

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
 Data File : VX040680.D
 Acq On : 16 Mar 2024 01:56
 Operator : JC/MD
 Sample : P1754-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCL27

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\SFAMXML030724WMA.M
 Title : VOC Analysis

Signal : TIC: VX040680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	14	rBV2	1823	1951	0.33%	0.034%
2	1.270	27	30	33	rBV	4115	4235	0.71%	0.073%
3	1.374	41	47	58	rBV2	181950	233751	39.10%	4.042%
4	1.666	91	95	109	rVB	53660	79257	13.26%	1.370%
5	2.136	167	172	181	rVB2	13114	22362	3.74%	0.387%
6	2.312	194	201	208	rBV3	188408	357854	59.85%	6.188%
7	2.380	208	212	219	rVB	33147	52978	8.86%	0.916%
8	2.532	230	237	252	rBV	70268	134293	22.46%	2.322%
9	2.953	302	306	312	rVB2	1879	3150	0.53%	0.054%
10	3.099	325	330	332	rBV3	795	1081	0.18%	0.019%
11	3.282	359	360	362	rBV	216	182	0.03%	0.003%
12	3.324	365	367	369	rVV2	301	267	0.04%	0.005%
13	3.477	390	392	395	rVB	256	230	0.04%	0.004%
14	3.507	395	397	399	rBV2	193	161	0.03%	0.003%
15	3.611	405	414	427	rVB2	24613	57108	9.55%	0.987%
16	3.727	432	433	434	rBV2	249	175	0.03%	0.003%
17	4.050	484	486	487	rBV	180	156	0.03%	0.003%
18	4.196	507	510	511	rBV	319	250	0.04%	0.004%
19	4.233	515	516	518	rBV	306	173	0.03%	0.003%
20	4.483	543	557	569	rBV3	99370	394531	65.99%	6.822%
21	5.056	636	651	667	rBV	86279	273669	45.77%	4.732%
22	5.385	695	705	717	rVB3	15936	49654	8.30%	0.859%
23	5.477	717	720	721	rBV	209	152	0.03%	0.003%
24	5.556	731	733	736	rVV3	231	217	0.04%	0.004%
25	5.873	780	785	788	rBV3	630	1295	0.22%	0.022%
26	5.970	789	801	815	rBV2	195142	597901	100.00%	10.339%
27	6.226	841	843	844	rBV	245	173	0.03%	0.003%
28	6.513	888	890	894	rBB	138	159	0.03%	0.003%
29	6.549	894	896	901	rVB	283	395	0.07%	0.007%
30	6.647	909	912	913	rBV	273	300	0.05%	0.005%
31	6.763	922	931	946	rBV	157452	380417	63.63%	6.578%
32	6.952	961	962	965	rVB	288	179	0.03%	0.003%
33	6.982	965	967	970	rBV	194	168	0.03%	0.003%
34	7.007	970	971	974	rVB2	226	168	0.03%	0.003%
35	7.062	978	980	983	rBV2	242	263	0.04%	0.005%
36	7.129	983	991	1000	rBV	21327	47859	8.00%	0.828%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
Data File : VX040680.D
Acq On : 16 Mar 2024 01:56
Operator : JC/MD
Sample : P1754-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCL27

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\SFAMXML030724WMA.M
Title : VOC Analysis

