

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049370.D
 Acq On : 23 Jun 2022 11:38
 Operator : SY/MD
 Sample : N3392-21 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ6

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: VU049370.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	41	46	50	rBV4	2688	3584	0.57%	0.058%
2	1.597	73	80	93	rBV	56470	67110	10.69%	1.084%
3	1.906	168	176	195	rVB	52262	70606	11.25%	1.141%
4	2.565	370	381	395	rBV	91181	147683	23.53%	2.386%
5	2.633	395	402	413	rVB3	2641	5072	0.81%	0.082%
6	2.716	425	428	430	rBV2	334	223	0.04%	0.004%
7	2.777	439	447	448	rBV3	1352	1165	0.19%	0.019%
8	2.957	499	503	505	rBV2	530	374	0.06%	0.006%
9	3.044	517	530	543	rBV2	16031	29371	4.68%	0.474%
10	3.099	543	547	550	rBV2	299	230	0.04%	0.004%
11	3.186	558	574	597	rBV	30455	71595	11.41%	1.157%
12	3.314	611	614	617	rVB2	335	208	0.03%	0.003%
13	3.944	805	810	817	rBV2	413	477	0.08%	0.008%
14	4.395	947	950	952	rBV	356	221	0.04%	0.004%
15	4.427	957	960	965	rVB2	250	214	0.03%	0.003%
16	4.543	991	996	999	rBV2	363	352	0.06%	0.006%
17	4.623	1007	1021	1060	rBV2	128472	341907	54.48%	5.523%
18	4.909	1107	1110	1113	rBV3	324	219	0.03%	0.004%
19	4.932	1113	1117	1120	rVB4	437	338	0.05%	0.005%
