

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049363.D
 Acq On : 22 Jun 2022 19:41
 Operator : SY/MD
 Sample : N3392-18 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ3

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: VU049363.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	39	45	51	rBV3	5214	7863	1.17%	0.117%
2	1.597	73	80	93	rBV	64880	75295	11.21%	1.121%
3	1.906	168	176	192	rVB	56884	74944	11.16%	1.116%
4	2.565	369	381	394	rBV	106547	172686	25.71%	2.571%
5	2.626	395	400	413	rVB3	2603	4729	0.70%	0.070%
6	2.748	434	438	439	rBV2	543	364	0.05%	0.005%
7	2.835	459	465	467	rBV2	312	272	0.04%	0.004%
8	2.867	472	475	480	rVB2	275	253	0.04%	0.004%
9	3.044	520	530	543	rVV4	4160	7812	1.16%	0.116%
10	3.186	556	574	592	rVB	24045	55191	8.22%	0.822%
11	3.263	593	598	602	rVB2	271	307	0.05%	0.005%
12	3.301	606	610	613	rBV2	224	203	0.03%	0.003%
13	3.420	643	647	650	rVB3	240	185	0.03%	0.003%
14	3.668	721	724	728	rBV2	421	257	0.04%	0.004%
15	4.112	858	862	867	rBV	202	226	0.03%	0.003%
16	4.273	908	912	916	rBV2	205	229	0.03%	0.003%
17	4.485	975	978	980	rBV	247	190	0.03%	0.003%
18	4.620	1006	1020	1048	rBV	119509	295512	44.00%	4.400%
19	4.890	1101	1104	1110	rVB4	473	468	0.07%	0.007%
20	4.941	1116	1120	1122	rVB3	303	188	0.03%	0.003%
21	4.957	1122	1125	1130	rVB2	282	246	0.04%	0.004%
22	5.060	1141	1157	1179	rBV	132793	288315	42.93%	4.293%
23	5.292	1226	1229	1236	rVB3	578	602	0.09%	0.009%
24	5.337	1236	1243	1247	rBV2	193	256	0.04%	0.004%
25	5.414	1263	1267	1270	rBV	248	178	0.03%	0.003%
26	5.565	1311	1314	1319	rVB2	324	215	0.03%	0.003%
27	5.723	1342	1363	1386	rBV3	239635	671564	100.00%	10.000%
28	5.800	1386	1387	1389	rVB2	553	180	0.03%	0.003%
29	5.912	1405	1422	1434	rBV2	10057	19913	2.97%	0.297%
30	6.163	1497	1500	1502	rBV2	373	268	0.04%	0.004%
31	6.247	1513	1526	1549	rBV	293356	558261	83.13%	8.313%
32	6.530	1606	1614	1622	rVB6	1417	2252	0.34%	0.034%
33	6.594	1630	1634	1638	rVB3	590	614	0.09%	0.009%
34	6.690	1649	1664	1683	rBV	177284	342292	50.97%	5.097%
35	6.925	1727	1737	1758	rVB	5423	11320	1.69%	0.169%
36	7.038	1760	1772	1793	rBV	111921	200638	29.88%	2.988%

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

37	7.169	1810	1813	1814	rBV	1138	629	0.09%	0.009%
38	7.288	1847	1850	1854	rVB2	445	272	0.04%	0.004%
39	7.391	1879	1882	1887	rVB2	274	185	0.03%	0.003%
40	7.417	1887	1890	1895	rVB3	302	278	0.04%	0.004%
41	7.446	1895	1899	1901	rBV	441	322	0.05%	0.005%
42	7.565	1924	1936	1950	rBV2	89042	155164	23.10%	2.311%
43	7.645	1959	1961	1965	rVB3	442	194	0.03%	0.003%
44	7.687	1968	1974	1975	rBV3	689	640	0.10%	0.010%
45	7.739	1980	1990	2002	rVV	21047	33412	4.98%	0.498%
46	7.896	2024	2039	2059	rBV	280294	485011	72.22%	7.222%
47	8.073	2091	2094	2101	rVB4	566	488	0.07%	0.007%
48	8.176	2107	2126	2148	rVV2	69890	150922	22.47%	2.247%
49	8.279	2155	2158	2163	rBV3	583	640	0.10%	0.010%
50	8.333	2174	2175	2181	rVB2	437	345	0.05%	0.005%
51	8.465	2204	2216	2229	rBV	25607	42108	6.27%	0.627%
52	8.575	2235	2250	2256	rBV7	5012	10652	1.59%	0.159%
53	8.632	2256	2268	2289	rVV	318089	576798	85.89%	8.589%
54	8.726	2289	2297	2316	rVB	50350	85236	12.69%	1.269%
55	8.835	2321	2331	2348	rVB	31130	51419	7.66%	0.766%
56	9.057	2398	2400	2405	rVB2	452	318	0.05%	0.005%
57	9.131	2418	2423	2426	rBV3	342	339	0.05%	0.005%
58	9.211	2436	2448	2460	rBV	72711	116648	17.37%	1.737%
59	9.304	2473	2477	2481	rVB3	405	326	0.05%	0.005%
60	9.366	2490	2496	2499	rBV2	1461	1503	0.22%	0.022%
61	9.417	2499	2512	2534	rVV	398169	656805	97.80%	9.780%
62	9.597	2565	2568	2572	rBV	221	187	0.03%	0.003%
63	9.626	2572	2577	2579	rBV3	554	469	0.07%	0.007%
64	9.809	2631	2634	2635	rBV2	356	181	0.03%	0.003%
65	9.832	2638	2641	2643	rVV3	261	189	0.03%	0.003%
66	9.886	2652	2658	2659	rBV	259	197	0.03%	0.003%
67	9.983	2683	2688	2690	rBV2	293	255	0.04%	0.004%
68	10.002	2692	2694	2699	rVB	408	208	0.03%	0.003%
69	10.073	2708	2716	2725	rBV4	5183	7716	1.15%	0.115%
70	10.240	2765	2768	2773	rVB2	244	261	0.04%	0.004%
71	10.337	2791	2798	2801	rBV	467	477	0.07%	0.007%
72	10.407	2818	2820	2823	rVV2	467	321	0.05%	0.005%
73	10.423	2823	2825	2828	rVV2	350	258	0.04%	0.004%
74	10.436	2828	2829	2832	rVV	404	180	0.03%	0.003%
75	10.468	2837	2839	2843	rVV	338	228	0.03%	0.003%
76	10.501	2847	2849	2854	rVB2	282	183	0.03%	0.003%

