

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
 Data File : VV029711.D
 Acq On : 19 Dec 2022 11:08
 Operator : SY/MD
 Sample : PB149723TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB723

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\SFAMVLM120722WMA.M
 Title : VOC Analysis

Signal : TIC: VV029711.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	100	rVB	228530	231250	15.54%	1.778%
2	1.564	156	163	179	rVB	184934	204619	13.75%	1.573%
3	2.105	321	331	344	rBV	358892	516003	34.67%	3.968%
4	2.503	445	455	470	rVB2	12850	20130	1.35%	0.155%
5	2.561	471	473	477	rVB	223	126	0.01%	0.001%
6	2.577	477	478	483	rVB2	235	139	0.01%	0.001%
7	2.597	483	484	487	rBV	212	135	0.01%	0.001%
8	2.625	490	493	495	rBV2	290	190	0.01%	0.001%
9	2.770	535	538	541	rVB2	523	310	0.02%	0.002%
10	2.931	584	588	592	rBV	151	159	0.01%	0.001%
11	2.992	604	607	608	rBV	203	96	0.01%	0.001%
12	3.021	614	616	620	rVB2	184	105	0.01%	0.001%
13	3.053	623	626	629	rBV2	147	136	0.01%	0.001%
14	3.137	649	652	654	rBV	152	97	0.01%	0.001%
15	3.188	664	668	671	rBV2	166	134	0.01%	0.001%
16	3.249	684	687	692	rVB2	262	214	0.01%	0.002%
17	3.420	733	740	742	rBV2	195	219	0.01%	0.002%
18	3.468	752	755	758	rVB2	162	98	0.01%	0.001%
19	3.510	766	768	772	rVB2	156	94	0.01%	0.001%
20	3.568	779	786	789	rBV	162	181	0.01%	0.001%
21	3.619	799	802	807	rBV	116	141	0.01%	0.001%
22	3.725	832	835	840	rVB	162	125	0.01%	0.001%
23	3.876	871	882	913	rBV	89758	263732	17.72%	2.028%
24	4.339	1008	1026	1067	rBV	230558	573736	38.54%	4.412%
25	4.561	1092	1095	1098	rVB3	359	211	0.01%	0.002%
26	4.590	1101	1104	1112	rVB4	275	280	0.02%	0.002%
27	4.767	1154	1159	1163	rBV	144	112	0.01%	0.001%
28	4.918	1202	1206	1207	rBV2	252	127	0.01%	0.001%
29	5.040	1226	1244	1292	rBV2	560052	1488515	100.00%	11.446%
30	5.281	1310	1319	1334	rBV	10664	24645	1.66%	0.190%
31	5.477	1377	1380	1385	rVB2	293	233	0.02%	0.002%
32	5.500	1385	1387	1389	rBV	395	213	0.01%	0.002%
33	5.542	1395	1400	1401	rBV2	413	186	0.01%	0.001%
34	5.555	1401	1404	1406	rBV	170	129	0.01%	0.001%
35	5.609	1408	1421	1451	rBV	529542	1082335	72.71%	8.322%
36	5.902	1502	1512	1533	rVB4	5590	13011	0.87%	0.100%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
 Title : VOC Analysis

