

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112621\
 Data File : VX025347.D
 Acq On : 26 Nov 2021 11:29
 Operator : JC/MD
 Sample : M4799-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0P63

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025347.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	55	rVB	79692	78844	14.45%	1.806%
2	1.666	90	95	104	rBV	60511	80679	14.79%	1.848%
3	2.306	193	200	209	rBV	115088	184845	33.89%	4.235%
4	2.380	209	212	220	rVB	3514	5777	1.06%	0.132%
5	2.514	229	234	236	rBV2	760	1135	0.21%	0.026%
6	2.697	263	264	271	rVB3	410	665	0.12%	0.015%
7	2.788	275	279	284	rVB2	850	1249	0.23%	0.029%
8	2.965	301	308	313	rVB	826	1423	0.26%	0.033%
9	3.099	325	330	332	rBV5	729	1279	0.23%	0.029%
10	3.215	346	349	350	rBV	217	157	0.03%	0.004%
11	3.605	409	413	416	rBV2	330	486	0.09%	0.011%
12	3.971	470	473	477	rVV2	160	263	0.05%	0.006%
13	4.227	513	515	522	rVB3	148	210	0.04%	0.005%
14	4.458	543	553	567	rBV	47242	133394	24.46%	3.056%
15	4.721	589	596	609	rBV	1701	4780	0.88%	0.110%
16	4.818	610	612	615	rVB	210	151	0.03%	0.003%
17	4.891	621	624	625	rBV	158	194	0.04%	0.004%
18	5.062	637	652	669	rBV	72641	229933	42.15%	5.267%
19	5.379	700	704	705	rBV2	424	456	0.08%	0.010%
20	5.464	712	718	719	rBV3	545	720	0.13%	0.016%
21	5.666	748	751	752	rBV2	260	261	0.05%	0.006%
22	5.970	789	801	820	rBV2	183831	545464	100.00%	12.496%
23	6.287	851	853	856	rVB	192	176	0.03%	0.004%
24	6.586	899	902	906	rBV2	106	188	0.03%	0.004%
25	6.763	921	931	944	rBV	134257	319039	58.49%	7.309%
26	6.952	961	962	967	rVB2	167	242	0.04%	0.006%
27	7.117	982	989	996	rBV5	3873	8435	1.55%	0.193%
28	7.220	1001	1006	1011	rBV3	329	552	0.10%	0.013%
29	7.312	1011	1021	1031	rBV	113856	246256	45.15%	5.641%
30	7.421	1033	1039	1053	rVB	20706	45570	8.35%	1.044%
31	7.586	1060	1066	1074	rVB3	519	1066	0.20%	0.024%
32	7.659	1076	1078	1081	rBV2	133	153	0.03%	0.004%
33	7.793	1098	1100	1101	rBV	239	168	0.03%	0.004%
34	7.927	1117	1122	1126	rBV3	899	1547	0.28%	0.035%
35	8.324	1181	1187	1200	rVV	80969	134949	24.74%	3.091%
36	8.446	1204	1207	1208	rBV2	157	193	0.04%	0.004%

