

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122123\
 Data File : VV033531.D
 Acq On : 21 Dec 2023 13:51
 Operator : SY/MD
 Sample : 05895-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCLS8

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\SFAMVLM121523WMA.M

Title : VOC Analysis

Signal : TIC: VV033531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.281	69	75	89	rVB	128905	134043	13.49%	1.714%
2	1.535	147	154	165	rVB	120803	141282	14.22%	1.807%
3	2.063	309	318	331	rBV	229709	332250	33.43%	4.249%
4	2.349	404	407	410	rBV5	1040	990	0.10%	0.013%
5	2.452	432	439	449	rVB3	6004	9597	0.97%	0.123%
6	2.635	493	496	499	rBV5	1203	897	0.09%	0.011%
7	2.687	509	512	514	rBV3	941	681	0.07%	0.009%
8	2.918	581	584	585	rBV3	1369	759	0.08%	0.010%
9	2.957	593	596	600	rBV4	1438	1156	0.12%	0.015%
10	3.018	613	615	617	rVB3	1249	540	0.05%	0.007%
11	3.066	627	630	634	rVB5	1238	506	0.05%	0.006%
12	3.117	640	646	647	rBV4	1308	1022	0.10%	0.013%
13	3.137	651	652	656	rBV3	835	643	0.06%	0.008%
14	3.416	735	739	744	rBV7	1214	990	0.10%	0.013%
15	3.461	751	753	755	rBV3	852	564	0.06%	0.007%
16	3.545	773	779	780	rBV6	774	775	0.08%	0.010%
17	3.645	805	810	812	rVV6	1192	999	0.10%	0.013%
