

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051023\
 Data File : VU054143.D
 Acq On : 10 May 2023 14:26
 Operator : JC/MD
 Sample : 02694-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JREP7

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\SFAMULM042923WMA.M
 Title : VOC Analysis

Signal : TIC: VU054143.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	98	rVB	96111	118349	10.91%	1.441%
2	1.684	98	107	128	rBV	318232	415009	38.24%	5.052%
3	1.906	169	176	194	rVB	76787	110377	10.17%	1.344%
4	2.359	291	317	354	rVB3	220087	1085230	100.00%	13.210%
5	3.044	524	530	535	rVB4	1042	1400	0.13%	0.017%
6	3.179	560	572	590	rBV	7443	17350	1.60%	0.211%
7	3.282	598	604	607	rBV	381	377	0.03%	0.005%
8	3.305	607	611	613	rBV	441	342	0.03%	0.004%
9	3.356	625	627	630	rBV2	224	144	0.01%	0.002%
10	3.523	677	679	681	rVB	156	46	0.00%	0.001%
11	3.565	688	692	694	rBV3	928	855	0.08%	0.010%
12	3.745	744	748	751	rBV	346	268	0.02%	0.003%
13	3.838	776	777	778	rBV	117	33	0.00%	0.000%
14	3.877	785	789	792	rBV2	250	226	0.02%	0.003%
15	3.941	807	809	814	rVB	199	95	0.01%	0.001%
16	4.125	835	866	894	rBV7	23387	127989	11.79%	1.558%
17	4.620	1008	1020	1042	rBV	68870	175051	16.13%	2.131%
18	4.993	1134	1136	1137	rBV	217	67	0.01%	0.001%