20	5.063	1141	1158	1181	rVV	127457	276108	44.00%	4.461%
21	5.337	1237	1243	1253	rVB2	401	538	0.09%	0.009%
22	5.723	1338	1363	1389	rBV2	222967	627559	100.00%	10.138%
23	5.813	1389	1391	1393	rVB2	423	200	0.03%	0.003%
24	5.915	1409	1423	1436	rBV3	9533	19124	3.05%	0.309%
25	5.977	1440	1442	1444	rVV3	439	244	0.04%	0.004%
26	5.999	1447	1449	1455	rVB3	269	225	0.04%	0.004%
27	6.141	1488	1493	1496	rBB2	242	212	0.03%	0.003%
28	6.247	1510	1526	1550	rBV	254189	482074	76.82%	7.788%
29	6.401	1572	1574	1577	rVB2	373	198	0.03%	0.003%
30	6.530	1606	1614	1623	rVB4	1705	2851	0.45%	0.046%
31	6.690	1650	1664	1682	rBV	166407	324289	51.67%	5.239%
32	6.787	1692	1694	1697	rBV2	388	289	0.05%	0.005%
33	6.861	1713	1717	1722	rVB	317	195	0.03%	0.003%
34	6.925	1726	1737	1751	rBV2	4838	10511	1.67%	0.170%
35	7.041	1761	1773	1795	rBV	104503	189999	30.28%	3.069%
36	7.179	1810	1816	1826	rVB6	1764	3288	0.52%	0.053%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049370.D
 Acq On : 23 Jun 2022 11:38
 Operator : SY/MD
 Sample : N3392-21 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ6

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

37	7.314	1856	1858	1863	rVB2	392	289	0.05%	0.005%
38	7.343	1863	1867	1872	rVB2	307	290	0.05%	0.005%
39	7.394	1878	1883	1887	rBV2	336	282	0.04%	0.005%