37	7.305	1012	1020	1034	rBV	127945	280978	46.99%	4.859%
38	7.433	1034	1041	1050	rVB3	11480	23875	3.99%	0.413%
39	7.574	1063	1064	1067	rBV	189	176	0.03%	0.003%
40	7.799	1100	1101	1105	rBV	180	214	0.04%	0.004%
41	7.848	1107	1109	1110	rBV	163	158	0.03%	0.003%
42	7.933	1121	1123	1124	rBV	325	314	0.05%	0.005%
43	8.013	1134	1136	1138	rBV	180	172	0.03%	0.003%
44	8.196	1162	1166	1169	rBV	199	274	0.05%	0.005%
45	8.324	1179	1187	1195	rBV	84230	134900	22.56%	2.333%
46	8.647	1234	1240	1250	rBV	277708	429431	71.82%	7.425%
47	8.872	1274	1277	1279	rVB	173	183	0.03%	0.003%
48	8.952	1284	1290	1299	rBV	60553	93985	15.72%	1.625%
49	9.037	1302	1304	1307	rVV2	213	220	0.04%	0.004%
50	9.275	1338	1343	1351	rVB4	1684	2312	0.39%	0.040%
51	9.384	1355	1361	1375	rBV	260452	381406	63.79%	6.595%
52	9.671	1405	1408	1410	rBV	294	375	0.06%	0.006%
53	9.915	1444	1448	1451	rVB2	315	396	0.07%	0.007%
54	9.957	1451	1455	1457	rBV2	184	195	0.03%	0.003%
55	10.055	1465	1471	1484	rBV	341482	474163	79.30%	8.199%
56	10.293	1507	1510	1511	rBV2	202	185	0.03%	0.003%
57	10.482	1538	1541	1543	rBV2	198	192	0.03%	0.003%
58	10.646	1566	1568	1570	rBV	244	231	0.04%	0.004%
59	10.732	1580	1582	1587	rBV2	131	213	0.04%	0.004%
60	10.787	1589	1591	1593	rBV2	148	184	0.03%	0.003%
61	10.878	1603	1606	1609	rBV2	190	272	0.05%	0.005%
62	10.963	1618	1620	1624	rVB	284	351	0.06%	0.006%
63	11.091	1639	1641	1644	rVB3	501	517	0.09%	0.009%
64	11.189	1652	1657	1667	rVB	264129	336911	56.35%	5.826%
65	11.311	1674	1677	1684	rVB	1253	1563	0.26%	0.027%
66	11.482	1704	1705	1707	rBV	159	159	0.03%	0.003%
67	11.695	1736	1740	1741	rBV2	126	155	0.03%	0.003%
68	11.756	1749	1750	1752	rVB	263	152	0.03%	0.003%
69	12.018	1788	1793	1801	rBV	364171	466907	78.09%	8.073%
70	12.158	1812	1816	1818	rBV	195	211	0.04%	0.004%
71	12.250	1827	1831	1832	rBV2	165	206	0.03%	0.004%
72	12.317	1837	1842	1858	rVB	347083	445689	74.54%	7.707%
73	12.579	1882	1885	1891	rVV2	287	455	0.08%	0.008%
74	12.634	1891	1894	1897	rBV2	171	243	0.04%	0.004%
75	12.689	1901	1903	1911	rVB3	207	360	0.06%	0.006%
76	13.097	1967	1970	1973	rBV2	141	184	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
 Data File : VX040680.D
 Acq On : 16 Mar 2024 01:56
 Operator : JC/MD
 Sample : P1754-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCL27

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\SFAMXML030724WMA.M
 Title : VOC Analysis

77	13.250	1988	1995	1996	rBV2	315	515	0.09%	0.009%
78	13.737	2072	2075	2078	rBV2	257	259	0.04%	0.004%
79	13.890	2097	2100	2101	rBV	167	159	0.03%	0.003%
80	13.926	2104	2106	2107	rBV2	208	184	0.03%	0.003%
81	13.957	2110	2111	2114	rVB	262	188	0.03%	0.003%
82	13.987	2114	2116	2118	rVB2	279	219	0.04%	0.004%
83	14.024	2120	2122	2126	rBV2	179	276	0.05%	0.005%
84	14.194	2149	2150	2153	rVB	275	277	0.05%	0.005%
85	14.310	2168	2169	2172	rBV2	151	169	0.03%	0.003%
86	14.414	2183	2186	2187	rVV	291	267	0.04%	0.005%
87	14.560	2208	2210	2214	rBV2	246	267	0.04%	0.005%
88	14.609	2214	2218	2221	rVB2	657	874	0.15%	0.015%
89	14.865	2258	2260	2264	rVB2	252	274	0.05%	0.005%
90	14.908	2264	2267	2270	rBV3	230	340	0.06%	0.006%
91	15.152	2304	2307	2308	rBV2	229	203	0.03%	0.004%
92	15.316	2332	2334	2335	rVB	278	188	0.03%	0.003%
93	15.335	2335	2337	2338	rBV	246	208	0.03%	0.004%
94	15.389	2344	2346	2349	rBV2	342	341	0.06%	0.006%
95	15.652	2385	2389	2393	rVB2	322	430	0.07%	0.007%
96	15.700	2396	2397	2399	rBV2	265	164	0.03%	0.003%
97	15.743	2402	2404	2405	rBV2	377	283	0.05%	0.005%
98	15.810	2413	2415	2418	rBV2	230	261	0.04%	0.005%
99	16.542	2529	2535	2536	rBV3	267	518	0.09%	0.009%
100	16.706	2560	2562	2564	rVB	272	164	0.03%	0.003%

