

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055768.D
 Acq On : 16 Oct 2023 13:37
 Operator : MD/SY
 Sample : PB156380TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB380

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_U\Method\SFAMULM101023WMA.M

Title : VOC Analysis

Signal : TIC: VU055768.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	109	rBV	207832	243244	12.53%	1.608%
2	1.891	179	187	206	rVB	177561	259488	13.37%	1.715%
3	2.486	369	372	377	rBV4	612	591	0.03%	0.004%
4	2.560	382	395	409	rBV	358883	592634	30.53%	3.917%
5	2.779	458	463	468	rBV4	914	1144	0.06%	0.008%
6	2.850	482	485	489	rBV2	647	515	0.03%	0.003%
7	2.949	513	516	519	rVB4	571	323	0.02%	0.002%
8	2.969	520	522	528	rVB2	732	693	0.04%	0.005%
9	2.994	528	530	533	rBV2	429	356	0.02%	0.002%
10	3.036	534	543	559	rVB3	10270	19990	1.03%	0.132%
11	3.178	575	587	599	rBV	14959	33699	1.74%	0.223%
12	3.624	720	726	728	rBV2	339	339	0.02%	0.002%
13	3.814	780	785	788	rVB2	361	334	0.02%	0.002%
14	3.833	788	791	793	rBV2	776	593	0.03%	0.004%
15	3.969	825	833	837	rVV3	456	425	0.02%	0.003%
16	4.001	837	843	848	rVB2	491	491	0.03%	0.003%
17	4.049	855	858	862	rVB	488	328	0.02%	0.002%
18	4.081	862	868	872	rBV2	389	416	0.02%	0.003%
19	4.512	997	1002	1006	rBV2	379	410	0.02%	0.003%
20	4.615	1023	1034	1078	rBV	135143	368732	18.99%	2.437%
21	4.895	1118	1121	1125	rVB3	666	508	0.03%	0.003%
22	5.055	1155	1171	1198	rBV	351575	788603	40.62%	5.212%
23	5.277	1238	1240	1247	rVB5	798	649	0.03%	0.004%
24	5.325	1247	1255	1257	rVV8	1461	1630	0.08%	0.011%
25	5.351	1261	1263	1268	rVB4	1126	709	0.04%	0.005%
26	5.721	1356	1378	1404	rBV2	695619	1941432	100.00%	12.831%
27	5.911	1429	1437	1451	rVB3	12653	24638	1.27%	0.163%
28	6.020	1466	1471	1472	rBV3	536	429	0.02%	0.003%
29	6.129	1501	1505	1509	rVB3	447	366	0.02%	0.002%
30	6.181	1519	1521	1528	rVB3	574	470	0.02%	0.003%
31	6.245	1528	1541	1571	rBV	504444	992447	51.12%	6.559%
32	6.528	1618	1629	1644	rBV4	19534	39442	2.03%	0.261%
33	6.589	1644	1648	1652	rBV5	722	811	0.04%	0.005%
34	6.685	1664	1678	1701	rBV	445808	879283	45.29%	5.811%
35	6.882	1736	1739	1741	rBV3	489	385	0.02%	0.003%
36	6.930	1744	1754	1773	rBV2	6749	17077	0.88%	0.113%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055768.D
 Acq On : 16 Oct 2023 13:37
 Operator : MD/SY
 Sample : PB156380TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB380

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_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	7.036	1777	1787	1819	rBV	139127	262782	13.54%	1.737%
38	7.187	1825	1834	1850	rBV6	6218	12803	0.66%	0.085%
39	7.325	1875	1877	1880	rBV2	585	427	0.02%	0.003%
40	7.374	1890	1892	1899	rVB2	658	587	0.03%	0.004%
41	7.560	1935	1950	1970	rBV	230867	421605	21.72%	2.786%
42	7.695	1985	1992	1994	rBV4	3636	3979	0.20%	0.026%
43	7.737	1996	2005	2016	rVB	30995	54368	2.80%	0.359%
44	7.894	2041	2054	2089	rBV	840465	1486694	76.58%	9.826%
45	8.110	2117	2121	2125	rVB3	588	490	0.03%	0.003%
46	8.174	2125	2141	2166	rBV2	181865	365294	18.82%	2.414%
47	8.460	2220	2230	2248	rBV	41624	71081	3.66%	0.470%
48	8.576	2251	2266	2272	rBV9	7948	17699	0.91%	0.117%
49	8.634	2272	2284	2305	rVV3	350392	837272	43.13%	5.534%
50	8.724	2307	2312	2336	rVV	75946	133407	6.87%	0.882%
51	8.833	2338	2346	2361	rVB	40133	67622	3.48%	0.447%
52	8.991	2389	2395	2399	rBV3	883	861	0.04%	0.006%
53	9.010	2399	2401	2405	rVB3	748	456	0.02%	0.003%
54	9.045	2409	2412	2414	rBV	687	338	0.02%	0.002%
55	9.074	2419	2421	2424	rBV2	595	390	0.02%	0.003%
56	9.209	2450	2463	2480	rBV	119215	197537	10.17%	1.306%
57	9.328	2497	2500	2502	rBV	643	382	0.02%	0.003%
58	9.367	2508	2512	2514	rVV4	1420	1288	0.07%	0.009%
59	9.415	2514	2527	2554	rVV	773509	1298140	66.87%	8.580%
60	9.650	2594	2600	2608	rVB6	1455	1900	0.10%	0.013%
61	9.856	2660	2664	2666	rBV2	517	386	0.02%	0.003%
62	9.907	2675	2680	2681	rBV2	543	365	0.02%	0.002%
63	9.923	2681	2685	2687	rBV3	924	703	0.04%	0.005%
64	10.074	2723	2732	2746	rBV4	7736	14553	0.75%	0.096%
65	10.152	2751	2756	2759	rVV2	688	604	0.03%	0.004%
66	10.251	2782	2787	2790	rBV2	383	348	0.02%	0.002%
67	10.325	2807	2810	2812	rBV	385	305	0.02%	0.002%
68	10.435	2839	2844	2850	rBV	380	405	0.02%	0.003%
69	10.480	2850	2858	2860	rBV	624	687	0.04%	0.005%
70	10.579	2885	2889	2895	rVB2	340	370	0.02%	0.002%
71	10.650	2906	2911	2914	rBV2	482	454	0.02%	0.003%
72	10.708	2917	2929	2930	rBV2	495	784	0.04%	0.005%
73	10.753	2931	2943	2965	rVV	657904	1079197	55.59%	7.133%
74	10.971	3006	3011	3013	rBV2	485	405	0.02%	0.003%
75	11.023	3023	3027	3034	rBV3	365	573	0.03%	0.004%
76	11.129	3057	3060	3064	rBV3	543	403	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055768.D
 Acq On : 16 Oct 2023 13:37
 Operator : MD/SY
 Sample : PB156380TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB380

