

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
 Data File : VX025919.D
 Acq On : 20 Dec 2021 17:08
 Operator : JC/MD
 Sample : M5150-28
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBBY4

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\SFAMXML122021WMA.M
 Title : VOC Analysis

Signal : TIC: VX025919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	10	13	22	rVB	79337	73732	4.74%	0.487%
2	1.258	25	28	31	rVV	27785	26428	1.70%	0.175%
3	1.294	31	34	43	rVB	62417	66487	4.27%	0.439%
4	1.373	43	47	55	rBV2	236754	252284	16.22%	1.666%
5	1.599	80	84	86	rBV	52740	54302	3.49%	0.359%
6	1.629	86	89	91	rBV	172652	180341	11.59%	1.191%
7	1.879	124	130	142	rVB	195103	275061	17.68%	1.817%
8	2.312	193	201	209	rBV4	353879	748105	48.09%	4.942%
9	2.392	209	214	227	rVB	996713	1555711	100.00%	10.276%
10	2.702	262	265	270	rVB3	1294	1953	0.13%	0.013%
11	2.788	272	279	294	rVV	135478	254083	16.33%	1.678%
12	2.946	302	305	311	rVB2	585	867	0.06%	0.006%
13	3.087	321	328	339	rBV	67616	134414	8.64%	0.888%
14	3.611	404	414	425	rVV	141145	337573	21.70%	2.230%
15	3.708	428	430	434	rVB2	310	353	0.02%	0.002%
16	4.214	508	513	514	rVV2	209	318	0.02%	0.002%
17	4.294	524	526	528	rBV	265	315	0.02%	0.002%
18	4.483	544	557	572	rVV2	124966	430881	27.70%	2.846%
