

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV020422\
 Data File : VV024558.D
 Acq On : 04 Feb 2022 11:54
 Operator : SY/MD
 Sample : N1352-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0HQ5

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_V\Method\SFAMVLM020222WMA.M
 Title : VOC Analysis

Signal : TIC: VV024558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	96	rVB	157106	154562	13.36%	1.471%
2	1.568	157	164	173	rBV	165941	183147	15.83%	1.743%
3	2.105	322	331	357	rVB	294366	445935	38.55%	4.243%
4	2.700	512	516	518	rBV3	404	267	0.02%	0.003%
5	2.767	530	537	541	rBV3	445	508	0.04%	0.005%
6	2.815	549	552	557	rVB4	376	289	0.02%	0.003%
7	2.883	570	573	574	rBV	499	179	0.02%	0.002%
8	2.970	596	600	601	rBV2	445	253	0.02%	0.002%
9	2.992	605	607	612	rVB3	280	191	0.02%	0.002%
10	3.018	612	615	616	rBV2	425	258	0.02%	0.002%
11	3.053	624	626	629	rVB	484	207	0.02%	0.002%
12	3.121	637	647	648	rBV2	593	820	0.07%	0.008%
13	3.153	654	657	658	rBV	166	78	0.01%	0.001%
14	3.320	707	709	710	rBV2	230	67	0.01%	0.001%
15	3.343	715	716	718	rVB2	330	124	0.01%	0.001%
