

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111221\
 Data File : VX025157.D
 Acq On : 12 Nov 2021 16:46
 Operator : JC/MD
 Sample : M4615-08
 Misc : 2.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0V14

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\SFAMXLM11121WMA.M
 Title : VOC Analysis

Signal : TIC: VX025157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	42	46	57	rVB	78248	93698	14.24%	1.455%
2	1.666	91	95	101	rBV	39899	57938	8.81%	0.900%
3	2.288	191	197	206	rBV	128195	212110	32.24%	3.295%
4	2.416	211	218	243	rVB	135865	477961	72.65%	7.424%
5	2.721	263	268	272	rBV	2472	4067	0.62%	0.063%
6	2.782	275	278	281	rVV4	1246	1637	0.25%	0.025%
7	2.953	299	306	318	rBV2	2787	7769	1.18%	0.121%
8	3.117	330	333	334	rBV2	634	723	0.11%	0.011%
9	4.495	548	559	569	rBV2	26969	116509	17.71%	1.810%
10	5.062	641	652	668	rVV	78187	259556	39.45%	4.032%
11	5.495	718	723	725	rBV4	1068	1895	0.29%	0.029%
12	5.629	736	745	754	rVB2	3776	12863	1.96%	0.200%
13	5.812	768	775	786	rVB6	2181	6672	1.01%	0.104%
14	5.970	789	801	816	rBV2	227990	657855	100.00%	10.218%
15	6.367	856	866	877	rBV3	2794	9093	1.38%	0.141%
16	6.598	897	904	913	rVV2	3830	10162	1.54%	0.158%
17	6.763	919	931	944	rBV	186980	466705	70.94%	7.249%
18	7.116	976	989	999	rBV10	2652	8624	1.31%	0.134%
19	7.214	1001	1005	1006	rBV3	868	1268	0.19%	0.020%
20	7.312	1012	1021	1032	rBV	131971	294759	44.81%	4.578%
21	7.433	1034	1041	1058	rVB2	23809	66032	10.04%	1.026%
22	7.659	1074	1078	1083	rVB5	452	722	0.11%	0.011%
23	8.324	1181	1187	1201	rBV	95846	175083	26.61%	2.719%
24	8.586	1226	1230	1232	rBV3	1318	1987	0.30%	0.031%
25	8.653	1234	1241	1248	rVV	343150	564853	85.86%	8.774%
26	8.720	1248	1252	1256	rVB	4762	7073	1.08%	0.110%
27	8.951	1284	1290	1302	rVV	68579	116657	17.73%	1.812%
28	9.128	1313	1319	1321	rBV4	473	754	0.11%	0.012%
29	9.281	1340	1344	1347	rBV3	808	1145	0.17%	0.018%
30	9.409	1357	1365	1378	rBV	164947	314301	47.78%	4.882%
31	9.549	1384	1388	1391	rVB4	621	1016	0.15%	0.016%
32	9.714	1413	1415	1423	rVB4	979	1559	0.24%	0.024%
33	9.829	1431	1434	1438	rBV3	513	642	0.10%	0.010%
34	9.903	1442	1446	1449	rBV4	994	1454	0.22%	0.023%
35	10.006	1459	1463	1465	rVV4	589	723	0.11%	0.011%
36	10.055	1465	1471	1486	rVV	361754	555752	84.48%	8.632%

