

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW101221\
 Data File : VW022755.D
 Acq On : 12 Oct 2021 15:51
 Operator : SY/MD
 Sample : M4126-17
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AC7

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\SFAMVLM100121WMA.M

Title : VOC Analysis

Signal : TIC: VW022755.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	77	83	95	rVB	88315	88990	14.66%	1.763%
2	1.568	157	164	175	rBV	77915	84764	13.96%	1.679%
3	2.108	322	332	348	rBV	159016	232974	38.37%	4.615%
4	2.355	382	409	410	rBV2	8675	25287	4.17%	0.501%
5	2.667	502	506	507	rBV2	244	181	0.03%	0.004%
6	2.712	517	520	521	rBV	238	130	0.02%	0.003%
7	2.722	521	523	525	rVV	346	149	0.02%	0.003%
8	2.953	593	595	601	rVB3	260	142	0.02%	0.003%
9	3.018	611	615	621	rBV2	232	312	0.05%	0.006%
10	3.130	646	650	653	rVB	252	156	0.03%	0.003%
11	3.150	653	656	657	rBV	297	133	0.02%	0.003%
12	3.175	662	664	667	rVB2	362	151	0.02%	0.003%
13	3.249	685	687	697	rVB2	401	319	0.05%	0.006%
14	3.375	722	726	728	rVB3	325	196	0.03%	0.004%
15	3.391	729	731	735	rBV2	227	117	0.02%	0.002%
16	3.468	751	755	757	rBV2	344	261	0.04%	0.005%
17	3.712	822	831	837	rBV3	330	607	0.10%	0.012%
18	3.892	876	887	920	rBV2	45609	144648	23.83%	2.865%
19	4.352	1014	1030	1058	rBV2	99451	250865	41.32%	4.969%
20	4.516	1080	1081	1085	rVB2	436	231	0.04%	0.005%
21	4.539	1085	1088	1092	rVB3	231	189	0.03%	0.004%
22	4.561	1092	1095	1097	rBV2	340	161	0.03%	0.003%
23	4.635	1116	1118	1124	rVB3	483	429	0.07%	0.008%
24	4.667	1124	1128	1130	rBV2	418	301	0.05%	0.006%
25	4.683	1130	1133	1136	rVV	173	128	0.02%	0.003%
26	4.709	1139	1141	1144	rVB2	209	112	0.02%	0.002%
27	4.732	1146	1148	1150	rVV	265	116	0.02%	0.002%
28	4.744	1150	1152	1154	rVV	366	121	0.02%	0.002%
29	4.789	1161	1166	1168	rBV2	246	280	0.05%	0.006%
30	4.905	1199	1202	1204	rBV	260	109	0.02%	0.002%
31	5.050	1231	1247	1283	rBV2	235212	607126	100.00%	12.027%
32	5.320	1328	1331	1337	rBV2	540	522	0.09%	0.010%
33	5.426	1362	1364	1366	rBV	202	110	0.02%	0.002%
34	5.455	1371	1373	1377	rVV	206	117	0.02%	0.002%
35	5.535	1395	1398	1401	rBV2	308	215	0.04%	0.004%
36	5.619	1412	1424	1452	rBV	240941	489953	80.70%	9.705%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW101221\
 Data File : VW022755.D
 Acq On : 12 Oct 2021 15:51
 Operator : SY/MD
 Sample : M4126-17
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AC7

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\SFAMVLM100121WMA.M
 Title : VOC Analysis

