

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

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\SFAMVLM041723WMA.M
 Title : VOC Analysis

Signal : TIC: VV030613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.285	69	76	91	rVB	111051	120938	14.70%	1.699%
2	1.535	148	154	167	rVB	100214	121245	14.73%	1.704%
3	2.066	310	319	332	rBV	216504	309776	37.64%	4.352%
4	2.384	414	418	424	rBV6	2141	2703	0.33%	0.038%
5	2.455	433	440	447	rBV4	5515	8703	1.06%	0.122%
6	2.776	538	540	543	rVB4	1455	836	0.10%	0.012%
7	2.850	561	563	568	rVB5	1534	852	0.10%	0.012%
8	3.027	616	618	621	rVV4	1559	1051	0.13%	0.015%
9	3.063	624	629	632	rBV7	1222	914	0.11%	0.013%
10	3.088	634	637	641	rVB7	1427	958	0.12%	0.013%
11	3.162	658	660	665	rVB6	1547	1093	0.13%	0.015%
12	3.256	687	689	692	rVB4	2074	1146	0.14%	0.016%
13	3.346	715	717	721	rBV5	1152	774	0.09%	0.011%
14	3.403	732	735	741	rBV7	1578	1573	0.19%	0.022%
15	3.596	792	795	796	rBV2	1349	884	0.11%	0.012%
16	3.667	813	817	821	rBV7	1670	1298	0.16%	0.018%
17	3.686	821	823	826	rBV4	1245	773	0.09%	0.011%
18	3.799	849	858	876	rBV	46294	123381	14.99%	1.734%
19	4.262	988	1002	1027	rVB	134514	342524	41.62%	4.813%
20	4.493	1071	1074	1077	rBV4	1649	1141	0.14%	0.016%
21	4.667	1125	1128	1132	rBV5	946	1013	0.12%	0.014%
22	4.844	1179	1183	1186	rBV4	1459	1206	0.15%	0.017%
23	4.882	1193	1195	1201	rBV7	1111	1120	0.14%	0.016%
24	4.966	1204	1221	1242	rBV2	310941	822926	100.00%	11.562%
25	5.542	1388	1400	1425	rBV2	274556	583274	70.88%	8.195%
26	5.847	1486	1495	1506	rBV2	6487	14416	1.75%	0.203%
27	5.998	1530	1542	1560	rBV	185914	382287	46.45%	5.371%
28	6.400	1658	1667	1687	rBV2	99648	194814	23.67%	2.737%
29	6.693	1756	1758	1761	rBV4	1671	1197	0.15%	0.017%
30	6.841	1799	1804	1807	rBV6	1984	1968	0.24%	0.028%
31	6.921	1819	1829	1847	rBV	94841	178479	21.69%	2.508%
32	7.127	1883	1893	1907	rBV2	24205	46357	5.63%	0.651%
33	7.252	1920	1932	1950	rBV	367026	649370	78.91%	9.124%
34	7.561	2019	2028	2044	rBV	98682	173608	21.10%	2.439%
35	7.870	2114	2124	2136	rBV	32881	56339	6.85%	0.792%
36	8.033	2165	2175	2199	rBV2	173738	338959	41.19%	4.762%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW041823\
 Data File : VW030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Title : VOC Analysis