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

37	10.195	1492	1494	1499	rVV2	605	905	0.14%	0.014%
38	10.244	1499	1502	1506	rVV2	772	1245	0.19%	0.019%
39	10.311	1509	1513	1518	rVV4	1817	3481	0.53%	0.054%
40	10.360	1518	1521	1526	rVV3	2700	3612	0.55%	0.056%
41	10.585	1553	1558	1562	rBB5	1028	1598	0.24%	0.025%
42	10.756	1583	1586	1587	rBV3	738	854	0.13%	0.013%
43	10.780	1587	1590	1594	rVV3	2178	2804	0.43%	0.044%
44	10.823	1594	1597	1599	rVV3	675	769	0.12%	0.012%
45	10.860	1599	1603	1606	rVV3	1633	2345	0.36%	0.036%
46	10.896	1606	1609	1613	rVB5	901	1145	0.17%	0.018%
47	10.945	1613	1617	1624	rVB4	2229	3824	0.58%	0.059%
48	11.030	1627	1631	1635	rBV5	1084	1700	0.26%	0.026%
49	11.085	1635	1640	1642	rBV4	1921	2865	0.44%	0.045%
50	11.122	1642	1646	1650	rVB2	4900	7765	1.18%	0.121%
51	11.201	1650	1659	1666	rBV	236330	311524	47.35%	4.839%
52	11.317	1672	1678	1684	rVB	83353	116294	17.68%	1.806%
53	11.384	1686	1689	1693	rVB5	800	1131	0.17%	0.018%
54	11.433	1693	1697	1700	rBV2	2401	3396	0.52%	0.053%
55	11.482	1700	1705	1711	rVB	17910	23464	3.57%	0.364%
56	11.542	1711	1715	1719	rBV5	765	1017	0.15%	0.016%
57	11.628	1726	1729	1734	rVB5	1379	2102	0.32%	0.033%
58	11.683	1734	1738	1740	rBV4	1271	1918	0.29%	0.030%
59	11.713	1740	1743	1747	rVV	5038	6076	0.92%	0.094%
60	11.750	1747	1749	1753	rVB4	3076	3956	0.60%	0.061%
61	11.841	1761	1764	1767	rBV4	1629	2248	0.34%	0.035%
62	11.890	1769	1772	1776	rVV3	1873	2805	0.43%	0.044%
63	11.945	1776	1781	1784	rVV3	3559	5999	0.91%	0.093%
64	11.975	1784	1786	1789	rVB2	1868	1939	0.29%	0.030%
65	12.024	1789	1794	1800	rBV	457767	582036	88.47%	9.041%
66	12.073	1800	1802	1805	rVV4	3032	3349	0.51%	0.052%
67	12.103	1805	1807	1812	rVV3	2842	3877	0.59%	0.060%
68	12.152	1812	1815	1817	rVV2	2151	2407	0.37%	0.037%
69	12.177	1817	1819	1824	rVB2	2171	2144	0.33%	0.033%
70	12.225	1824	1827	1828	rBV2	1137	1242	0.19%	0.019%
71	12.323	1837	1843	1850	rBV	393141	503885	76.60%	7.827%
72	12.426	1856	1860	1864	rVV	20320	22899	3.48%	0.356%
73	12.469	1864	1867	1873	rVB6	1873	4137	0.63%	0.064%
74	12.585	1883	1886	1891	rVB5	1699	2834	0.43%	0.044%
75	12.683	1899	1902	1908	rVB5	1508	2456	0.37%	0.038%
76	12.768	1911	1916	1920	rVV2	26459	36954	5.62%	0.574%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML111121WMA.M
 Title : VOC Analysis

77	12.823	1922	1925	1928	rVB4	886	1043	0.16%	0.016%
78	12.859	1928	1931	1933	rBV4	676	988	0.15%	0.015%
79	12.884	1933	1935	1943	rVB5	2163	3837	0.58%	0.060%
80	13.048	1958	1962	1967	rBV5	1240	1721	0.26%	0.027%
81	13.237	1990	1993	1996	rBV4	3967	4482	0.68%	0.070%
82	13.268	1996	1998	2001	rVV2	3261	3533	0.54%	0.055%
83	13.298	2001	2003	2008	rVB4	1744	2039	0.31%	0.032%
84	13.347	2008	2011	2015	rBV3	550	963	0.15%	0.015%
85	13.390	2015	2018	2020	rBV3	1079	1162	0.18%	0.018%
86	13.499	2035	2036	2040	rVB2	854	800	0.12%	0.012%
87	13.701	2064	2069	2072	rVV5	1199	1975	0.30%	0.031%
88	13.737	2073	2075	2080	rVB3	1019	1286	0.20%	0.020%
89	13.804	2083	2086	2088	rBV4	878	921	0.14%	0.014%
90	13.847	2090	2093	2098	rVB6	1174	1674	0.25%	0.026%
91	13.981	2111	2115	2118	rBV6	900	1641	0.25%	0.025%
92	14.042	2122	2125	2127	rVB3	1495	1730	0.26%	0.027%
93	14.133	2136	2140	2143	rVB	4284	6012	0.91%	0.093%
94	14.353	2173	2176	2180	rBV5	1418	1898	0.29%	0.029%
95	14.444	2188	2191	2194	rVB4	2472	2629	0.40%	0.041%
96	14.560	2207	2210	2212	rBV4	1518	2180	0.33%	0.034%
97	14.615	2217	2219	2226	rVV8	2334	4050	0.62%	0.063%
98	15.420	2348	2351	2356	rVB2	8803	12318	1.87%	0.191%
99	15.566	2370	2375	2380	rVB	101755	145892	22.18%	2.266%
100	16.097	2458	2462	2468	rBV	17460	34683	5.27%	0.539%

