

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021930.D
 Acq On : 23 Aug 2021 12:43
 Operator : SY/MD
 Sample : M3487-02 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AB8

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

Signal : TIC: VV021930.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	99	rVB	196329	199747	15.07%	1.845%
2	1.564	156	163	178	rVB	154043	178418	13.46%	1.648%
3	2.105	321	331	346	rBV	299335	436720	32.95%	4.035%
4	2.429	430	432	435	rBV2	793	521	0.04%	0.005%
5	2.507	447	456	470	rVB	20406	35792	2.70%	0.331%
6	2.674	506	508	511	rVB	450	201	0.02%	0.002%
7	2.709	517	519	523	rBV2	571	338	0.03%	0.003%
8	2.744	528	530	532	rBV	279	163	0.01%	0.002%
9	2.783	540	542	544	rBV3	270	135	0.01%	0.001%
10	2.796	544	546	548	rVB2	338	164	0.01%	0.002%
11	2.825	553	555	558	rBV2	352	210	0.02%	0.002%
12	2.995	606	608	611	rBV2	268	204	0.02%	0.002%
13	3.076	631	633	634	rBV	329	143	0.01%	0.001%
14	3.159	655	659	662	rBV2	328	238	0.02%	0.002%
15	3.179	662	665	667	rBV2	359	285	0.02%	0.003%
16	3.275	694	695	698	rVB	371	177	0.01%	0.002%
17	3.404	732	735	736	rBV	308	196	0.01%	0.002%