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_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

77	11.303	3110	3114	3121	rBV2	697	891	0.05%	0.006%
78	11.377	3131	3137	3139	rBV2	583	499	0.03%	0.003%
79	11.402	3142	3145	3150	rVV	585	574	0.03%	0.004%
80	11.750	3248	3253	3256	rBV2	496	500	0.03%	0.003%
81	11.811	3260	3272	3303	rBV	742394	1209953	62.32%	7.997%
82	12.065	3349	3351	3355	rVB	869	524	0.03%	0.003%
83	12.090	3355	3359	3364	rBV2	604	600	0.03%	0.004%
84	12.190	3376	3390	3419	rBV	813407	1355604	69.82%	8.959%
85	12.332	3431	3434	3437	rBV4	980	702	0.04%	0.005%
86	12.637	3526	3529	3532	rBV	507	307	0.02%	0.002%
87	12.868	3596	3601	3602	rBV3	612	488	0.03%	0.003%
88	13.029	3649	3651	3655	rBV3	411	334	0.02%	0.002%
89	13.139	3680	3685	3689	rBV2	583	728	0.04%	0.005%
90	13.724	3864	3867	3870	rBV	598	516	0.03%	0.003%
91	13.769	3878	3881	3885	rBV	469	480	0.02%	0.003%
92	13.791	3885	3888	3892	rVV2	460	358	0.02%	0.002%
93	14.122	3986	3991	3996	rBV4	1344	1490	0.08%	0.010%
94	14.145	3996	3998	4001	rVV3	682	416	0.02%	0.003%
95	14.444	4088	4091	4097	rVB3	587	531	0.03%	0.004%
96	14.849	4214	4217	4218	rBV2	503	314	0.02%	0.002%
97	15.026	4269	4272	4273	rBV2	702	414	0.02%	0.003%
98	15.161	4311	4314	4316	rBV2	804	560	0.03%	0.004%
99	15.277	4347	4350	4354	rBV4	742	560	0.03%	0.004%
100	16.016	4578	4580	4590	rBV9	1369	1756	0.09%	0.012%

