

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049373.D
 Acq On : 23 Jun 2022 12:48
 Operator : SY/MD
 Sample : N3392-16 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ1

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: VU049373.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	40	46	48	rBV4	2854	3253	0.38%	0.043%
2	1.597	73	80	97	rBV	96843	114522	13.43%	1.520%
3	1.906	168	176	192	rVB	77436	102066	11.97%	1.355%
4	2.565	369	381	395	rBV	159543	254971	29.90%	3.385%
5	2.636	398	403	415	rVB4	2119	3551	0.42%	0.047%
6	2.768	441	444	447	rVB2	353	223	0.03%	0.003%
7	2.960	501	504	508	rBV2	263	211	0.02%	0.003%
8	3.044	521	530	543	rVB3	5668	10187	1.19%	0.135%
9	3.108	547	550	553	rVB2	292	193	0.02%	0.003%
10	3.189	563	575	586	rVB2	1697	3976	0.47%	0.053%
11	3.301	605	610	615	rBV	284	262	0.03%	0.003%
12	3.620	706	709	712	rBV2	266	185	0.02%	0.002%
13	3.748	746	749	755	rBV3	294	293	0.03%	0.004%
14	3.906	794	798	801	rVB2	207	192	0.02%	0.003%
15	4.102	855	859	865	rBV2	173	195	0.02%	0.003%
16	4.285	913	916	920	rVB2	366	267	0.03%	0.004%
17	4.388	941	948	951	rBV2	256	331	0.04%	0.004%
18	4.452	963	968	970	rBV	210	198	0.02%	0.003%
19	4.507	981	985	989	rVB2	265	220	0.03%	0.003%
20	4.623	1009	1021	1048	rBV	113231	283461	33.25%	3.763%
21	4.986	1132	1134	1138	rVB2	494	358	0.04%	0.005%
22	5.063	1142	1158	1180	rVV	162938	357352	41.91%	4.744%
23	5.173	1189	1192	1196	rVB4	337	199	0.02%	0.003%
24	5.192	1196	1198	1203	rVB2	283	207	0.02%	0.003%
25	5.285	1222	1227	1232	rVB3	659	763	0.09%	0.010%
26	5.330	1238	1241	1244	rBV	295	187	0.02%	0.002%
27	5.726	1343	1364	1390	rBV2	313947	852630	100.00%	11.320%
28	5.845	1399	1401	1408	rVB2	513	385	0.05%	0.005%
29	5.912	1409	1422	1435	rBV2	9515	19794	2.32%	0.263%
30	6.009	1449	1452	1457	rVB3	338	297	0.03%	0.004%
31	6.115	1482	1485	1487	rBV	344	225	0.03%	0.003%
32	6.156	1495	1498	1502	rBV3	325	235	0.03%	0.003%
33	6.246	1511	1526	1546	rBV	297331	563791	66.12%	7.485%
34	6.398	1570	1573	1576	rBV4	412	286	0.03%	0.004%
35	6.449	1586	1589	1592	rBV2	309	236	0.03%	0.003%
36	6.526	1607	1613	1622	rBV4	1594	2767	0.32%	0.037%