37	5.770	1469	1471	1473	rBV3	412	275	0.05%	0.005%
38	5.908	1502	1514	1531	rBV3	25517	52686	8.68%	1.044%
39	6.072	1551	1565	1585	rBV	135719	277602	45.72%	5.499%
40	6.198	1601	1604	1605	rBV2	689	334	0.06%	0.007%
41	6.294	1632	1634	1639	rVB2	415	267	0.04%	0.005%
42	6.490	1693	1695	1698	rVB3	195	120	0.02%	0.002%
43	6.622	1730	1736	1738	rBV2	303	280	0.05%	0.006%
44	6.641	1738	1742	1743	rBV	324	192	0.03%	0.004%
45	6.696	1756	1759	1768	rVB3	542	557	0.09%	0.011%
46	6.741	1771	1773	1775	rVV	181	124	0.02%	0.002%
47	6.989	1838	1850	1872	rBV	67500	126014	20.76%	2.496%
48	7.320	1941	1953	1971	rBV	267698	471711	77.70%	9.344%
49	7.551	2024	2025	2028	rVB	365	115	0.02%	0.002%
50	7.577	2032	2033	2036	rBV	228	112	0.02%	0.002%
51	7.625	2038	2048	2072	rBV	47781	84596	13.93%	1.676%
52	7.879	2124	2127	2130	rBV2	242	159	0.03%	0.003%
53	8.091	2184	2193	2233	rBV2	118119	265422	43.72%	5.258%
54	8.362	2275	2277	2278	rBV	334	152	0.03%	0.003%
55	8.452	2303	2305	2307	rVB	318	108	0.02%	0.002%
56	8.632	2358	2361	2364	rBV	247	202	0.03%	0.004%
57	8.690	2375	2379	2383	rBV2	258	203	0.03%	0.004%
58	8.754	2397	2399	2402	rBV2	276	122	0.02%	0.002%
59	8.770	2402	2404	2407	rBV	225	129	0.02%	0.003%
60	8.854	2419	2430	2458	rVV	373660	604897	99.63%	11.982%
61	9.265	2556	2558	2561	rBV2	163	125	0.02%	0.002%
62	9.313	2571	2573	2577	rVB3	312	131	0.02%	0.003%
63	9.445	2608	2614	2617	rVB2	300	357	0.06%	0.007%
64	9.461	2617	2619	2622	rVB	169	109	0.02%	0.002%
65	9.487	2622	2627	2630	rBV	350	298	0.05%	0.006%
66	9.850	2738	2740	2743	rBV	215	151	0.02%	0.003%
67	9.921	2757	2762	2765	rBV	253	279	0.05%	0.006%
68	10.043	2798	2800	2807	rBV2	296	280	0.05%	0.006%
69	10.079	2807	2811	2815	rBV2	230	258	0.04%	0.005%
70	10.130	2821	2827	2833	rVB4	1213	1641	0.27%	0.033%
71	10.217	2843	2854	2871	rBV	157368	245854	40.49%	4.870%
72	10.641	2984	2986	2989	rBV2	313	205	0.03%	0.004%
73	10.821	3039	3042	3045	rBV	309	262	0.04%	0.005%
74	10.879	3058	3060	3063	rVB	254	138	0.02%	0.003%
75	10.915	3064	3071	3073	rBV2	992	1006	0.17%	0.020%
76	10.972	3086	3089	3093	rBV2	208	196	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
 Data File : VV022755.D
 Acq On : 12 Oct 2021 15:51
 Operator : SY/MD
 Sample : M4126-17
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AC7

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\SFAMVLM100121WMA.M
 Title : VOC Analysis

77	11.037	3106	3109	3112	rBV2	531	277	0.05%	0.005%
78	11.117	3129	3134	3136	rBV2	142	159	0.03%	0.003%
79	11.249	3165	3175	3196	rBV	354478	538068	88.63%	10.659%
80	11.429	3226	3231	3239	rVB7	929	1357	0.22%	0.027%
81	11.461	3239	3241	3246	rVB2	245	133	0.02%	0.003%
82	11.535	3261	3264	3269	rBV4	866	963	0.16%	0.019%
83	11.574	3275	3276	3279	rVB2	453	189	0.03%	0.004%
84	11.625	3280	3292	3314	rVV	271641	435530	71.74%	8.627%
85	11.960	3394	3396	3398	rBV	338	168	0.03%	0.003%
86	12.059	3424	3427	3431	rVB2	268	188	0.03%	0.004%
87	12.075	3431	3432	3437	rBV2	237	180	0.03%	0.004%
88	12.133	3448	3450	3451	rBV	281	136	0.02%	0.003%
89	12.169	3459	3461	3464	rBV2	285	122	0.02%	0.002%
90	12.230	3476	3480	3482	rBV2	297	226	0.04%	0.004%
91	12.432	3540	3543	3546	rBV2	356	256	0.04%	0.005%
92	12.506	3564	3566	3568	rBV2	299	123	0.02%	0.002%
93	12.583	3587	3590	3592	rBV	174	122	0.02%	0.002%
94	12.596	3592	3594	3600	rVB2	442	322	0.05%	0.006%
95	12.628	3600	3604	3606	rBV	314	280	0.05%	0.006%
96	12.664	3611	3615	3616	rBV2	316	239	0.04%	0.005%
97	12.927	3694	3697	3699	rBV2	238	132	0.02%	0.003%
98	13.143	3761	3764	3765	rBV	409	221	0.04%	0.004%
99	13.413	3844	3848	3850	rBV2	390	324	0.05%	0.006%
100	14.480	4177	4180	4182	rBV2	407	236	0.04%	0.005%

