

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021929.D
 Acq On : 23 Aug 2021 12:19
 Operator : SY/MD
 Sample : M3487-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AB7

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: VV021929.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	97	rVB	205920	208027	15.26%	1.873%
2	1.561	155	162	176	rBV	157129	180647	13.25%	1.626%
3	2.101	321	330	345	rBV	298868	443333	32.52%	3.991%
4	2.503	445	455	467	rBV	26167	44636	3.27%	0.402%
5	2.764	534	536	541	rVB2	435	246	0.02%	0.002%
6	2.793	541	545	546	rBV2	281	182	0.01%	0.002%
7	2.880	569	572	573	rBV	331	129	0.01%	0.001%
8	2.954	592	595	597	rBV	220	129	0.01%	0.001%
9	2.966	597	599	605	rVB	420	301	0.02%	0.003%
10	3.040	619	622	625	rVB2	484	280	0.02%	0.003%
11	3.066	628	630	634	rVB2	337	198	0.01%	0.002%
12	3.085	634	636	639	rBV	180	136	0.01%	0.001%
13	3.101	639	641	644	rVB2	338	204	0.01%	0.002%
14	3.150	652	656	657	rBV	209	159	0.01%	0.001%
15	3.204	670	673	675	rBV2	173	119	0.01%	0.001%
16	3.253	686	688	690	rVB2	287	113	0.01%	0.001%
17	3.265	690	692	694	rBV2	252	135	0.01%	0.001%
18	3.281	694	697	701	rVV2	425	325	0.02%	0.003%
19	3.320	705	709	710	rBV	308	138	0.01%	0.001%
20	3.462	751	753	755	rBV2	299	134	0.01%	0.001%
21	3.487	755	761	762	rBV3	541	408	0.03%	0.004%
22	3.548	776	780	781	rBV2	163	114	0.01%	0.001%
23	3.609	798	799	802	rVV2	265	133	0.01%	0.001%
24	3.677	816	820	824	rBV2	329	313	0.02%	0.003%
25	3.696	824	826	828	rBV	275	141	0.01%	0.001%
26	3.764	844	847	849	rBV2	211	150	0.01%	0.001%
27	3.812	855	862	866	rBV3	426	481	0.04%	0.004%
28	3.870	869	880	912	rBV	100764	265278	19.46%	2.388%
29	4.343	1010	1027	1056	rBV	211739	537924	39.46%	4.843%
30	4.728	1144	1147	1150	rBV2	449	315	0.02%	0.003%
31	4.767	1157	1159	1162	rVB	291	135	0.01%	0.001%
32	4.786	1162	1165	1167	rBV	342	204	0.01%	0.002%
33	4.876	1189	1193	1196	rVB3	287	219	0.02%	0.002%
34	5.043	1224	1245	1274	rBV2	533069	1363279	100.00%	12.273%
35	5.413	1358	1360	1368	rVB4	900	934	0.07%	0.008%
36	5.478	1376	1380	1384	rBV4	472	462	0.03%	0.004%

