

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049372.D
 Acq On : 23 Jun 2022 12:25
 Operator : SY/MD
 Sample : N3392-20RE 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ5RE

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: VU049372.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	38	44	52	rBV2	7809	11195	1.88%	0.188%
2	1.597	74	80	91	rBV	51865	59894	10.05%	1.005%
3	1.899	166	174	191	rVB	46443	64685	10.86%	1.086%
4	2.562	369	380	393	rBV	82076	131765	22.12%	2.211%
5	2.620	393	398	414	rVB3	2860	5113	0.86%	0.086%
6	2.697	419	422	426	rVB3	379	306	0.05%	0.005%
7	2.742	433	436	437	rBV	433	220	0.04%	0.004%
8	2.761	438	442	444	rBV4	852	726	0.12%	0.012%
9	3.044	517	530	543	rBV2	14499	27936	4.69%	0.469%
10	3.182	557	573	594	rBV	46095	112610	18.90%	1.890%
11	3.665	718	723	724	rBV	249	226	0.04%	0.004%
12	3.674	724	726	732	rVB2	332	294	0.05%	0.005%
13	3.748	746	749	753	rVB2	416	329	0.06%	0.006%
14	3.777	753	758	761	rBV2	394	465	0.08%	0.008%
15	3.874	784	788	791	rBV	289	250	0.04%	0.004%
16	4.176	880	882	889	rVB3	234	260	0.04%	0.004%
17	4.491	976	980	985	rBV3	228	208	0.03%	0.003%
18	4.616	1006	1019	1044	rBV	123671	302131	50.71%	5.070%
19	4.809	1075	1079	1090	rVB5	1625	2710	0.45%	0.045%
20	4.877	1098	1100	1106	rBV3	220	194	0.03%	0.003%
21	4.938	1117	1119	1125	rVB	429	425	0.07%	0.007%
22	5.060	1141	1157	1183	rBV2	117823	258512	43.39%	4.338%
23	5.150	1183	1185	1190	rVB2	335	265	0.04%	0.004%
24	5.324	1233	1239	1241	rBV3	424	465	0.08%	0.008%
25	5.452	1275	1279	1282	rBV2	290	223	0.04%	0.004%
26	5.722	1343	1363	1385	rBV2	209640	595772	100.00%	9.998%
27	5.909	1412	1421	1438	rVV2	9149	17693	2.97%	0.297%
28	5.970	1438	1440	1444	rVB2	553	311	0.05%	0.005%
29	6.044	1458	1463	1464	rBV2	237	197	0.03%	0.003%
30	6.105	1478	1482	1485	rBV2	223	230	0.04%	0.004%
31	6.153	1494	1497	1501	rVB2	435	316	0.05%	0.005%
32	6.246	1513	1526	1550	rVV	238659	450537	75.62%	7.561%
33	6.465	1591	1594	1597	rBV3	604	412	0.07%	0.007%
34	6.526	1606	1613	1620	rVB5	1901	2777	0.47%	0.047%
35	6.568	1620	1626	1627	rBV3	283	227	0.04%	0.004%
36	6.632	1642	1646	1650	rVB2	239	279	0.05%	0.005%

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Integrator: RTE

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

37	6.690	1650	1664	1686	rBV	158110	308931	51.85%	5.184%
38	6.771	1686	1689	1691	rVV2	580	440	0.07%	0.007%
39	6.783	1691	1693	1697	rVV	621	499	0.08%	0.008%
40	6.806	1697	1700	1707	rVB5	1086	940	0.16%	0.016%
41	6.870	1716	1720	1722	rBV2	267	177	0.03%	0.003%
42	6.925	1725	1737	1749	rBV	4949	10766	1.81%	0.181%
43	7.037	1759	1772	1793	rBV	106557	186478	31.30%	3.129%
44	7.185	1809	1818	1826	rVB6	2310	3731	0.63%	0.063%
45	7.256	1837	1840	1844	rVB2	252	182	0.03%	0.003%
46	7.298	1849	1853	1860	rVB3	418	499	0.08%	0.008%
47	7.443	1895	1898	1902	rBV2	187	168	0.03%	0.003%
48	7.565	1924	1936	1951	rBV	78558	134534	22.58%	2.258%
49	7.655	1962	1964	1967	rBV2	240	180	0.03%	0.003%
50	7.684	1967	1973	1975	rVV3	638	570	0.10%	0.010%
51	7.700	1975	1978	1979	rVV2	659	441	0.07%	0.007%
52	7.738	1981	1990	2001	rVV2	18895	31485	5.28%	0.528%
53	7.790	2001	2006	2017	rVB4	2562	3971	0.67%	0.067%
54	7.896	2026	2039	2058	rBV	225496	385931	64.78%	6.477%
55	8.034	2078	2082	2085	rVB2	470	352	0.06%	0.006%
56	8.095	2100	2101	2108	rBV2	250	190	0.03%	0.003%
57	8.176	2108	2126	2140	rBV2	60956	130789	21.95%	2.195%
58	8.282	2153	2159	2161	rBV3	407	437	0.07%	0.007%
59	8.401	2191	2196	2200	rVB2	234	221	0.04%	0.004%
60	8.465	2204	2216	2229	rBV	21797	35900	6.03%	0.602%
61	8.571	2235	2249	2256	rBV9	4129	8708	1.46%	0.146%
62	8.632	2256	2268	2289	rVV2	313898	584015	98.03%	9.801%
63	8.725	2290	2297	2315	rVB	47636	75094	12.60%	1.260%
64	8.835	2322	2331	2350	rVB	28647	46536	7.81%	0.781%
65	8.912	2352	2355	2357	rVB3	431	200	0.03%	0.003%
66	8.957	2365	2369	2372	rBV2	291	270	0.05%	0.005%
67	9.041	2389	2395	2396	rBV2	279	271	0.05%	0.005%
68	9.208	2433	2447	2465	rBV2	63810	101759	17.08%	1.708%
69	9.369	2491	2497	2500	rBV3	1025	1208	0.20%	0.020%
70	9.417	2500	2512	2536	rVV	320952	526965	88.45%	8.843%
71	9.574	2555	2561	2563	rVB2	387	371	0.06%	0.006%
72	9.635	2576	2580	2582	rBV	772	640	0.11%	0.011%
73	9.922	2661	2669	2676	rBV3	1132	1645	0.28%	0.028%
74	9.986	2685	2689	2692	rBV2	316	222	0.04%	0.004%
75	10.073	2708	2716	2726	rVB3	4315	6959	1.17%	0.117%
76	10.314	2786	2791	2792	rBV	228	170	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M