16	3.378	722	727	731	rBV4	376	351	0.03%	0.003%
17	3.417	735	739	741	rBV3	285	215	0.02%	0.002%
18	3.449	747	749	751	rVB3	208	73	0.01%	0.001%
19	3.474	751	757	758	rBV3	385	311	0.03%	0.003%
20	3.677	817	820	823	rBV3	489	433	0.04%	0.004%
21	3.777	849	851	853	rBV2	284	154	0.01%	0.001%
22	3.819	859	864	865	rBV	305	227	0.02%	0.002%
23	3.876	872	882	926	rBV	82241	244042	21.10%	2.322%
24	4.343	1012	1027	1052	rBV	185921	456730	39.48%	4.346%
25	4.529	1083	1085	1087	rBV2	399	199	0.02%	0.002%
26	4.587	1101	1103	1104	rBV	181	93	0.01%	0.001%
27	4.626	1111	1115	1118	rBV	289	182	0.02%	0.002%
28	4.741	1147	1151	1154	rBV3	285	234	0.02%	0.002%
29	4.786	1162	1165	1166	rBV	157	76	0.01%	0.001%
30	4.835	1178	1180	1182	rVB2	348	157	0.01%	0.001%
31	4.857	1184	1187	1189	rVV2	213	128	0.01%	0.001%
32	4.886	1194	1196	1198	rBV3	364	175	0.02%	0.002%
33	5.040	1227	1244	1276	rBV2	449368	1156790	100.00%	11.006%
34	5.442	1368	1369	1371	rBV	311	162	0.01%	0.002%
35	5.519	1390	1393	1395	rBV3	287	210	0.02%	0.002%
36	5.529	1395	1396	1399	rVV2	200	96	0.01%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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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_V\Method\SFAMVLM020222WMA.M
