

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111221\
 Data File : VX025144.D
 Acq On : 12 Nov 2021 10:32
 Operator : JC/MD
 Sample : M4615-01 40X
 Misc : 4.34g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0V00

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\SFAMXLM111121WMA.M
 Title : VOC Analysis

Signal : TIC: VX025144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.361	41	45	60	rBV	2360606	2824768	5.87%	4.987%
2	1.666	92	95	102	rVB	61971	76744	0.16%	0.135%
3	2.306	194	200	216	rVB	146144	237731	0.49%	0.420%
4	2.501	230	232	233	rBV	668	546	0.00%	0.001%
5	2.660	256	258	260	rBV2	545	270	0.00%	0.000%
6	2.684	260	262	263	rBV2	383	387	0.00%	0.001%
7	2.782	271	278	286	rVB2	8460	18048	0.04%	0.032%
8	3.007	304	315	329	rBV2	47567	188417	0.39%	0.333%
9	3.245	353	354	356	rBV2	417	347	0.00%	0.001%
10	3.416	377	382	384	rBV3	353	670	0.00%	0.001%
11	3.459	386	389	390	rBV2	387	292	0.00%	0.001%
12	3.513	395	398	400	rBV4	324	495	0.00%	0.001%
13	3.715	426	431	435	rBV4	263	508	0.00%	0.001%
14	3.751	435	437	438	rBV2	517	340	0.00%	0.001%
15	3.782	438	442	444	rBV3	434	554	0.00%	0.001%
16	3.806	444	446	448	rBV2	239	281	0.00%	0.000%
17	4.099	492	494	497	rVB2	499	488	0.00%	0.001%
18	4.123	497	498	500	rBV2	338	262	0.00%	0.000%
19	4.288	524	525	530	rBV4	508	661	0.00%	0.001%
20	4.465	545	554	570	rBV	52996	156919	0.33%	0.277%
21	4.654	582	585	587	rBV2	475	522	0.00%	0.001%
22	5.062	638	652	670	rVV	84533	264549	0.55%	0.467%
23	5.269	684	686	688	rVB3	377	264	0.00%	0.000%
24	5.300	688	691	693	rBV3	287	305	0.00%	0.001%
25	5.385	702	705	706	rBV2	553	582	0.00%	0.001%
26	5.531	727	729	731	rBV2	342	320	0.00%	0.001%
27	5.556	731	733	734	rBV	435	315	0.00%	0.001%
28	5.745	761	764	766	rBV3	227	321	0.00%	0.001%
29	5.818	773	776	777	rBV3	341	314	0.00%	0.001%
30	5.976	789	802	817	rBV2	225305	671675	1.40%	1.186%
31	6.458	879	881	884	rBV4	473	332	0.00%	0.001%
32	6.592	899	903	905	rBV3	219	278	0.00%	0.000%
33	6.629	908	909	912	rVB3	374	284	0.00%	0.001%
34	6.769	921	932	947	rBV	186658	450668	0.94%	0.796%
35	6.995	967	969	971	rBV2	410	469	0.00%	0.001%
36	7.104	974	987	995	rBV	33014	88626	0.18%	0.156%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM11121WMA.M
 Title : VOC Analysis