37	6.014	1544	1547	1548	rBV	163	107	0.01%	0.001%
38	6.063	1548	1562	1600	rVV	318508	660622	44.38%	5.080%
39	6.278	1626	1629	1635	rVB2	343	272	0.02%	0.002%
40	6.307	1635	1638	1640	rBV	226	129	0.01%	0.001%
41	6.355	1640	1653	1660	rBV2	4327	9684	0.65%	0.074%
42	6.461	1676	1686	1718	rBV	132046	261395	17.56%	2.010%
43	6.712	1762	1764	1768	rVB	469	253	0.02%	0.002%
44	6.744	1771	1774	1775	rBV	262	135	0.01%	0.001%
45	6.931	1830	1832	1834	rBV3	218	149	0.01%	0.001%
46	6.979	1835	1847	1870	rBV	163665	301858	20.28%	2.321%
47	7.182	1900	1910	1923	rBV	32069	57745	3.88%	0.444%
48	7.307	1937	1949	1991	rBV	703056	1248827	83.90%	9.603%
49	7.571	2029	2031	2033	rBV2	515	188	0.01%	0.001%
50	7.612	2033	2044	2071	rVV2	154948	275993	18.54%	2.122%
51	7.876	2124	2126	2127	rBV	242	92	0.01%	0.001%
52	7.921	2128	2140	2160	rVV	46293	80110	5.38%	0.616%
53	8.082	2181	2190	2214	rBV	339206	620133	41.66%	4.768%
54	8.188	2216	2223	2248	rVB	74776	127742	8.58%	0.982%
55	8.297	2249	2257	2279	rVB2	42224	72832	4.89%	0.560%
56	8.577	2342	2344	2347	rBV2	169	108	0.01%	0.001%
57	8.596	2347	2350	2353	rBV	495	342	0.02%	0.003%
58	8.673	2363	2374	2398	rBV	139749	223761	15.03%	1.721%
59	8.844	2414	2427	2456	rBV	792181	1311636	88.12%	10.086%
60	9.117	2502	2512	2517	rBV6	1598	2875	0.19%	0.022%
61	9.223	2542	2545	2548	rBV2	241	131	0.01%	0.001%
62	9.239	2548	2550	2557	rVB2	181	111	0.01%	0.001%
63	9.275	2557	2561	2564	rBV2	270	235	0.02%	0.002%
64	9.291	2564	2566	2570	rVB	222	119	0.01%	0.001%
65	9.384	2587	2595	2596	rBV4	1361	1436	0.10%	0.011%
66	9.542	2634	2644	2655	rBV3	11590	19041	1.28%	0.146%
67	9.657	2674	2680	2683	rBV2	169	171	0.01%	0.001%
68	9.680	2683	2687	2690	rBV2	205	205	0.01%	0.002%
69	9.722	2698	2700	2706	rBV3	154	153	0.01%	0.001%
70	9.751	2707	2709	2711	rVB2	253	101	0.01%	0.001%
71	9.799	2722	2724	2726	rBV	355	177	0.01%	0.001%
72	9.895	2751	2754	2756	rBV	154	119	0.01%	0.001%
73	9.915	2758	2760	2772	rVB3	581	806	0.05%	0.006%
74	9.966	2772	2776	2781	rBV2	273	200	0.01%	0.002%
75	9.998	2784	2786	2788	rBV	194	127	0.01%	0.001%
76	10.088	2810	2814	2817	rBV2	131	107	0.01%	0.001%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	10.162	2827	2837	2841	rBV	19467	27886	1.87%	0.214%
78	10.207	2842	2851	2874	rVB	451782	706301	47.45%	5.431%
79	10.378	2896	2904	2910	rBV4	1388	2103	0.14%	0.016%
80	10.497	2935	2941	2944	rBV	247	226	0.02%	0.002%
81	10.535	2944	2953	2956	rBV2	813	998	0.07%	0.008%
82	10.567	2956	2963	2976	rVB2	8870	14150	0.95%	0.109%
83	10.644	2985	2987	2991	rBV	168	133	0.01%	0.001%
84	10.673	2994	2996	3001	rVB2	189	96	0.01%	0.001%
85	10.734	3013	3015	3019	rVB2	271	142	0.01%	0.001%
86	10.853	3050	3052	3055	rVB2	549	248	0.02%	0.002%
87	10.886	3055	3062	3063	rBV	306	220	0.01%	0.002%
88	11.066	3116	3118	3120	rBV	212	122	0.01%	0.001%
89	11.130	3134	3138	3140	rBV2	207	156	0.01%	0.001%
90	11.236	3159	3171	3198	rBV	880074	1367722	91.88%	10.517%
91	11.484	3246	3248	3251	rBV2	329	206	0.01%	0.002%
92	11.522	3257	3260	3261	rBV2	307	174	0.01%	0.001%
93	11.612	3275	3288	3312	rBV	745784	1168605	78.51%	8.986%
94	11.831	3354	3356	3358	rBV2	415	221	0.01%	0.002%
95	11.898	3374	3377	3384	rBV2	291	303	0.02%	0.002%
96	12.114	3441	3444	3446	rBV	240	130	0.01%	0.001%
97	12.214	3472	3475	3476	rBV	421	282	0.02%	0.002%
98	12.683	3619	3621	3625	rBV2	551	361	0.02%	0.003%
99	12.709	3625	3629	3632	rBV3	365	319	0.02%	0.002%
100	13.493	3867	3873	3889	rVB	6823	11526	0.77%	0.089%

