

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030660.D
 Acq On : 17 Aug 2022 15:15
 Operator : JC/MD
 Sample : N4221-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN2

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: VX030660.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB	84918	75038	0.49%	0.181%
2	1.264	25	29	39	rVB	22928	35994	0.23%	0.087%
3	1.368	42	46	54	rVB2	426038	477647	3.09%	1.154%
4	1.666	90	95	105	rVB	133012	165807	1.07%	0.400%
5	1.746	105	108	114	rBV4	4230	6209	0.04%	0.015%
6	1.996	146	149	154	rVB	12291	14038	0.09%	0.034%
7	2.319	194	202	217	rBV	3802083	6104384	39.46%	14.745%
8	2.477	227	228	231	rBV	789	488	0.00%	0.001%
9	2.709	264	266	269	rVV2	592	709	0.00%	0.002%
10	2.794	274	280	286	rBV	5720	10905	0.07%	0.026%
11	2.959	300	307	308	rBV3	1218	2463	0.02%	0.006%
12	3.093	323	329	336	rBV5	7832	16037	0.10%	0.039%
13	3.209	346	348	350	rBV	589	460	0.00%	0.001%
14	3.331	363	368	375	rBV4	948	2017	0.01%	0.005%
15	3.404	378	380	383	rBV2	401	428	0.00%	0.001%
16	3.617	404	415	431	rBV	215328	509262	3.29%	1.230%
17	3.837	449	451	455	rVB2	465	616	0.00%	0.001%
18	3.879	455	458	462	rBV2	615	994	0.01%	0.002%
19	4.245	517	518	521	rBV	527	481	0.00%	0.001%
20	4.495	545	559	581	rBV2	750487	2215679	14.32%	5.352%
21	4.867	617	620	623	rBV	655	780	0.01%	0.002%
22	5.062	639	652	670	rVV	176967	541081	3.50%	1.307%
23	5.294	688	690	694	rBV2	399	455	0.00%	0.001%