19	4.635	580	582	584	rVB3	563	387	0.02%	0.003%
20	4.666	584	587	590	rBV2	384	446	0.03%	0.003%
21	4.745	598	600	604	rBV2	255	304	0.02%	0.002%
22	4.897	615	625	639	rBV2	75873	224178	14.41%	1.481%
23	5.086	639	656	673	rVB3	156085	698793	44.92%	4.616%
24	5.379	693	704	716	rBV2	47250	146894	9.44%	0.970%
25	5.671	740	752	768	rBV	129146	382864	24.61%	2.529%
26	5.854	779	782	786	rBV4	393	539	0.03%	0.004%
27	5.970	788	801	807	rBV2	255181	774308	49.77%	5.115%
28	6.263	846	849	853	rVB2	280	321	0.02%	0.002%
29	6.513	883	890	898	rBV4	1229	3163	0.20%	0.021%
30	6.763	920	931	948	rBV	176356	423681	27.23%	2.799%
31	7.013	969	972	973	rBV	335	290	0.02%	0.002%
32	7.122	981	990	1007	rBV	328835	713611	45.87%	4.714%
33	7.311	1012	1021	1032	rVV	152460	345153	22.19%	2.280%
34	7.433	1033	1041	1051	rVB	147392	306496	19.70%	2.025%
35	7.555	1058	1061	1063	rBV2	300	454	0.03%	0.003%
36	7.824	1098	1105	1113	rBV	59327	109945	7.07%	0.726%

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37	7.964	1120	1128	1138	rBV2	9412	17879	1.15%	0.118%
38	8.323	1181	1187	1191	rBV	106959	181456	11.66%	1.199%
39	8.366	1191	1194	1207	rVB	101133	158379	10.18%	1.046%
40	8.494	1209	1215	1222	rBV	20191	32578	2.09%	0.215%
