

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039270.D
 Acq On : 16 Dec 2023 07:20
 Operator : JC/MD
 Sample : 05845-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHJ0

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_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.179	12	15	21	rVB	7480	8914	0.96%	0.119%
2	1.246	23	26	27	rVV	2593	3037	0.33%	0.041%
3	1.270	27	30	42	rVV	157288	170125	18.29%	2.270%
4	1.368	43	46	56	rVB	112803	124262	13.36%	1.658%
5	1.672	91	96	108	rBV	73901	107020	11.51%	1.428%
6	2.313	194	201	208	rBV2	262550	494905	53.21%	6.602%
7	2.373	208	211	221	rVB	40163	64386	6.92%	0.859%
8	2.526	230	236	247	rBV	56463	102562	11.03%	1.368%
9	2.794	276	280	284	rVB3	799	1354	0.15%	0.018%
10	2.947	298	305	315	rBV2	7637	17419	1.87%	0.232%
11	3.093	325	329	332	rBV2	785	1181	0.13%	0.016%
12	3.343	366	370	372	rVB2	193	215	0.02%	0.003%
13	3.520	395	399	401	rBV2	188	323	0.03%	0.004%
14	3.611	406	414	424	rVV2	4669	10711	1.15%	0.143%
15	3.733	430	434	435	rVV2	207	265	0.03%	0.004%
16	4.178	502	507	510	rBV	264	410	0.04%	0.005%
17	4.446	543	551	565	rBV	78161	237725	25.56%	3.171%
18	4.812	609	611	613	rVB	337	264	0.03%	0.004%
19	4.836	613	615	617	rBV	307	270	0.03%	0.004%