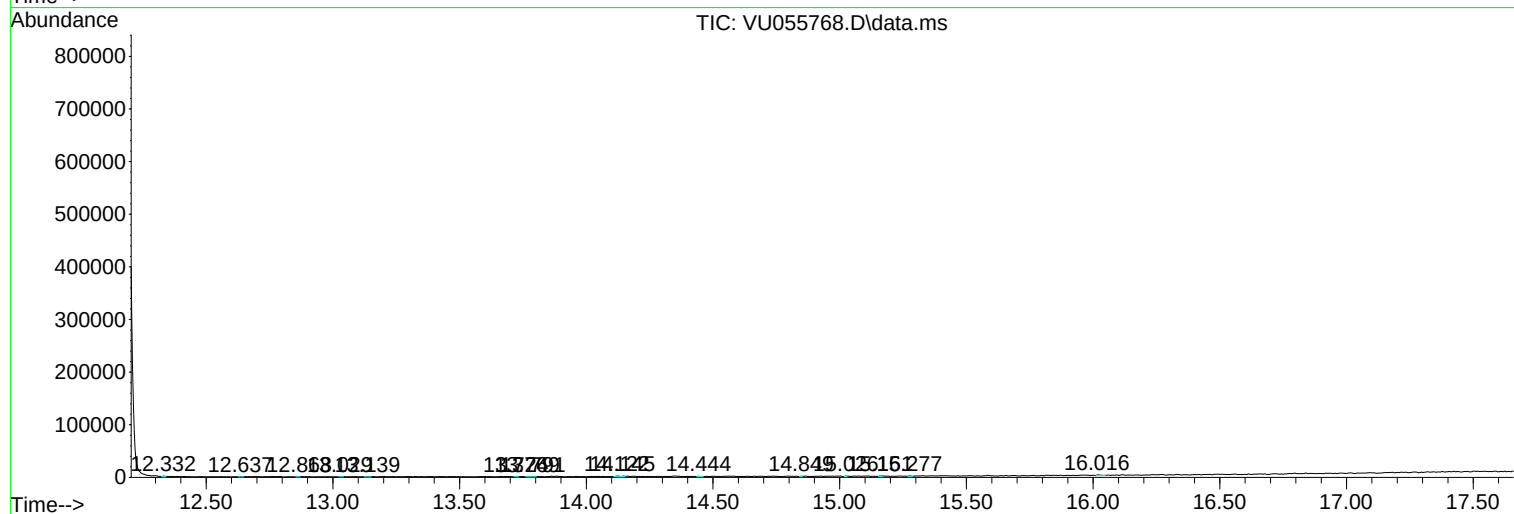
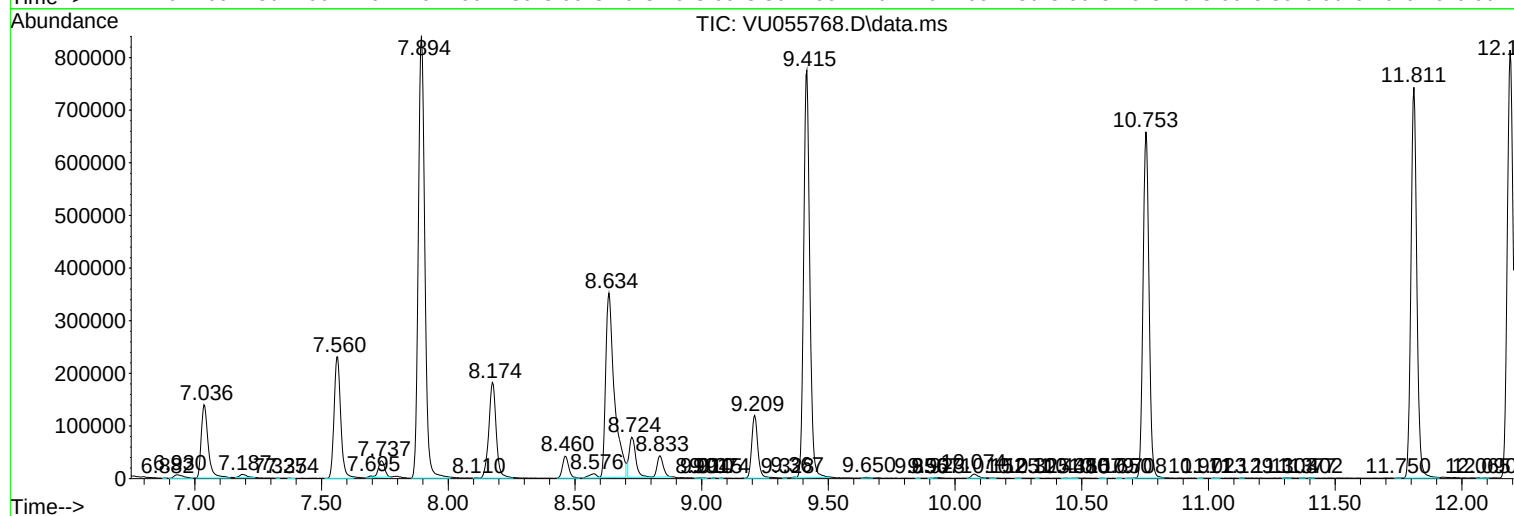
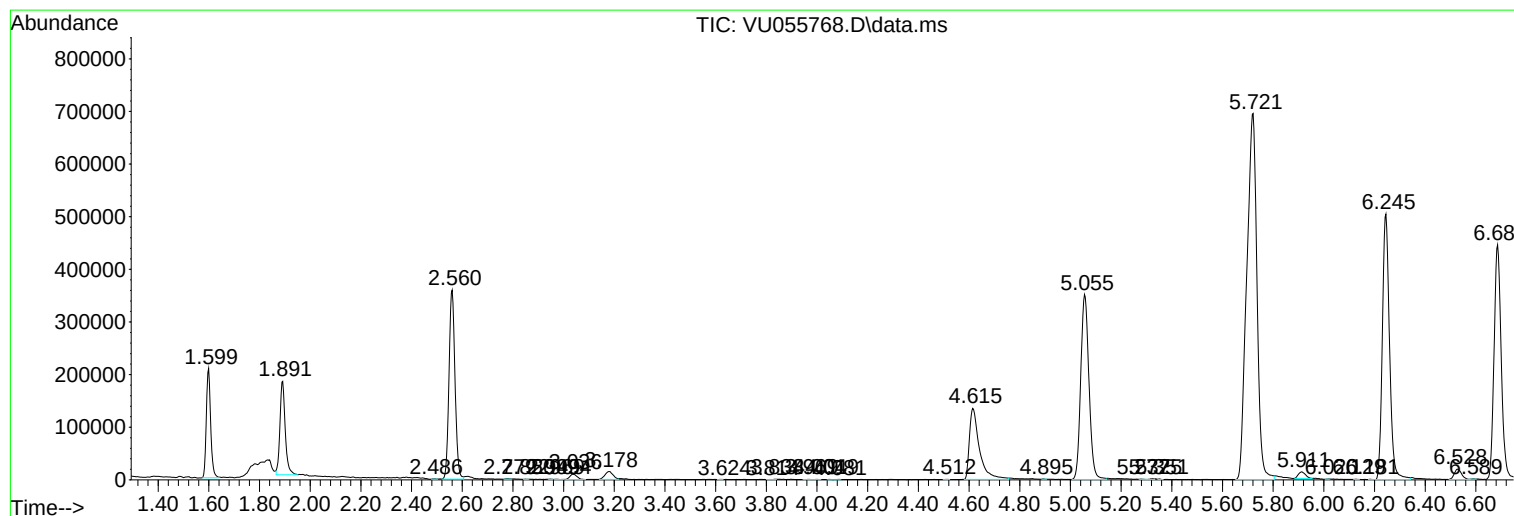
Sum of corrected areas: 15130667

