

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035136.D
 Acq On : 18 Apr 2023 20:42
 Operator : JC/MD
 Sample : VX0418WBL03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK623

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.167	11	13	16	rVB3	1650	1290	0.07%	0.009%
2	1.264	24	29	42	rBV	50787	165553	9.00%	1.206%
3	1.368	42	46	58	rVB	228130	257865	14.02%	1.879%
4	1.673	92	96	110	rVB	161005	214919	11.68%	1.566%
5	2.307	194	200	211	rBV	423020	653443	35.53%	4.761%
6	2.514	229	234	239	rVB2	2942	4475	0.24%	0.033%
7	2.599	246	248	254	rBV3	363	665	0.04%	0.005%
8	2.715	258	267	272	rBV4	821	1828	0.10%	0.013%
9	2.788	274	279	284	rBV3	5052	9308	0.51%	0.068%
10	2.959	305	307	309	rVV	286	206	0.01%	0.002%
11	3.038	318	320	323	rVB2	366	311	0.02%	0.002%
12	3.105	323	331	340	rBV6	3115	8628	0.47%	0.063%
13	3.197	345	346	349	rBV2	166	220	0.01%	0.002%
14	3.319	364	366	371	rVB3	287	349	0.02%	0.003%
15	3.404	378	380	383	rVB	304	249	0.01%	0.002%
16	3.611	407	414	421	rBV4	1047	2499	0.14%	0.018%
17	3.727	431	433	437	rVB2	314	271	0.01%	0.002%
18	3.812	445	447	452	rVB2	227	233	0.01%	0.002%
19	3.892	457	460	463	rBV2	205	244	0.01%	0.002%
20	4.178	505	507	510	rVB2	389	314	0.02%	0.002%
21	4.306	524	528	530	rBV	150	230	0.01%	0.002%