Title : VOC Analysis

77	10.754	2916	2928	2953	rVB	272804	448641	75.30%	7.529%
78	11.037	3012	3016	3020	rBV2	269	264	0.04%	0.004%
79	11.394	3125	3127	3131	rVB	375	175	0.03%	0.003%
80	11.610	3192	3194	3198	rBV	254	211	0.04%	0.004%
81	11.812	3244	3257	3274	rBV	289353	459399	77.11%	7.709%
82	11.954	3298	3301	3308	rVB4	341	368	0.06%	0.006%
83	11.986	3308	3311	3314	rBV	377	231	0.04%	0.004%
84	12.192	3363	3375	3391	rBV	246903	401434	67.38%	6.737%
85	12.359	3424	3427	3429	rVB	311	196	0.03%	0.003%
86	12.523	3475	3478	3482	rVB	354	225	0.04%	0.004%
87	12.729	3540	3542	3545	rVB	361	185	0.03%	0.003%
88	13.050	3639	3642	3644	rBV2	285	184	0.03%	0.003%
89	13.298	3713	3719	3721	rBV	317	406	0.07%	0.007%
90	13.539	3790	3794	3796	rBV	414	336	0.06%	0.006%
91	13.709	3845	3847	3853	rVV2	314	279	0.05%	0.005%
92	13.899	3903	3906	3911	rBV2	489	403	0.07%	0.007%
93	13.982	3930	3932	3936	rVB2	333	189	0.03%	0.003%
94	14.050	3948	3953	3958	rBV2	353	484	0.08%	0.008%
95	14.343	4041	4044	4048	rVB2	452	295	0.05%	0.005%
96	14.417	4064	4067	4071	rBV	348	282	0.05%	0.005%
97	14.500	4090	4093	4097	rBV2	340	218	0.04%	0.004%
98	14.822	4189	4193	4195	rBV3	431	340	0.06%	0.006%
99	15.240	4320	4323	4327	rBV2	411	366	0.06%	0.006%
100	16.117	4592	4596	4600	rBV3	676	793	0.13%	0.013%