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

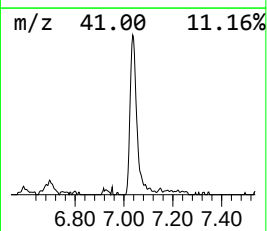
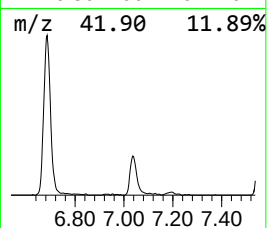
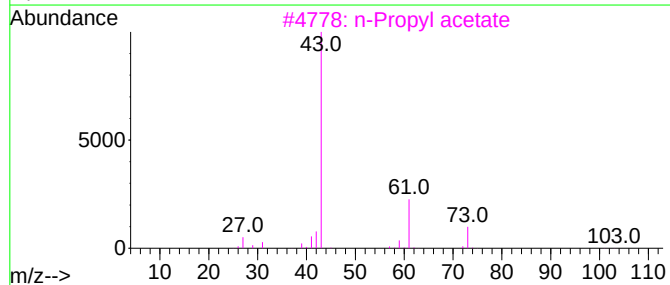
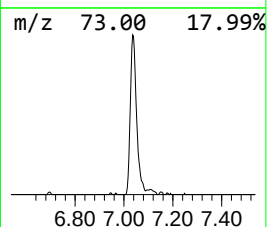
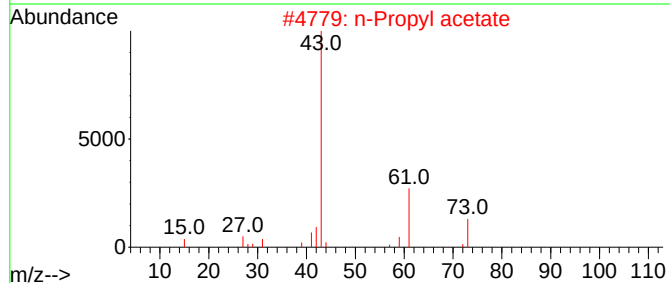
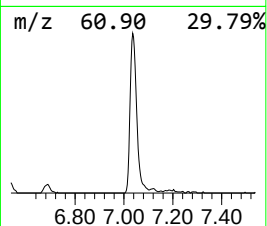
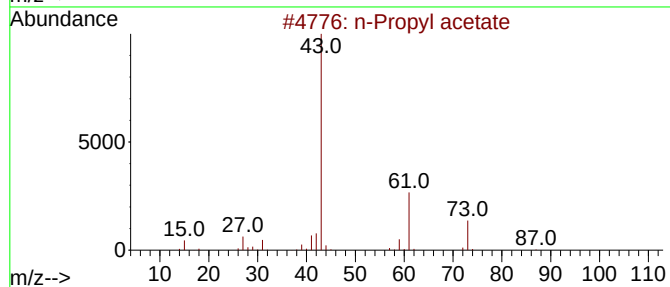
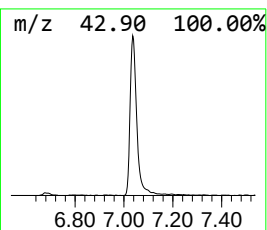
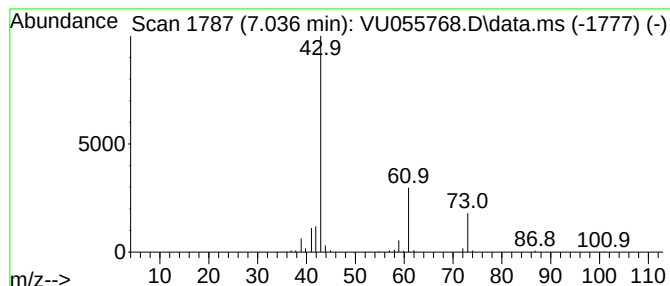
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
7.036	13.24 ug/L	262782	1,4-Difluorobenzene	6.245