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Integrator: RTE

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

37	5.519	1391	1393	1396	rBV	329	141	0.01%	0.001%
38	5.568	1403	1408	1409	rVB2	265	213	0.02%	0.002%
39	5.613	1409	1422	1451	rBV	478023	962621	70.61%	8.666%
40	5.905	1502	1513	1531	rBV2	26402	56018	4.11%	0.504%
41	6.066	1550	1563	1586	rBV	290507	603924	44.30%	5.437%
42	6.465	1677	1687	1723	rBV	57365	119320	8.75%	1.074%
43	6.802	1790	1792	1794	rBV2	408	266	0.02%	0.002%
44	6.931	1830	1832	1835	rBV3	349	195	0.01%	0.002%
45	6.986	1837	1849	1871	rBV	166734	303799	22.28%	2.735%
46	7.188	1903	1912	1924	rBV2	12803	22502	1.65%	0.203%
47	7.313	1939	1951	1971	rBV	646834	1130189	82.90%	10.175%
48	7.619	2035	2046	2073	rBV	110229	199312	14.62%	1.794%
49	7.873	2122	2125	2128	rBV2	334	206	0.02%	0.002%
50	7.889	2128	2130	2132	rBV	367	190	0.01%	0.002%
51	7.931	2134	2143	2153	rVV4	2728	5556	0.41%	0.050%
52	7.998	2161	2164	2167	rVB	446	243	0.02%	0.002%
53	8.037	2167	2176	2183	rBV2	7950	11665	0.86%	0.105%
54	8.088	2183	2192	2216	rVV2	256982	490994	36.02%	4.420%
55	8.191	2217	2224	2254	rVB	94255	160978	11.81%	1.449%
56	8.394	2286	2287	2289	rBV	367	184	0.01%	0.002%
57	8.635	2359	2362	2365	rBV2	371	268	0.02%	0.002%
58	8.680	2365	2376	2397	rBV	59006	98113	7.20%	0.883%
59	8.850	2417	2429	2454	rBV	711244	1148487	84.24%	10.340%
60	9.108	2507	2509	2513	rVB3	546	344	0.03%	0.003%
61	9.153	2518	2523	2528	rBV5	1067	1285	0.09%	0.012%
62	9.207	2538	2540	2542	rBV	287	127	0.01%	0.001%
63	9.310	2570	2572	2576	rBV2	257	253	0.02%	0.002%
64	9.391	2595	2597	2599	rBV2	188	114	0.01%	0.001%
65	9.555	2642	2648	2649	rBV4	1329	1110	0.08%	0.010%
66	9.741	2703	2706	2708	rBV2	181	120	0.01%	0.001%
67	9.815	2722	2729	2732	rBV2	352	434	0.03%	0.004%
68	9.956	2771	2773	2779	rVB2	297	203	0.01%	0.002%
69	10.024	2790	2794	2796	rBV2	551	340	0.02%	0.003%
70	10.130	2819	2827	2836	rVB4	3647	5756	0.42%	0.052%
71	10.217	2841	2854	2876	rBV	367586	590367	43.30%	5.315%
72	10.423	2916	2918	2922	rBV	269	161	0.01%	0.001%
73	10.545	2953	2956	2958	rBV	494	272	0.02%	0.002%
74	10.571	2958	2964	2965	rBV4	860	784	0.06%	0.007%
75	10.635	2980	2984	2987	rBV3	372	249	0.02%	0.002%
76	10.657	2987	2991	2998	rVB3	565	679	0.05%	0.006%

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Title : VOC Analysis

77	10.693	2998	3002	3004	rBV2	294	237	0.02%	0.002%
78	10.789	3028	3032	3035	rVB2	374	254	0.02%	0.002%
79	10.857	3050	3053	3054	rBV2	392	176	0.01%	0.002%
80	10.918	3064	3072	3083	rVB7	3415	5654	0.41%	0.051%
81	10.960	3083	3085	3088	rVB2	267	120	0.01%	0.001%
82	11.104	3127	3130	3131	rBV2	296	153	0.01%	0.001%
83	11.146	3138	3143	3148	rBV4	1684	1904	0.14%	0.017%
84	11.249	3164	3175	3204	rBV	731483	1135928	83.32%	10.227%
85	11.551	3263	3269	3271	rBV4	775	785	0.06%	0.007%
86	11.625	3279	3292	3312	rBV	635199	990302	72.64%	8.916%
87	11.821	3349	3353	3354	rBV	437	284	0.02%	0.003%
88	11.944	3387	3391	3392	rBV2	306	233	0.02%	0.002%
89	11.985	3402	3404	3407	rVB2	286	115	0.01%	0.001%
90	12.403	3531	3534	3541	rVB2	334	218	0.02%	0.002%
91	12.442	3544	3546	3549	rBV2	230	138	0.01%	0.001%
92	12.535	3573	3575	3578	rBV2	553	284	0.02%	0.003%
93	12.661	3610	3614	3618	rBV5	415	379	0.03%	0.003%
94	12.715	3627	3631	3634	rBV2	556	491	0.04%	0.004%
95	12.866	3675	3678	3681	rBV	322	224	0.02%	0.002%
96	12.902	3686	3689	3691	rBV	519	303	0.02%	0.003%
97	12.943	3701	3702	3706	rBV	240	135	0.01%	0.001%
98	13.069	3737	3741	3743	rBV	392	293	0.02%	0.003%
99	13.178	3771	3775	3779	rBV2	624	568	0.04%	0.005%
100	13.635	3914	3917	3920	rBV	409	348	0.03%	0.003%