41	8.647	1234	1240	1248	rBV	401633	631931	40.62%	4.174%
42	8.787	1261	1263	1267	rVB3	603	734	0.05%	0.005%
43	8.866	1274	1276	1279	rBV	334	364	0.02%	0.002%
44	8.951	1284	1290	1291	rBV	75724	97427	6.26%	0.644%
45	8.976	1291	1294	1305	rVB	189606	283150	18.20%	1.870%
46	9.153	1317	1323	1331	rBV	145318	212289	13.65%	1.402%
47	9.213	1331	1333	1336	rVV3	834	1022	0.07%	0.007%
48	9.274	1336	1343	1356	rVV	449197	661983	42.55%	4.373%
49	9.384	1356	1361	1375	rVV	241855	364762	23.45%	2.409%
50	9.524	1378	1384	1390	rVV	130941	192270	12.36%	1.270%
51	9.610	1392	1398	1404	rVV	87100	119519	7.68%	0.789%
52	9.841	1432	1436	1438	rBV2	286	297	0.02%	0.002%
53	9.890	1442	1444	1448	rVB2	235	272	0.02%	0.002%
54	10.055	1465	1471	1483	rBV	406732	546534	35.13%	3.610%
55	10.165	1483	1489	1499	rVB	341494	473118	30.41%	3.125%
56	10.305	1507	1512	1517	rBV2	2529	3580	0.23%	0.024%
57	10.512	1541	1546	1547	rVB3	424	605	0.04%	0.004%
58	10.530	1547	1549	1551	rBV2	348	420	0.03%	0.003%
59	10.658	1564	1570	1574	rVB4	2152	4226	0.27%	0.028%
60	10.750	1582	1585	1588	rBV3	217	312	0.02%	0.002%
61	10.799	1588	1593	1603	rVV	129816	177765	11.43%	1.174%
62	10.914	1611	1612	1614	rBV	432	306	0.02%	0.002%
63	10.963	1616	1620	1624	rVV2	2652	3089	0.20%	0.020%
64	11.000	1624	1626	1630	rVB2	342	360	0.02%	0.002%