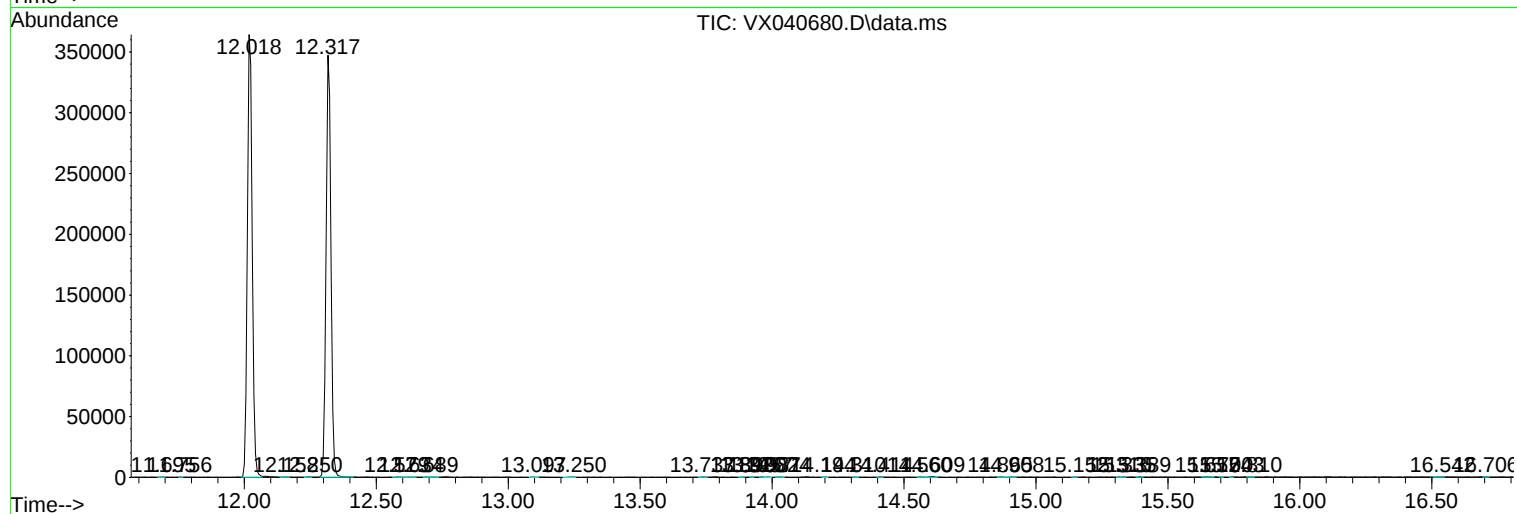
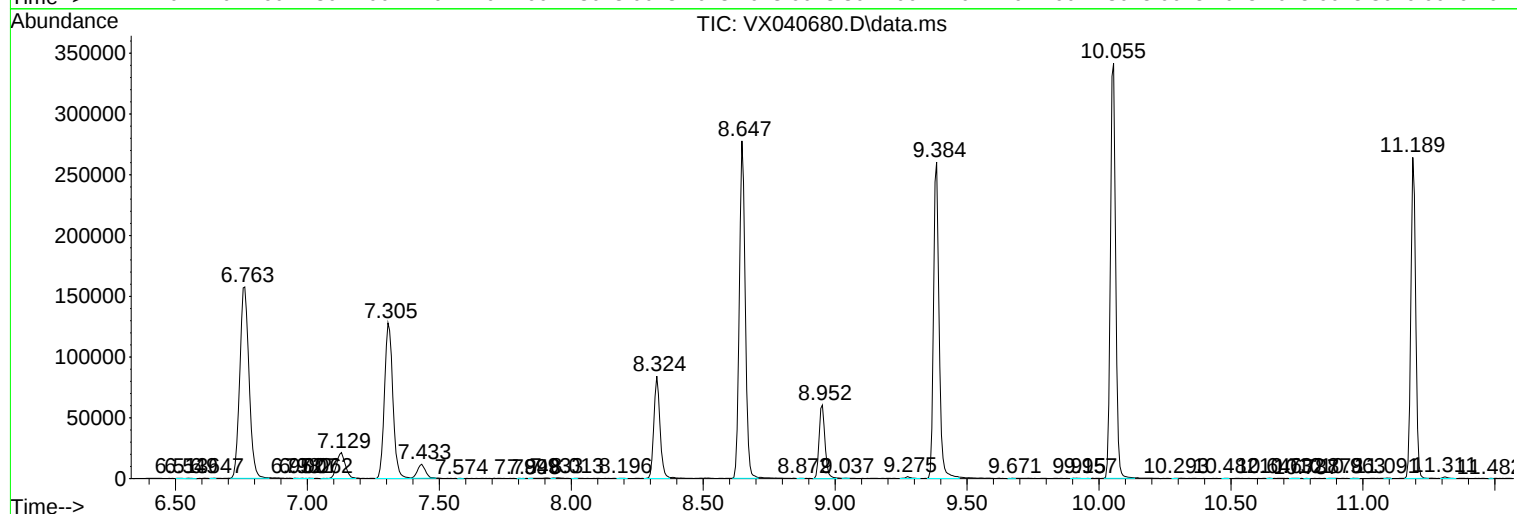