22	4.465	545	554	573	rBV	117563	361060	19.63%	2.630%
23	4.745	599	600	602	rBV	404	249	0.01%	0.002%
24	4.891	622	624	626	rBV2	596	612	0.03%	0.004%
25	5.056	639	651	667	rBV	239464	712284	38.72%	5.189%
26	5.294	686	690	693	rBV2	353	683	0.04%	0.005%
27	5.349	698	699	700	rBV	489	213	0.01%	0.002%
28	5.379	700	704	705	rBV2	1593	1664	0.09%	0.012%
29	5.550	727	732	743	rVB4	1841	4579	0.25%	0.033%
30	5.641	746	747	749	rVV2	289	280	0.02%	0.002%
31	5.678	749	753	760	rVB6	895	2412	0.13%	0.018%
32	5.745	762	764	767	rBV2	336	384	0.02%	0.003%
33	5.806	772	774	779	rVB2	407	411	0.02%	0.003%
34	5.971	788	801	819	rBV2	613606	1839350	100.00%	13.400%
35	6.324	858	859	860	rBV	406	215	0.01%	0.002%
36	6.385	868	869	872	rBV2	337	276	0.02%	0.002%

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 Title : VOC Analysis

37	6.483	882	885	887	rBV2	277	269	0.01%	0.002%
38	6.763	921	931	949	rBV	472373	1139124	61.93%	8.299%
39	7.013	970	972	976	rVB3	429	576	0.03%	0.004%
40	7.062	976	980	982	rBV3	341	409	0.02%	0.003%
41	7.129	982	991	1000	rBV6	4174	11981	0.65%	0.087%
42	7.306	1011	1020	1037	rBV	371433	832227	45.25%	6.063%
43	7.562	1060	1062	1064	rVB2	256	207	0.01%	0.002%
44	7.598	1064	1068	1070	rVB	378	469	0.03%	0.003%
45	7.641	1070	1075	1079	rBV2	226	476	0.03%	0.003%
