

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049352.D
 Acq On : 22 Jun 2022 15:22
 Operator : SY/MD
 Sample : N3392-06 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEY1

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\SFAMULM061022WMA.M
 Title : VOC Analysis

Signal : TIC: VU049352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	23	rVB	65593	59246	7.57%	0.814%
2	1.485	41	45	50	rBV5	2759	3239	0.41%	0.045%
3	1.597	73	80	94	rBV	75145	87129	11.13%	1.198%
4	1.906	168	176	192	rVB	66809	88837	11.35%	1.221%
5	2.327	304	307	311	rBV5	966	959	0.12%	0.013%
6	2.565	369	381	394	rBV	129394	205062	26.20%	2.818%
7	2.629	394	401	412	rVB2	4948	8381	1.07%	0.115%
8	2.755	437	440	443	rBV2	298	217	0.03%	0.003%
9	2.774	443	446	447	rBV	713	412	0.05%	0.006%
10	2.993	512	514	518	rVB3	339	190	0.02%	0.003%
11	3.044	520	530	540	rVV3	4197	6893	0.88%	0.095%
12	3.186	560	574	601	rVB2	20814	51573	6.59%	0.709%
13	3.363	626	629	633	rVB2	367	238	0.03%	0.003%
14	3.388	633	637	640	rBV2	327	238	0.03%	0.003%
15	3.408	640	643	649	rVB2	375	269	0.03%	0.004%
16	3.552	685	688	692	rBV3	287	232	0.03%	0.003%
17	3.703	730	735	738	rBV	214	187	0.02%	0.003%
18	3.906	792	798	800	rBV2	326	380	0.05%	0.005%
19	4.108	857	861	867	rVB	326	302	0.04%	0.004%
20	4.163	871	878	886	rBV2	318	500	0.06%	0.007%
21	4.436	960	963	969	rBV3	281	287	0.04%	0.004%
22	4.494	977	981	984	rBV2	247	204	0.03%	0.003%
23	4.549	995	998	1000	rBV2	419	220	0.03%	0.003%
24	4.578	1001	1007	1008	rBV2	339	312	0.04%	0.004%
25	4.623	1008	1021	1047	rBV	124971	317910	40.61%	4.369%
26	5.063	1141	1158	1183	rBV	150544	328698	41.99%	4.518%
27	5.240	1208	1213	1219	rBV2	156	232	0.03%	0.003%
28	5.285	1225	1227	1234	rVB3	376	294	0.04%	0.004%
29	5.726	1338	1364	1391	rBV2	281958	782748	100.00%	10.758%
30	5.915	1412	1423	1437	rVV3	9013	18786	2.40%	0.258%
31	5.973	1438	1441	1445	rVV4	450	316	0.04%	0.004%
32	6.247	1513	1526	1549	rBV	300933	572430	73.13%	7.867%
33	6.530	1606	1614	1615	rBV4	2143	2391	0.31%	0.033%
34	6.620	1639	1642	1646	rBV3	391	299	0.04%	0.004%
35	6.690	1650	1664	1682	rVV	199350	387816	49.55%	5.330%
36	6.758	1682	1685	1688	rVB5	578	365	0.05%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
 Title : VOC Analysis

37	6.793	1694	1696	1698	rBV2	430	203	0.03%	0.003%
38	6.825	1704	1706	1710	rVB2	647	371	0.05%	0.005%
39	6.867	1716	1719	1723	rBV4	491	473	0.06%	0.007%
40	6.925	1724	1737	1751	rVV2	5134	10594	1.35%	0.146%
41	7.041	1761	1773	1792	rBV	106182	189177	24.17%	2.600%
42	7.153	1806	1808	1811	rBV3	305	202	0.03%	0.003%
43	7.179	1811	1816	1817	rBV4	1437	1207	0.15%	0.017%
44	7.218	1825	1828	1834	rVB5	511	510	0.07%	0.007%
45	7.285	1847	1849	1858	rVB3	297	370	0.05%	0.005%
46	7.407	1884	1887	1891	rVB2	337	211	0.03%	0.003%
47	7.446	1896	1899	1901	rBV	350	214	0.03%	0.003%
48	7.565	1922	1936	1953	rBV	106003	184980	23.63%	2.542%
49	7.690	1968	1975	1979	rBV3	980	1162	0.15%	0.016%
50	7.739	1979	1990	2001	rBV	20710	34644	4.43%	0.476%
51	7.793	2003	2007	2014	rVB3	1625	1930	0.25%	0.027%
52	7.896	2026	2039	2055	rBV	329948	574882	73.44%	7.901%
53	8.060	2085	2090	2097	rVB3	544	550	0.07%	0.008%
54	8.179	2108	2127	2145	rBV3	77349	152191	19.44%	2.092%
55	8.407	2195	2198	2200	rBV2	290	189	0.02%	0.003%
56	8.465	2206	2216	2232	rBV2	23101	38726	4.95%	0.532%
57	8.575	2236	2250	2256	rVV7	4484	9423	1.20%	0.130%
58	8.632	2256	2268	2289	rVV	343502	619659	79.16%	8.517%
59	8.726	2289	2297	2320	rVV	54011	93379	11.93%	1.283%
60	8.835	2322	2331	2344	rVB	12669	21231	2.71%	0.292%
61	8.931	2359	2361	2366	rVB2	427	317	0.04%	0.004%
62	8.967	2369	2372	2378	rBV2	430	431	0.06%	0.006%
63	8.992	2378	2380	2389	rBV3	213	187	0.02%	0.003%
64	9.153	2427	2430	2431	rBV	298	207	0.03%	0.003%
65	9.163	2431	2433	2436	rVV2	385	257	0.03%	0.004%
66	9.211	2436	2448	2466	rVV	72816	115199	14.72%	1.583%
67	9.279	2466	2469	2472	rVB3	572	402	0.05%	0.006%
68	9.369	2491	2497	2499	rBV3	1185	1250	0.16%	0.017%
69	9.417	2499	2512	2530	rVV	407562	675046	86.24%	9.278%
70	9.552	2548	2554	2563	rVB8	970	1688	0.22%	0.023%
71	9.645	2579	2583	2584	rBV	405	224	0.03%	0.003%
72	9.928	2661	2671	2676	rBV	718	1145	0.15%	0.016%
73	10.066	2710	2714	2717	rBV2	477	360	0.05%	0.005%
74	10.481	2840	2843	2846	rVB2	259	186	0.02%	0.003%
75	10.520	2852	2855	2857	rVB	349	209	0.03%	0.003%
76	10.549	2857	2864	2867	rBV2	257	279	0.04%	0.004%