40	7.494	1911	1914	1916	rBV	267	212	0.03%	0.003%
41	7.565	1924	1936	1957	rBV	79684	141845	22.60%	2.291%
42	7.694	1971	1976	1980	rBV3	823	824	0.13%	0.013%
43	7.739	1980	1990	2000	rBV	18858	30965	4.93%	0.500%
44	7.896	2026	2039	2060	rBV	241341	417025	66.45%	6.737%
45	8.179	2109	2127	2150	rBV3	63493	137527	21.91%	2.222%
46	8.388	2188	2192	2194	rBV	287	203	0.03%	0.003%
47	8.465	2206	2216	2229	rVV	22453	37200	5.93%	0.601%
48	8.571	2234	2249	2256	rBV5	4431	9856	1.57%	0.159%
49	8.632	2256	2268	2289	rVV2	321678	590341	94.07%	9.537%
50	8.726	2290	2297	2317	rVB	46261	79994	12.75%	1.292%
51	8.835	2322	2331	2350	rVB	28469	46859	7.47%	0.757%
52	8.906	2350	2353	2354	rBV	641	343	0.05%	0.006%
53	8.951	2363	2367	2370	rVB3	389	353	0.06%	0.006%
54	8.967	2370	2372	2377	rBV	286	195	0.03%	0.003%
55	9.031	2386	2392	2395	rBV2	260	332	0.05%	0.005%
56	9.044	2395	2396	2402	rVB2	434	320	0.05%	0.005%
57	9.211	2437	2448	2465	rBV	67061	106973	17.05%	1.728%
58	9.369	2489	2497	2500	rBV3	1064	1555	0.25%	0.025%
59	9.417	2500	2512	2542	rVB	339488	557498	88.84%	9.006%
60	9.571	2557	2560	2563	rBV	381	289	0.05%	0.005%
61	9.607	2569	2571	2575	rBV	214	193	0.03%	0.003%
62	9.645	2576	2583	2587	rBV	723	854	0.14%	0.014%
63	9.918	2663	2668	2682	rVB3	913	1272	0.20%	0.021%