 Title : VOC Analysis

37	5.609	1409	1421	1447	rBV	409952	808775	69.92%	7.695%
38	5.902	1500	1512	1535	rBV4	29892	72080	6.23%	0.686%
39	6.063	1550	1562	1588	rVB2	263872	534898	46.24%	5.089%
40	6.455	1674	1684	1717	rBV	180019	329078	28.45%	3.131%
41	6.867	1809	1812	1818	rVB5	490	401	0.03%	0.004%
42	6.979	1837	1847	1870	rBV	161083	292866	25.32%	2.786%
43	7.182	1900	1910	1922	rBV	31992	53974	4.67%	0.514%
44	7.310	1938	1950	1969	rBV	543659	946784	81.85%	9.008%
45	7.616	2036	2045	2069	rBV	112380	193940	16.77%	1.845%
46	7.924	2133	2141	2151	rBV2	7542	12261	1.06%	0.117%
47	8.031	2165	2174	2181	rBV2	21137	30382	2.63%	0.289%
48	8.082	2182	2190	2213	rVV	312641	575740	49.77%	5.478%
49	8.185	2214	2222	2244	rVB	301712	472777	40.87%	4.498%
50	8.301	2250	2258	2280	rVB	24872	44699	3.86%	0.425%
51	8.677	2364	2375	2394	rBV	185187	282496	24.42%	2.688%
52	8.847	2417	2428	2452	rBV	610464	976395	84.41%	9.290%
53	9.095	2503	2505	2510	rBV2	472	353	0.03%	0.003%
54	9.407	2599	2602	2605	rBV3	472	339	0.03%	0.003%