20	5.056	634	651	670	rBV	115282	375496	40.37%	5.009%
21	5.294	685	690	695	rBV2	197	478	0.05%	0.006%
22	5.385	695	705	716	rBV4	9674	28523	3.07%	0.381%
23	5.531	727	729	731	rBV	354	237	0.03%	0.003%
24	5.733	759	762	765	rBV2	212	238	0.03%	0.003%
25	5.970	785	801	820	rBV2	306267	930089	100.00%	12.408%
26	6.233	840	844	845	rBV2	936	873	0.09%	0.012%
27	6.318	856	858	859	rBV	284	223	0.02%	0.003%
28	6.659	913	914	918	rBV2	174	203	0.02%	0.003%
29	6.757	921	930	952	rVV	196546	481572	51.78%	6.425%
30	7.019	971	973	976	rBV3	240	238	0.03%	0.003%
31	7.104	983	987	988	rBV	205	256	0.03%	0.003%
32	7.123	988	990	993	rVB2	439	345	0.04%	0.005%
33	7.306	1008	1020	1036	rBV	189340	419273	45.08%	5.593%
34	7.482	1047	1049	1051	rBV2	487	492	0.05%	0.007%
35	7.714	1085	1087	1089	rBV2	289	322	0.03%	0.004%
36	7.812	1101	1103	1107	rBV	259	277	0.03%	0.004%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	7.897	1113	1117	1123	rVB3	1261	2348	0.25%	0.031%
38	8.324	1180	1187	1198	rBV	126654	209934	22.57%	2.801%
39	8.500	1212	1216	1217	rBV2	205	292	0.03%	0.004%
40	8.574	1225	1228	1230	rBV4	359	502	0.05%	0.007%
41	8.647	1234	1240	1261	rVV	464704	736888	79.23%	9.831%
42	8.952	1284	1290	1301	rBV	90343	138754	14.92%	1.851%