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 Title : VOC Analysis

77	10.539	2854	2861	2865	rBV2	234	309	0.05%	0.005%
78	10.671	2897	2902	2904	rBV2	271	203	0.03%	0.003%
79	10.755	2916	2928	2952	rVB	280050	450533	67.09%	6.709%
80	11.092	3030	3033	3037	rVB2	238	182	0.03%	0.003%
81	11.224	3071	3074	3079	rVB3	251	240	0.04%	0.004%
82	11.420	3132	3135	3138	rVB2	320	229	0.03%	0.003%
83	11.552	3170	3176	3179	rBV3	316	276	0.04%	0.004%
84	11.812	3245	3257	3280	rBV	373976	597452	88.96%	8.897%
85	12.192	3363	3375	3394	rBV	295856	485068	72.23%	7.223%
86	12.848	3577	3579	3586	rVB	379	301	0.04%	0.004%
87	13.005	3624	3628	3632	rBV2	350	344	0.05%	0.005%
88	13.025	3632	3634	3640	rVB2	369	316	0.05%	0.005%
89	13.066	3643	3647	3651	rBV3	385	352	0.05%	0.005%
90	13.089	3651	3654	3658	rVB3	319	271	0.04%	0.004%
91	13.549	3794	3797	3799	rBV2	266	183	0.03%	0.003%
92	13.806	3874	3877	3882	rBV3	349	279	0.04%	0.004%
93	13.844	3885	3889	3891	rBV3	294	258	0.04%	0.004%
94	14.089	3962	3965	3970	rBV4	387	500	0.07%	0.007%
95	14.269	4018	4021	4025	rVB3	311	213	0.03%	0.003%
96	14.417	4064	4067	4068	rBV	270	184	0.03%	0.003%
97	14.626	4129	4132	4135	rBV	378	295	0.04%	0.004%
98	15.050	4260	4264	4265	rBV2	354	258	0.04%	0.004%
99	15.748	4478	4481	4487	rVB2	566	483	0.07%	0.007%
100	16.150	4603	4606	4610	rBV4	584	486	0.07%	0.007%