55	9.551	2639	2647	2655	rBV4	4915	7441	0.64%	0.071%
56	9.748	2705	2708	2712	rBV2	285	304	0.03%	0.003%
57	9.960	2773	2774	2776	rBV	269	124	0.01%	0.001%
58	10.014	2782	2791	2793	rBV3	430	601	0.05%	0.006%
59	10.127	2818	2826	2835	rVB3	3335	5197	0.45%	0.049%
60	10.214	2841	2853	2871	rBV	311838	490450	42.40%	4.666%
61	10.320	2881	2886	2888	rBV3	586	635	0.05%	0.006%
62	10.416	2913	2916	2920	rVB2	459	344	0.03%	0.003%
63	10.503	2941	2943	2946	rBV2	185	105	0.01%	0.001%
64	10.519	2946	2948	2951	rBV3	299	179	0.02%	0.002%
65	10.539	2951	2954	2958	rBV2	421	433	0.04%	0.004%
66	10.728	3010	3013	3017	rBV2	247	183	0.02%	0.002%
67	10.751	3017	3020	3024	rVV2	284	216	0.02%	0.002%
68	10.821	3040	3042	3043	rBV2	314	143	0.01%	0.001%
69	10.876	3056	3059	3061	rBV3	387	247	0.02%	0.002%
70	10.911	3065	3070	3082	rVB6	3261	5202	0.45%	0.049%
71	11.034	3104	3108	3113	rVB5	861	852	0.07%	0.008%
72	11.111	3128	3132	3133	rBV2	341	255	0.02%	0.002%
73	11.246	3163	3174	3191	rBV	595501	909388	78.61%	8.652%
74	11.622	3279	3291	3312	rBV	515528	810388	70.05%	7.710%
75	12.088	3433	3436	3444	rVB4	876	1028	0.09%	0.010%
