

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039240.D
 Acq On : 15 Dec 2023 19:53
 Operator : JC/MD
 Sample : 05844-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHG4

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: VX039240.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	7	9	17	rVB3	3588	4116	0.05%	0.024%
2	1.264	27	29	33	rVB2	3321	3000	0.04%	0.017%
3	1.373	42	47	57	rBV2	239875	290408	3.50%	1.667%
4	1.666	91	95	111	rVB	65297	107904	1.30%	0.619%
5	1.916	133	136	141	rVB	9091	11735	0.14%	0.067%
6	2.135	167	172	182	rVB	19136	33970	0.41%	0.195%
7	2.318	194	202	210	rBV	5066604	8287676	100.00%	47.580%
8	2.526	230	236	250	rBV	390830	688961	8.31%	3.955%
9	2.952	299	306	317	rVB	7871	17919	0.22%	0.103%
10	3.099	323	330	332	rBV6	1448	2421	0.03%	0.014%
11	3.160	338	340	342	rBV2	273	221	0.00%	0.001%
12	3.202	345	347	349	rBV2	336	360	0.00%	0.002%
13	3.507	393	397	400	rVV	559	689	0.01%	0.004%
14	3.611	404	414	430	rBV	234614	540708	6.52%	3.104%
15	3.757	431	438	453	rVB2	9715	27769	0.34%	0.159%
16	3.946	467	469	472	rVB2	246	281	0.00%	0.002%
17	3.976	472	474	475	rBV	284	228	0.00%	0.001%
18	4.019	479	481	483	rVB2	214	215	0.00%	0.001%
19	4.105	491	495	496	rBV	177	270	0.00%	0.002%
20	4.178	505	507	511	rVB2	249	260	0.00%	0.001%
21	4.226	513	515	517	rBV2	196	207	0.00%	0.001%
22	4.336	530	533	535	rBV2	222	345	0.00%	0.002%
23	4.379	538	540	543	rBV2	143	218	0.00%	0.001%
24	4.476	543	556	566	rBV2	102470	470214	5.67%	2.700%
25	4.897	624	625	627	rBV	394	255	0.00%	0.001%
26	5.056	630	651	671	rBV	123394	411125	4.96%	2.360%
27	5.263	683	685	687	rVB2	316	251	0.00%	0.001%
28	5.385	694	705	716	rVV3	24805	73687	0.89%	0.423%
29	5.543	727	731	732	rBV2	563	492	0.01%	0.003%
30	5.629	742	745	747	rVB2	195	249	0.00%	0.001%
31	5.970	789	801	810	rBV2	308896	943892	11.39%	5.419%
32	6.208	839	840	843	rVB2	293	208	0.00%	0.001%
33	6.238	843	845	849	rVB2	380	521	0.01%	0.003%
34	6.348	860	863	866	rBV	296	432	0.01%	0.002%
35	6.763	921	931	944	rBV	225651	551818	6.66%	3.168%
36	7.122	982	990	1012	rBV	144517	322754	3.89%	1.853%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039240.D
 Acq On : 15 Dec 2023 19:53
 Operator : JC/MD
 Sample : 05844-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHG4