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Integrator: RTE

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

37	6.574	1626	1628	1632	rVB	425	222	0.03%	0.003%
38	6.613	1637	1640	1643	rBV2	362	223	0.03%	0.003%
39	6.690	1647	1664	1681	rBV	215808	415582	48.74%	5.517%
40	6.780	1687	1692	1696	rBV3	624	720	0.08%	0.010%
41	6.806	1696	1700	1703	rVV3	364	344	0.04%	0.005%
42	6.928	1727	1738	1755	rBV2	4934	11284	1.32%	0.150%
43	7.041	1759	1773	1790	rBV	111526	200460	23.51%	2.661%
44	7.185	1810	1818	1833	rVB6	2915	5457	0.64%	0.072%
45	7.375	1873	1877	1881	rBV2	272	221	0.03%	0.003%
46	7.398	1881	1884	1888	rVB2	316	227	0.03%	0.003%
47	7.507	1912	1918	1920	rBV3	347	292	0.03%	0.004%
48	7.565	1924	1936	1954	rVV2	110603	197335	23.14%	2.620%
49	7.671	1966	1969	1970	rBV	315	192	0.02%	0.003%
50	7.687	1970	1974	1980	rVV3	926	1196	0.14%	0.016%
51	7.738	1980	1990	2001	rVV2	19599	33144	3.89%	0.440%
52	7.896	2020	2039	2062	rBV	374627	647456	75.94%	8.596%
53	8.079	2094	2096	2100	rBV3	327	272	0.03%	0.004%
54	8.176	2107	2126	2143	rBV2	83113	175504	20.58%	2.330%
55	8.385	2188	2191	2197	rVB2	403	337	0.04%	0.004%
56	8.465	2205	2216	2232	rVV	25595	42456	4.98%	0.564%
57	8.632	2257	2268	2289	rBV	335052	616090	72.26%	8.179%
58	8.725	2290	2297	2321	rVV	51405	87297	10.24%	1.159%
59	8.835	2321	2331	2350	rVB2	30042	50295	5.90%	0.668%
60	9.211	2437	2448	2469	rBV	75651	120389	14.12%	1.598%
61	9.365	2489	2496	2499	rBV4	1610	1780	0.21%	0.024%
62	9.417	2499	2512	2534	rVV	406381	666656	78.19%	8.851%
63	9.561	2554	2557	2559	rBV2	340	230	0.03%	0.003%
64	9.574	2559	2561	2565	rVB3	301	229	0.03%	0.003%
65	9.642	2577	2582	2591	rVB3	1078	1364	0.16%	0.018%
66	9.754	2611	2617	2620	rVB2	346	335	0.04%	0.004%
67	9.790	2620	2628	2629	rBV2	309	376	0.04%	0.005%
68	9.873	2650	2654	2656	rBV	233	197	0.02%	0.003%
69	9.912	2662	2666	2667	rBV2	561	389	0.05%	0.005%
70	10.073	2708	2716	2725	rVB3	5205	7772	0.91%	0.103%
71	10.179	2747	2749	2755	rVB2	285	214	0.03%	0.003%
72	10.233	2762	2766	2769	rVV2	301	268	0.03%	0.004%
73	10.253	2770	2772	2779	rVB2	308	257	0.03%	0.003%
74	10.365	2804	2807	2812	rVB	231	209	0.02%	0.003%
75	10.754	2916	2928	2951	rVB	305111	495711	58.14%	6.581%
76	11.153	3050	3052	3057	rVB	343	222	0.03%	0.003%

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Max Peaks: 100

Stop Thrs : 0

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 Title : VOC Analysis

77	11.243	3078	3080	3087	rVB2	260	219	0.03%	0.003%
78	11.275	3087	3090	3092	rBV2	332	214	0.03%	0.003%
79	11.394	3122	3127	3130	rBV2	235	225	0.03%	0.003%
80	11.484	3151	3155	3159	rBV2	232	186	0.02%	0.002%
81	11.565	3175	3180	3183	rBV	404	437	0.05%	0.006%
82	11.748	3232	3237	3240	rVB2	405	405	0.05%	0.005%
83	11.812	3240	3257	3276	rBV	375349	596902	70.01%	7.925%
84	11.970	3303	3306	3309	rBV	266	207	0.02%	0.003%
85	12.192	3363	3375	3392	rBV	351467	566662	66.46%	7.523%
86	12.381	3431	3434	3444	rVB	390	431	0.05%	0.006%
87	12.439	3449	3452	3454	rBV	270	185	0.02%	0.002%
88	12.889	3590	3592	3596	rBV2	255	185	0.02%	0.002%
89	13.442	3761	3764	3767	rBV	532	330	0.04%	0.004%
90	13.465	3769	3771	3776	rVV2	241	221	0.03%	0.003%
91	13.693	3838	3842	3845	rBV2	353	336	0.04%	0.004%
92	13.757	3859	3862	3865	rBV3	261	204	0.02%	0.003%
93	13.815	3876	3880	3884	rBV2	340	306	0.04%	0.004%
94	13.847	3887	3890	3893	rBV3	281	222	0.03%	0.003%
95	14.095	3964	3967	3972	rBV3	802	539	0.06%	0.007%
96	14.581	4115	4118	4119	rBV	349	243	0.03%	0.003%
97	14.876	4208	4210	4214	rBV3	295	258	0.03%	0.003%
98	14.970	4236	4239	4241	rBV2	392	228	0.03%	0.003%
99	15.722	4470	4473	4475	rBV3	450	339	0.04%	0.005%
100	16.172	4608	4613	4616	rBV3	797	995	0.12%	0.013%