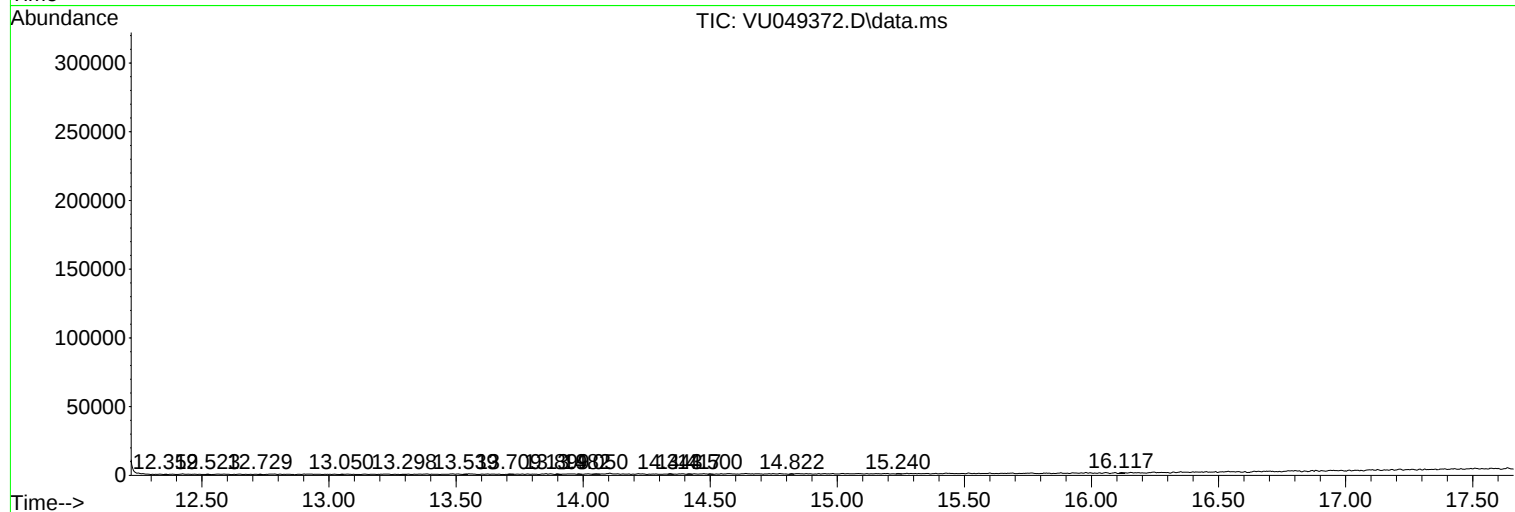
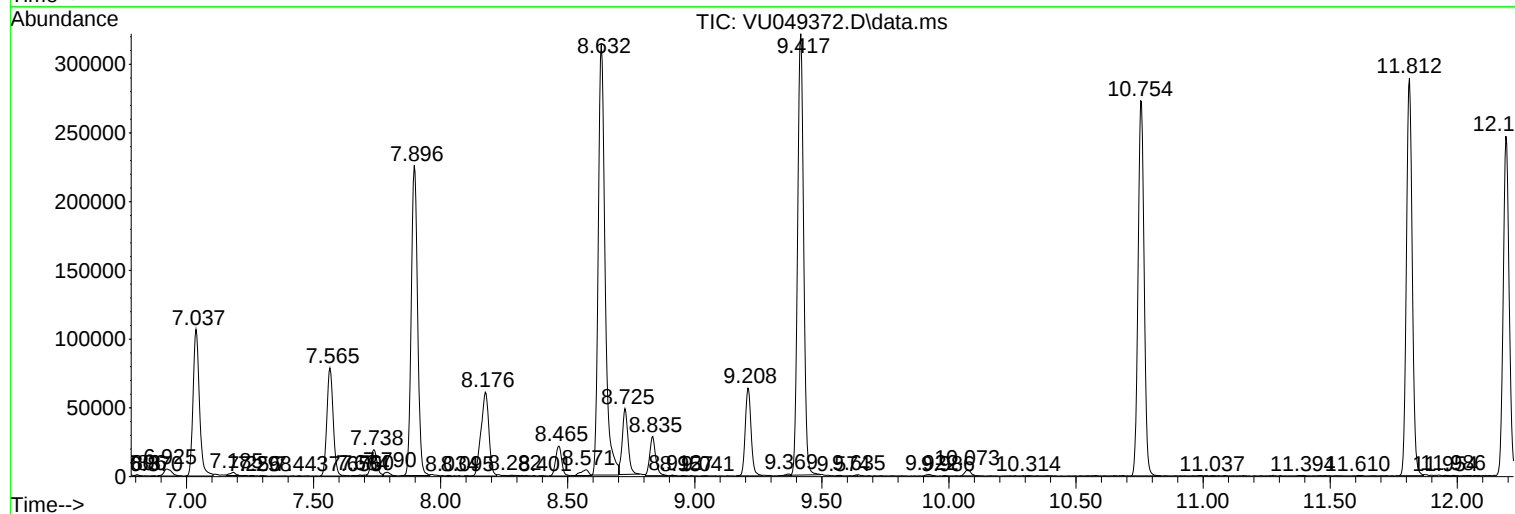
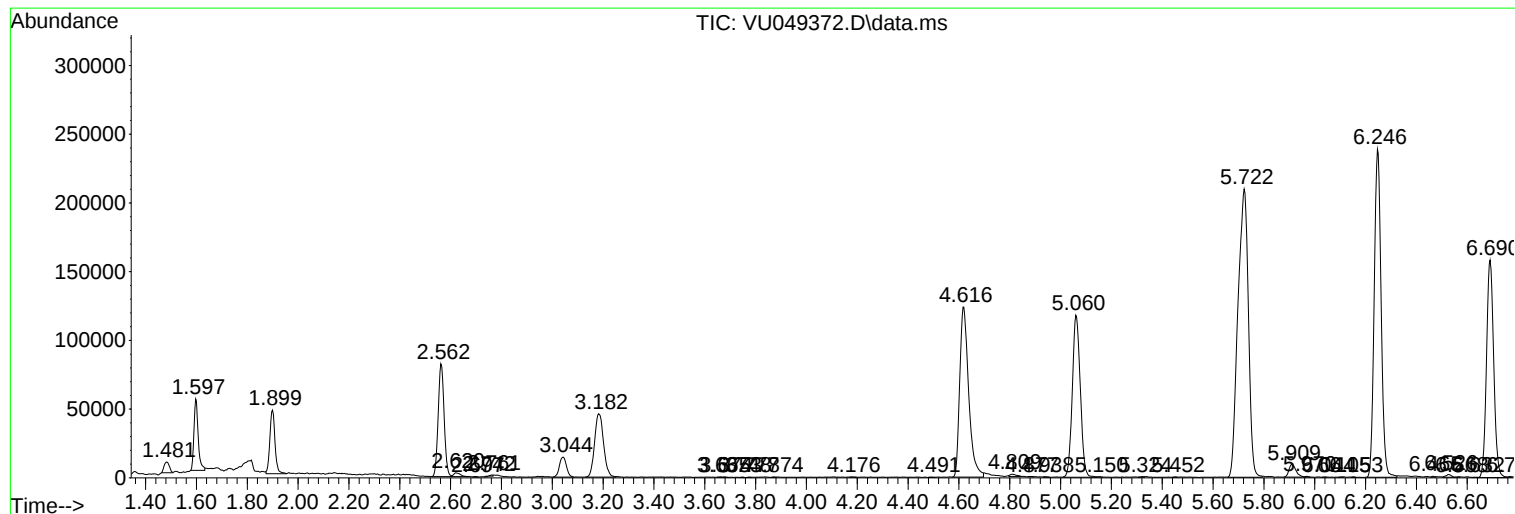
Sum of corrected areas: 5958907