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

37	7.305	1012	1020	1034	rBV	191159	428212	5.17%	2.458%
38	7.433	1036	1041	1048	rVB3	4659	10131	0.12%	0.058%
39	7.604	1066	1069	1070	rBV	253	211	0.00%	0.001%
40	7.854	1107	1110	1111	rVB2	438	331	0.00%	0.002%
41	7.884	1114	1115	1116	rBV	447	318	0.00%	0.002%
42	8.256	1174	1176	1179	rBV2	195	304	0.00%	0.002%
43	8.323	1181	1187	1204	rVV	137492	229677	2.77%	1.319%
44	8.646	1234	1240	1257	rVV	464326	737669	8.90%	4.235%
45	8.951	1284	1290	1298	rBV	98495	152172	1.84%	0.874%
46	9.098	1312	1314	1317	rVB3	441	342	0.00%	0.002%
47	9.274	1337	1343	1352	rVB2	16101	24320	0.29%	0.140%
48	9.384	1355	1361	1384	rVV	403922	579629	6.99%	3.328%
49	9.622	1398	1400	1401	rBV	330	233	0.00%	0.001%
50	9.725	1415	1417	1418	rBV	262	229	0.00%	0.001%
51	9.744	1418	1420	1422	rVV2	218	218	0.00%	0.001%
52	9.853	1432	1438	1439	rBV2	187	310	0.00%	0.002%
53	10.055	1465	1471	1482	rBV	485468	667494	8.05%	3.832%
54	10.244	1501	1502	1505	rBV2	239	276	0.00%	0.002%
55	10.299	1509	1511	1517	rVV3	470	722	0.01%	0.004%
56	10.359	1519	1521	1523	rBV2	242	236	0.00%	0.001%
57	10.512	1542	1546	1548	rBV	171	218	0.00%	0.001%
58	10.585	1556	1558	1560	rBV2	239	245	0.00%	0.001%
59	10.646	1565	1568	1573	rVV3	245	430	0.01%	0.002%
60	11.018	1624	1629	1637	rVV	2861	4372	0.05%	0.025%
61	11.085	1637	1640	1646	rVB3	1481	2181	0.03%	0.013%
62	11.189	1652	1657	1667	rVV	364373	471844	5.69%	2.709%
63	11.262	1667	1669	1671	rVV	648	521	0.01%	0.003%
64	11.280	1671	1672	1674	rVV	358	262	0.00%	0.002%
65	11.311	1674	1677	1684	rVB3	2168	3110	0.04%	0.018%
66	11.439	1694	1698	1699	rVV2	205	226	0.00%	0.001%
67	11.457	1699	1701	1704	rVB3	405	358	0.00%	0.002%
68	11.487	1704	1706	1708	rBV2	338	330	0.00%	0.002%
69	11.591	1720	1723	1729	rVB2	210	354	0.00%	0.002%
70	11.707	1740	1742	1744	rVV	385	308	0.00%	0.002%
71	11.749	1747	1749	1754	rVV3	532	754	0.01%	0.004%
72	11.792	1754	1756	1758	rVV	387	276	0.00%	0.002%
73	11.817	1758	1760	1762	rVB2	259	224	0.00%	0.001%
74	11.975	1778	1786	1788	rBV3	425	865	0.01%	0.005%
75	12.018	1788	1793	1804	rBV	485777	644610	7.78%	3.701%
76	12.225	1824	1827	1828	rBV	489	408	0.00%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039240.D
 Acq On : 15 Dec 2023 19:53
 Operator : JC/MD
 Sample : 05844-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHG4

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

77	12.316	1837	1842	1851	rBV	508317	647965	7.82%	3.720%
78	12.591	1884	1887	1888	rVB	433	344	0.00%	0.002%
79	12.682	1899	1902	1904	rBV2	169	224	0.00%	0.001%
80	12.755	1912	1914	1919	rVB2	647	1036	0.01%	0.006%
81	13.103	1969	1971	1976	rVB2	377	348	0.00%	0.002%
82	13.286	1999	2001	2003	rVV	295	220	0.00%	0.001%
83	13.322	2005	2007	2010	rBV2	189	226	0.00%	0.001%
84	13.359	2010	2013	2015	rBV	217	213	0.00%	0.001%
85	13.432	2021	2025	2030	rBV2	879	1267	0.02%	0.007%
86	13.591	2049	2051	2056	rVB3	553	640	0.01%	0.004%
87	13.780	2078	2082	2087	rBV3	555	988	0.01%	0.006%
88	13.834	2089	2091	2093	rBV2	348	356	0.00%	0.002%
89	13.926	2103	2106	2107	rBV2	187	240	0.00%	0.001%
90	13.969	2110	2113	2116	rVV2	208	318	0.00%	0.002%
91	14.261	2158	2161	2166	rBV2	187	334	0.00%	0.002%
92	14.493	2197	2199	2201	rVB	426	232	0.00%	0.001%
93	14.853	2255	2258	2259	rBV2	215	231	0.00%	0.001%
94	14.962	2274	2276	2278	rBV2	205	210	0.00%	0.001%
95	15.121	2299	2302	2305	rBV3	258	389	0.00%	0.002%
96	15.651	2386	2389	2390	rBV3	433	418	0.01%	0.002%
97	15.737	2401	2403	2408	rVB2	294	338	0.00%	0.002%
98	16.182	2474	2476	2480	rBV2	413	564	0.01%	0.003%
99	16.218	2480	2482	2486	rVB3	313	365	0.00%	0.002%
100	16.523	2530	2532	2534	rBV2	267	213	0.00%	0.001%