37	8.249	2235	2242	2258	rVB2	30280	50652	6.16%	0.712%
38	8.628	2350	2360	2377	rBV	96023	155621	18.91%	2.187%
39	8.728	2389	2391	2393	rBV3	1937	773	0.09%	0.011%
40	8.792	2400	2411	2438	rBV	447486	742638	90.24%	10.434%
41	9.127	2513	2515	2517	rBV3	1730	821	0.10%	0.012%
42	9.172	2526	2529	2531	rBV4	1817	1071	0.13%	0.015%
43	9.294	2564	2567	2571	rVB6	3075	1925	0.23%	0.027%
44	9.336	2575	2580	2584	rBV7	2016	2717	0.33%	0.038%
45	9.468	2617	2621	2622	rBV4	1177	823	0.10%	0.012%
46	9.496	2623	2630	2640	rBV10	7250	13309	1.62%	0.187%
47	9.699	2691	2693	2702	rVB8	2797	3157	0.38%	0.044%
48	9.744	2702	2707	2709	rBV5	1397	975	0.12%	0.014%
49	9.760	2709	2712	2713	rBV3	1522	755	0.09%	0.011%
50	9.802	2723	2725	2730	rVB6	1799	1141	0.14%	0.016%
51	9.824	2730	2732	2735	rBV3	1613	1159	0.14%	0.016%
52	9.966	2771	2776	2778	rBV5	2380	1861	0.23%	0.026%
53	10.098	2814	2817	2822	rBV6	1780	1119	0.14%	0.016%
54	10.162	2826	2837	2856	rVB	249680	395474	48.06%	5.556%
55	10.316	2882	2885	2887	rBV3	2292	1215	0.15%	0.017%
56	10.451	2925	2927	2929	rBV3	1565	893	0.11%	0.013%
57	10.525	2947	2950	2953	rBV4	1822	1012	0.12%	0.014%
58	10.574	2964	2965	2969	rVV4	1558	965	0.12%	0.014%
59	10.593	2969	2971	2974	rVB5	1448	797	0.10%	0.011%
60	10.612	2974	2977	2980	rVB5	1745	834	0.10%	0.012%
61	10.631	2980	2983	2986	rBV5	1894	1010	0.12%	0.014%
62	10.789	3028	3032	3036	rVV6	1058	1181	0.14%	0.017%
63	10.869	3053	3057	3058	rBV3	1595	857	0.10%	0.012%
64	10.889	3061	3063	3065	rBV3	1186	745	0.09%	0.010%
65	10.953	3081	3083	3089	rBV6	1957	1448	0.18%	0.020%
66	10.985	3089	3093	3096	rVB6	1258	996	0.12%	0.014%
67	11.001	3096	3098	3099	rBV2	1395	775	0.09%	0.011%
68	11.037	3106	3109	3112	rBV5	1593	1178	0.14%	0.017%
69	11.111	3127	3132	3135	rBV7	1188	1098	0.13%	0.015%
70	11.152	3143	3145	3147	rBV3	1695	1047	0.13%	0.015%
71	11.194	3147	3158	3173	rVV	388624	626615	76.14%	8.804%
72	11.332	3198	3201	3204	rVB4	2508	1366	0.17%	0.019%
73	11.503	3252	3254	3259	rVB5	1983	1642	0.20%	0.023%
74	11.570	3262	3275	3290	rBV	356104	569955	69.26%	8.008%
75	11.998	3406	3408	3411	rBV4	1478	858	0.10%	0.012%
76	12.136	3446	3451	3454	rBV6	1773	1749	0.21%	0.025%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

Integration Parameters: LSCINT.P
 Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs : 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Title : VOC Analysis

77	12.413	3529	3537	3538	rBV7	2027	2390	0.29%	0.034%
78	12.535	3573	3575	3578	rBV4	1263	934	0.11%	0.013%
79	12.619	3599	3601	3605	rVB5	2015	1336	0.16%	0.019%
80	12.641	3605	3608	3610	rBV5	1324	961	0.12%	0.014%
81	12.692	3622	3624	3630	rBV7	1409	1285	0.16%	0.018%
82	12.837	3662	3669	3672	rBV8	1984	2563	0.31%	0.036%
83	12.927	3694	3697	3700	rBV5	1669	782	0.10%	0.011%
84	12.943	3700	3702	3706	rVV4	1216	929	0.11%	0.013%
85	12.959	3706	3707	3713	rVB6	1283	911	0.11%	0.013%
86	13.030	3725	3729	3734	rBV7	1095	1329	0.16%	0.019%
87	13.059	3734	3738	3740	rBV4	2030	1332	0.16%	0.019%
88	13.104	3750	3752	3754	rBV3	1979	1169	0.14%	0.016%
89	13.152	3764	3767	3768	rBV3	1652	780	0.09%	0.011%
90	13.204	3780	3783	3786	rBV5	1951	1569	0.19%	0.022%
91	13.368	3830	3834	3836	rBV4	1656	1354	0.16%	0.019%
92	13.426	3847	3852	3855	rBV6	1713	1900	0.23%	0.027%
93	13.448	3855	3859	3860	rBV4	3110	1932	0.23%	0.027%
94	13.686	3928	3933	3935	rBV5	2438	2182	0.27%	0.031%
95	13.750	3949	3953	3957	rBV6	1238	1095	0.13%	0.015%
96	13.882	3992	3994	4000	rVB8	2212	1136	0.14%	0.016%
97	14.008	4032	4033	4037	rBV4	1218	982	0.12%	0.014%
98	14.631	4225	4227	4231	rBV5	1154	921	0.11%	0.013%
99	14.808	4277	4282	4284	rBV6	2194	2098	0.25%	0.029%
100	15.564	4515	4517	4521	rBV5	2064	1342	0.16%	0.019%