18	3.722	832	834	836	rBV3	1149	541	0.05%	0.007%
19	3.751	841	843	844	rBV2	1157	457	0.05%	0.006%
20	3.786	845	854	876	rBV	53582	146437	14.74%	1.873%
21	4.249	985	998	1022	rBV	163744	417406	42.00%	5.339%
22	4.445	1056	1059	1061	rBV3	1977	1212	0.12%	0.016%
23	4.735	1145	1149	1150	rBV3	971	715	0.07%	0.009%
24	4.773	1157	1161	1166	rBV6	1495	1449	0.15%	0.019%
25	4.812	1171	1173	1175	rBV3	1224	619	0.06%	0.008%
26	4.866	1188	1190	1192	rBV2	1425	558	0.06%	0.007%
27	4.879	1192	1194	1197	rVB4	1604	786	0.08%	0.010%
28	4.892	1197	1198	1201	rBV3	1349	808	0.08%	0.010%
29	4.960	1201	1219	1241	rBV2	369767	993761	100.00%	12.710%
30	5.535	1387	1398	1429	rBV	299882	626723	63.07%	8.016%
31	5.770	1469	1471	1473	rBV3	1105	565	0.06%	0.007%
32	5.989	1527	1539	1561	rBV	227276	470774	47.37%	6.021%
33	6.265	1622	1625	1627	rBV4	1570	981	0.10%	0.013%
34	6.400	1659	1667	1691	rBV	38849	82412	8.29%	1.054%
35	6.915	1815	1827	1847	rBV	110186	211885	21.32%	2.710%
36	7.124	1885	1892	1900	rBV2	16482	24646	2.48%	0.315%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMVLM121523WMA.M
 Title : VOC Analysis

37	7.243	1919	1929	1955	rBV	413028	740598	74.52%	9.472%
38	7.554	2018	2026	2047	rBV	81913	147095	14.80%	1.881%
