

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030631.D
 Acq On : 15 Aug 2022 16:34
 Operator : JC/MD
 Sample : N4181-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 X3C26

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	26	28	32	rBV2	5008	4727	0.24%	0.017%
2	1.368	42	46	58	rVB2	373234	444792	22.59%	1.587%
3	1.557	73	77	84	rBV	142503	152973	7.77%	0.546%
4	1.642	87	91	93	rVV	77483	95362	4.84%	0.340%
5	1.666	93	95	102	rVB	75843	84388	4.29%	0.301%
6	1.880	125	130	139	rVB	447938	611262	31.05%	2.181%
7	2.313	193	201	209	rBV3	480045	859899	43.68%	3.069%
8	2.398	209	215	223	rVV	635638	1008141	51.21%	3.598%
9	2.471	223	227	239	rVB	110930	187808	9.54%	0.670%
10	2.715	263	267	273	rVB	4964	8955	0.45%	0.032%
11	2.788	274	279	287	rVB5	3671	8015	0.41%	0.029%
12	2.904	296	298	299	rBV	587	503	0.03%	0.002%
13	2.934	300	303	304	rBV2	980	836	0.04%	0.003%
14	3.123	323	334	349	rBV	513709	1193052	60.60%	4.257%
15	3.440	380	386	392	rBV5	2478	5968	0.30%	0.021%
16	3.520	396	399	402	rBV2	536	903	0.05%	0.003%
17	3.550	402	404	407	rVB2	441	455	0.02%	0.002%
18	3.599	409	412	413	rBV3	780	705	0.04%	0.003%
19	3.959	467	471	475	rBV2	356	553	0.03%	0.002%
20	4.489	547	558	573	rBV3	232097	717357	36.44%	2.560%
21	4.739	597	599	603	rVB3	554	541	0.03%	0.002%
22	5.062	641	652	667	rVV	126239	405507	20.60%	1.447%
23	5.306	690	692	695	rVB3	833	849	0.04%	0.003%
24	5.379	699	704	705	rBV2	909	1252	0.06%	0.004%
25	5.550	726	732	734	rBV4	1265	2513	0.13%	0.009%
26	5.977	787	802	808	rBV2	323210	953230	48.42%	3.402%
27	6.227	841	843	846	rBV2	644	700	0.04%	0.002%
28	6.251	846	847	850	rVB3	1034	735	0.04%	0.003%
29	6.373	865	867	872	rVB4	664	733	0.04%	0.003%
30	6.446	878	879	883	rBV	428	536	0.03%	0.002%
31	6.604	901	905	907	rVB2	454	509	0.03%	0.002%
32	6.769	922	932	946	rBV	293834	709499	36.04%	2.532%
33	7.001	968	970	972	rBV2	540	697	0.04%	0.002%
34	7.129	981	991	1011	rVB	432675	936735	47.58%	3.343%
35	7.318	1013	1022	1026	rBV	208476	452560	22.99%	1.615%
36	7.385	1026	1033	1039	rBV	733261	1519090	77.17%	5.421%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030631.D
 Acq On : 15 Aug 2022 16:34
 Operator : JC/MD
 Sample : N4181-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 X3C26

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\SFAMXMLM080422WMA.M
 Title : VOC Analysis

37	7.604	1067	1069	1072	rVB3	588	610	0.03%	0.002%
38	7.940	1117	1124	1126	rBV3	2672	4390	0.22%	0.016%
39	8.019	1135	1137	1140	rBV	338	493	0.03%	0.002%
40	8.165	1155	1161	1162	rBV3	1440	2392	0.12%	0.009%
41	8.330	1182	1188	1196	rBV	131845	213417	10.84%	0.762%
42	8.482	1209	1213	1215	rBV4	1380	2299	0.12%	0.008%
43	8.580	1222	1229	1235	rBV	785265	1227900	62.38%	4.382%
44	8.653	1235	1241	1251	rVB	452984	704498	35.79%	2.514%
45	8.805	1263	1266	1268	rBV4	1209	1629	0.08%	0.006%
46	8.860	1273	1275	1279	rBV4	930	1139	0.06%	0.004%
47	8.909	1279	1283	1285	rBV4	2006	2721	0.14%	0.010%
48	8.952	1285	1290	1299	rVV	95096	145710	7.40%	0.520%
49	9.153	1317	1323	1336	rVB	258542	386475	19.63%	1.379%
50	9.275	1336	1343	1356	rBV	467188	676065	34.34%	2.413%
51	9.391	1356	1362	1366	rVV	465827	647442	32.89%	2.310%
52	9.439	1366	1370	1378	rVV	501044	725594	36.86%	2.589%
53	9.525	1379	1384	1393	rVV	200560	290929	14.78%	1.038%
54	9.616	1393	1399	1411	rVB	490498	717396	36.44%	2.560%
55	9.787	1426	1427	1431	rVB2	752	580	0.03%	0.002%
56	9.897	1442	1445	1446	rBV2	711	802	0.04%	0.003%
57	9.945	1451	1453	1456	rBV4	474	663	0.03%	0.002%
58	9.988	1456	1460	1462	rVV4	955	1330	0.07%	0.005%
59	10.055	1466	1471	1484	rVB	620765	834874	42.41%	2.979%
60	10.195	1489	1494	1502	rVB	1374338	1740175	88.40%	6.210%
61	10.305	1509	1512	1518	rVB	7209	10149	0.52%	0.036%
62	10.579	1555	1557	1561	rVB2	449	521	0.03%	0.002%
63	10.646	1562	1568	1579	rBV	562710	721367	36.64%	2.574%
64	10.799	1590	1593	1598	rVB5	932	1532	0.08%	0.005%
65	10.963	1614	1620	1630	rBV	1613619	1968576	100.00%	7.025%
66	11.195	1653	1658	1666	rBV	421484	520216	26.43%	1.856%
67	11.372	1684	1687	1693	rVB2	2390	3420	0.17%	0.012%
68	11.433	1693	1697	1699	rBV3	511	556	0.03%	0.002%
69	11.482	1700	1705	1714	rVB	420715	476832	24.22%	1.702%
70	11.652	1728	1733	1741	rVB	30710	44368	2.25%	0.158%
71	11.713	1741	1743	1747	rVB2	1541	1595	0.08%	0.006%
72	11.750	1747	1749	1750	rBV2	916	775	0.04%	0.003%
73	11.793	1753	1756	1759	rBV3	761	901	0.05%	0.003%
74	11.866	1763	1768	1772	rVB5	1833	2677	0.14%	0.010%
75	11.927	1772	1778	1780	rBV	6492	8248	0.42%	0.029%
76	11.969	1780	1785	1790	rVV	848937	1061166	53.91%	3.787%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030631.D
 Acq On : 15 Aug 2022 16:34
 Operator : JC/MD
 Sample : N4181-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 X3C26