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 Title : VOC Analysis

37	8.482	1208	1213	1216	rVB3	620	963	0.18%	0.022%
38	8.580	1223	1229	1234	rBV3	1713	2623	0.48%	0.060%
39	8.653	1234	1241	1248	rBV	282509	446154	81.79%	10.221%
40	8.720	1249	1252	1260	rVB	5671	8486	1.56%	0.194%
41	8.811	1265	1267	1271	rVB2	170	177	0.03%	0.004%
42	8.952	1284	1290	1302	rBV	60873	87942	16.12%	2.015%
43	9.159	1320	1324	1328	rVB3	762	913	0.17%	0.021%
44	9.238	1334	1337	1340	rVV2	1567	2436	0.45%	0.056%
45	9.275	1340	1343	1348	rVB2	2239	3187	0.58%	0.073%
46	9.384	1355	1361	1379	rBV	208890	299242	54.86%	6.855%
47	9.525	1380	1384	1391	rVB2	2835	4040	0.74%	0.093%
48	9.610	1395	1398	1404	rVB2	518	799	0.15%	0.018%
49	9.903	1443	1446	1449	rBV2	131	167	0.03%	0.004%
50	10.055	1465	1471	1486	rVV	283961	377708	69.25%	8.653%
51	10.195	1491	1494	1499	rVV2	1755	2379	0.44%	0.054%
52	10.244	1499	1502	1505	rVV3	278	336	0.06%	0.008%
53	10.305	1508	1512	1519	rVB	2330	3005	0.55%	0.069%
54	10.592	1555	1559	1564	rVB4	583	773	0.14%	0.018%
55	10.646	1564	1568	1574	rVB3	2958	4684	0.86%	0.107%
56	10.768	1585	1588	1592	rBV3	662	869	0.16%	0.020%
57	10.799	1592	1593	1597	rVB2	428	368	0.07%	0.008%
58	10.860	1601	1603	1605	rBV2	282	266	0.05%	0.006%
59	10.963	1617	1620	1624	rBV2	2190	2435	0.45%	0.056%
60	11.122	1641	1646	1650	rVB2	1018	1487	0.27%	0.034%
61	11.195	1652	1658	1664	rBV	223805	281724	51.65%	6.454%
62	11.280	1670	1672	1675	rVB2	264	188	0.03%	0.004%
63	11.311	1675	1677	1684	rVB2	983	1281	0.23%	0.029%
64	11.378	1687	1688	1691	rBV2	217	204	0.04%	0.005%
65	11.451	1697	1700	1705	rBV	1990	2279	0.42%	0.052%
66	11.610	1723	1726	1728	rBV2	145	224	0.04%	0.005%
67	11.665	1730	1735	1742	rBV3	2516	4014	0.74%	0.092%
68	11.756	1742	1750	1756	rVV3	4896	7329	1.34%	0.168%
69	11.847	1761	1765	1766	rBV3	276	289	0.05%	0.007%
70	11.927	1774	1778	1782	rBV2	868	1243	0.23%	0.028%
71	11.969	1782	1785	1789	rVV	1354	1597	0.29%	0.037%
72	12.024	1789	1794	1801	rVV	293090	355597	65.19%	8.146%
73	12.122	1809	1810	1811	rBV	308	188	0.03%	0.004%
74	12.225	1822	1827	1833	rBV	8113	12249	2.25%	0.281%
75	12.323	1837	1843	1850	rVB	316074	398785	73.11%	9.136%
76	12.585	1883	1886	1894	rVB3	1447	2122	0.39%	0.049%

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 Title : VOC Analysis

77	12.670	1897	1900	1904	rBV2	229	370	0.07%	0.008%
78	12.768	1911	1916	1919	rBV4	409	593	0.11%	0.014%
79	12.811	1920	1923	1925	rVV	374	350	0.06%	0.008%
80	12.853	1926	1930	1935	rVB2	919	1450	0.27%	0.033%
81	12.945	1943	1945	1950	rVB3	349	360	0.07%	0.008%
82	12.994	1950	1953	1956	rVB2	117	157	0.03%	0.004%
83	13.115	1969	1973	1976	rBV3	1143	1404	0.26%	0.032%
84	13.170	1979	1982	1986	rVB4	555	669	0.12%	0.015%
85	13.512	2036	2038	2041	rBV2	453	443	0.08%	0.010%
86	13.591	2047	2051	2056	rVB2	1315	1631	0.30%	0.037%
87	13.640	2056	2059	2060	rBV	178	159	0.03%	0.004%
88	13.737	2071	2075	2077	rBV2	366	427	0.08%	0.010%
89	13.780	2078	2082	2087	rVV2	1200	1626	0.30%	0.037%
90	13.963	2108	2112	2116	rBV2	801	967	0.18%	0.022%
91	14.140	2136	2141	2143	rBV2	752	968	0.18%	0.022%
92	14.329	2168	2172	2176	rBV3	164	231	0.04%	0.005%
93	14.432	2186	2189	2190	rBV	158	163	0.03%	0.004%
94	14.493	2194	2199	2200	rBB	266	253	0.05%	0.006%
95	14.755	2240	2242	2245	rBV2	318	290	0.05%	0.007%
96	15.268	2323	2326	2327	rBV2	313	240	0.04%	0.005%
97	15.755	2404	2406	2408	rBV	240	150	0.03%	0.003%
98	16.572	2538	2540	2543	rBV2	236	258	0.05%	0.006%
99	16.651	2551	2553	2555	rBV2	241	168	0.03%	0.004%
100	16.670	2555	2556	2559	rBV2	232	206	0.04%	0.005%