39	7.783	2095	2097	2101	rVB4	1036	470	0.05%	0.006%
40	7.799	2101	2102	2104	rBV2	1373	482	0.05%	0.006%
41	7.863	2113	2122	2133	rBV2	26301	44062	4.43%	0.564%
42	8.024	2164	2172	2198	rBV	183895	378531	38.09%	4.841%
43	8.506	2321	2322	2325	rBV2	1028	521	0.05%	0.007%
44	8.622	2349	2358	2376	rVB	56953	95443	9.60%	1.221%
45	8.786	2398	2409	2433	rBV	514307	856257	86.16%	10.952%
46	9.329	2575	2578	2585	rVB7	1685	1973	0.20%	0.025%
47	9.432	2608	2610	2613	rBV3	984	624	0.06%	0.008%
48	9.493	2626	2629	2631	rBV4	2371	1421	0.14%	0.018%
49	9.664	2679	2682	2683	rBV3	894	580	0.06%	0.007%
50	9.715	2690	2698	2699	rBV7	1951	2002	0.20%	0.026%
51	9.808	2723	2727	2729	rBV4	1526	1359	0.14%	0.017%
52	10.152	2822	2834	2853	rVV	299437	479093	48.21%	6.128%
53	10.262	2864	2868	2870	rBV4	1630	1098	0.11%	0.014%
54	10.532	2944	2952	2954	rBV8	1717	2235	0.22%	0.029%
55	10.545	2954	2956	2961	rVV7	1486	1109	0.11%	0.014%
56	10.570	2961	2964	2967	rVV4	851	684	0.07%	0.009%
57	10.657	2987	2991	2993	rVB4	916	720	0.07%	0.009%
58	10.677	2993	2997	3000	rVB5	1264	808	0.08%	0.010%
59	10.779	3025	3029	3032	rBV6	755	685	0.07%	0.009%
60	10.886	3059	3062	3063	rBV3	875	492	0.05%	0.006%
61	10.927	3072	3075	3079	rBV6	1340	913	0.09%	0.012%