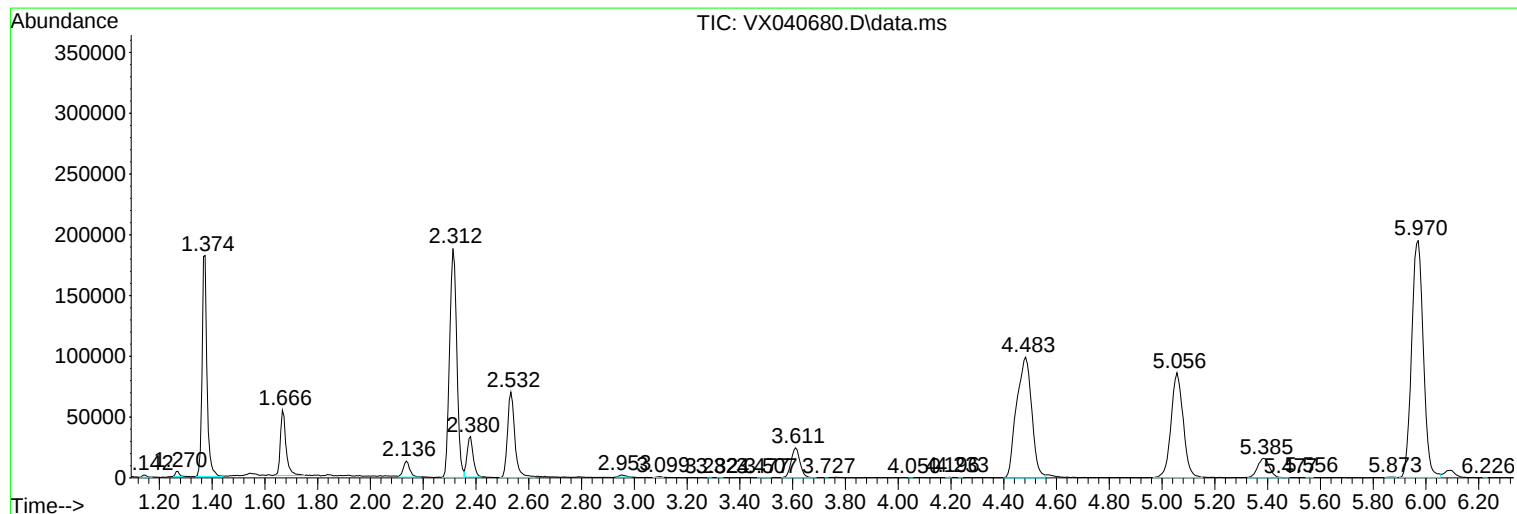
Sum of corrected areas: 5783209