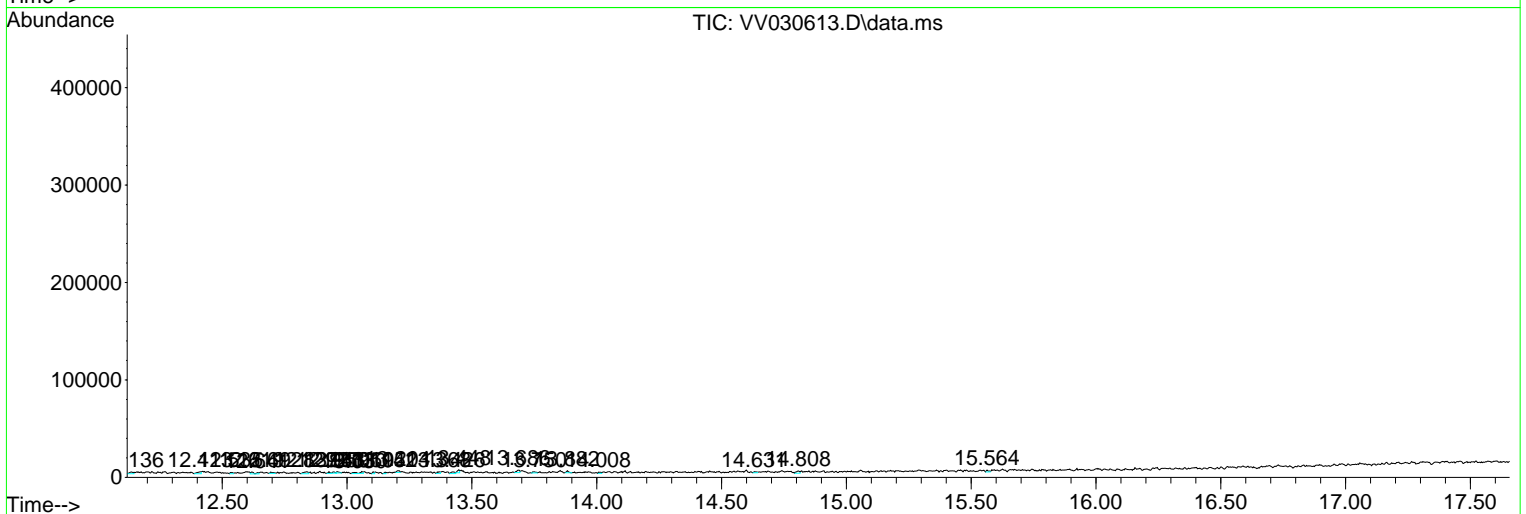
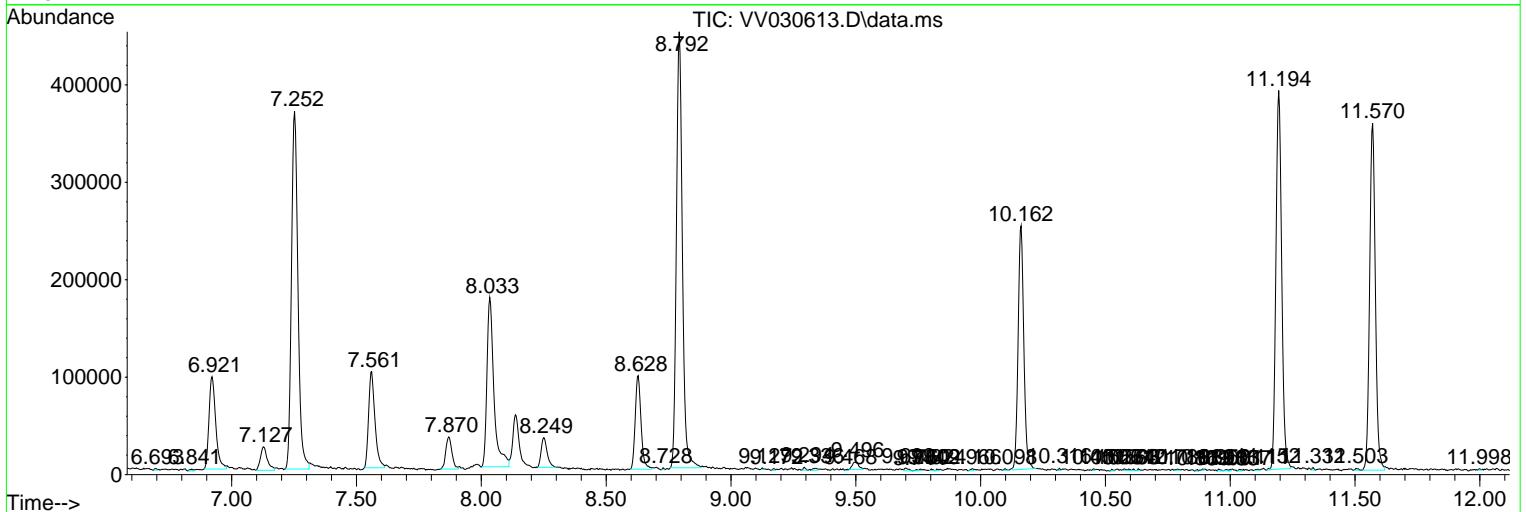