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 ClientSampleId :
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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

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 Title : VOC Analysis

77	10.571	2867	2871	2876	rVV	152	188	0.02%	0.003%
78	10.754	2916	2928	2950	rBV	295514	479407	61.25%	6.589%
79	11.037	3013	3016	3021	rVB2	623	565	0.07%	0.008%
80	11.070	3021	3026	3028	rBV2	399	388	0.05%	0.005%
81	11.343	3106	3111	3112	rBV	279	199	0.03%	0.003%
82	11.388	3122	3125	3130	rVB	385	298	0.04%	0.004%
83	11.552	3174	3176	3181	rVB2	355	205	0.03%	0.003%
84	11.661	3206	3210	3215	rBV2	561	475	0.06%	0.007%
85	11.812	3245	3257	3279	rBV	374648	601167	76.80%	8.262%
86	11.918	3289	3290	3296	rVB2	459	345	0.04%	0.005%
87	11.967	3302	3305	3310	rVB2	334	213	0.03%	0.003%
88	12.060	3326	3334	3338	rBV2	366	548	0.07%	0.008%
89	12.192	3362	3375	3396	rBV	322953	526710	67.29%	7.239%
90	12.285	3401	3404	3408	rVB3	521	500	0.06%	0.007%
91	12.343	3419	3422	3423	rBV	350	230	0.03%	0.003%
92	12.539	3480	3483	3487	rVB2	328	220	0.03%	0.003%
93	12.758	3548	3551	3552	rBV2	338	189	0.02%	0.003%
94	12.770	3552	3555	3559	rVB	642	527	0.07%	0.007%
95	12.848	3576	3579	3583	rVB	363	221	0.03%	0.003%
96	12.934	3602	3606	3608	rBV	322	253	0.03%	0.003%
97	13.272	3705	3711	3714	rBV2	333	421	0.05%	0.006%
98	14.182	3991	3994	3997	rVB2	563	354	0.05%	0.005%
99	14.291	4025	4028	4030	rBV3	309	190	0.02%	0.003%
100	15.886	4521	4524	4527	rBV2	596	436	0.06%	0.006%