24	5.385	694	705	719	rVB2	40834	131749	0.85%	0.318%
25	5.538	728	730	731	rBV	744	505	0.00%	0.001%
26	5.977	789	802	817	rBV2	462461	1360549	8.80%	3.286%
27	6.184	834	836	838	rBV	542	377	0.00%	0.001%
28	6.239	841	845	846	rBV2	1171	1252	0.01%	0.003%
29	6.330	857	860	861	rBV	554	424	0.00%	0.001%
30	6.385	862	869	880	rVV2	7168	18869	0.12%	0.046%
31	6.580	899	901	903	rBV2	328	433	0.00%	0.001%
32	6.665	910	915	916	rVB2	406	379	0.00%	0.001%
33	6.702	919	921	922	rBV	665	464	0.00%	0.001%
34	6.769	922	932	946	rBV	307885	727475	4.70%	1.757%
35	6.909	953	955	957	rBV3	705	459	0.00%	0.001%
36	7.129	979	991	1013	rBV	7099888	15469393	100.00%	37.365%

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 Title : VOC Analysis

37	7.312	1013	1021	1038	rVB	271792	606637	3.92%	1.465%
38	7.574	1063	1064	1066	rBV2	710	505	0.00%	0.001%
39	7.677	1074	1081	1091	rBV2	42825	92189	0.60%	0.223%
40	7.909	1115	1119	1120	rBV2	933	1272	0.01%	0.003%
41	7.976	1126	1130	1138	rVB4	4682	8406	0.05%	0.020%
42	8.055	1141	1143	1146	rBV2	444	582	0.00%	0.001%
43	8.135	1151	1156	1162	rVB5	708	1718	0.01%	0.004%
44	8.251	1171	1175	1176	rBV	691	563	0.00%	0.001%
45	8.330	1181	1188	1201	rVV	188596	308467	1.99%	0.745%
46	8.494	1211	1215	1216	rBV2	1072	1388	0.01%	0.003%
47	8.653	1234	1241	1250	rBV	694377	1090075	7.05%	2.633%
48	8.848	1268	1273	1279	rVB5	5762	11061	0.07%	0.027%