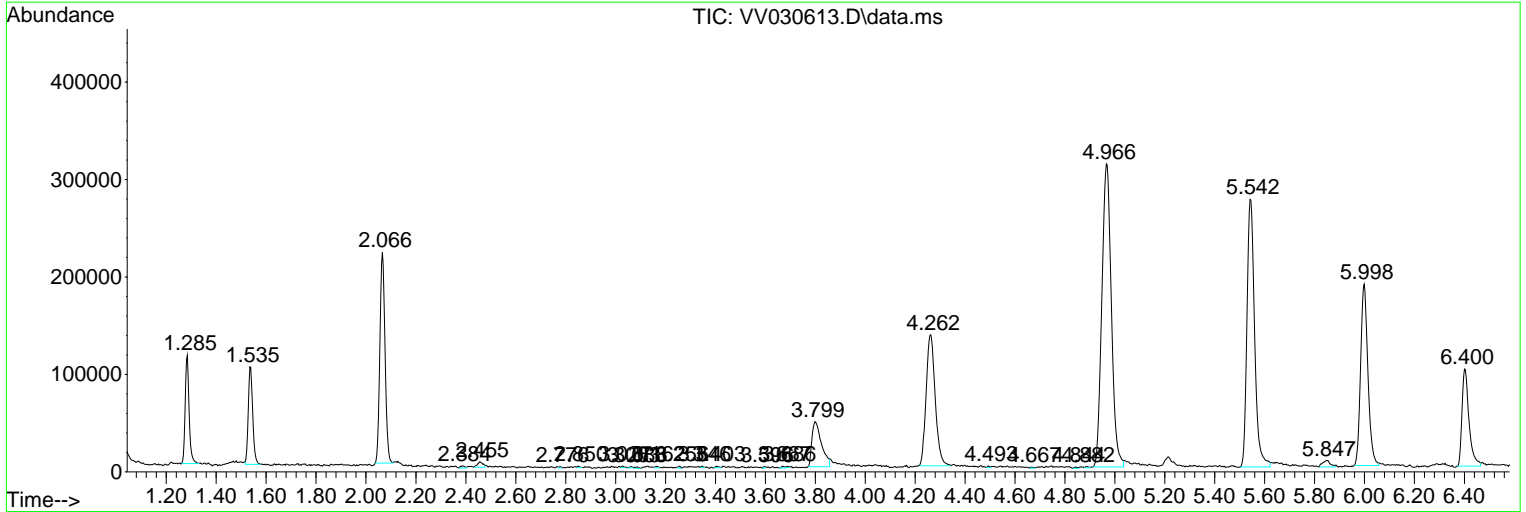
Sum of corrected areas: 7117335