64	10.073	2705	2716	2728	rBV3	4565	7255	1.16%	0.117%
65	10.128	2730	2733	2738	rVB2	403	245	0.04%	0.004%
66	10.382	2809	2812	2815	rVV3	281	231	0.04%	0.004%
67	10.565	2867	2869	2873	rBV3	263	209	0.03%	0.003%
68	10.754	2916	2928	2947	rBV	275066	437788	69.76%	7.072%
69	11.089	3030	3032	3038	rVB	287	209	0.03%	0.003%
70	11.121	3038	3042	3046	rVB3	408	353	0.06%	0.006%
71	11.144	3046	3049	3054	rBV	282	234	0.04%	0.004%
72	11.201	3063	3067	3072	rBV2	176	220	0.04%	0.004%
73	11.285	3087	3093	3096	rBV2	380	364	0.06%	0.006%
74	11.677	3210	3215	3218	rBV2	295	305	0.05%	0.005%
75	11.812	3244	3257	3273	rBV	299427	480298	76.53%	7.759%
76	11.986	3306	3311	3318	rBV2	284	349	0.06%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049370.D
 Acq On : 23 Jun 2022 11:38
 Operator : SY/MD
 Sample : N3392-21 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ6

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

77	12.192	3363	3375	3394	rBV	247442	407267	64.90%	6.579%
78	12.398	3436	3439	3442	rVB2	305	203	0.03%	0.003%
79	12.516	3472	3476	3480	rBV3	419	394	0.06%	0.006%
80	12.555	3485	3488	3495	rVB2	307	342	0.05%	0.006%
81	13.076	3645	3650	3653	rVB3	345	336	0.05%	0.005%
82	13.095	3653	3656	3659	rVB2	304	201	0.03%	0.003%