37	7.318	1012	1022	1030	rBV	133077	304118	0.63%	0.537%
38	7.458	1030	1045	1052	rBV	17204694	48143101	100.00%	84.988%
39	8.330	1181	1188	1197	rBV	110526	181091	0.38%	0.320%
40	8.470	1210	1211	1217	rVB4	935	1067	0.00%	0.002%
41	8.653	1234	1241	1249	rBV	378658	582130	1.21%	1.028%
42	8.720	1249	1252	1261	rVB	6047	10075	0.02%	0.018%
43	8.952	1284	1290	1299	rBV	84020	118210	0.25%	0.209%
44	9.110	1309	1316	1321	rBV	2913	5135	0.01%	0.009%
45	9.384	1356	1361	1374	rBV	259218	365817	0.76%	0.646%
46	9.592	1393	1395	1398	rVB3	408	345	0.00%	0.001%
47	9.622	1398	1400	1403	rBV4	250	327	0.00%	0.001%
48	9.787	1425	1427	1429	rBV3	325	389	0.00%	0.001%
49	9.933	1449	1451	1454	rBV3	264	322	0.00%	0.001%
50	10.055	1465	1471	1485	rVB	403006	539602	1.12%	0.953%
51	10.195	1491	1494	1499	rVB4	804	955	0.00%	0.002%
52	10.305	1508	1512	1518	rBV3	1106	1542	0.00%	0.003%
53	10.506	1541	1545	1547	rBV5	428	588	0.00%	0.001%
54	10.610	1558	1562	1565	rBV3	430	588	0.00%	0.001%
55	10.652	1567	1569	1573	rVB4	818	952	0.00%	0.002%
56	10.909	1609	1611	1613	rBV2	336	393	0.00%	0.001%
57	10.945	1615	1617	1625	rVB8	632	1212	0.00%	0.002%
58	11.055	1633	1635	1639	rBV3	402	510	0.00%	0.001%
59	11.091	1639	1641	1643	rVV2	590	487	0.00%	0.001%
60	11.122	1643	1646	1650	rVB3	2557	3094	0.01%	0.005%
61	11.195	1652	1658	1666	rBV	261399	334251	0.69%	0.590%
62	11.384	1687	1689	1690	rBV2	387	299	0.00%	0.001%
63	11.555	1713	1717	1719	rBV2	632	987	0.00%	0.002%
64	11.750	1745	1749	1755	rVB2	2624	3618	0.01%	0.006%
65	11.841	1761	1764	1768	rVB4	585	827	0.00%	0.001%
66	11.939	1776	1780	1783	rBV4	1381	1565	0.00%	0.003%
67	11.975	1783	1786	1789	rVB4	893	1160	0.00%	0.002%
68	12.024	1789	1794	1806	rBV	421711	530297	1.10%	0.936%
69	12.110	1806	1808	1809	rBV2	561	516	0.00%	0.001%
70	12.323	1837	1843	1851	rVB	408853	508247	1.06%	0.897%
71	12.427	1858	1860	1867	rVB3	850	894	0.00%	0.002%
72	12.542	1876	1879	1880	rBV3	307	284	0.00%	0.001%
73	12.774	1914	1917	1920	rBV5	316	364	0.00%	0.001%
74	12.865	1928	1932	1935	rBV3	375	616	0.00%	0.001%
75	12.951	1942	1946	1948	rBV3	399	567	0.00%	0.001%
76	12.981	1950	1951	1957	rVV4	307	409	0.00%	0.001%

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Integrator: RTE

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 Title : VOC Analysis

77	13.054	1960	1963	1967	rVV4	462	736	0.00%	0.001%
78	13.109	1970	1972	1977	rVB4	578	758	0.00%	0.001%
79	13.219	1988	1990	1992	rVB3	391	338	0.00%	0.001%
80	13.250	1992	1995	1996	rBV2	302	264	0.00%	0.000%
81	13.280	1996	2000	2001	rVV3	422	406	0.00%	0.001%
82	13.591	2046	2051	2055	rBV4	804	1275	0.00%	0.002%
83	13.786	2079	2083	2087	rVB2	595	918	0.00%	0.002%
84	13.920	2104	2105	2107	rBV2	338	289	0.00%	0.001%
85	13.963	2110	2112	2115	rVV3	586	570	0.00%	0.001%
86	14.030	2121	2123	2126	rVV	641	521	0.00%	0.001%
87	14.091	2131	2133	2137	rVB3	300	309	0.00%	0.001%
88	14.127	2137	2139	2142	rBV3	353	358	0.00%	0.001%
89	14.213	2151	2153	2156	rVB3	410	448	0.00%	0.001%
90	14.249	2156	2159	2161	rBV3	399	379	0.00%	0.001%
91	14.396	2181	2183	2187	rBV4	471	554	0.00%	0.001%
92	14.438	2187	2190	2191	rBV3	303	392	0.00%	0.001%
93	14.688	2229	2231	2232	rBV2	360	294	0.00%	0.001%
94	14.822	2251	2253	2256	rBV2	338	296	0.00%	0.001%
95	14.883	2260	2263	2265	rBV4	410	440	0.00%	0.001%
96	14.981	2277	2279	2280	rBV	312	276	0.00%	0.000%
97	15.018	2283	2285	2287	rBV2	346	292	0.00%	0.001%
98	15.280	2327	2328	2333	rBV4	287	422	0.00%	0.001%
99	15.828	2416	2418	2420	rBV3	391	292	0.00%	0.001%
100	16.115	2461	2465	2466	rBV2	444	419	0.00%	0.001%