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

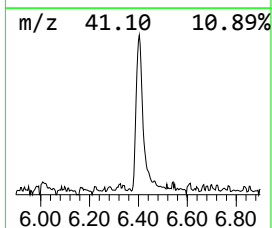
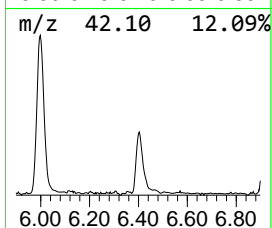
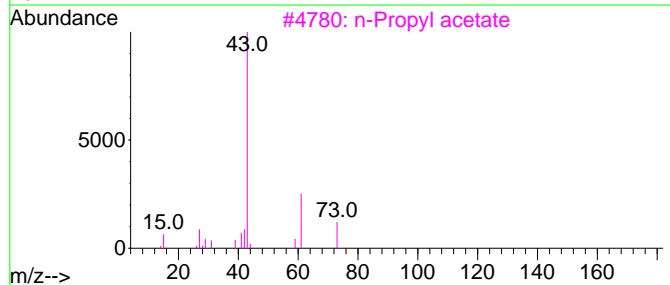
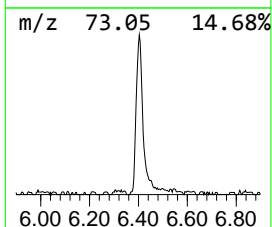
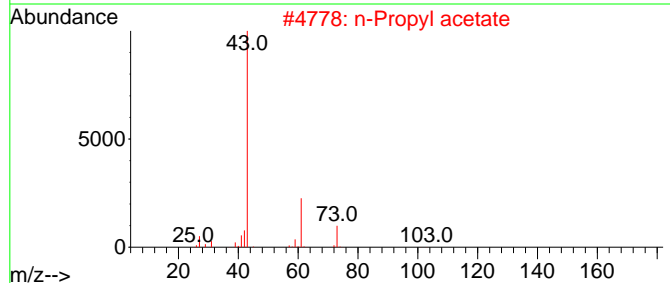
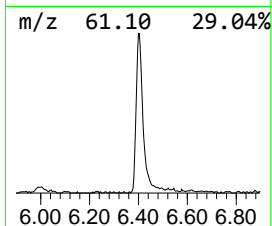
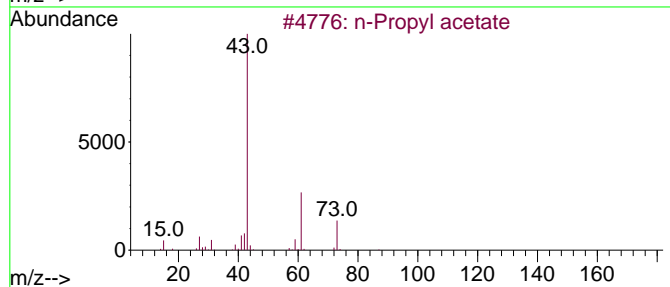
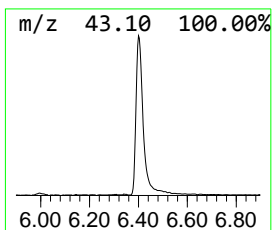
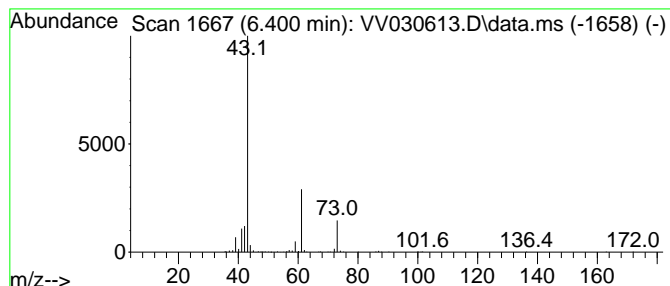
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.400	16.70 ug/L	194814	1,4-Difluorobenzene	5.542

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	56
5			n-Propyl acetate	102	C5H10O2	000109-60-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

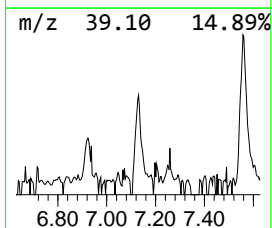
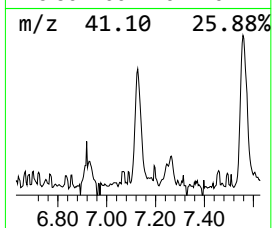
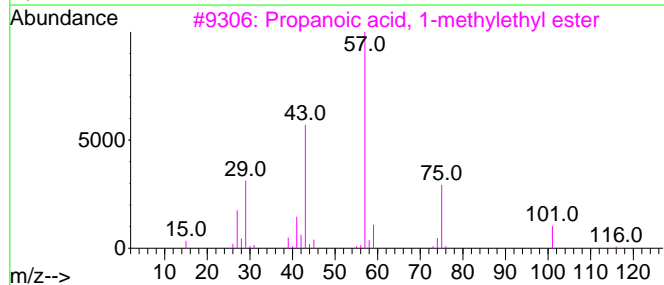
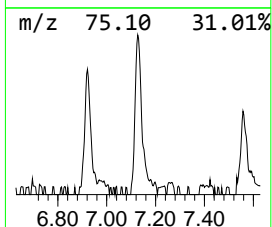
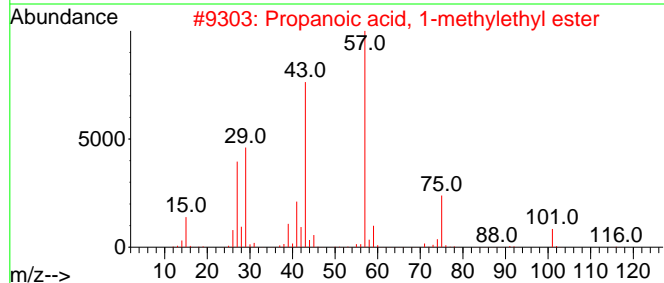
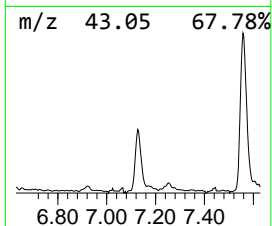
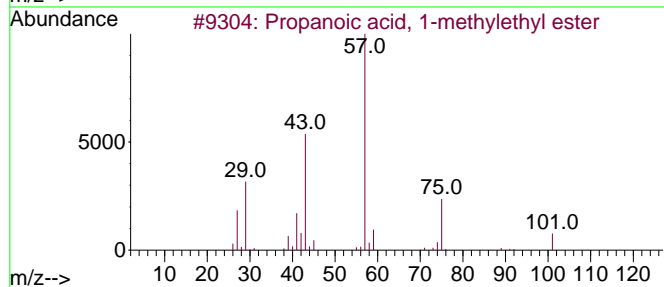
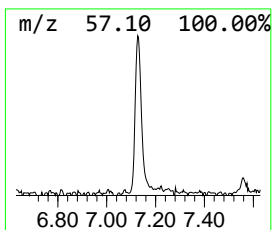
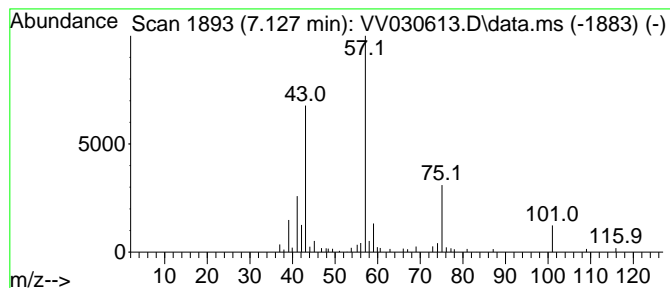
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.97 ug/L	46357	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

