

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
 Data File : VX030629.D
 Acq On : 15 Aug 2022 15:48
 Operator : JC/MD
 Sample : N4181-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 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: VX030629.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	rVB2	5243	5230	0.27%	0.018%
2	1.368	42	46	57	rVB2	423917	507230	25.75%	1.776%
3	1.557	73	77	83	rBV	141711	154616	7.85%	0.541%
4	1.642	87	91	93	rVV	79682	98940	5.02%	0.346%
5	1.666	93	95	102	rVB	109725	118603	6.02%	0.415%
6	1.880	125	130	142	rVB	447949	630827	32.03%	2.208%
7	2.136	168	172	176	rBV4	1559	2871	0.15%	0.010%
8	2.313	193	201	209	rBV3	536847	982676	49.89%	3.440%
9	2.398	209	215	222	rVV	615609	991922	50.36%	3.473%
10	2.471	222	227	240	rVB	111190	192611	9.78%	0.674%
11	2.715	262	267	275	rVV	5027	9155	0.46%	0.032%
12	2.788	275	279	284	rVB4	2206	3879	0.20%	0.014%
13	2.947	299	305	311	rVV4	2551	6143	0.31%	0.022%
14	3.124	321	334	349	rBV	511799	1190509	60.45%	4.168%
15	3.398	377	379	381	rVV	480	506	0.03%	0.002%
16	3.447	381	387	393	rVV4	2718	5532	0.28%	0.019%
17	4.489	545	558	571	rBV3	219018	681242	34.59%	2.385%
18	4.715	592	595	599	rVB4	534	625	0.03%	0.002%
19	4.843	615	616	619	rBV	508	480	0.02%	0.002%
20	5.062	640	652	670	rBV	155502	470207	23.87%	1.646%
21	5.221	676	678	681	rBV2	724	1085	0.06%	0.004%
22	5.385	702	705	706	rVV2	892	671	0.03%	0.002%
23	5.526	725	728	729	rBV2	850	788	0.04%	0.003%
24	5.977	789	802	809	rBV2	391978	1180605	59.94%	4.133%
25	6.251	841	847	849	rBV3	1357	2429	0.12%	0.009%
26	6.367	864	866	870	rVB2	364	513	0.03%	0.002%
27	6.458	877	881	882	rBV2	620	791	0.04%	0.003%
28	6.562	894	898	901	rVB2	409	500	0.03%	0.002%
29	6.708	919	922	923	rBV	482	516	0.03%	0.002%
30	6.769	923	932	947	rVV	273627	653398	33.18%	2.287%
31	7.013	969	972	975	rBV3	626	999	0.05%	0.003%
32	7.129	981	991	1004	rBV	433686	929091	47.17%	3.253%
33	7.312	1012	1021	1026	rBV	234918	509424	25.87%	1.783%
34	7.385	1027	1033	1039	rVV	733975	1496970	76.01%	5.241%
35	7.659	1076	1078	1083	rVB4	659	596	0.03%	0.002%
36	7.946	1119	1125	1126	rBV2	1145	1466	0.07%	0.005%

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Integrator: RTE

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

37	8.153	1155	1159	1160	rBV2	1298	1111	0.06%	0.004%
38	8.330	1182	1188	1199	rBV	156031	262122	13.31%	0.918%
39	8.482	1211	1213	1216	rBV3	662	902	0.05%	0.003%
40	8.580	1222	1229	1235	rBV	783624	1223683	62.13%	4.284%
41	8.653	1235	1241	1249	rVB	600447	924978	46.97%	3.238%
42	8.952	1285	1290	1299	rBV	114937	175744	8.92%	0.615%
43	9.153	1317	1323	1336	rVB	257838	385086	19.55%	1.348%
44	9.275	1336	1343	1356	rBV	476775	678176	34.43%	2.374%
45	9.391	1356	1362	1366	rBV	437093	598072	30.37%	2.094%
46	9.433	1366	1369	1378	rVV	505505	707561	35.93%	2.477%
47	9.525	1379	1384	1392	rVV	197054	286758	14.56%	1.004%
48	9.610	1393	1398	1408	rVB	499298	721523	36.63%	2.526%
49	9.903	1443	1446	1449	rVB2	991	918	0.05%	0.003%
50	9.982	1454	1459	1461	rBV	1091	1365	0.07%	0.005%
51	10.013	1461	1464	1465	rBV2	572	524	0.03%	0.002%
52	10.055	1466	1471	1483	rVV	581181	779174	39.56%	2.728%
53	10.195	1488	1494	1505	rVV	1358835	1749740	88.84%	6.126%
54	10.305	1509	1512	1518	rVB3	7685	10481	0.53%	0.037%
55	10.647	1562	1568	1581	rVB	562651	721996	36.66%	2.528%
56	10.799	1589	1593	1599	rVB4	1369	2185	0.11%	0.008%
57	10.866	1599	1604	1606	rBV	673	847	0.04%	0.003%
58	10.915	1610	1612	1614	rBV	478	603	0.03%	0.002%
59	10.964	1615	1620	1634	rVB	1619097	1969497	100.00%	6.895%
60	11.079	1634	1639	1643	rBV3	1082	2229	0.11%	0.008%
61	11.195	1652	1658	1669	rBV	411743	516796	26.24%	1.809%
62	11.329	1678	1680	1683	rVB3	727	709	0.04%	0.002%
63	11.372	1683	1687	1694	rVB4	2028	3630	0.18%	0.013%
64	11.482	1700	1705	1713	rVB	410302	474130	24.07%	1.660%
65	11.652	1728	1733	1741	rBV	30518	44489	2.26%	0.156%
66	11.866	1765	1768	1771	rVB3	1667	1837	0.09%	0.006%
67	11.927	1774	1778	1780	rVV2	6154	8009	0.41%	0.028%
68	11.970	1780	1785	1790	rVV	874623	1055703	53.60%	3.696%
69	12.024	1790	1794	1806	rVB	630736	776717	39.44%	2.719%
70	12.165	1813	1817	1819	rBV3	8384	10660	0.54%	0.037%
71	12.189	1819	1821	1826	rVB	20194	23492	1.19%	0.082%
72	12.329	1837	1844	1851	rBV2	1230420	1895612	96.25%	6.636%
73	12.421	1856	1859	1863	rVV5	5290	6938	0.35%	0.024%
74	12.555	1877	1881	1882	rBV3	658	583	0.03%	0.002%
75	12.652	1894	1897	1898	rVV	757	802	0.04%	0.003%
76	12.671	1898	1900	1903	rVV3	1691	1828	0.09%	0.006%