83	13.250	3700	3704	3708	rVB2	409	315	0.05%	0.005%
84	13.275	3708	3712	3714	rBV	336	289	0.05%	0.005%
85	13.304	3719	3721	3724	rVV2	334	203	0.03%	0.003%
86	13.327	3724	3728	3731	rVB	345	258	0.04%	0.004%
87	13.684	3832	3839	3844	rBV2	522	745	0.12%	0.012%
88	13.709	3844	3847	3850	rBV2	415	343	0.05%	0.006%
89	13.754	3859	3861	3866	rVB2	339	263	0.04%	0.004%
90	13.844	3885	3889	3890	rBV	726	460	0.07%	0.007%
91	13.909	3905	3909	3914	rBV3	329	370	0.06%	0.006%
92	13.986	3931	3933	3935	rBV	339	208	0.03%	0.003%
93	14.098	3959	3968	3979	rBV4	1908	3952	0.63%	0.064%
94	14.323	4035	4038	4039	rBV2	513	292	0.05%	0.005%
95	14.397	4058	4061	4064	rVB	548	385	0.06%	0.006%
96	14.439	4064	4074	4077	rBV3	481	728	0.12%	0.012%
97	14.803	4182	4187	4191	rVB2	368	382	0.06%	0.006%
98	15.385	4366	4368	4372	rBV3	356	252	0.04%	0.004%
99	15.719	4467	4472	4475	rBV4	645	664	0.11%	0.011%
100	15.963	4546	4548	4552	rBV3	496	406	0.06%	0.007%

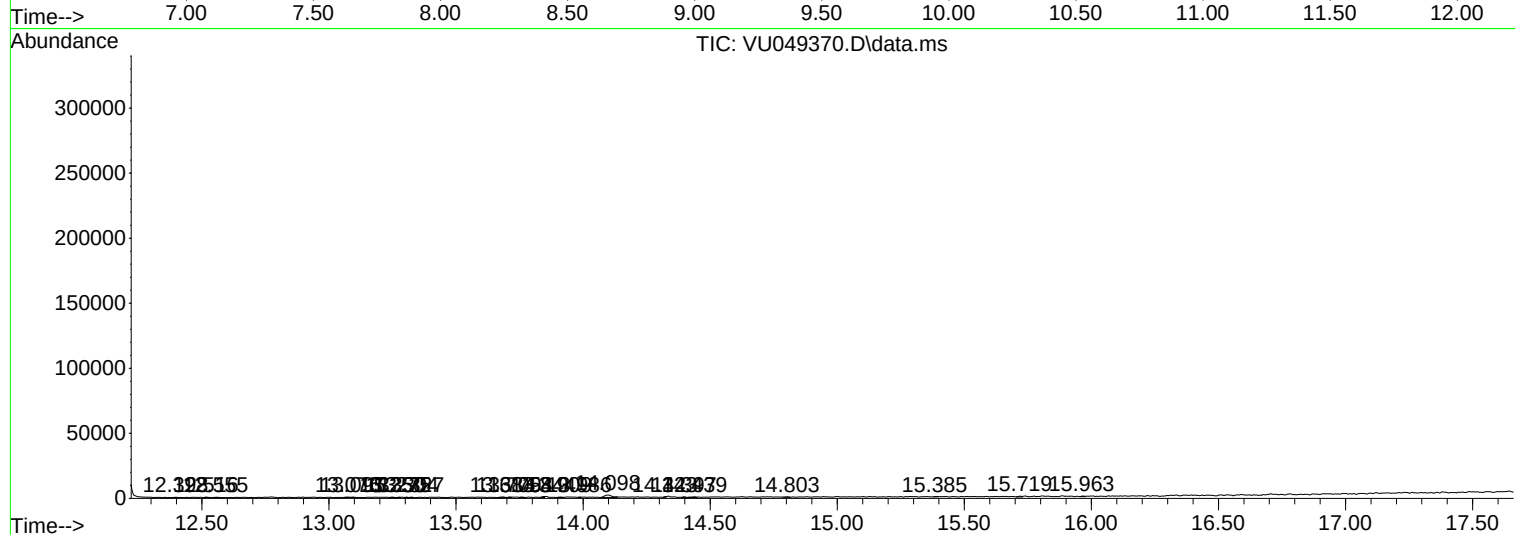
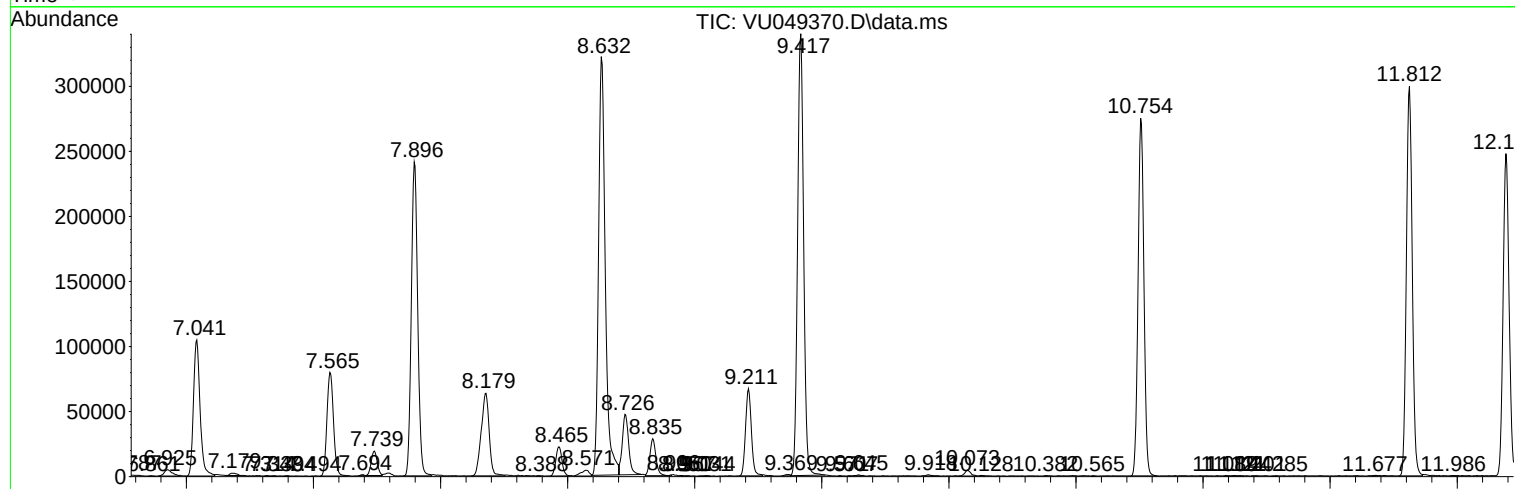
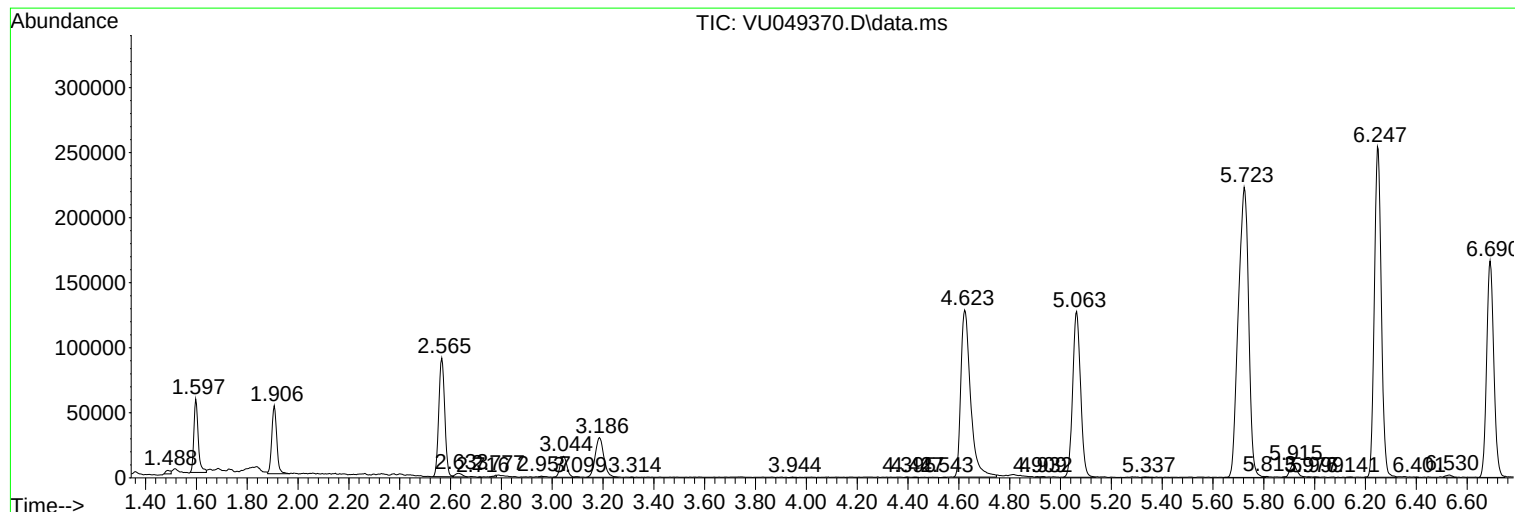
Sum of corrected areas: 6190060

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

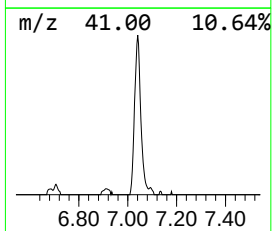
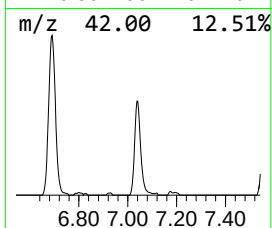
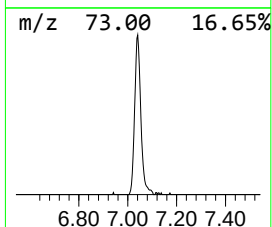