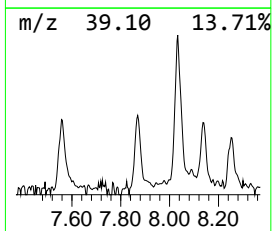
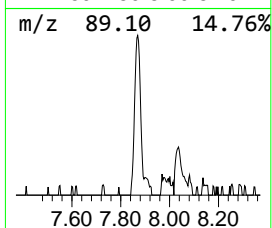
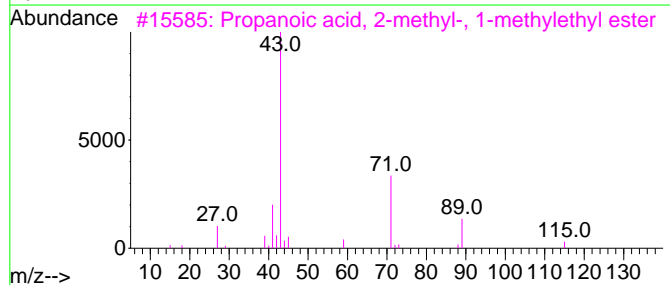
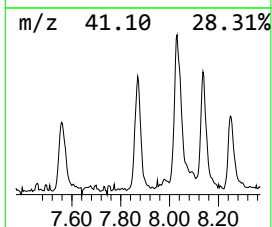
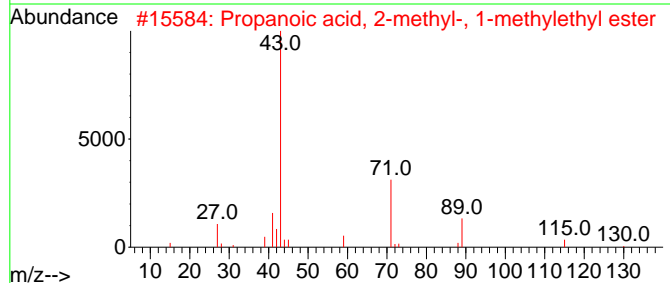
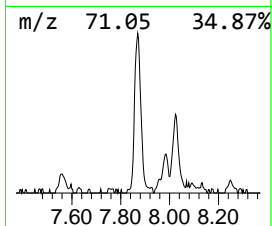
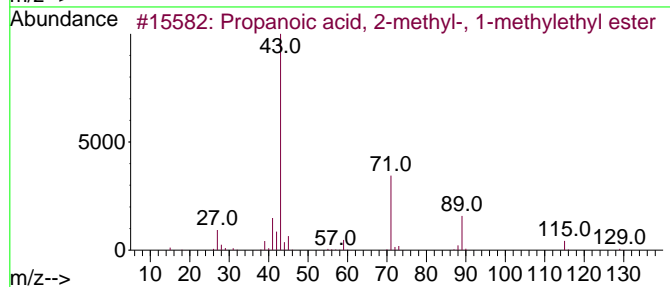
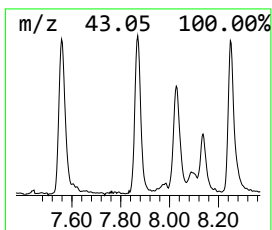
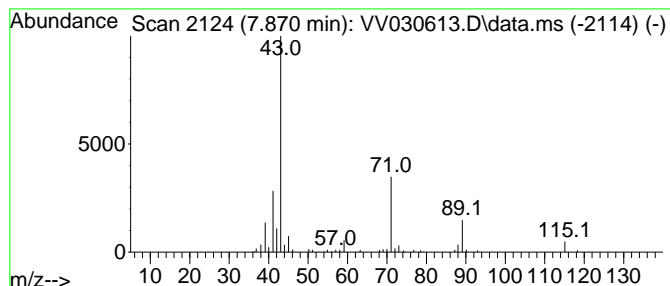
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Quant Title : VOC Analysis