65	11.122	1642	1646	1650	rVB	2881	3396	0.22%	0.022%
66	11.195	1652	1658	1660	rBV	302780	438126	28.16%	2.894%
67	11.378	1686	1688	1694	rVV3	275	397	0.03%	0.003%
68	11.451	1697	1700	1707	rBV3	2820	4380	0.28%	0.029%
69	11.616	1723	1727	1731	rVB	3035	3461	0.22%	0.023%
70	11.756	1740	1750	1759	rBV	609720	777676	49.99%	5.137%
71	11.872	1766	1769	1771	rVB3	541	530	0.03%	0.004%
72	11.896	1771	1773	1775	rBV2	427	371	0.02%	0.002%
73	11.933	1777	1779	1782	rVB3	1356	1328	0.09%	0.009%
74	11.975	1782	1786	1789	rVB2	2491	2790	0.18%	0.018%
75	12.024	1789	1794	1801	rBV	431466	532947	34.26%	3.520%
76	12.128	1808	1811	1812	rBV2	1078	1301	0.08%	0.009%

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77	12.152	1812	1815	1819	rVB3	1657	2077	0.13%	0.014%
78	12.243	1827	1830	1832	rBV3	397	430	0.03%	0.003%
79	12.268	1832	1834	1836	rVV2	494	400	0.03%	0.003%
80	12.323	1836	1843	1856	rVB	426923	554396	35.64%	3.662%
81	12.457	1864	1865	1868	rVB	430	313	0.02%	0.002%
82	12.487	1868	1870	1873	rBV2	436	439	0.03%	0.003%
83	12.536	1877	1878	1880	rBV	519	365	0.02%	0.002%
84	12.664	1898	1899	1906	rVB3	381	487	0.03%	0.003%
85	12.859	1927	1931	1934	rBV2	312	433	0.03%	0.003%
86	12.945	1939	1945	1955	rBV	88492	111717	7.18%	0.738%