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\SFAMXML080422WMA.M
 Title : VOC Analysis

77	12.024	1790	1794	1805	rVB	701146	858409	43.61%	3.063%
78	12.189	1819	1821	1826	rVB2	22100	25985	1.32%	0.093%
79	12.335	1837	1845	1851	rBV2	1108671	1817642	92.33%	6.486%
80	12.427	1856	1860	1863	rVV5	4805	6840	0.35%	0.024%
81	12.561	1878	1882	1884	rVB4	658	853	0.04%	0.003%
82	12.646	1894	1896	1898	rBV2	979	926	0.05%	0.003%
83	12.762	1912	1915	1917	rBV2	1041	1361	0.07%	0.005%
84	13.067	1963	1965	1967	rBV2	467	503	0.03%	0.002%
85	13.116	1967	1973	1984	rVV	704269	850645	43.21%	3.036%
86	13.201	1984	1987	1991	rVB3	1667	2259	0.11%	0.008%
87	13.359	2009	2013	2020	rBV	90570	119348	6.06%	0.426%
88	13.433	2020	2025	2029	rBV2	19218	25826	1.31%	0.092%
89	13.591	2045	2051	2056	rBV	608354	742933	37.74%	2.651%
90	13.646	2056	2060	2066	rVB3	25262	31971	1.62%	0.114%
91	13.847	2091	2093	2097	rVB2	549	682	0.03%	0.002%
92	13.902	2100	2102	2104	rBV2	461	496	0.03%	0.002%
93	13.963	2109	2112	2117	rVB3	3229	3751	0.19%	0.013%
94	14.134	2136	2140	2144	rVB2	2058	2353	0.12%	0.008%
95	14.213	2149	2153	2156	rVB5	521	813	0.04%	0.003%
96	14.280	2159	2164	2170	rBV5	849	1896	0.10%	0.007%
97	14.335	2171	2173	2177	rVB3	974	1110	0.06%	0.004%
98	14.902	2265	2266	2268	rVB2	994	510	0.03%	0.002%
99	15.103	2297	2299	2303	rVB3	789	536	0.03%	0.002%
100	16.036	2450	2452	2453	rBV2	768	751	0.04%	0.003%