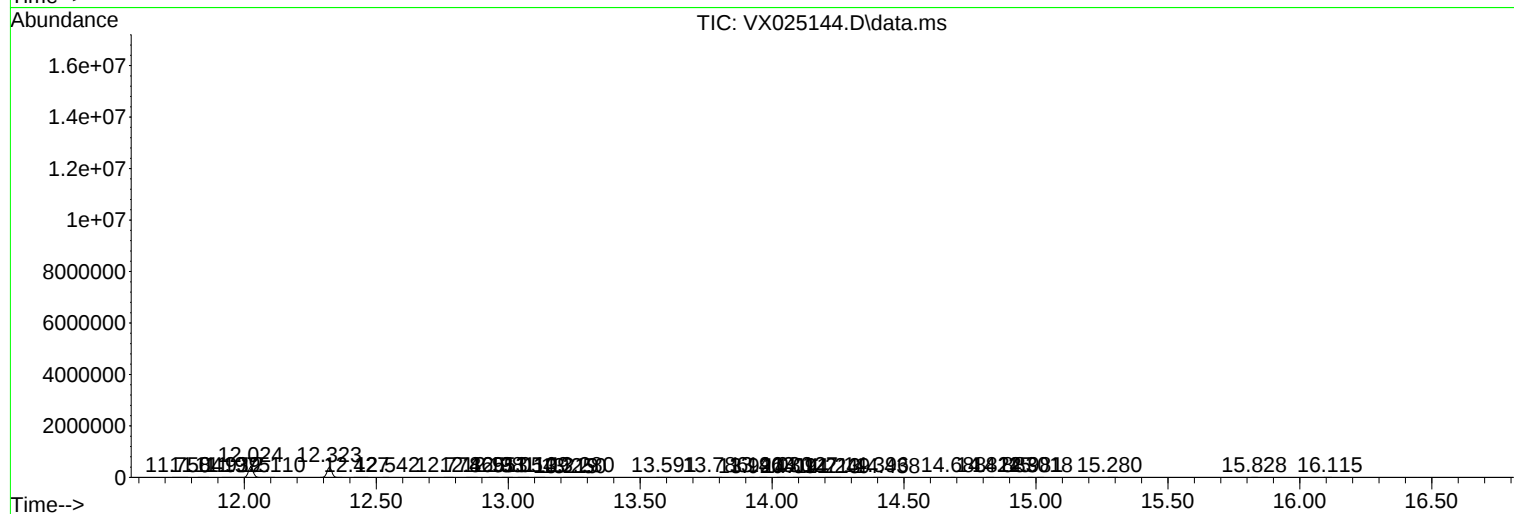
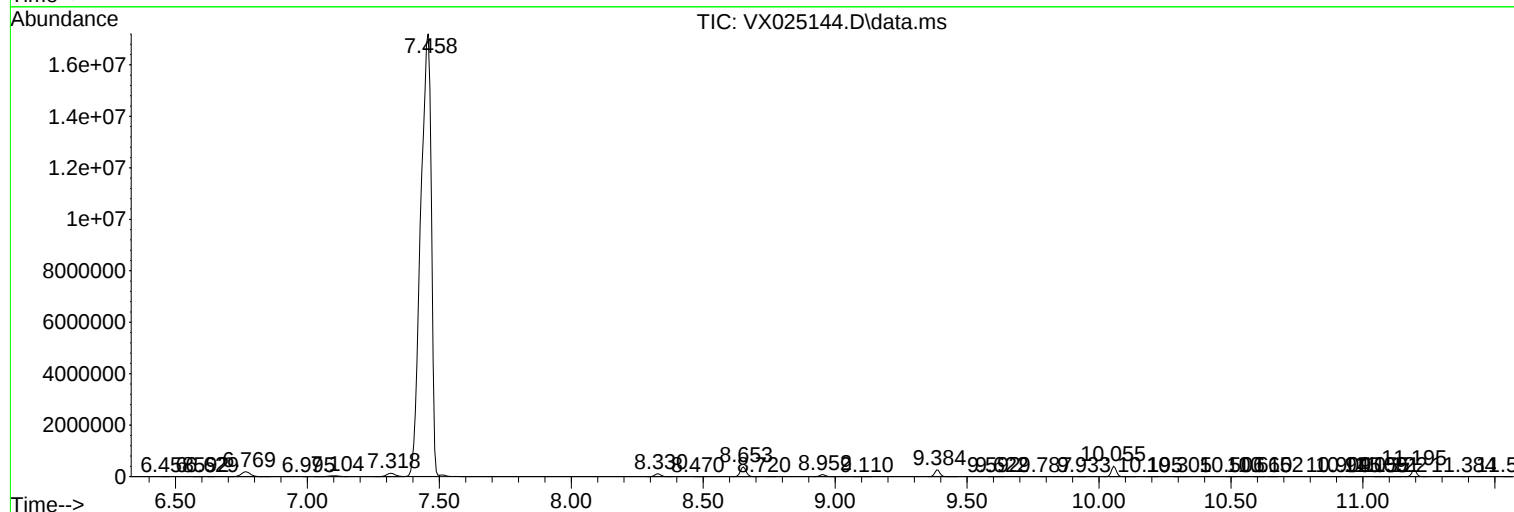