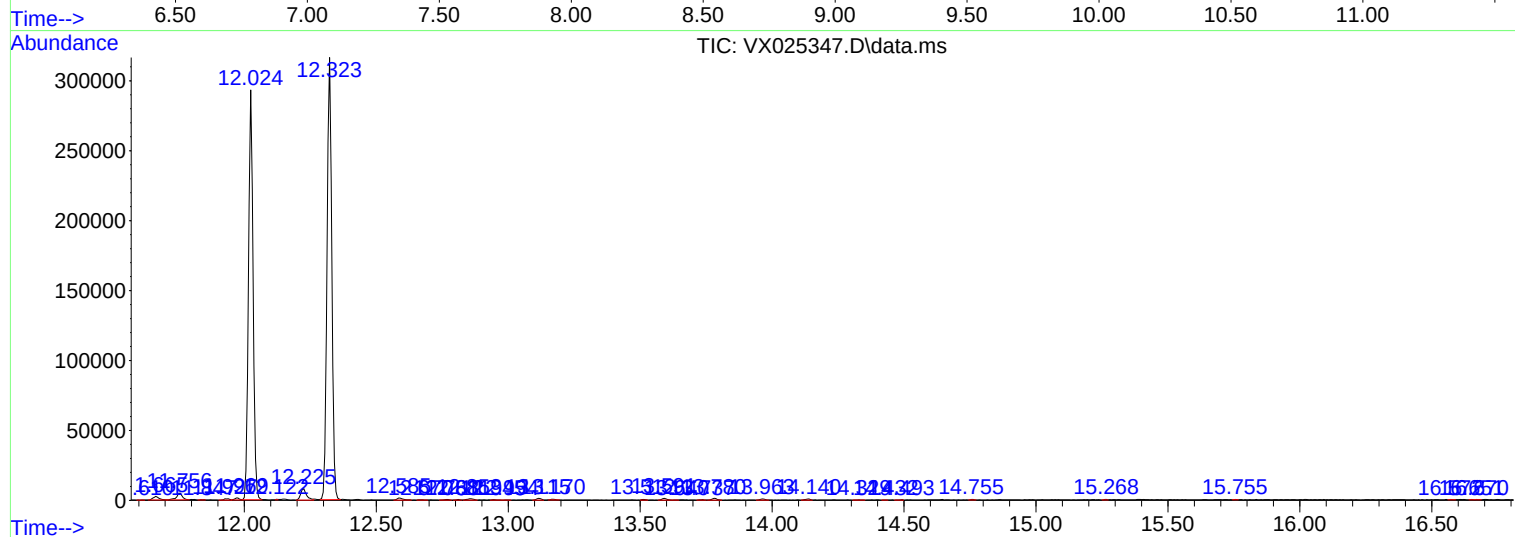
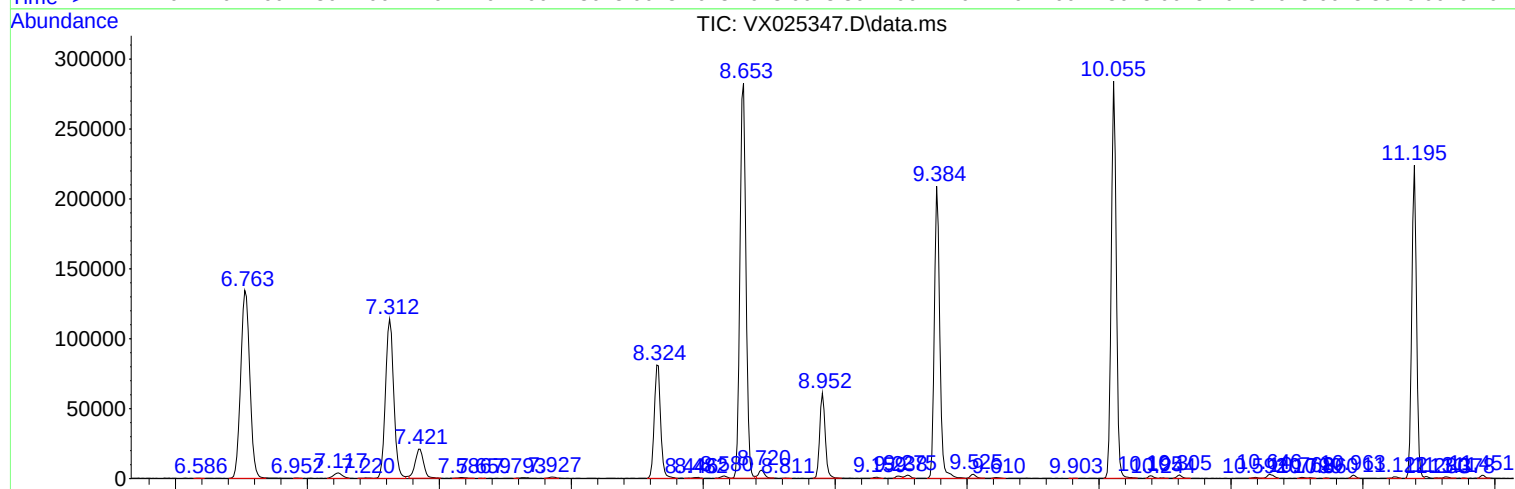