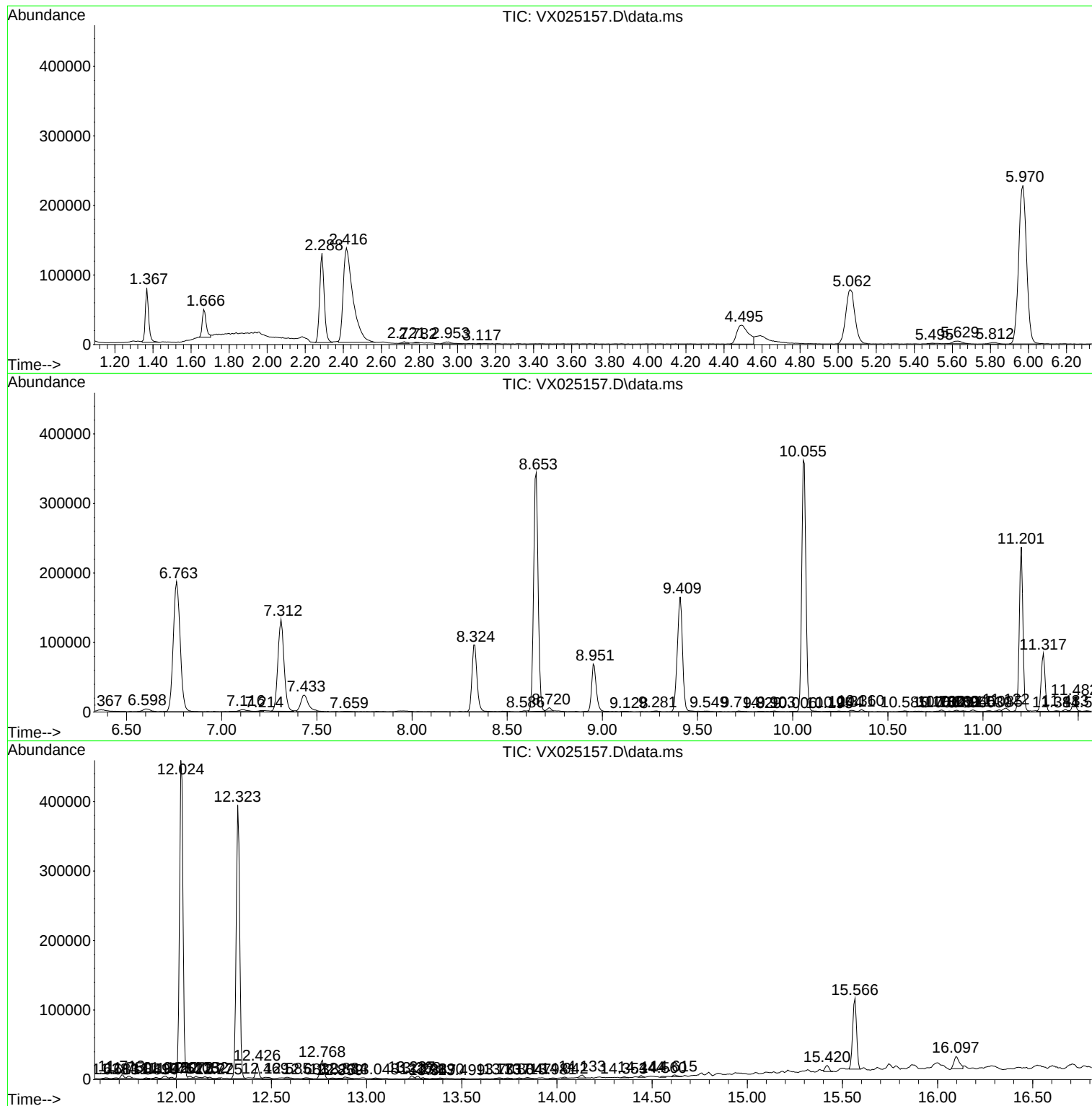
Sum of corrected areas: 6438075

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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