Sum of corrected areas: 28023161

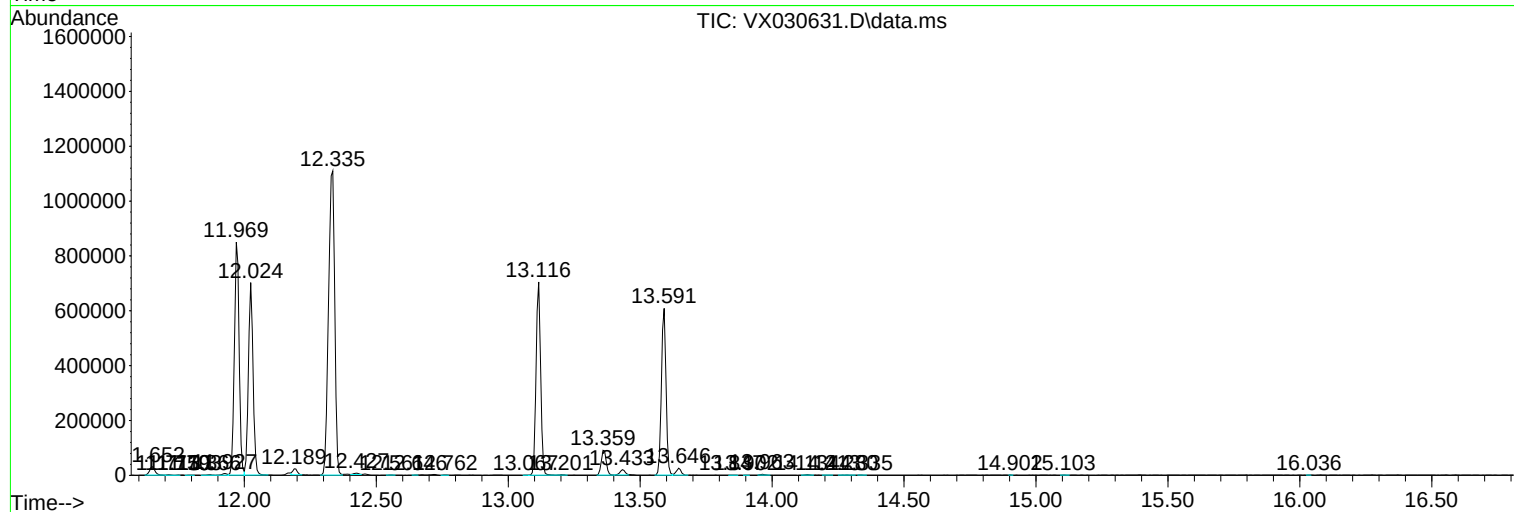
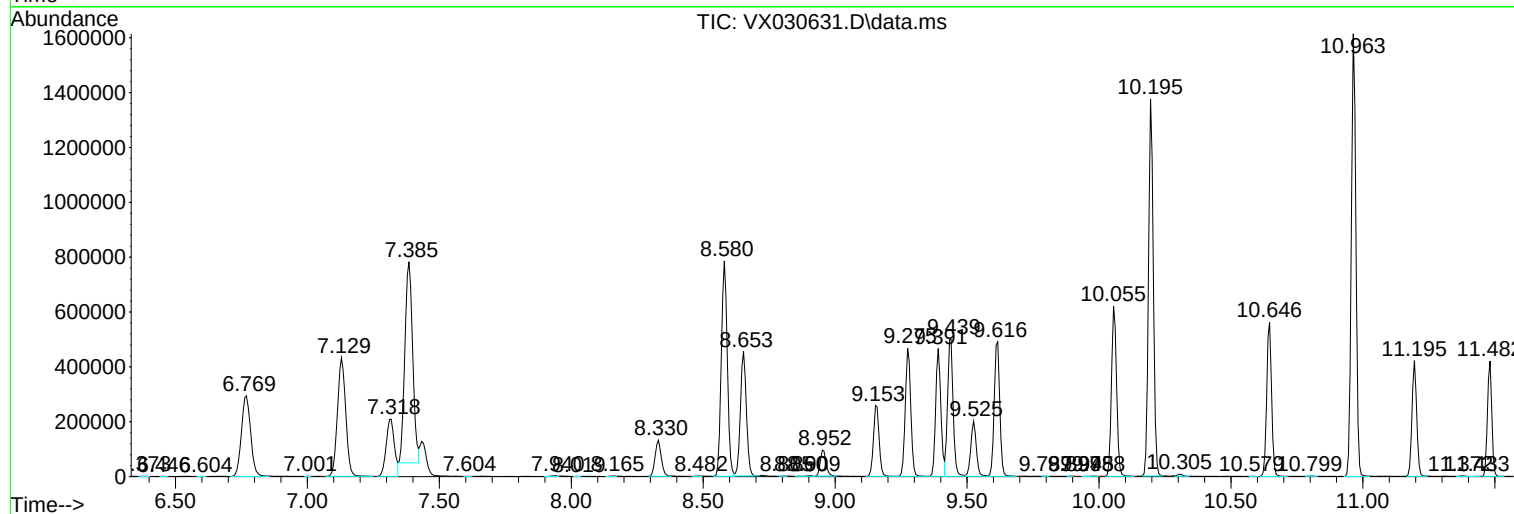
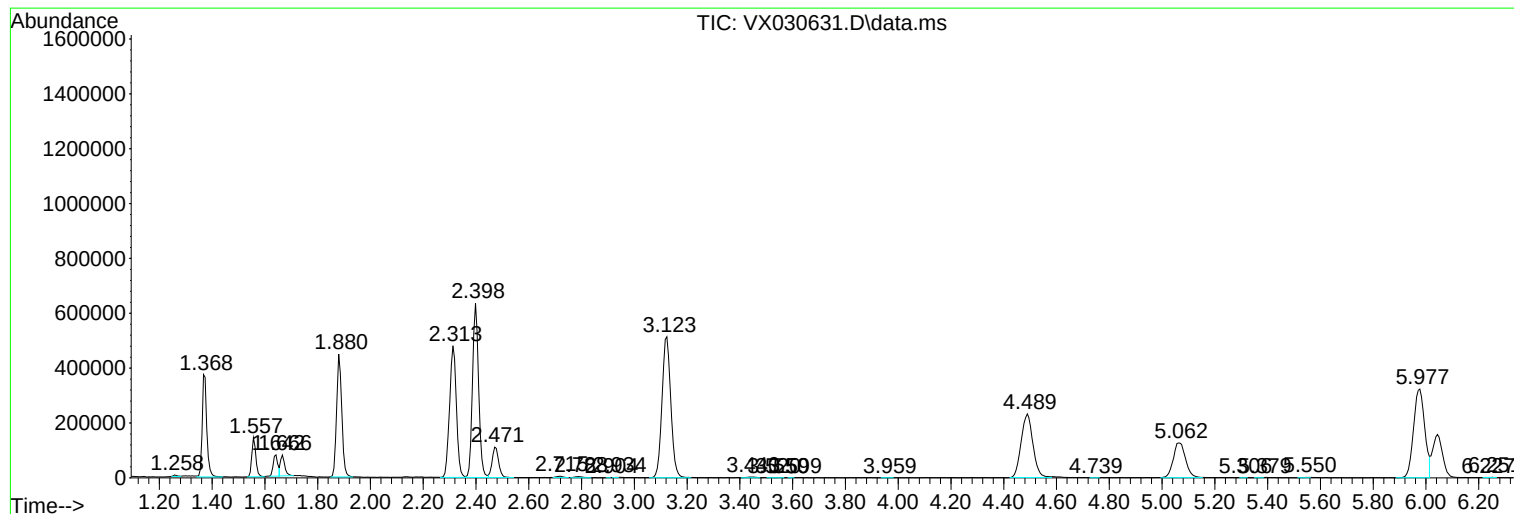
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