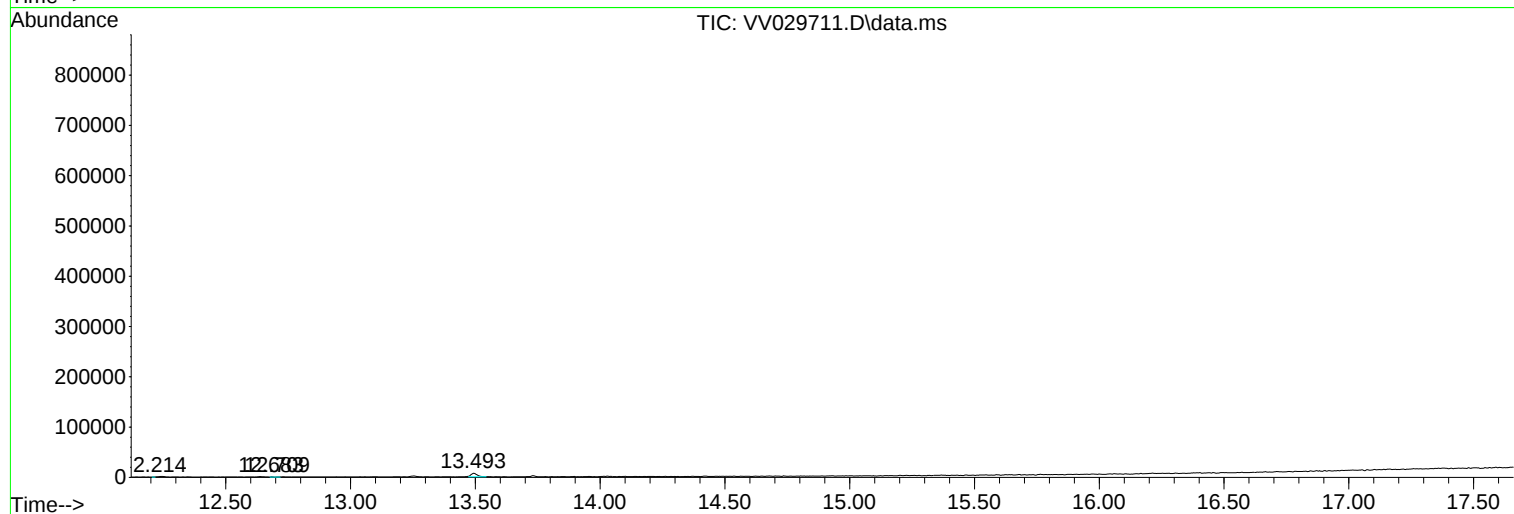
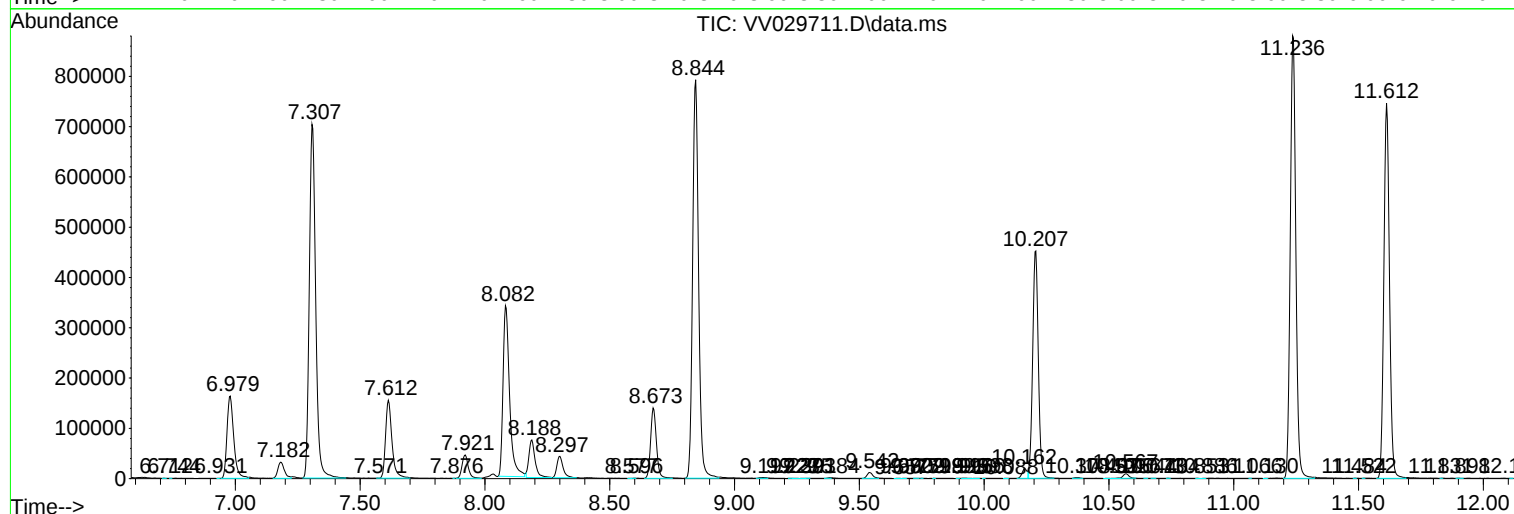
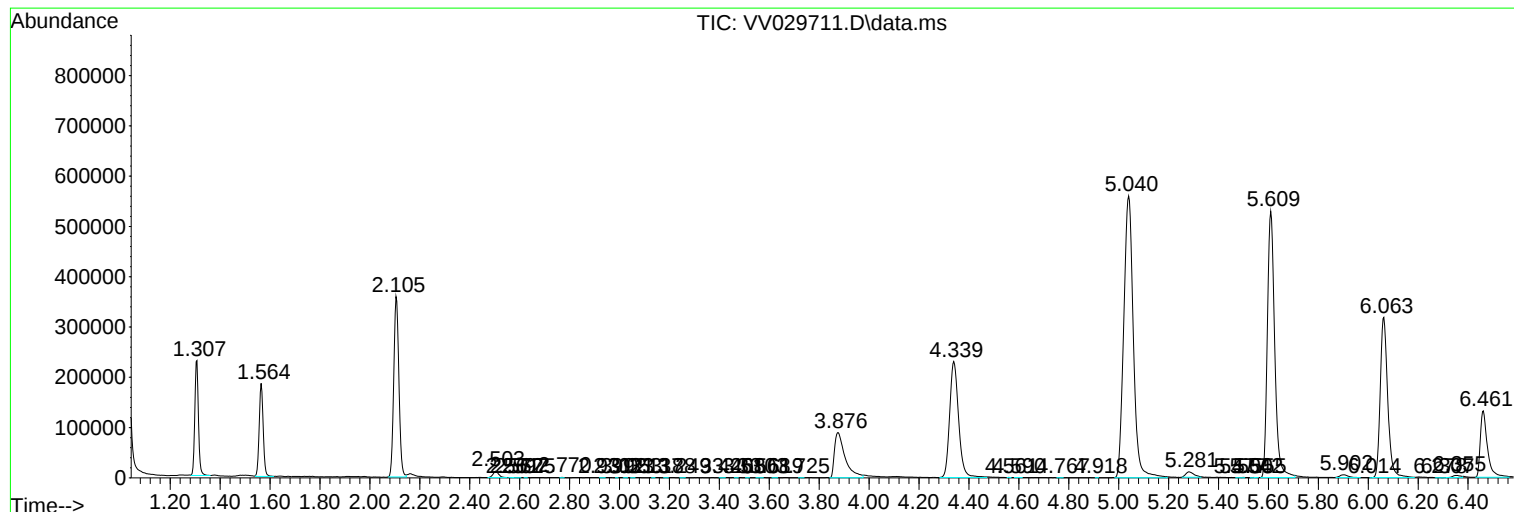
Sum of corrected areas: 13005023