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
Data File : VX040680.D
Acq On : 16 Mar 2024 01:56
Operator : JC/MD
Sample : P1754-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCL27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML030724WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
Data File : VX040680.D
Acq On : 16 Mar 2024 01:56
Operator : JC/MD
Sample : P1754-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCL27

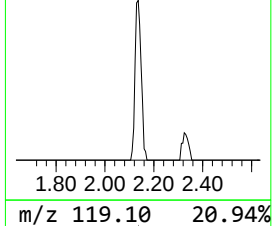
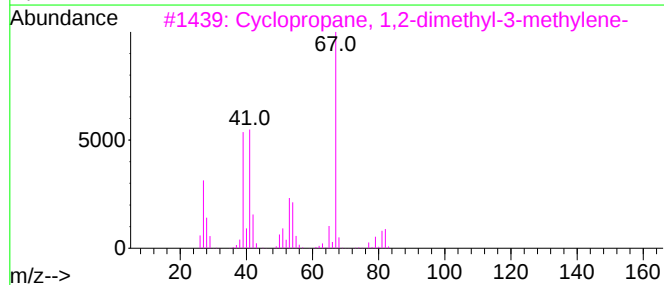
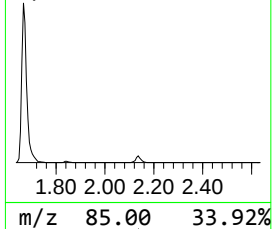
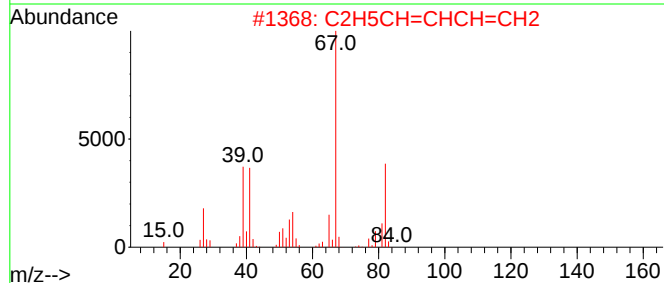
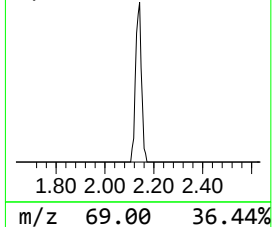
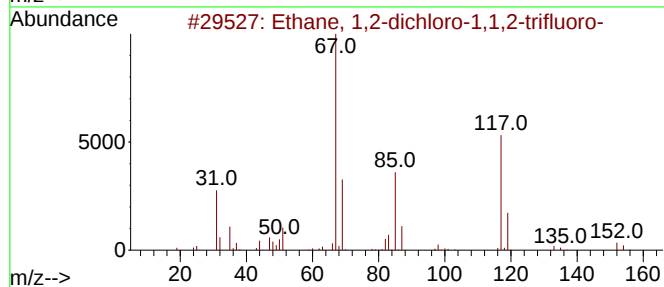
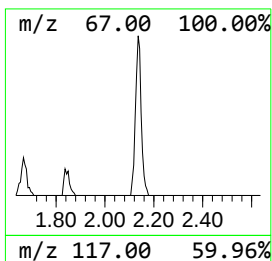
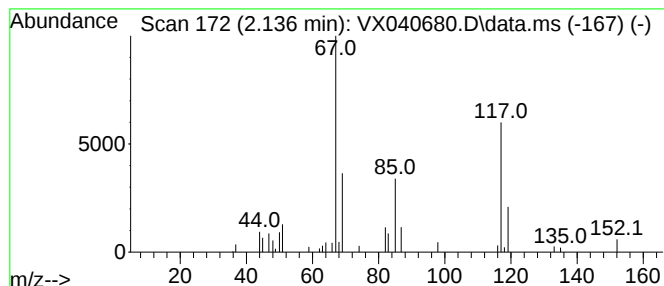
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML030724WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethane, 1,2-dichloro-1,1,2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.136	2.94 ug/L	22362	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	93
2			C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	35
3			Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	35
4			2-Pentyn-4-one	82	C5H6O	007299-55-0	25
5			1,3,3-Trimethylcyclopropene	82	C6H10	003664-56-0	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
Data File : VX040680.D
Acq On : 16 Mar 2024 01:56
Operator : JC/MD
Sample : P1754-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCL27