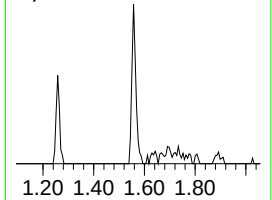
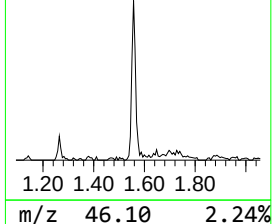
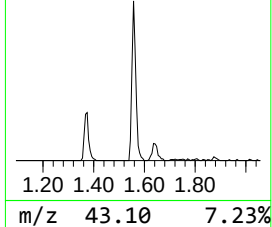
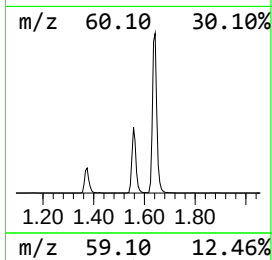
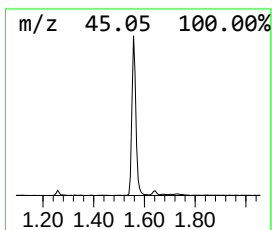
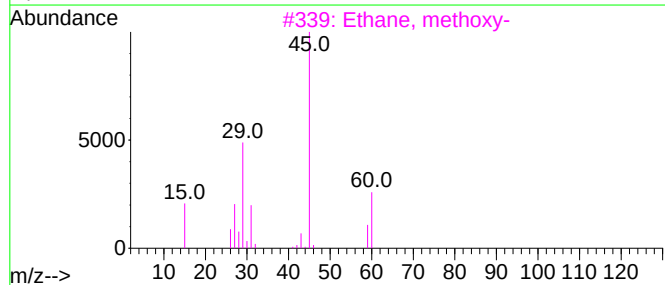
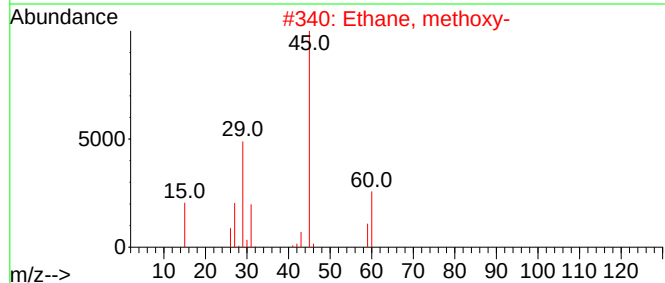
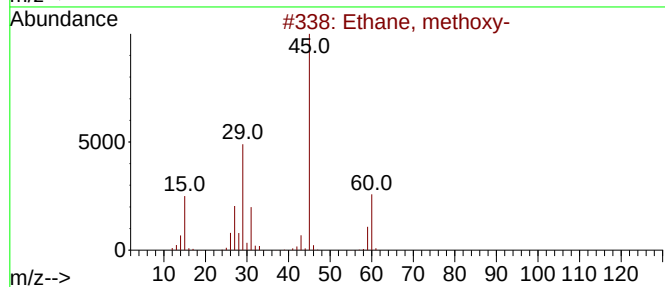
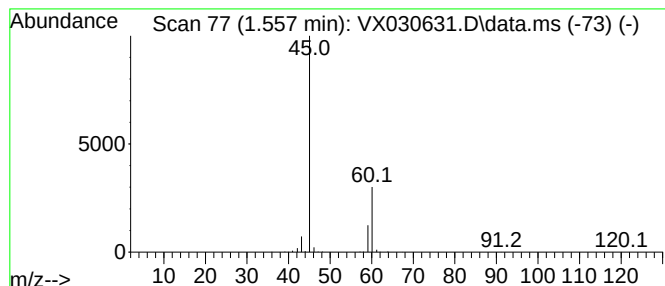
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethane, methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.557	10.78 ug/L	152973	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, methoxy-	60	C3H8O	000540-67-0	78
2			Ethane, methoxy-	60	C3H8O	000540-67-0	78
3			Ethane, methoxy-	60	C3H8O	000540-67-0	78
4			Ethane, methoxy-	60	C3H8O	000540-67-0	56
5			2-Butanol, (R)-	74	C4H10O	014898-79-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

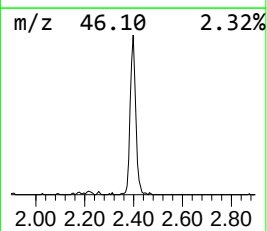
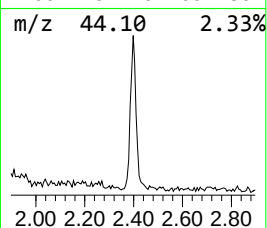
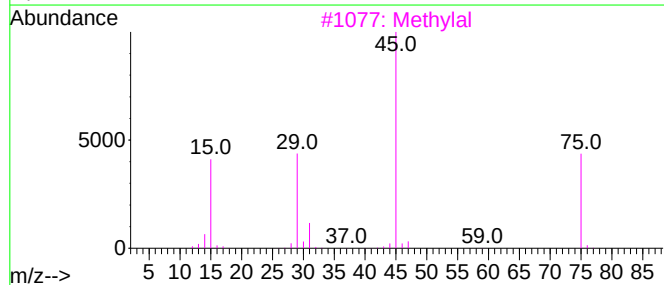
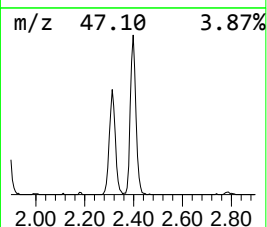
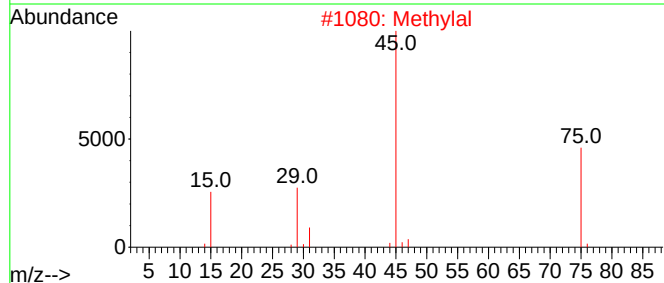
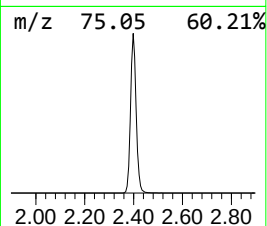
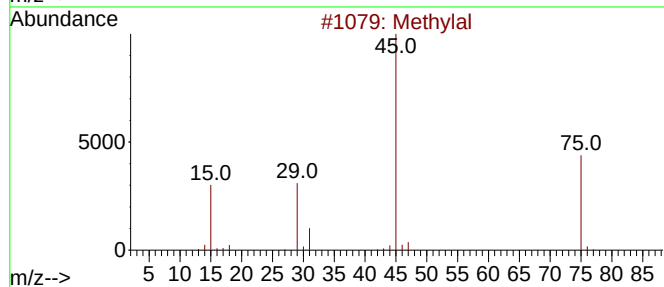
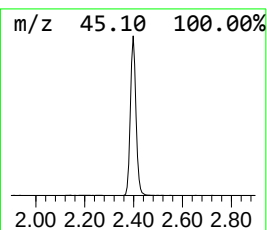
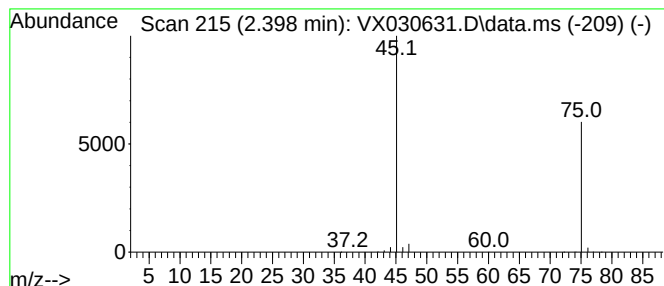
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methylal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.398	71.05 ug/L	1008140	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylal			76	C3H8O2	000109-87-5	78
2	Methylal			76	C3H8O2	000109-87-5	78
3	Methylal			76	C3H8O2	000109-87-5	78
4	Methylal			76	C3H8O2	000109-87-5	59
5	Methanamine, N,N-dimethyl-, N-oxide			75	C3H9NO	001184-78-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