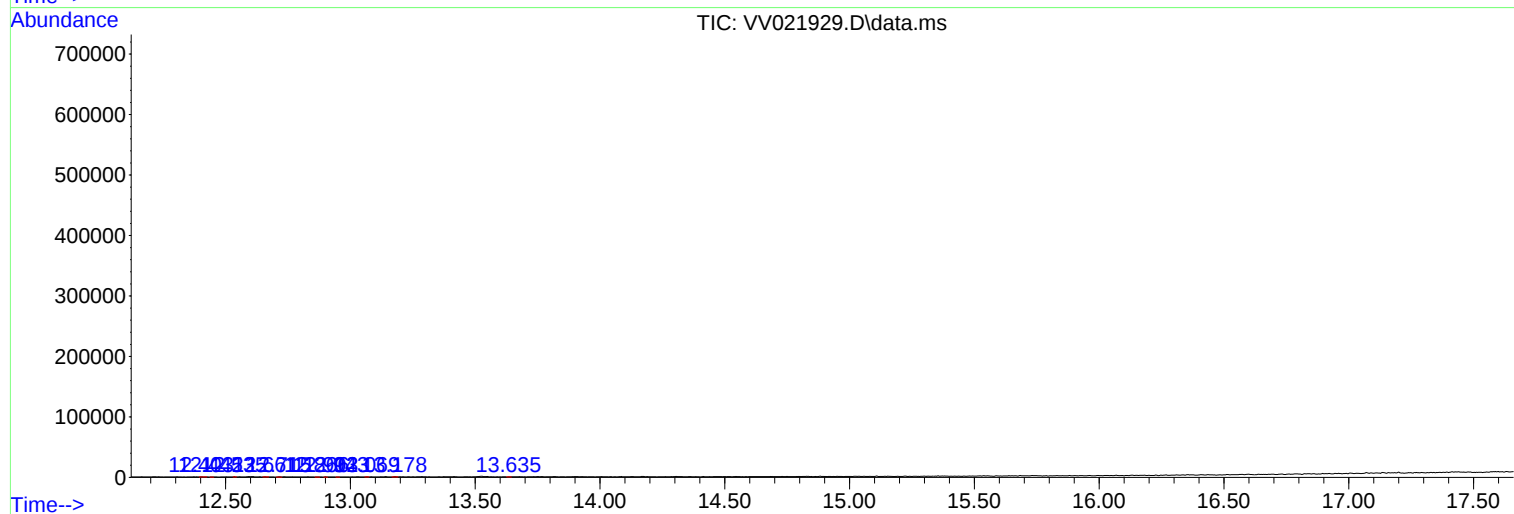
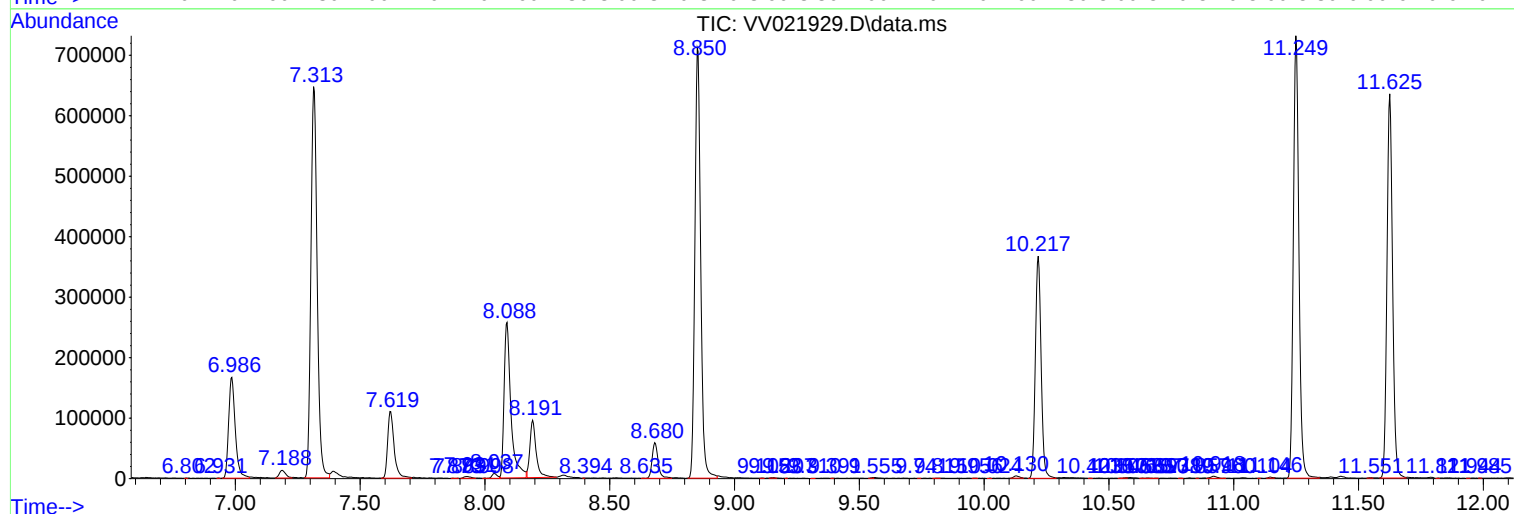