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77	12.719	1905	1908	1912	rVB2	2716	3187	0.16%	0.011%
78	12.768	1912	1916	1920	rVB3	559	965	0.05%	0.003%
79	12.805	1920	1922	1928	rBV3	766	1337	0.07%	0.005%
80	12.933	1940	1943	1944	rBV	413	478	0.02%	0.002%
81	12.951	1944	1946	1949	rVB3	765	650	0.03%	0.002%
82	13.116	1967	1973	1984	rVV	637064	790844	40.15%	2.769%
83	13.201	1984	1987	1991	rBV4	1490	2155	0.11%	0.008%
84	13.359	2008	2013	2020	rBV2	89536	114389	5.81%	0.400%
85	13.433	2021	2025	2030	rVB2	16431	22316	1.13%	0.078%
86	13.591	2045	2051	2056	rBV	577763	723014	36.71%	2.531%
87	13.646	2056	2060	2065	rVB2	24247	30510	1.55%	0.107%
88	13.811	2086	2087	2089	rBV	758	548	0.03%	0.002%
89	13.963	2109	2112	2116	rBV5	3244	4001	0.20%	0.014%
90	14.097	2131	2134	2136	rBV2	637	513	0.03%	0.002%
91	14.134	2136	2140	2145	rVB5	1142	2042	0.10%	0.007%
92	14.286	2162	2165	2166	rBV2	697	787	0.04%	0.003%
93	14.542	2205	2207	2209	rBV3	617	584	0.03%	0.002%
94	14.932	2270	2271	2273	rBV2	805	504	0.03%	0.002%
95	15.268	2324	2326	2329	rBV4	715	613	0.03%	0.002%
96	15.396	2342	2347	2349	rBV3	929	1467	0.07%	0.005%
97	15.444	2354	2355	2357	rBV	776	569	0.03%	0.002%
98	16.030	2449	2451	2454	rVB3	806	600	0.03%	0.002%
99	16.079	2457	2459	2461	rBV2	812	590	0.03%	0.002%
100	16.774	2571	2573	2575	rBV2	691	650	0.03%	0.002%