46	7.684	1079	1082	1085	rVB2	234	349	0.02%	0.003%
47	7.781	1095	1098	1101	rBV2	337	565	0.03%	0.004%
48	7.824	1101	1105	1110	rVV4	772	1366	0.07%	0.010%
49	7.946	1118	1125	1132	rBV5	1021	2669	0.15%	0.019%
50	8.025	1134	1138	1140	rVV4	352	436	0.02%	0.003%
51	8.324	1180	1187	1207	rBV	232722	380877	20.71%	2.775%
52	8.494	1212	1215	1216	rBV2	800	671	0.04%	0.005%
53	8.580	1224	1229	1233	rBV3	2790	4295	0.23%	0.031%
54	8.647	1234	1240	1249	rBV	950407	1499443	81.52%	10.924%
55	8.952	1284	1290	1304	rBV	153607	239803	13.04%	1.747%
56	9.165	1320	1325	1328	rVB3	2104	3273	0.18%	0.024%
57	9.226	1331	1335	1337	rBV	361	449	0.02%	0.003%
58	9.275	1339	1343	1348	rVB5	3703	5375	0.29%	0.039%
59	9.385	1355	1361	1377	rBV	555264	785272	42.69%	5.721%
60	9.720	1414	1416	1420	rBV3	277	312	0.02%	0.002%
61	9.793	1426	1428	1430	rVB	558	346	0.02%	0.003%
62	9.830	1430	1434	1436	rBV2	213	315	0.02%	0.002%
63	9.903	1444	1446	1449	rBV3	336	243	0.01%	0.002%
64	9.927	1449	1450	1453	rVV2	290	210	0.01%	0.002%
65	9.970	1456	1457	1461	rVB	396	269	0.01%	0.002%
66	10.055	1465	1471	1488	rVV	936149	1289848	70.13%	9.397%
67	10.195	1491	1494	1500	rVB2	4644	7128	0.39%	0.052%
68	10.305	1508	1512	1517	rVB2	4640	6524	0.35%	0.048%
69	10.610	1559	1562	1563	rBV2	269	260	0.01%	0.002%