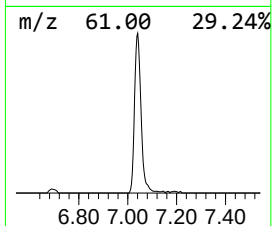
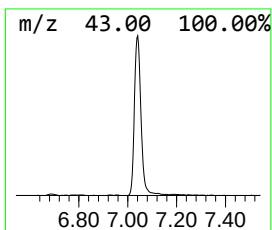
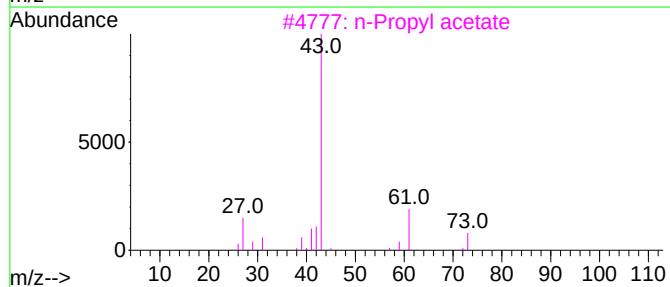
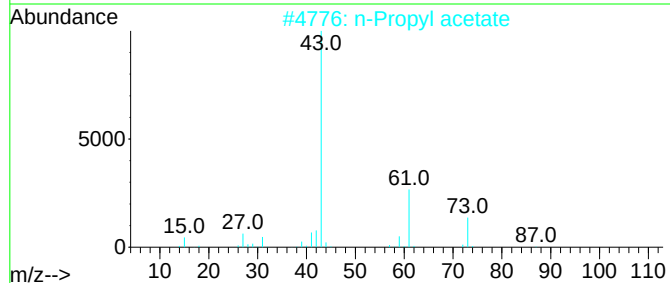
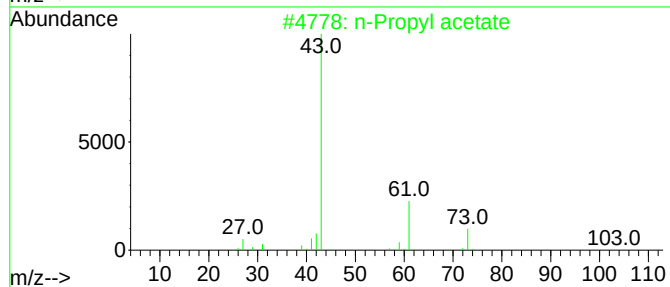
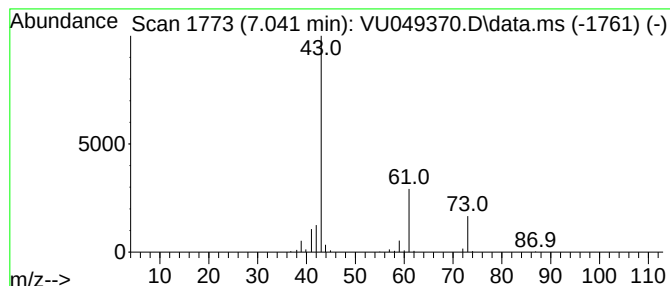
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	19.71 ug/L	189999	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

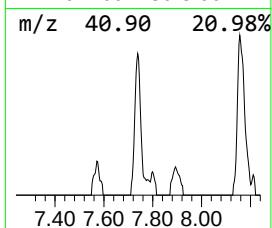
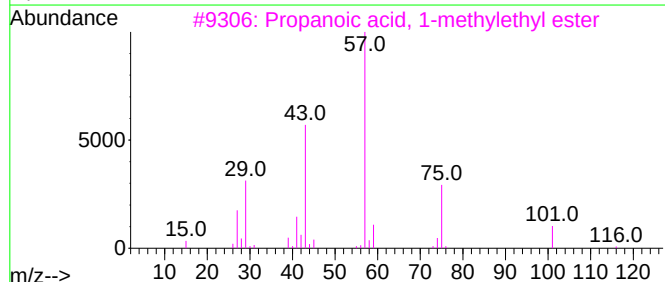
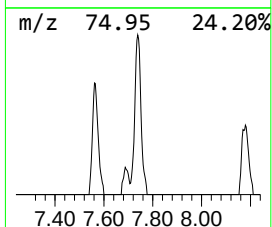
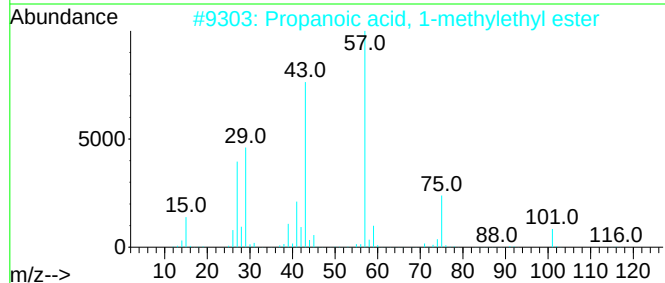
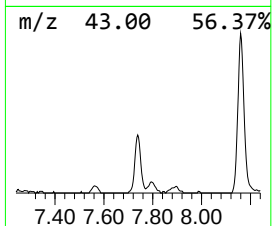
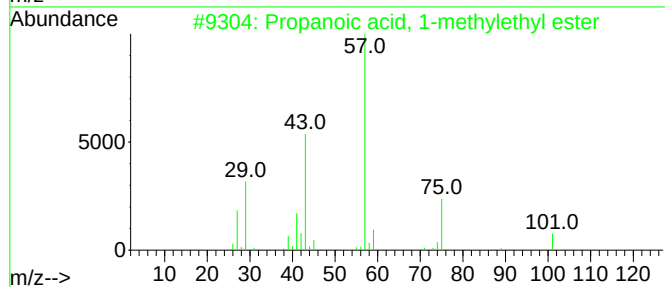
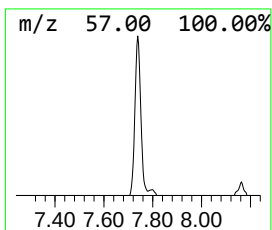
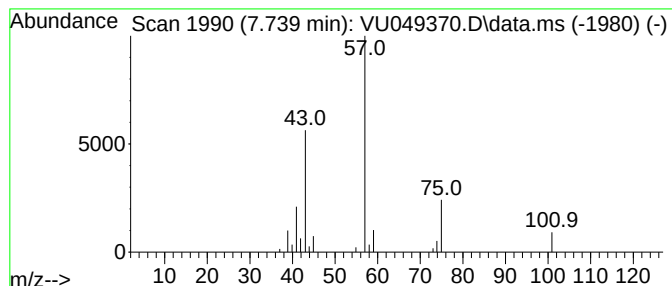
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	3.21 ug/L	30965	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	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

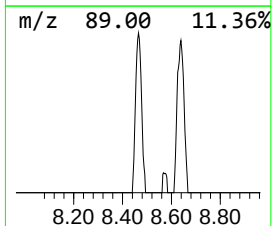
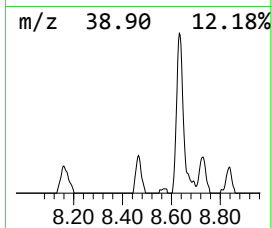
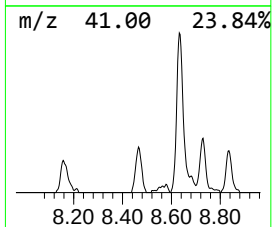
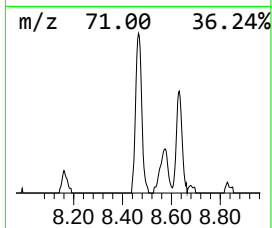
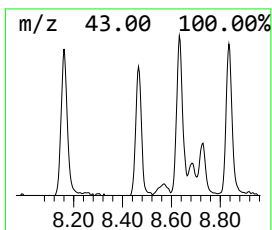
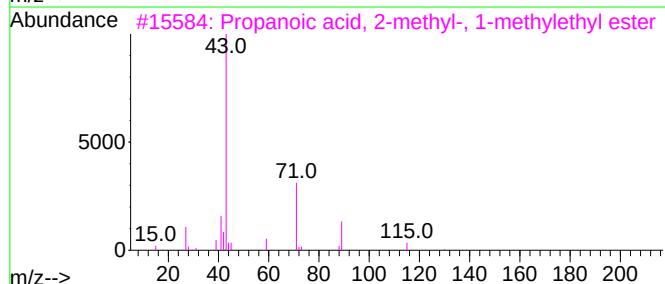
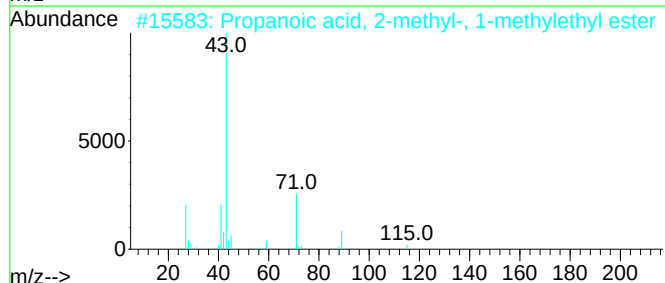
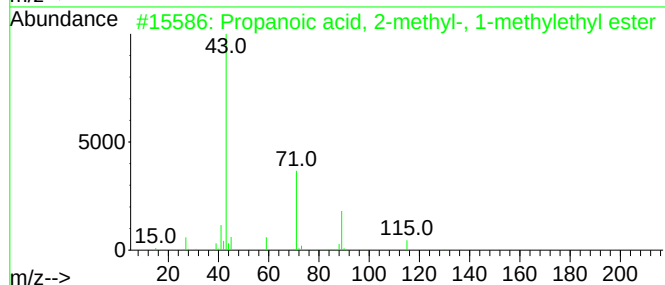