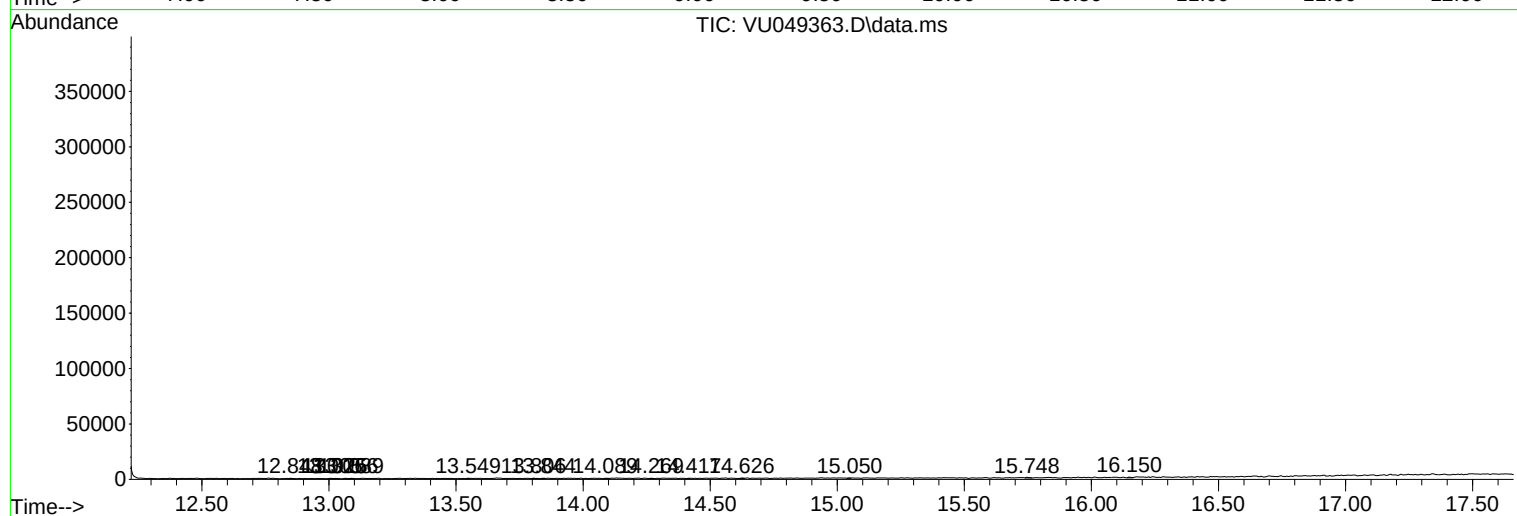
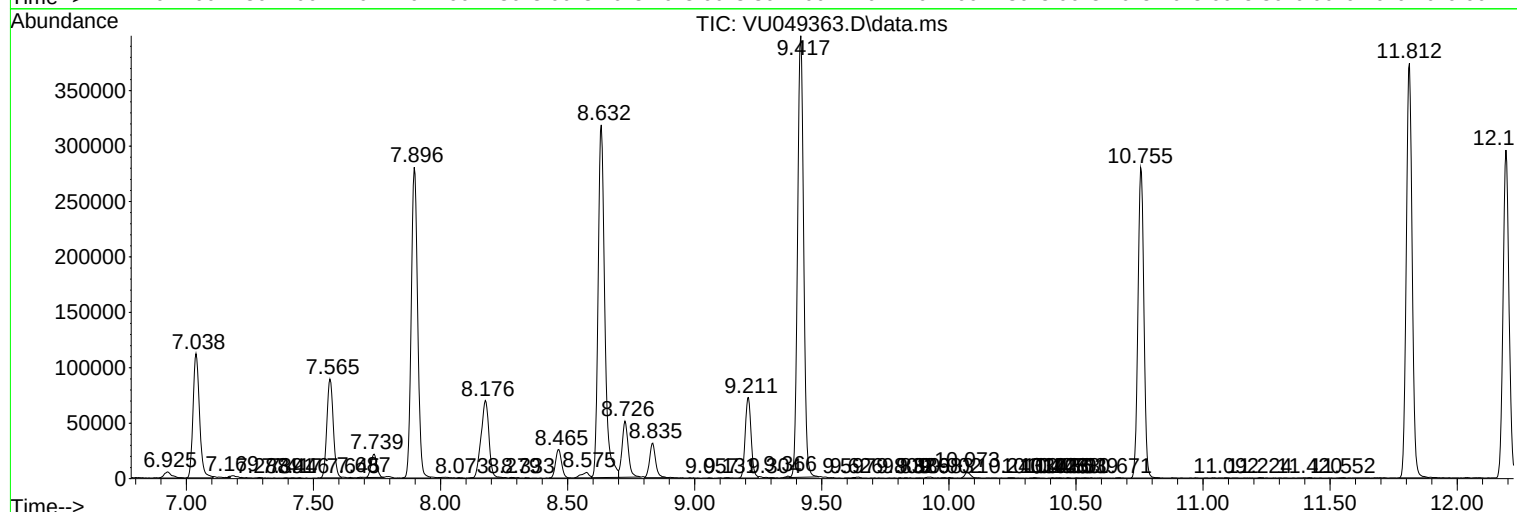
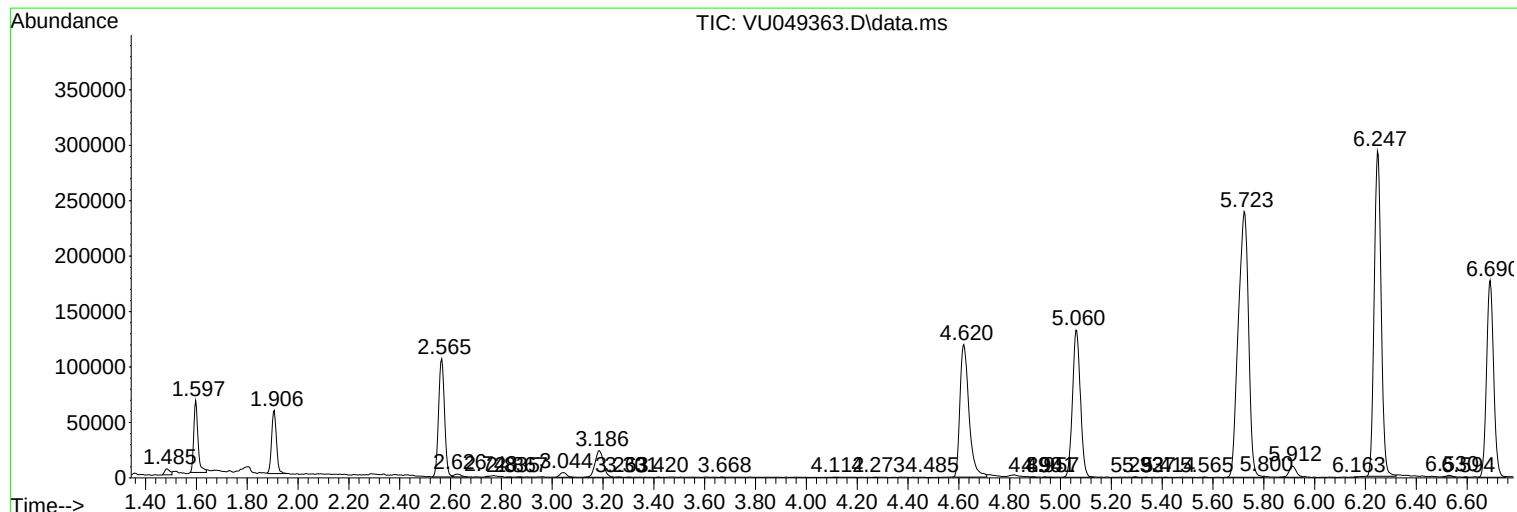
Sum of corrected areas: 6715467