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Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_V
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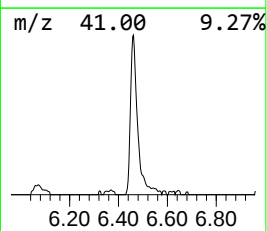
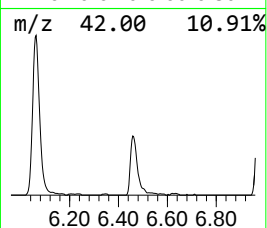
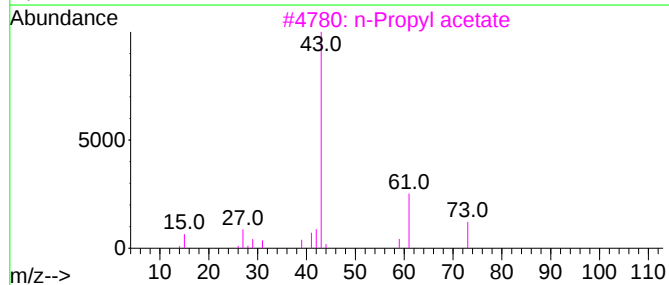
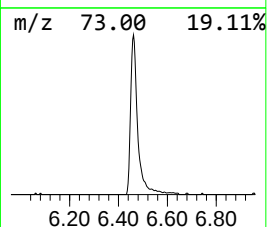
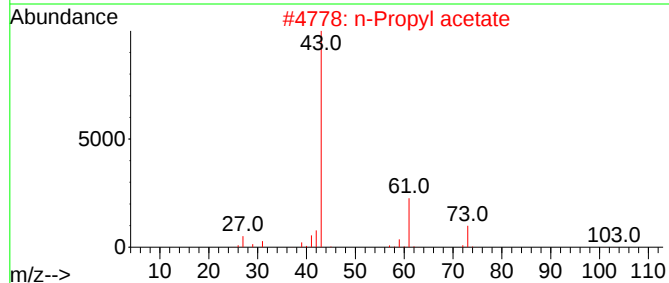
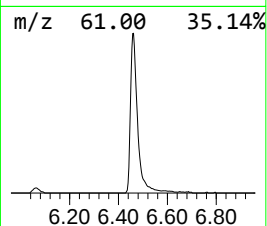
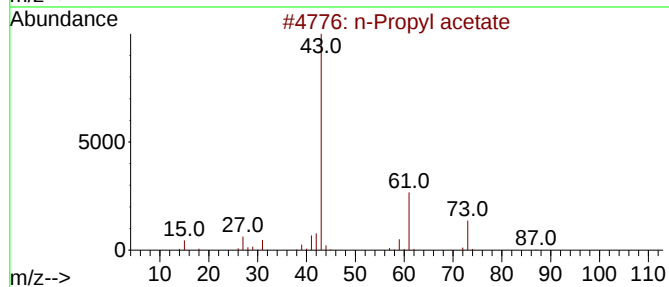
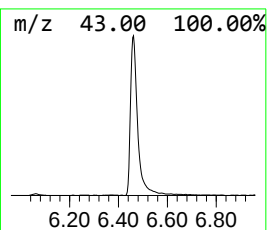
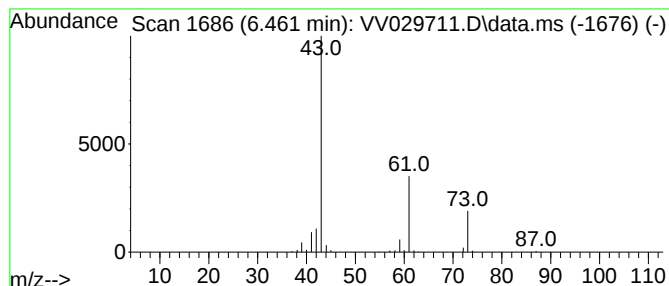
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
6.461	12.08 ug/L	261395	1,4-Difluorobenzene	5.609

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	74
3		n-Propyl acetate	102	C5H10O2	000109-60-4	72
4		n-Propyl acetate	102	C5H10O2	000109-60-4	40
5		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38