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	72
5	Isopropyl acetate			102	C5H10O2	000108-21-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

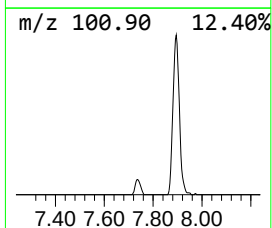
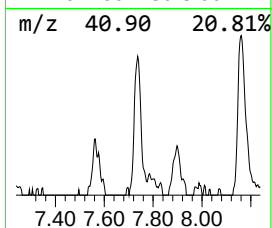
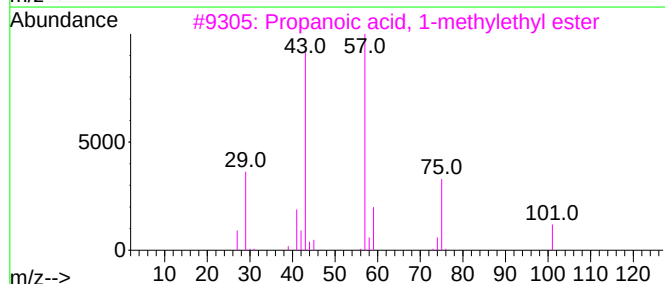
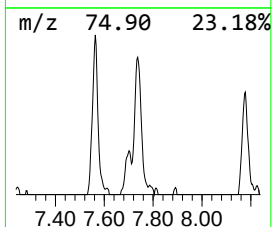
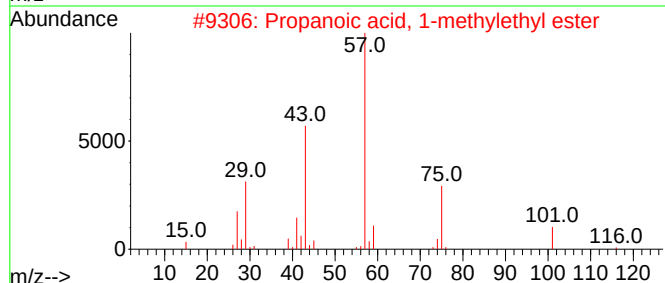
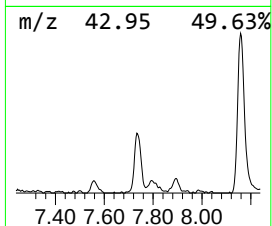
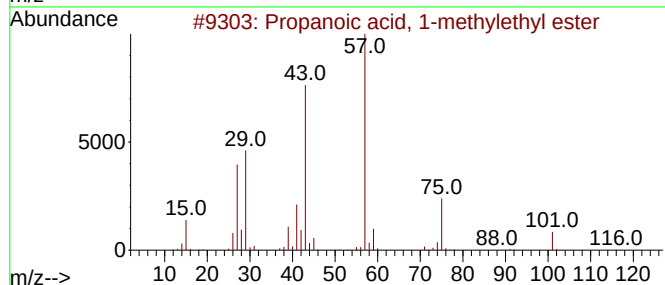
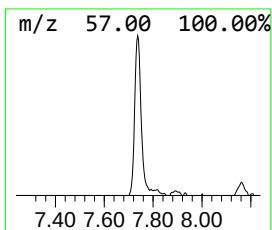
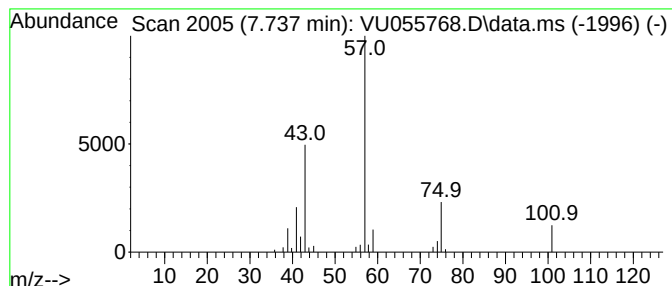
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
7.737	2.74 ug/L	54368	1,4-Difluorobenzene	6.245

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	64
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_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