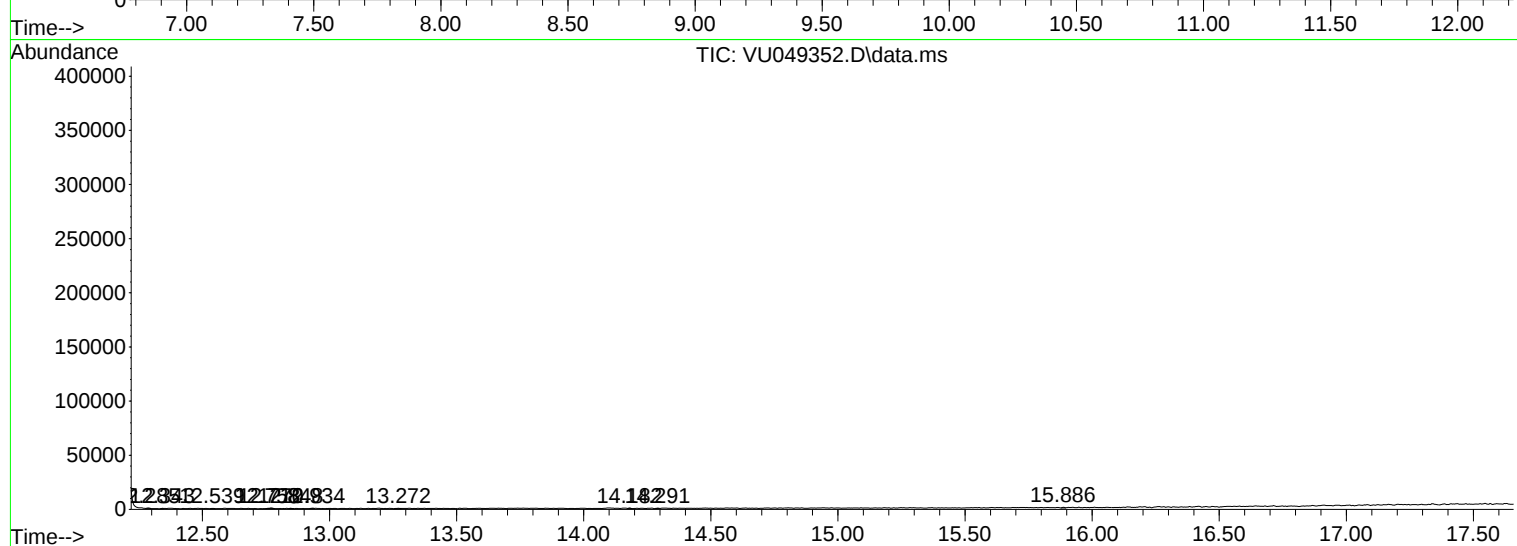
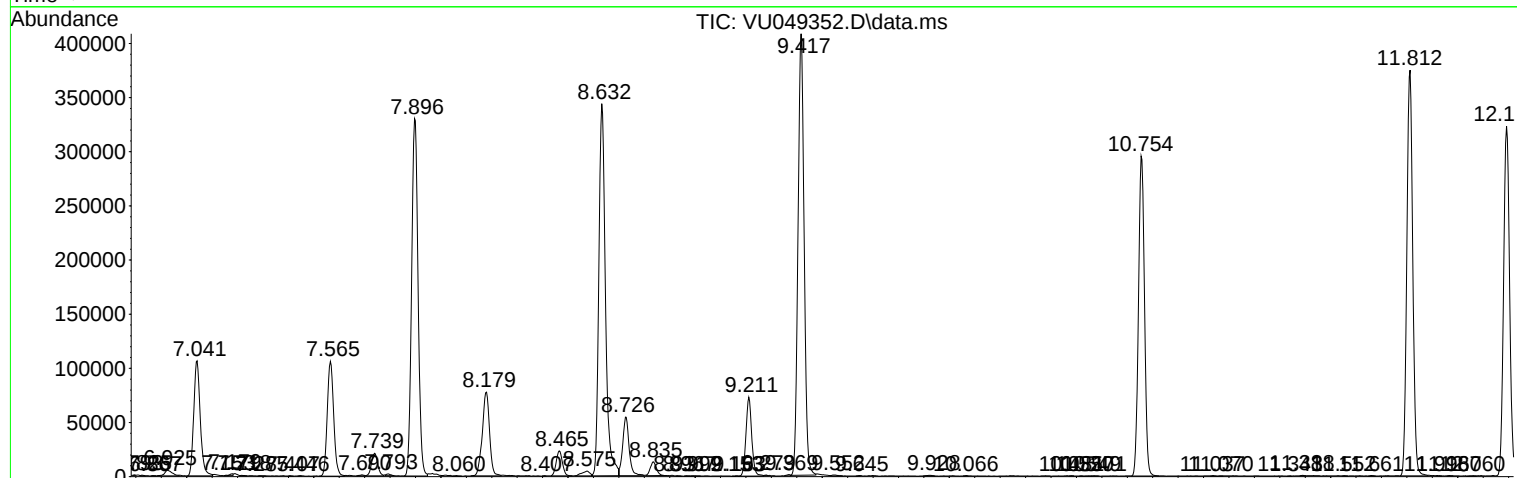
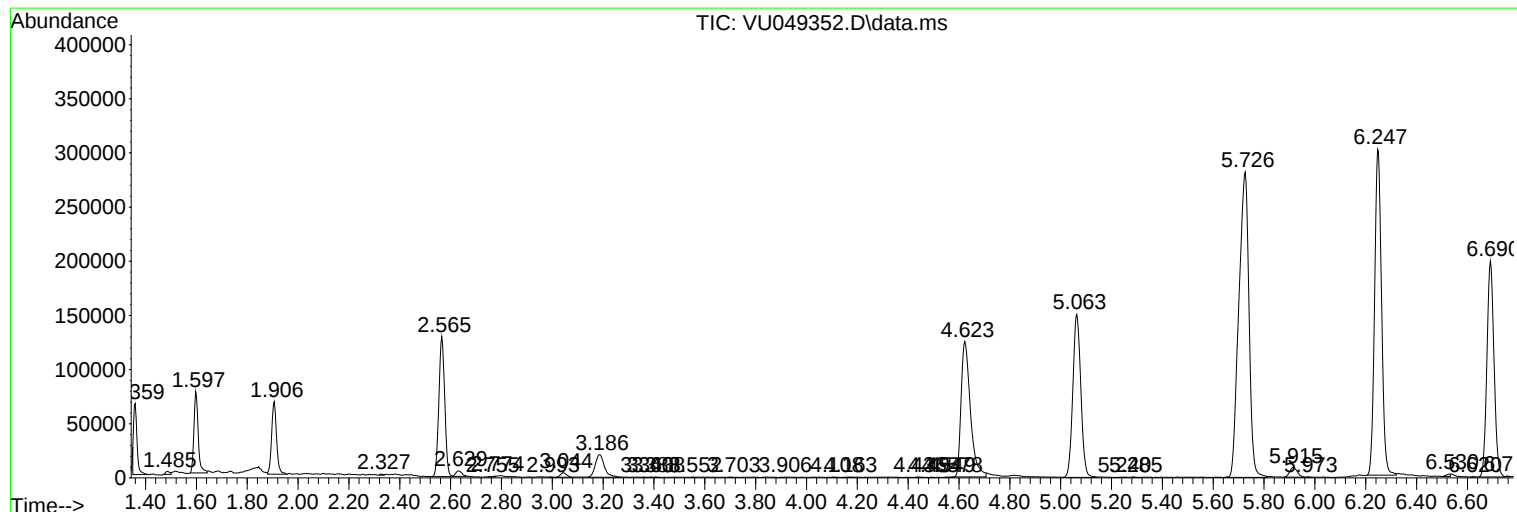
Sum of corrected areas: 7275906