19	5.057	1137	1156	1174	rBV	158578	352969	32.52%	4.297%
20	5.314	1229	1236	1238	rBV3	438	377	0.03%	0.005%
21	5.395	1259	1261	1263	rBV2	243	133	0.01%	0.002%
22	5.472	1283	1285	1290	rVB	168	70	0.01%	0.001%
23	5.517	1296	1299	1302	rVB	214	127	0.01%	0.002%
24	5.539	1302	1306	1309	rBV	271	252	0.02%	0.003%
25	5.572	1315	1316	1320	rVB	151	47	0.00%	0.001%
26	5.600	1322	1325	1331	rBV	364	252	0.02%	0.003%
27	5.626	1331	1333	1335	rBV	133	68	0.01%	0.001%
28	5.719	1341	1362	1385	rBV2	312600	857914	79.05%	10.443%
29	5.941	1429	1431	1432	rBV2	468	198	0.02%	0.002%
30	5.964	1432	1438	1443	rVV4	976	1403	0.13%	0.017%
31	6.031	1457	1459	1461	rBV2	261	140	0.01%	0.002%
32	6.244	1511	1525	1544	rBV	303643	574656	52.95%	6.995%
33	6.526	1605	1613	1617	rBV5	2193	3320	0.31%	0.040%
34	6.684	1650	1662	1684	rVB	200143	386310	35.60%	4.702%
35	7.002	1759	1761	1762	rBV	279	93	0.01%	0.001%
36	7.022	1765	1767	1769	rBV	337	148	0.01%	0.002%

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37	7.073	1781	1783	1785	rVB	302	136	0.01%	0.002%
38	7.086	1785	1787	1791	rBV	268	224	0.02%	0.003%
39	7.150	1804	1807	1811	rBV3	414	426	0.04%	0.005%
40	7.224	1829	1830	1832	rBV	229	73	0.01%	0.001%
41	7.362	1869	1873	1876	rVB2	302	196	0.02%	0.002%
42	7.379	1876	1878	1881	rBV2	229	112	0.01%	0.001%