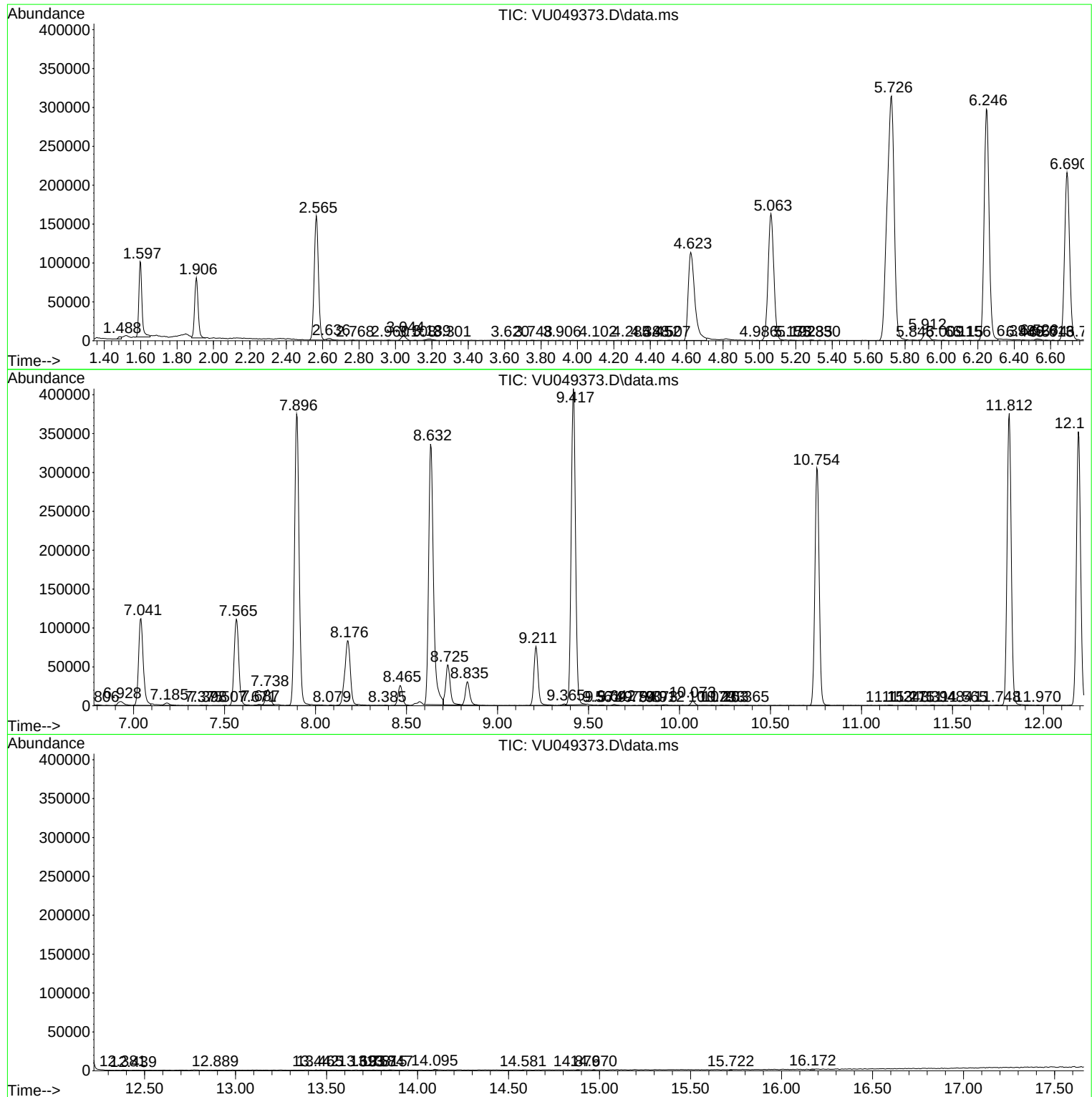
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