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
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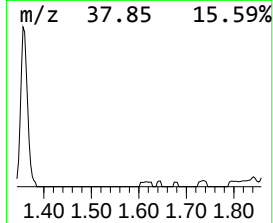
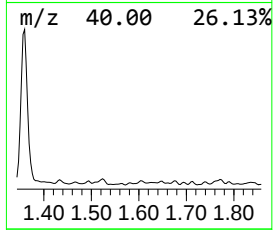
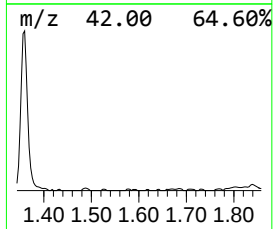
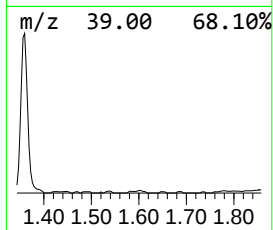
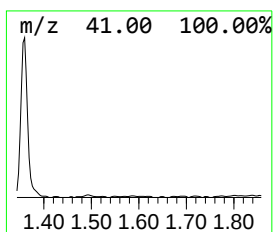
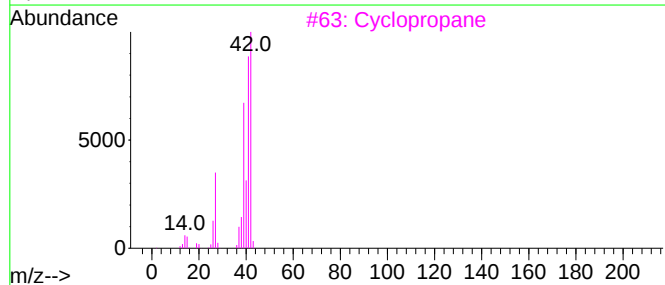
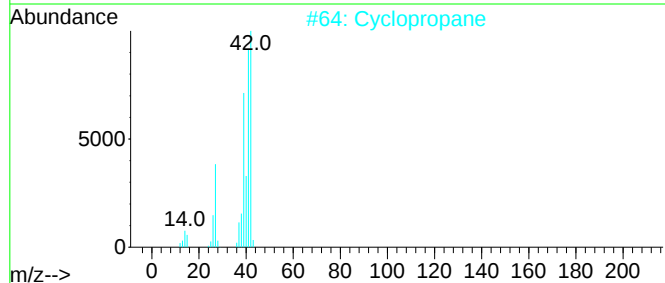
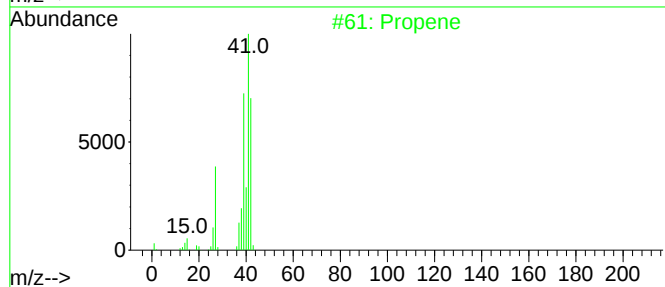
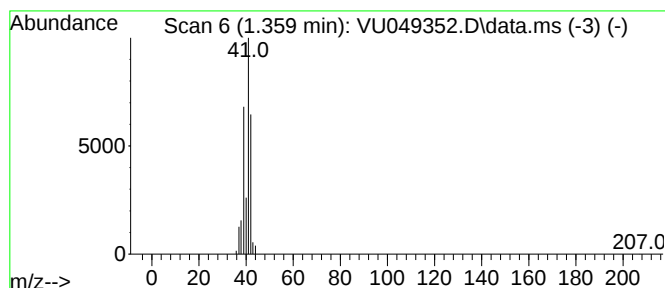
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	5.17 ug/L	59246	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propene	42	C3H6	000115-07-1	90
2		Cyclopropane	42	C3H6	000075-19-4	78
3		Cyclopropane	42	C3H6	000075-19-4	78
4		Propene	42	C3H6	000115-07-1	40
5		Cyclopropane	42	C3H6	000075-19-4	37