76	12.442	3544	3546	3548	rBV2	283	142	0.01%	0.001%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Title : VOC Analysis

77	13.082	3743	3745	3746	rBV	415	196	0.02%	0.002%
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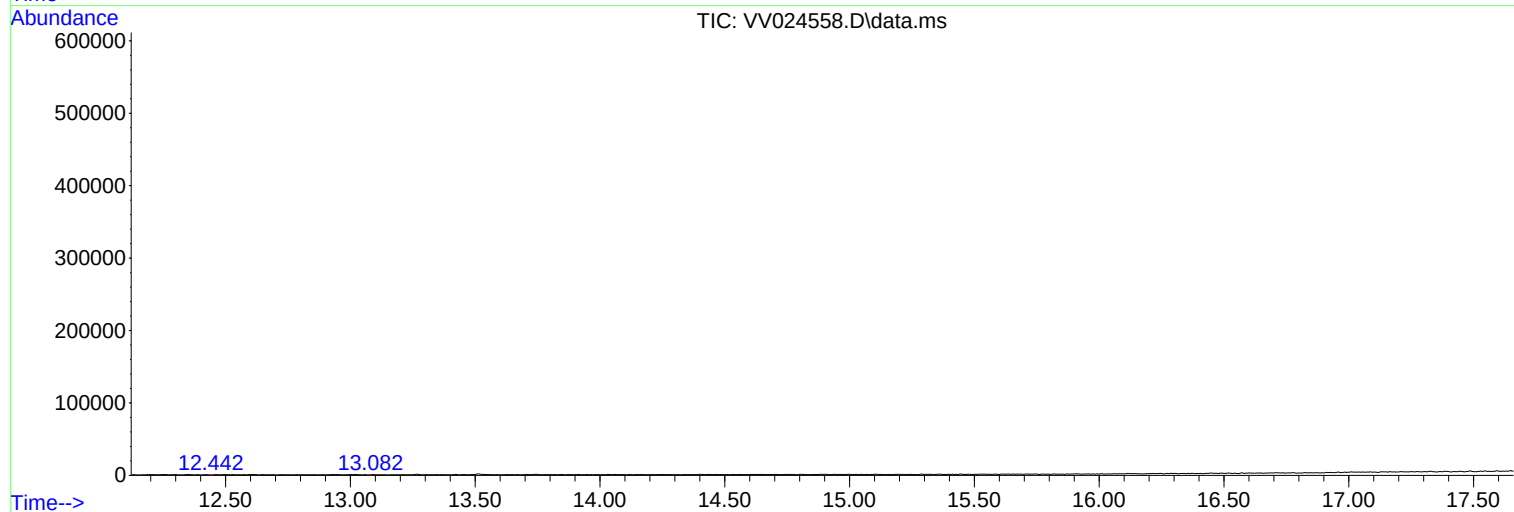
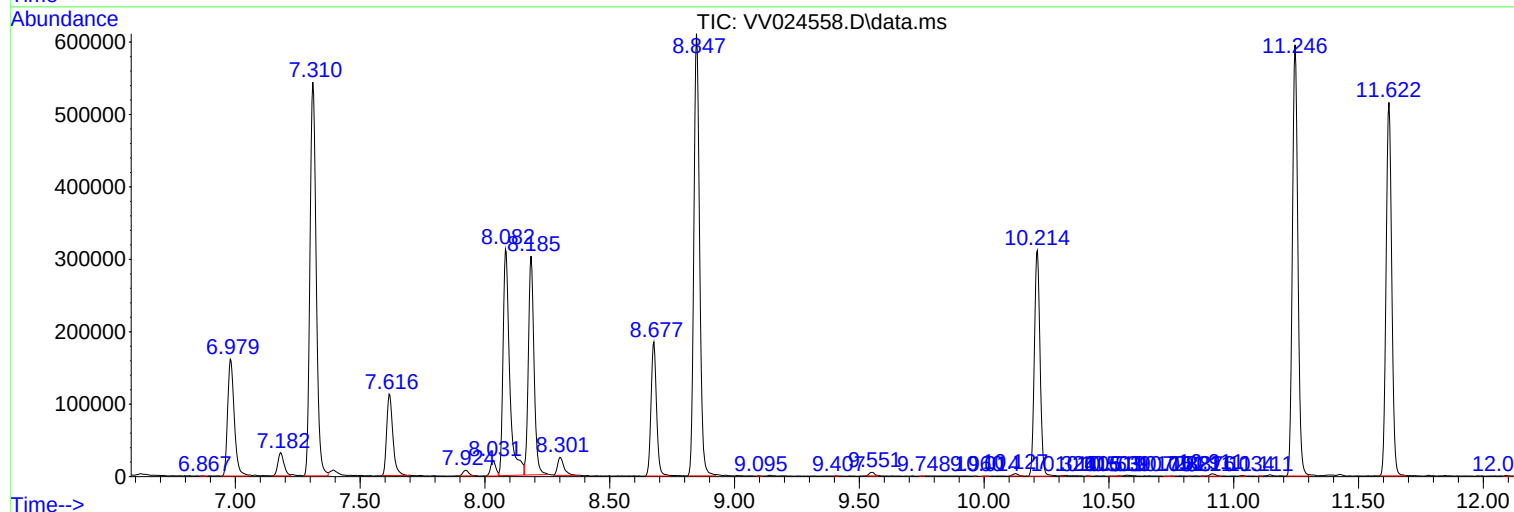
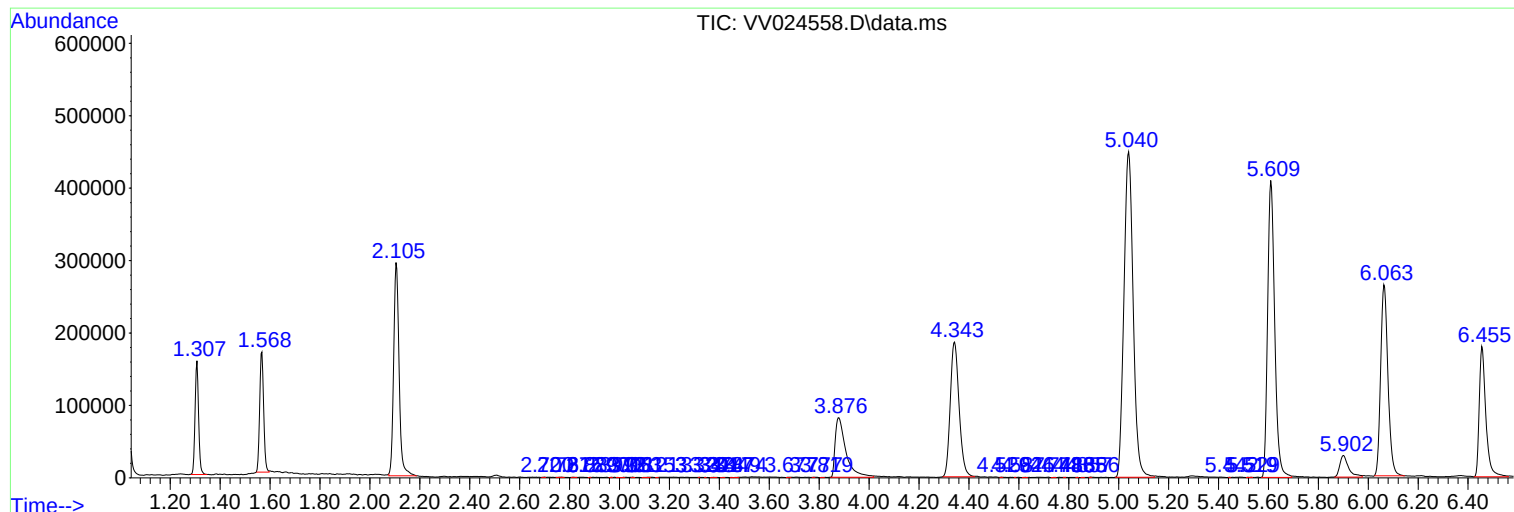
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0HQ5

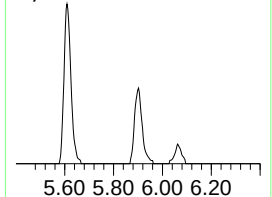
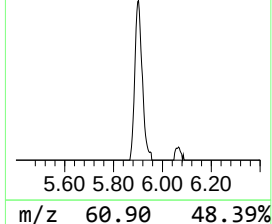
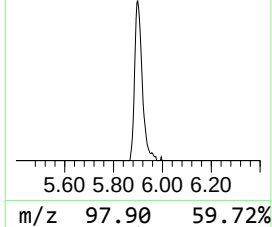
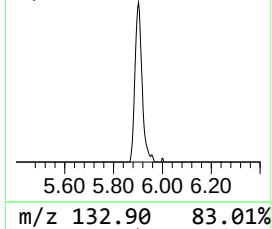
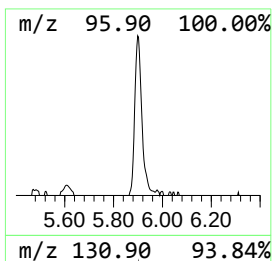
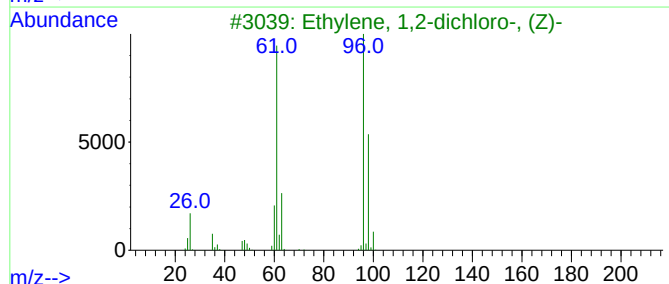
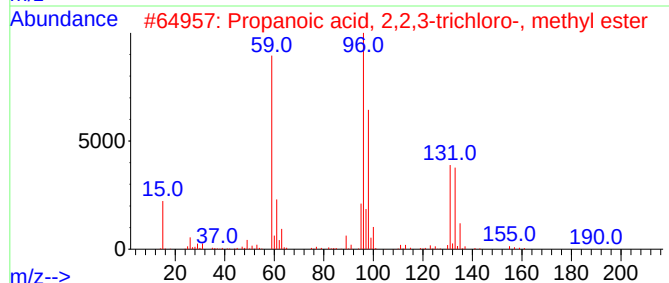
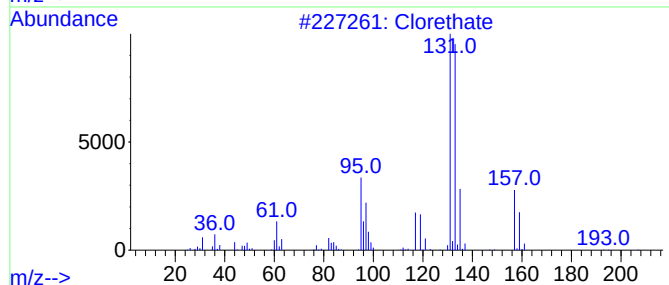
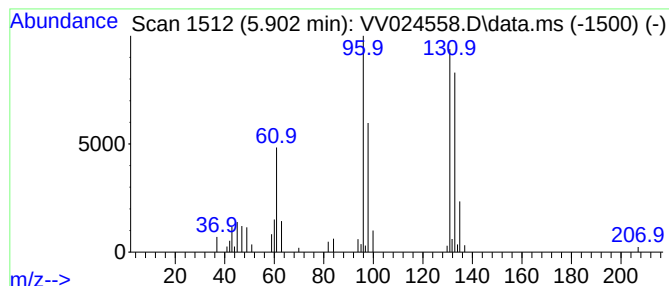
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Clorethate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	4.46 ug/L	72080	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Clorethate	322	C5H4Cl6O3	005634-37-7	50
2			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	42
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25