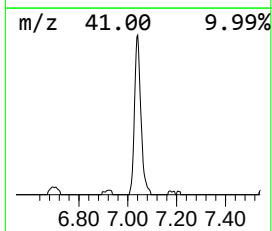
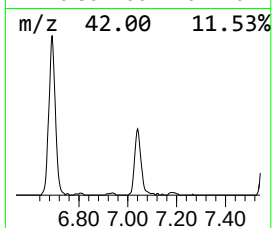
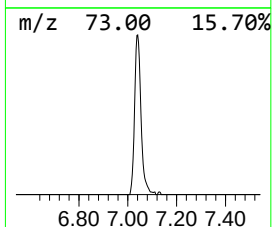
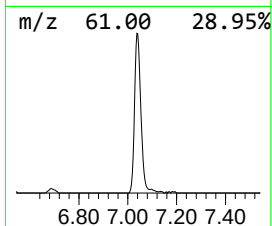
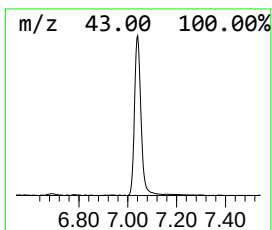
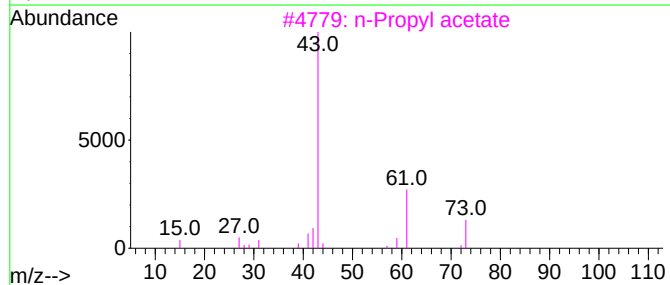
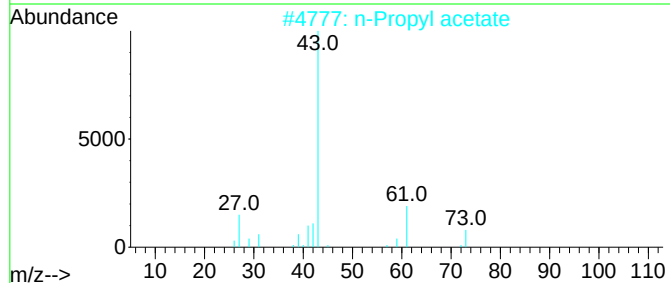
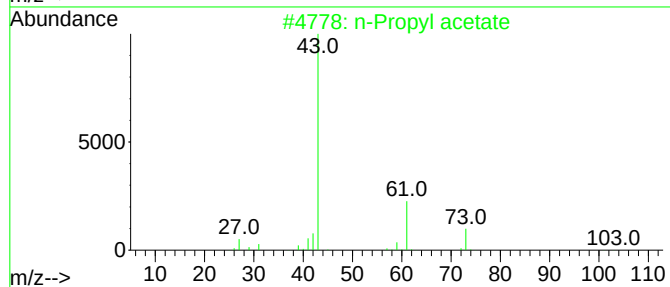
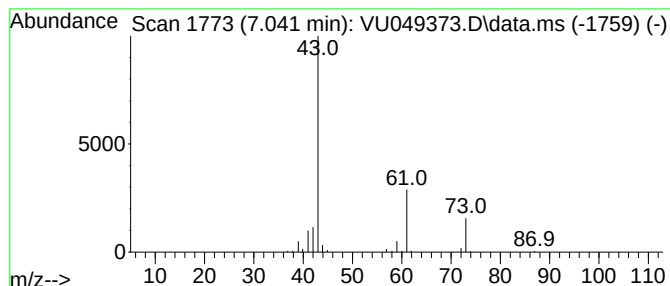
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	17.78 ug/L	200460	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	78
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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Instrument :
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EXEZ1