62	11.104	3127	3130	3133	rBV4	707	582	0.06%	0.007%
63	11.185	3144	3155	3178	rBV	458722	719170	72.37%	9.198%
64	11.500	3251	3253	3255	rBV2	1255	562	0.06%	0.007%
65	11.561	3261	3272	3294	rBV	441395	698965	70.34%	8.940%
66	11.908	3375	3380	3383	rBV5	1131	1322	0.13%	0.017%
67	12.291	3496	3499	3500	rBV3	799	490	0.05%	0.006%
68	12.358	3517	3520	3523	rBV4	1012	874	0.09%	0.011%
69	12.413	3534	3537	3539	rBV4	1204	782	0.08%	0.010%
70	12.461	3550	3552	3555	rVB3	1276	660	0.07%	0.008%
71	12.477	3555	3557	3560	rVB3	863	507	0.05%	0.006%
72	12.548	3576	3579	3582	rBV5	815	609	0.06%	0.008%
73	12.577	3584	3588	3589	rBV2	989	679	0.07%	0.009%
74	12.712	3626	3630	3635	rVV6	1297	968	0.10%	0.012%
75	12.750	3640	3642	3648	rVB7	1427	992	0.10%	0.013%
76	12.779	3648	3651	3653	rBV3	951	656	0.07%	0.008%

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
 Title : VOC Analysis

77	12.876	3679	3681	3685	rBV4	1014	491	0.05%	0.006%
78	12.934	3693	3699	3701	rBV5	1514	1416	0.14%	0.018%
79	12.985	3712	3715	3716	rBV2	764	444	0.04%	0.006%
80	13.062	3736	3739	3741	rBV3	910	620	0.06%	0.008%
81	13.178	3772	3775	3777	rBV3	1212	788	0.08%	0.010%
82	13.236	3790	3793	3794	rBV3	793	490	0.05%	0.006%
83	13.278	3803	3806	3808	rBV4	1157	787	0.08%	0.010%