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Instrument :
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EXEZ3

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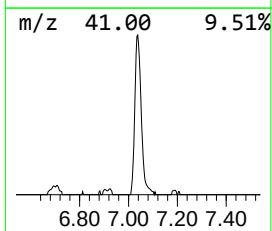
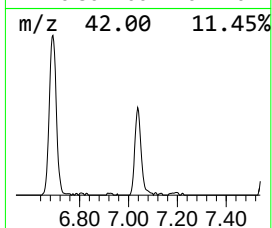
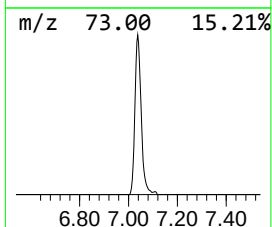
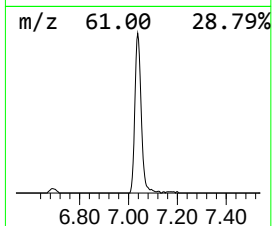
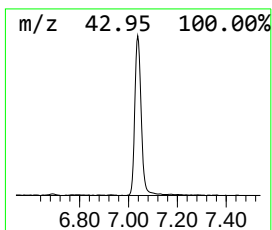
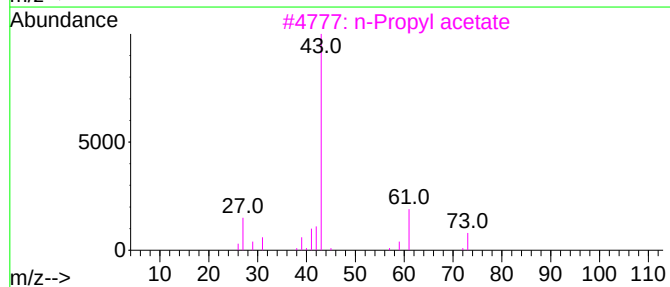
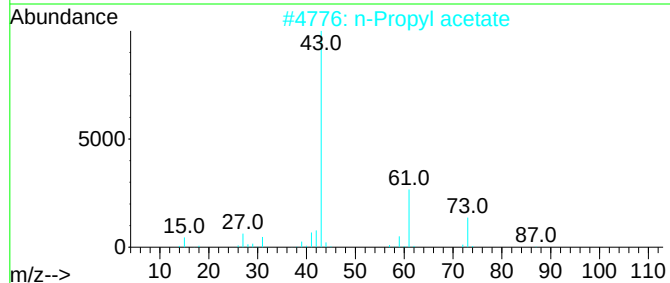
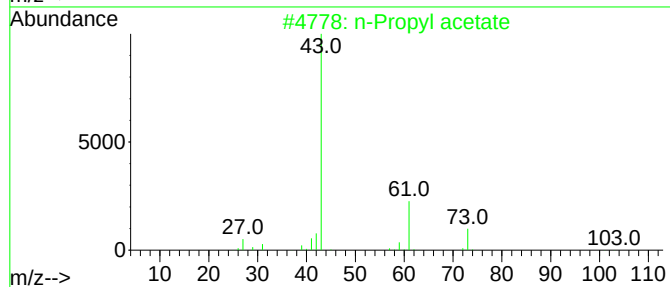
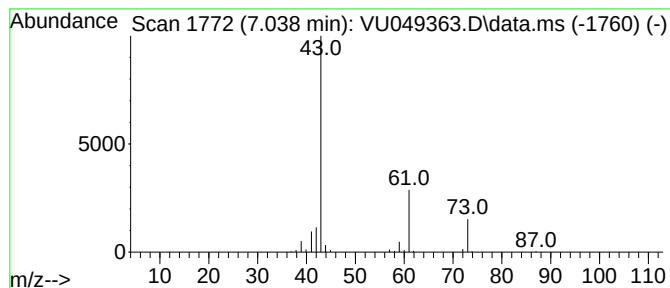
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	17.97 ug/L	200638	1,4-Difluorobenzene	6.247