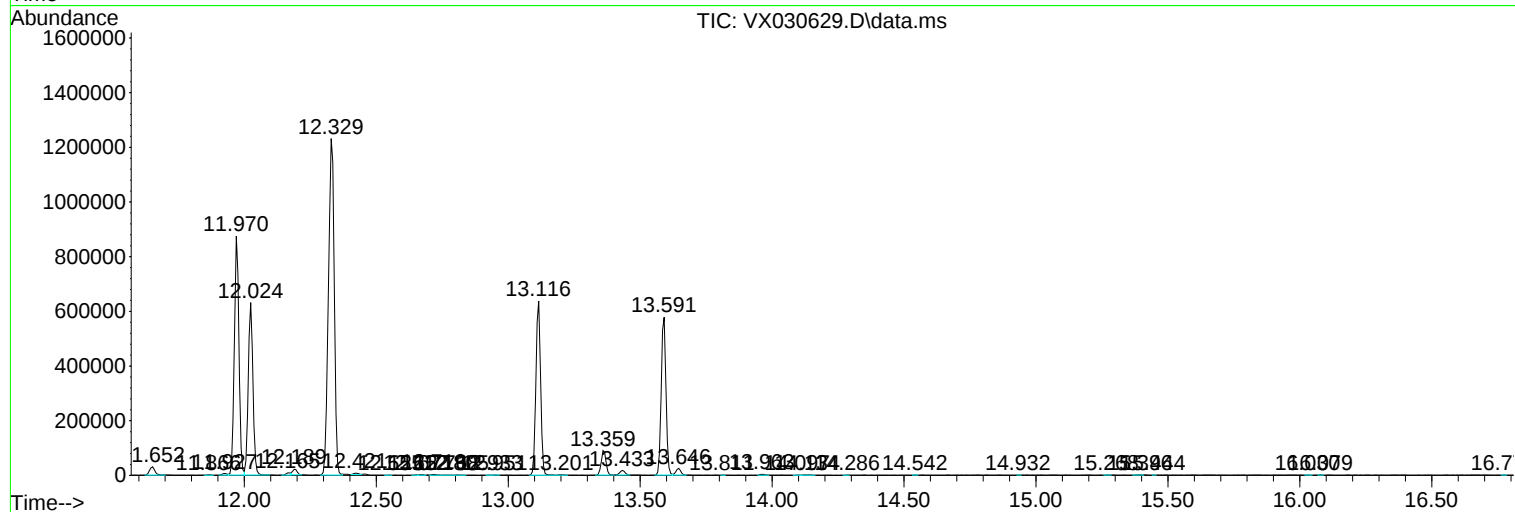
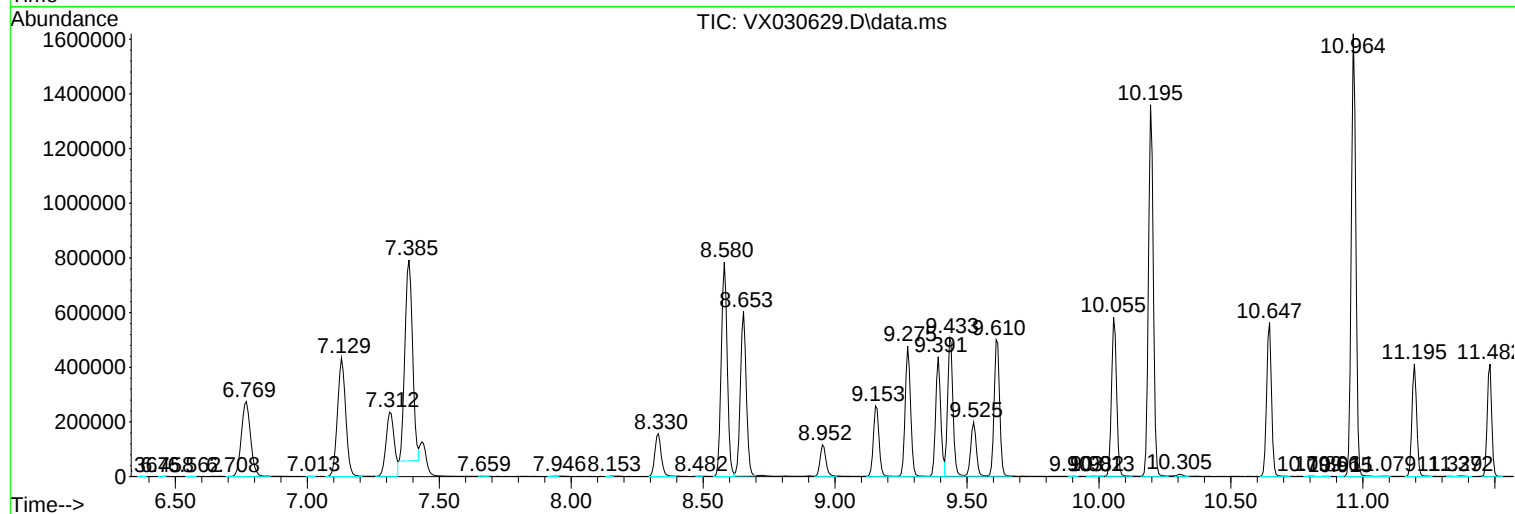
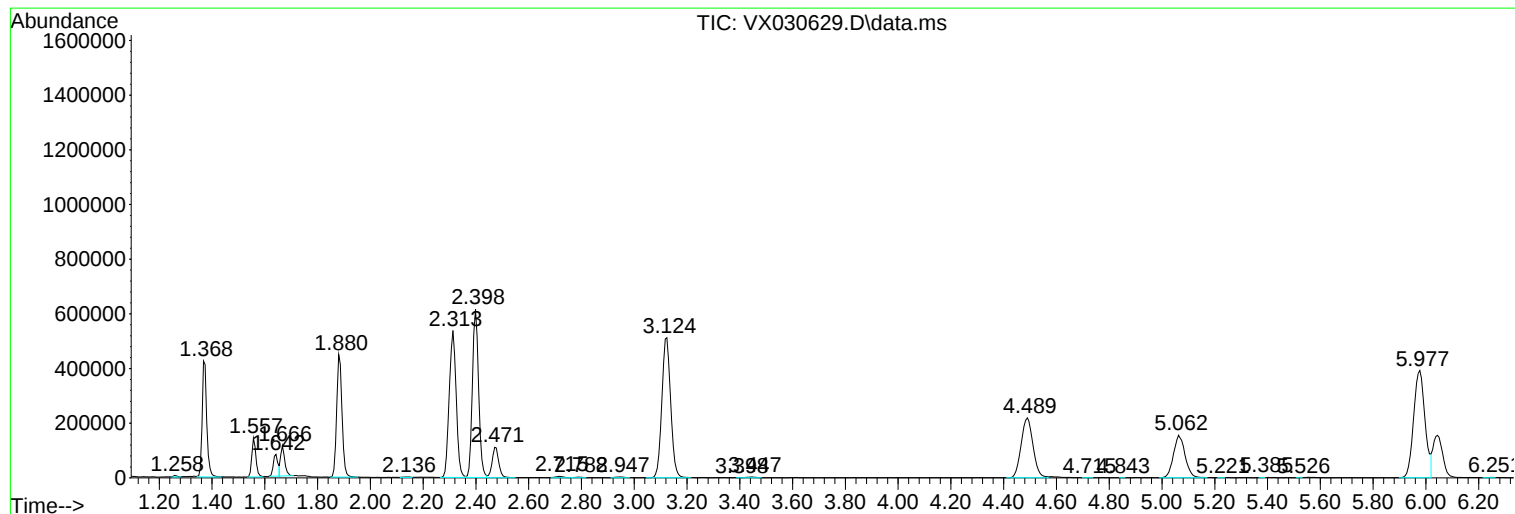
Sum of corrected areas: 28564169

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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