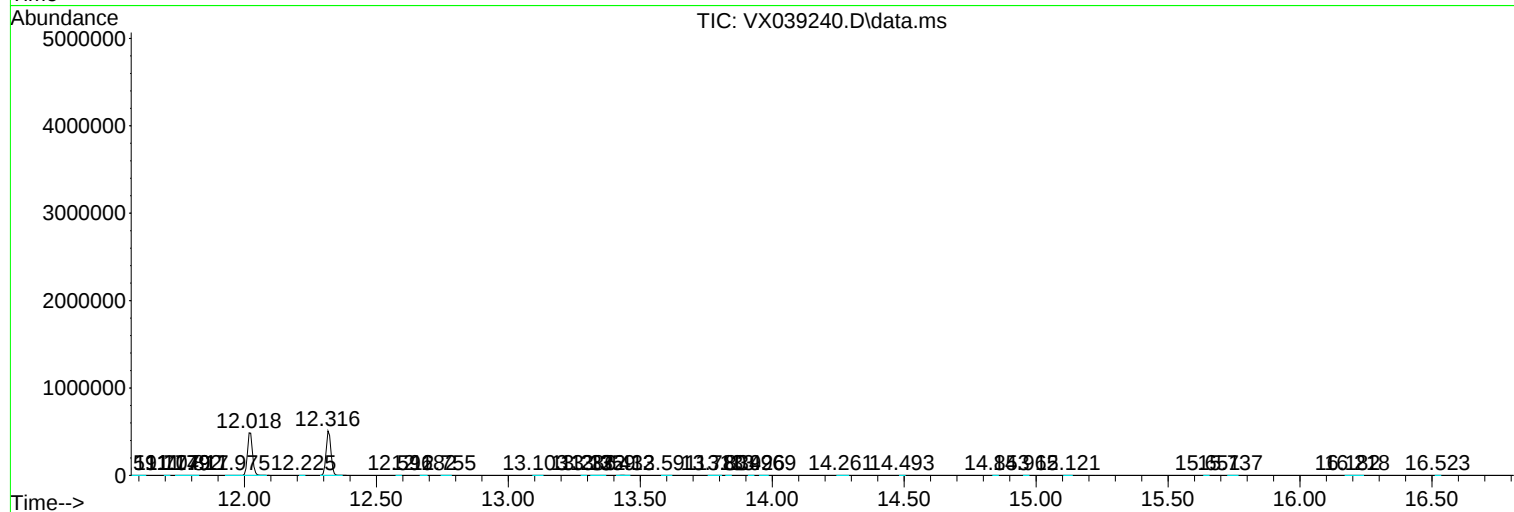
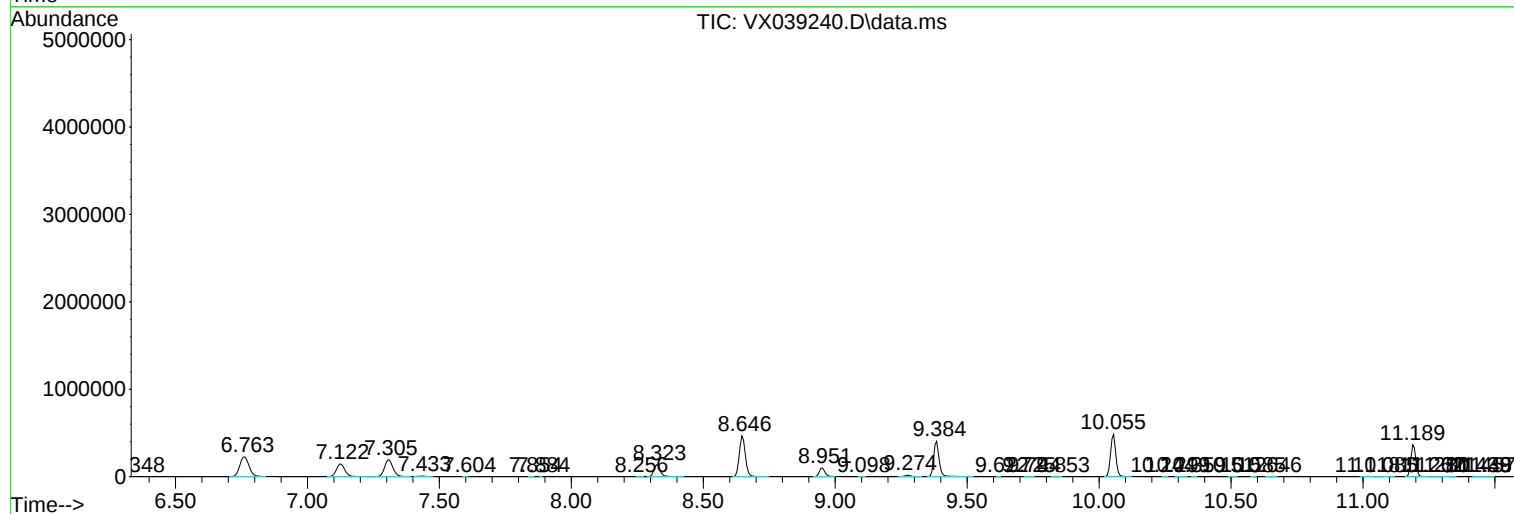