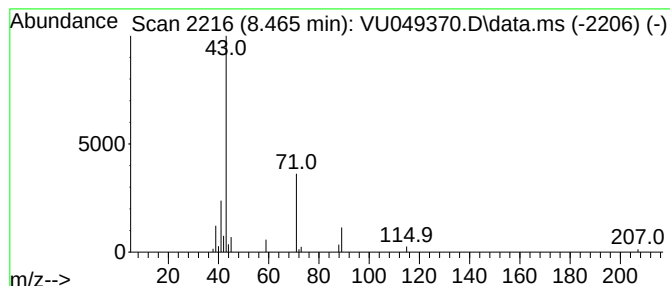
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.34 ug/L	37200	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	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	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

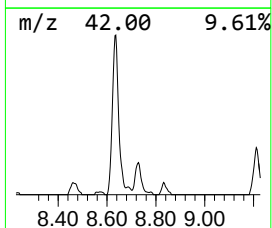
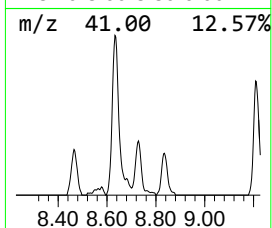
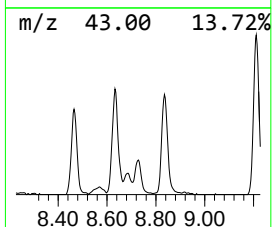
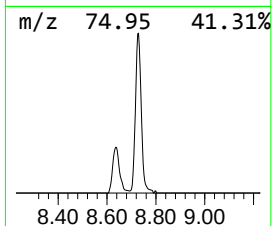
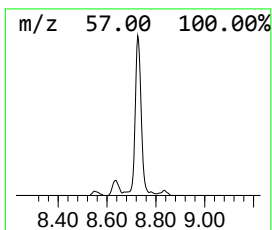
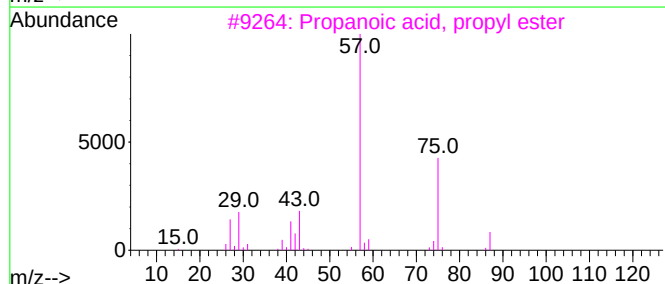
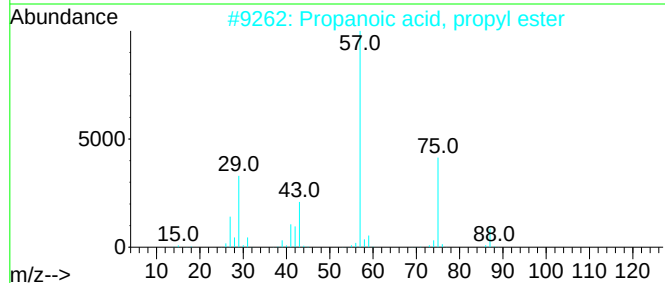
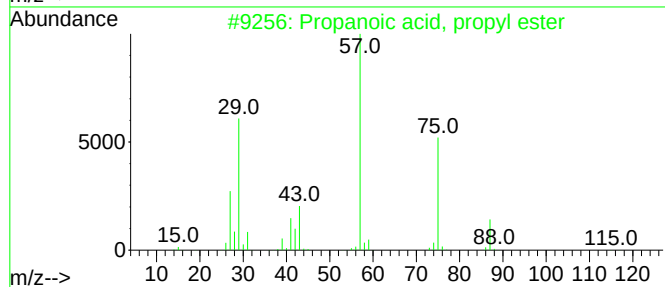
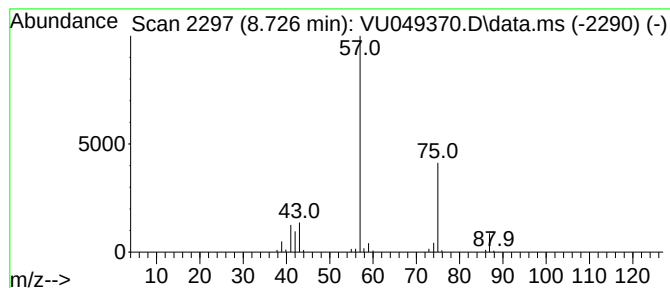
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	7.17 ug/L	79994	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	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

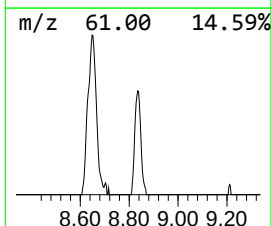
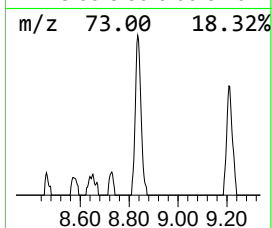
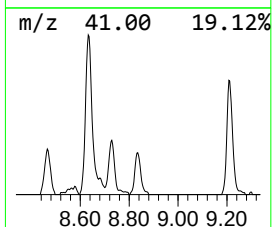
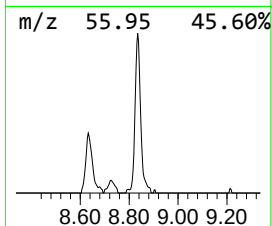
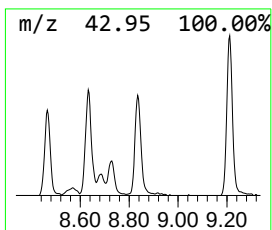
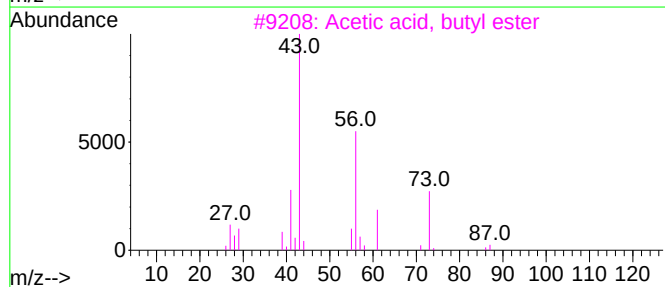
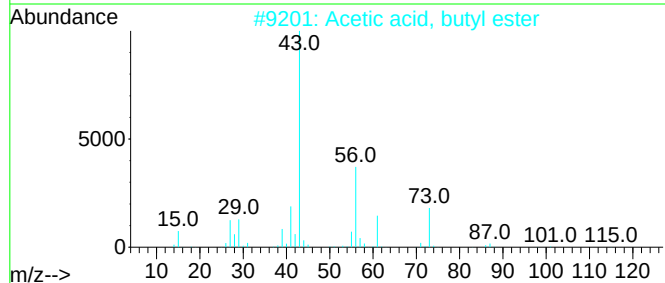
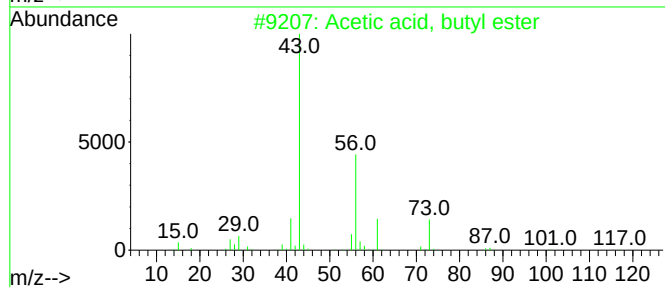
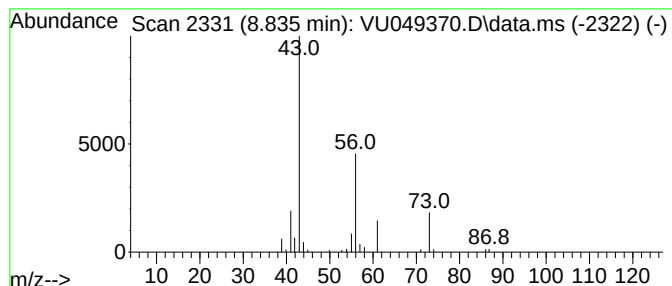
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	4.20 ug/L	46859	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	53