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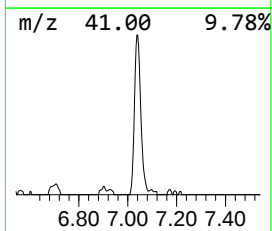
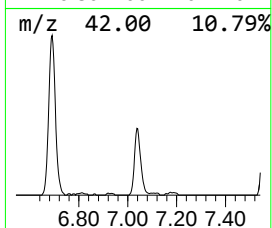
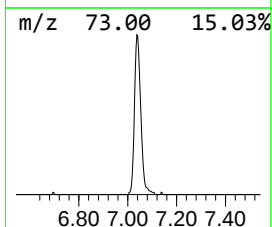
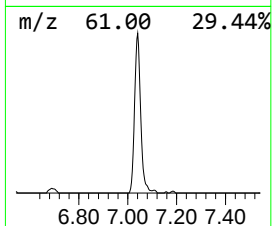
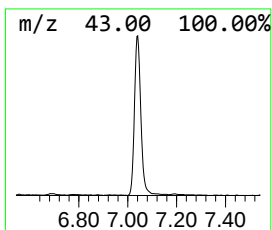
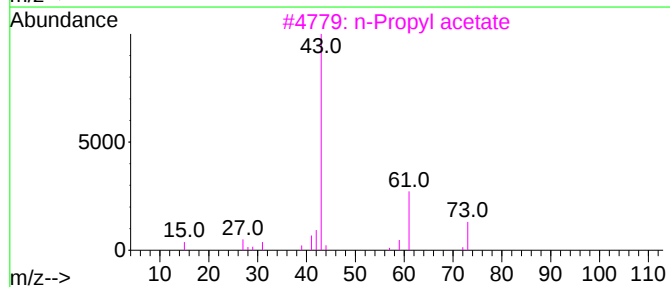
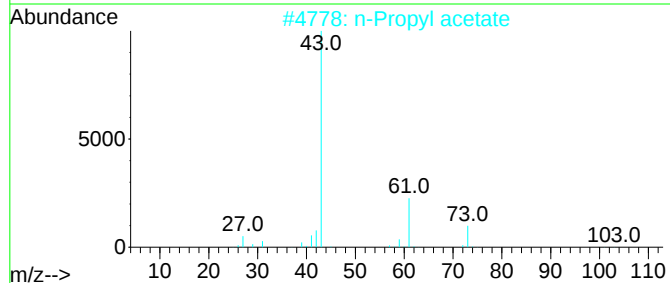
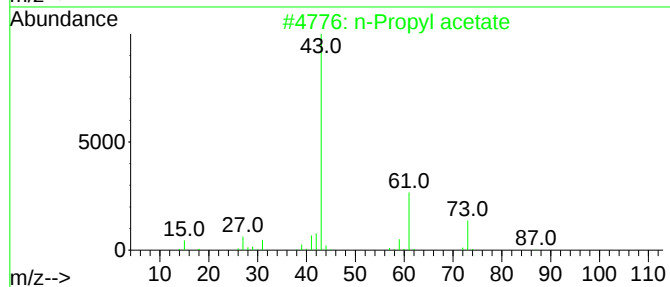
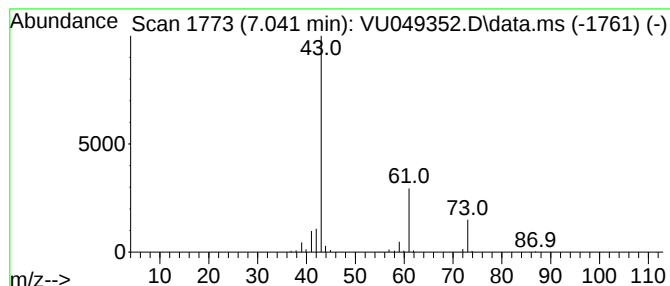
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	16.52 ug/L	189177	1,4-Difluorobenzene	6.250