87	13.115	1969	1973	1977	rBV2	1296	1570	0.10%	0.010%
88	13.194	1985	1986	1989	rBV3	302	274	0.02%	0.002%
89	13.591	2048	2051	2055	rVB3	1390	1709	0.11%	0.011%
90	13.786	2079	2083	2087	rVV3	1172	1582	0.10%	0.010%
91	13.829	2089	2090	2094	rBV2	249	315	0.02%	0.002%
92	13.963	2108	2112	2115	rVV3	1140	1311	0.08%	0.009%
93	14.030	2121	2123	2126	rBV2	361	370	0.02%	0.002%
94	14.060	2126	2128	2131	rVV	236	264	0.02%	0.002%
95	14.139	2140	2141	2145	rVB2	436	316	0.02%	0.002%
96	14.627	2219	2221	2225	rBV2	215	308	0.02%	0.002%
97	14.700	2229	2233	2234	rBV2	339	300	0.02%	0.002%
98	14.853	2254	2258	2260	rBV2	350	527	0.03%	0.003%
99	15.383	2343	2345	2346	rBV2	337	264	0.02%	0.002%
100	16.560	2536	2538	2540	rVB2	337	275	0.02%	0.002%

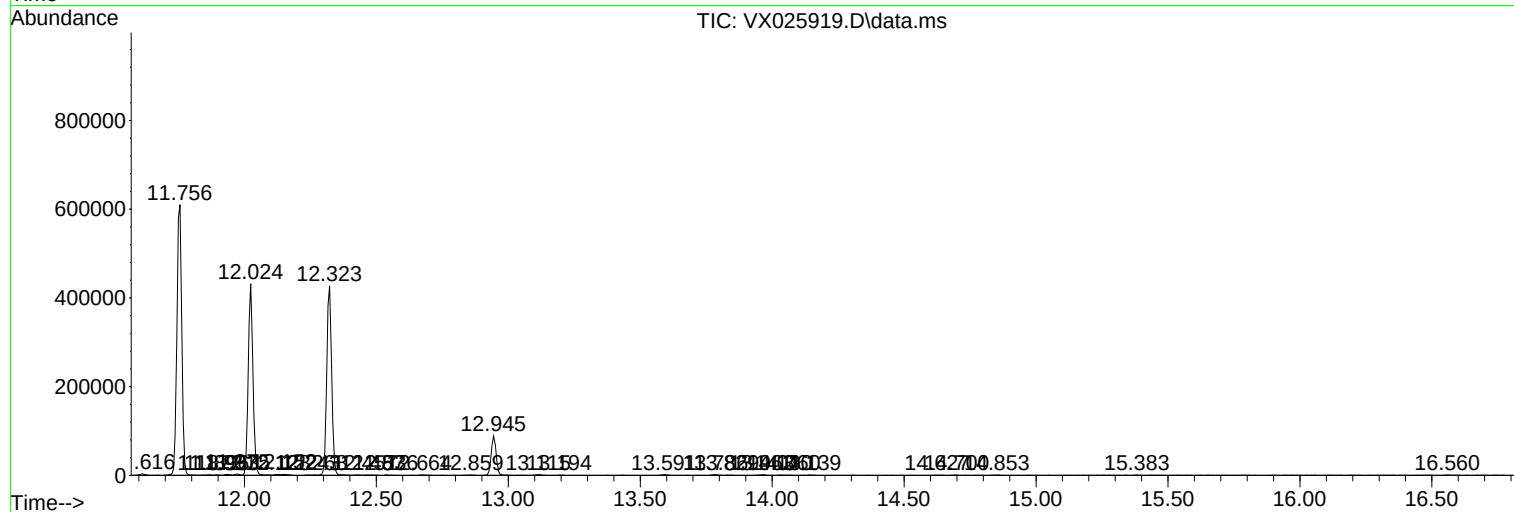
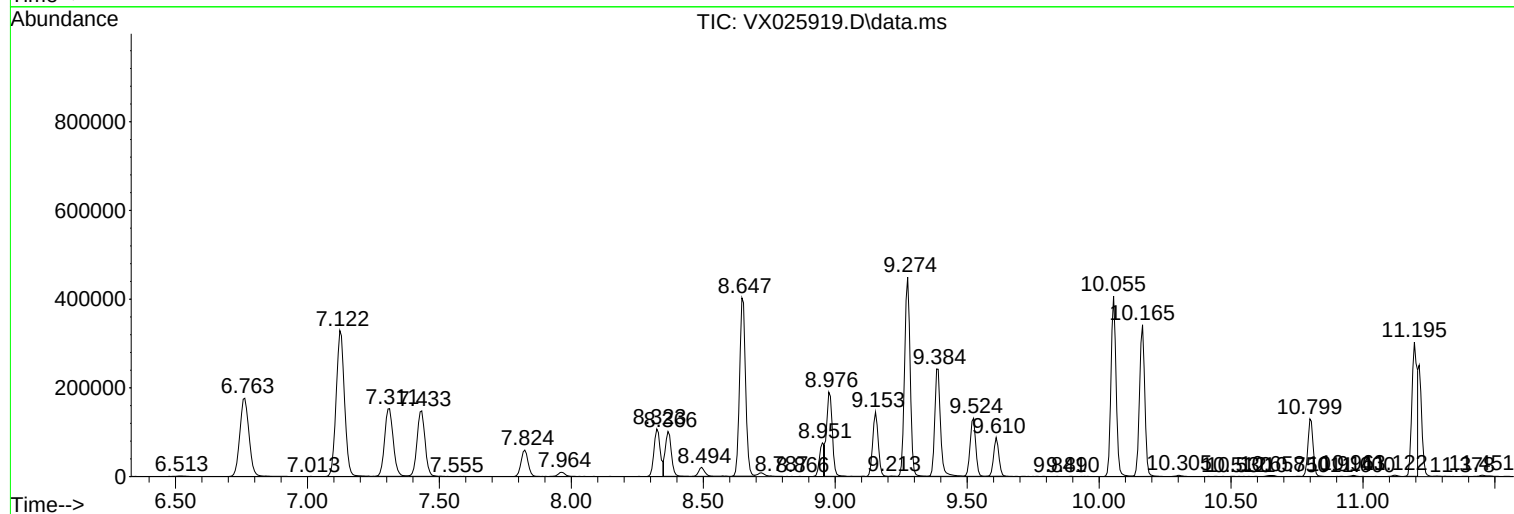
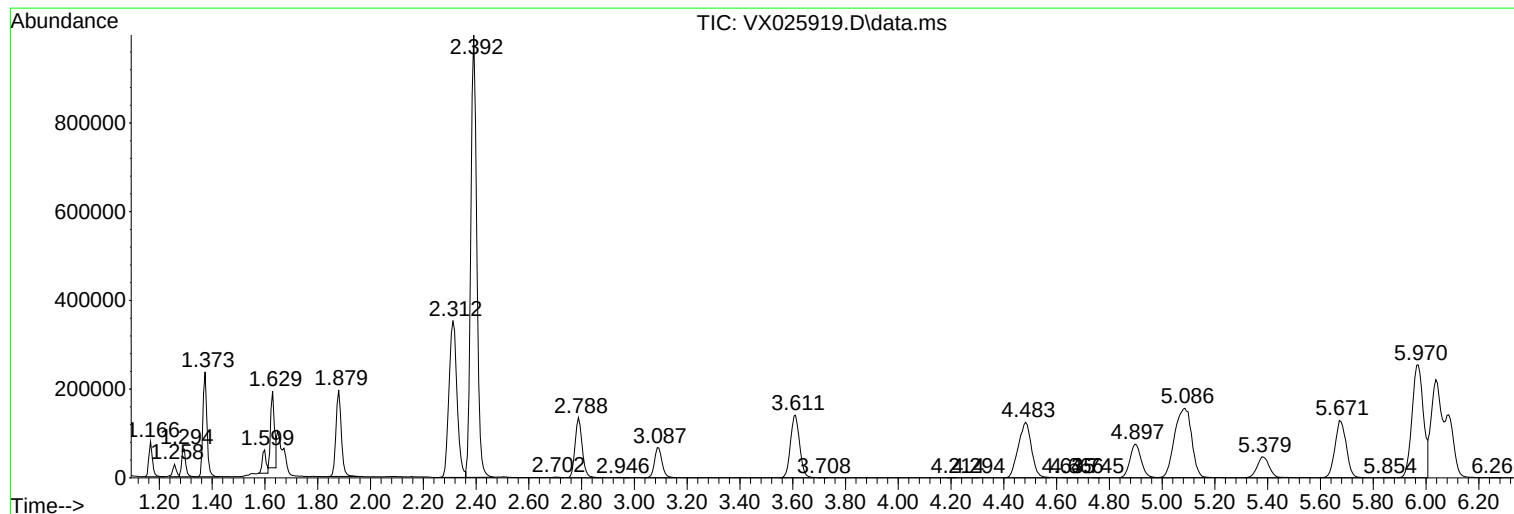
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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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



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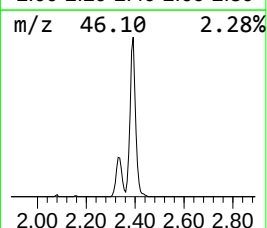
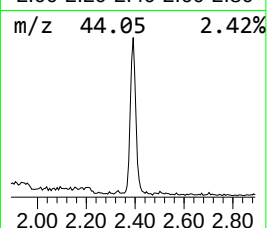
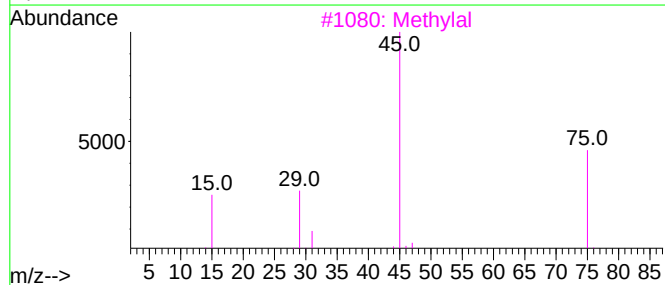
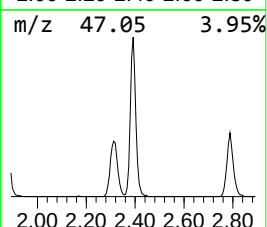