43	9.141	1319	1321	1326	rVB2	239	364	0.04%	0.005%
44	9.384	1355	1361	1370	rBV	370178	535764	57.60%	7.147%
45	9.988	1458	1460	1463	rVB	192	204	0.02%	0.003%
46	10.055	1465	1471	1484	rBV	428672	592706	63.73%	7.907%
47	10.207	1492	1496	1498	rVB3	456	600	0.06%	0.008%
48	10.305	1509	1512	1516	rVB	677	634	0.07%	0.008%
49	10.384	1523	1525	1529	rVB3	392	463	0.05%	0.006%
50	10.457	1534	1537	1541	rBV2	170	316	0.03%	0.004%
51	10.555	1550	1553	1557	rBV2	262	300	0.03%	0.004%
52	10.646	1563	1568	1571	rBV2	349	592	0.06%	0.008%
53	10.829	1596	1598	1600	rBV	304	249	0.03%	0.003%
54	10.963	1618	1620	1621	rBV2	263	244	0.03%	0.003%
55	11.018	1624	1629	1635	rBV	3005	4156	0.45%	0.055%
56	11.091	1638	1641	1645	rVB5	1538	1999	0.21%	0.027%
57	11.152	1649	1651	1652	rBV	911	887	0.10%	0.012%
58	11.189	1652	1657	1667	rVB	345975	438712	47.17%	5.853%
59	11.280	1668	1672	1674	rVB3	1190	1456	0.16%	0.019%
60	11.457	1697	1701	1705	rVB2	682	793	0.09%	0.011%
61	11.494	1705	1707	1710	rBV	178	207	0.02%	0.003%
62	11.530	1710	1713	1716	rBV2	224	279	0.03%	0.004%
63	11.677	1732	1737	1740	rBV2	193	342	0.04%	0.005%
64	11.701	1740	1741	1746	rVV	340	355	0.04%	0.005%
65	11.756	1747	1750	1753	rVV2	570	638	0.07%	0.009%