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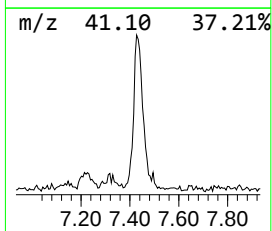
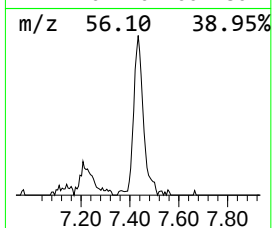
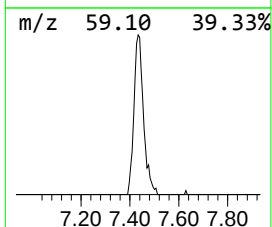
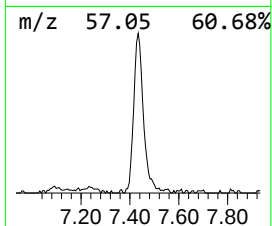
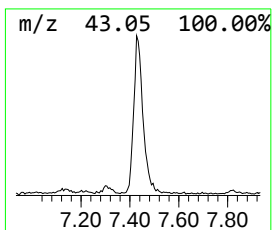
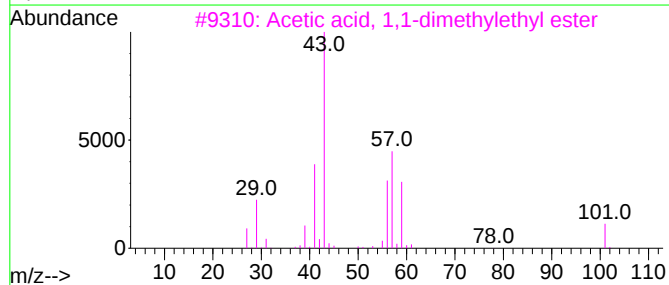
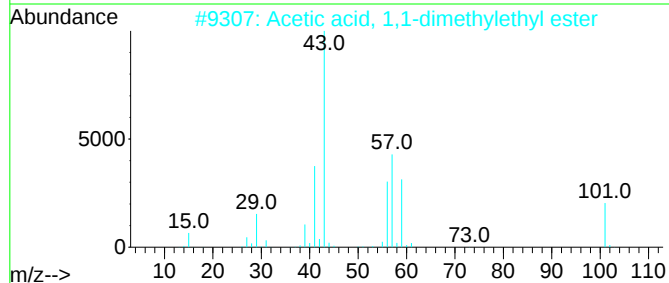
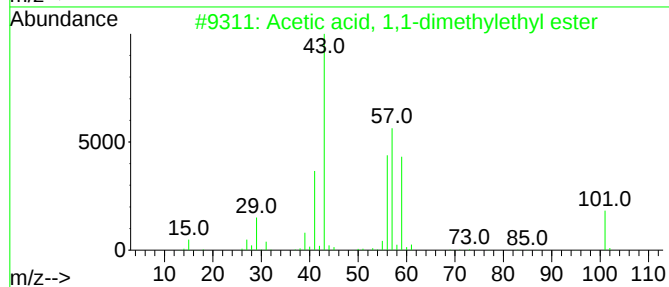
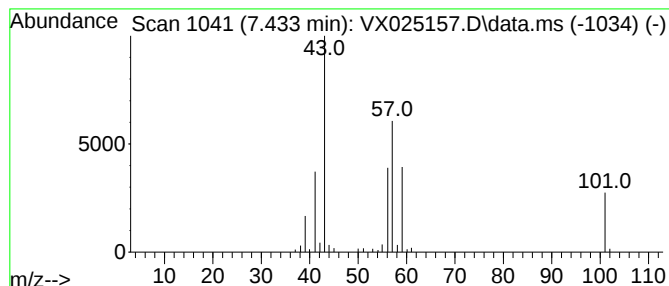
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetic acid, 1,1-dimethylet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.433	7.07 ug/L	66032	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	90
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	83
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	83
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	78
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40