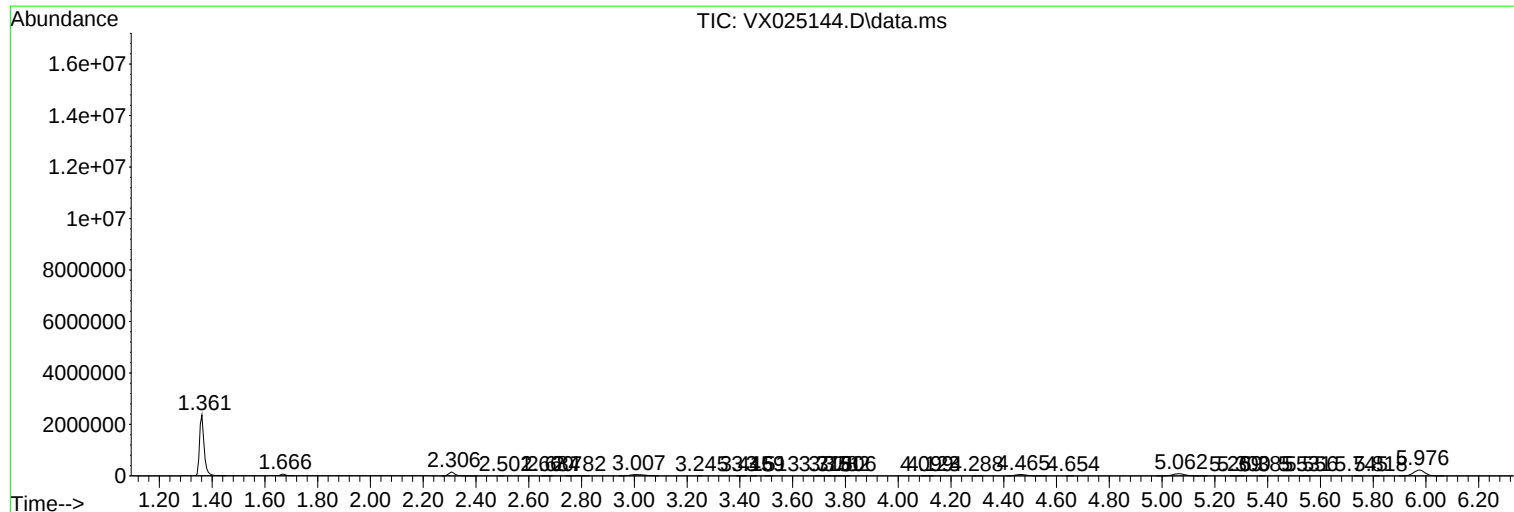
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V00