43	7.417	1889	1890	1892	rVB	130	29	0.00%	0.000%
44	7.433	1892	1895	1897	rBV	141	58	0.01%	0.001%
45	7.469	1905	1906	1911	rBV	248	205	0.02%	0.002%
46	7.497	1914	1915	1916	rBV	132	38	0.00%	0.000%
47	7.517	1919	1921	1923	rBV	190	114	0.01%	0.001%
48	7.559	1923	1934	1954	rBV	111439	199370	18.37%	2.427%
49	7.745	1988	1992	1995	rBV	200	185	0.02%	0.002%
50	7.790	1995	2006	2015	rBV4	5884	10304	0.95%	0.125%
51	7.893	2025	2038	2053	rBV	399961	697350	64.26%	8.489%
52	8.102	2100	2103	2107	rVB3	447	306	0.03%	0.004%
53	8.173	2114	2125	2147	rBV	78932	138246	12.74%	1.683%
54	8.288	2158	2161	2164	rBV	270	137	0.01%	0.002%
55	8.308	2164	2167	2168	rVV	312	167	0.02%	0.002%
56	8.337	2172	2176	2179	rVB2	191	151	0.01%	0.002%
57	8.427	2202	2204	2205	rBV2	253	109	0.01%	0.001%
58	8.462	2209	2215	2217	rBV	1382	1305	0.12%	0.016%
59	8.629	2254	2267	2294	rBV2	193845	377890	34.82%	4.600%
60	8.790	2311	2317	2319	rBV5	746	824	0.08%	0.010%
61	8.864	2337	2340	2342	rBV2	223	124	0.01%	0.002%
62	9.002	2379	2383	2389	rVB2	432	407	0.04%	0.005%
63	9.041	2391	2395	2399	rBV2	403	328	0.03%	0.004%
64	9.147	2426	2428	2429	rBV	163	45	0.00%	0.001%
65	9.186	2439	2440	2441	rBV	129	29	0.00%	0.000%
66	9.243	2457	2458	2460	rVB	238	62	0.01%	0.001%
67	9.411	2497	2510	2531	rBV	414969	695275	64.07%	8.463%