18	3.426	739	742	743	rBV	505	278	0.02%	0.003%
19	3.497	761	764	767	rBV	248	144	0.01%	0.001%
20	3.542	777	778	782	rVB3	427	203	0.02%	0.002%
21	3.564	782	785	787	rBV2	418	232	0.02%	0.002%
22	3.757	842	845	850	rVB	272	218	0.02%	0.002%
23	3.789	852	855	859	rVB	274	165	0.01%	0.002%
24	3.812	859	862	865	rBV2	386	223	0.02%	0.002%
25	3.876	873	882	922	rBV	105731	284346	21.46%	2.627%
26	4.352	1013	1030	1062	rBV	207728	521158	39.32%	4.815%
27	4.690	1130	1135	1140	rVB3	649	616	0.05%	0.006%
28	4.728	1143	1147	1150	rBV2	363	264	0.02%	0.002%
29	4.793	1163	1167	1169	rVB2	353	256	0.02%	0.002%
30	4.805	1169	1171	1175	rBV2	325	132	0.01%	0.001%
31	4.831	1177	1179	1182	rVB2	383	235	0.02%	0.002%
32	4.847	1182	1184	1188	rBV	162	131	0.01%	0.001%
33	4.883	1191	1195	1196	rVB	333	218	0.02%	0.002%
34	4.892	1196	1198	1203	rVB2	384	333	0.03%	0.003%
35	4.918	1203	1206	1207	rBV	303	184	0.01%	0.002%
36	5.047	1229	1246	1274	rBV2	521504	1325306	100.00%	12.244%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	5.522	1389	1394	1397	rBV2	509	447	0.03%	0.004%
38	5.558	1403	1405	1408	rVB	298	131	0.01%	0.001%
39	5.619	1410	1424	1461	rBV	453932	916450	69.15%	8.467%