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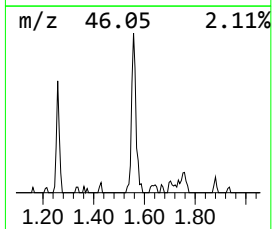
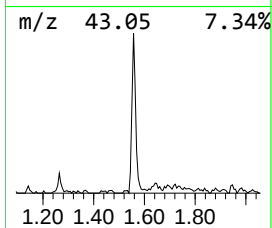
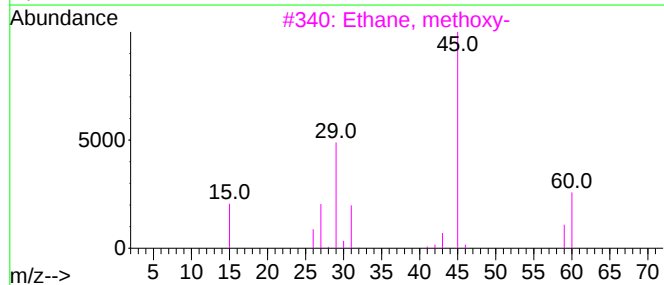
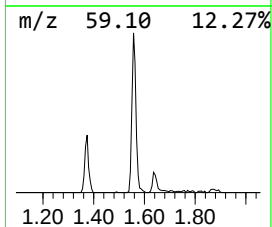
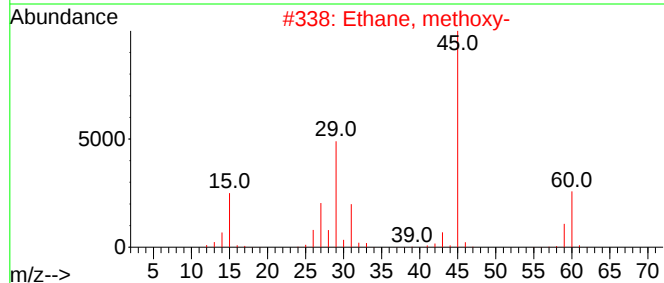
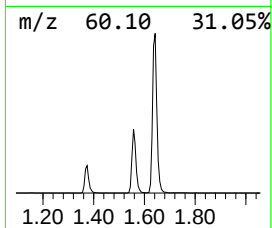
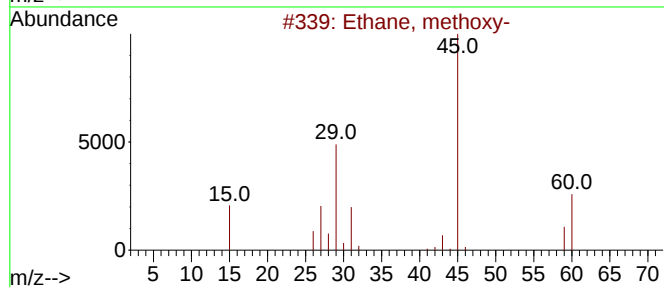
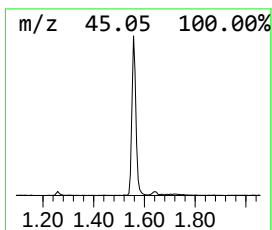
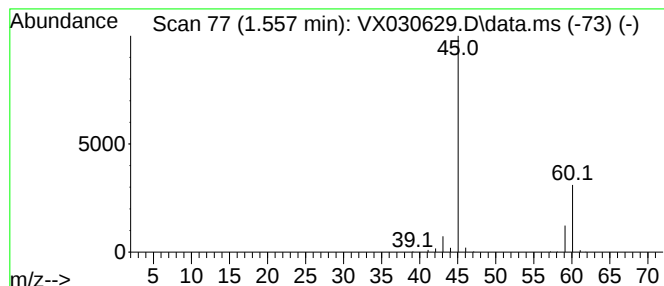
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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	11.83 ug/L	154616	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			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9



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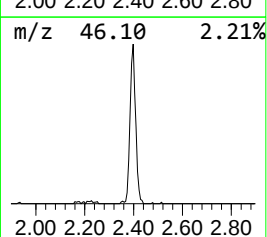
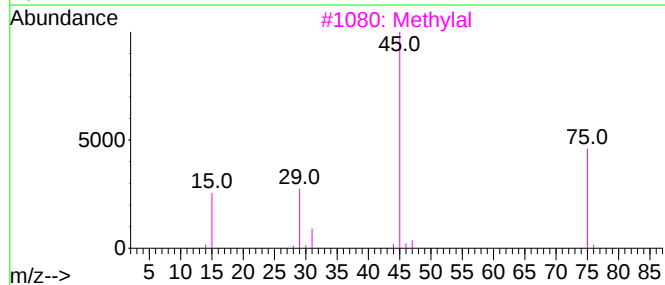
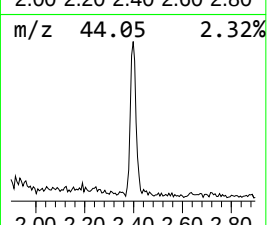
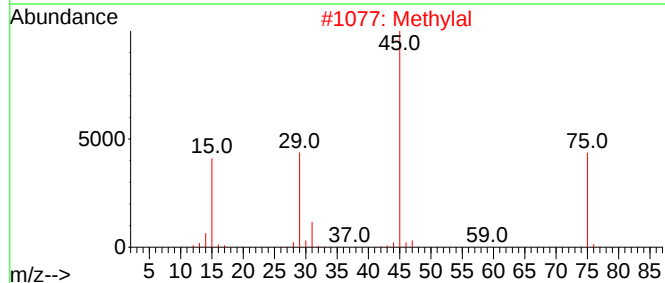
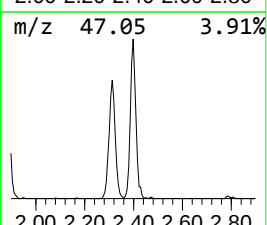
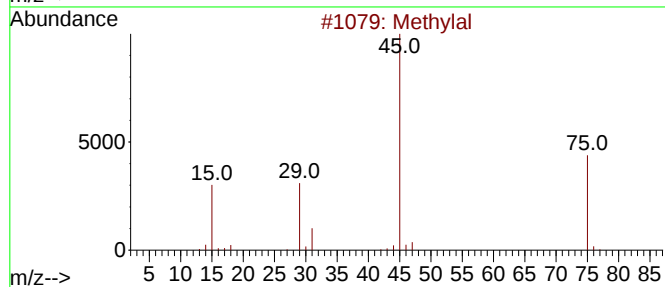
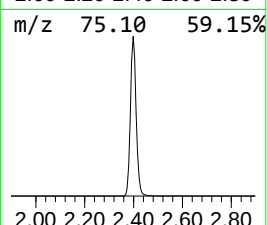
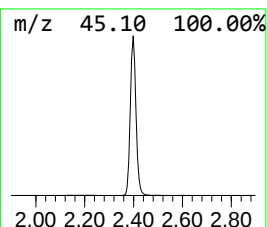
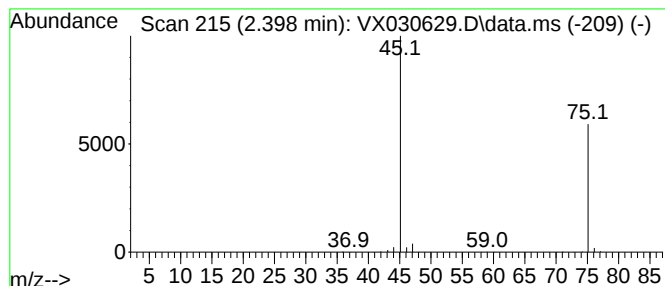
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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	75.90 ug/L	991922	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylal			76	C3H8O2	000109-87-5	83
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	7