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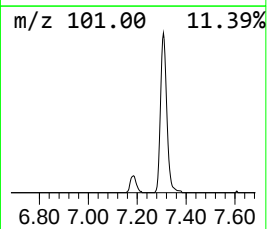
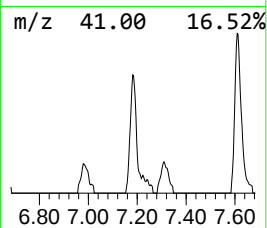
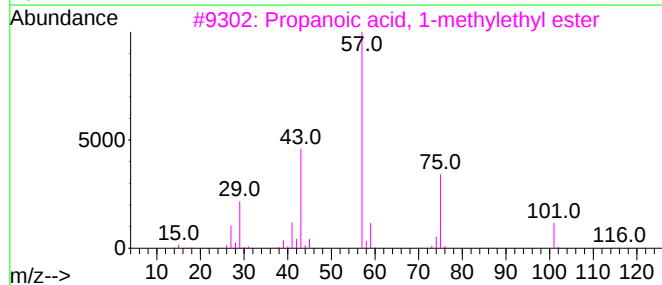
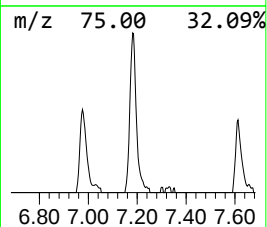
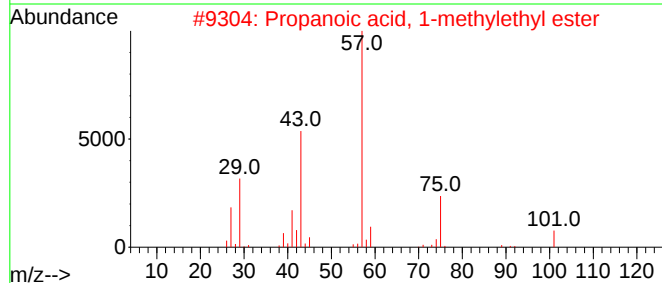
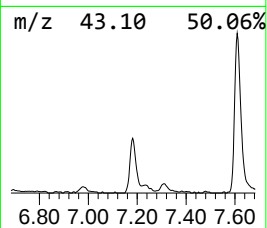
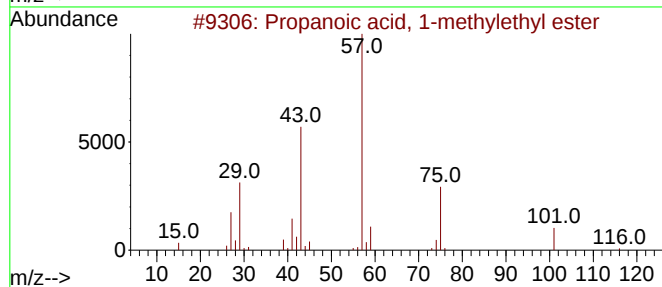
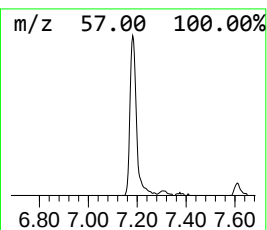
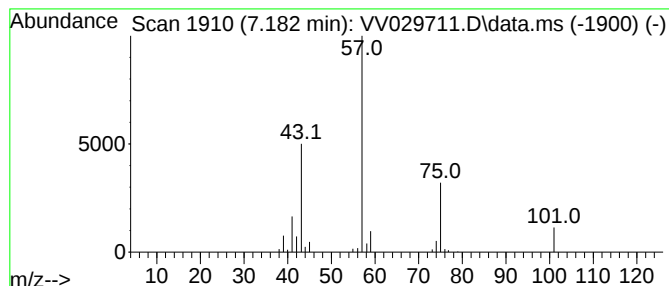
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	2.67 ug/L	57745	1,4-Difluorobenzene	5.609