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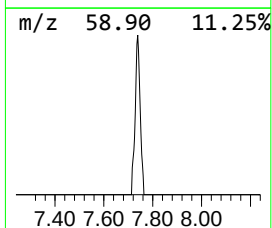
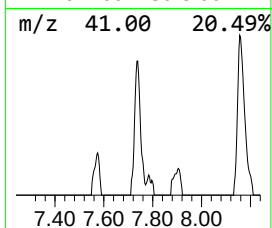
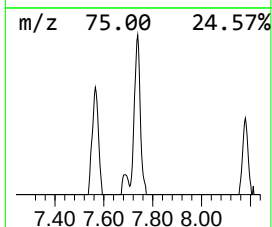
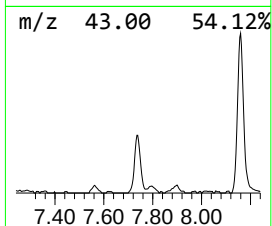
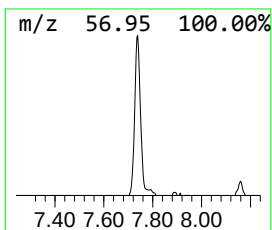
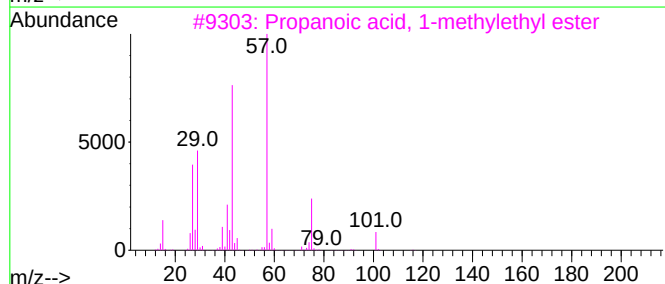
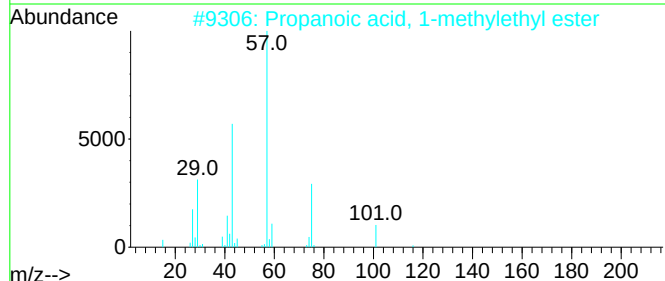
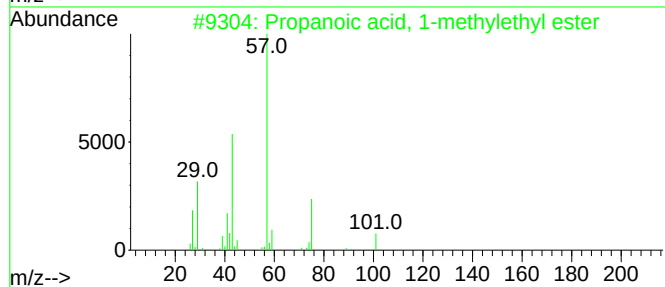
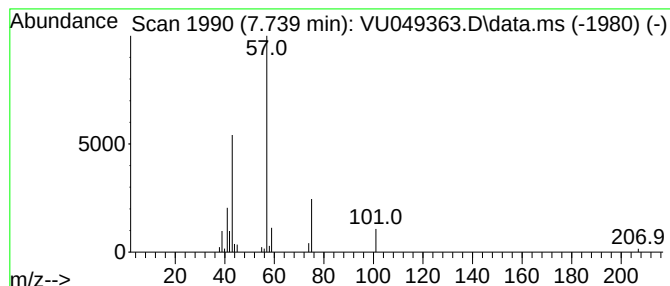
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	2.99 ug/L	33412	1,4-Difluorobenzene	6.247

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	72
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36