68	9.719	2604	2606	2611	rVB2	459	343	0.03%	0.004%
69	9.748	2611	2615	2616	rBV	301	212	0.02%	0.003%
70	10.118	2722	2730	2735	rBV6	1313	2103	0.19%	0.026%
71	10.240	2764	2768	2770	rBV	598	541	0.05%	0.007%
72	10.285	2780	2782	2785	rBV	178	85	0.01%	0.001%
73	10.359	2803	2805	2808	rBV2	311	151	0.01%	0.002%
74	10.462	2834	2837	2844	rBV3	511	402	0.04%	0.005%
75	10.497	2845	2848	2850	rBV2	275	200	0.02%	0.002%
76	10.620	2884	2886	2889	rBV	188	72	0.01%	0.001%

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77	10.642	2891	2893	2895	rBV	202	70	0.01%	0.001%
78	10.700	2908	2911	2913	rBV2	209	144	0.01%	0.002%
79	10.751	2915	2927	2949	rVV	271711	448028	41.28%	5.454%
80	11.285	3091	3093	3096	rBV	347	170	0.02%	0.002%
81	11.394	3125	3127	3128	rBV	236	77	0.01%	0.001%
82	11.465	3144	3149	3150	rBV	754	541	0.05%	0.007%
83	11.501	3158	3160	3163	rBV2	271	150	0.01%	0.002%
84	11.806	3242	3255	3276	rBV	454099	708718	65.31%	8.627%
85	12.037	3325	3327	3332	rVB	253	156	0.01%	0.002%
86	12.086	3334	3342	3347	rBV4	951	1199	0.11%	0.015%
87	12.189	3361	3374	3400	rBV	426567	694364	63.98%	8.452%
88	12.430	3447	3449	3453	rBV2	366	205	0.02%	0.002%
89	12.494	3466	3469	3471	rBV2	389	252	0.02%	0.003%
90	12.896	3592	3594	3596	rBV2	301	129	0.01%	0.002%
91	13.410	3751	3754	3755	rBV	336	214	0.02%	0.003%