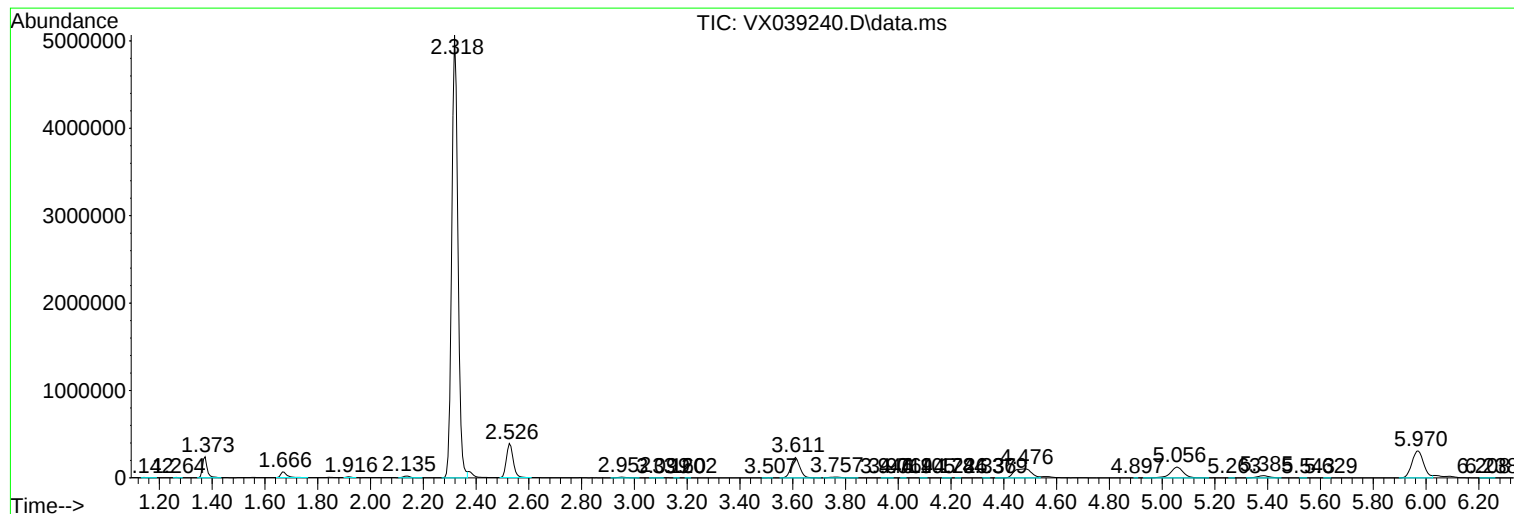
Sum of corrected areas: 17418388