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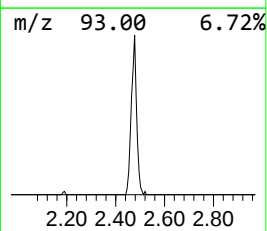
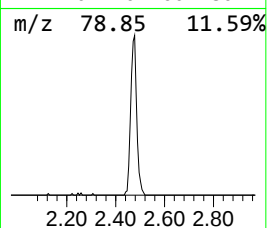
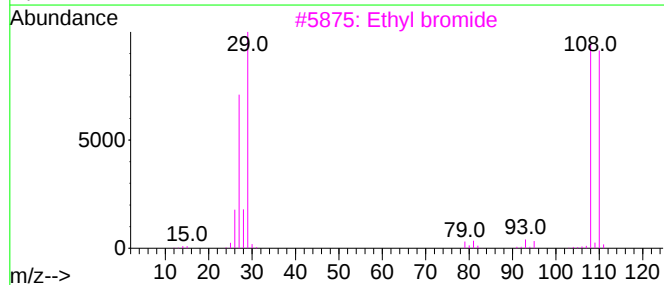
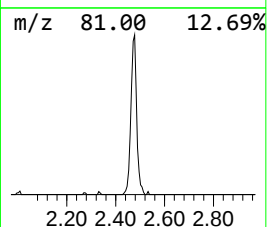
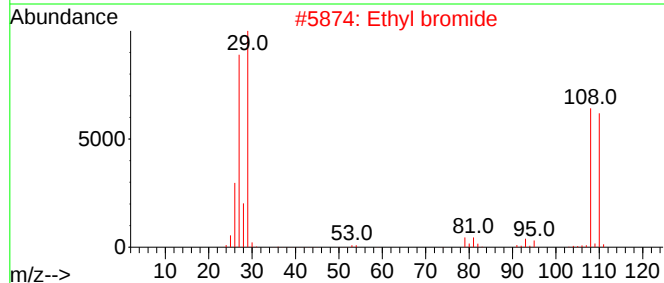
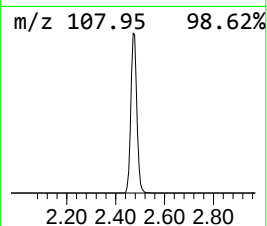
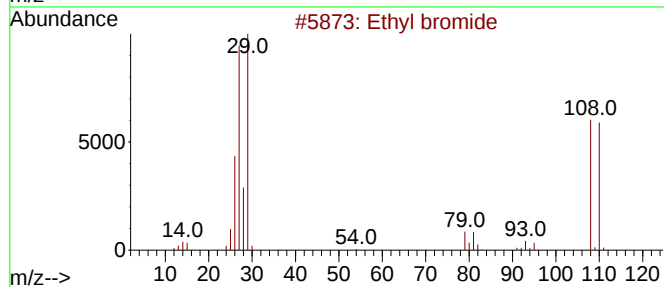
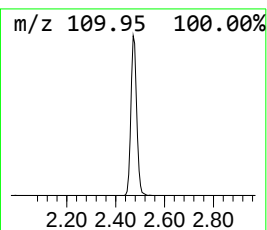
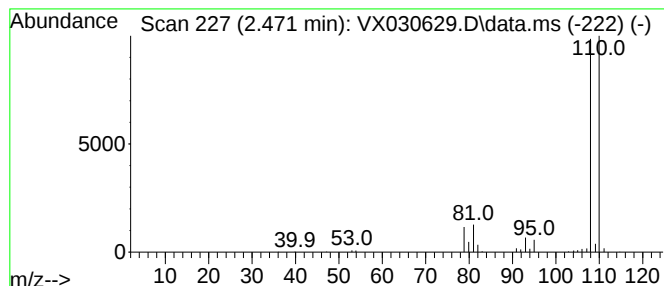
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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	14.74 ug/L	192611	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 : VX030629.D
Acq On : 15 Aug 2022 15:48
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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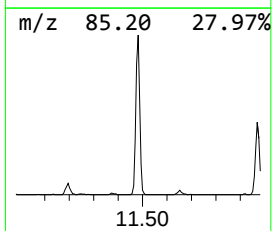
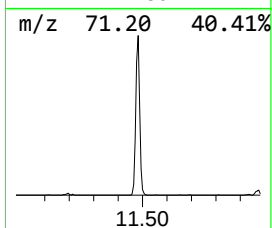
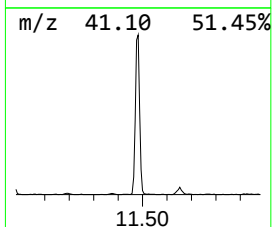
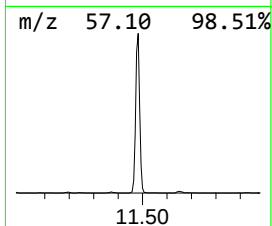
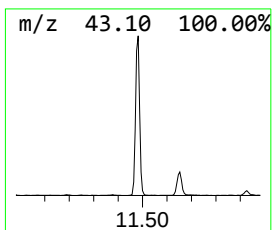
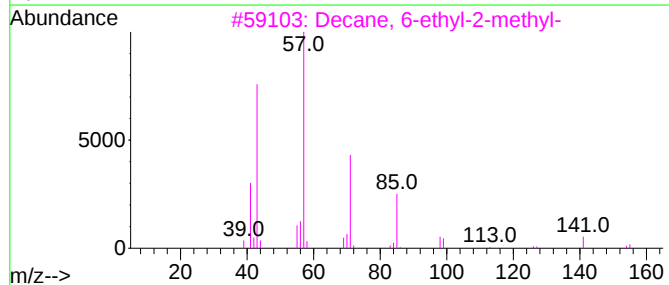
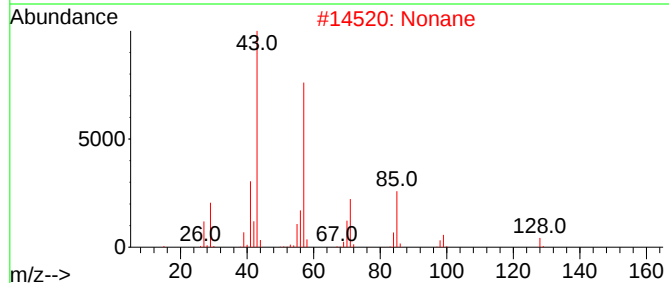
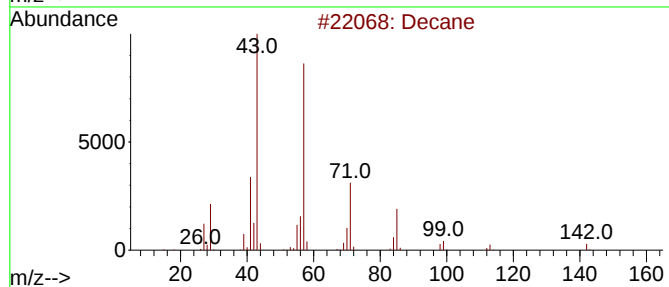
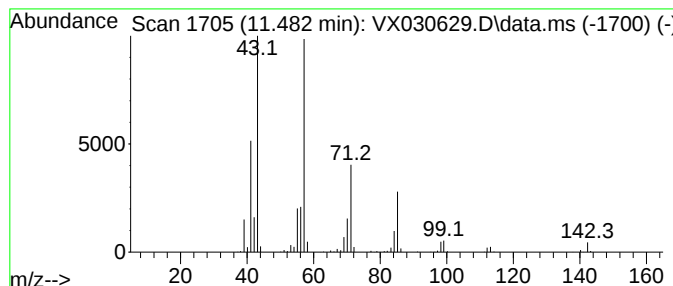
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Quant Title : VOC Analysis

