	0.04%	0.005%
75	12.297	3496	3501	3503	rBV4	1090	920	0.09%	0.011%
76	12.320	3503	3508	3515	rVB5	787	884	0.09%	0.010%

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 Title : VOC Analysis

77	12.403	3531	3534	3540	rVB5	805	746	0.08%	0.009%
78	12.474	3553	3556	3559	rBV3	515	380	0.04%	0.004%
79	12.545	3574	3578	3581	rBV4	423	347	0.04%	0.004%
80	12.590	3590	3592	3596	rBV3	567	335	0.03%	0.004%
81	12.667	3615	3616	3621	rBV4	383	313	0.03%	0.004%
82	12.718	3628	3632	3636	rVB6	715	641	0.07%	0.007%
83	12.741	3636	3639	3641	rBV2	630	470	0.05%	0.005%
84	12.834	3665	3668	3672	rVV3	836	648	0.07%	0.008%
85	12.940	3698	3701	3703	rBV2	454	346	0.04%	0.004%
86	12.969	3707	3710	3711	rBV2	678	343	0.04%	0.004%
87	12.992	3715	3717	3721	rVB3	559	311	0.03%	0.004%
88	13.091	3743	3748	3751	rBV3	593	395	0.04%	0.005%
89	13.165	3769	3771	3777	rVB3	511	374	0.04%	0.004%
90	13.213	3779	3786	3792	rVB10	847	990	0.10%	0.012%
91	13.451	3856	3860	3864	rBV2	1307	1293	0.13%	0.015%
92	13.676	3926	3930	3933	rBV5	615	570	0.06%	0.007%
93	13.696	3933	3936	3939	rVB3	952	612	0.06%	0.007%
94	13.988	4023	4027	4037	rVB6	1407	2117	0.22%	0.025%
95	14.027	4037	4039	4043	rVB4	536	335	0.03%	0.004%
96	14.599	4209	4217	4218	rBV4	579	735	0.08%	0.009%
97	14.680	4239	4242	4245	rBV4	556	552	0.06%	0.006%
98	14.824	4285	4287	4290	rVB4	641	356	0.04%	0.004%
99	14.914	4313	4315	4320	rVV3	757	361	0.04%	0.004%
100	15.323	4439	4442	4446	rBV5	894	806	0.08%	0.009%

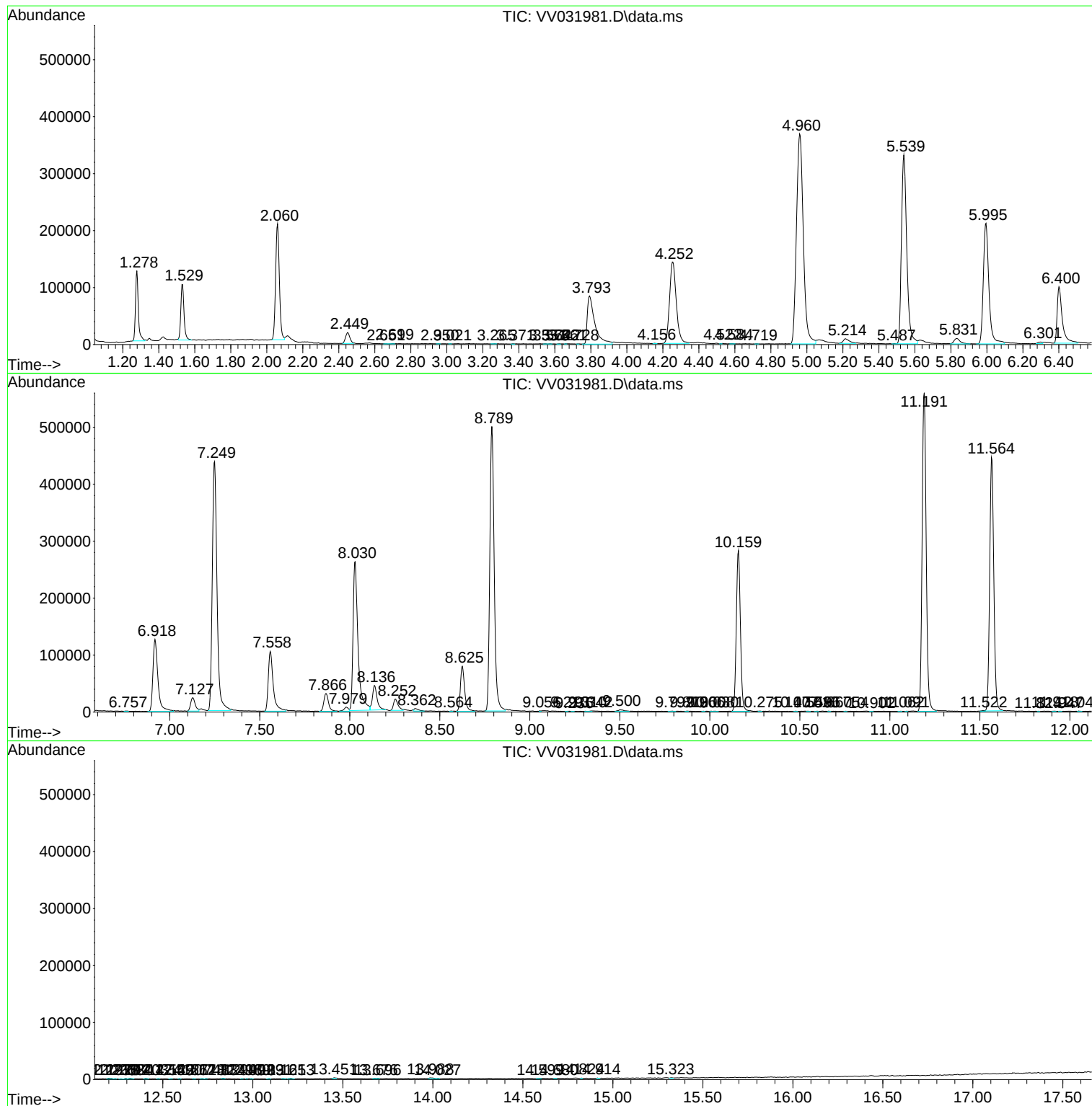
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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



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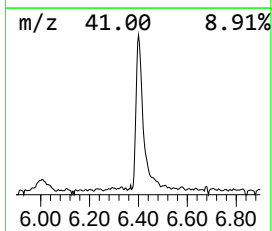