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039240.D
Acq On : 15 Dec 2023 19:53
Operator : JC/MD
Sample : 05844-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHG4

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039240.D
Acq On : 15 Dec 2023 19:53
Operator : JC/MD
Sample : 05844-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHG4

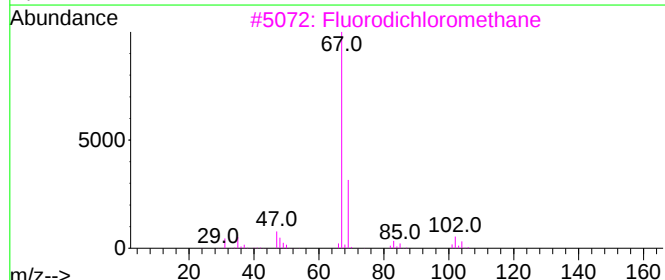
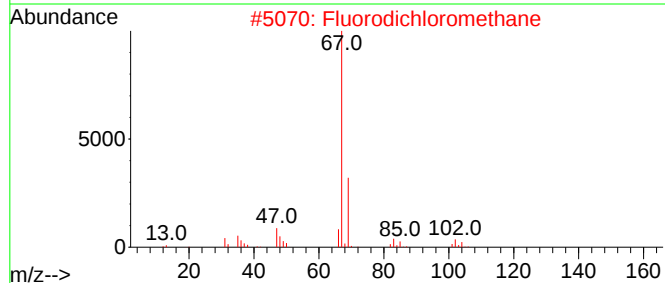
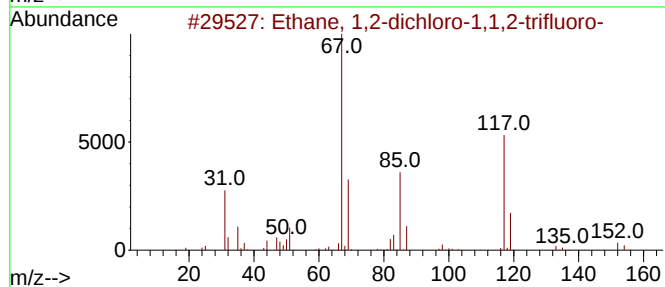
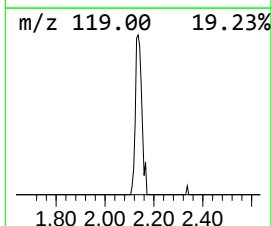
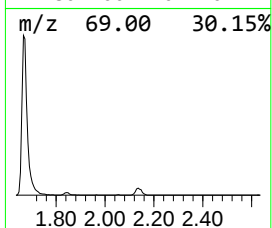
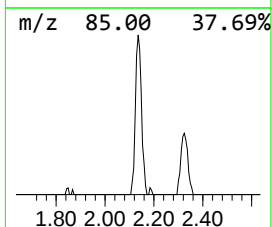
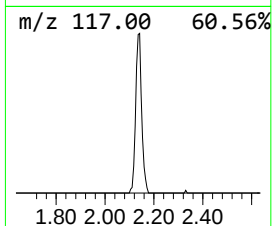
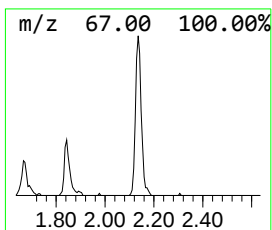
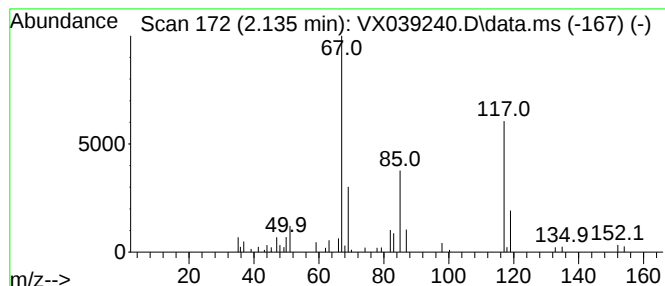
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.135	3.08 ug/L	33970	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	46
2			Fluorodichloromethane	102	CHCl2F	000075-43-4	25
3			Fluorodichloromethane	102	CHCl2F	000075-43-4	17
4			1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	12
5			Benzyl nitrile	117	C8H7N	000140-29-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039240.D
Acq On : 15 Dec 2023 19:53
Operator : JC/MD
Sample : 05844-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHG4