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ClientSampleId :
EXEZ5RE

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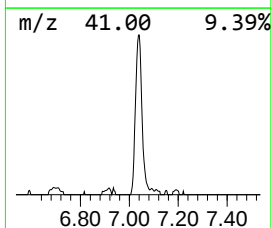
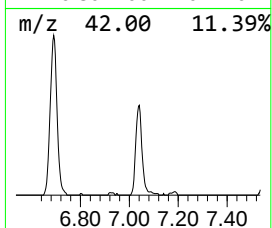
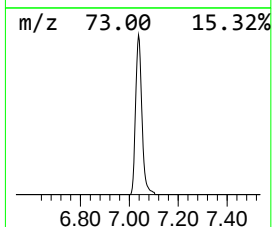
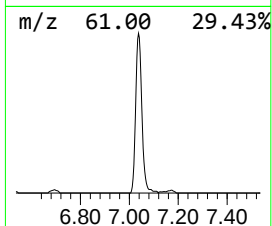
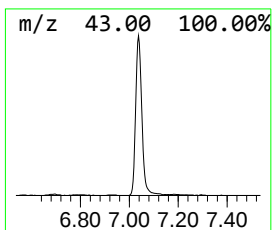
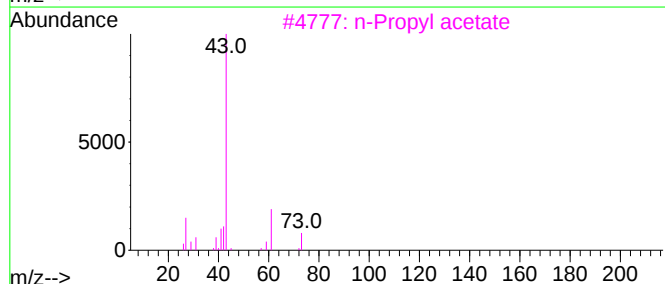
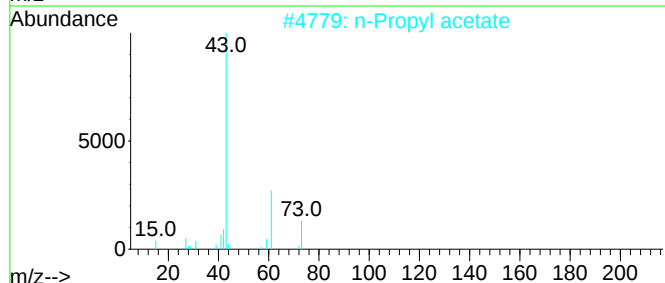
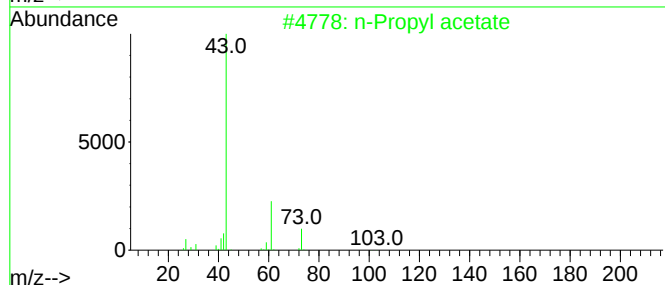
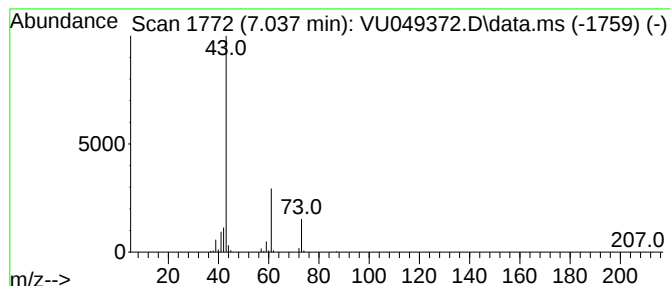
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
7.037	20.70 ug/L	186478	1,4-Difluorobenzene	6.246