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.
7.870	3.79 ug/L	56339	Chlorobenzene-d5	8.792

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-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

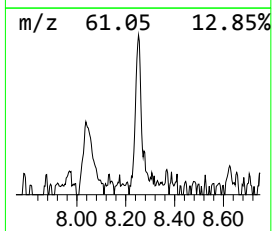
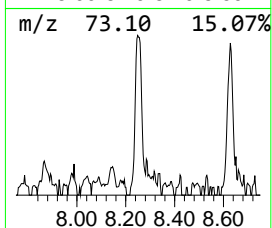
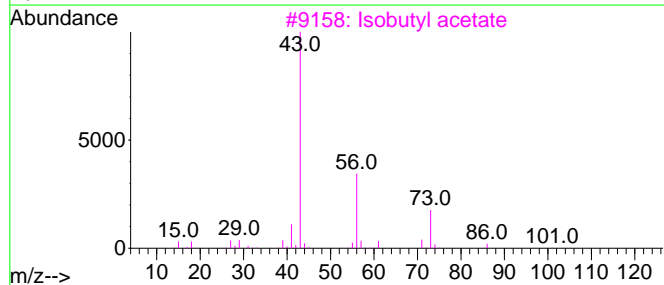
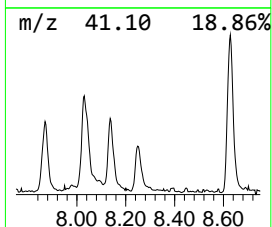
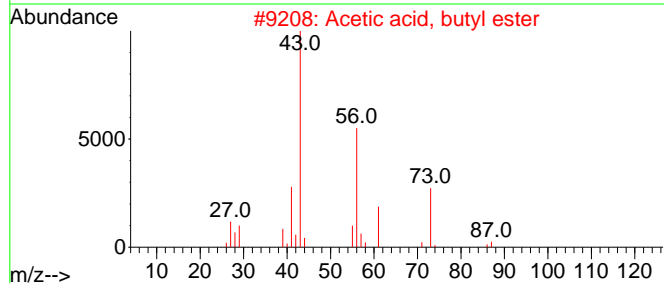
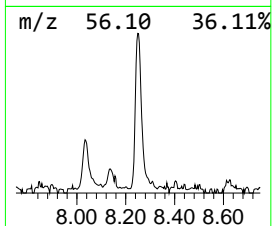
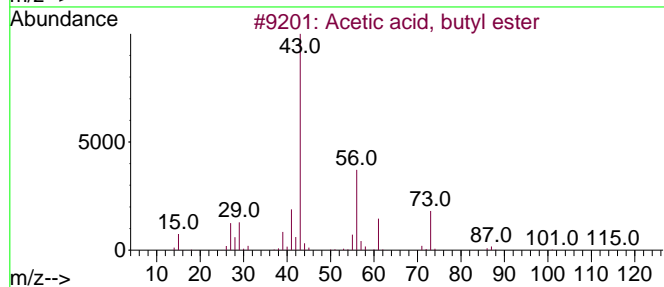
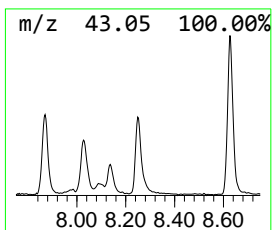
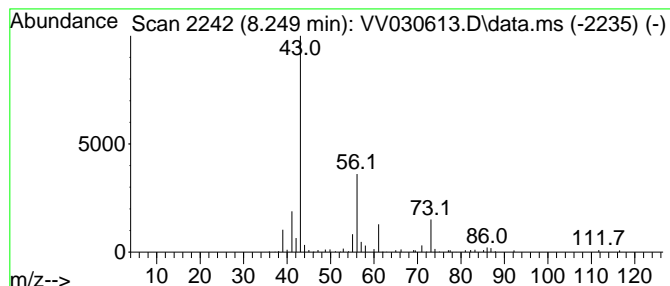
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 5 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	3.41 ug/L	50652	Chlorobenzene-d5	8.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
3			Isobutyl acetate	116	C6H12O2	000110-19-0	59
4			Isobutyl acetate	116	C6H12O2	000110-19-0	59
5			Isobutyl acetate	116	C6H12O2	000110-19-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041823\
 Data File : VV030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