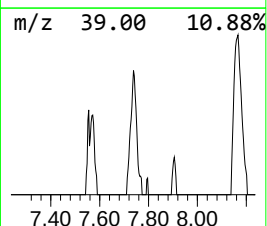
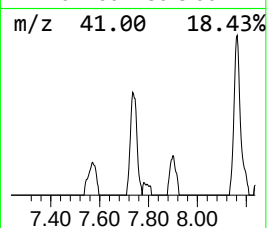
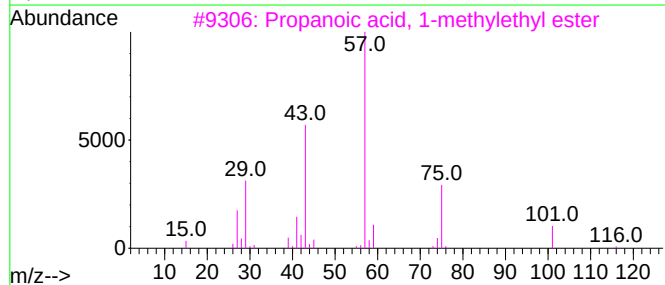
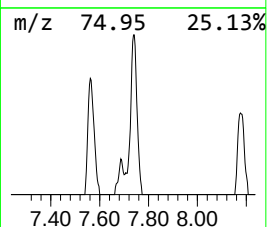
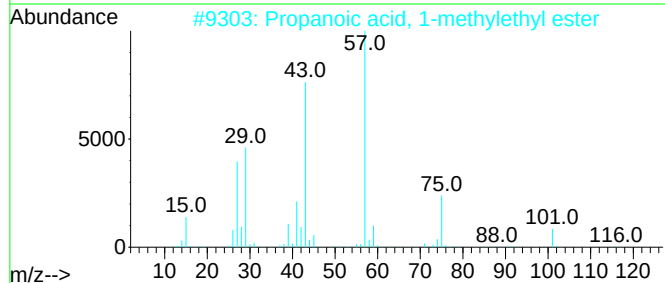
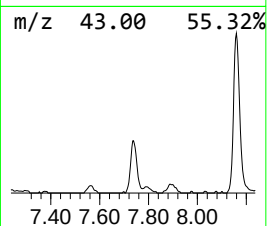
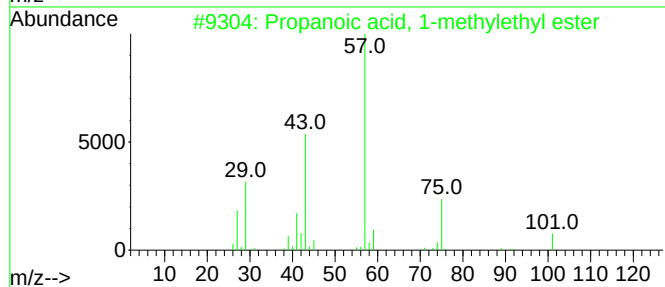
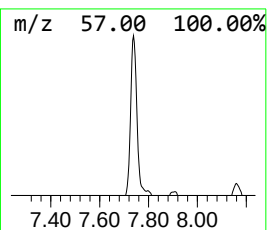
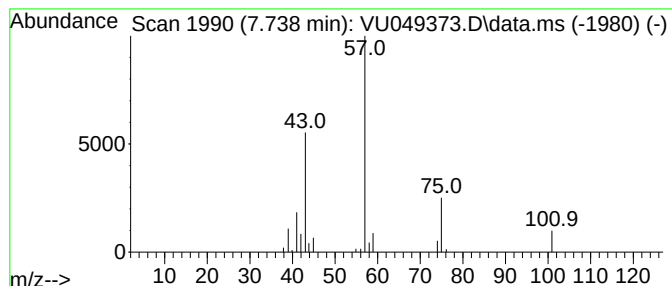
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.94 ug/L	33144	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	78
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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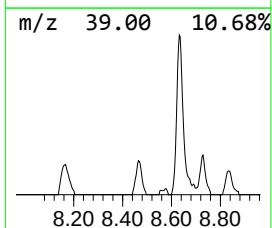
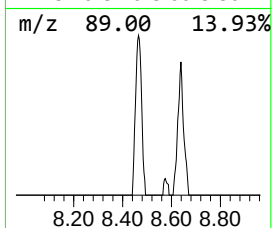
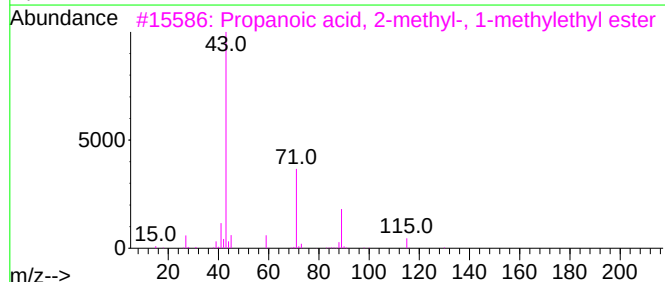
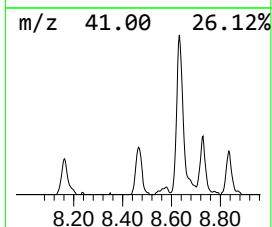
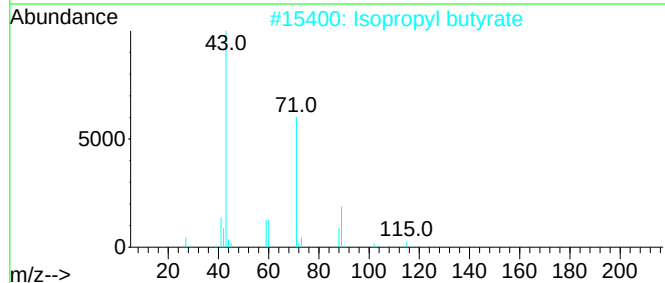
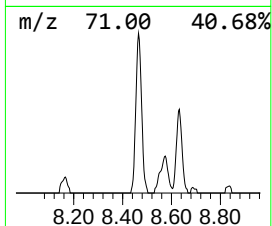
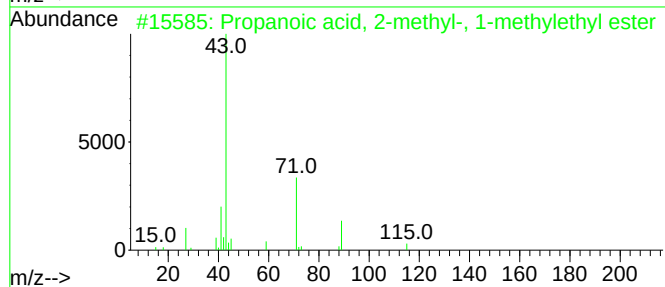
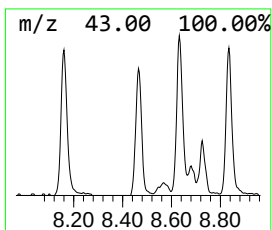
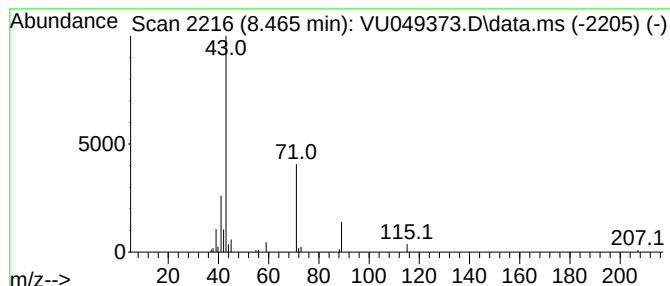
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.18 ug/L	42456	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049373.D
Acq On : 23 Jun 2022 12:48
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