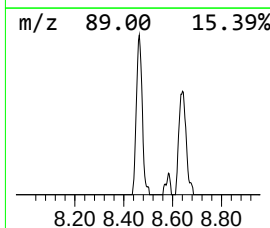
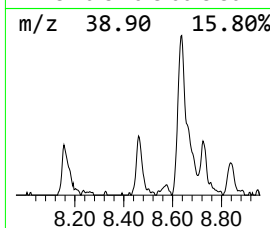
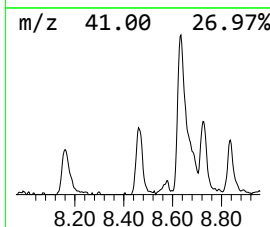
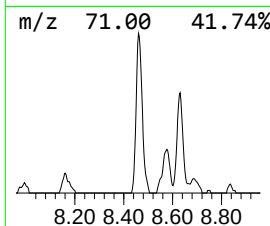
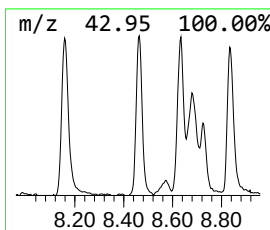
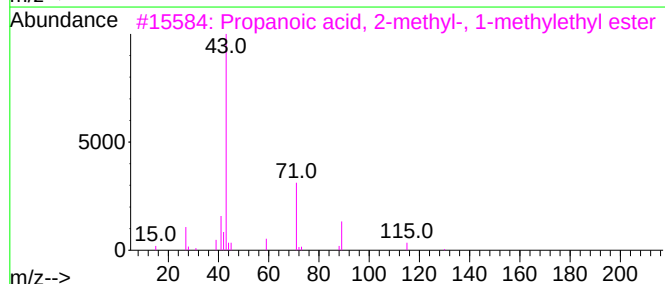
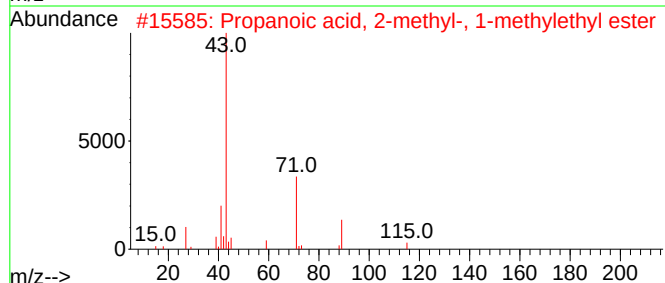
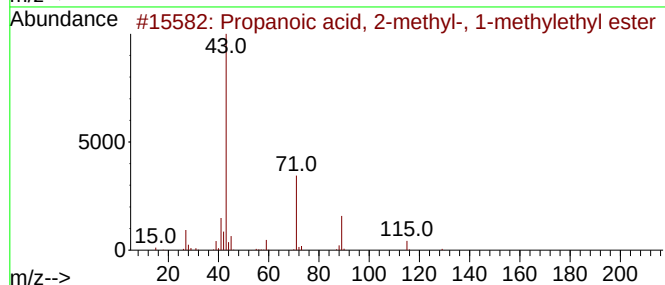
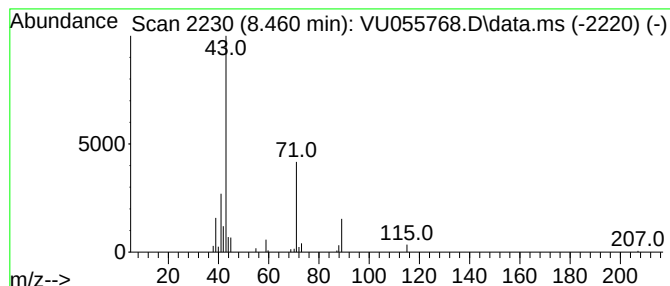
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.460	2.74 ug/L	71081	Chlorobenzene-d5	9.415

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	74
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

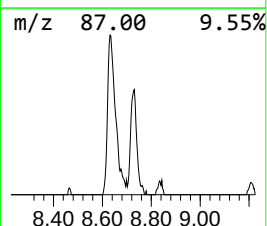
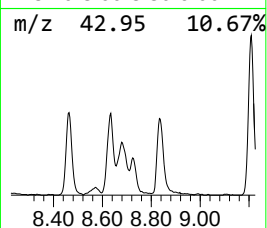
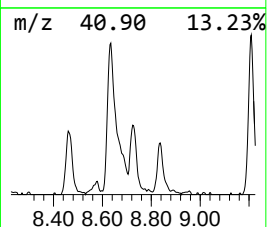
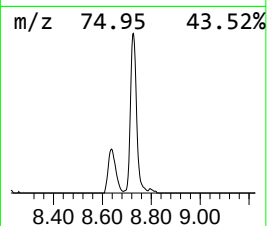
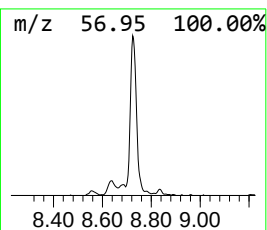
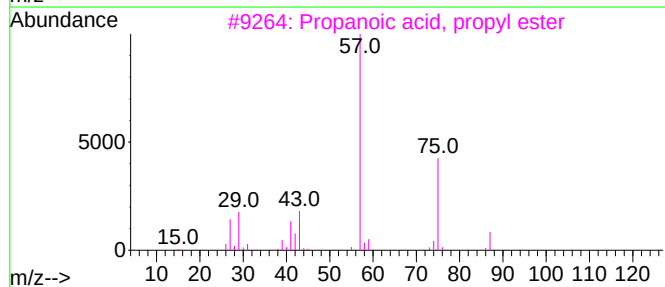
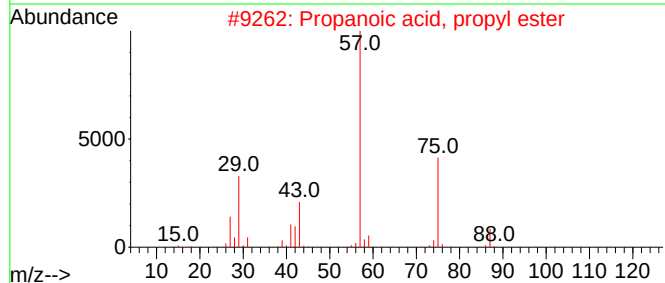
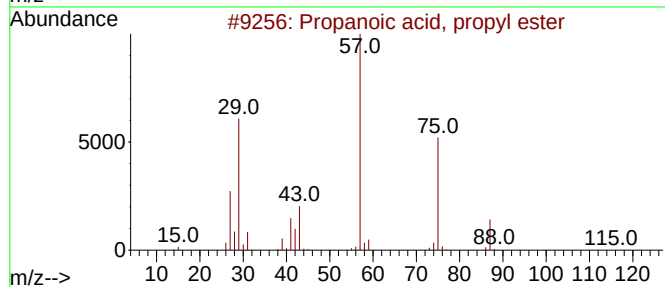
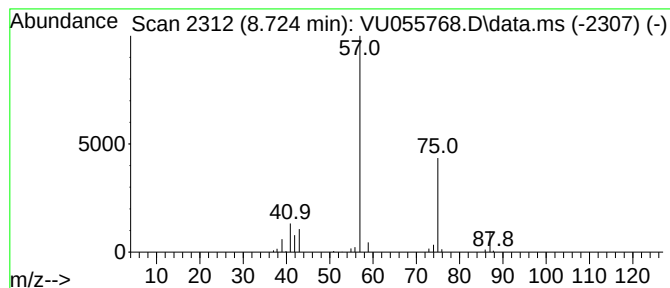
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
8.724	5.14 ug/L	133407	Chlorobenzene-d5	9.415