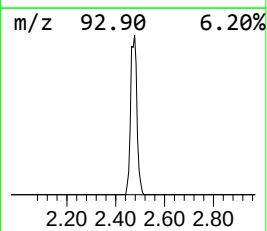
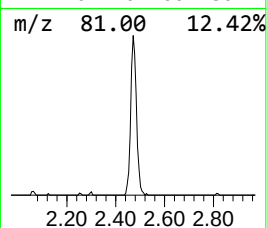
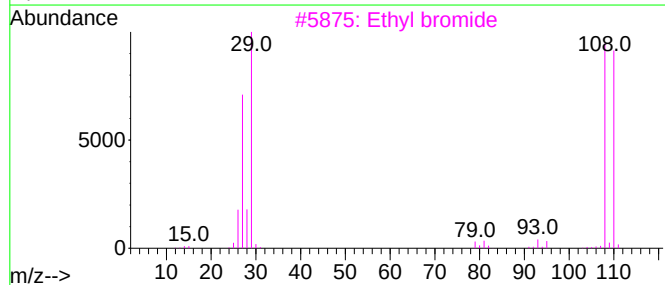
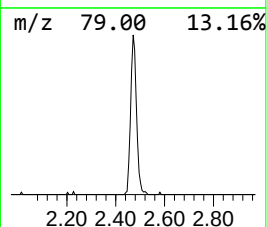
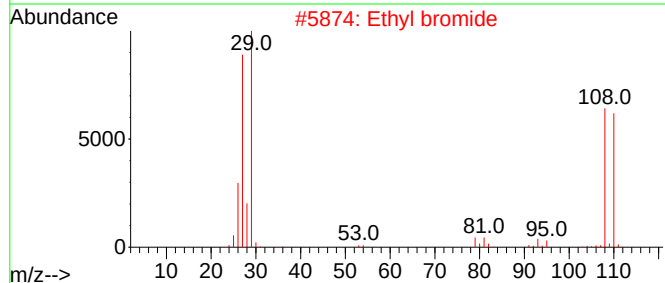
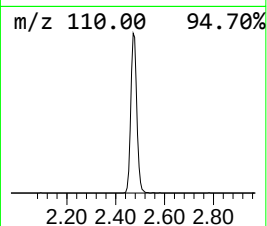
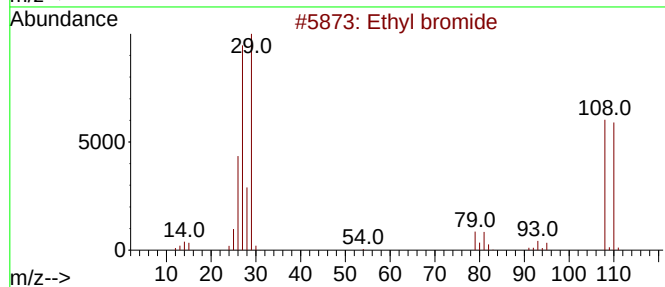
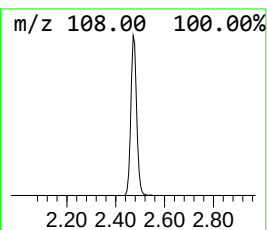
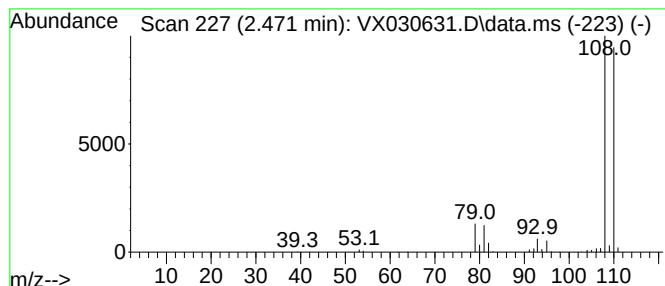
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Ethyl bromide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.471	13.24 ug/L	187808	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl bromide	108	C2H5Br	000074-96-4	90
2			Ethyl bromide	108	C2H5Br	000074-96-4	90
3			Ethyl bromide	108	C2H5Br	000074-96-4	86
4			Ethyl bromide	108	C2H5Br	000074-96-4	86
5			Ethyl bromide	108	C2H5Br	000074-96-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