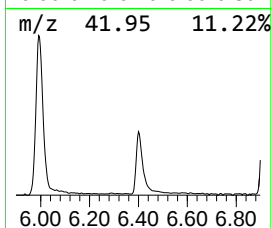
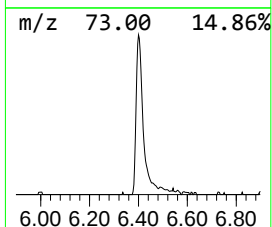
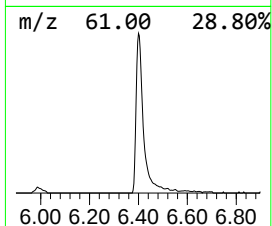
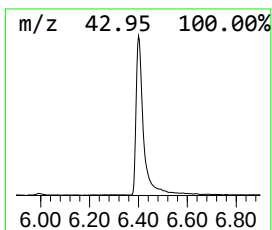
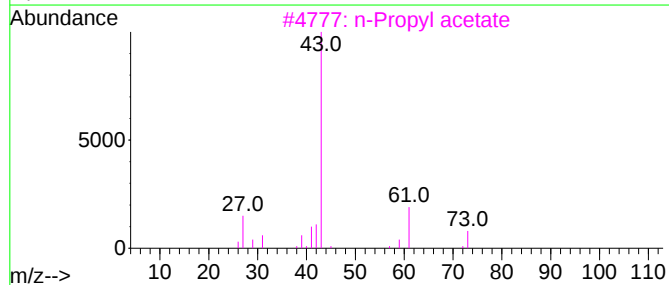
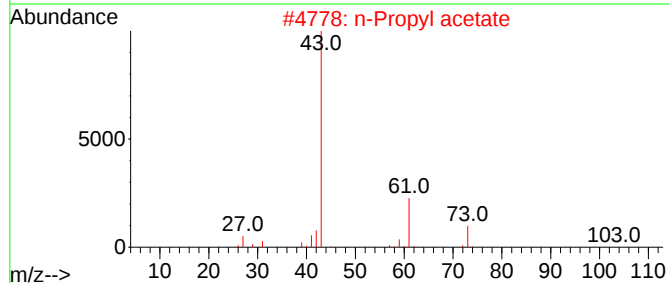
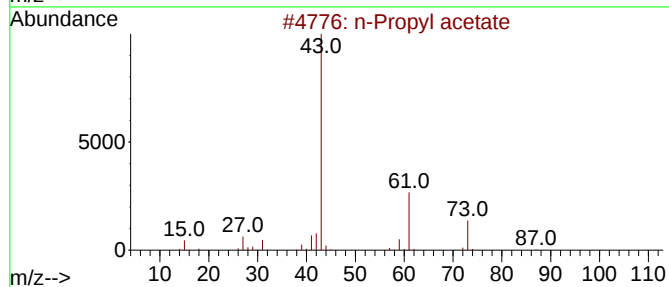
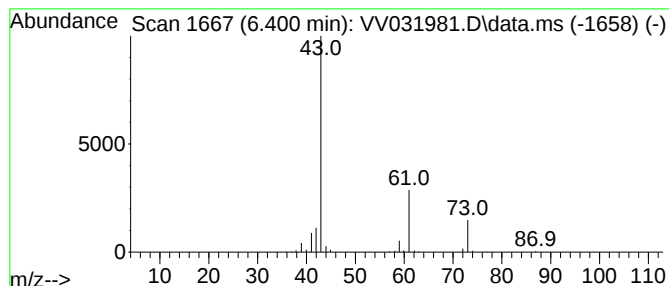
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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	14.37 ug/L	196021	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	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	56



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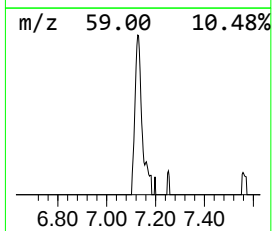
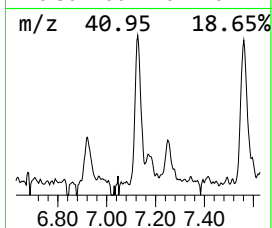
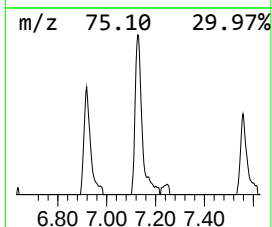
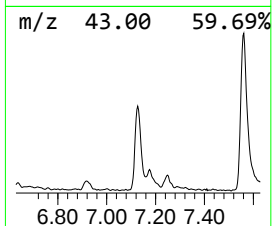