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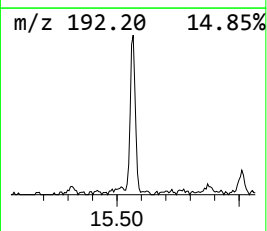
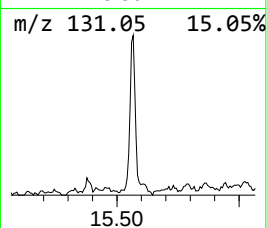
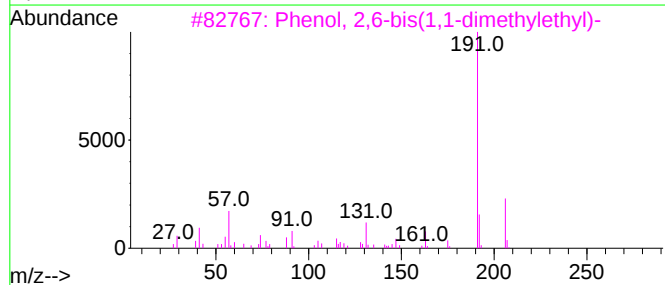
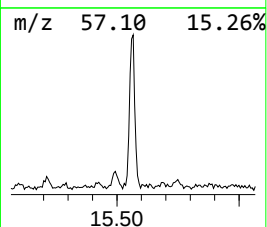
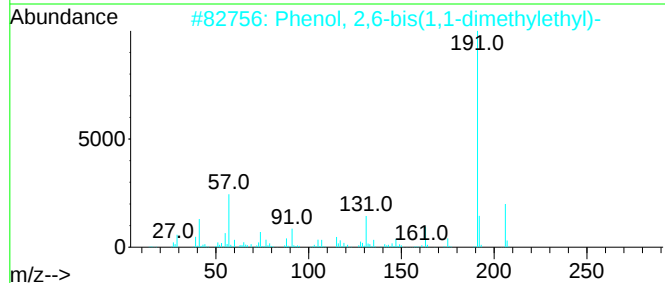
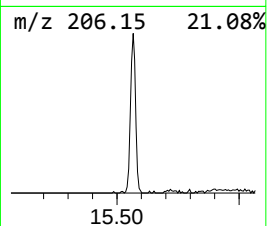
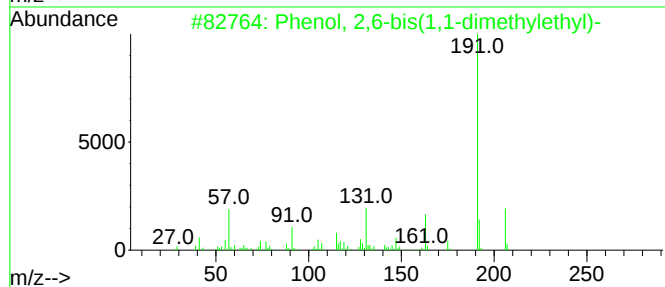
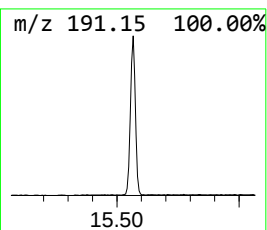
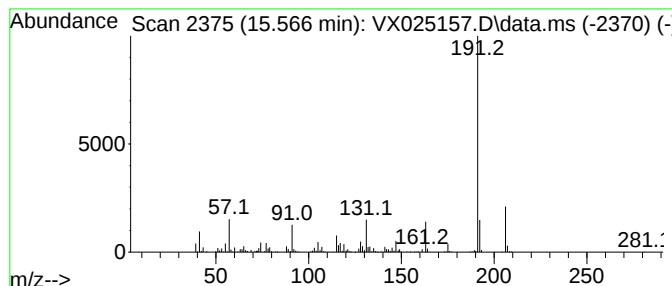
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML111121WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.566	12.53 ug/L	145892	1,4-Dichlorobenzene-d4	12.030

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	98
2			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
3			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
4			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
5			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	91