40	5.908	1503	1514	1531	rBV3	27836	58425	4.41%	0.540%
41	6.072	1552	1565	1589	rBV	290401	588355	44.39%	5.436%
42	6.468	1679	1688	1713	rBV	64624	127101	9.59%	1.174%
43	6.706	1761	1762	1767	rVB2	781	497	0.04%	0.005%
44	6.886	1815	1818	1824	rBV3	280	222	0.02%	0.002%
45	6.989	1839	1850	1873	rBV	160487	296085	22.34%	2.735%
46	7.191	1905	1913	1930	rBV2	12340	21094	1.59%	0.195%
47	7.317	1940	1952	1972	rBV	619551	1093700	82.52%	10.104%
48	7.625	2037	2048	2071	rBV	108069	191533	14.45%	1.770%
49	7.786	2097	2098	2100	rBV2	485	194	0.01%	0.002%
50	7.863	2120	2122	2128	rVB3	570	442	0.03%	0.004%
51	7.899	2131	2133	2136	rBV2	249	150	0.01%	0.001%
52	7.934	2136	2144	2152	rBV3	3640	5513	0.42%	0.051%
53	7.995	2160	2163	2166	rBV2	390	317	0.02%	0.003%
54	8.008	2166	2167	2169	rVB	444	136	0.01%	0.001%
55	8.040	2169	2177	2183	rBV4	8018	11554	0.87%	0.107%
56	8.091	2184	2193	2217	rVV2	274250	518186	39.10%	4.787%
57	8.194	2218	2225	2247	rVB	93122	155237	11.71%	1.434%
58	8.532	2327	2330	2331	rBV2	529	269	0.02%	0.002%
59	8.577	2341	2344	2346	rBV2	452	257	0.02%	0.002%
60	8.616	2351	2356	2357	rBV3	432	331	0.02%	0.003%