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
ClientSampleId :
COV00

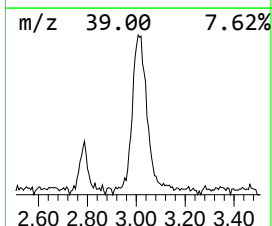
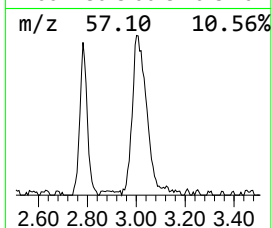
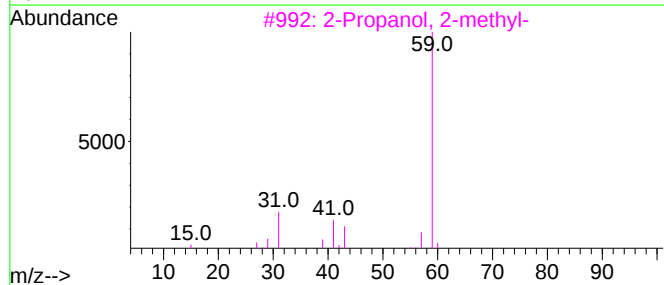
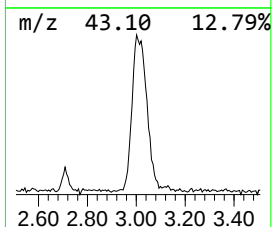
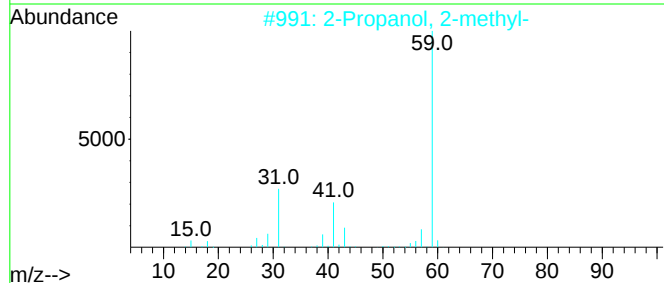
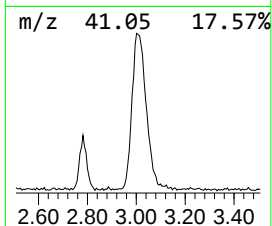
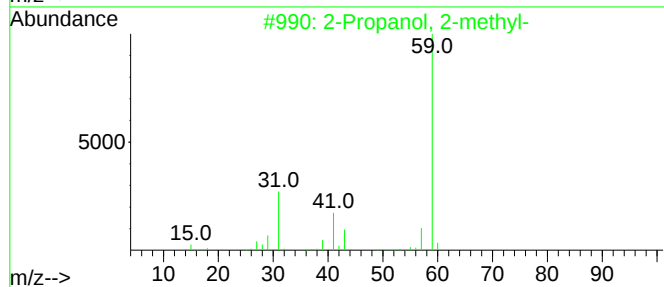
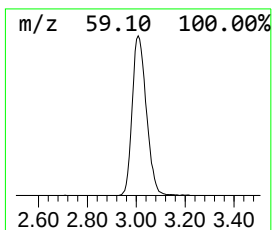
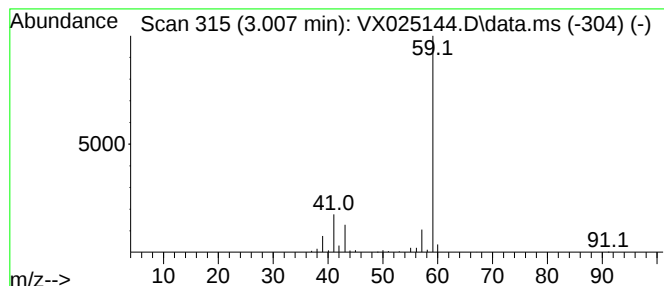
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.007	20.90 ug/L	188417	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	83
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	64
3	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	64
4	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	64
5	Propanoic acid, 2-hydroxy-2-methyl-			104	C4H8O3	000594-61-6	9