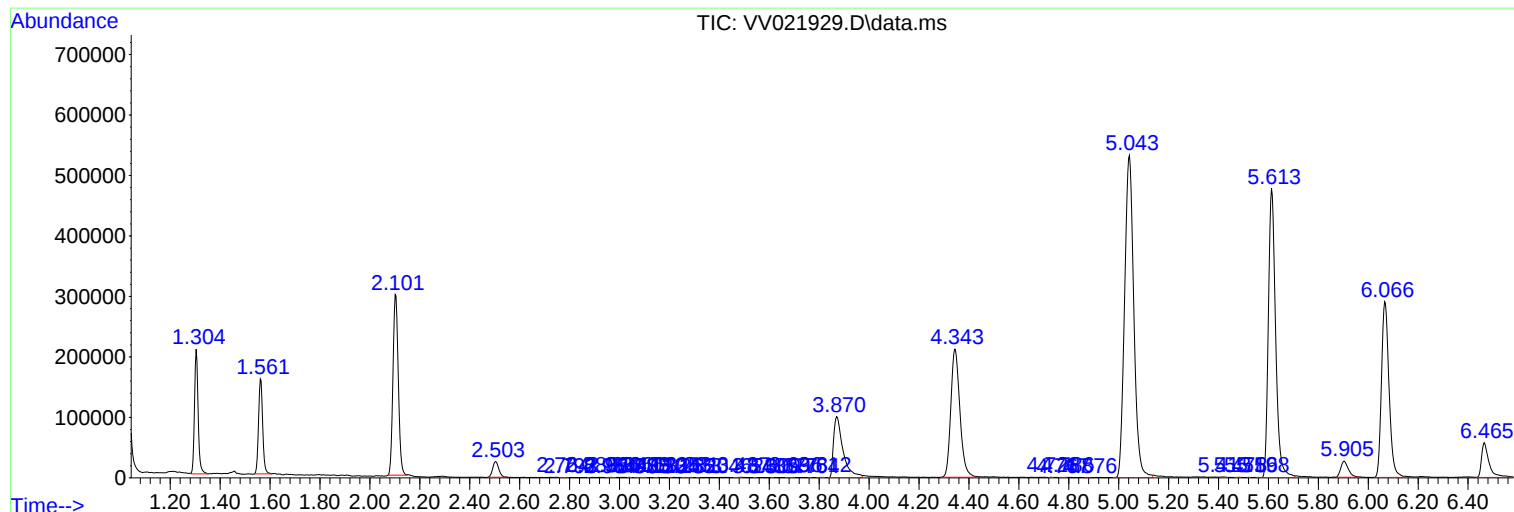
Sum of corrected areas: 11107569