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	83
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	78
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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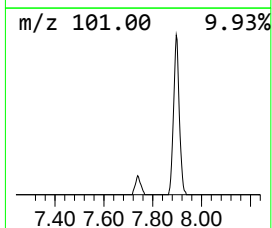
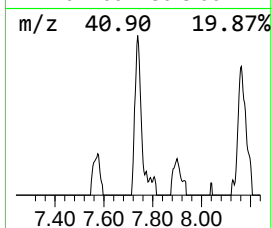
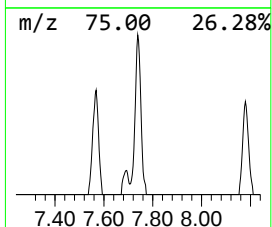
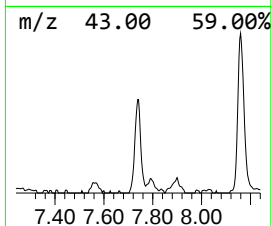
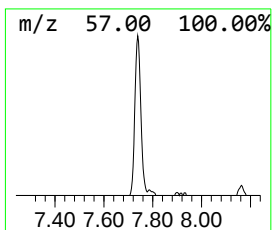
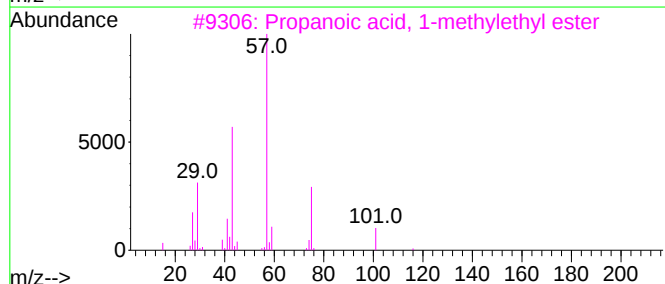
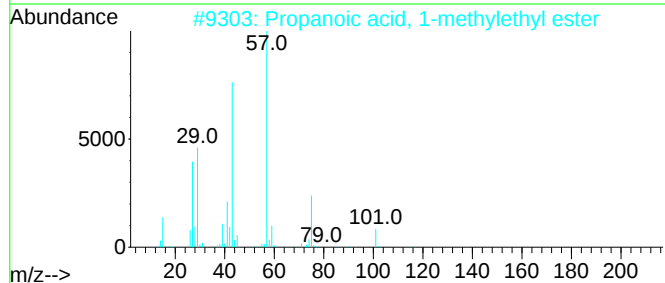
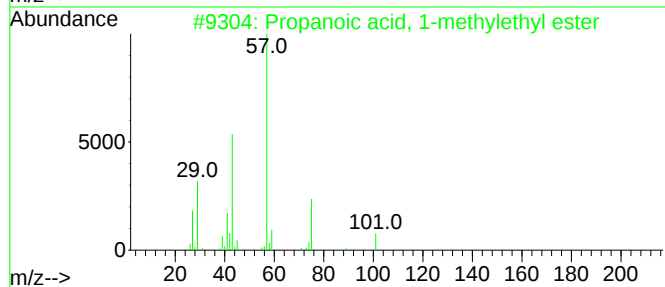
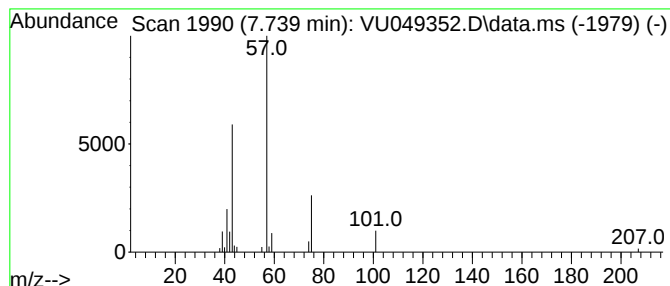
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	3.03 ug/L	34644	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	40
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049352.D
Acq On : 22 Jun 2022 15:22
Operator : SY/MD
Sample : N3392-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY1

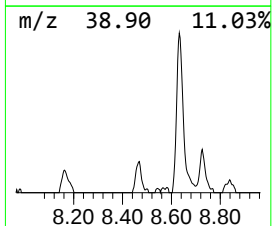
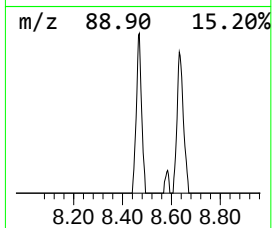
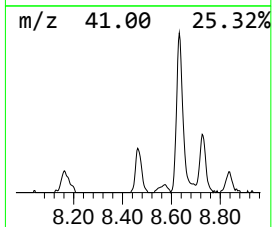
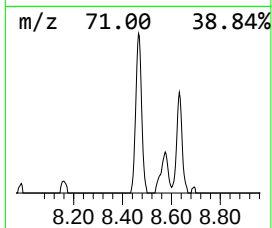
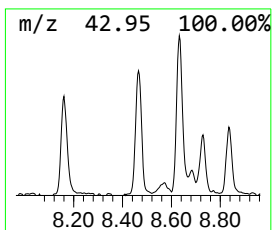
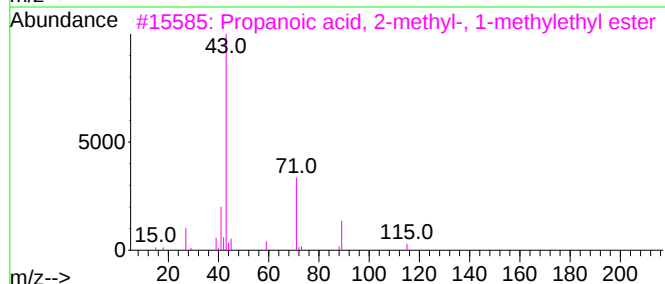
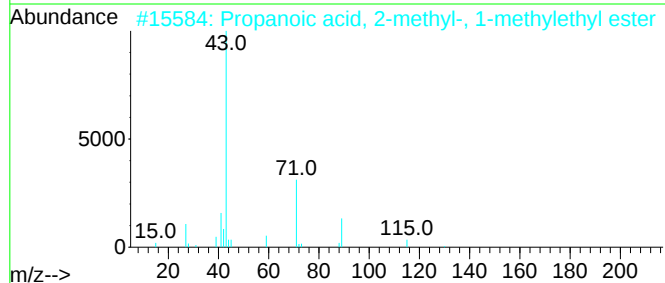
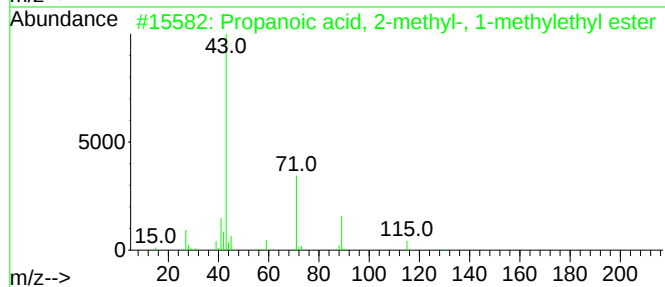
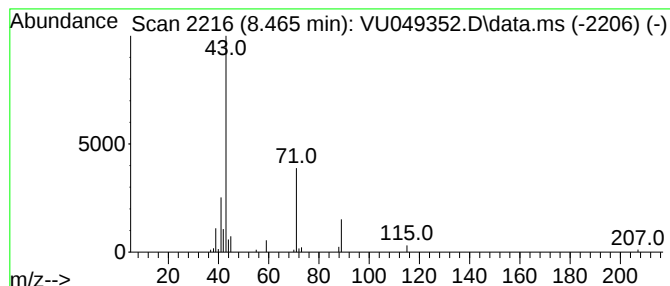
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.87 ug/L	38726	Chlorobenzene-d5	9.417