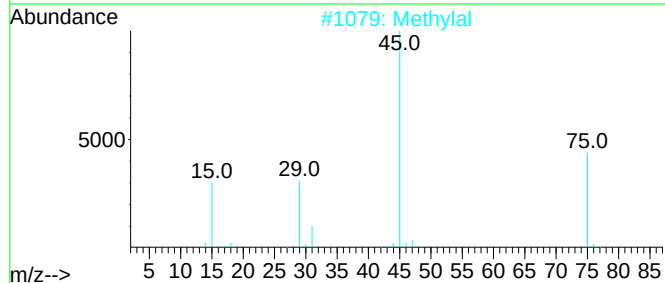
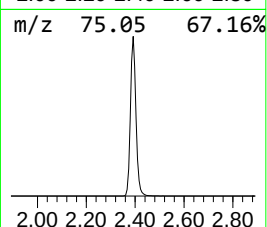
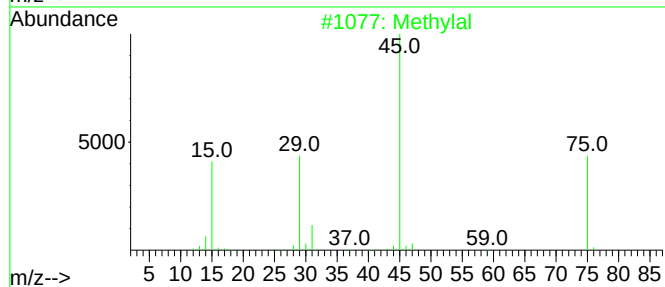
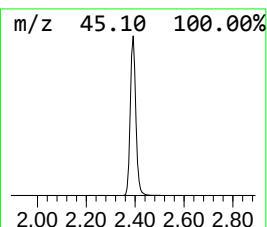
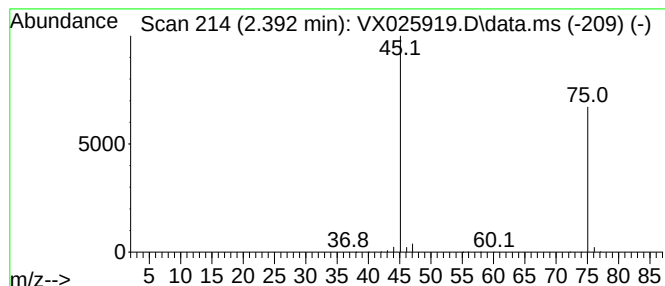
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methylal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.392	183.60 ug/L	1555710	1,4-Difluorobenzene	6.763

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



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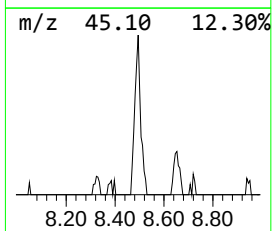
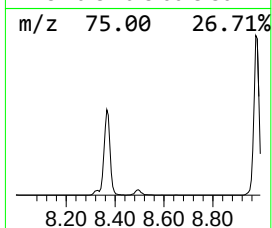
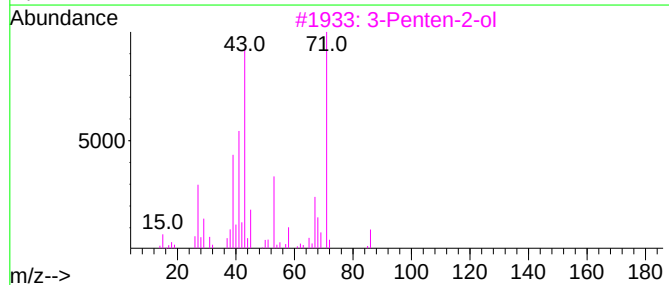
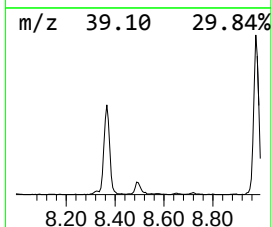
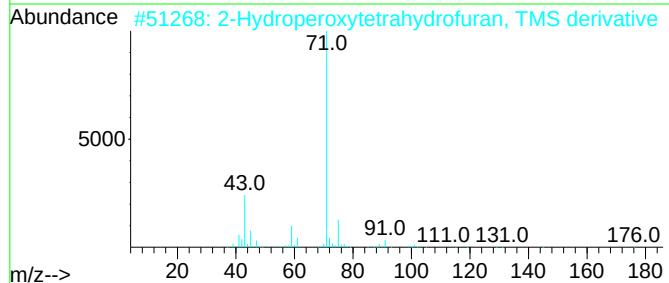
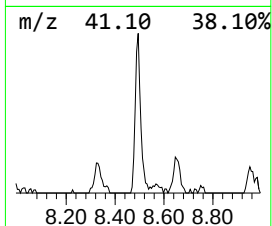
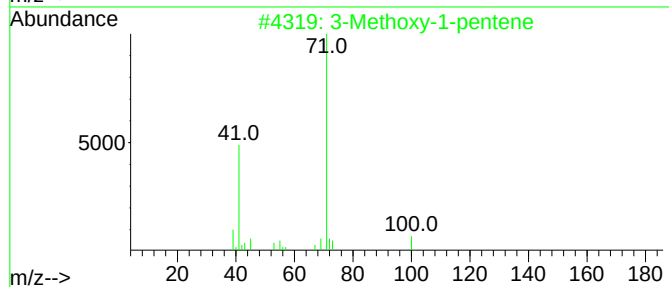
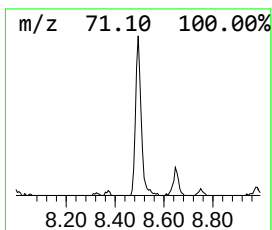
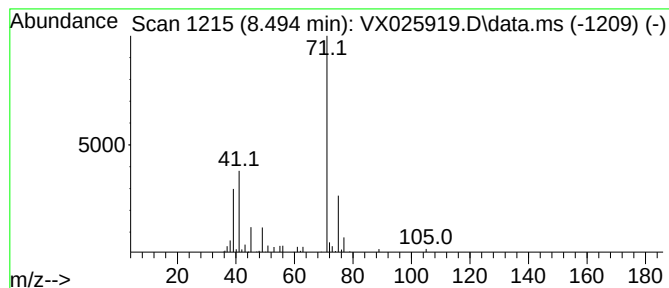
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 3-Methoxy-1-pentene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.494	2.98 ug/L	32578	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methoxy-1-pentene	100	C6H12O	014092-18-3	53
2			2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	39
3			3-Penten-2-ol	86	C5H10O	001569-50-2	36
4			Sulfurous acid, 2-pentyl pentyl ...	222	C10H22O3S	1000309-15-4	36