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Instrument :
MSVOA_V
ClientSampleId :
C0AB7

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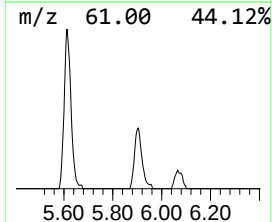
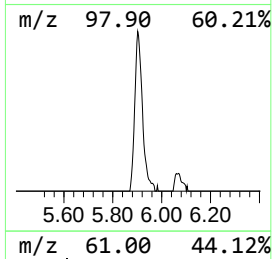
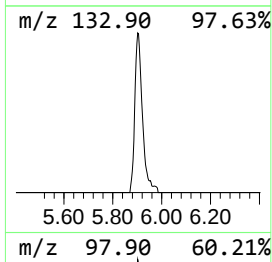
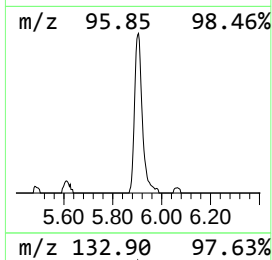
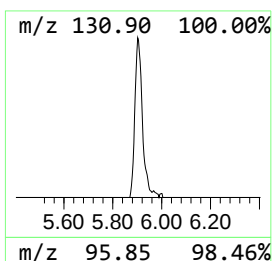
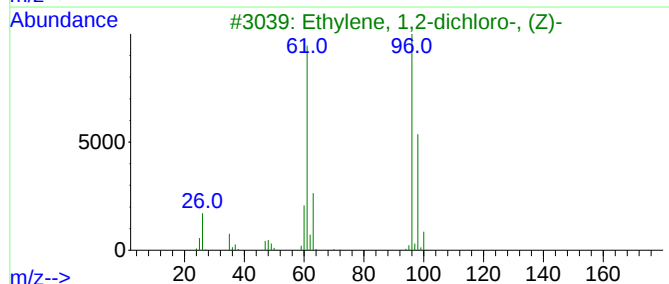
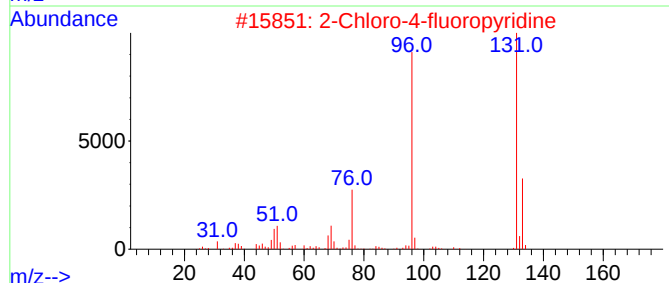
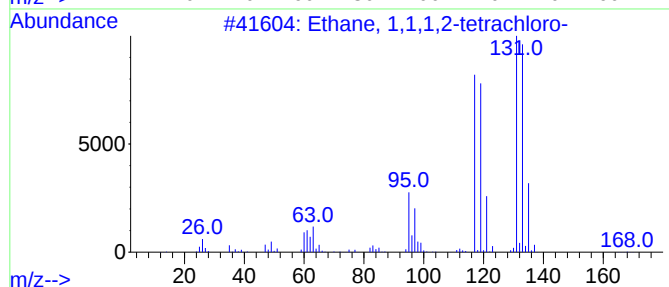
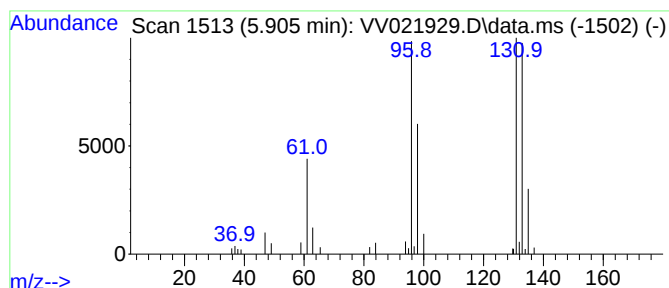
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
5.905	2.91 ug/L	56018	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	43
2			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	27