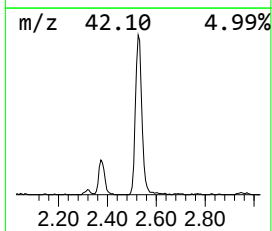
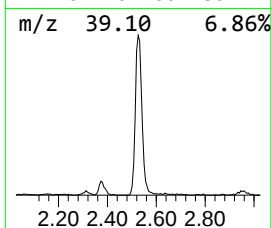
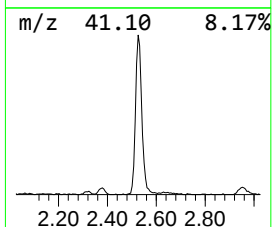
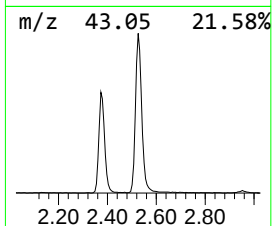
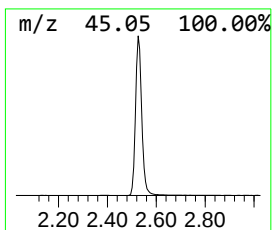
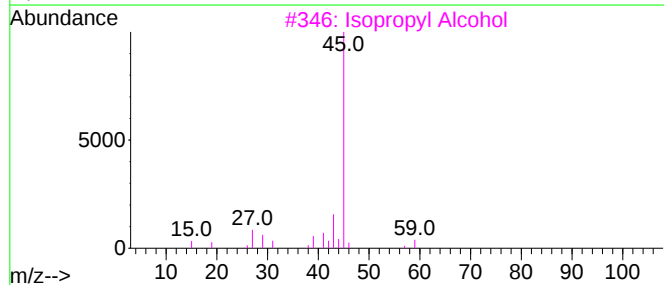
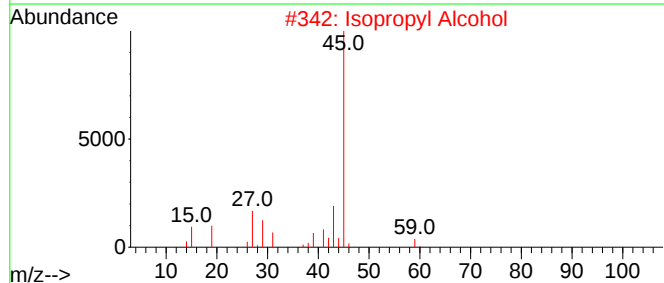
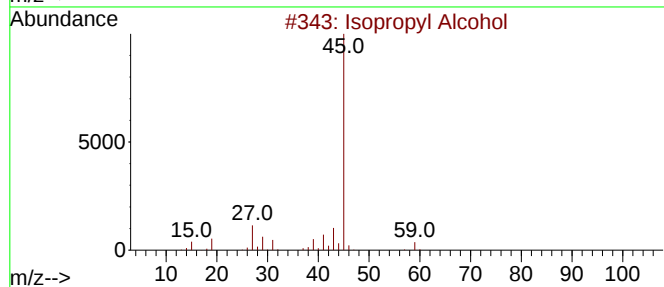
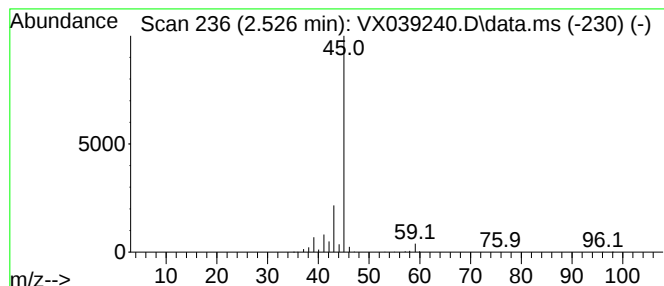
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.526	62.43 ug/L	688961	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	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039240.D
Acq On : 15 Dec 2023 19:53
Operator : JC/MD
Sample : 05844-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHG4