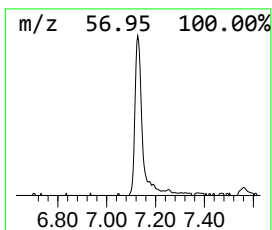
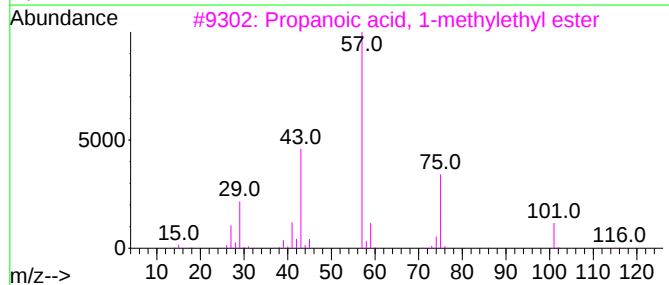
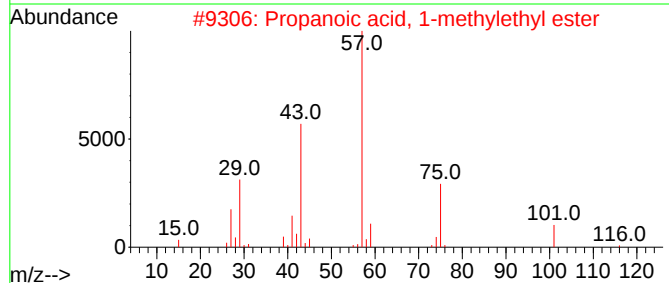
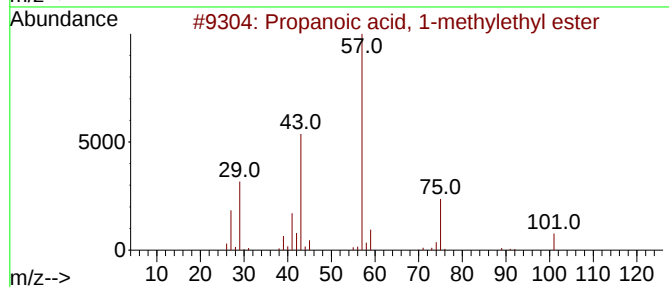
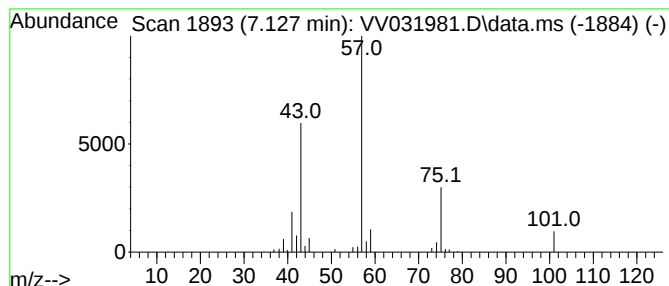
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.06 ug/L	41715	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	90
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	53



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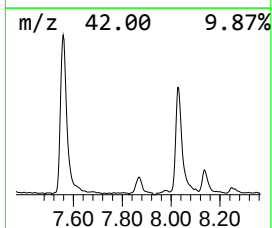
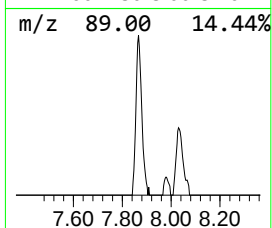
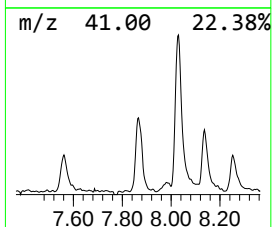
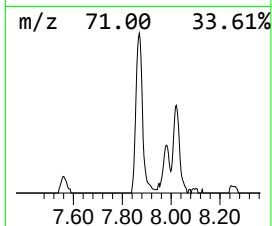
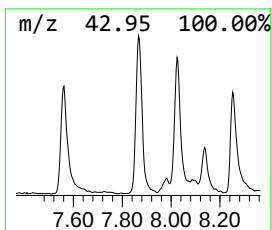
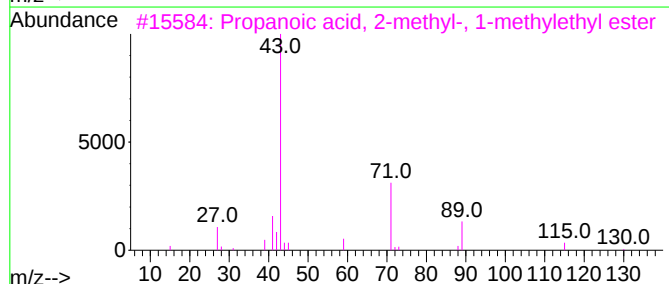
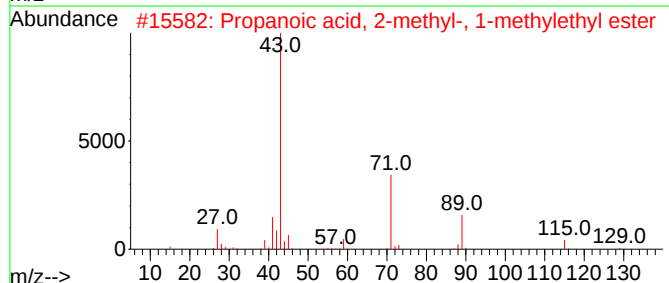
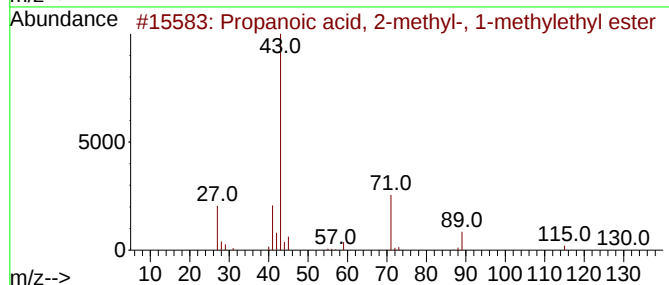
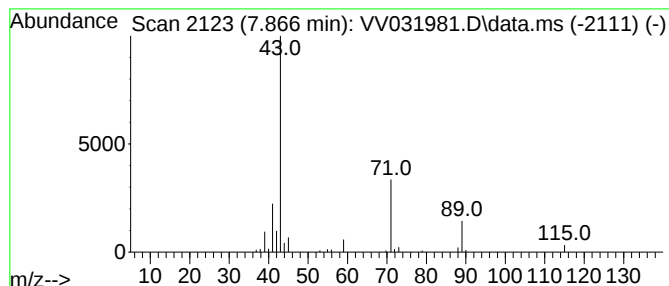