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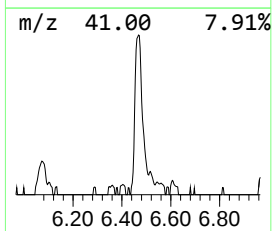
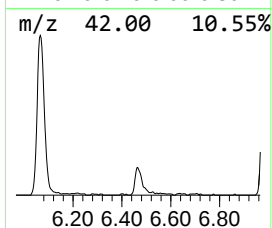
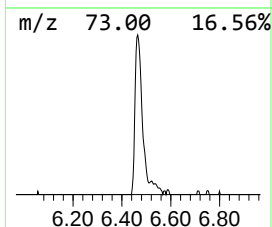
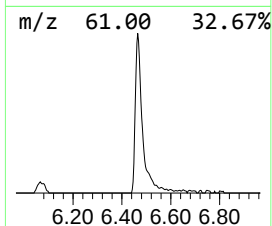
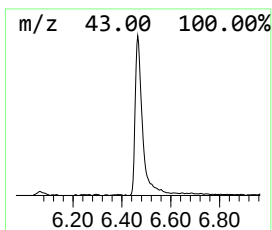
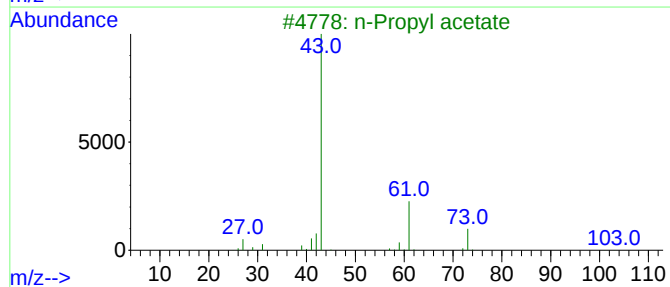
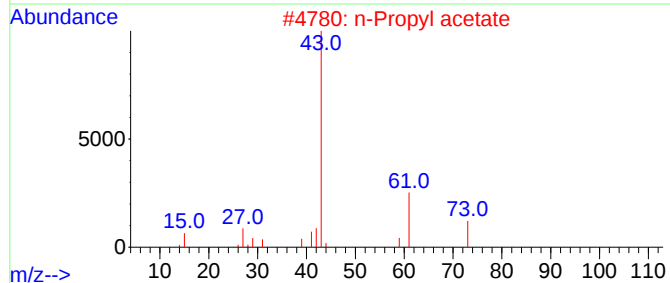
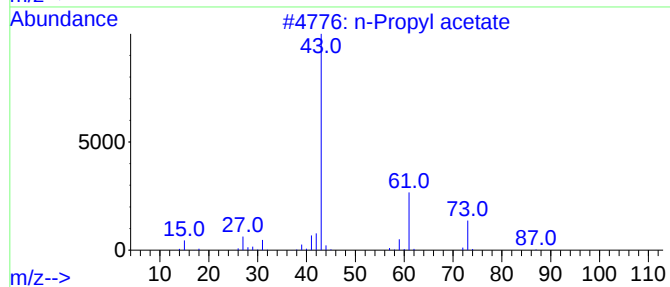
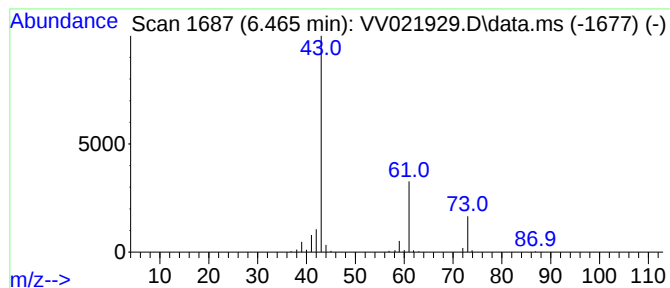
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
6.465	6.20 ug/L	119320	1,4-Difluorobenzene	5.613

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	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	64
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	Isopropyl acetate			102	C5H10O2	000108-21-4	38