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	30.52 ug/L	474130	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	87
2			Nonane	128	C9H20	000111-84-2	72
3			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	64
4			Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64
5			Nonane	128	C9H20	000111-84-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030629.D
Acq On : 15 Aug 2022 15:48
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

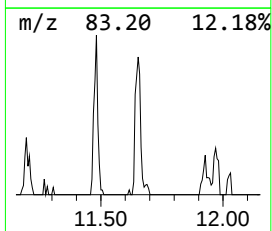
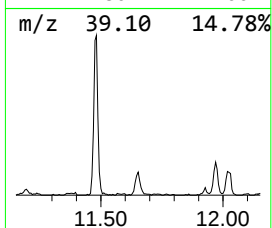
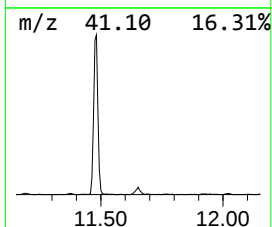
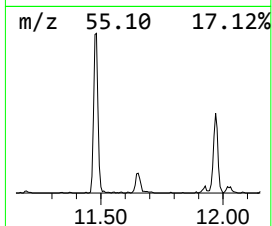
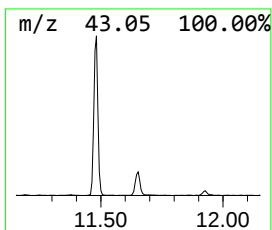
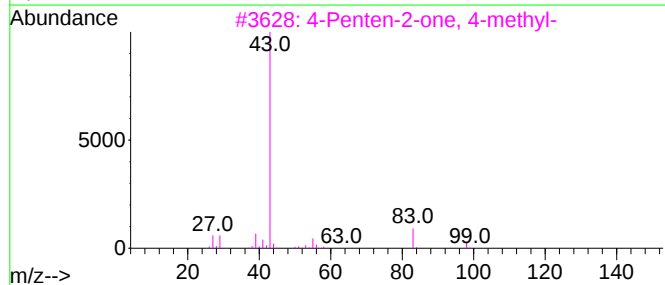
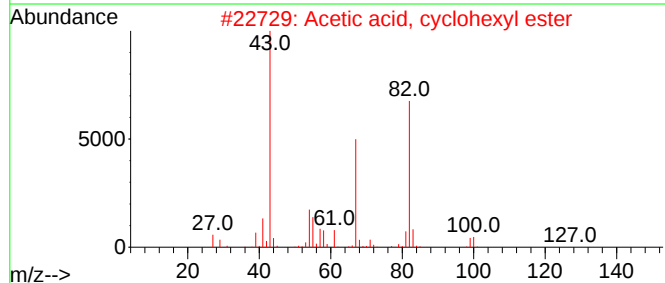
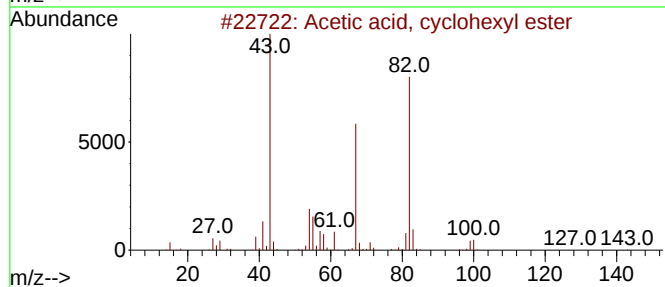
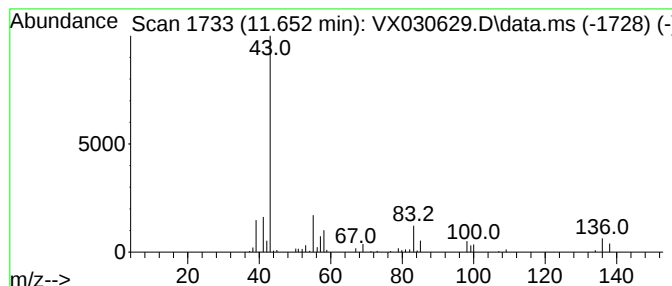
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Quant Title : VOC Analysis