70	10.647	1563	1568	1579	rVV3	6215	13088	0.71%	0.095%
71	10.799	1590	1593	1599	rVB2	812	1104	0.06%	0.008%
72	10.909	1609	1611	1613	rBV2	273	273	0.01%	0.002%
73	10.964	1616	1620	1628	rVB2	5787	7785	0.42%	0.057%
74	11.079	1637	1639	1640	rBV	268	229	0.01%	0.002%
75	11.189	1652	1657	1664	rBV	601754	794133	43.17%	5.786%
76	11.451	1697	1700	1707	rVB	5506	6668	0.36%	0.049%

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 Title : VOC Analysis

77	11.756	1745	1750	1755	rVB	5322	6321	0.34%	0.046%
78	11.829	1757	1762	1763	rBV2	206	248	0.01%	0.002%
79	11.884	1768	1771	1772	rBV2	196	224	0.01%	0.002%
80	11.969	1780	1785	1788	rBV	4981	6521	0.35%	0.048%
81	12.024	1788	1794	1806	rVB	899297	1174516	63.85%	8.557%
82	12.146	1813	1814	1819	rVB2	728	688	0.04%	0.005%
83	12.238	1827	1829	1831	rBV2	301	219	0.01%	0.002%
84	12.317	1837	1842	1861	rVB	956574	1216657	66.15%	8.864%
85	12.683	1900	1902	1905	rVV2	257	239	0.01%	0.002%
86	12.829	1922	1926	1930	rBV3	302	705	0.04%	0.005%
87	12.866	1930	1932	1935	rVB	286	273	0.01%	0.002%
88	12.945	1943	1945	1948	rVV2	750	896	0.05%	0.007%
89	12.975	1948	1950	1955	rVV2	261	401	0.02%	0.003%
90	13.024	1956	1958	1960	rVV	288	210	0.01%	0.002%
91	13.116	1968	1973	1979	rVB	7086	9322	0.51%	0.068%