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	3.36 ug/L	56588	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	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031981.D
Acq On : 08 Sep 2023 13:29
Operator : SY/MD
Sample : 04280-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD2

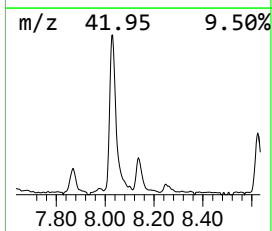
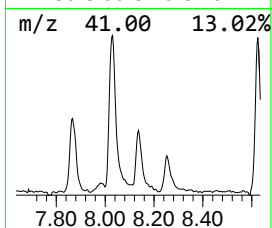
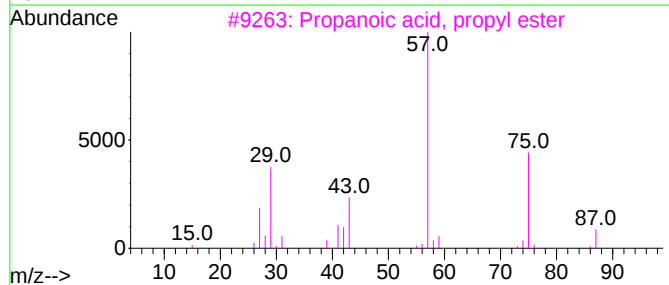
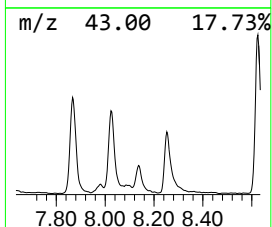
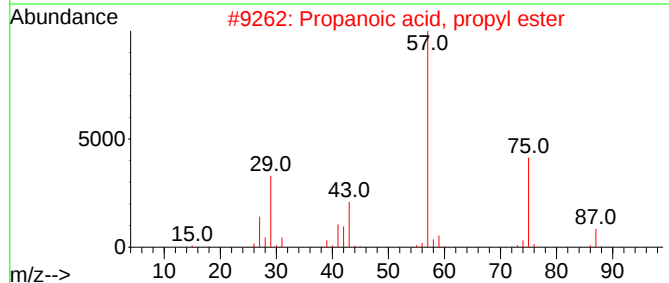
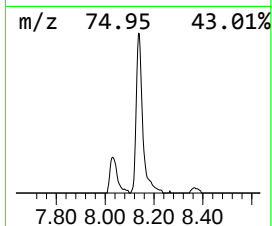
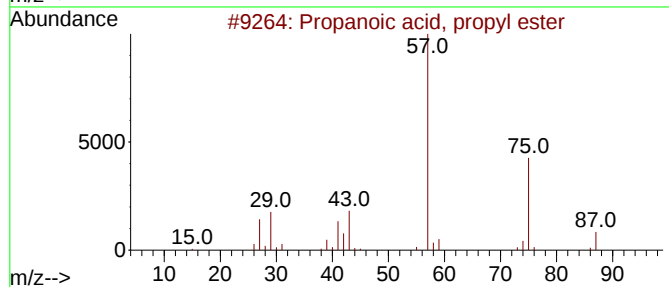
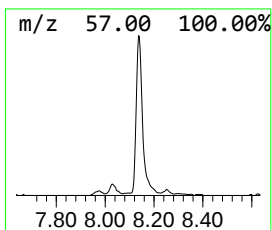
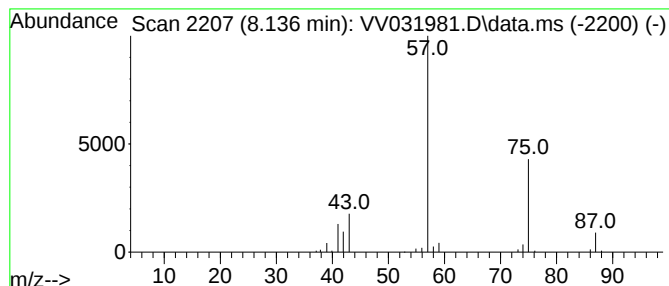
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Quant Title : VOC Analysis

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.