61	8.683	2366	2377	2400	rBV	62183	103473	7.81%	0.956%
62	8.854	2418	2430	2460	rBV	667483	1101039	83.08%	10.172%
63	9.018	2479	2481	2489	rVB3	788	674	0.05%	0.006%
64	9.069	2493	2497	2500	rBV3	532	432	0.03%	0.004%
65	9.101	2504	2507	2510	rBV3	284	185	0.01%	0.002%
66	9.127	2512	2515	2518	rBV2	343	278	0.02%	0.003%
67	9.146	2520	2521	2523	rBV	487	264	0.02%	0.002%
68	9.294	2564	2567	2569	rBV	308	153	0.01%	0.001%
69	9.307	2569	2571	2576	rBV2	240	143	0.01%	0.001%
70	9.349	2582	2584	2586	rBV	274	150	0.01%	0.001%
71	9.513	2632	2635	2638	rVB2	382	214	0.02%	0.002%
72	9.561	2644	2650	2659	rBV8	1143	1764	0.13%	0.016%
73	9.622	2667	2669	2672	rBV2	374	201	0.02%	0.002%
74	9.683	2685	2688	2691	rVB2	638	368	0.03%	0.003%
75	10.059	2802	2805	2809	rBV3	268	253	0.02%	0.002%
76	10.127	2818	2826	2837	rVB6	3634	6591	0.50%	0.061%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Peak separation: 5

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Title : VOC Analysis

77	10.217	2843	2854	2875	rBV	370316	593119	44.75%	5.480%
78	10.509	2942	2945	2947	rBV	326	166	0.01%	0.002%
79	10.580	2960	2967	2973	rBV6	1297	1867	0.14%	0.017%
80	10.657	2989	2991	2997	rBV3	380	344	0.03%	0.003%