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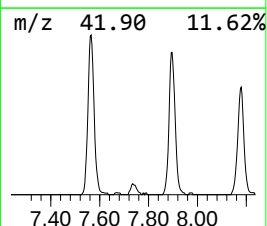
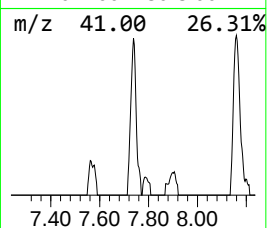
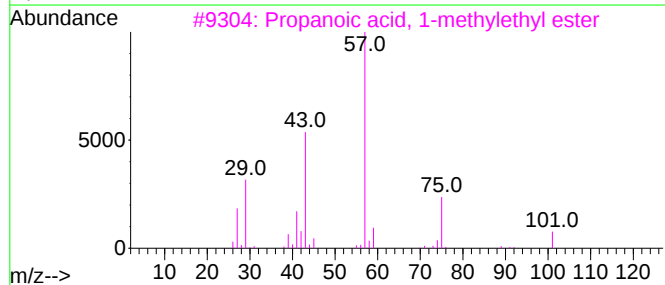
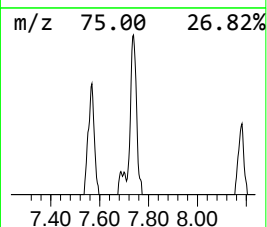
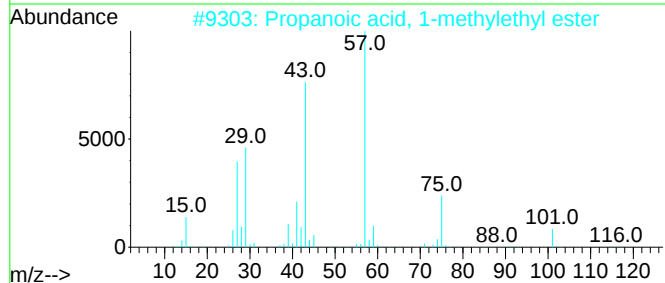
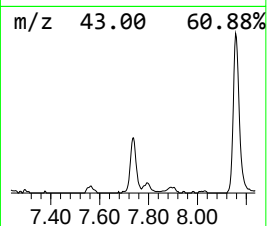
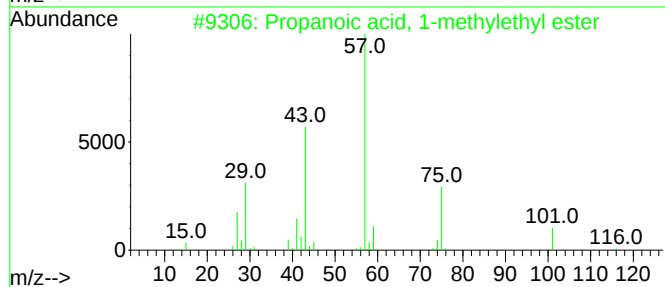
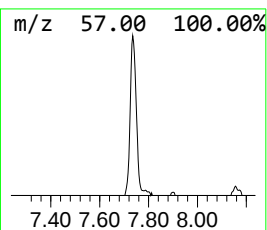
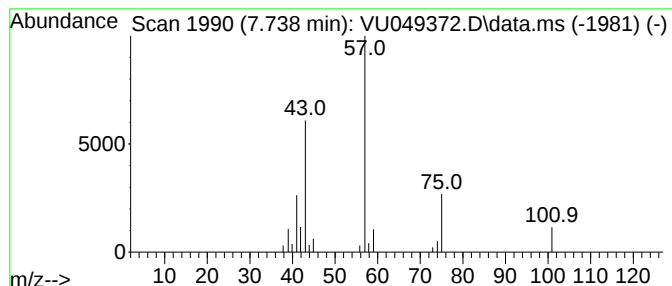
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
7.738	3.49 ug/L	31485	1,4-Difluorobenzene	6.246

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	72
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36