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	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049352.D
Acq On : 22 Jun 2022 15:22
Operator : SY/MD
Sample : N3392-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY1

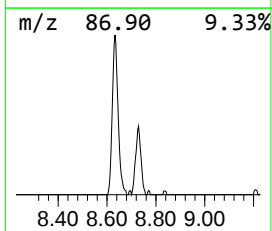
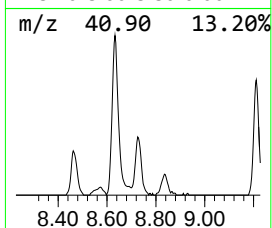
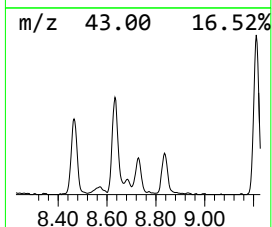
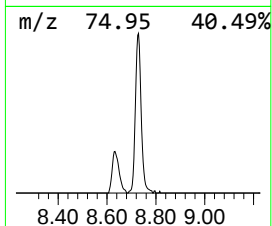
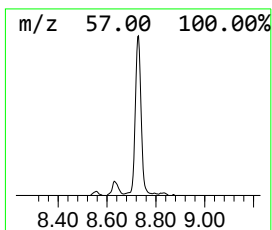
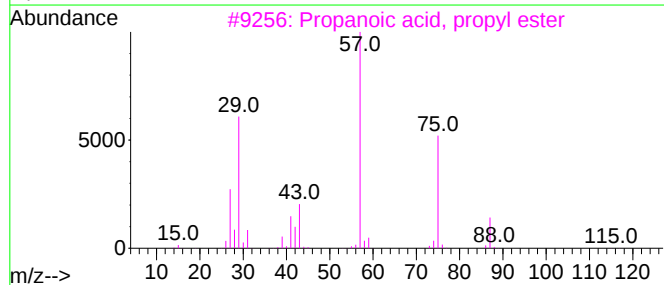
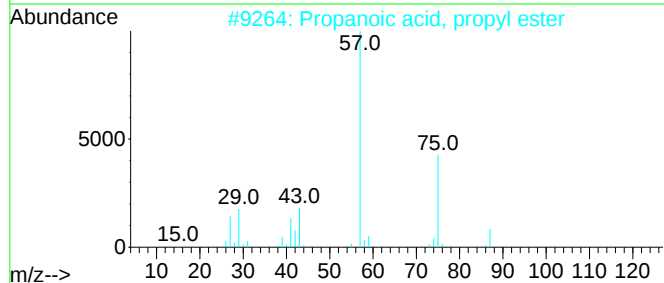
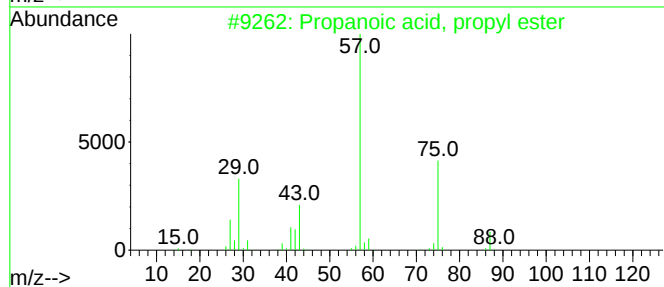
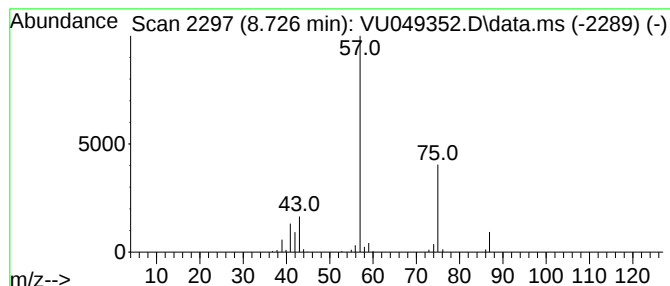
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Quant Title : VOC Analysis