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.
11.653	2.86 ug/L	44489	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, cyclohexyl ester	142	C8H14O2	000622-45-7	33
2			Acetic acid, cyclohexyl ester	142	C8H14O2	000622-45-7	33
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	32
4			5-Hexen-2-one	98	C6H10O	000109-49-9	30
5			5-Hexen-2-one	98	C6H10O	000109-49-9	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030629.D
Acq On : 15 Aug 2022 15:48
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

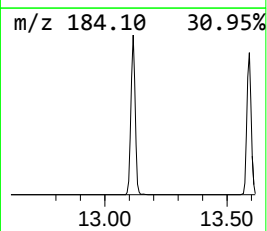
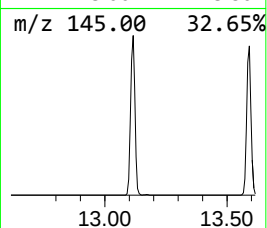
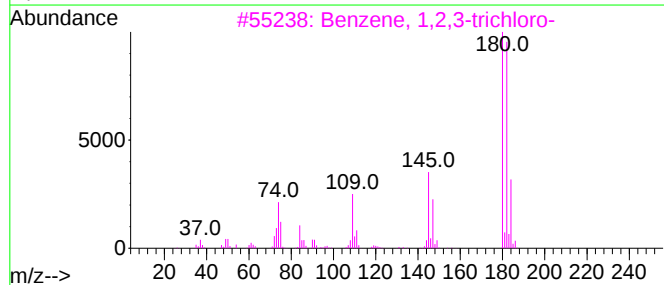
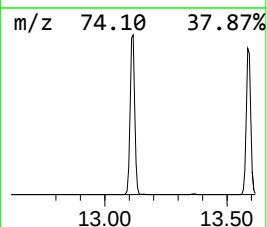
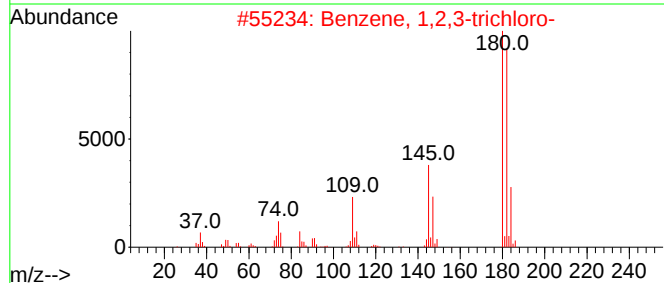
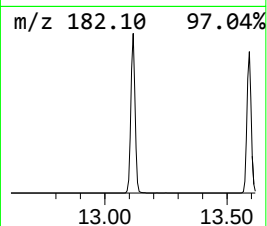
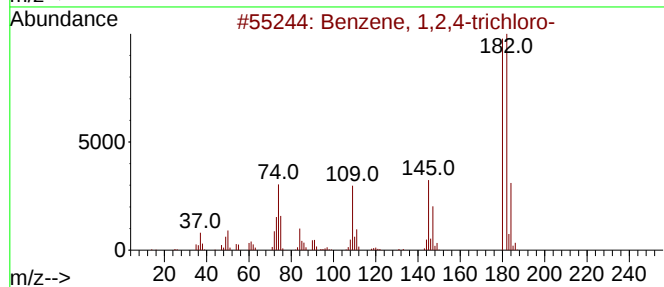
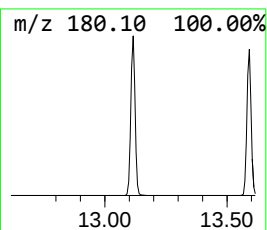
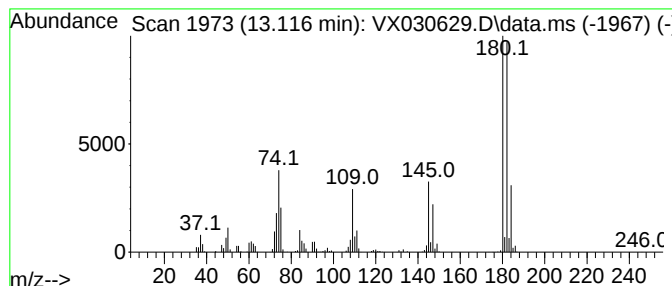
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Quant Title : VOC Analysis