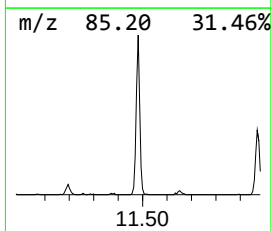
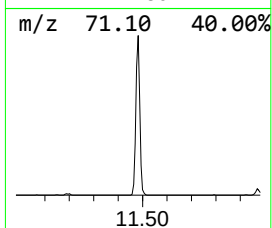
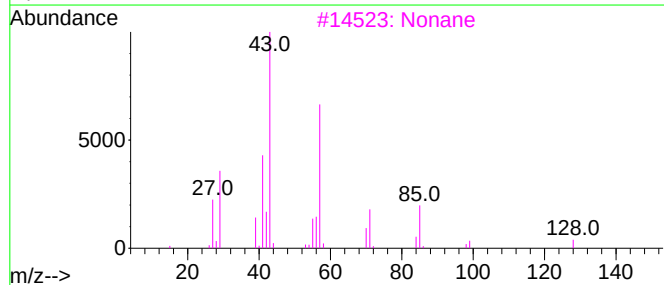
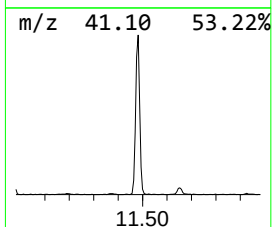
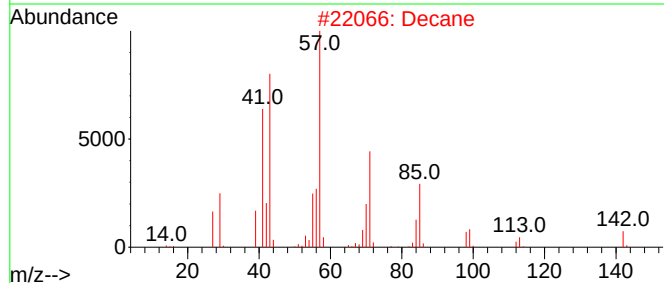
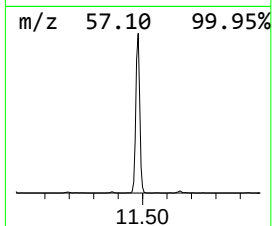
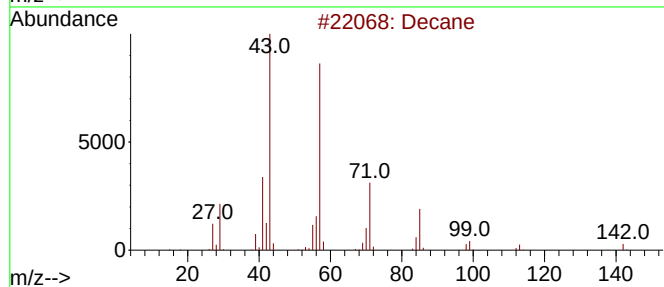
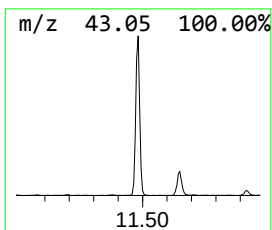
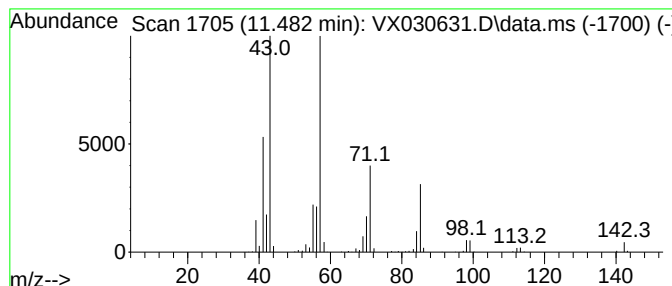
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.482	27.77 ug/L	476832	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	87
2			Decane	142	C10H22	000124-18-5	87
3			Nonane	128	C9H20	000111-84-2	83
4			Nonane	128	C9H20	000111-84-2	72
5			Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