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	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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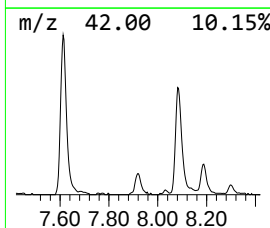
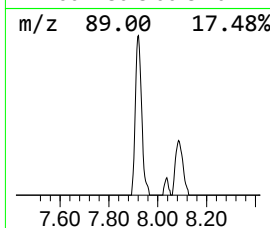
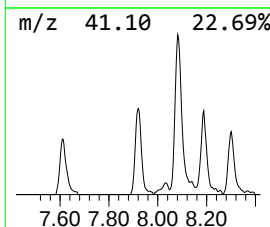
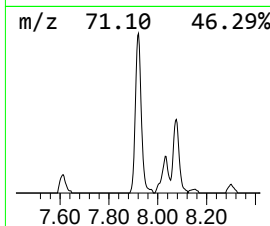
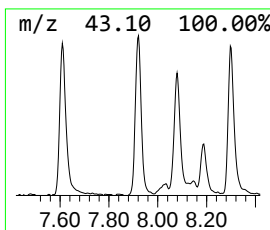
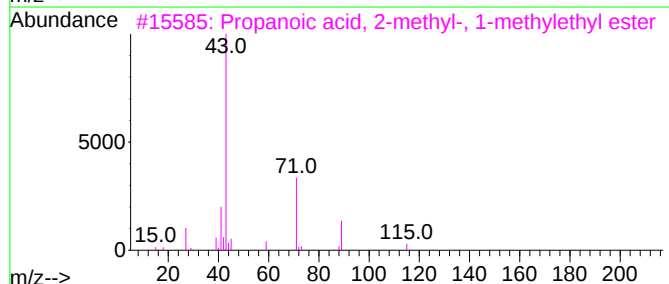
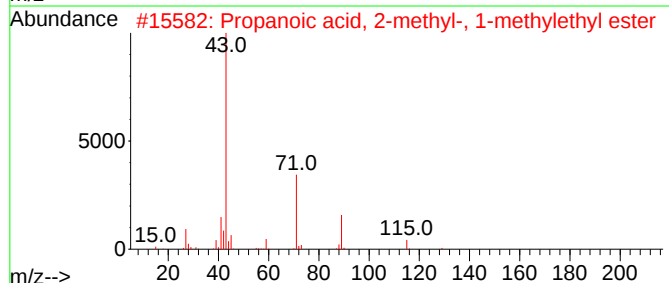
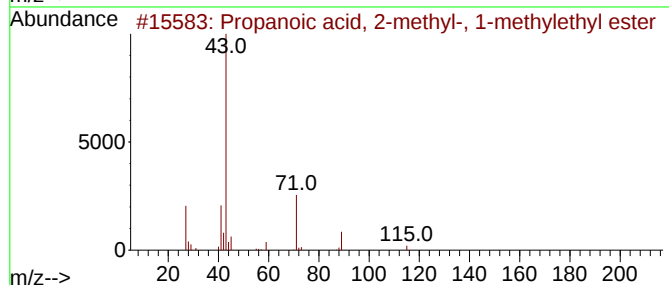
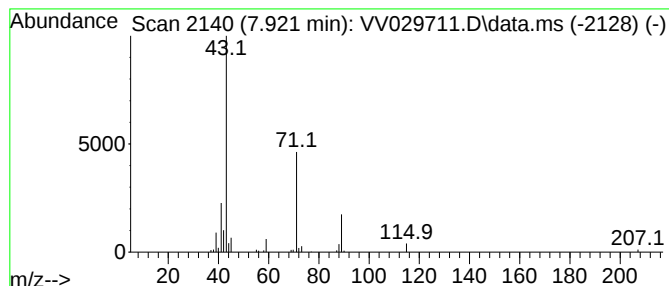
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
7.921	3.05 ug/L	80110	Chlorobenzene-d5	8.844

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-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029711.D
Acq On : 19 Dec 2022 11:08
Operator : SY/MD
Sample : PB149723TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB723

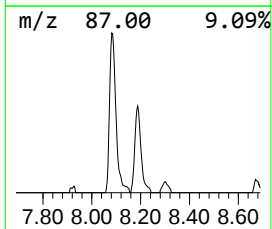
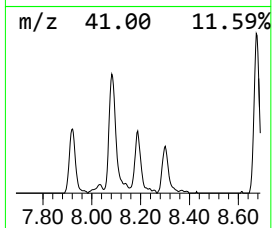
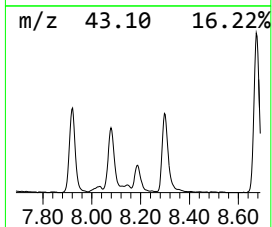
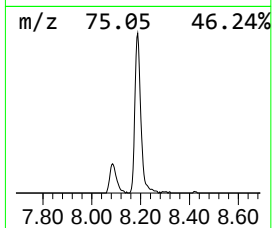
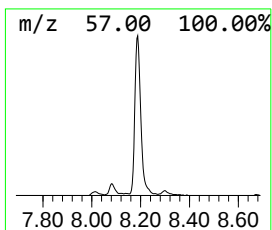
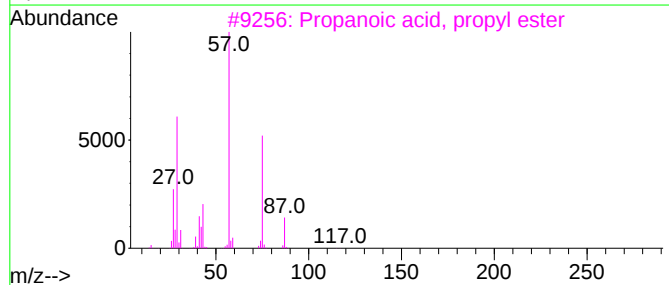
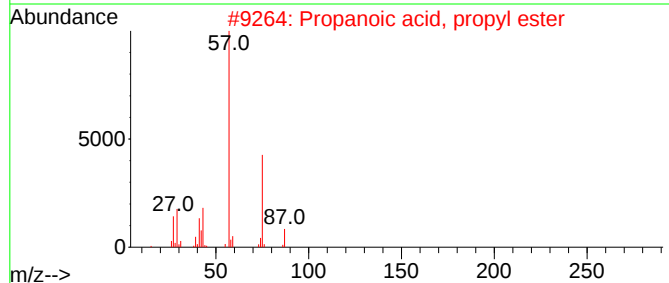
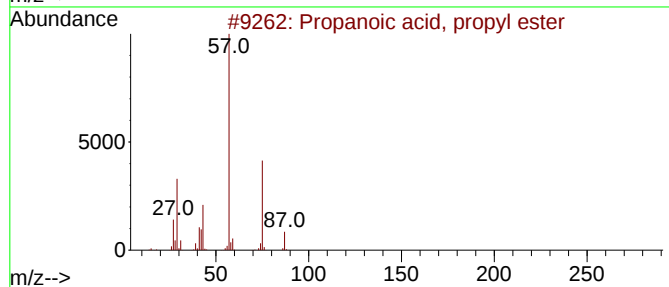
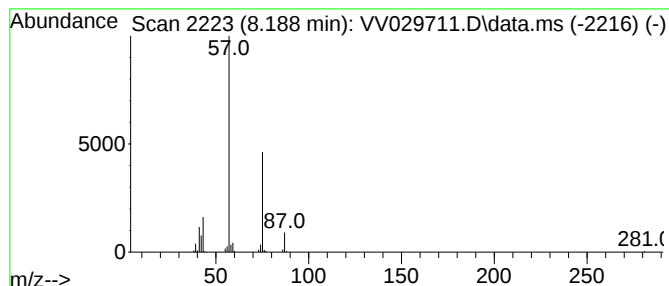
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Quant Title : VOC Analysis