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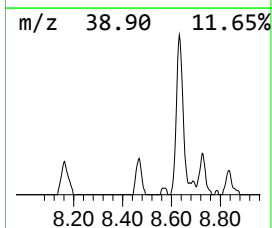
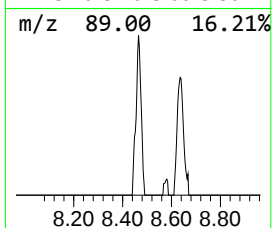
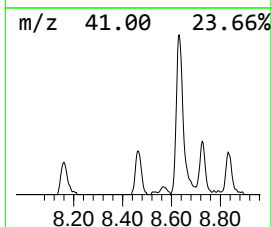
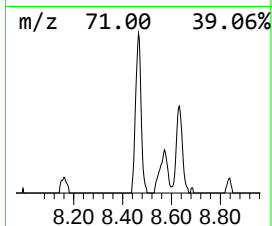
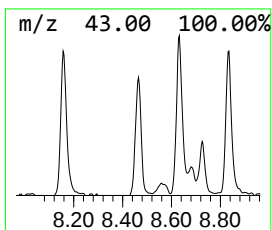
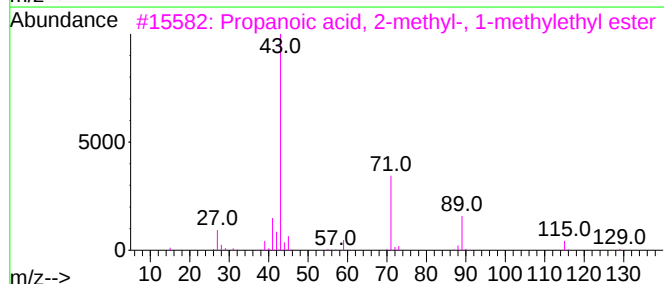
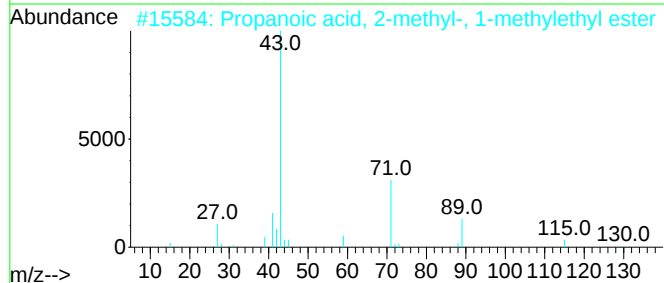
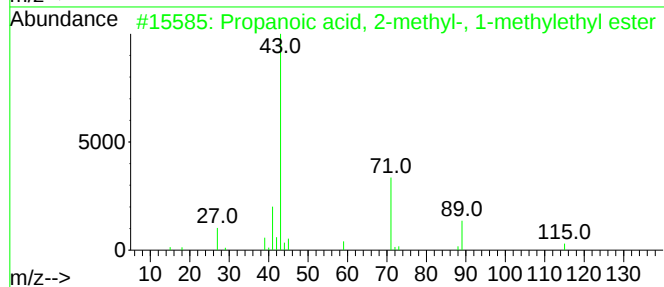
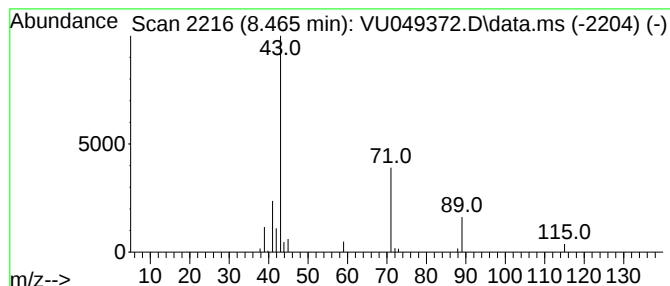
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.41 ug/L	35900	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	64
5			Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049372.D
Acq On : 23 Jun 2022 12:25
Operator : SY/MD
Sample : N3392-20RE 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5RE

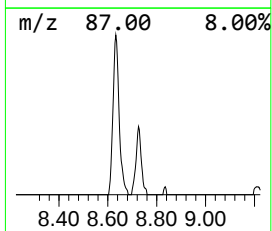
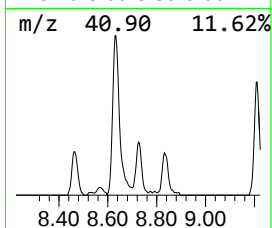
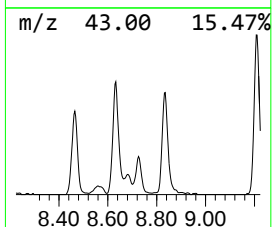
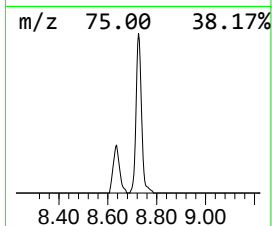
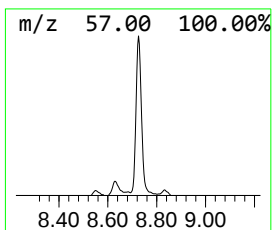
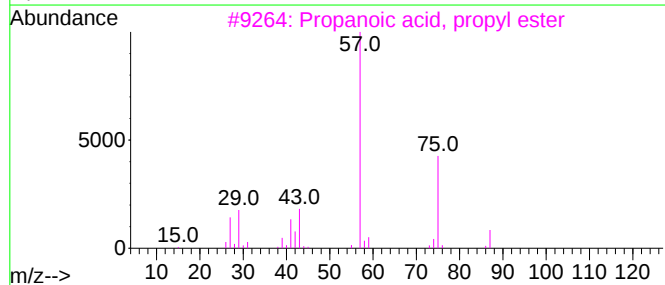
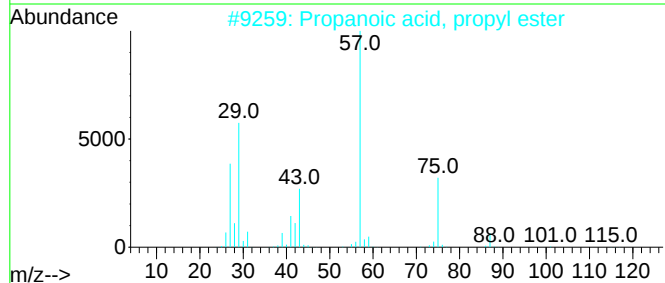
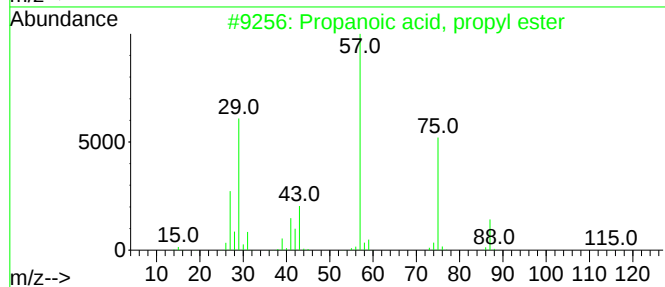
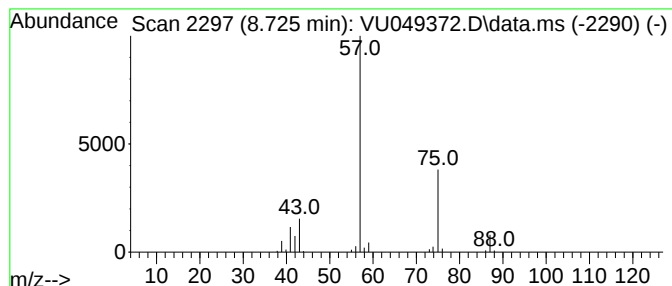
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Quant Title : VOC Analysis