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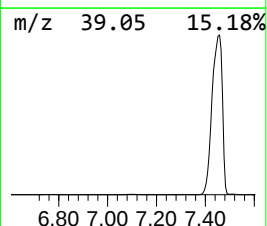
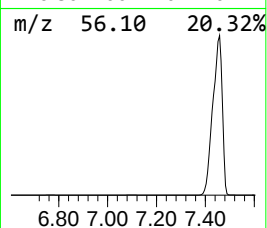
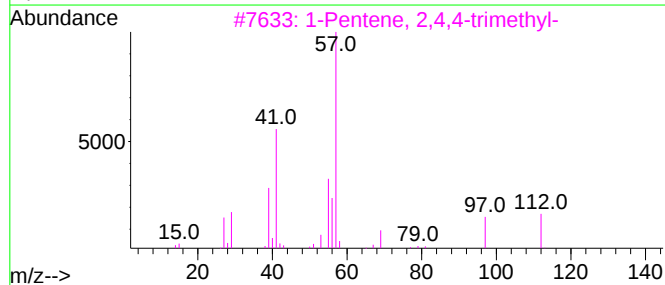
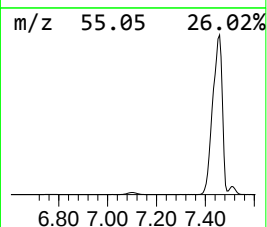
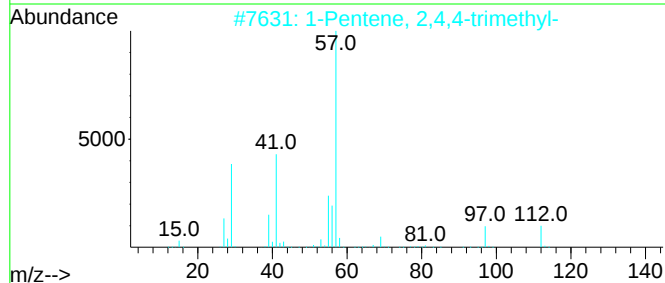
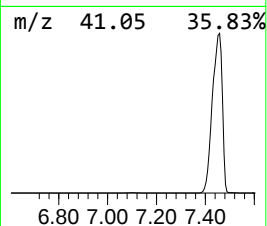
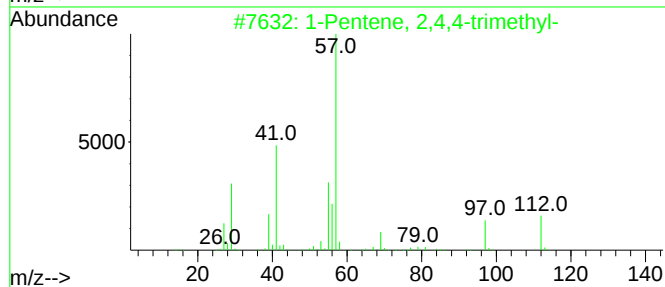
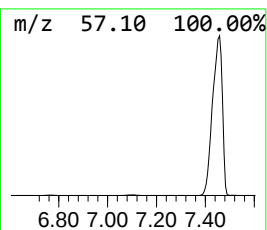
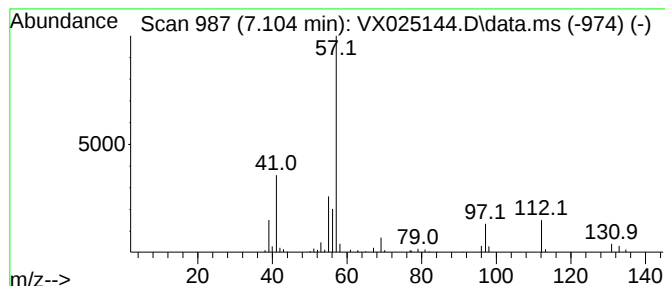
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.104	9.83 ug/L	88626	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2,4,4-trimethyl-		112	C8H16		000107-39-1	81
2	1-Pentene, 2,4,4-trimethyl-		112	C8H16		000107-39-1	68
3	1-Pentene, 2,4,4-trimethyl-		112	C8H16		000107-39-1	64
4	1-Pentene, 2,4,4-trimethyl-		112	C8H16		000107-39-1	52
5	1-Pentene, 2,4,4-trimethyl-		112	C8H16		000107-39-1	50