8.136	4.49 ug/L	75779	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	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031981.D
Acq On : 08 Sep 2023 13:29
Operator : SY/MD
Sample : 04280-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD2

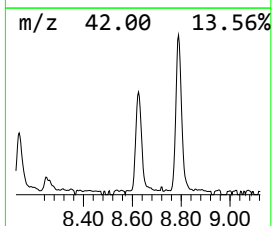
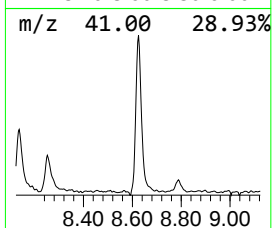
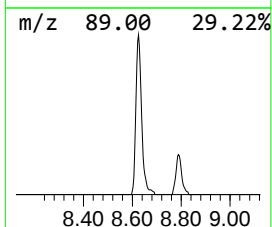
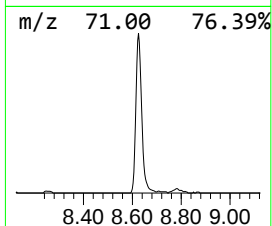
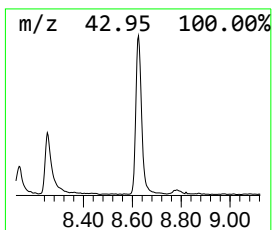
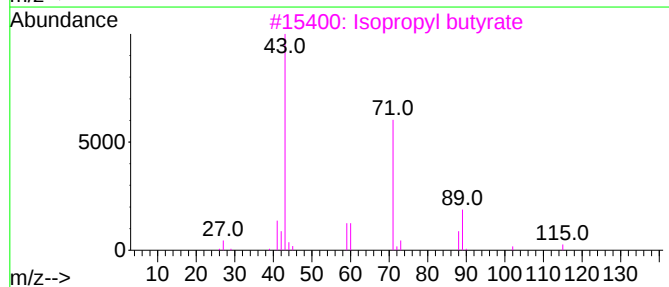
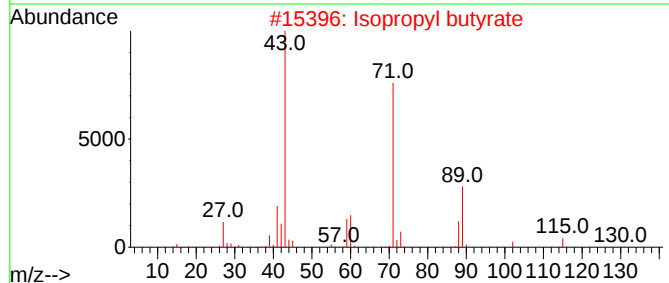
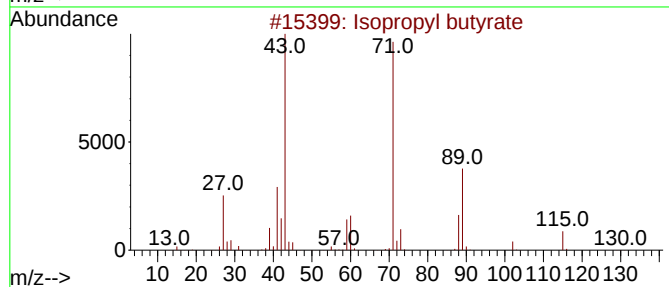
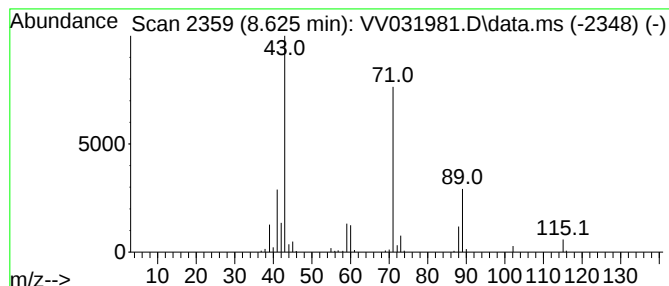
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.625	7.86 ug/L	132486	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			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090823\
Data File : VV031981.D
Acq On : 08 Sep 2023 13:29
Operator : SY/MD
Sample : 04280-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JLAD2

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	14.4	ug/L	196021	1	5.539	681901	50.0
Propanoic acid,...	7.127	3.1	ug/L	41715	1	5.539	681901	50.0
Propanoic acid,...	7.866	3.4	ug/L	56588	2	8.789	843279	50.0
Propanoic acid,...	8.136	4.5	ug/L	75779	2	8.789	843279	50.0
Isopropyl butyrate	8.625	7.9	ug/L	132486	2	8.789	843279	50.0