84	13.426	3849	3852	3856	rBV5	1746	1619	0.16%	0.021%
85	13.792	3963	3966	3969	rBV3	1638	911	0.09%	0.012%
86	13.837	3978	3980	3983	rVB2	1379	600	0.06%	0.008%
87	13.953	4013	4016	4019	rBV5	1009	846	0.09%	0.011%
88	14.107	4063	4064	4067	rVB3	1126	461	0.05%	0.006%
89	14.136	4067	4073	4075	rBV5	1323	1315	0.13%	0.017%
90	14.178	4081	4086	4087	rBV5	887	687	0.07%	0.009%
91	14.278	4113	4117	4119	rVV5	1060	763	0.08%	0.010%
92	14.307	4124	4126	4130	rVB5	1153	751	0.08%	0.010%
93	14.410	4155	4158	4163	rVB4	1646	1301	0.13%	0.017%
94	14.438	4163	4167	4170	rBV4	1492	1323	0.13%	0.017%
95	14.535	4194	4197	4198	rBV2	1145	686	0.07%	0.009%
96	14.824	4285	4287	4290	rBV4	1077	734	0.07%	0.009%
97	14.908	4311	4313	4318	rBV5	1074	757	0.08%	0.010%
98	15.114	4374	4377	4379	rBV4	1195	714	0.07%	0.009%
99	15.374	4454	4458	4461	rBV5	1607	1498	0.15%	0.019%
100	15.538	4507	4509	4513	rBV4	1592	1074	0.11%	0.014%

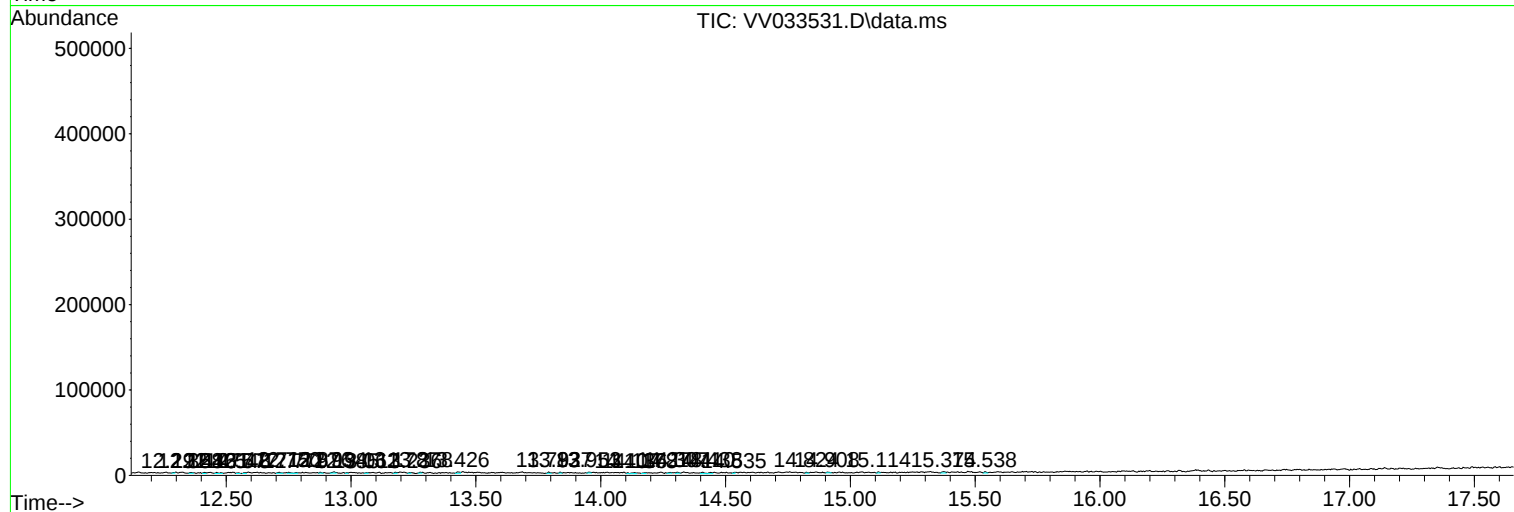
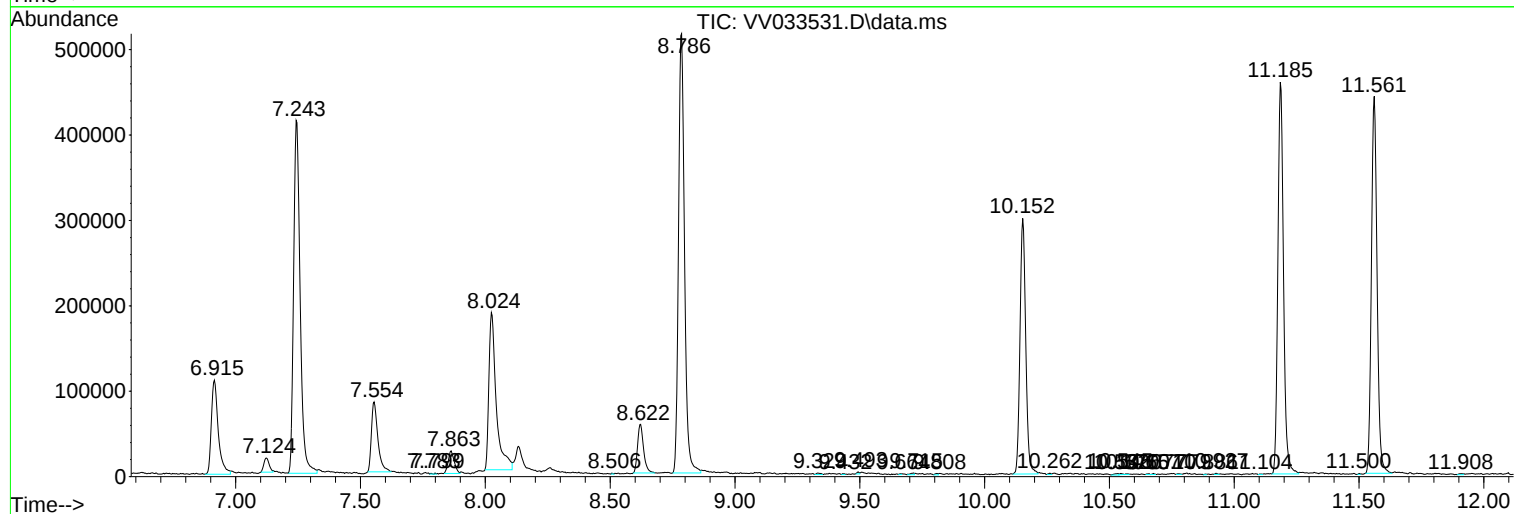
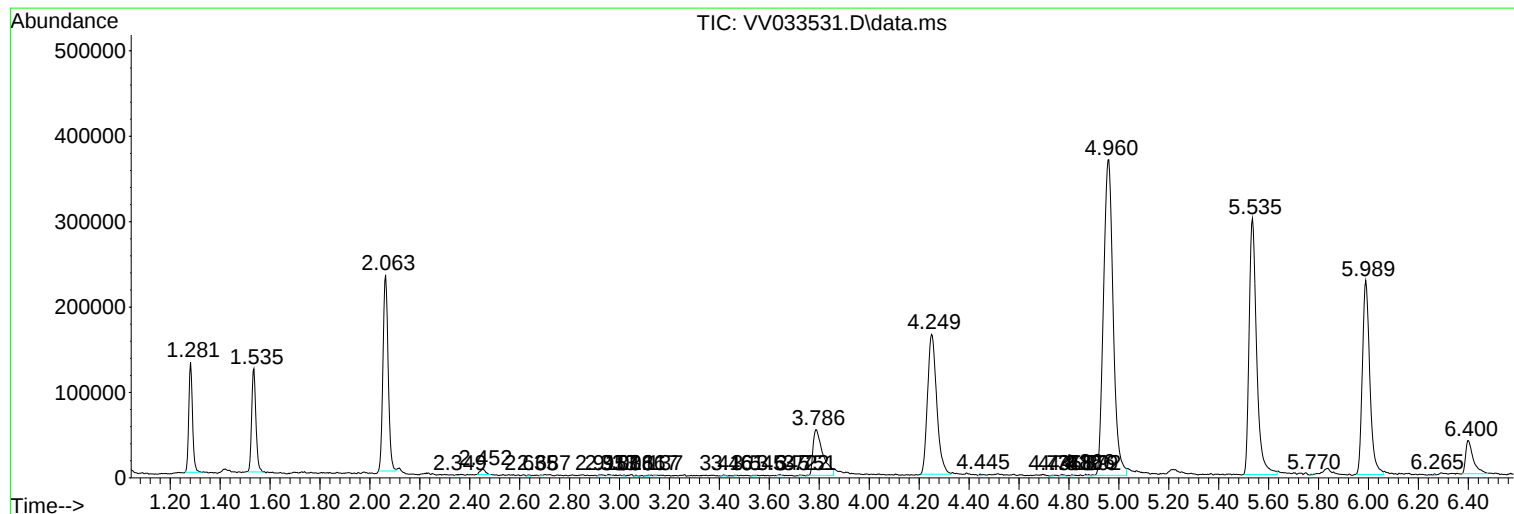
Sum of corrected areas: 7818578

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCLS8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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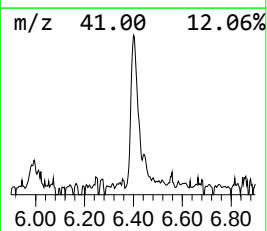