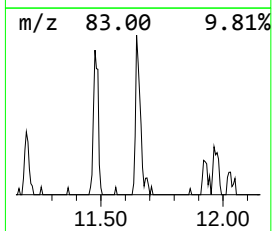
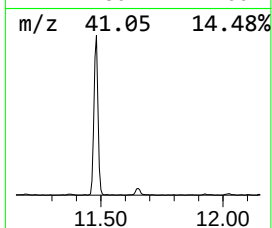
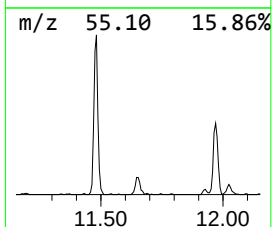
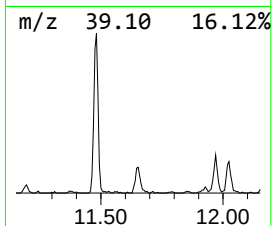
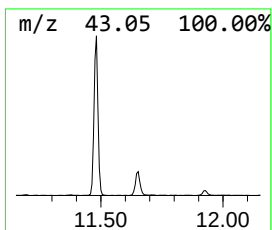
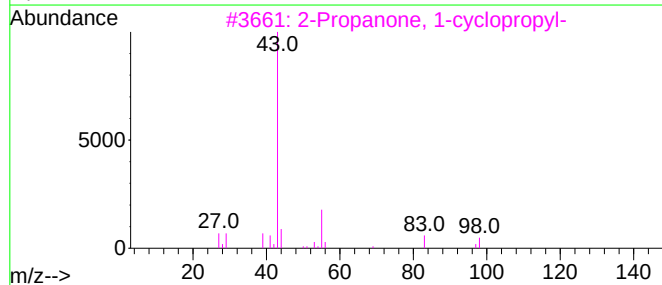
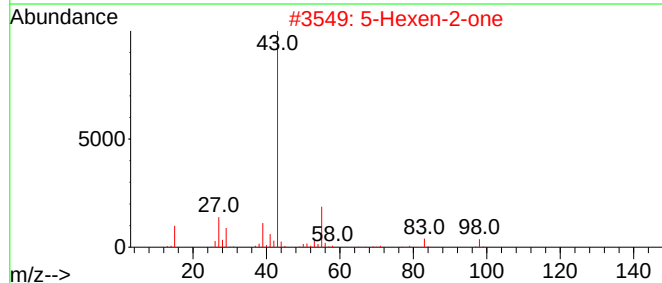
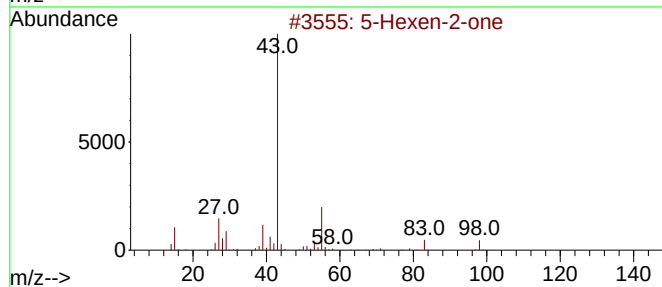
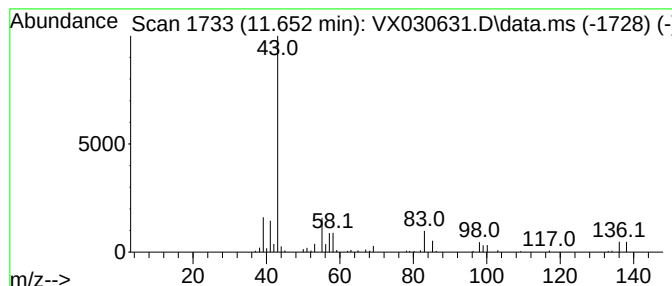
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.652	2.58 ug/L	44368	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hexen-2-one	98	C6H10O	000109-49-9	35
2		5-Hexen-2-one	98	C6H10O	000109-49-9	35
3		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	32
4		5-Hexen-2-one	98	C6H10O	000109-49-9	32
5		5-Hexen-2-one	98	C6H10O	000109-49-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

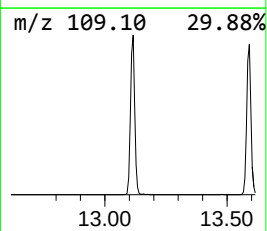
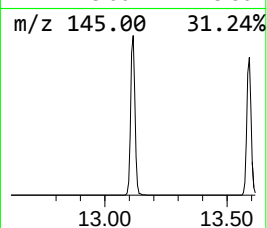
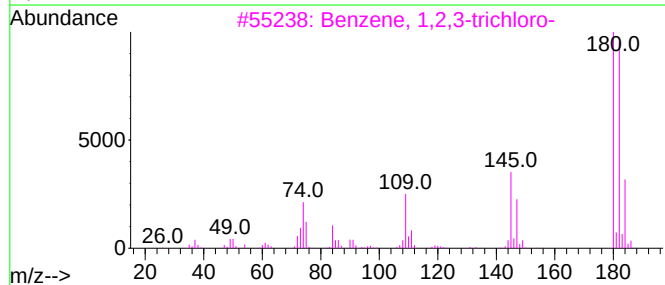
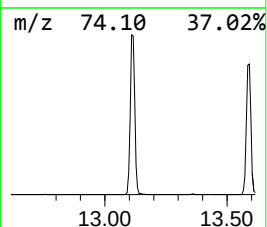
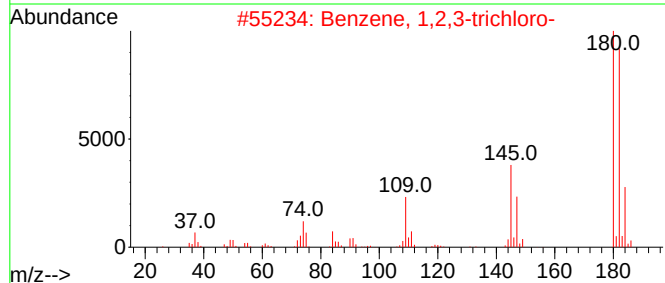
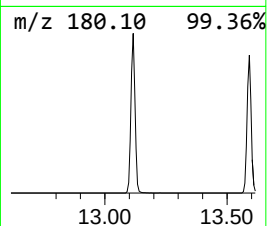
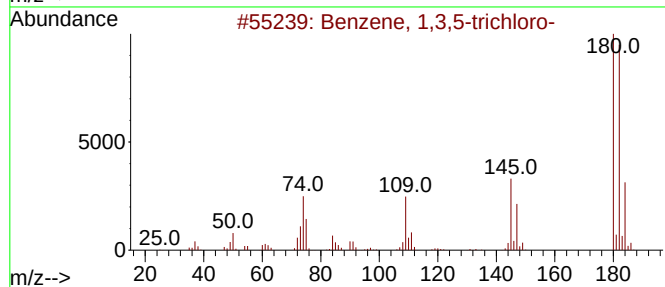
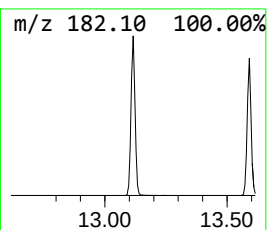
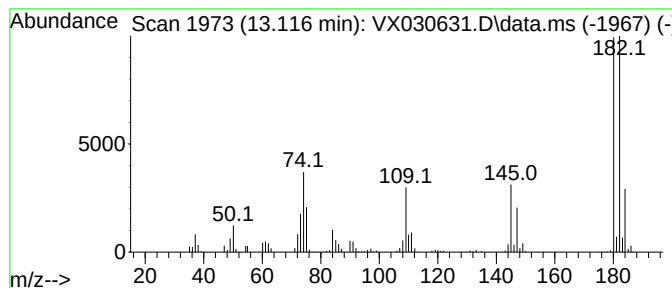
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Benzene, 1,3,5-trichloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.116	49.55 ug/L	850645	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	97
2			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	96
3			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	96
4			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	96
5			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