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.725	7.13 ug/L	75094	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049372.D
Acq On : 23 Jun 2022 12:25
Operator : SY/MD
Sample : N3392-20RE 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5RE

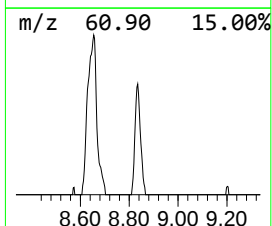
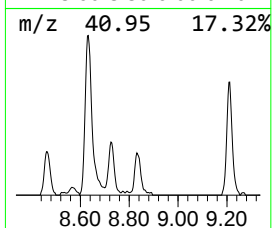
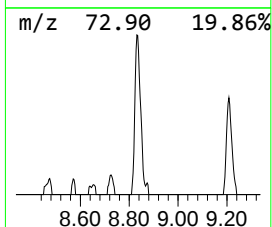
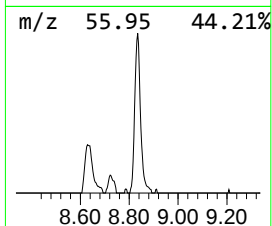
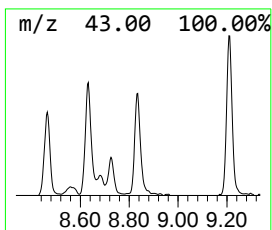
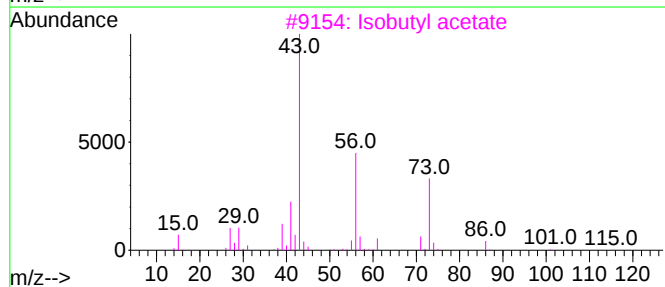
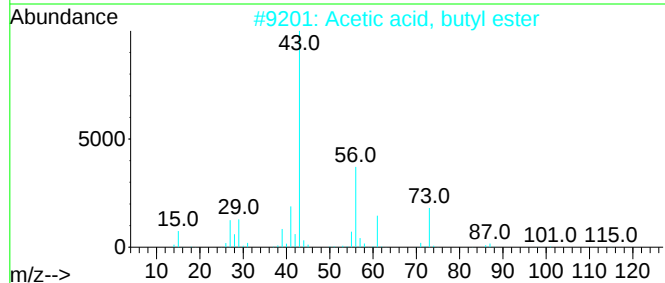
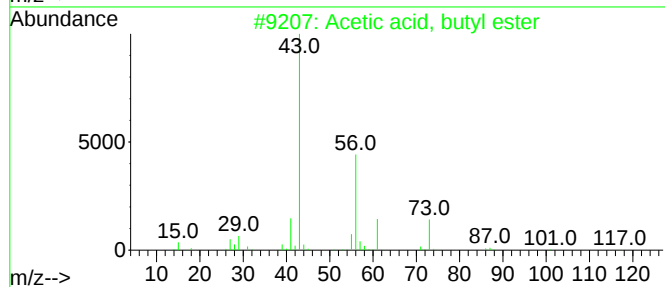
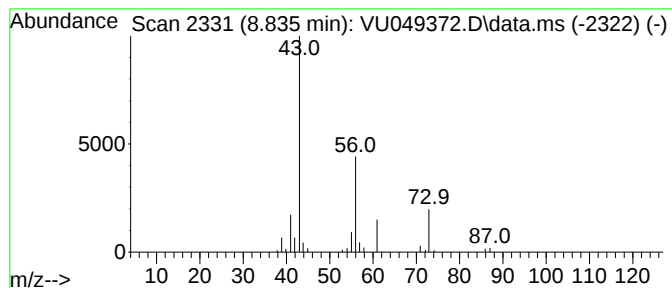
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Quant Title : VOC Analysis