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.
8.188	4.87 ug/L	127742	Chlorobenzene-d5	8.844

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	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029711.D
Acq On : 19 Dec 2022 11:08
Operator : SY/MD
Sample : PB149723TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB723

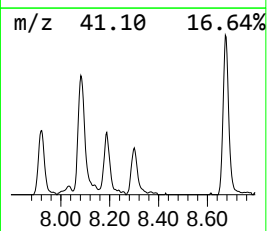
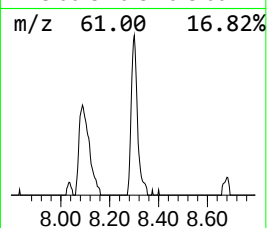
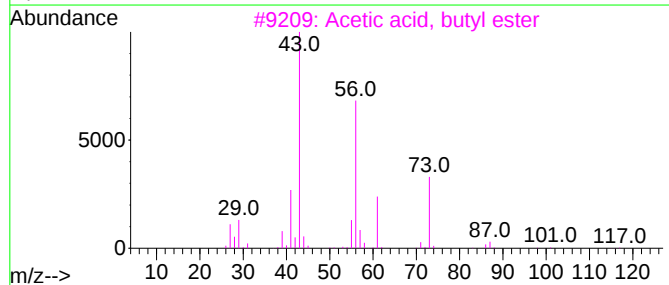
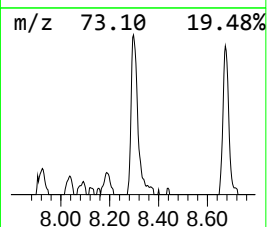
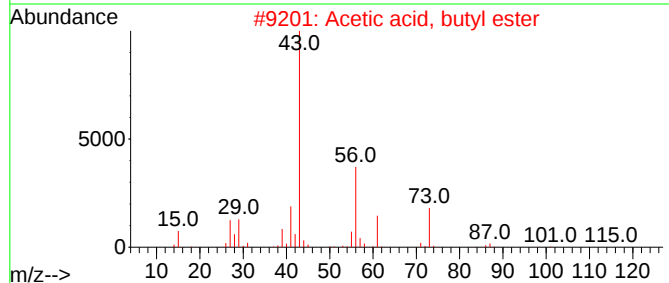
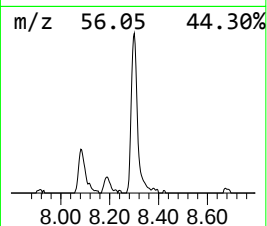
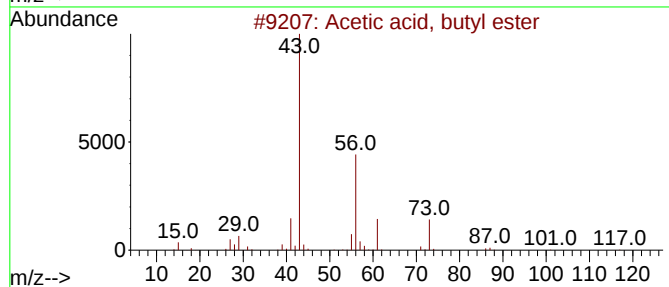
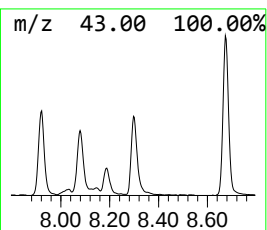
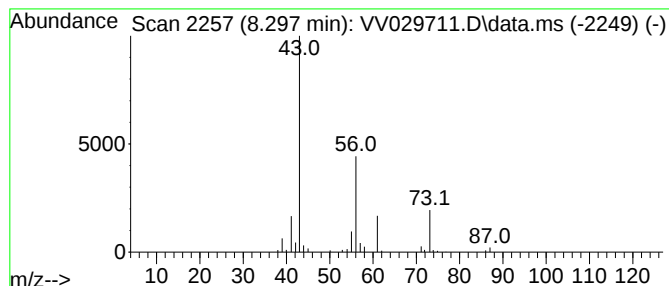
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	2.78 ug/L	72832	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78		
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	42		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029711.D
Acq On : 19 Dec 2022 11:08
Operator : SY/MD
Sample : PB149723TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB723