66	11.793	1754	1756	1760	rVB	217	211	0.02%	0.003%
67	11.969	1783	1785	1788	rVB3	272	225	0.02%	0.003%
68	12.018	1788	1793	1802	rBV	453538	594974	63.97%	7.937%
69	12.134	1809	1812	1815	rBV2	308	261	0.03%	0.003%
70	12.231	1826	1828	1831	rVB2	367	308	0.03%	0.004%
71	12.317	1837	1842	1852	rBV	494135	634847	68.26%	8.469%
72	12.481	1867	1869	1872	rVB	293	261	0.03%	0.003%
73	12.542	1877	1879	1881	rVB	408	303	0.03%	0.004%
74	12.567	1881	1883	1884	rBV2	359	256	0.03%	0.003%
75	12.591	1884	1887	1889	rVB	306	361	0.04%	0.005%
76	12.658	1895	1898	1899	rBV2	254	215	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	12.762	1910	1915	1918	rVB	474	738	0.08%	0.010%
78	12.926	1940	1942	1945	rVV	234	238	0.03%	0.003%
79	13.122	1972	1974	1976	rVB2	368	246	0.03%	0.003%
80	13.213	1986	1989	1991	rVB2	248	249	0.03%	0.003%
81	13.262	1995	1997	2001	rBV2	261	238	0.03%	0.003%
82	13.304	2001	2004	2006	rBV	247	230	0.02%	0.003%
83	13.432	2021	2025	2030	rVV3	806	1201	0.13%	0.016%
84	13.542	2040	2043	2046	rVV2	156	207	0.02%	0.003%
85	13.585	2049	2050	2054	rVB2	377	459	0.05%	0.006%
86	13.621	2054	2056	2060	rBV	291	345	0.04%	0.005%
87	13.780	2077	2082	2084	rBV2	435	567	0.06%	0.008%
88	13.969	2109	2113	2116	rVB	370	413	0.04%	0.006%