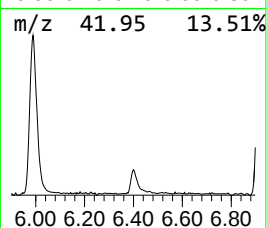
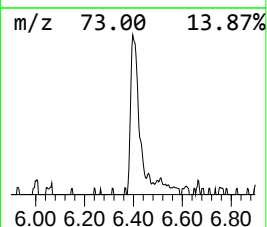
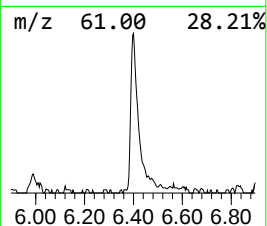
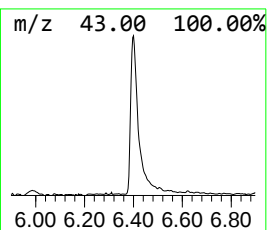
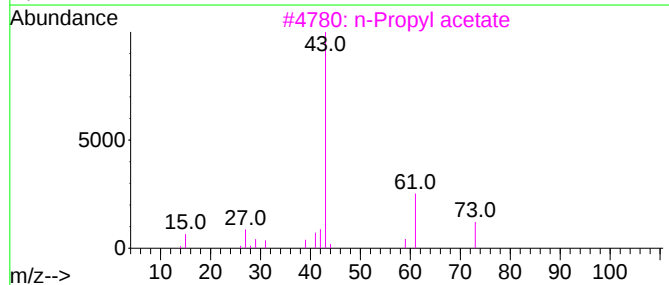
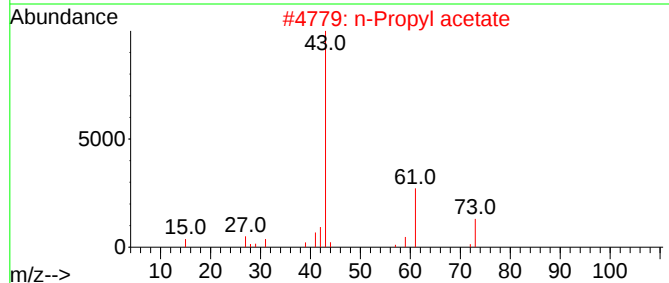
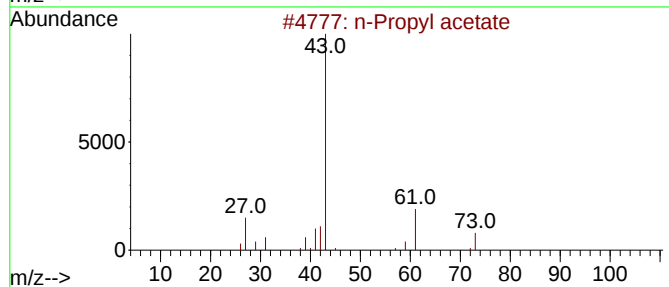
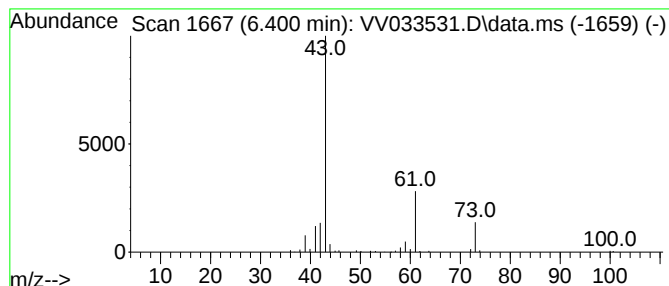
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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	6.57 ug/L	82412	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	72
2	n-Propyl acetate			102	C5H10O2	000109-60-4	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	64
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	56



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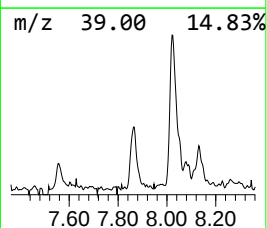
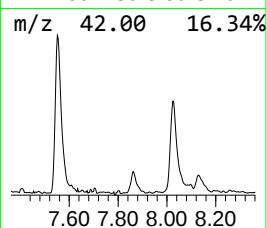
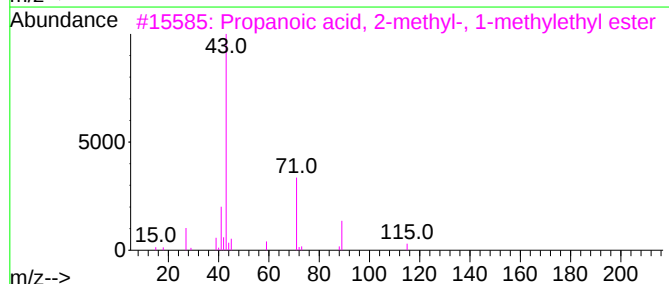
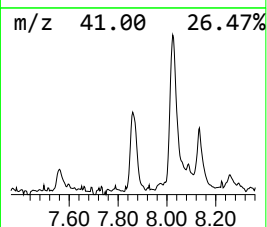
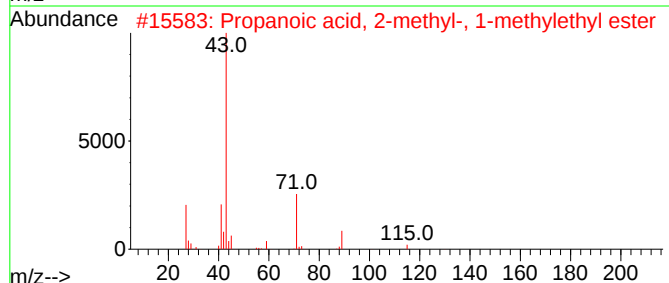
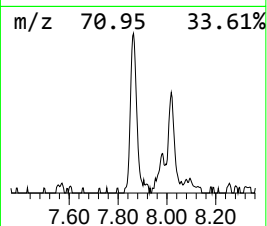
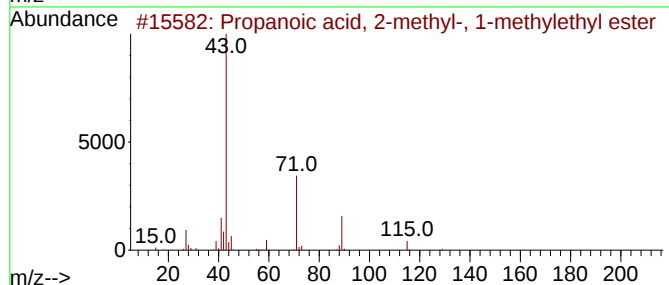
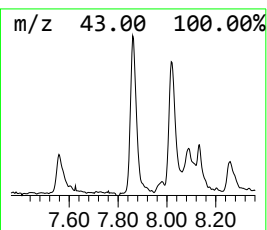
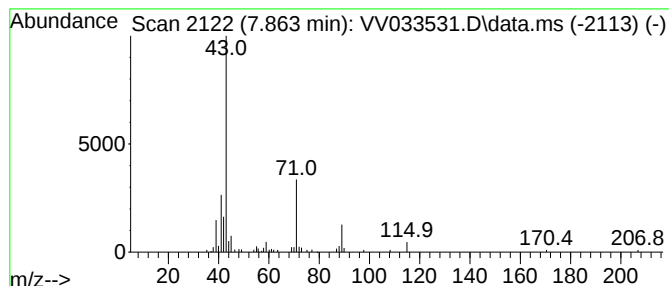