81	10.747	3016	3019	3020	rBV	315	156	0.01%	0.001%
82	10.886	3060	3062	3065	rBV2	324	217	0.02%	0.002%
83	10.915	3065	3071	3073	rBV3	2566	2416	0.18%	0.022%
84	11.001	3093	3098	3100	rBV2	270	181	0.01%	0.002%
85	11.030	3102	3107	3111	rBV3	643	752	0.06%	0.007%
86	11.252	3164	3176	3197	rBV	682739	1065312	80.38%	9.842%
87	11.477	3243	3246	3251	rBV3	506	442	0.03%	0.004%
88	11.529	3258	3262	3264	rBV3	887	636	0.05%	0.006%
89	11.625	3280	3292	3312	rBV	610112	964029	72.74%	8.906%
90	11.985	3402	3404	3407	rVB2	425	189	0.01%	0.002%
91	12.024	3414	3416	3422	rVB2	590	414	0.03%	0.004%
92	12.059	3422	3427	3429	rBV2	456	373	0.03%	0.003%
93	12.217	3472	3476	3479	rBV3	361	267	0.02%	0.002%
94	12.458	3549	3551	3554	rVB2	335	212	0.02%	0.002%
95	12.519	3568	3570	3574	rVB3	511	285	0.02%	0.003%
96	12.593	3589	3593	3596	rBV3	687	696	0.05%	0.006%
97	12.715	3628	3631	3633	rBV2	375	225	0.02%	0.002%
98	12.802	3655	3658	3662	rBV2	402	268	0.02%	0.002%
99	13.673	3927	3929	3931	rBV	388	178	0.01%	0.002%
100	14.085	4055	4057	4058	rBV	549	242	0.02%	0.002%

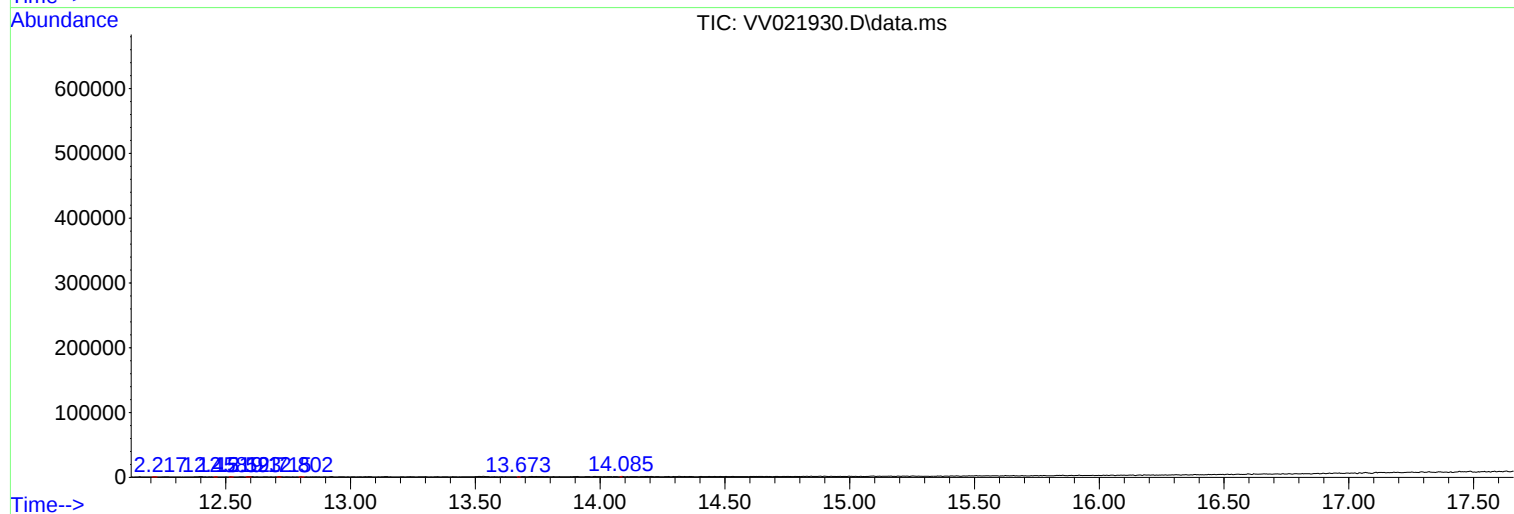
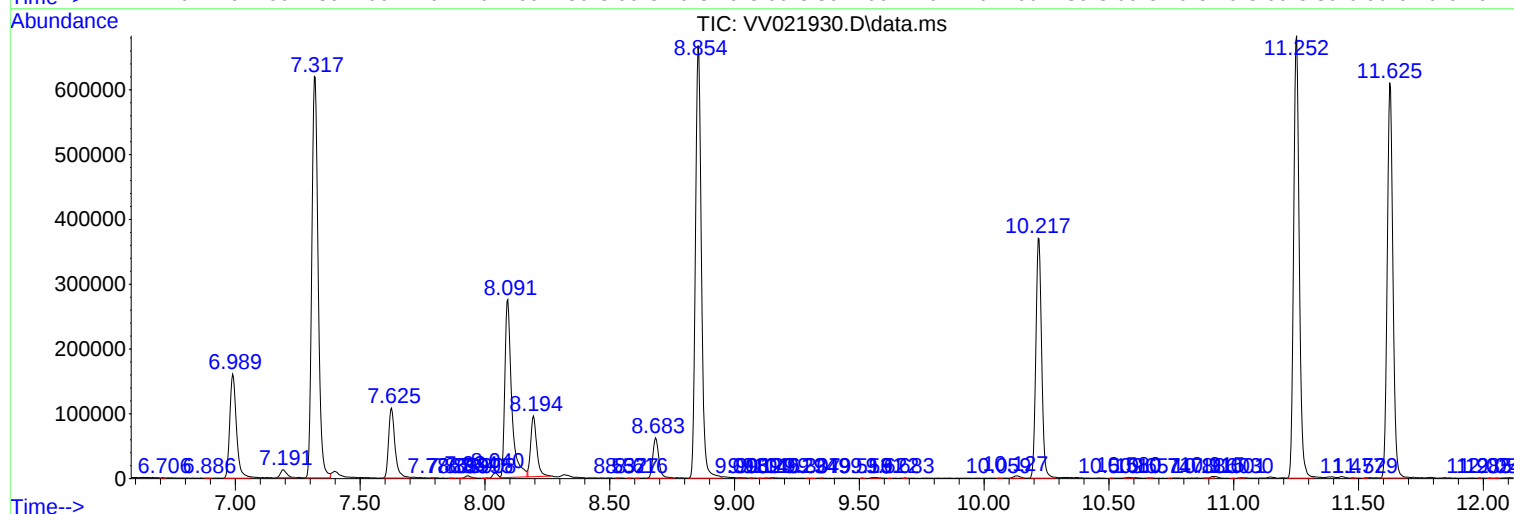