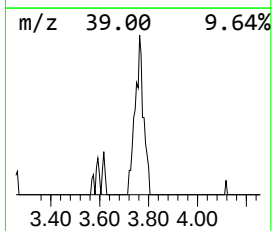
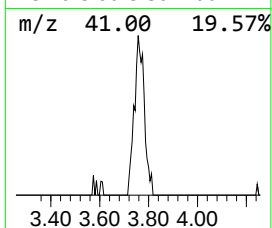
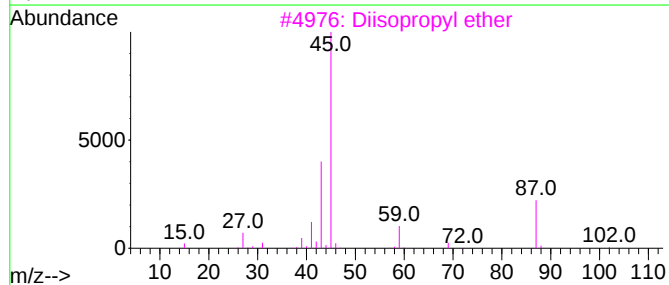
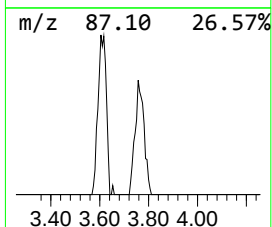
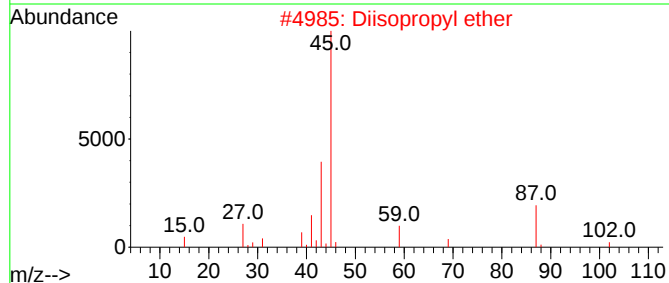
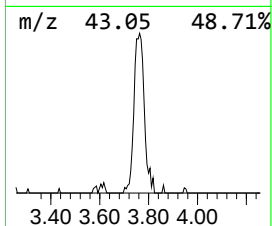
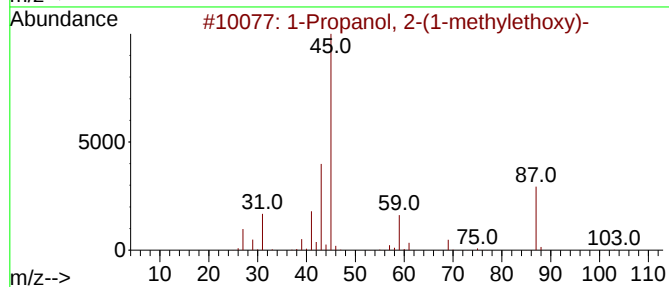
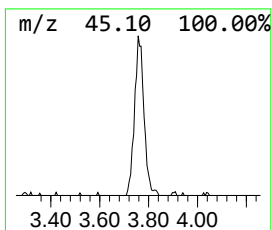
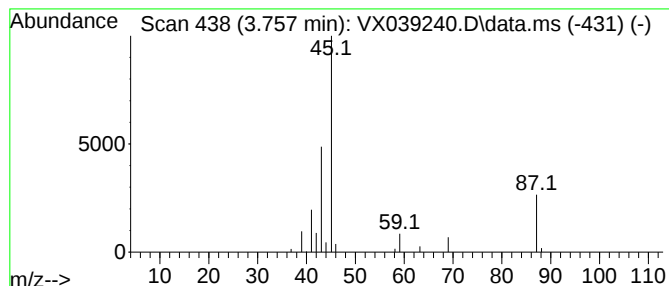
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Propanol, 2-(1-methyletho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.757	2.52 ug/L	27769	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	83
2		Diisopropyl ether	102	C6H14O	000108-20-3	78
3		Diisopropyl ether	102	C6H14O	000108-20-3	64
4		Diisopropyl ether	102	C6H14O	000108-20-3	64
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039240.D
Acq On : 15 Dec 2023 19:53
Operator : JC/MD
Sample : 05844-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHG4

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.135	3.1	ug/L	33970	1	6.763	551818	50.0
Isopropyl Alcohol	2.526	62.4	ug/L	688961	1	6.763	551818	50.0
1-Propanol, 2-(...	3.757	2.5	ug/L	27769	1	6.763	551818	50.0