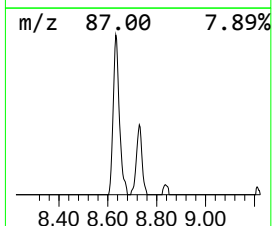
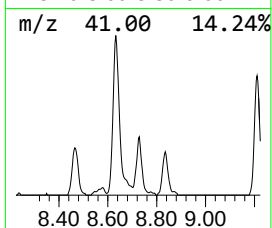
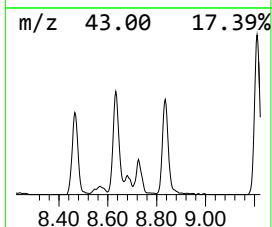
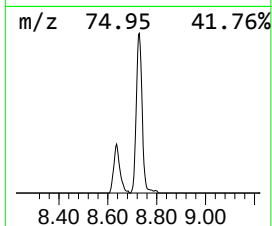
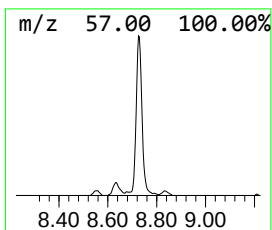
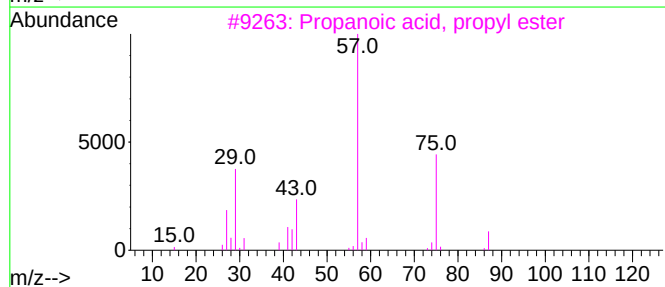
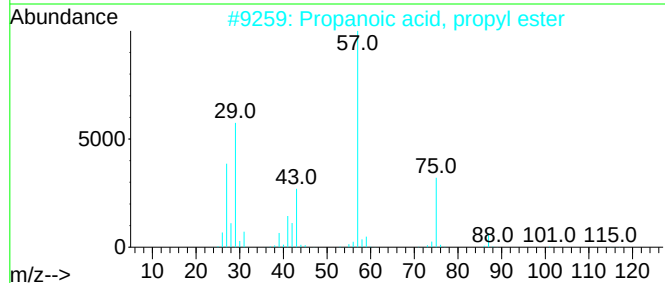
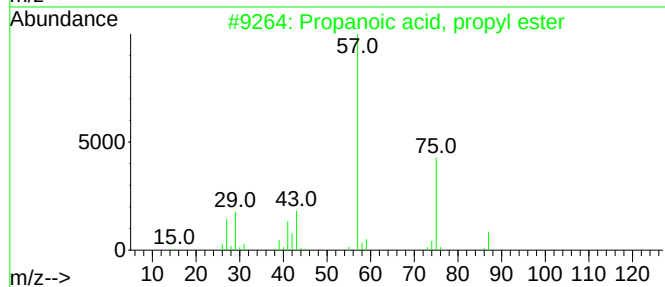
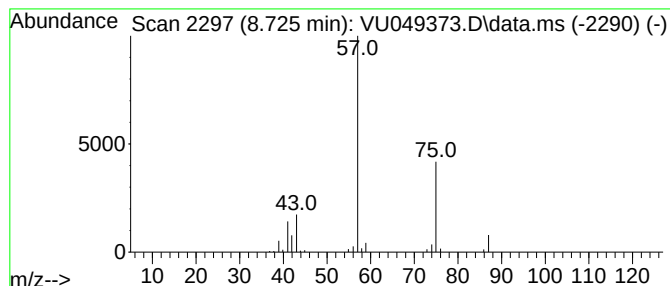
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Quant Title : VOC Analysis