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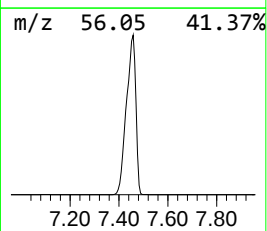
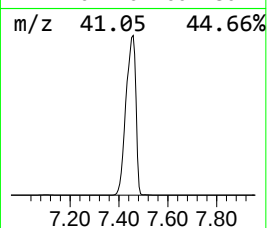
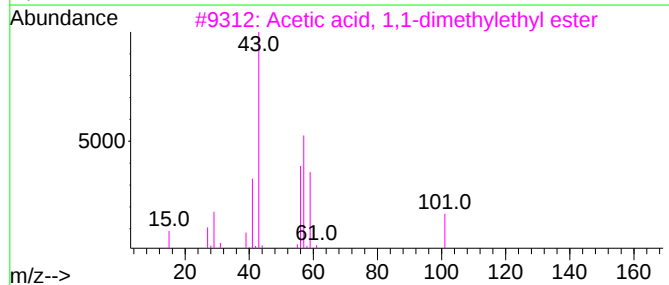
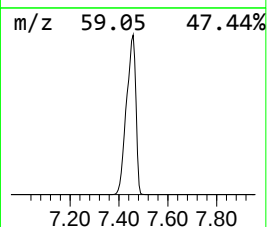
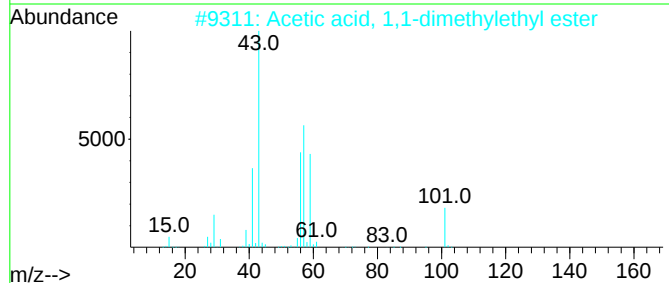
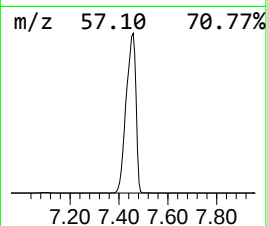
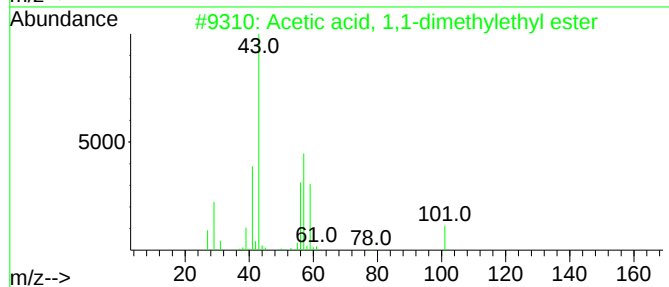
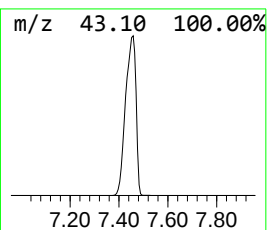
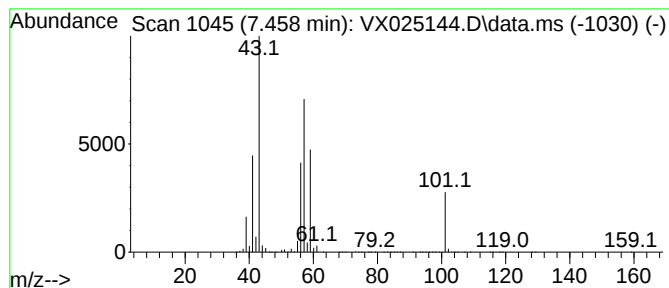
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Acetic acid, 1,1-dimethylet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	5341.30 ug/L	48143100	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	83
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	78
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	78
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	72
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111221\
Data File : VX025144.D
Acq On : 12 Nov 2021 10:32
Operator : JC/MD
Sample : M4615-01 40X
Misc : 4.34g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V00

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML111121WMA.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
2-Propanol, 2-m...	3.007	20.9	ug/L	188417	1	6.769	450668	50.0
(DEL) Alkane: S...	7.104	9.8	ug/L	88626	1	6.769	450668	50.0
Acetic acid, 1,...	7.458	5341.3	ug/L	48143100	1	6.769	450668	50.0