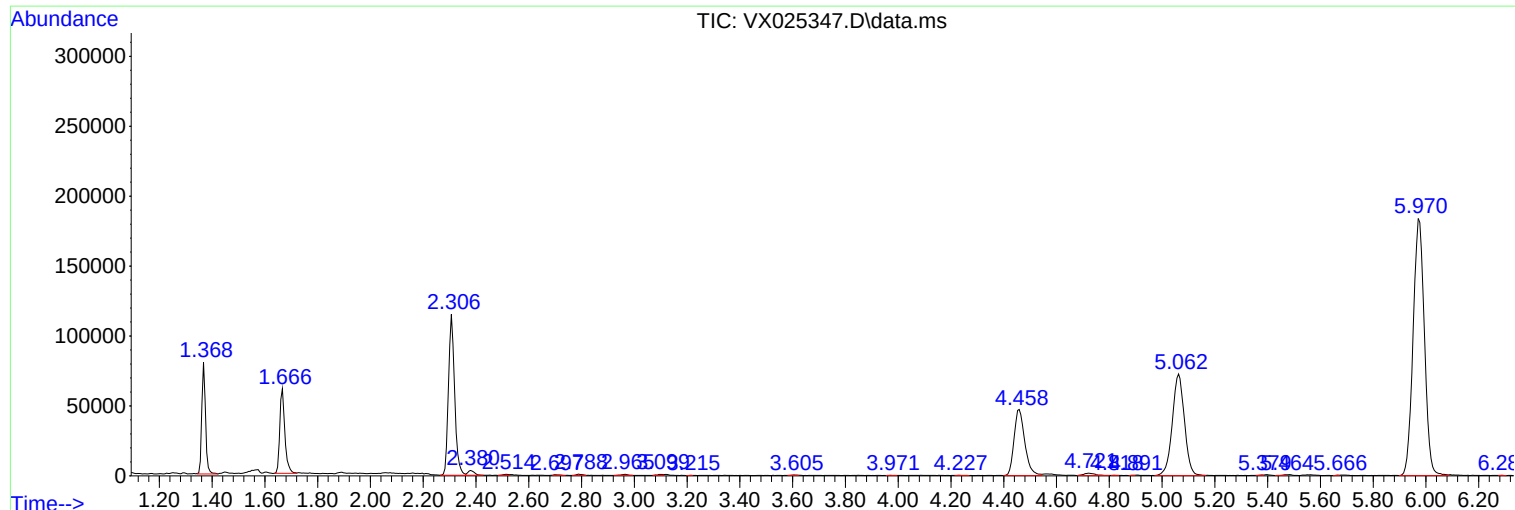
Sum of corrected areas: 4365184