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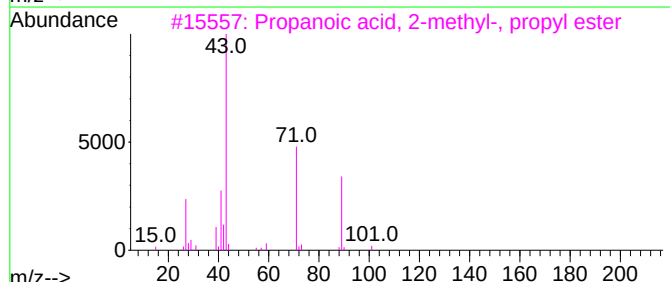
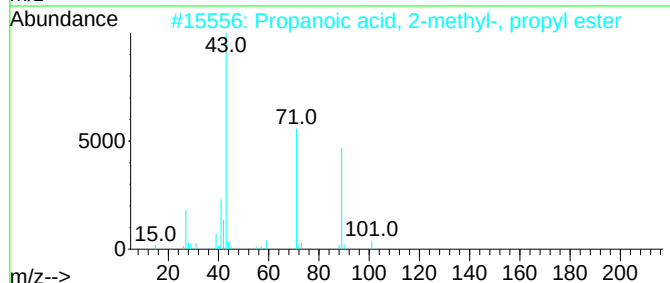
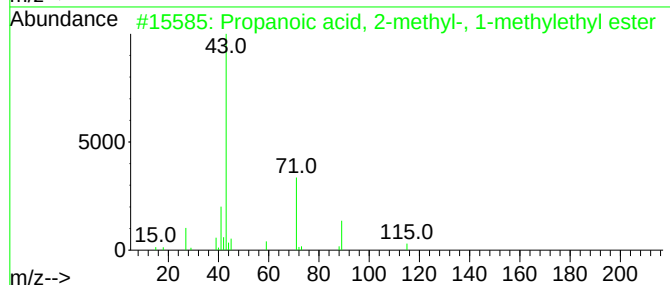
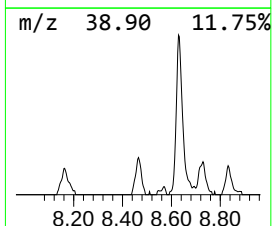
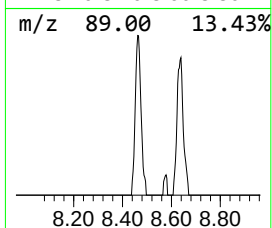
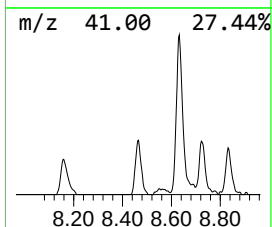
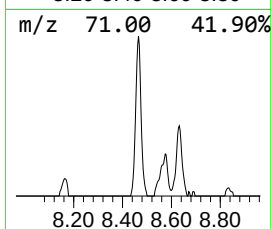
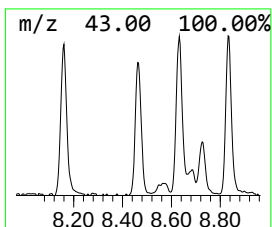
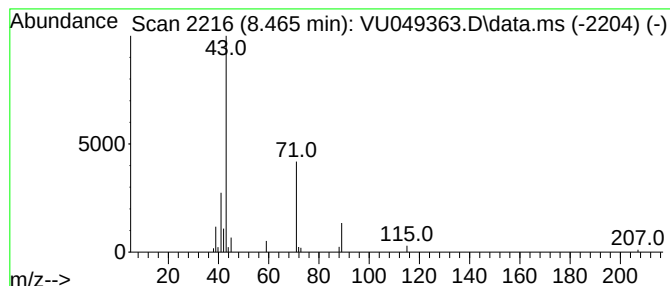
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.21 ug/L	42108	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-, propy...	130	C7H14O2	000644-49-5	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049363.D
Acq On : 22 Jun 2022 19:41
Operator : SY/MD
Sample : N3392-18 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ3

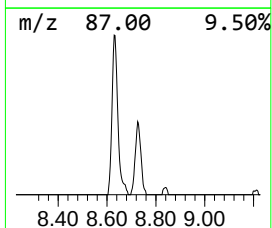
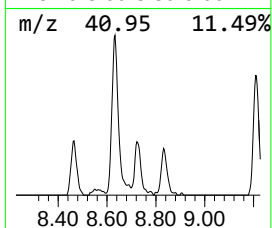
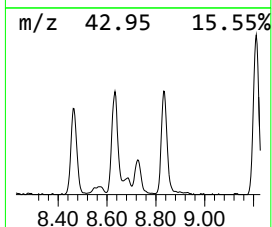
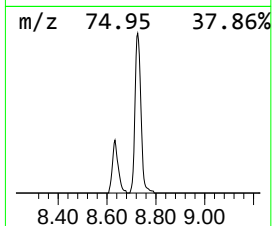
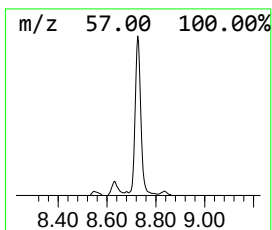
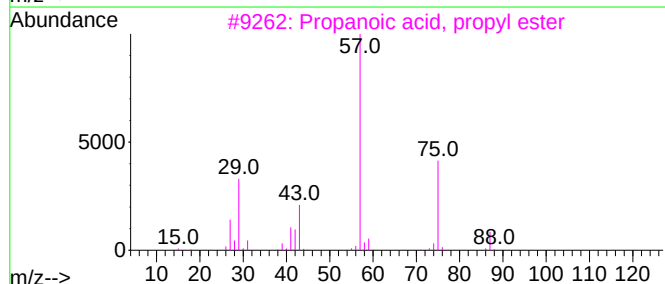
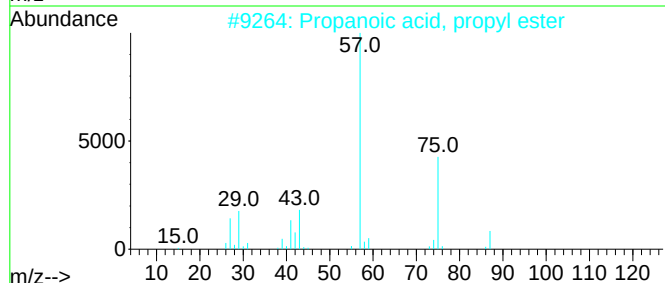
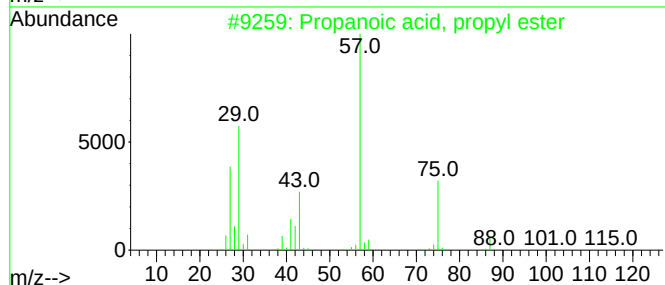
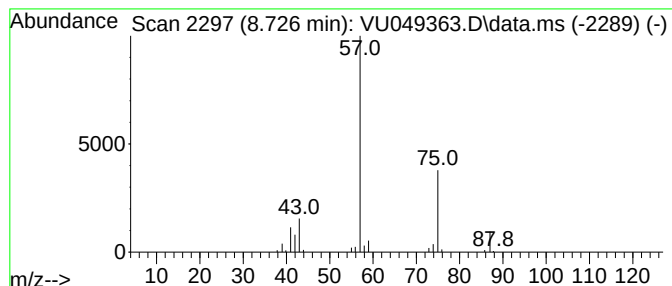
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	6.49 ug/L	85236	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	78
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049363.D
Acq On : 22 Jun 2022 19:41
Operator : SY/MD
Sample : N3392-18 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ3