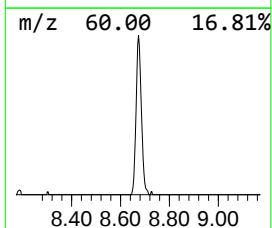
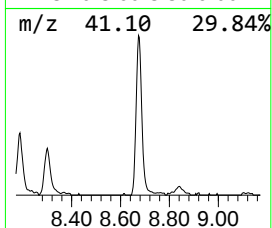
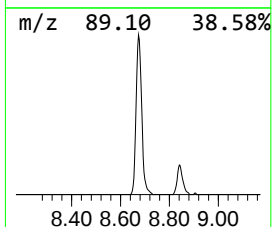
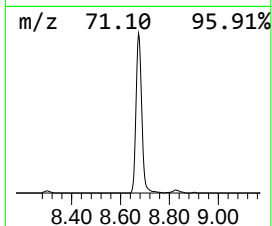
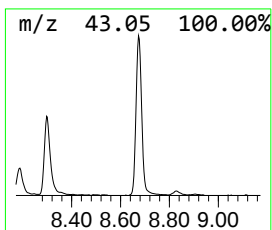
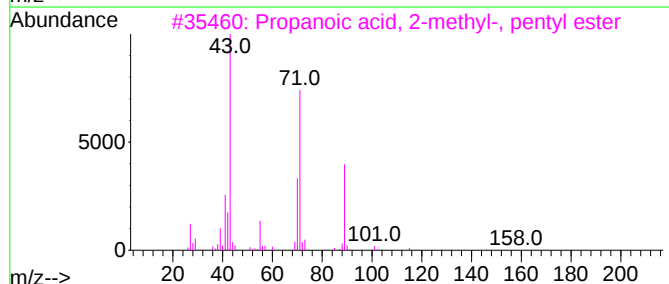
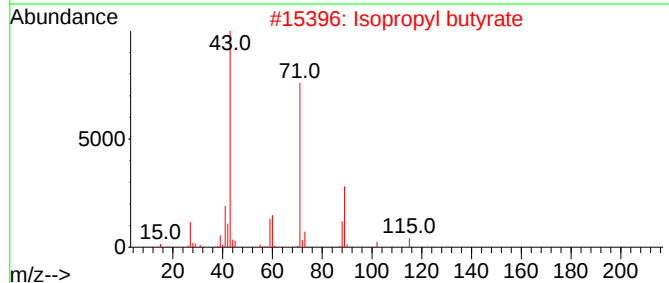
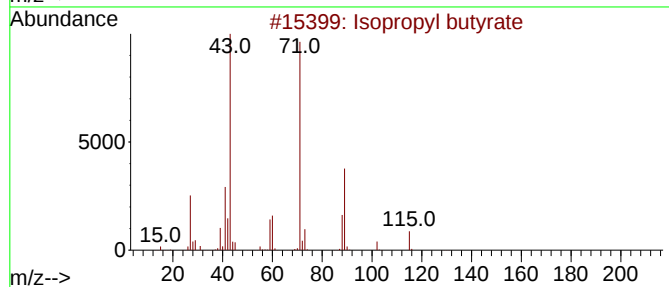
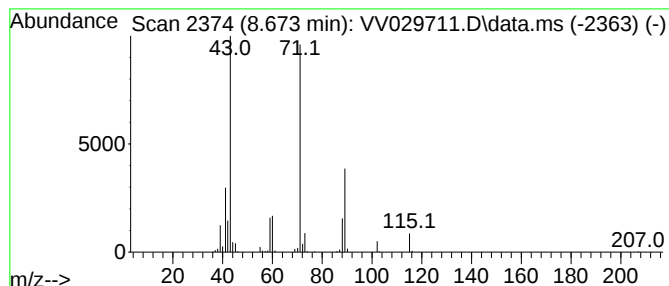
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
8.673	8.53 ug/L	223761	Chlorobenzene-d5	8.844

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			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029711.D
Acq On : 19 Dec 2022 11:08
Operator : SY/MD
Sample : PB149723TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB723

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.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	6.461	12.1	ug/L	261395	1	5.609	1082340	50.0
Propanoic acid,...	7.182	2.7	ug/L	57745	1	5.609	1082340	50.0
Propanoic acid,...	7.921	3.0	ug/L	80110	2	8.844	1311640	50.0
Propanoic acid,...	8.188	4.9	ug/L	127742	2	8.844	1311640	50.0
Acetic acid, bu...	8.297	2.8	ug/L	72832	2	8.844	1311640	50.0
Isopropyl butyrate	8.673	8.5	ug/L	223761	2	8.844	1311640	50.0