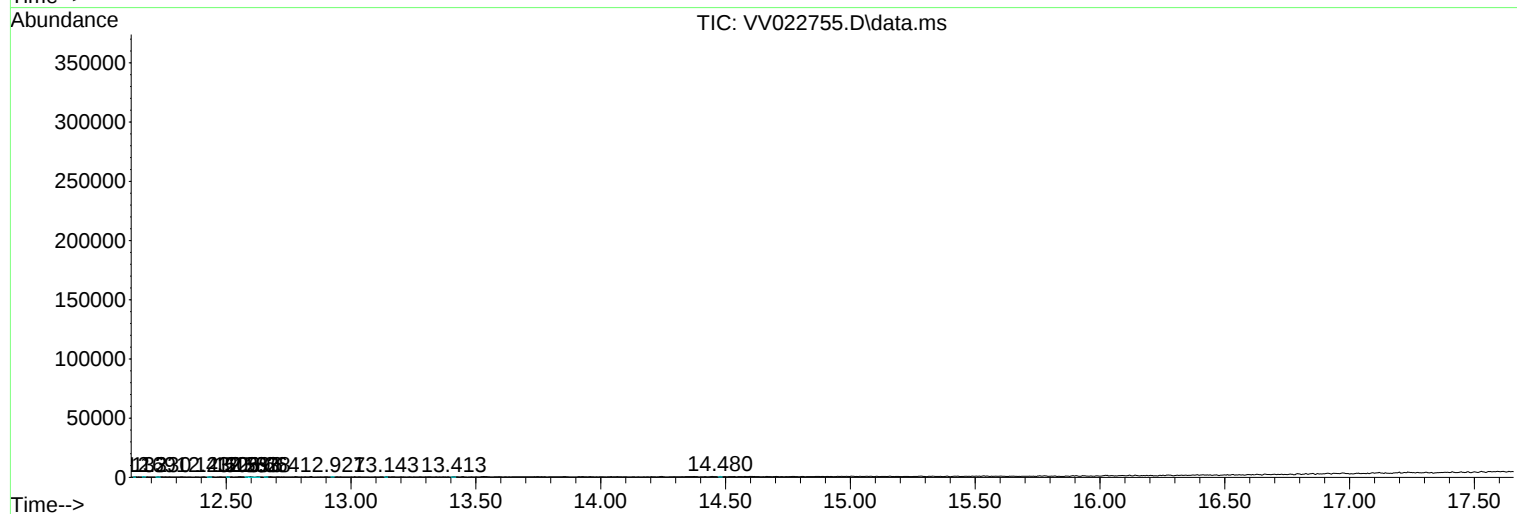
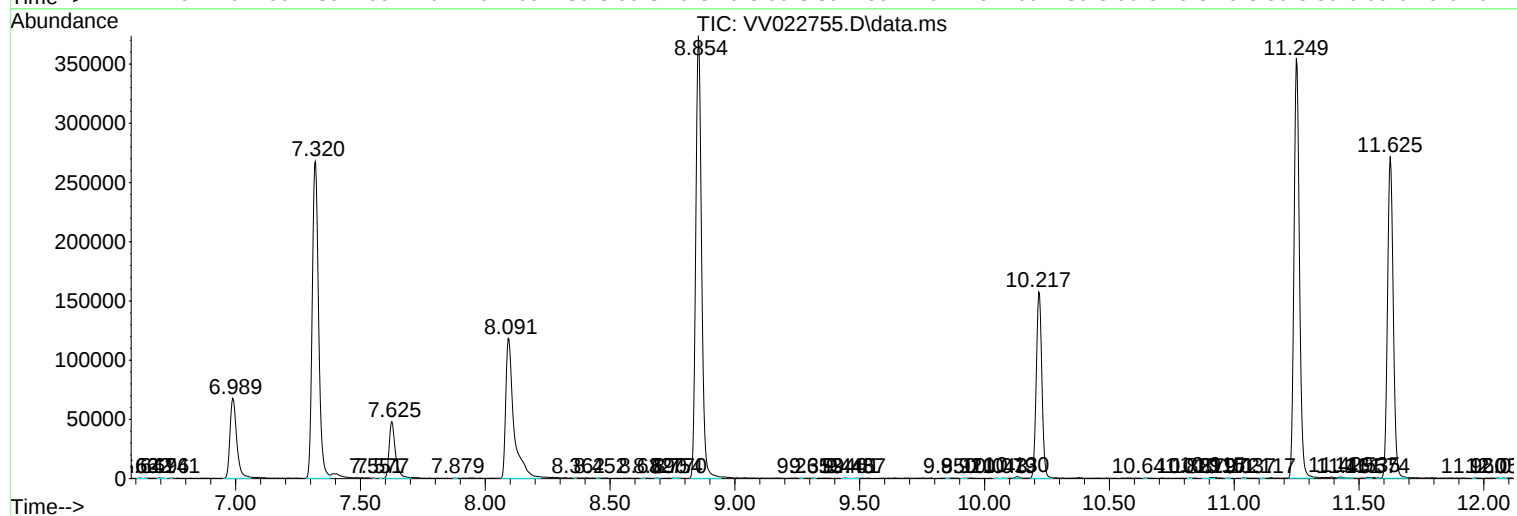