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Instrument :
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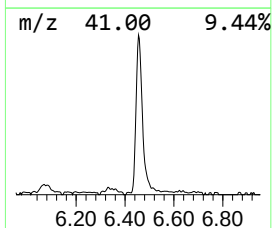
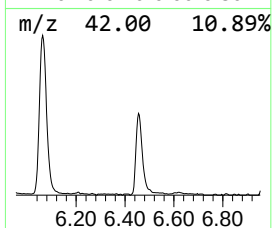
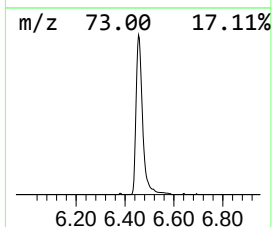
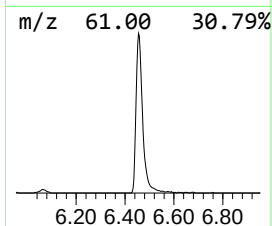
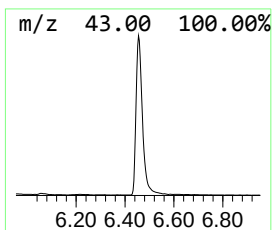
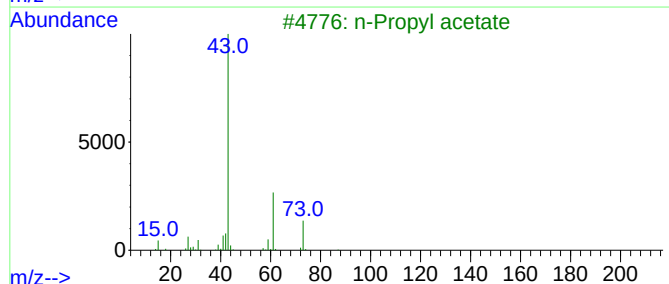
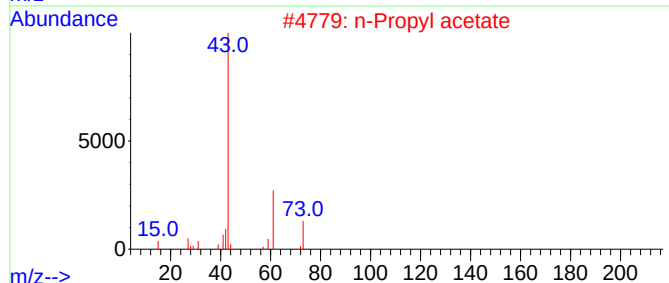
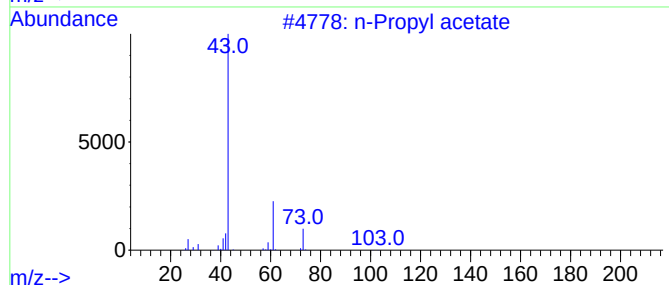
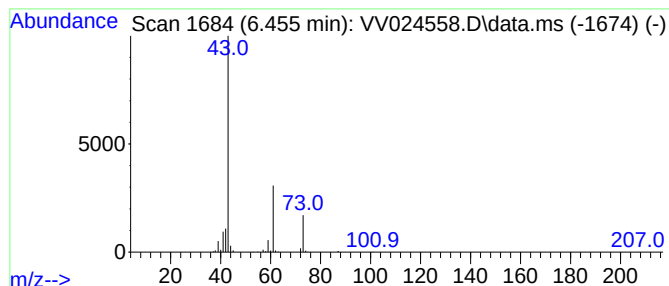
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.455	20.34 ug/L	329078	1,4-Difluorobenzene	5.609

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	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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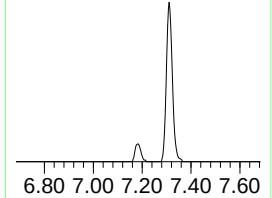
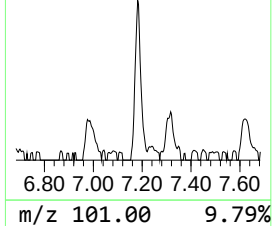
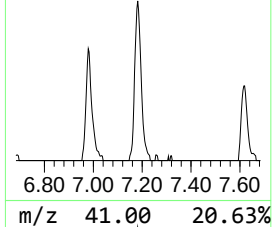
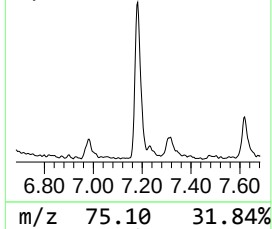
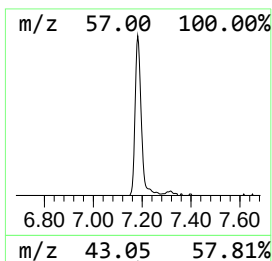
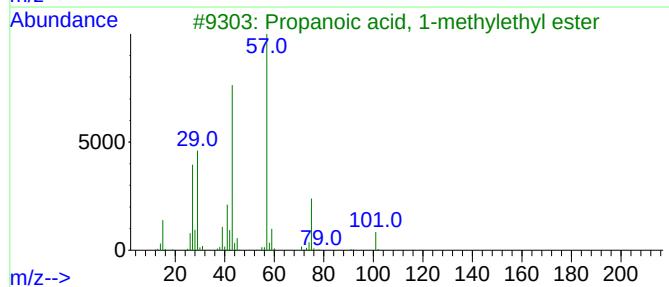
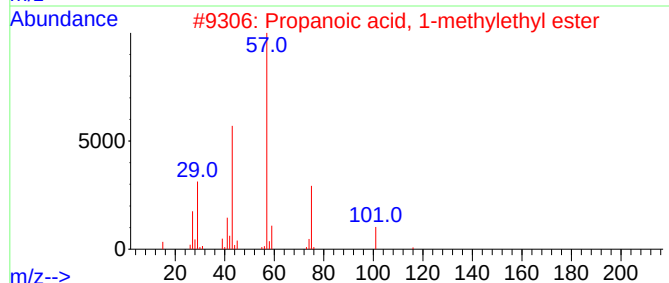
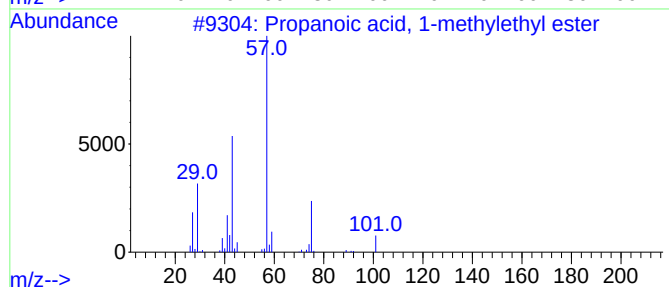