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	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

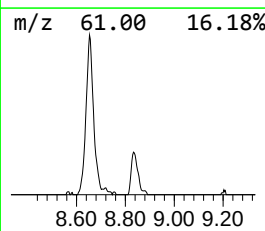
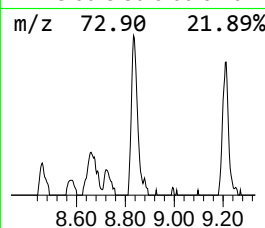
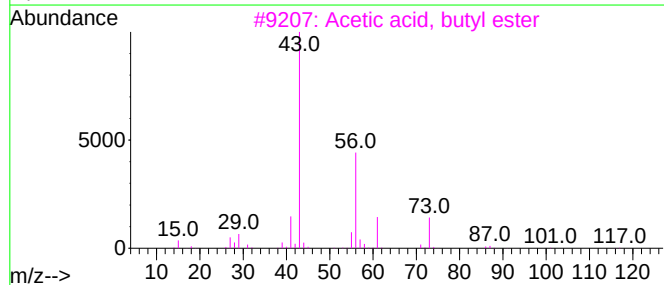
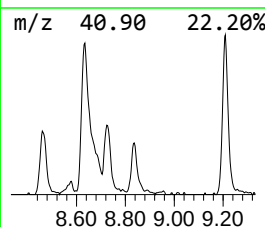
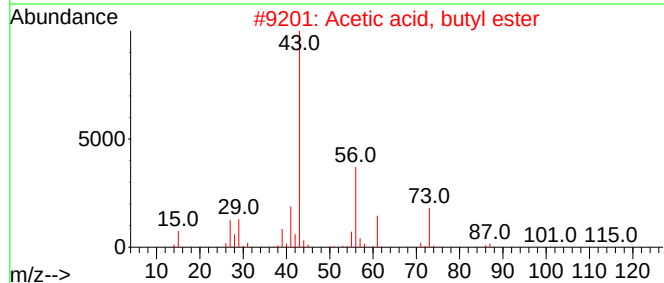
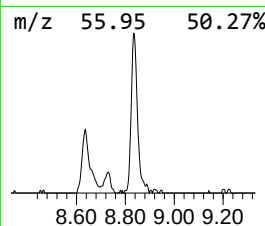
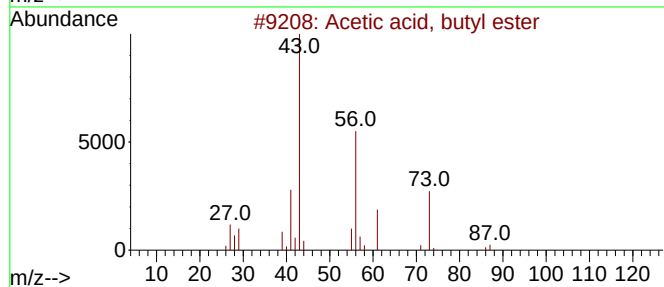
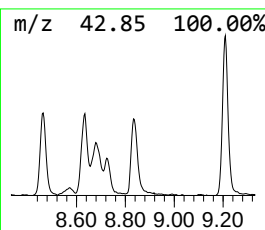
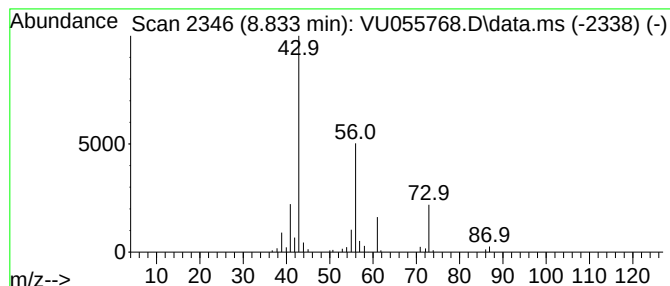
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
8.833	2.60 ug/L	67622	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