92	13.513	3781	3786	3788	rBV2	607	623	0.06%	0.008%
93	13.902	3905	3907	3909	rBV	343	119	0.01%	0.001%

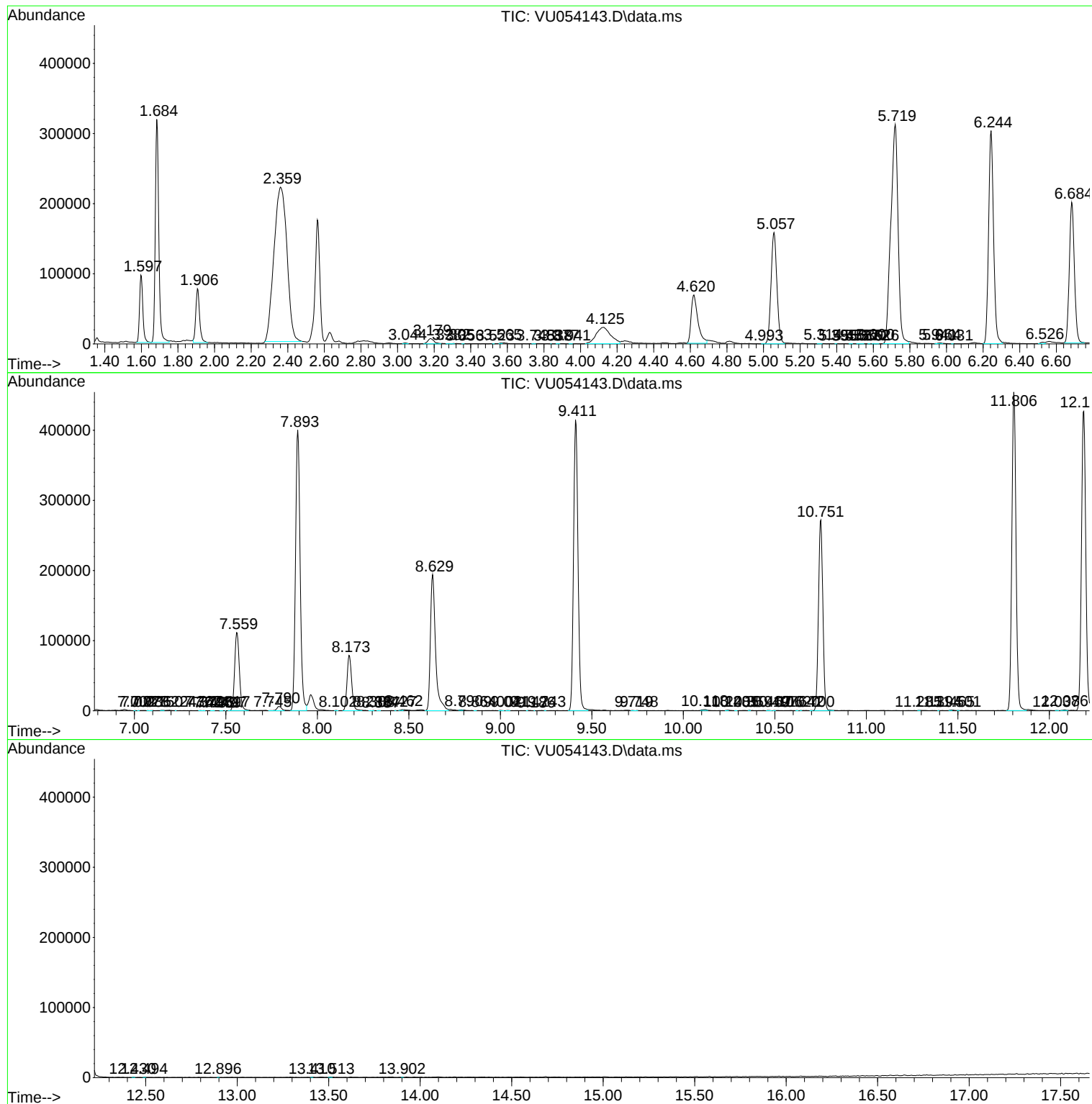
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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



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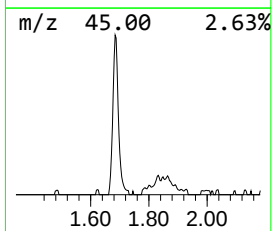
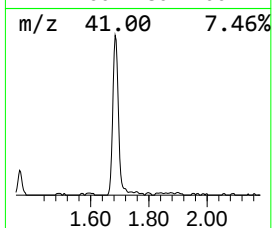
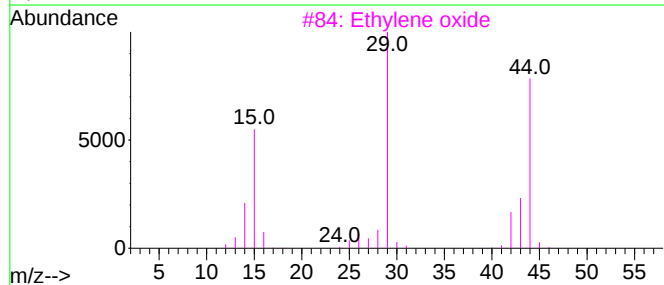
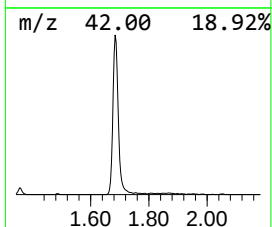
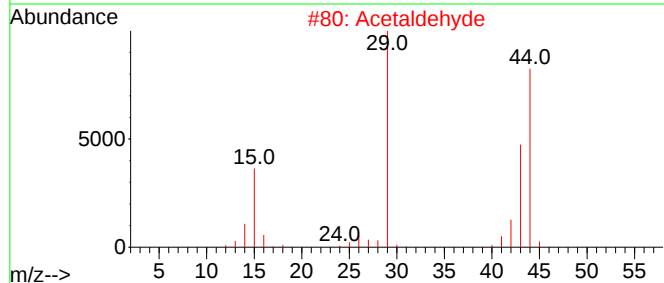
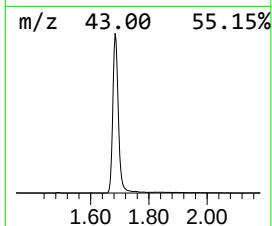
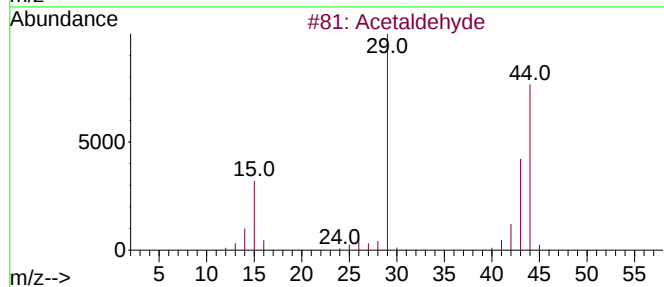
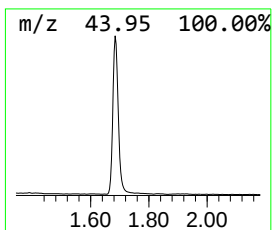
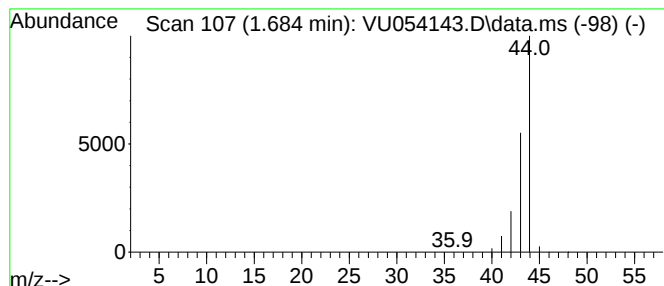
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.684	36.11 ug/L	415009	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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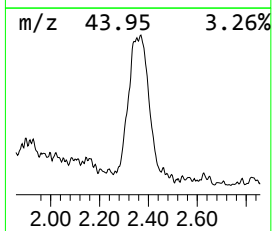
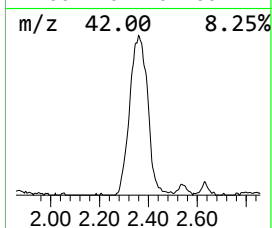
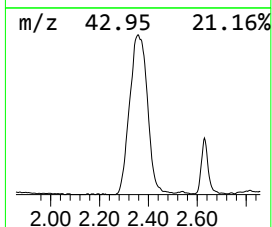
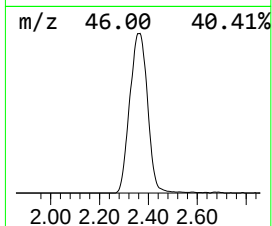
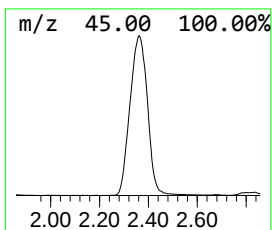
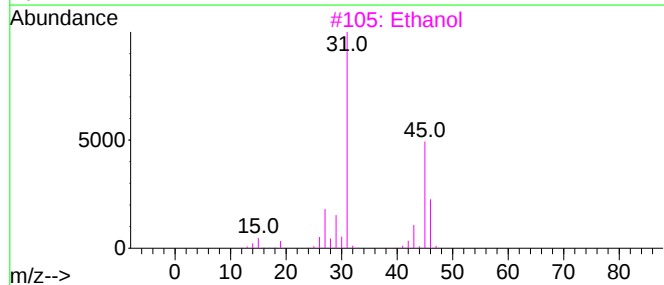
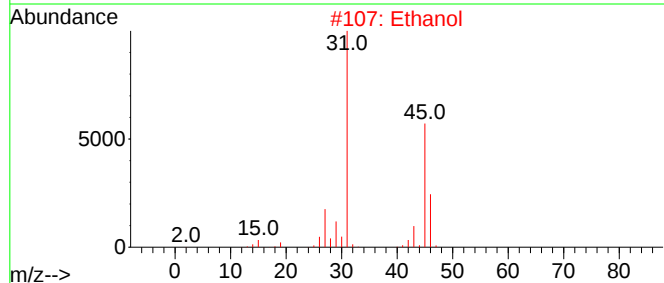
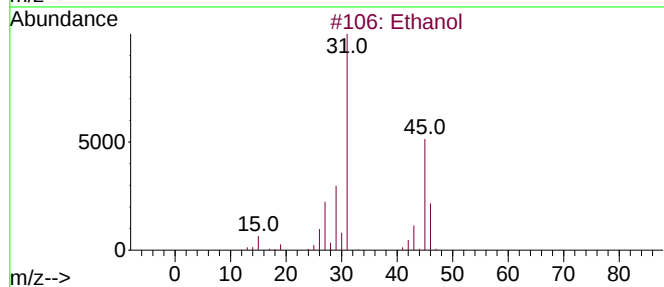
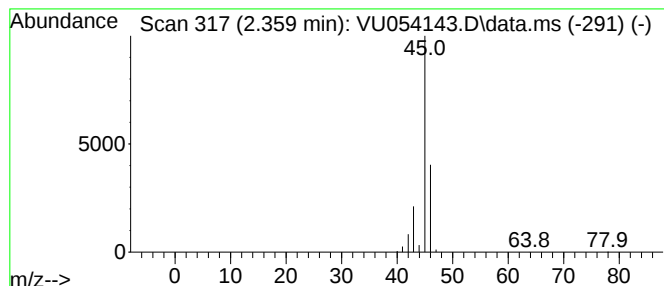