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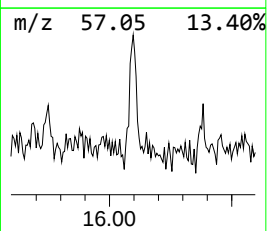
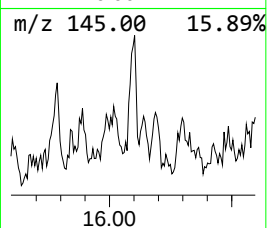
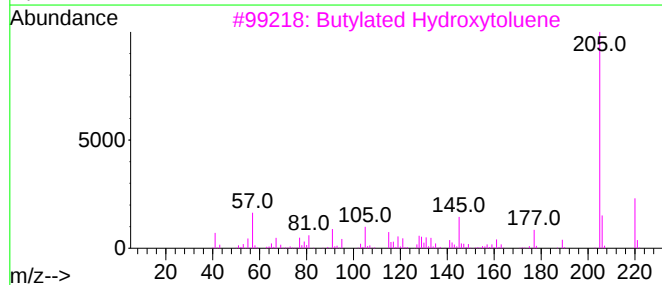
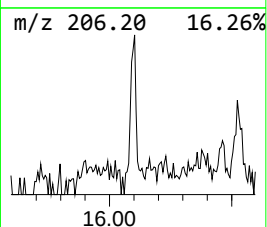
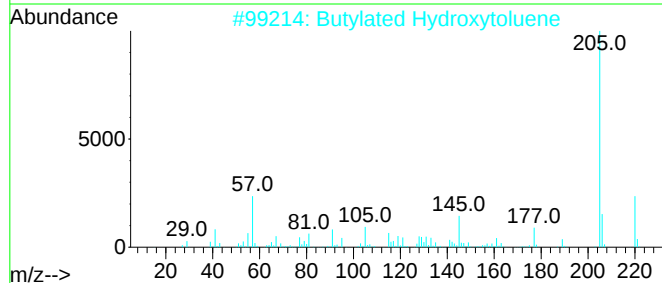
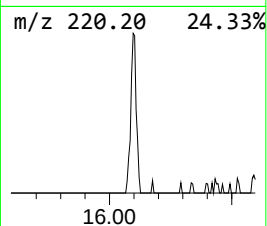
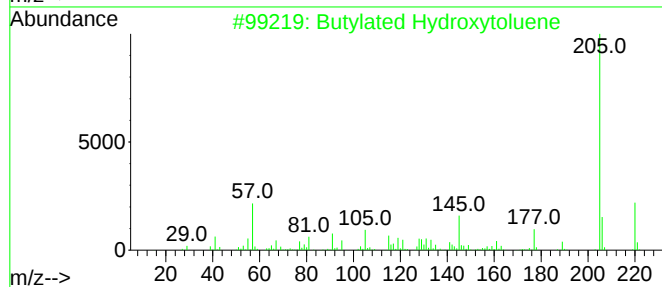
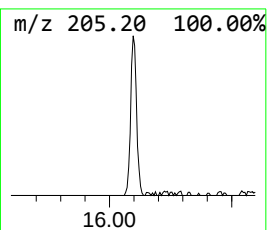
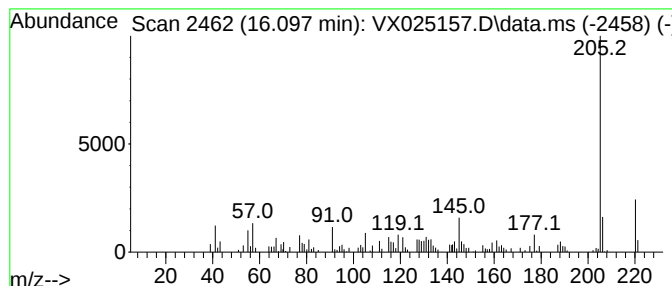
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.096	2.98 ug/L	34683	1,4-Dichlorobenzene-d4	12.030

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	90
5			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111221\
Data File : VX025157.D
Acq On : 12 Nov 2021 16:46
Operator : JC/MD
Sample : M4615-08
Misc : 2.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0V14

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
Acetic acid, 1,...	7.433	7.1	ug/L	66032	1	6.763	466705	50.0
Phenol, 2,6-bis...	15.566	12.5	ug/L	145892	3	12.030	582036	50.0
Butylated Hydro...	16.096	3.0	ug/L	34683	3	12.030	582036	50.0