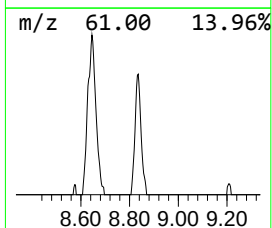
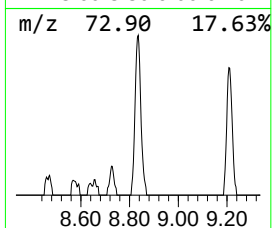
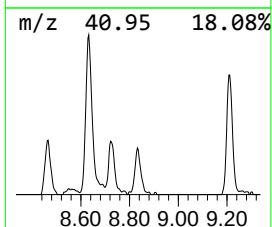
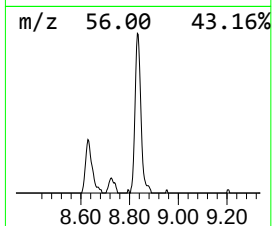
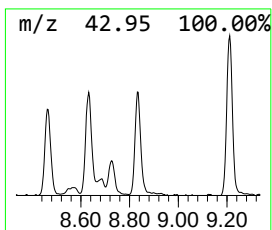
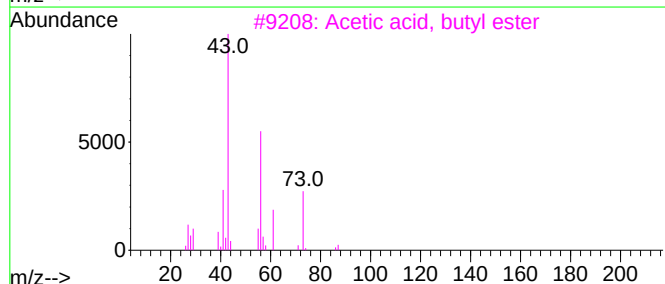
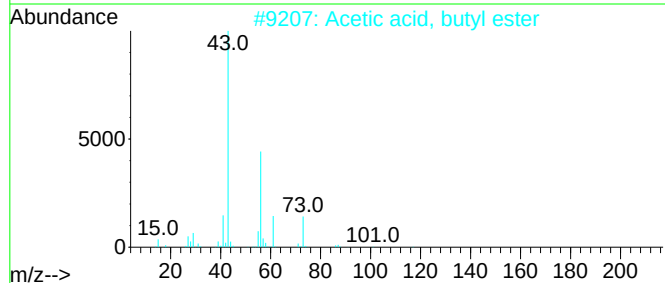
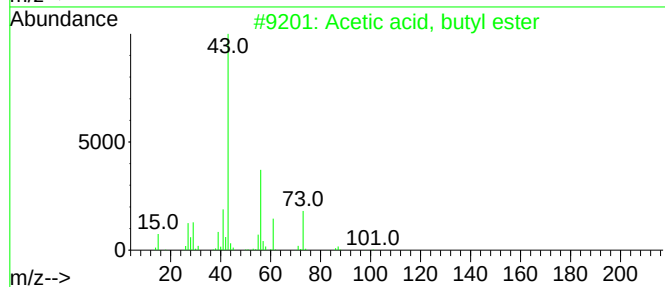
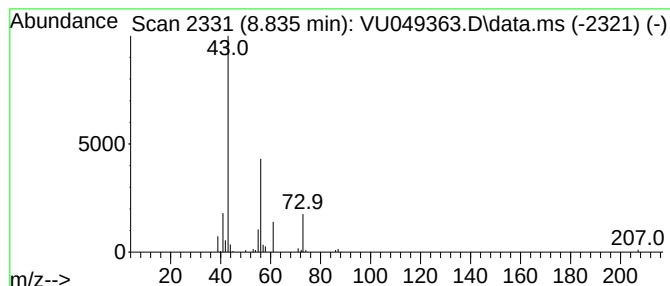
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Quant Title : VOC Analysis