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	6.92 ug/L	93379	Chlorobenzene-d5	9.417

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	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049352.D
Acq On : 22 Jun 2022 15:22
Operator : SY/MD
Sample : N3392-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY1

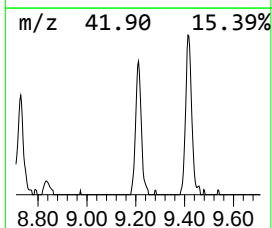
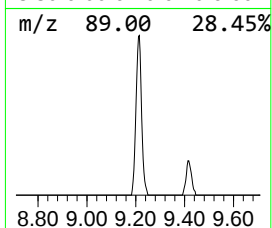
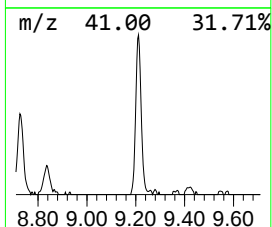
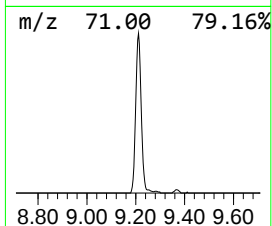
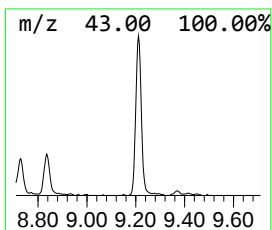
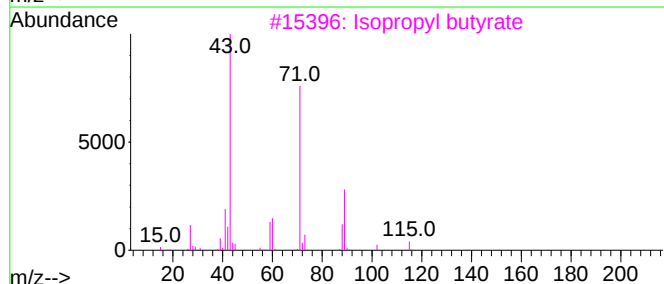
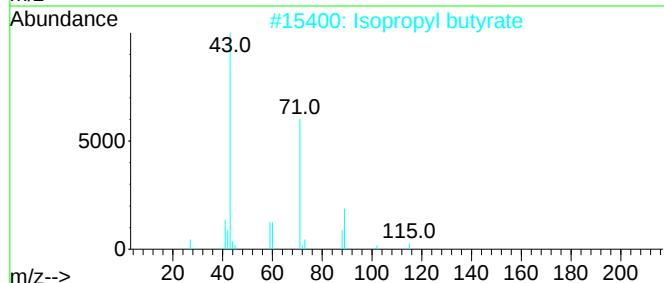
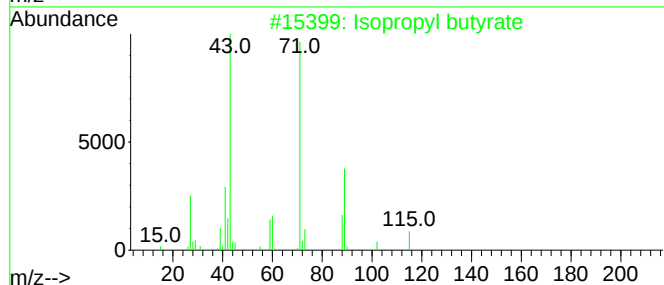
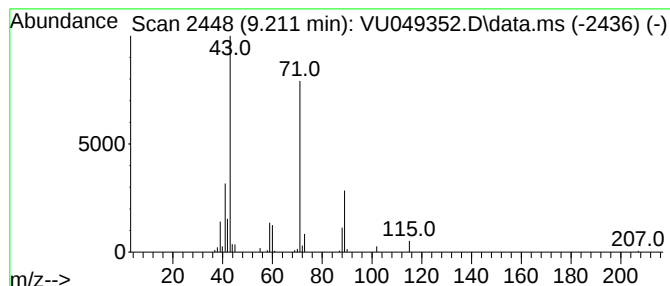
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	8.53 ug/L	115199	Chlorobenzene-d5	9.417

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	90
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\VU062222\
Data File : VU049352.D
Acq On : 22 Jun 2022 15:22
Operator : SY/MD
Sample : N3392-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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
(DEL) Alkane: S...	1.359	5.2	ug/L	59246	1	6.250	572430	50.0
n-Propyl acetate	7.041	16.5	ug/L	189177	1	6.250	572430	50.0
Propanoic acid,...	7.739	3.0	ug/L	34644	1	6.250	572430	50.0
Propanoic acid,...	8.465	2.9	ug/L	38726	2	9.417	675046	50.0
Propanoic acid,...	8.726	6.9	ug/L	93379	2	9.417	675046	50.0
Isopropyl butyrate	9.211	8.5	ug/L	115199	2	9.417	675046	50.0