89	14.213	2151	2153	2156	rVB	203	202	0.02%	0.003%
90	14.786	2244	2247	2249	rVB2	222	223	0.02%	0.003%
91	14.847	2255	2257	2259	rBV	239	213	0.02%	0.003%
92	15.085	2294	2296	2298	rBV	278	200	0.02%	0.003%
93	15.176	2308	2311	2313	rVB2	239	218	0.02%	0.003%
94	15.396	2346	2347	2354	rBV3	224	354	0.04%	0.005%
95	15.627	2383	2385	2387	rBV	354	313	0.03%	0.004%
96	15.859	2421	2423	2424	rBV	444	210	0.02%	0.003%
97	15.987	2442	2444	2448	rVB3	209	249	0.03%	0.003%
98	16.030	2448	2451	2453	rBV2	269	348	0.04%	0.005%
99	16.200	2478	2479	2482	rVB2	430	259	0.03%	0.003%
100	16.475	2522	2524	2525	rBV	331	249	0.03%	0.003%

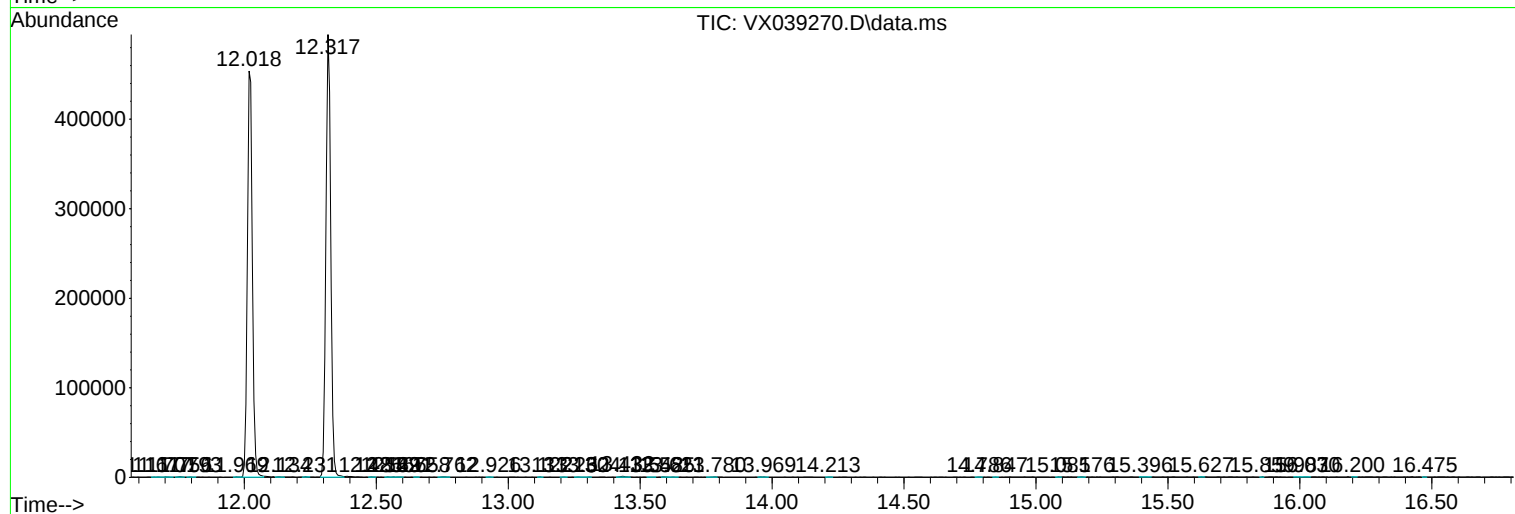
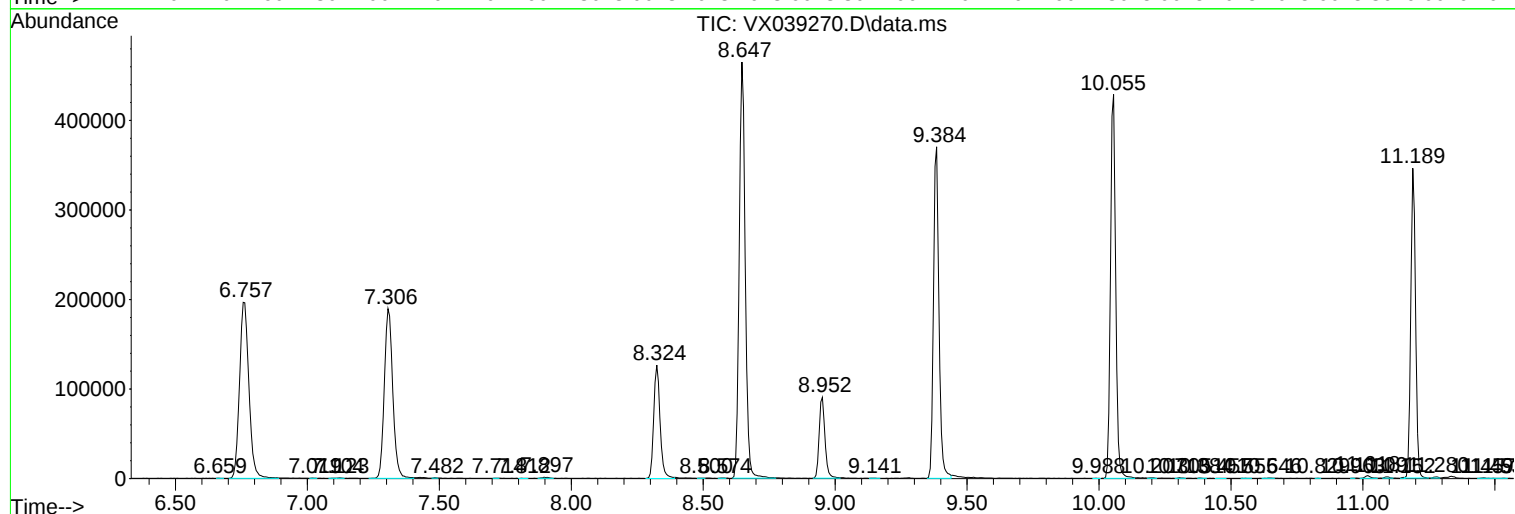
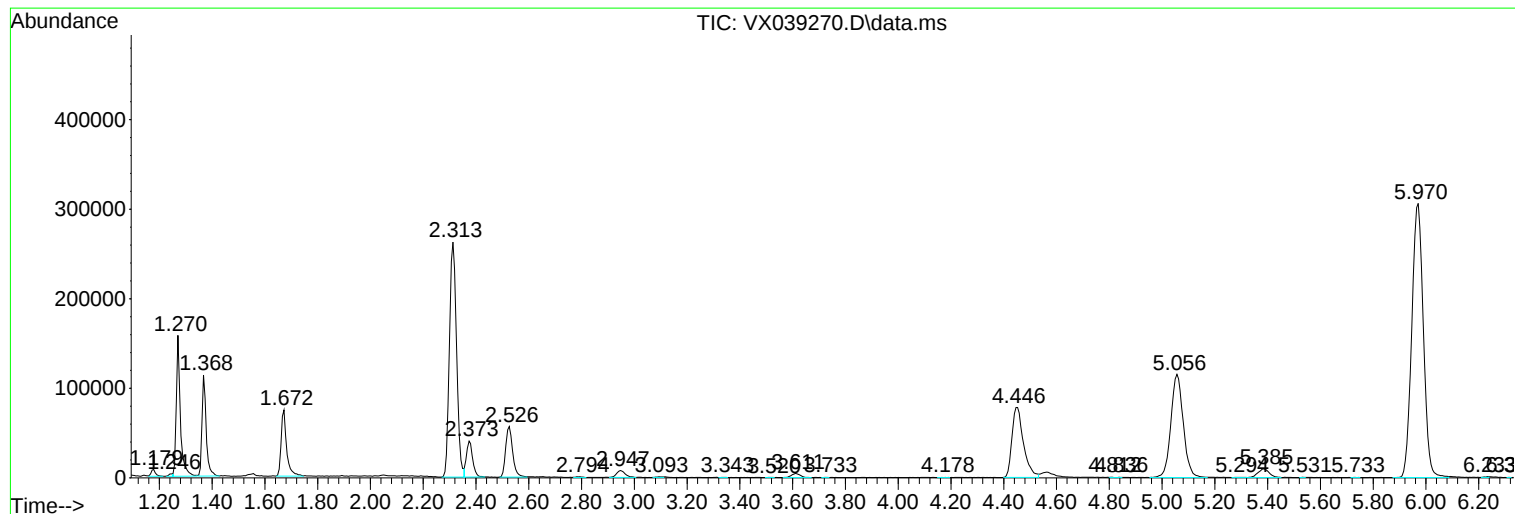
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

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



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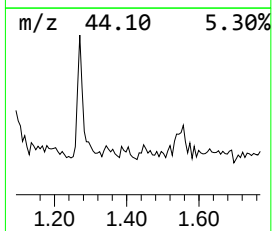
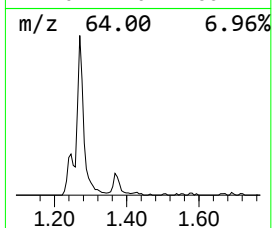
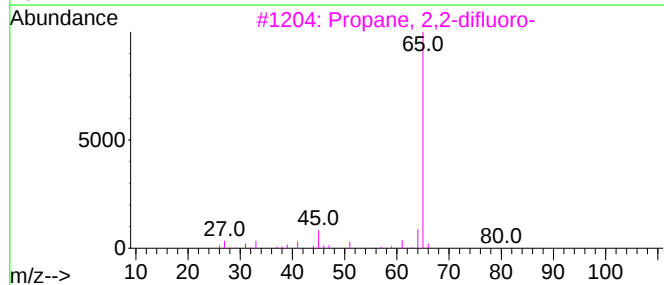
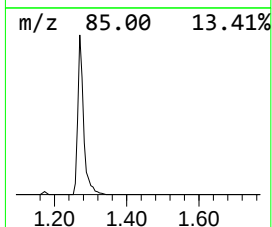
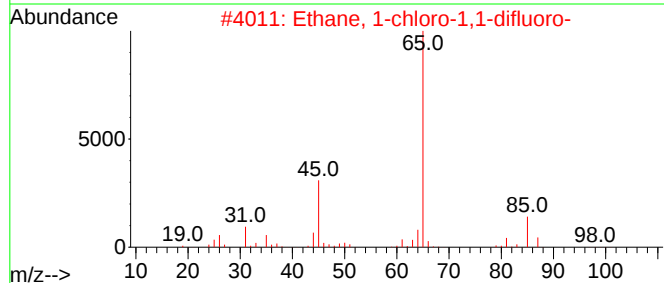
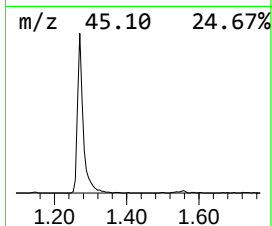
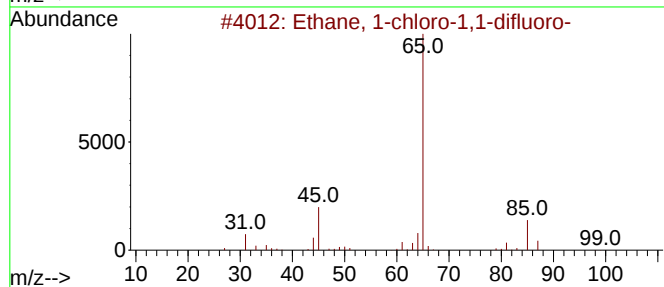
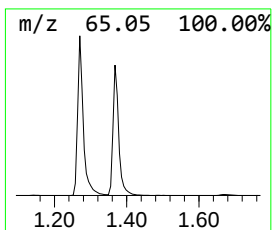