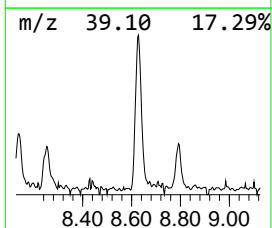
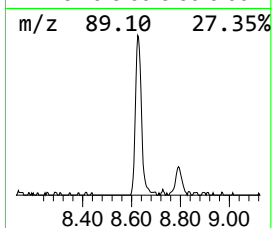
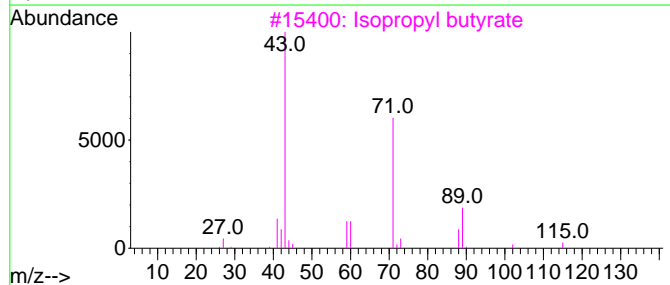
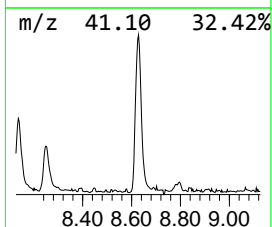
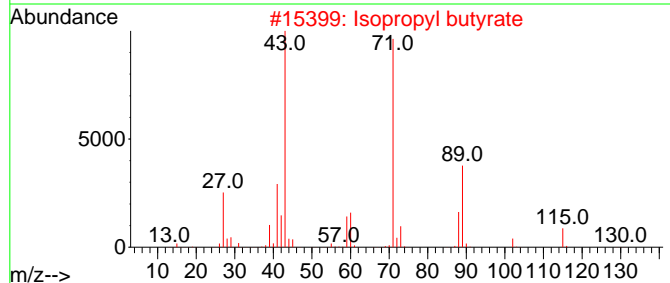
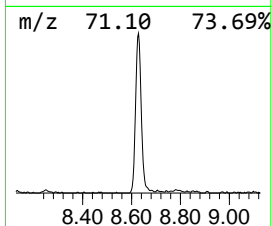
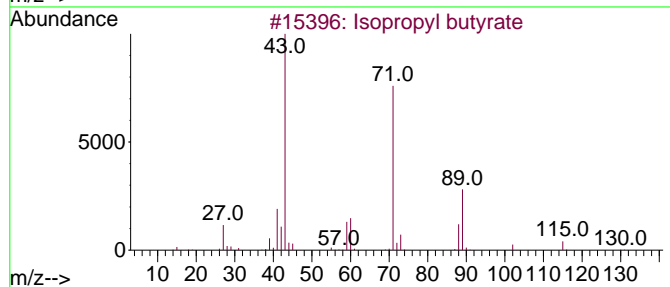
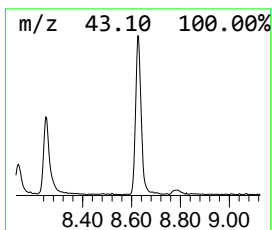
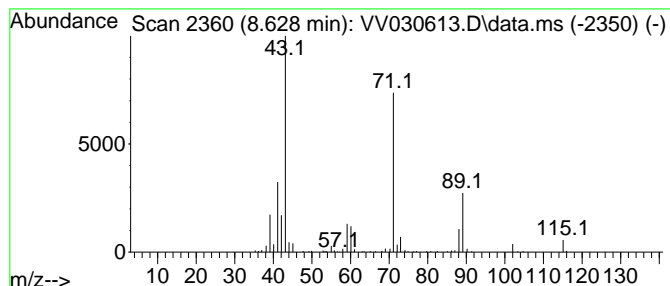
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
 Quant Title : VOC Analysis

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.
8.628	10.48 ug/L	155621	Chlorobenzene-d5	8.792

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	86
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW041823\
 Data File : VW030613.D
 Acq On : 18 Apr 2023 13:31
 Operator : SY/MD
 Sample : PB152132TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.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	16.7	ug/L	194814	1	5.542	583274	50.0
Propanoic acid,...	7.127	4.0	ug/L	46357	1	5.542	583274	50.0
Propanoic acid,...	7.870	3.8	ug/L	56339	2	8.792	742638	50.0
Acetic acid, bu...	8.249	3.4	ug/L	50652	2	8.792	742638	50.0
Isopropyl butyrate	8.628	10.5	ug/L	155621	2	8.792	742638	50.0