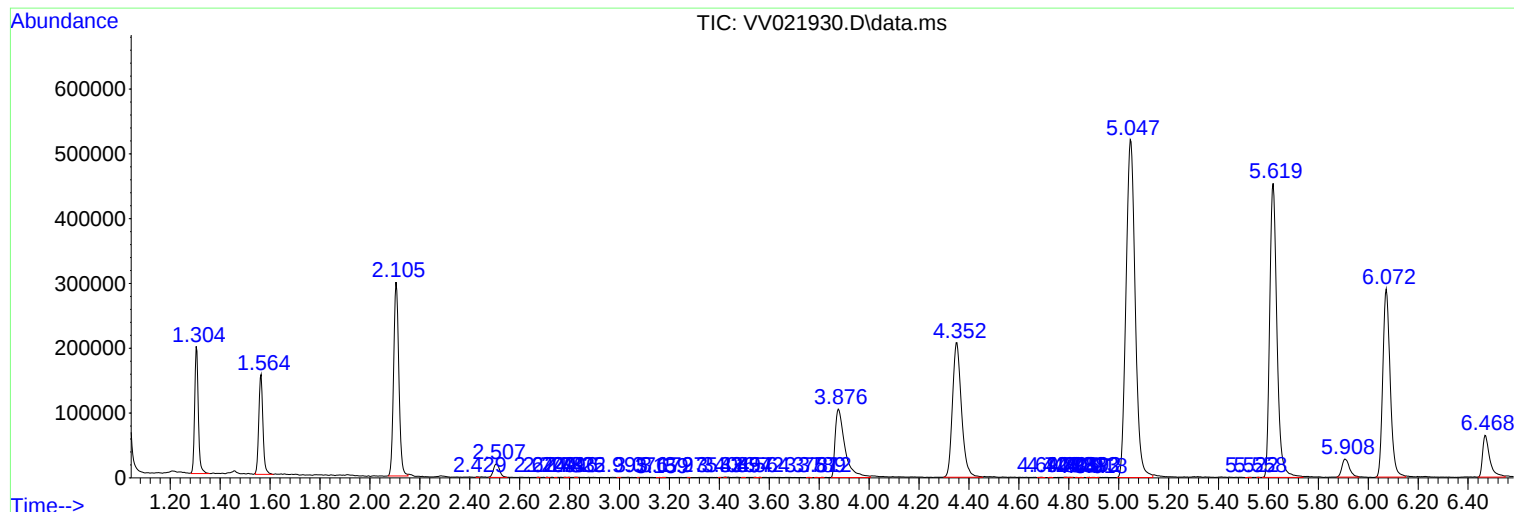
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.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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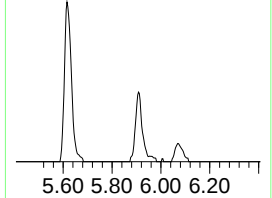
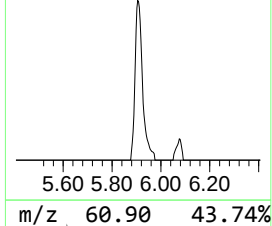
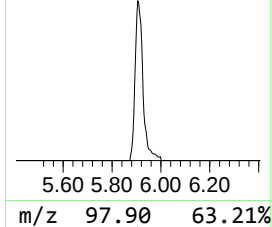
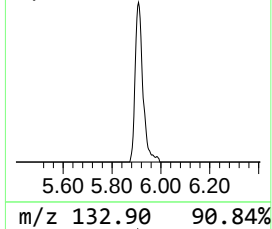
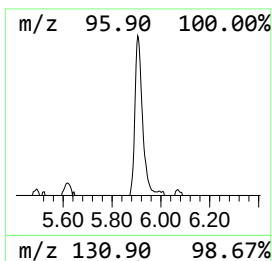
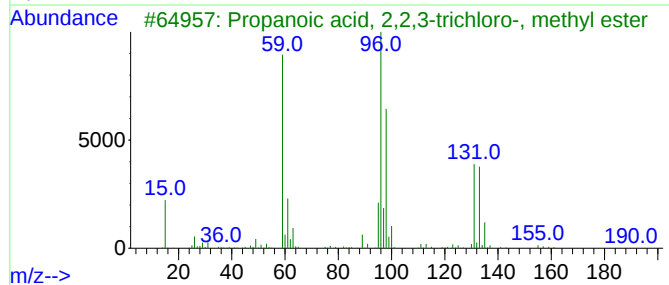
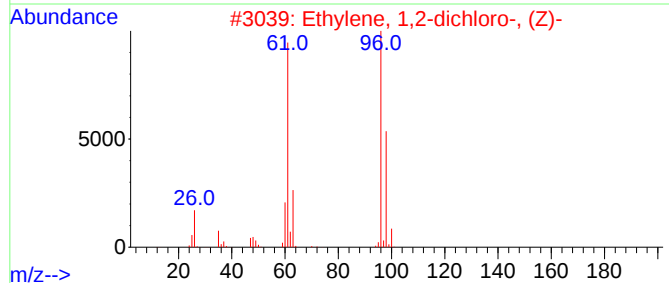
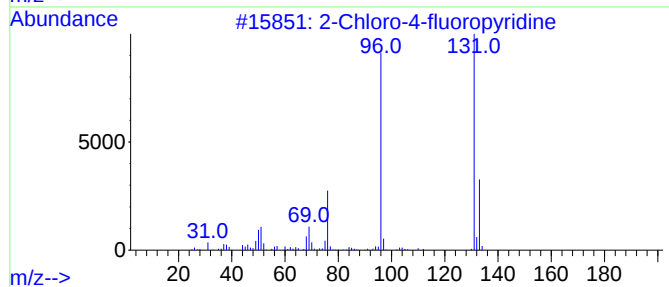
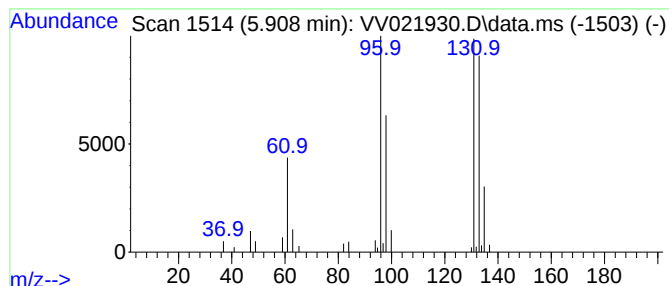
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	3.19 ug/L	58425	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
2		Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3		Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	38
4		4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5		Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25



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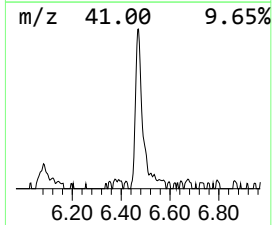
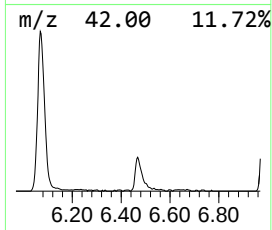
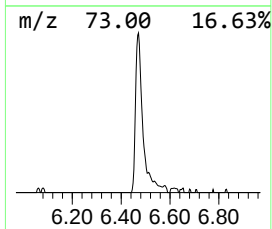