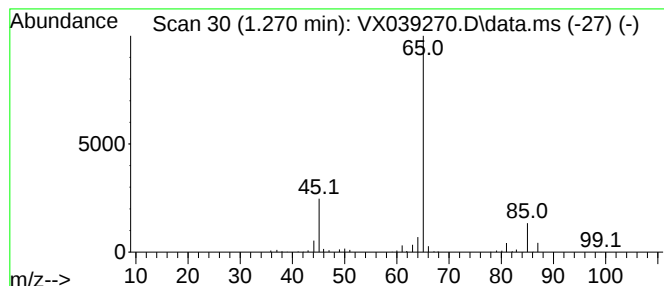
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	17.66 ug/L	170125	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	83
2			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	83
3			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	9
4			2,2-Difluoropropionic acid	110	C3H4F2O2	000373-96-6	4
5			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2



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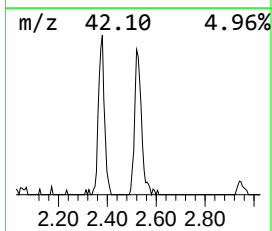
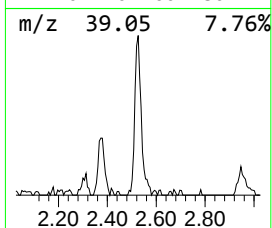
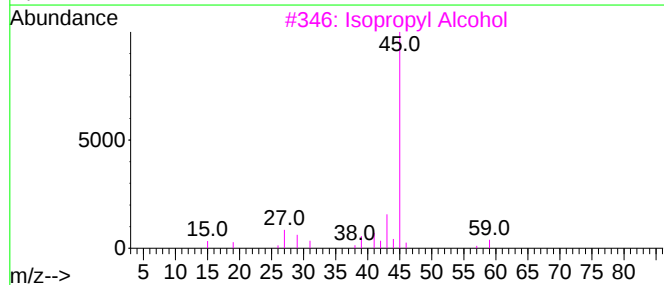
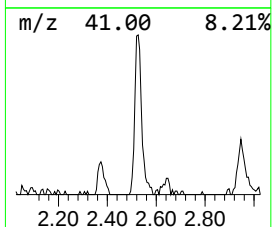
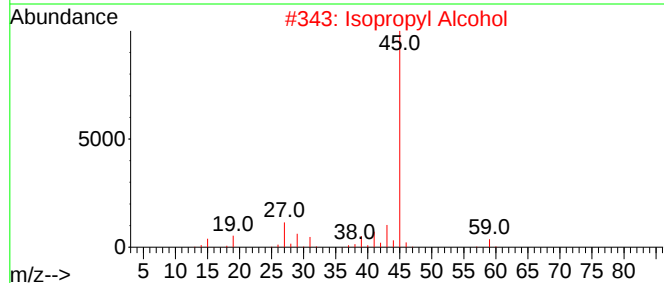
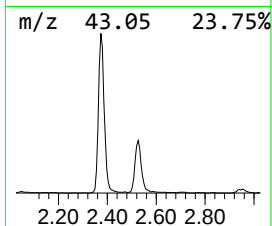
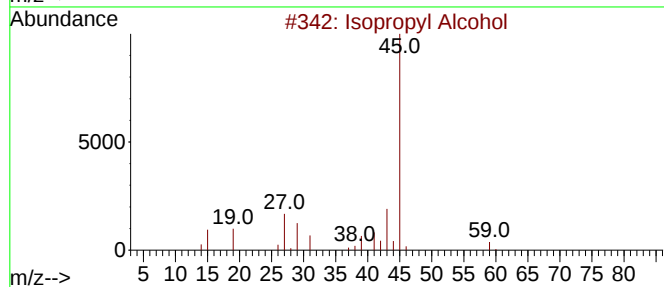
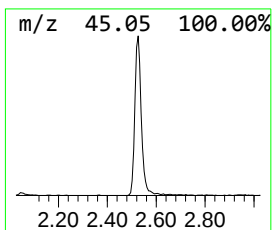
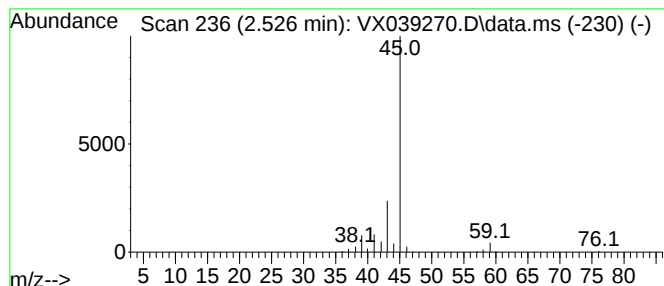
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.526	10.65 ug/L	102562	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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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
Ethane, 1-chlor...	1.270	17.7	ug/L	170125	1	6.763	481572	50.0
Isopropyl Alcohol	2.526	10.7	ug/L	102562	1	6.763	481572	50.0