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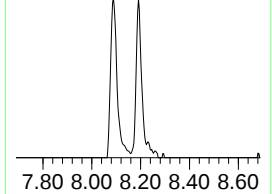
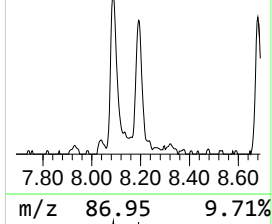
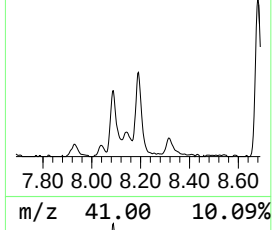
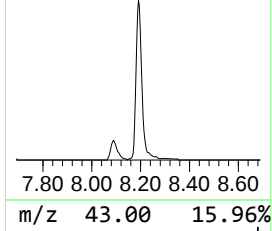
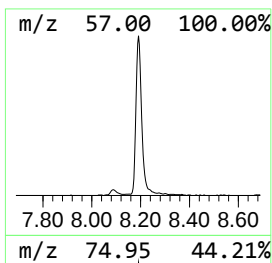
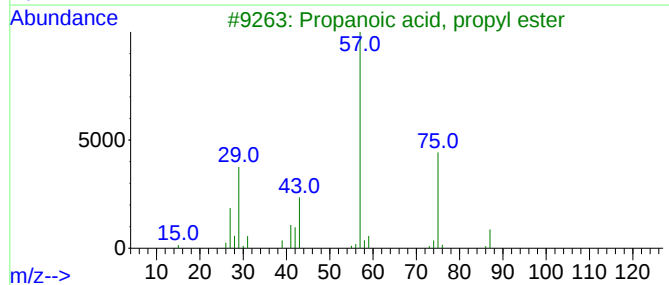
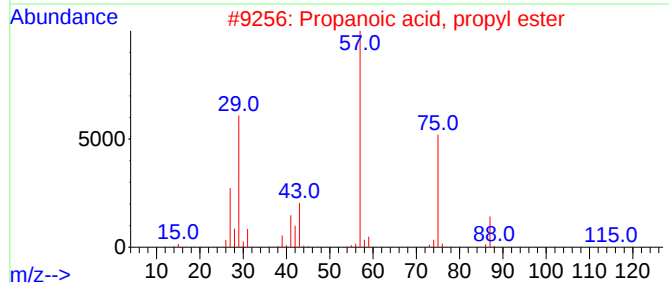
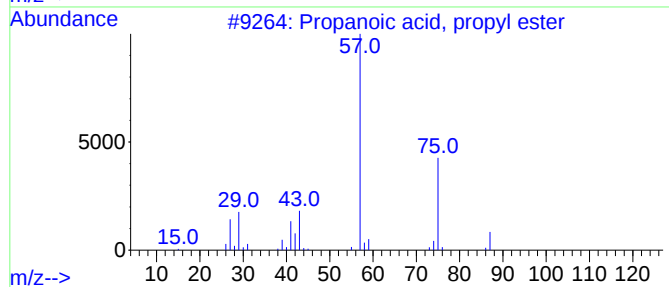
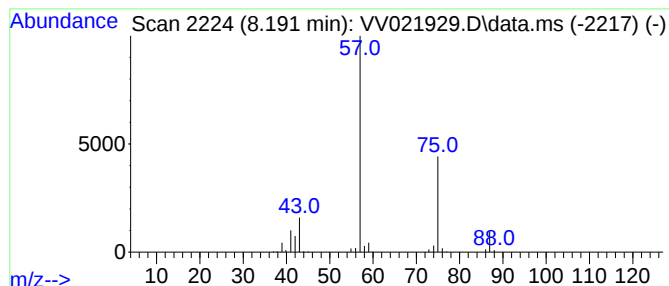
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
8.191	7.01 ug/L	160978	Chlorobenzene-d5	8.854

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			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021929.D
Acq On : 23 Aug 2021 12:19
Operator : SY/MD
Sample : M3487-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB7