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	2.57 ug/L	44062	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	59
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50



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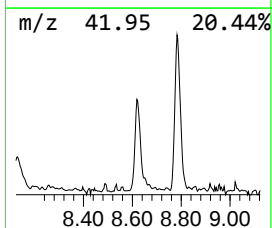
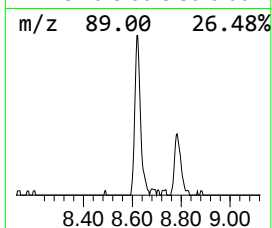
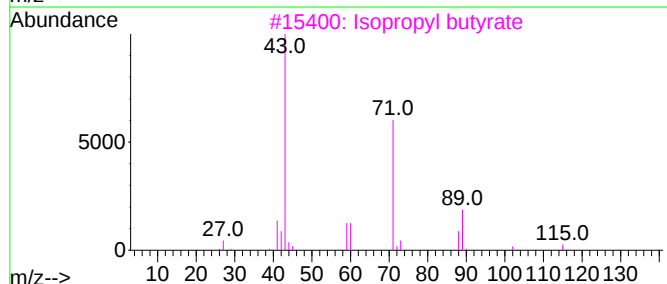
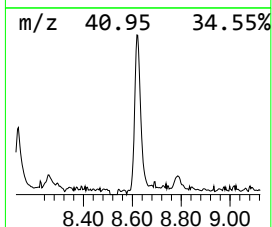
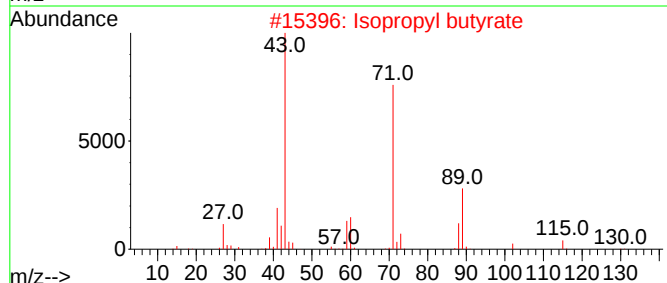
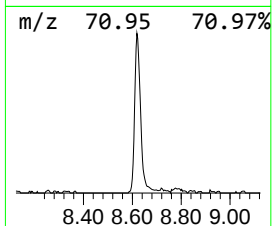
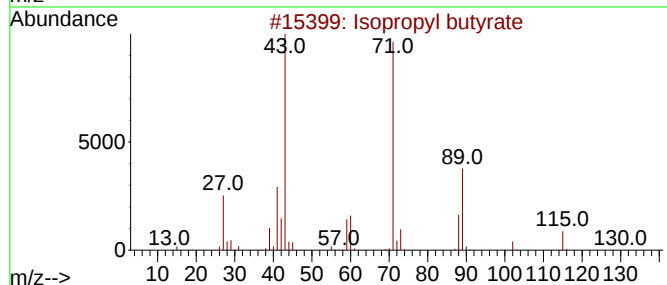
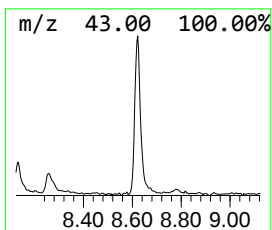
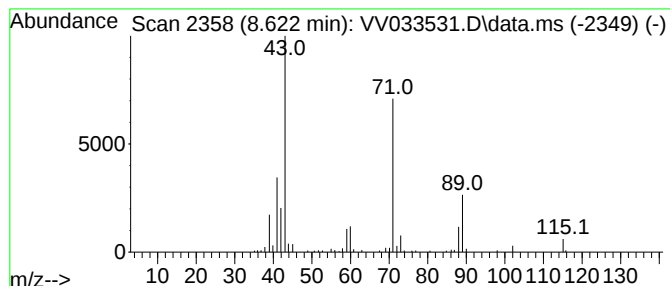
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	5.57 ug/L	95443	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	80
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	80
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122123\
Data File : VV033531.D
Acq On : 21 Dec 2023 13:51
Operator : SY/MD
Sample : 05895-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCLS8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.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	6.6	ug/L	82412	1	5.535	626723	50.0
Propanoic acid,...	7.863	2.6	ug/L	44062	2	8.786	856257	50.0
Isopropyl butyrate	8.622	5.6	ug/L	95443	2	8.786	856257	50.0