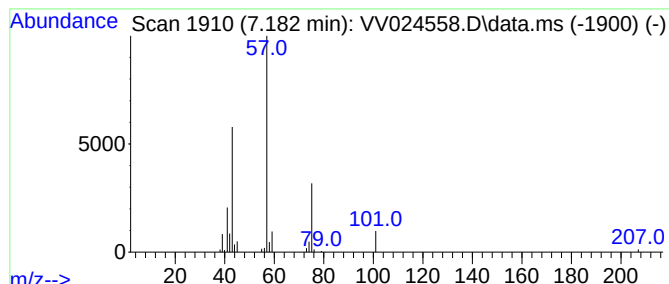
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	3.34 ug/L	53974	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	86
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56



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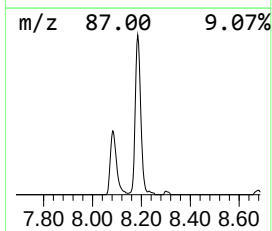
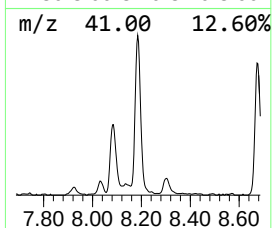
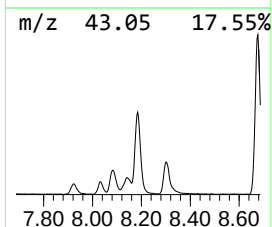
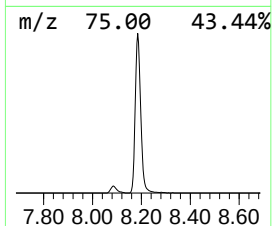
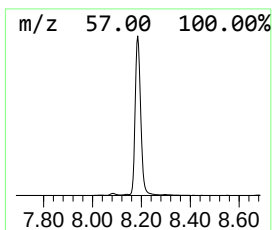
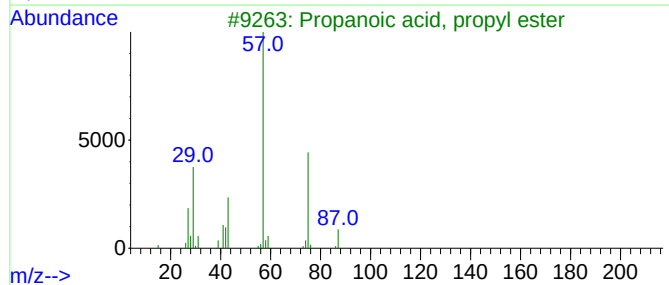
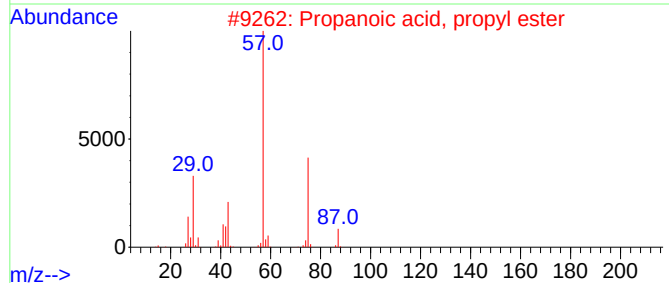
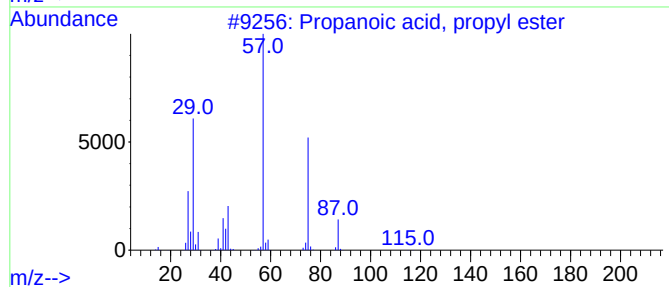
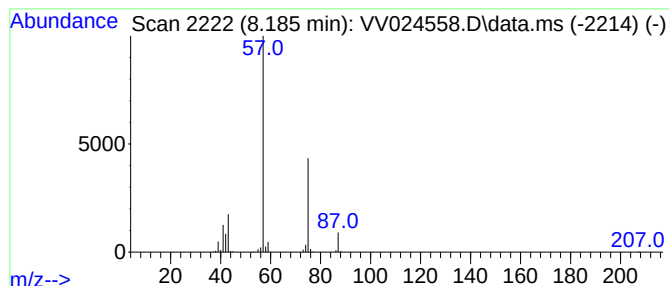
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.185	24.21 ug/L	472777	Chlorobenzene-d5	8.847

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	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV020422\
Data File : VV024558.D
Acq On : 04 Feb 2022 11:54
Operator : SY/MD
Sample : N1352-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0HQ5

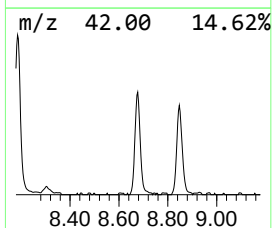
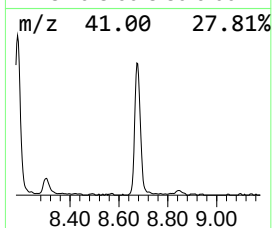