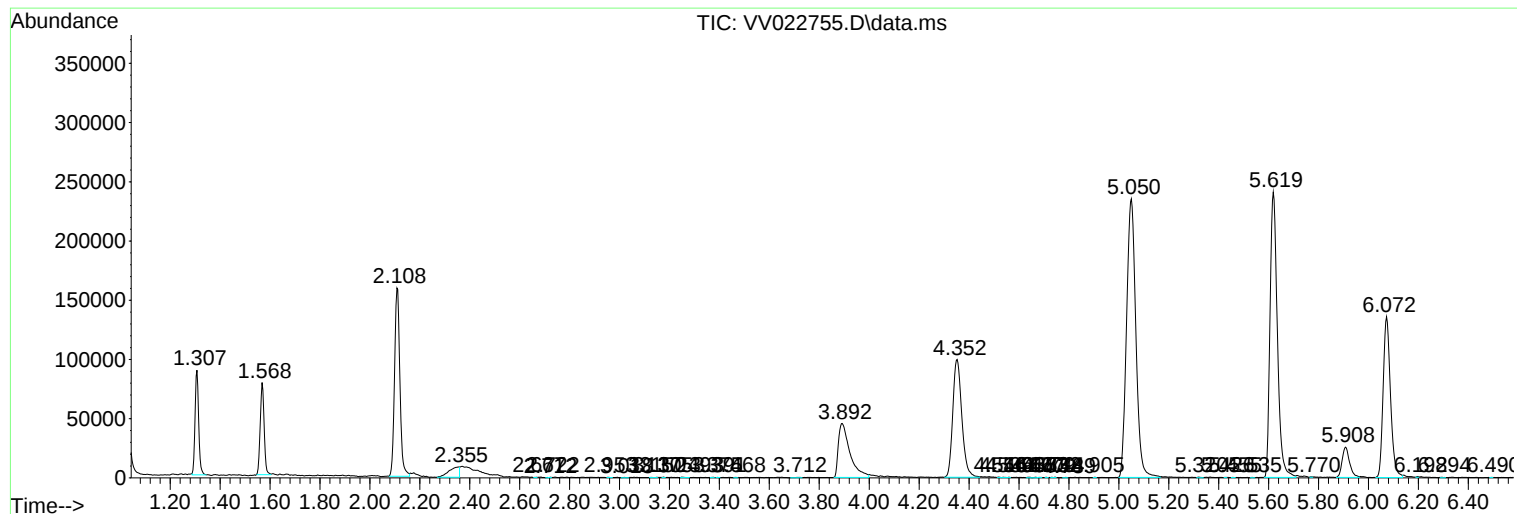
Sum of corrected areas: 5048222