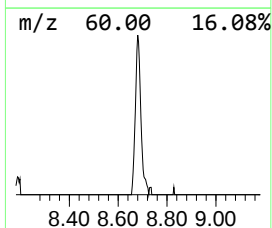
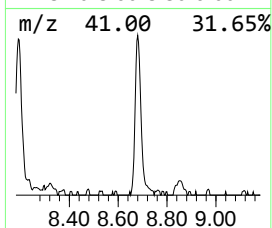
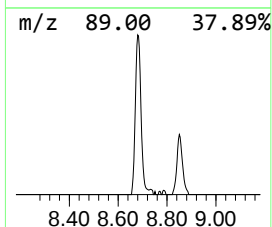
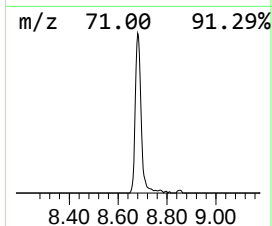
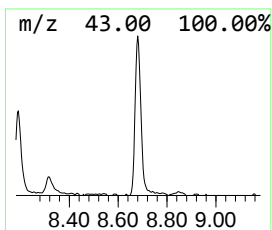
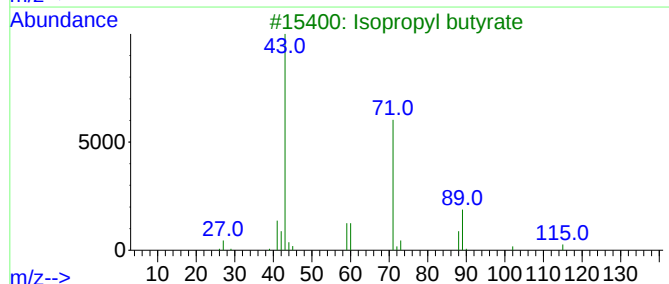
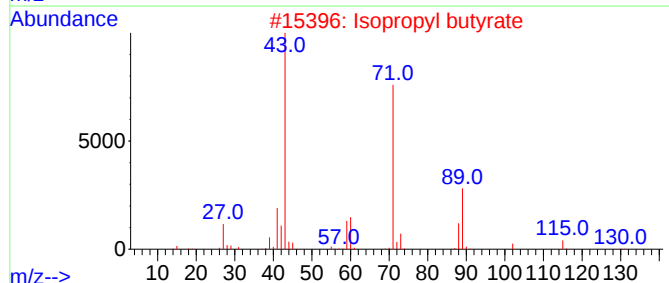
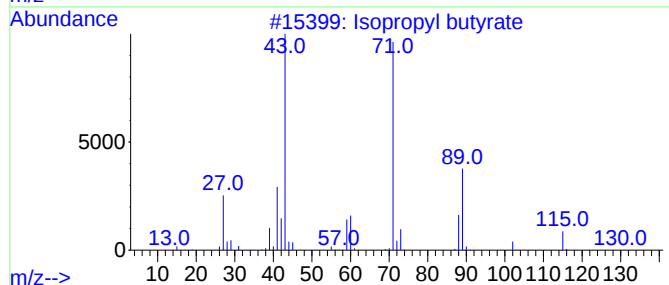
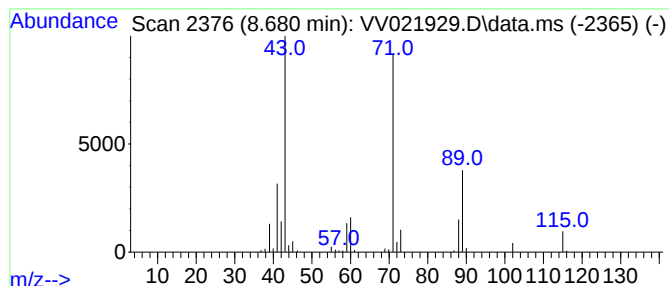
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Quant Title : VOC Analysis

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.
8.680	4.27 ug/L	98113	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			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021929.D
Acq On : 23 Aug 2021 12:19
Operator : SY/MD
Sample : M3487-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB7

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	5.905	2.9	ug/L	56018	1	5.613	962621	50.0
n-Propyl acetate	6.465	6.2	ug/L	119320	1	5.613	962621	50.0
Propanoic acid,...	8.191	7.0	ug/L	160978	2	8.854	1148490	50.0
Isopropyl butyrate	8.680	4.3	ug/L	98113	2	8.854	1148490	50.0