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	50.91 ug/L	790844	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	99
2			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
3			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
4			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	97
5			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030629.D
Acq On : 15 Aug 2022 15:48
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
X3C26

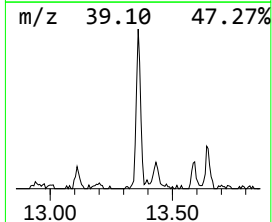
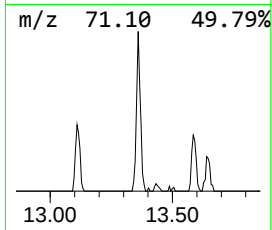
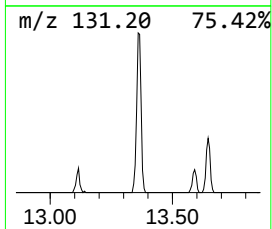
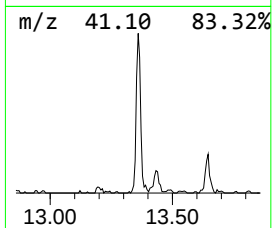
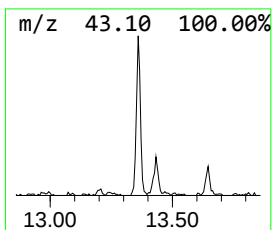
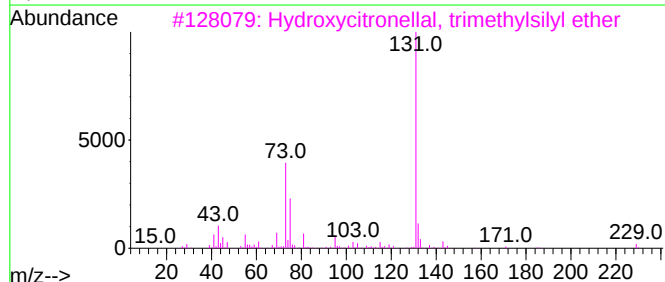
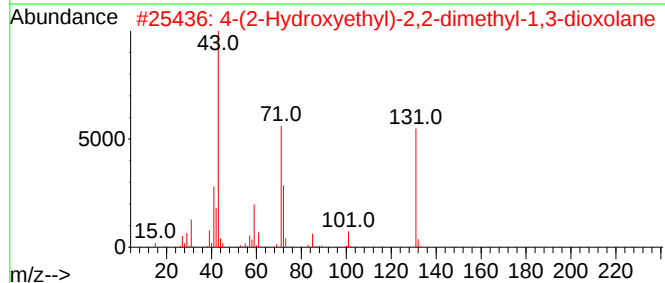
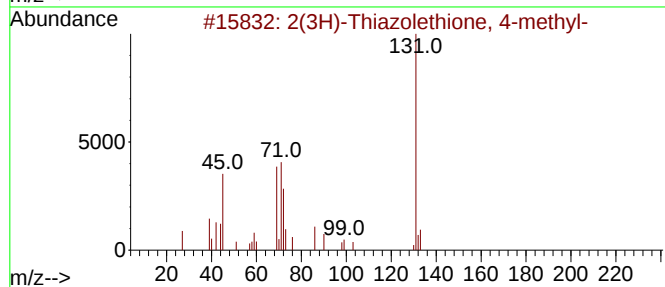
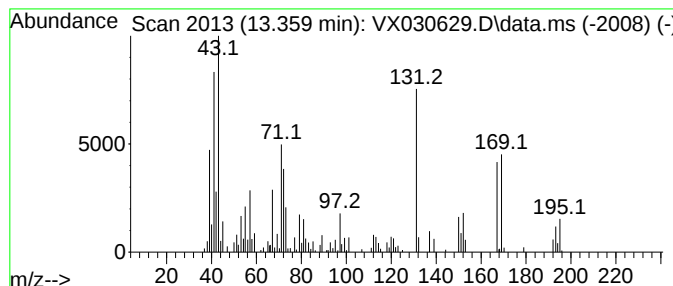
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Quant Title : VOC Analysis

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

Peak Number 8 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.360	7.36 ug/L	114389	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Thiazolethione, 4-methyl-	131	C4H5NS2	005685-06-3	32		
2	4-(2-Hydroxyethyl)-2,2-dimethyl-...	146	C7H14O3	005754-34-7	23		
3	Hydroxycitronellal, trimethylsilyl...	244	C13H28O2Si	1000463-76-6	22		
4	4-Propoxy-2-butanone	130	C7H14O2	089975-71-3	22		
5	1,5-Hexadiene-3,4-diol, 3,4-dime...	142	C8H14O2	002781-29-5	22		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081522\
Data File : VX030629.D
Acq On : 15 Aug 2022 15:48
Operator : JC/MD
Sample : N4181-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 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	11.8	ug/L	154616	1	6.769	653398	50.0
Methylal	2.398	75.9	ug/L	991922	1	6.769	653398	50.0
Ethyl bromide	2.471	14.7	ug/L	192611	1	6.769	653398	50.0
(DEL) Alkane: S...	11.482	30.5	ug/L	474130	3	12.024	776717	50.0
unknown-01	11.653	2.9	ug/L	44489	3	12.024	776717	50.0
Benzene, 1,3,5-...	13.116	50.9	ug/L	790844	3	12.024	776717	50.0
unknown-02	13.360	7.4	ug/L	114389	3	12.024	776717	50.0