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.359	94.42 ug/L	1085230	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
2	Ethanol			46	C2H6O	000064-17-5	74
3	Ethanol			46	C2H6O	000064-17-5	64
4	Ethanol			46	C2H6O	000064-17-5	9
5	Dimethyl ether			46	C2H6O	000115-10-6	9



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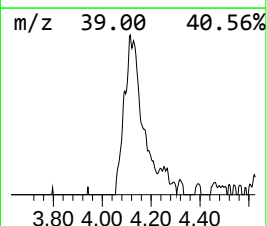
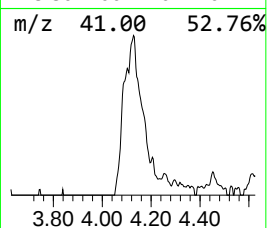
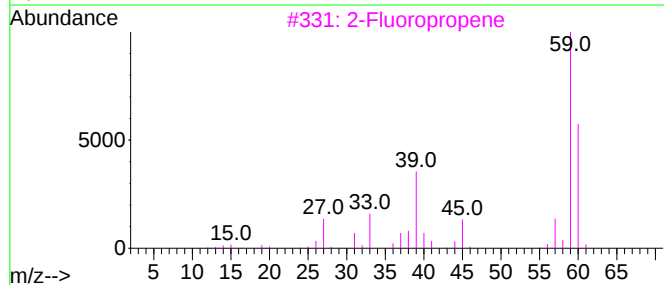
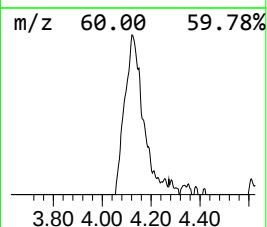
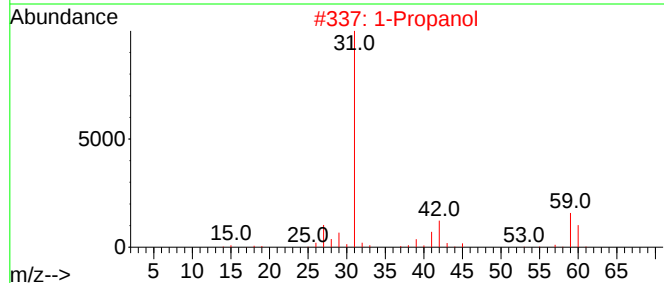
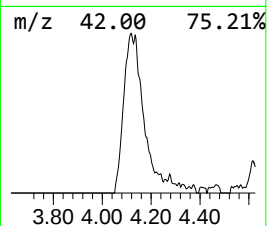
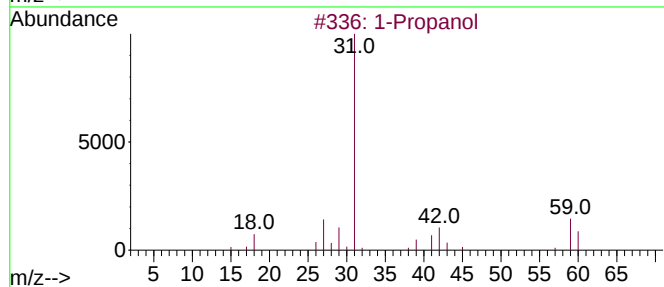
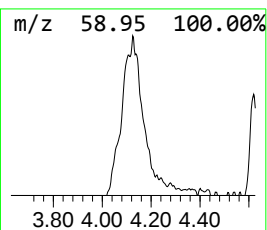
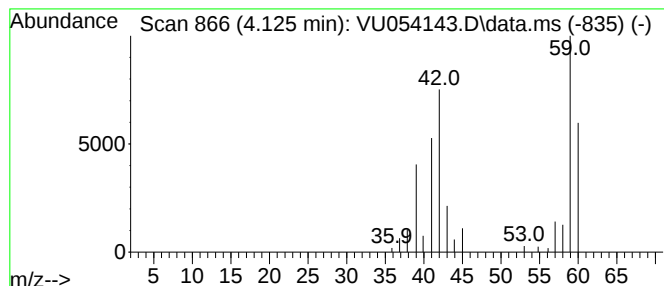
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.125	11.14 ug/L	127989	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	1-Propanol			60	C3H8O	000071-23-8	59
3	2-Fluoropropene			60	C3H5F	001184-60-7	52
4	2-Fluoropropene			60	C3H5F	001184-60-7	50
5	1-Propanol			60	C3H8O	000071-23-8	45



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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
Acetaldehyde	1.684	36.1	ug/L	415009	1	6.244	574656	50.0
Ethanol	2.359	94.4	ug/L	1085230	1	6.244	574656	50.0
1-Propanol	4.125	11.1	ug/L	127989	1	6.244	574656	50.0