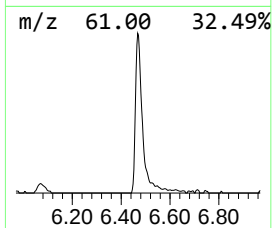
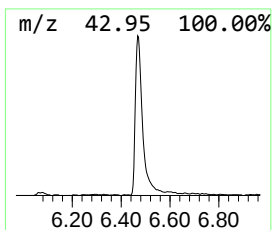
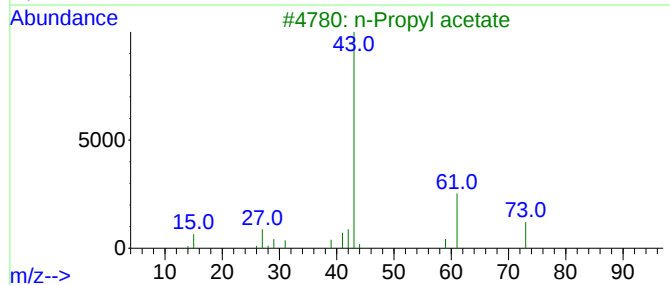
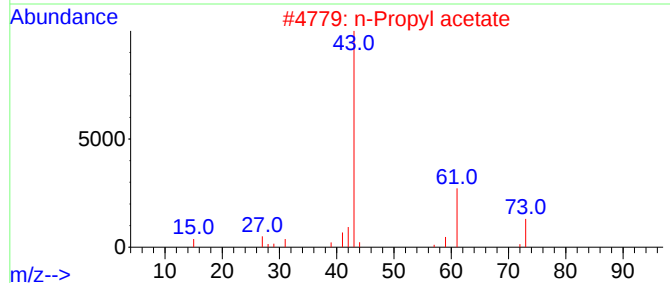
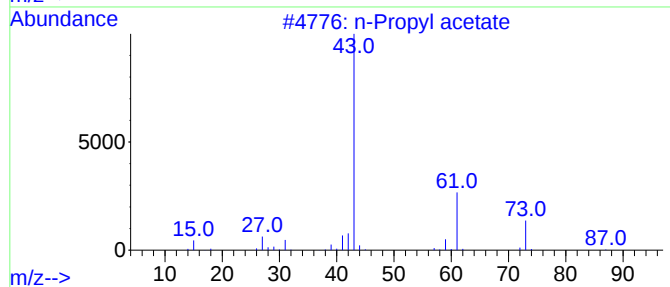
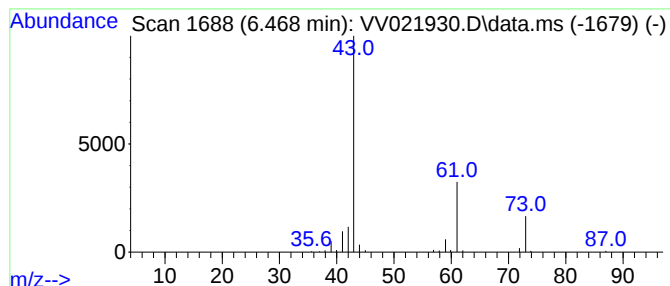
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.468	6.93 ug/L	127101	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	78
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	72



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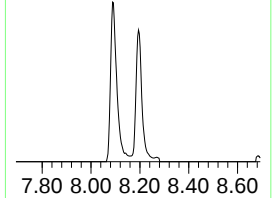
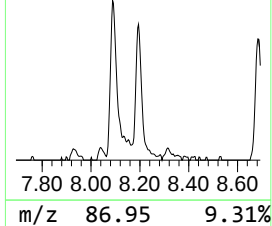
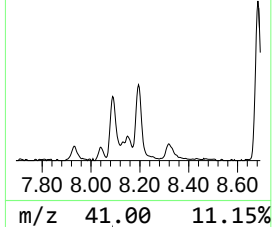
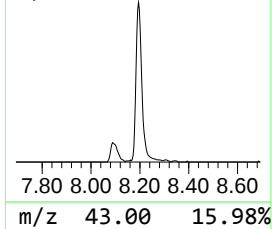
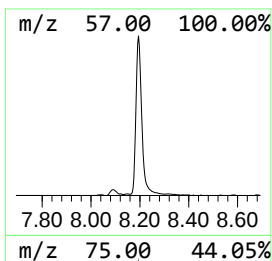
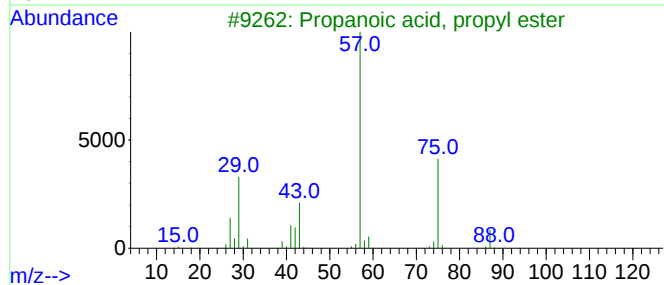
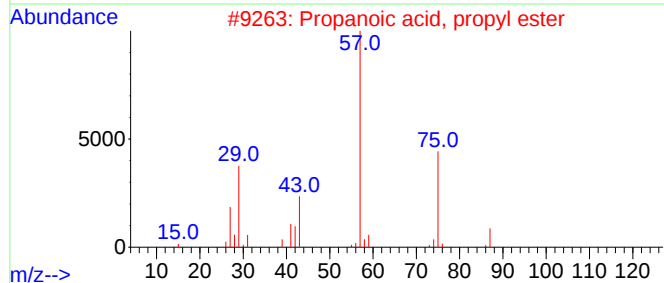
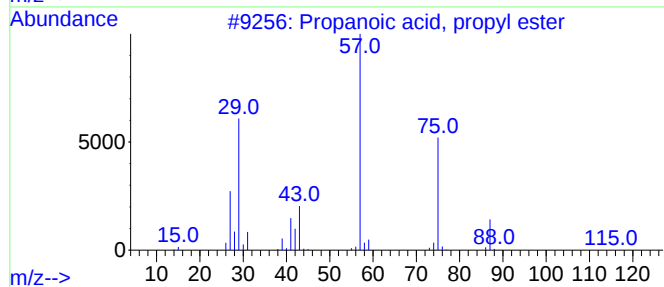
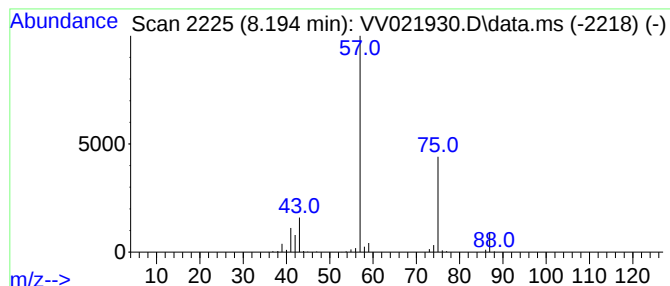
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.194	7.05 ug/L	155237	Chlorobenzene-d5	8.854

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	50
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, propyl ester	116	C6H12O2	000106-36-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021930.D