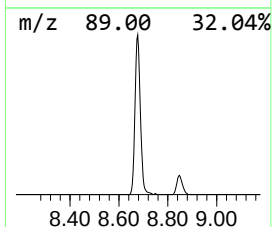
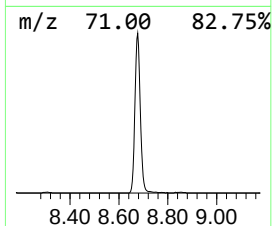
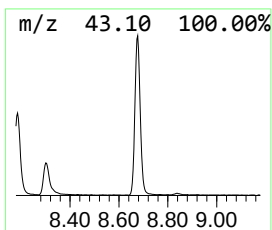
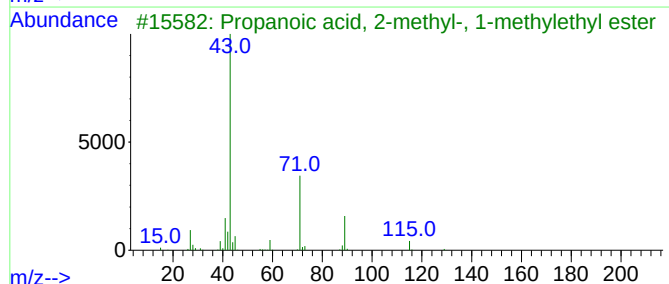
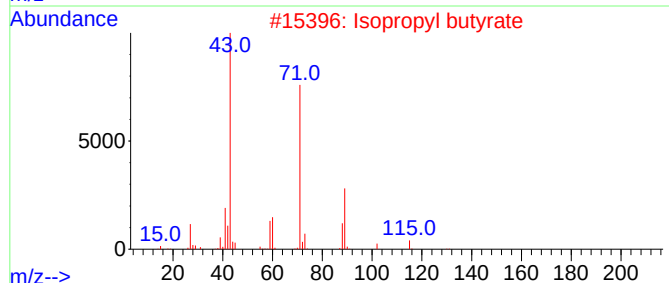
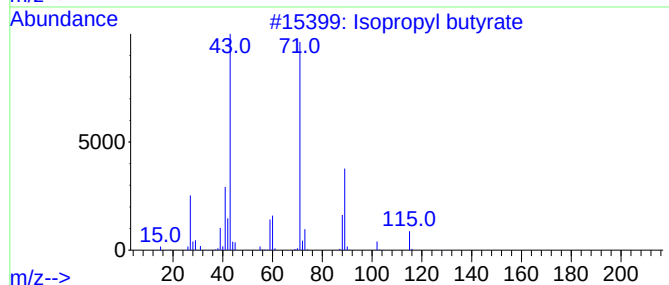
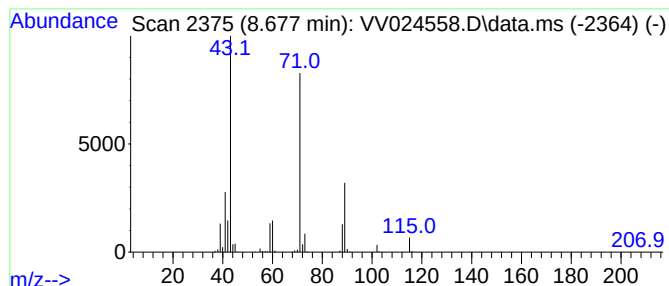
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Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.677	14.47 ug/L	282496	Chlorobenzene-d5	8.847

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			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV020422\
Data File : VV024558.D
Acq On : 04 Feb 2022 11:54
Operator : SY/MD
Sample : N1352-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0HQ5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.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
Clorethate	5.902	4.5	ug/L	72080	1	5.609	808775	50.0
n-Propyl acetate	6.455	20.3	ug/L	329078	1	5.609	808775	50.0
Propanoic acid,...	7.182	3.3	ug/L	53974	1	5.609	808775	50.0
Propanoic acid,...	8.185	24.2	ug/L	472777	2	8.847	976395	50.0
Isopropyl butyrate	8.677	14.5	ug/L	282496	2	8.847	976395	50.0