49	8.909	1279	1283	1284	rBV2	363	388	0.00%	0.001%
50	8.952	1284	1290	1298	rBV	138010	200543	1.30%	0.484%
51	9.159	1320	1324	1329	rVB4	6477	10258	0.07%	0.025%
52	9.275	1332	1343	1356	rBV	4635897	7001544	45.26%	16.912%
53	9.384	1356	1361	1373	rVB	447690	653302	4.22%	1.578%
54	9.732	1414	1418	1427	rVB3	11996	19351	0.13%	0.047%
55	9.939	1449	1452	1455	rVB3	529	549	0.00%	0.001%
56	10.018	1457	1465	1466	rBV6	2662	4651	0.03%	0.011%
57	10.055	1466	1471	1483	rVB	638856	850403	5.50%	2.054%
58	10.201	1492	1495	1500	rVB4	1576	2203	0.01%	0.005%
59	10.287	1508	1509	1510	rBV	817	436	0.00%	0.001%
60	10.378	1518	1524	1531	rBV	24048	33998	0.22%	0.082%
61	10.457	1534	1537	1539	rBV2	388	437	0.00%	0.001%
62	10.531	1545	1549	1551	rBV2	777	1148	0.01%	0.003%
63	10.646	1565	1568	1570	rBV3	1553	1353	0.01%	0.003%
64	10.695	1573	1576	1578	rBV2	1134	1268	0.01%	0.003%
65	10.787	1589	1591	1593	rBV3	717	772	0.00%	0.002%
66	10.909	1607	1611	1614	rVB2	1030	1282	0.01%	0.003%
67	10.963	1618	1620	1624	rBV3	563	709	0.00%	0.002%
68	11.091	1638	1641	1646	rVB3	1854	3043	0.02%	0.007%
69	11.134	1646	1648	1652	rBV4	734	967	0.01%	0.002%
70	11.195	1652	1658	1667	rVV	469665	590584	3.82%	1.426%
71	11.317	1673	1678	1685	rVB	99809	138718	0.90%	0.335%
72	11.402	1691	1692	1693	rBV	879	466	0.00%	0.001%
73	11.567	1717	1719	1721	rBV3	586	421	0.00%	0.001%
74	11.616	1724	1727	1728	rBV2	403	477	0.00%	0.001%