92	13.329	2006	2008	2010	rBV2	281	330	0.02%	0.002%
93	13.591	2046	2051	2058	rBV4	5203	7583	0.41%	0.055%
94	13.780	2078	2082	2087	rVB	4939	5779	0.31%	0.042%
95	13.963	2109	2112	2116	rBV2	4529	5436	0.30%	0.040%
96	14.128	2136	2139	2141	rBV3	813	849	0.05%	0.006%
97	14.195	2148	2150	2154	rVB3	379	429	0.02%	0.003%
98	14.640	2221	2223	2225	rBV2	418	290	0.02%	0.002%
99	14.664	2225	2227	2230	rVV	401	429	0.02%	0.003%
100	14.756	2240	2242	2243	rBV2	446	446	0.02%	0.003%

Sum of corrected areas: 13726099

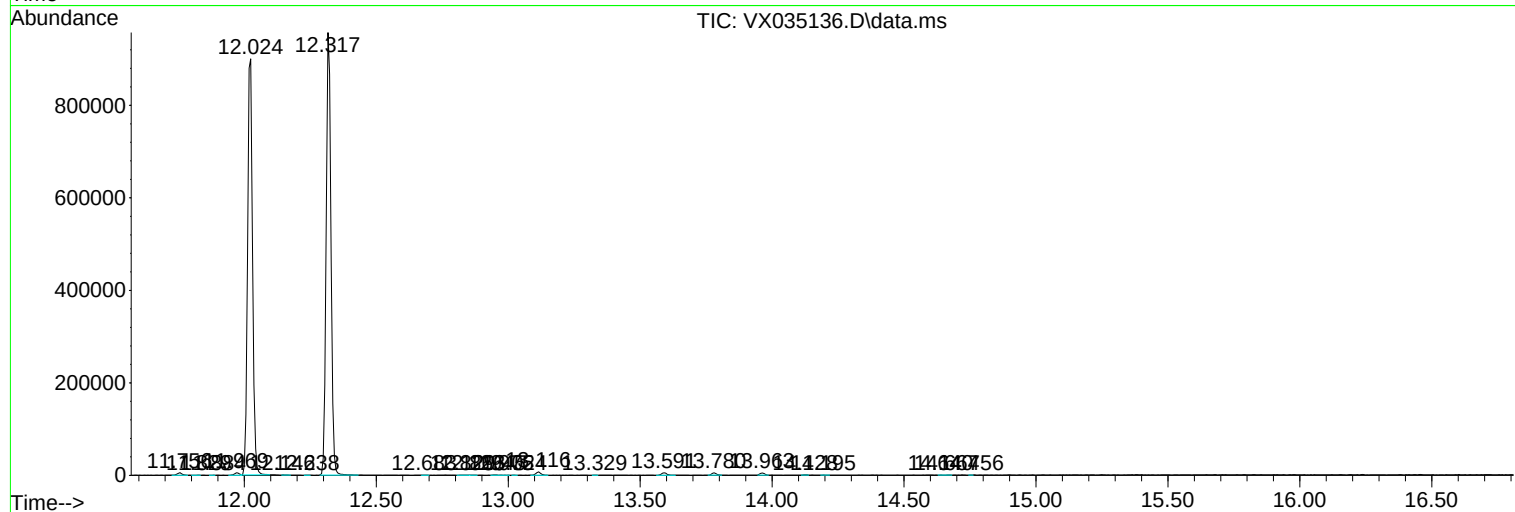
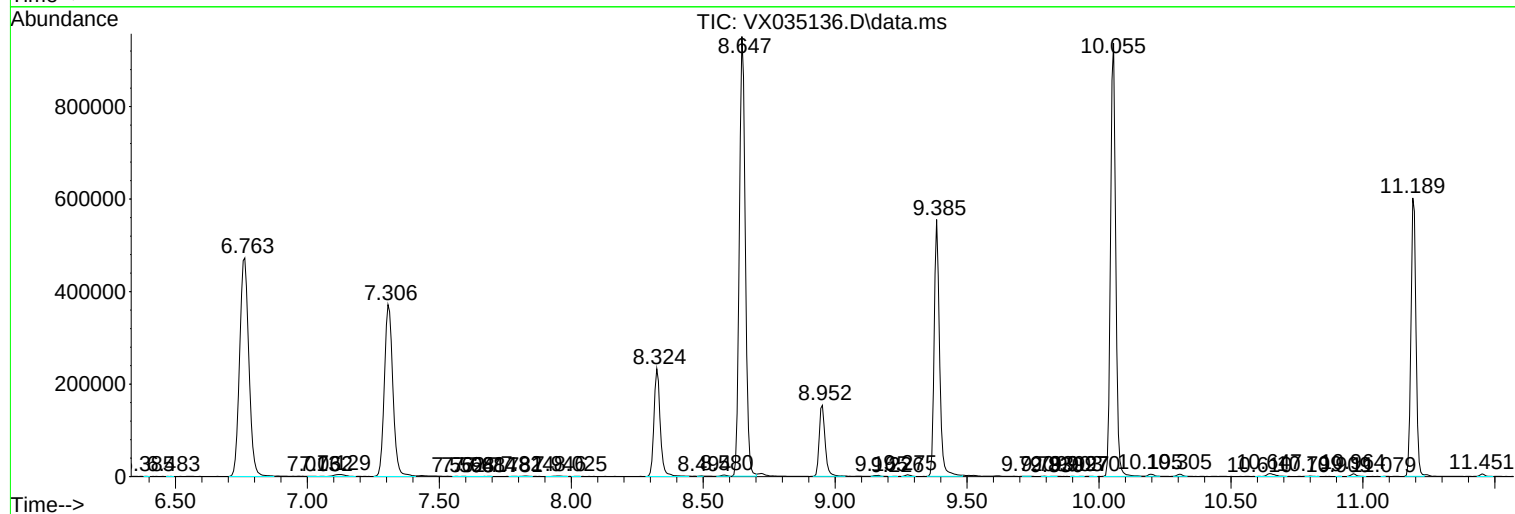
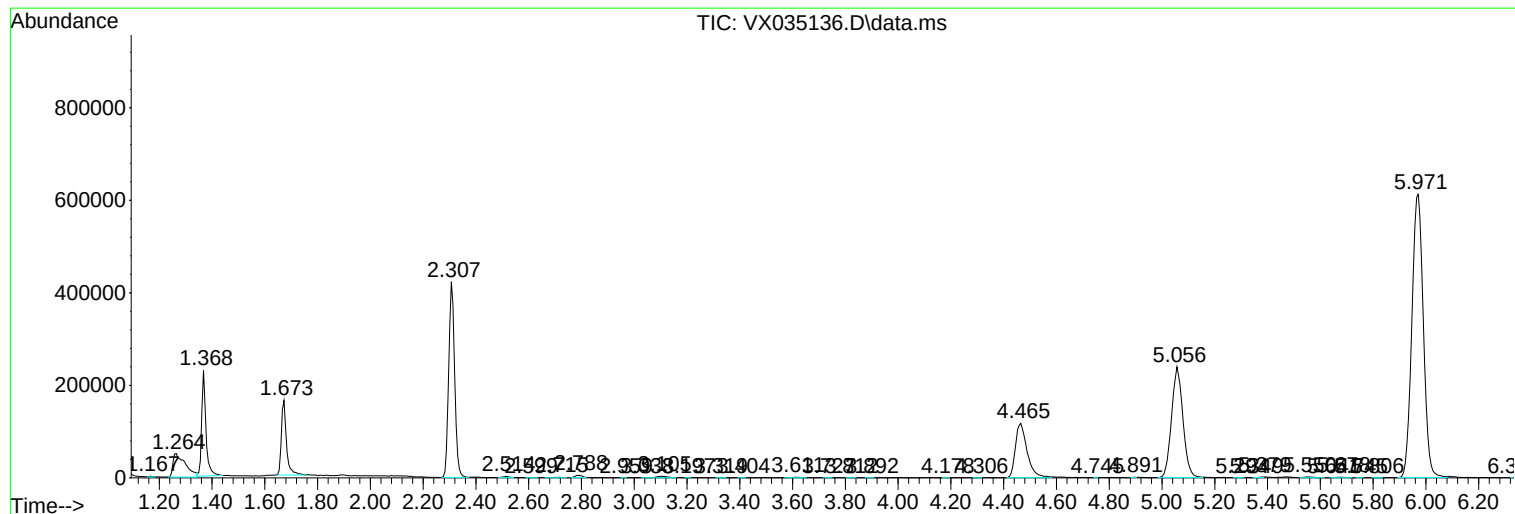
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
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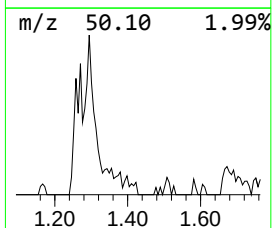
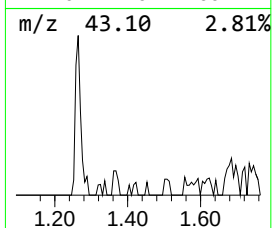
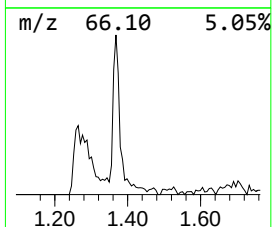
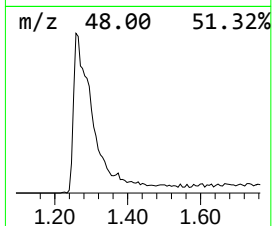
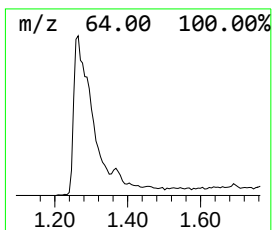
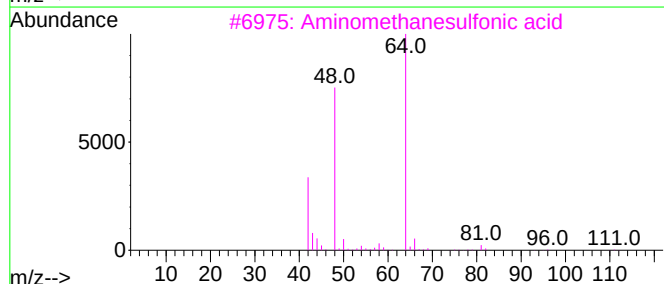
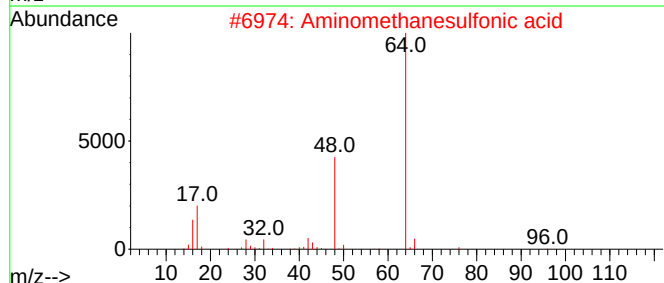
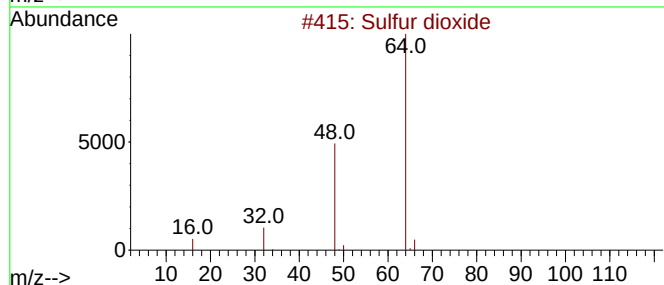
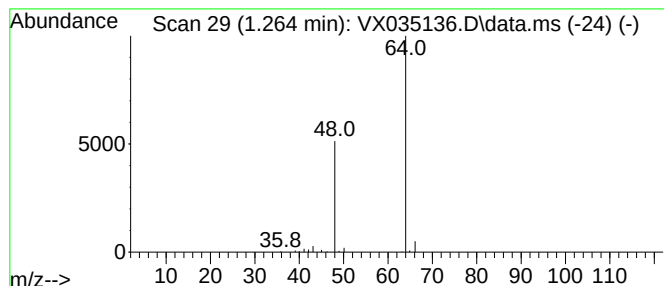
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	7.27 ug/L	165553	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.264	7.3	ug/L	165553	1	6.763	1139120	50.0