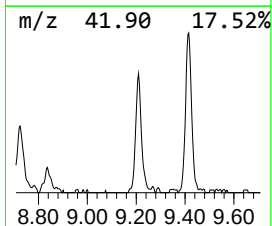
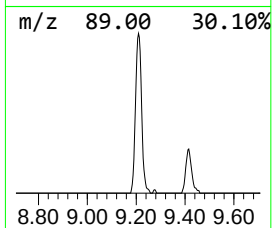
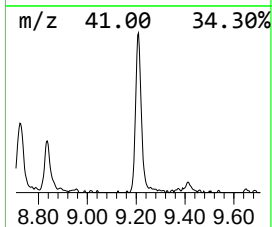
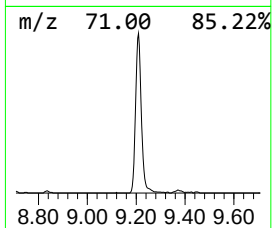
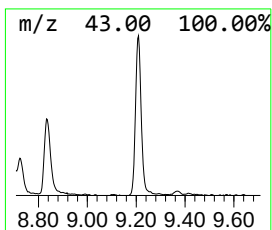
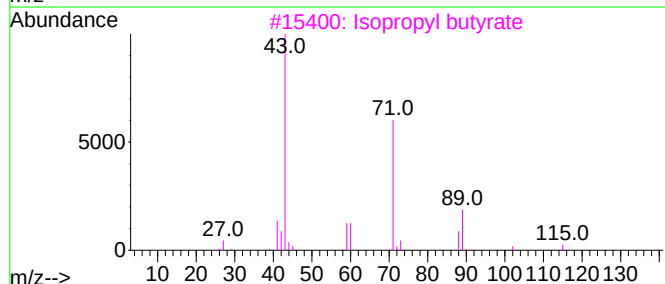
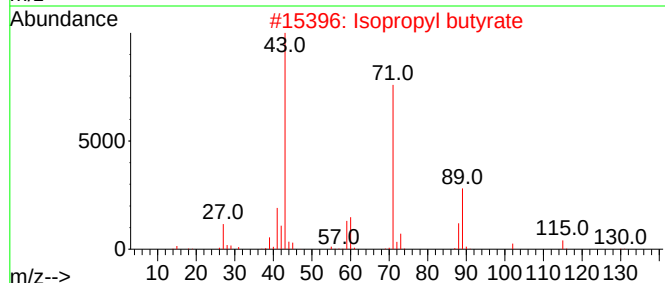
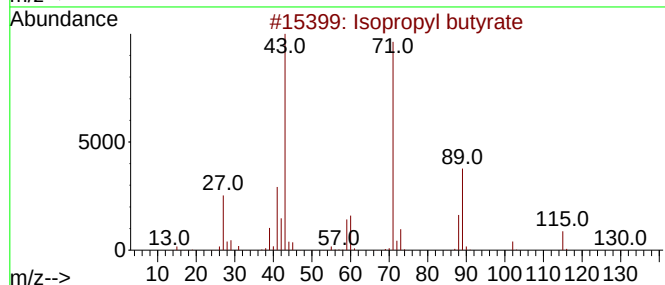
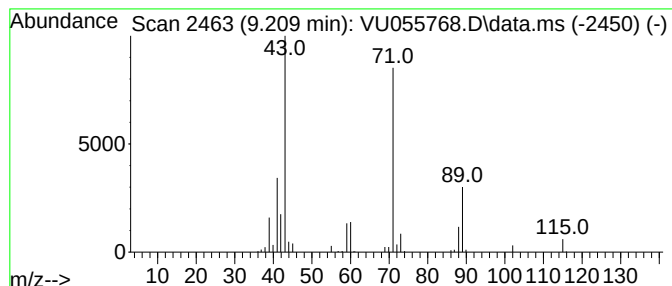
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
9.209	7.61 ug/L	197537	Chlorobenzene-d5	9.415

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	78
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_U\Data\VU101623\
Data File : VU055768.D
Acq On : 16 Oct 2023 13:37
Operator : MD/SY
Sample : PB156380TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB380

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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	7.036	13.2	ug/L	262782	1	6.245	992447	50.0
Propanoic acid,...	7.737	2.7	ug/L	54368	1	6.245	992447	50.0
Propanoic acid,...	8.460	2.7	ug/L	71081	2	9.415	1298140	50.0
Propanoic acid,...	8.724	5.1	ug/L	133407	2	9.415	1298140	50.0
Acetic acid, bu...	8.833	2.6	ug/L	67622	2	9.415	1298140	50.0
Isopropyl butyrate	9.209	7.6	ug/L	197537	2	9.415	1298140	50.0