75	11.695	1737	1740	1746	rVB6	1970	2728	0.02%	0.007%
76	11.793	1753	1756	1761	rVB4	1677	2158	0.01%	0.005%

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77	11.884	1768	1771	1775	rBV4	1301	1811	0.01%	0.004%
78	11.933	1776	1779	1781	rVB3	1543	1483	0.01%	0.004%
79	11.969	1783	1785	1789	rBV3	1148	1044	0.01%	0.003%
80	12.024	1789	1794	1804	rBV	676077	821567	5.31%	1.984%
81	12.219	1823	1826	1833	rBV2	9504	14207	0.09%	0.034%
82	12.323	1837	1843	1852	rVV	756177	934958	6.04%	2.258%
83	12.427	1855	1860	1863	rBV6	3411	4945	0.03%	0.012%
84	12.603	1886	1889	1890	rBV	648	536	0.00%	0.001%
85	12.701	1903	1905	1908	rVB3	576	551	0.00%	0.001%
86	12.768	1910	1916	1922	rVB2	41141	57163	0.37%	0.138%
87	12.853	1927	1930	1935	rVV3	3749	4576	0.03%	0.011%
88	13.225	1988	1991	1994	rBV4	906	1230	0.01%	0.003%
89	13.780	2079	2082	2086	rBV3	756	1210	0.01%	0.003%
90	13.963	2111	2112	2115	rVB	824	427	0.00%	0.001%
91	14.018	2119	2121	2123	rVB	739	440	0.00%	0.001%
92	14.042	2123	2125	2127	rBV2	553	554	0.00%	0.001%
93	14.073	2127	2130	2131	rBV	436	433	0.00%	0.001%
94	14.134	2136	2140	2143	rVV	6834	8663	0.06%	0.021%
95	14.237	2155	2157	2158	rBV2	625	461	0.00%	0.001%
96	14.420	2184	2187	2189	rBV2	736	518	0.00%	0.001%
97	14.445	2189	2191	2193	rVB2	642	585	0.00%	0.001%
98	15.560	2372	2374	2375	rBV	672	410	0.00%	0.001%
99	15.737	2401	2403	2406	rBV2	841	1048	0.01%	0.003%