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.
8.725	6.55 ug/L	87297	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	78
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049373.D
Acq On : 23 Jun 2022 12:48
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

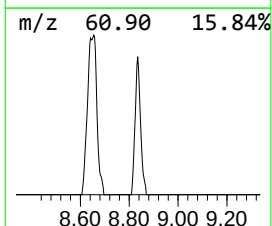
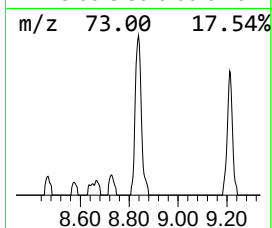
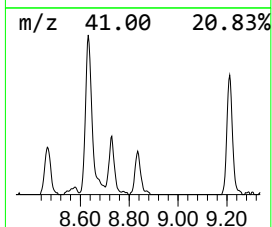
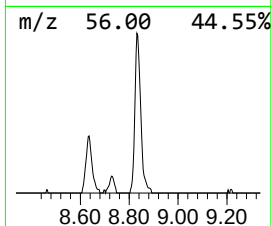
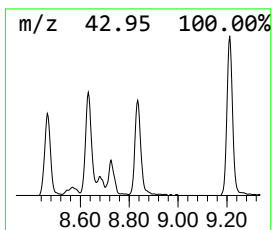
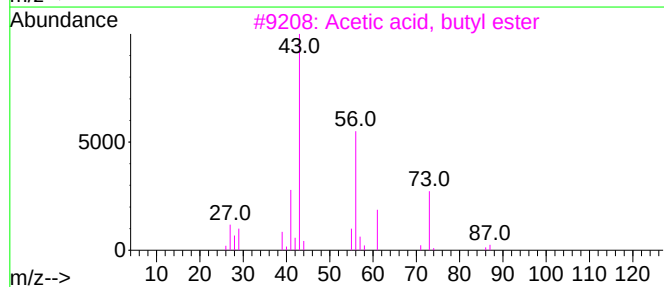
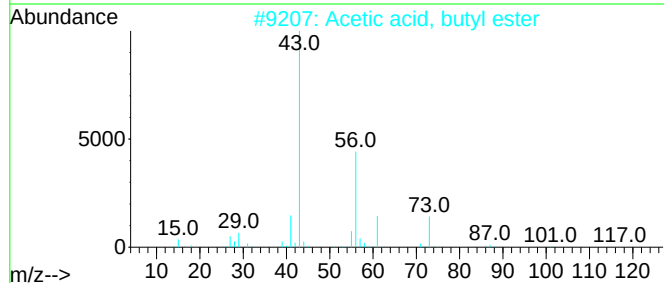
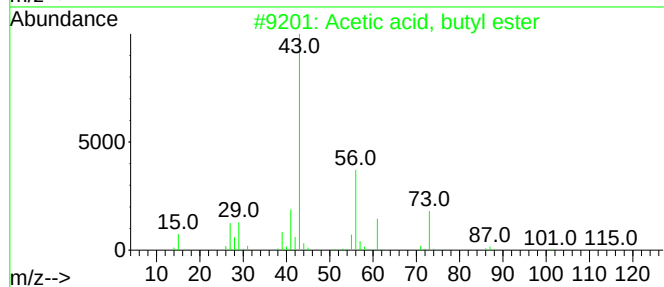
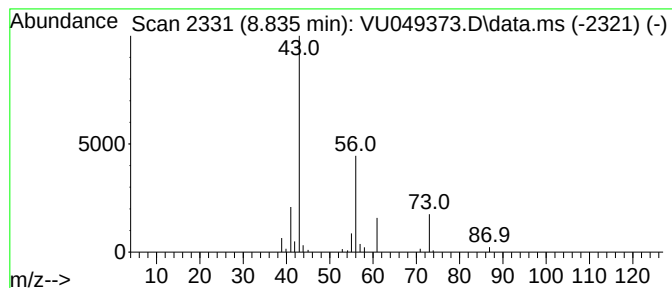
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.77 ug/L	50295	Chlorobenzene-d5	9.417