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
Data File : VV022755.D
Acq On : 12 Oct 2021 15:51
Operator : SY/MD
Sample : M4126-17
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AC7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
Data File : VV022755.D
Acq On : 12 Oct 2021 15:51
Operator : SY/MD
Sample : M4126-17
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AC7

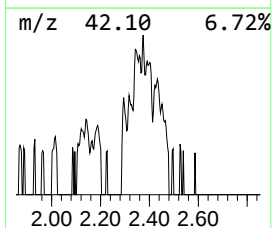
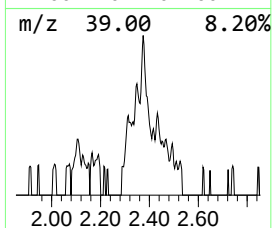
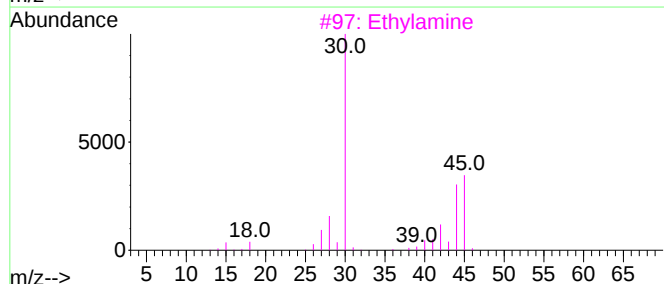
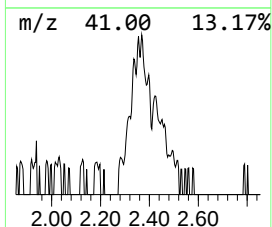
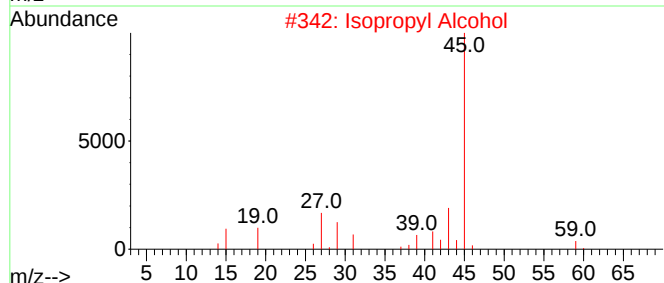
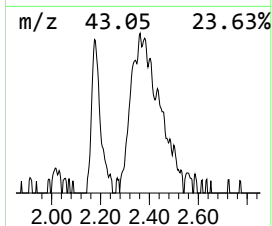
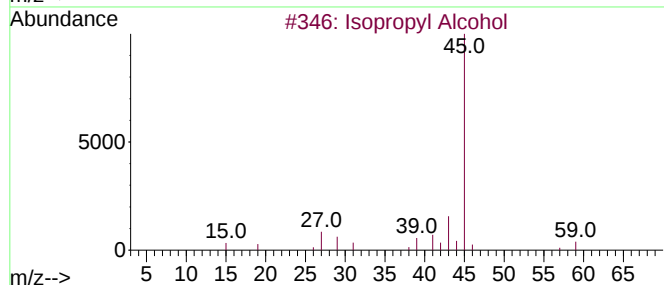
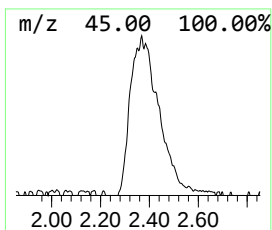
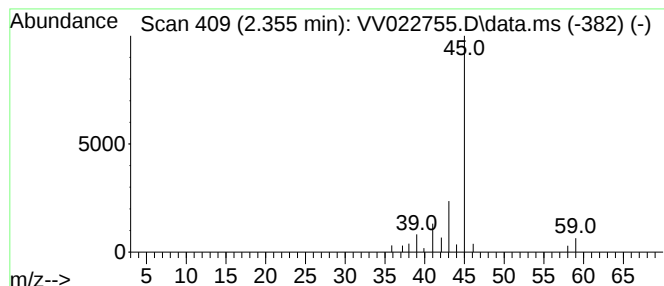
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.355	2.58 ug/L	25287	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3		Ethylamine	45	C2H7N	000075-04-7	7
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	4
5		Formamide	45	CH3NO	000075-12-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
Data File : VV022755.D
Acq On : 12 Oct 2021 15:51
Operator : SY/MD
Sample : M4126-17
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AC7