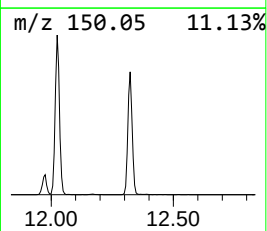
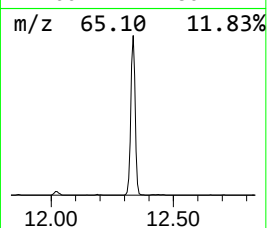
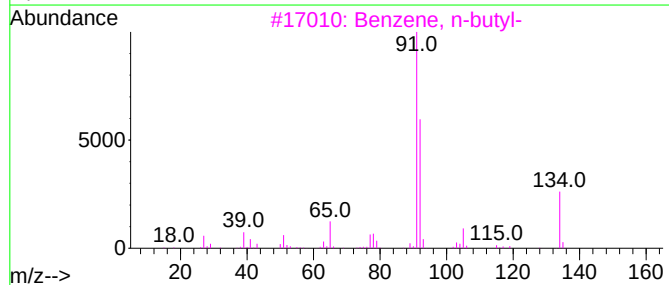
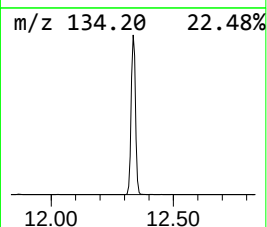
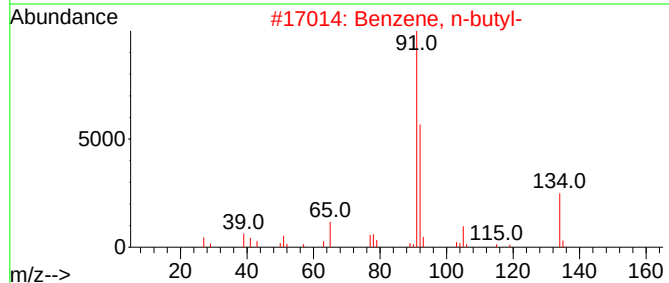
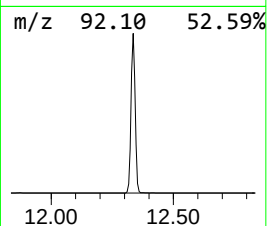
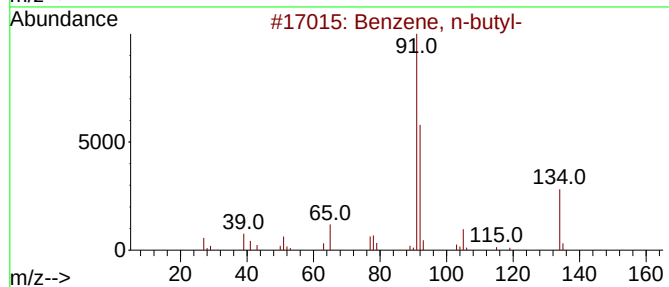
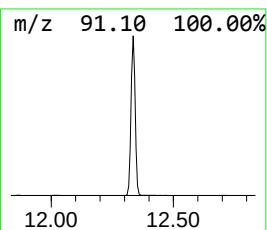
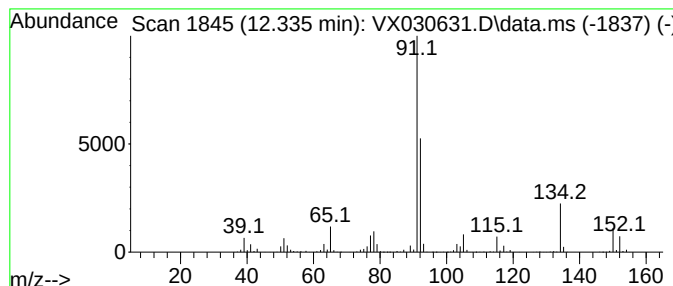
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 9 Benzene, n-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.335	105.87 ug/L	1817640	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, n-butyl-	134	C10H14	000104-51-8	94
2			Benzene, n-butyl-	134	C10H14	000104-51-8	94
3			Benzene, n-butyl-	134	C10H14	000104-51-8	94
4			Benzene, n-butyl-	134	C10H14	000104-51-8	81
5			Benzene, n-butyl-	134	C10H14	000104-51-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030631.D
Acq On : 15 Aug 2022 16:34
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.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, methoxy-	1.557	10.8	ug/L	152973	1	6.769	709499	50.0
Methylal	2.398	71.0	ug/L	1008140	1	6.769	709499	50.0
Ethyl bromide	2.471	13.2	ug/L	187808	1	6.769	709499	50.0
(DEL) Alkane: S...	11.482	27.8	ug/L	476832	3	12.024	858409	50.0
unknown-01	11.652	2.6	ug/L	44368	3	12.024	858409	50.0
Benzene, 1,3,5-...	13.116	49.5	ug/L	850645	3	12.024	858409	50.0
Benzene, n-butyl-	12.335	105.9	ug/L	1817640	3	12.024	858409	50.0