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	83		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56		
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049373.D
Acq On : 23 Jun 2022 12:48
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

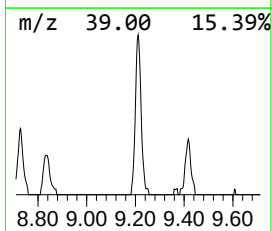
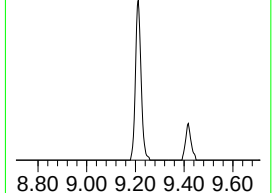
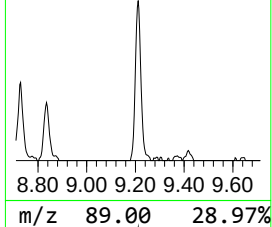
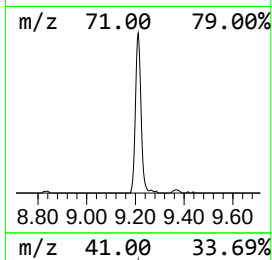
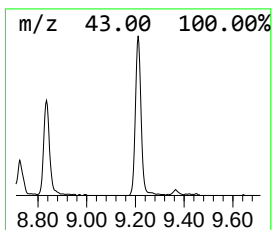
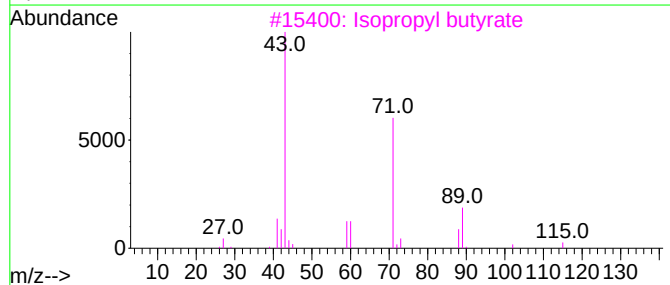
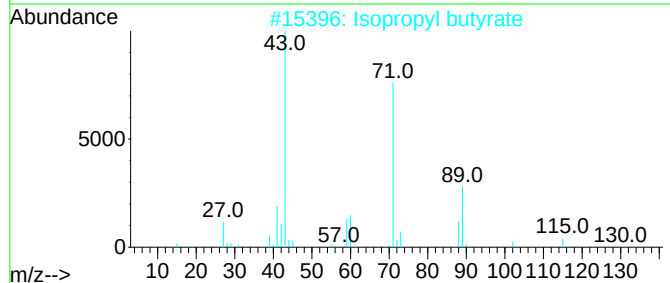
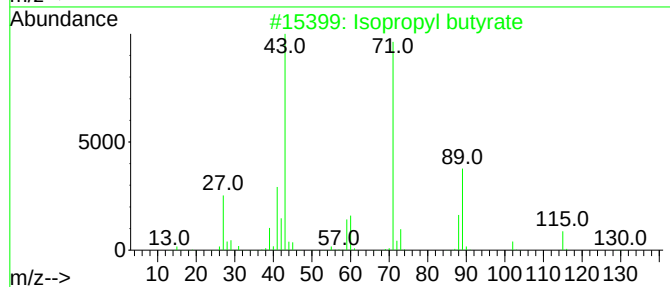
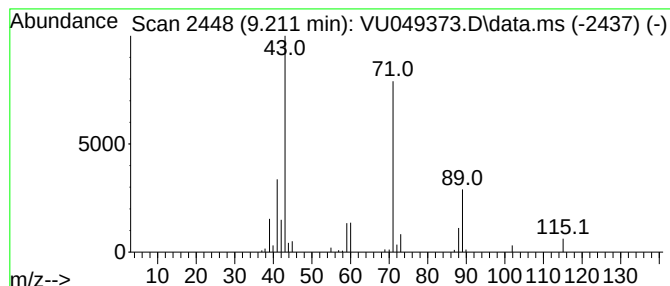
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	9.03 ug/L	120389	Chlorobenzene-d5	9.417

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			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	64
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049373.D
Acq On : 23 Jun 2022 12:48
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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
n-Propyl acetate	7.041	17.8	ug/L	200460	1	6.250	563791	50.0
Propanoic acid,...	7.738	2.9	ug/L	33144	1	6.250	563791	50.0
Propanoic acid,...	8.465	3.2	ug/L	42456	2	9.417	666656	50.0
Propanoic acid,...	8.725	6.5	ug/L	87297	2	9.417	666656	50.0
Acetic acid, bu...	8.835	3.8	ug/L	50295	2	9.417	666656	50.0
Isopropyl butyrate	9.211	9.0	ug/L	120389	2	9.417	666656	50.0