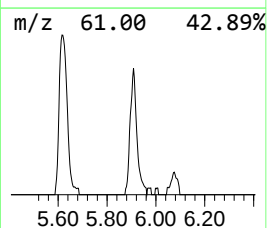
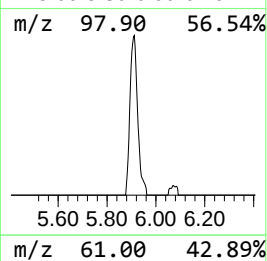
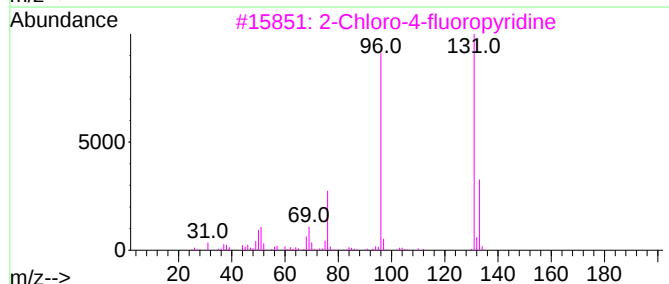
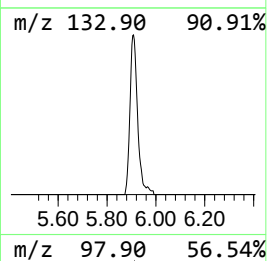
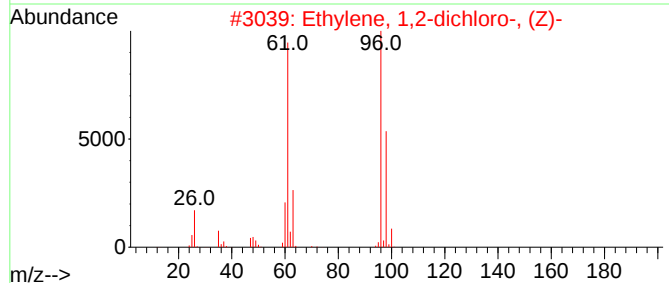
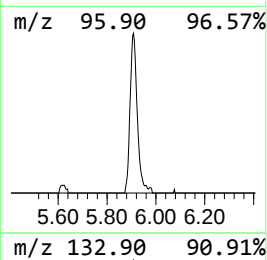
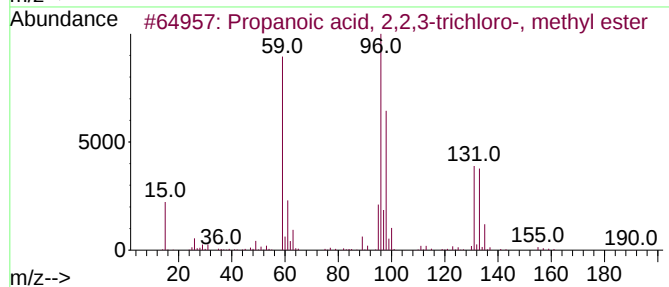
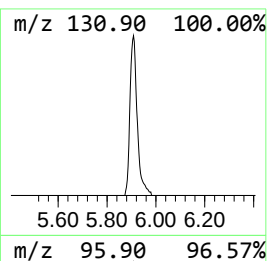
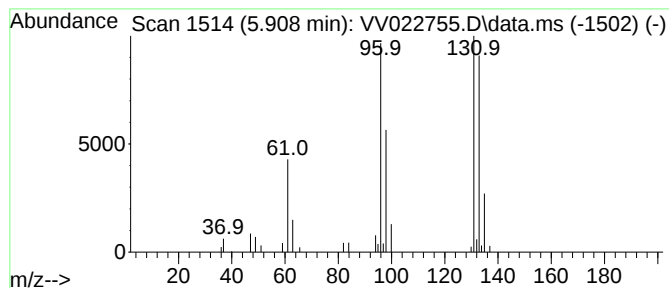
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	5.38 ug/L	52686	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	30
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101221\
Data File : VV022755.D
Acq On : 12 Oct 2021 15:51
Operator : SY/MD
Sample : M4126-17
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AC7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.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	2.355	2.6	ug/L	25287	1	5.619	489953	50.0
Propanoic acid,...	5.908	5.4	ug/L	52686	1	5.619	489953	50.0