Acq On : 23 Aug 2021 12:43
Operator : SY/MD
Sample : M3487-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB8

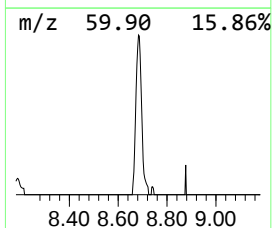
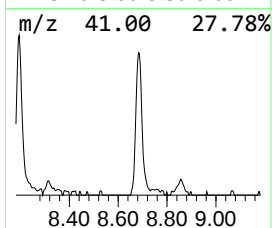
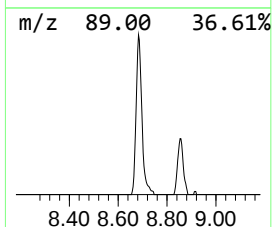
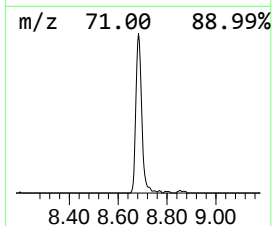
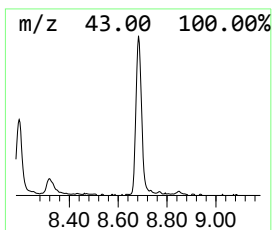
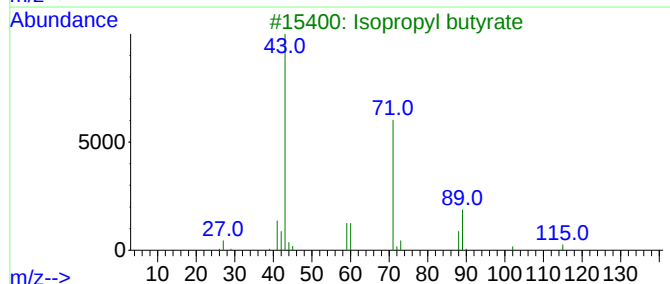
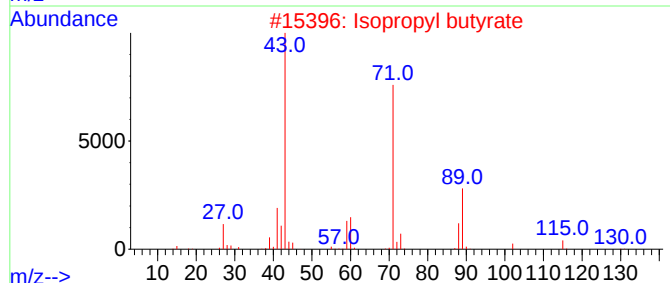
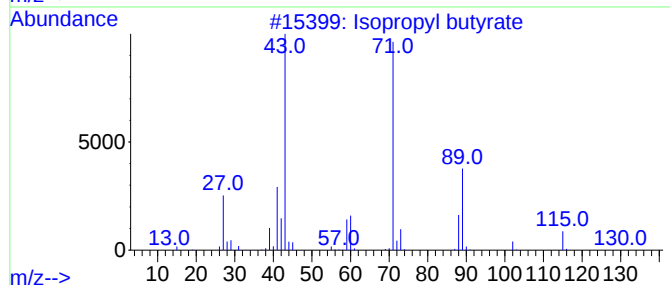
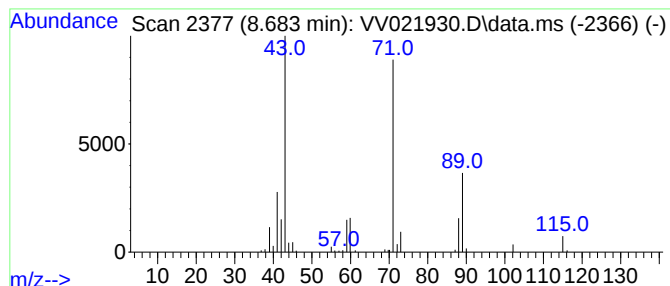
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.683	4.70 ug/L	103473	Chlorobenzene-d5	8.854

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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021930.D
Acq On : 23 Aug 2021 12:43
Operator : SY/MD
Sample : M3487-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.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
unknown-01	5.908	3.2	ug/L	58425	1	5.619	916450	50.0
n-Propyl acetate	6.468	6.9	ug/L	127101	1	5.619	916450	50.0
Propanoic acid,...	8.194	7.0	ug/L	155237	2	8.854	1101040	50.0
Isopropyl butyrate	8.683	4.7	ug/L	103473	2	8.854	1101040	50.0