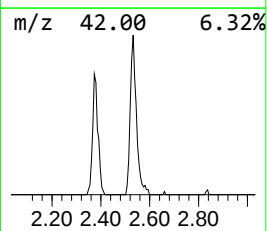
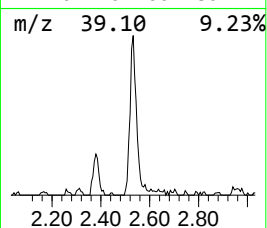
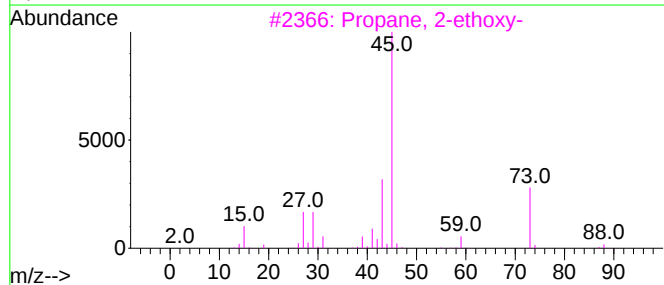
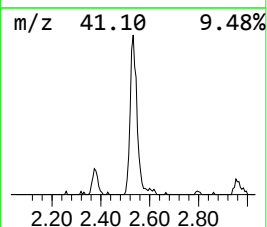
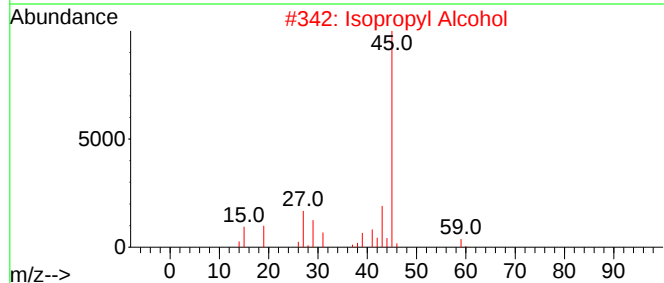
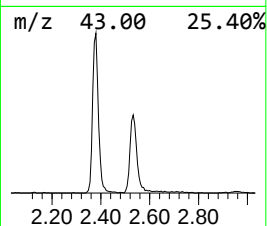
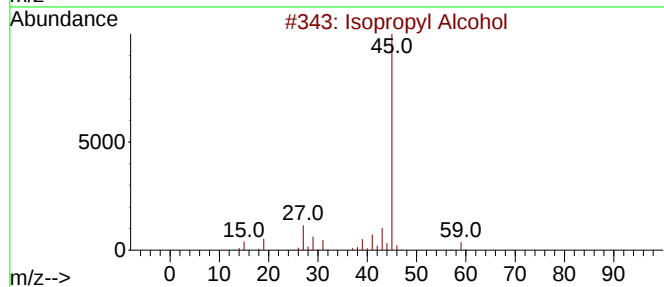
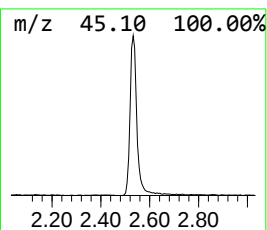
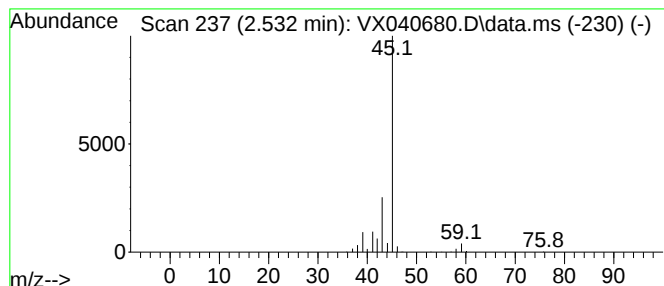
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML030724WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	17.65 ug/L	134293	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		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	64
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031524\
Data File : VX040680.D
Acq On : 16 Mar 2024 01:56
Operator : JC/MD
Sample : P1754-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCL27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML030724WMA.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
Ethane, 1,2-dic...	2.136	2.9	ug/L	22362	1	6.763	380417	50.0
Isopropyl Alcohol	2.532	17.6	ug/L	134293	1	6.763	380417	50.0