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	36



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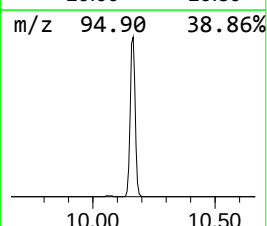
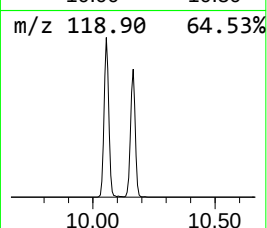
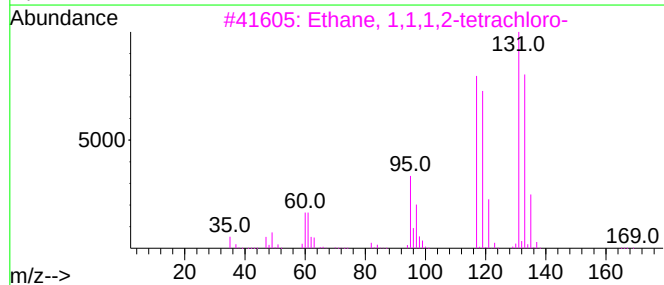
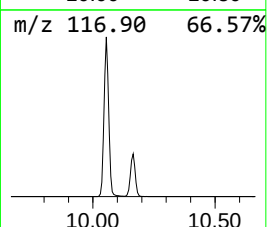
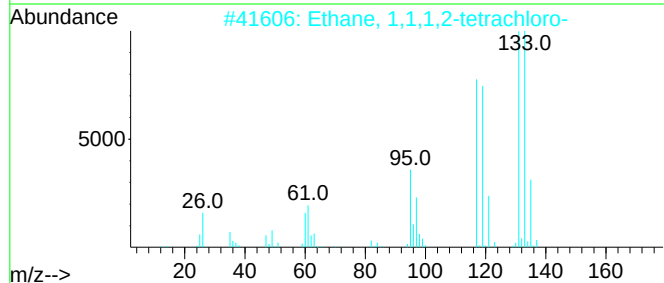
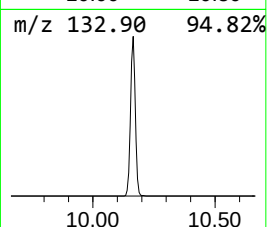
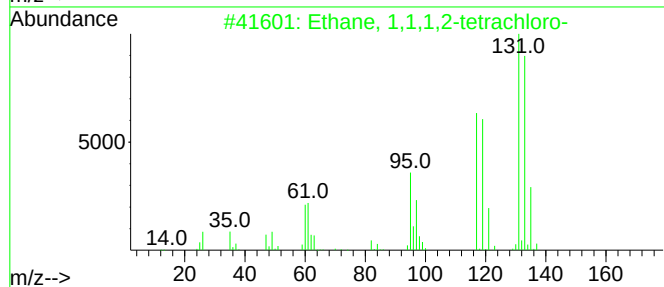
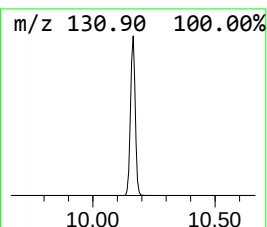
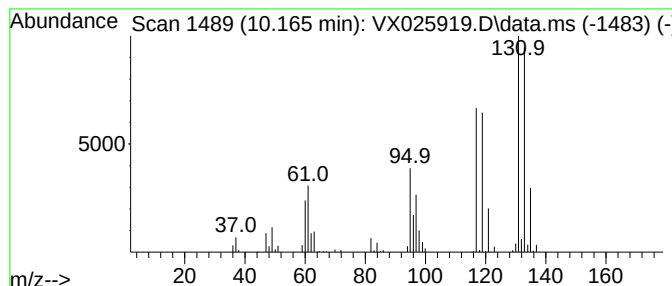
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.165	43.28 ug/L	473118	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	86
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	64
5			Benzonitrile, 4-methoxy-	133	C8H7NO	000874-90-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
Data File : VX025919.D
Acq On : 20 Dec 2021 17:08
Operator : JC/MD
Sample : M5150-28
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GBBY4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122021WMA.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
Methylal	2.392	183.6	ug/L	1555710	1	6.763	423681	50.0
3-Methoxy-1-pen...	8.494	3.0	ug/L	32578	2	10.055	546534	50.0
Ethane, 1,1,1,2...	10.165	43.3	ug/L	473118	2	10.055	546534	50.0