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.91 ug/L	51419	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	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
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 : VU049363.D
Acq On : 22 Jun 2022 19:41
Operator : SY/MD
Sample : N3392-18 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ3

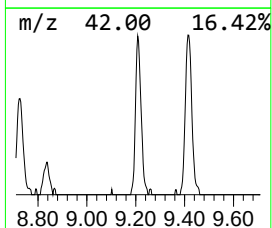
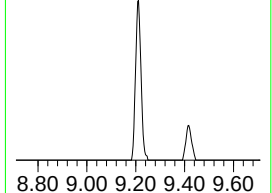
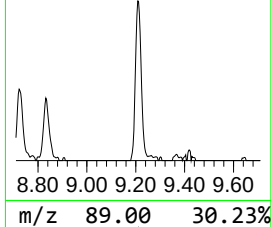
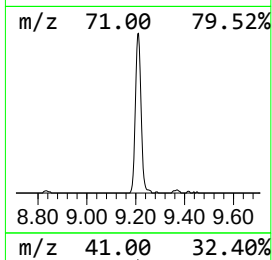
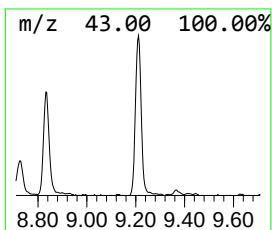
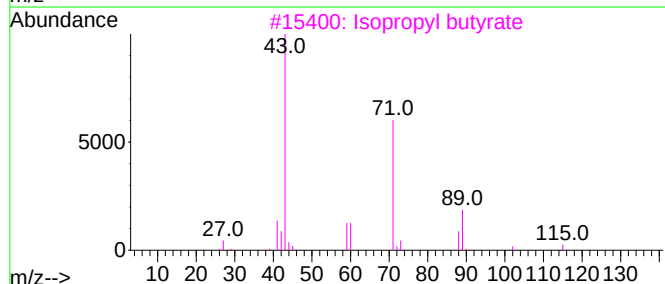
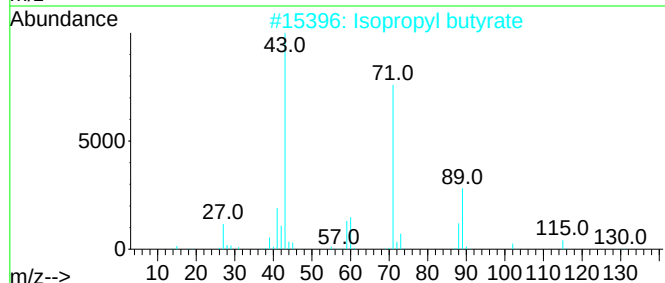
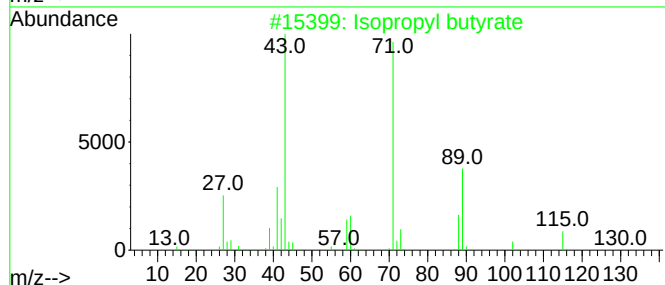
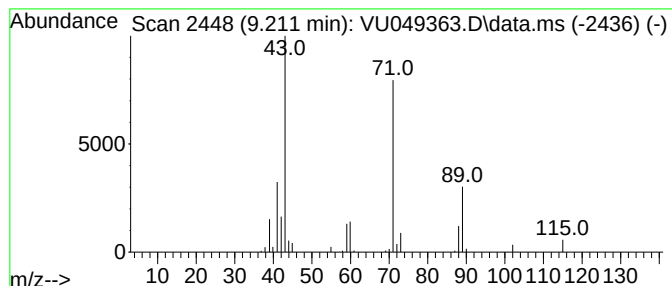
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	8.88 ug/L	116648	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-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049363.D
Acq On : 22 Jun 2022 19:41
Operator : SY/MD
Sample : N3392-18 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ3

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	7.038	18.0	ug/L	200638	1	6.247	558261	50.0
Propanoic acid,...	7.739	3.0	ug/L	33412	1	6.247	558261	50.0
Propanoic acid,...	8.465	3.2	ug/L	42108	2	9.417	656805	50.0
Propanoic acid,...	8.726	6.5	ug/L	85236	2	9.417	656805	50.0
Acetic acid, bu...	8.835	3.9	ug/L	51419	2	9.417	656805	50.0
Isopropyl butyrate	9.211	8.9	ug/L	116648	2	9.417	656805	50.0