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	4.42 ug/L	46536	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			Isobutyl acetate	116	C6H12O2	000110-19-0	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049372.D
Acq On : 23 Jun 2022 12:25
Operator : SY/MD
Sample : N3392-20RE 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5RE

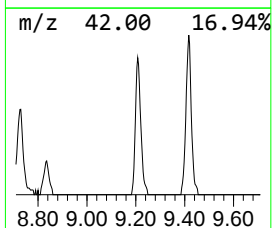
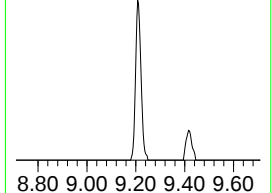
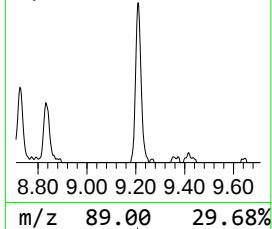
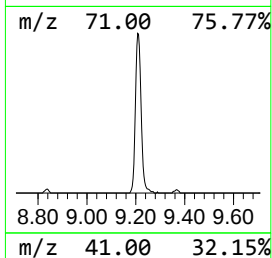
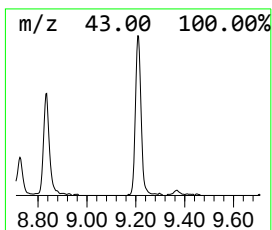
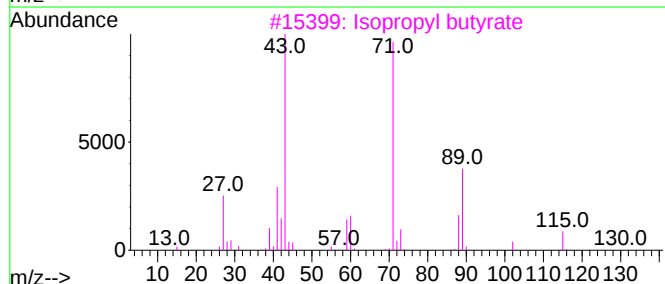
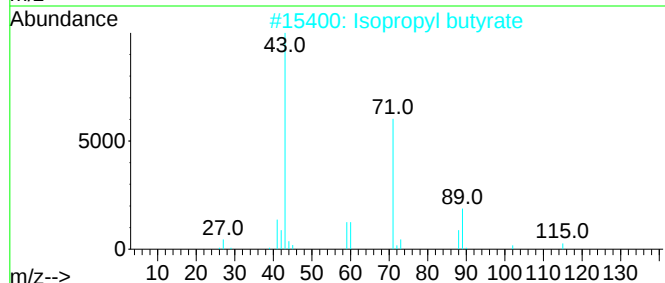
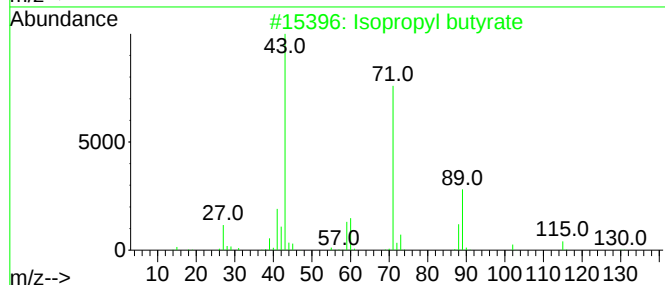
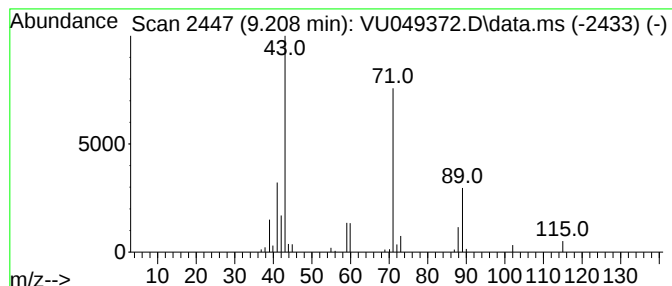
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Quant Title : VOC Analysis

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

Peak Number 9 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.208	9.66 ug/L	101759	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-, propy...	130	C7H14O2	000644-49-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049372.D
Acq On : 23 Jun 2022 12:25
Operator : SY/MD
Sample : N3392-20RE 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ5RE

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
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Propanoic acid,...	7.738	3.5	ug/L	31485	1	6.246	450537	50.0
Propanoic acid,...	8.465	3.4	ug/L	35900	2	9.417	526965	50.0
Propanoic acid,...	8.725	7.1	ug/L	75094	2	9.417	526965	50.0
Acetic acid, bu...	8.835	4.4	ug/L	46536	2	9.417	526965	50.0
Isopropyl butyrate	9.208	9.7	ug/L	101759	2	9.417	526965	50.0