100	16.670	2554	2556	2558	rBV2	996	811	0.01%	0.002%

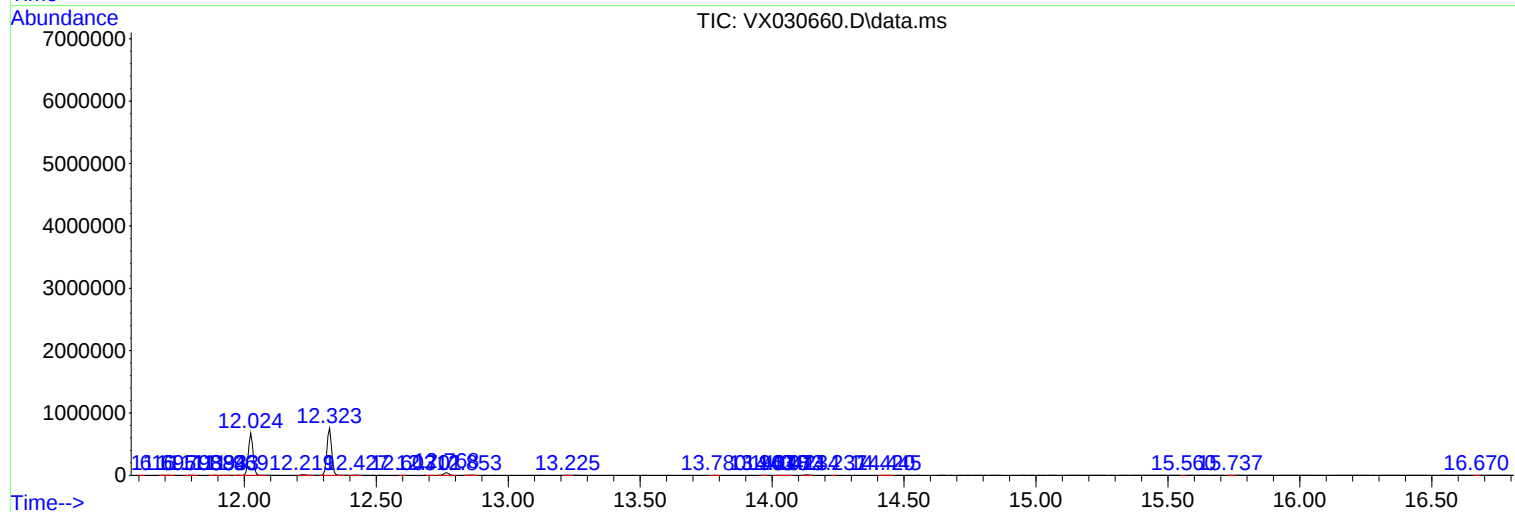
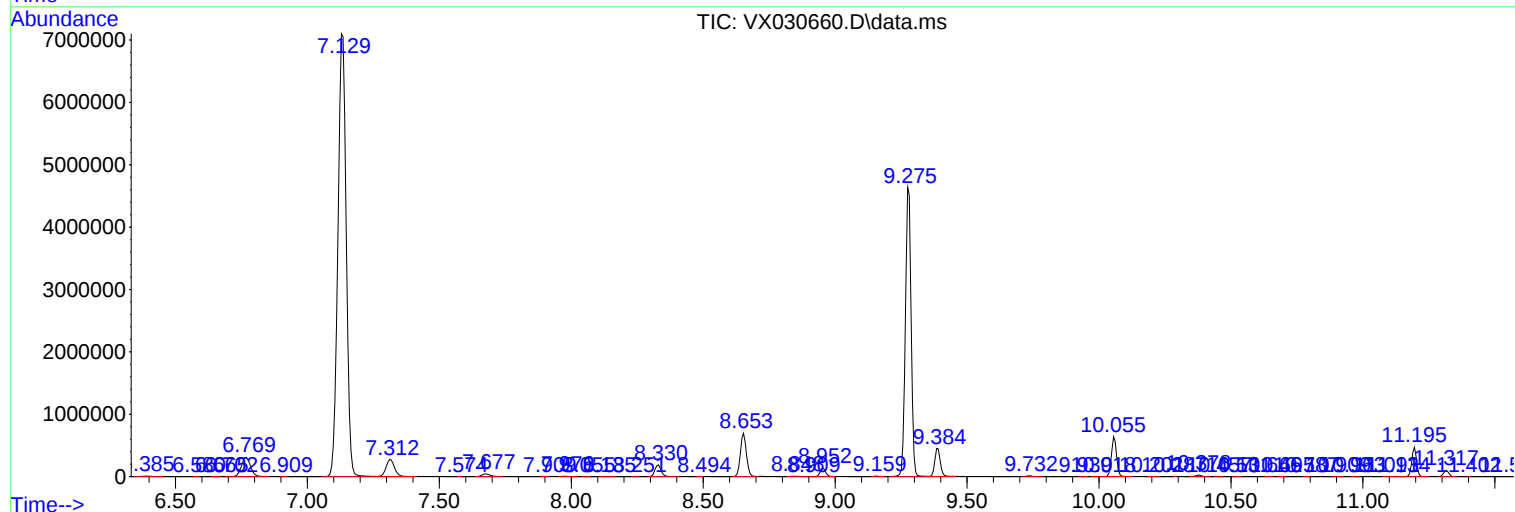
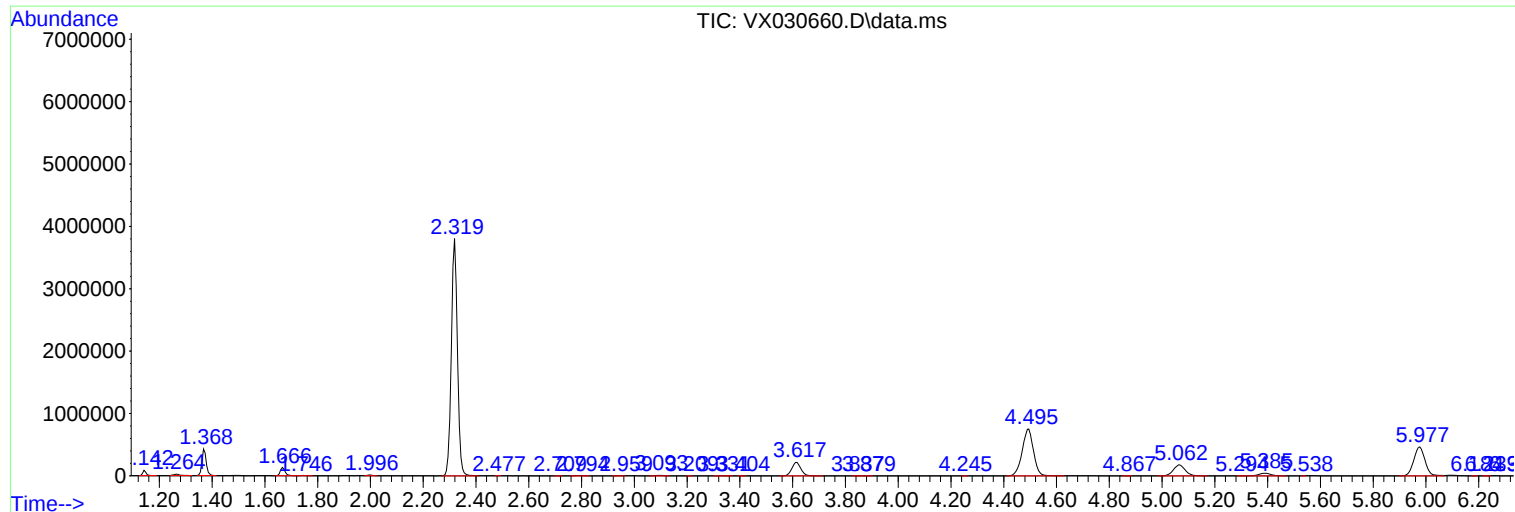
Sum of corrected areas: 41400951

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Instrument :
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ClientSampleId :
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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



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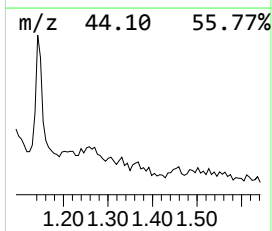
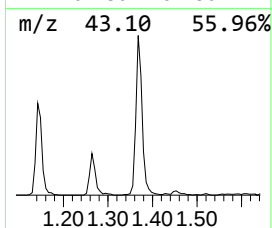
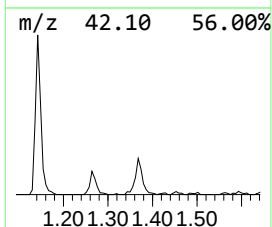
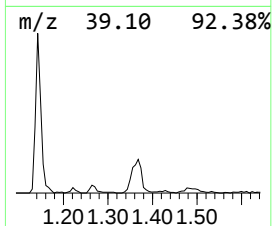
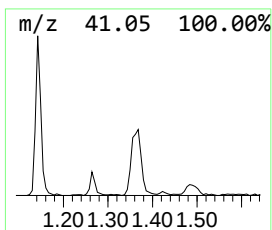
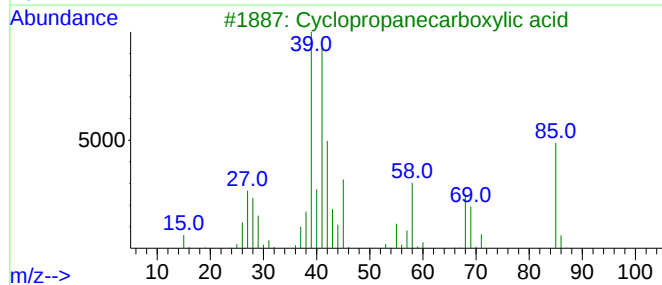
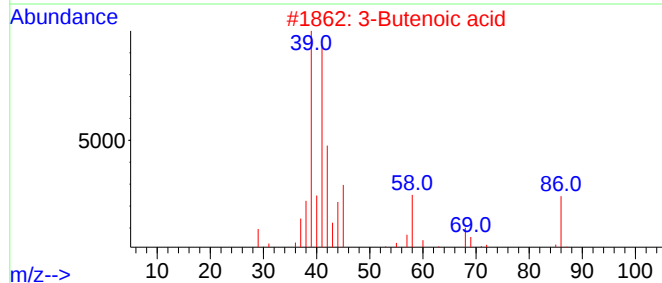
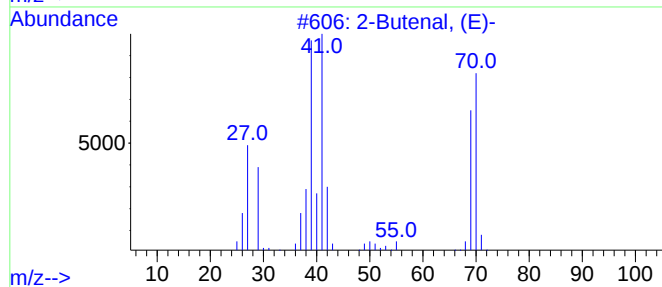
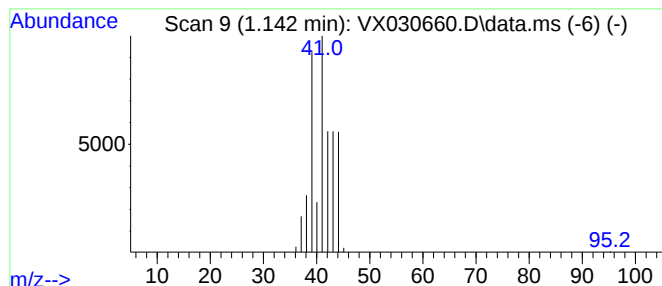
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Butenal, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	5.16 ug/L	75038	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-			70	C4H6O	000123-73-9	72
2	3-Butenoic acid			86	C4H6O2	000625-38-7	64
3	Cyclopropanecarboxylic acid			86	C4H6O2	001759-53-1	64
4	Furan, 2,5-dihydro-			70	C4H6O	001708-29-8	59
5	Cyclopropanecarboxylic acid			86	C4H6O2	001759-53-1	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butenal, (E)-	1.142	5.2	ug/L	75038	1	6.769	727475	50.0