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0P63

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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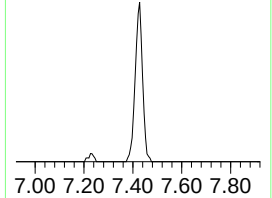
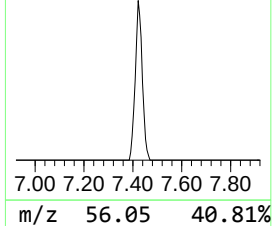
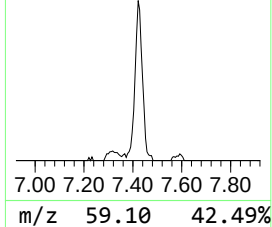
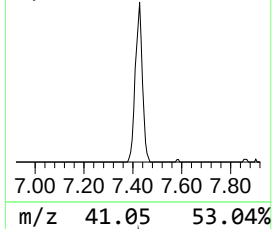
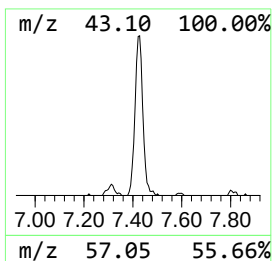
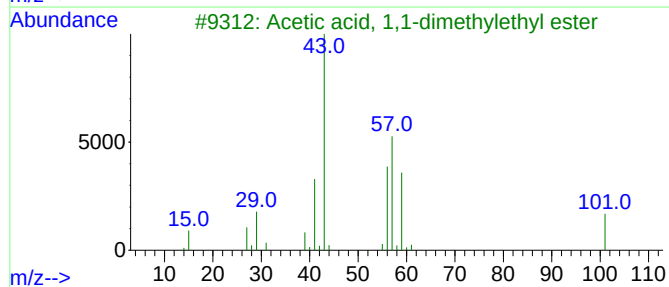
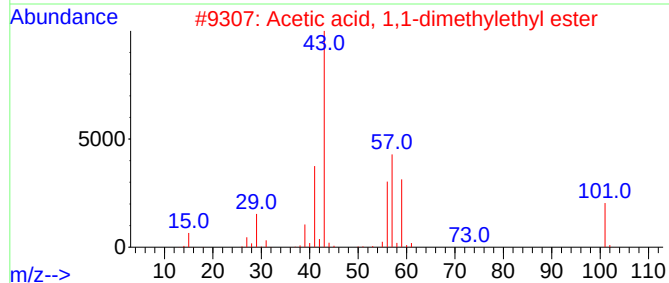
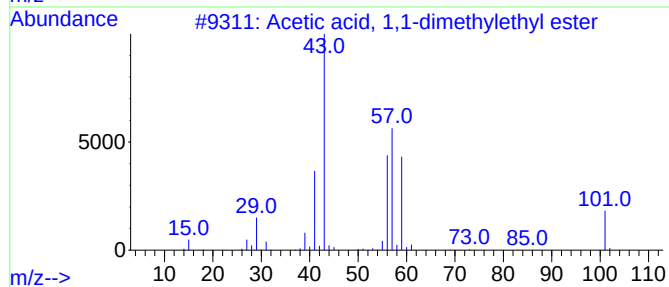
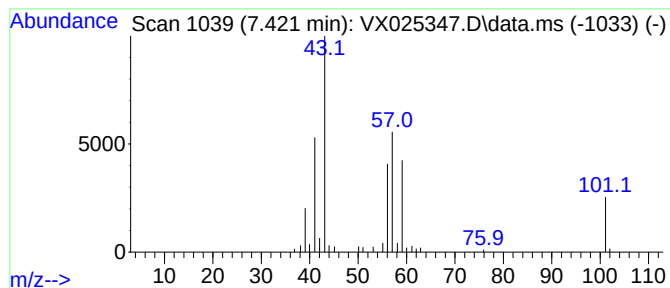
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetic acid, 1,1-dimethylet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.421	7.14 ug/L	45570	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	74
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	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, 1,...	7.421	7.1	ug/L	45570	1	6.763	319039	50.0