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

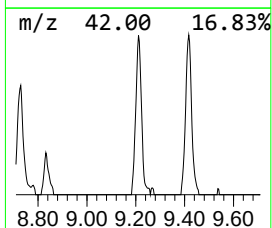
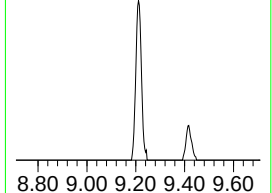
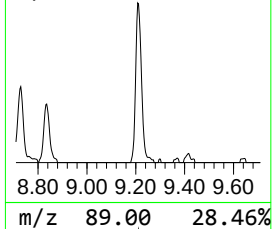
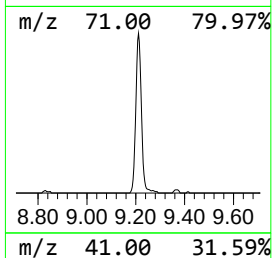
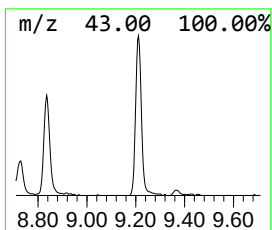
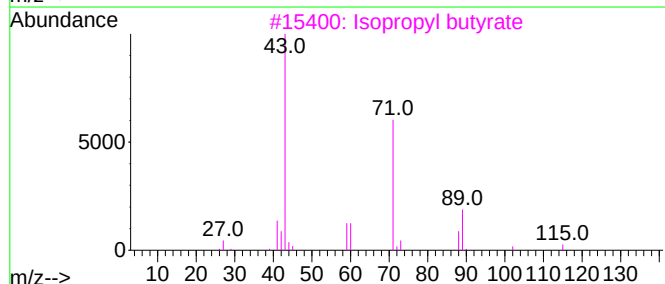
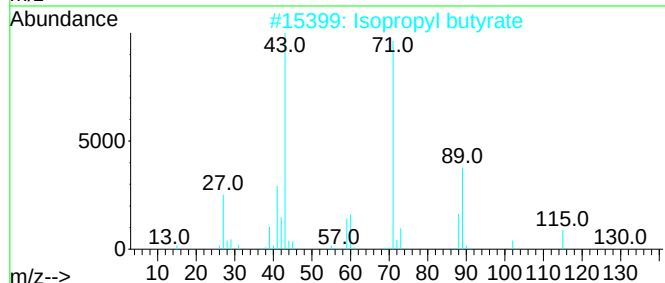
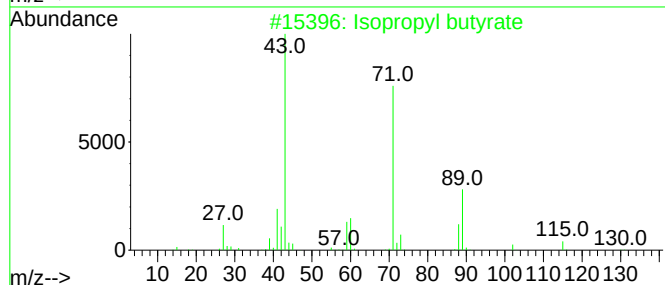
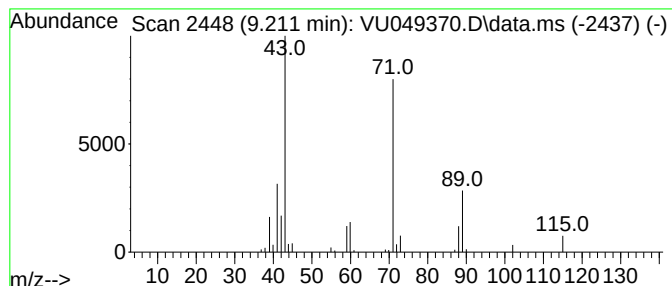
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 9 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	9.59 ug/L	106973	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	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049370.D
Acq On : 23 Jun 2022 11:38
Operator : SY/MD
Sample : N3392-21 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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	7.041	19.7	ug/L	189999	1	6.250	482074	50.0
Propanoic acid,...	7.739	3.2	ug/L	30965	1	6.250	482074	50.0
Propanoic acid,...	8.465	3.3	ug/L	37200	2	9.417	557498	50.0
Propanoic acid,...	8.726	7.2	ug/L	79994	2	9.417	557498	50.0
Acetic acid, bu...	8.835	4.2	ug/L	46859	2	9.417	557498	50.0
Isopropyl butyrate	9.211	9.6	ug/L	106973	2	9.417	557498	50.0