

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035134.D
 Acq On : 18 Apr 2023 19:33
 Operator : JC/MD
 Sample : 02333-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMG5

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: VX035134.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	18	rVB2	7375	7729	0.53%	0.065%
2	1.246	23	26	42	rBV	249842	477965	32.83%	4.016%
3	1.368	43	46	59	rVB	180230	206871	14.21%	1.738%
4	1.672	92	96	109	rVB	121717	159589	10.96%	1.341%
5	2.306	194	200	212	rBV	334720	516336	35.47%	4.339%
6	2.514	230	234	238	rBV3	1043	1575	0.11%	0.013%
7	2.642	253	255	258	rBV2	382	349	0.02%	0.003%
8	2.703	263	265	267	rBV	394	409	0.03%	0.003%
9	2.788	275	279	287	rVB4	1066	2028	0.14%	0.017%
10	2.886	293	295	300	rBV3	411	698	0.05%	0.006%
11	2.940	300	304	306	rVV2	582	679	0.05%	0.006%
12	2.977	309	310	312	rBV	315	234	0.02%	0.002%
13	3.111	324	332	343	rBV2	27282	63374	4.35%	0.533%
14	3.300	360	363	364	rBV	211	225	0.02%	0.002%
15	3.410	379	381	384	rVB3	270	245	0.02%	0.002%
16	3.440	384	386	392	rVB4	490	795	0.05%	0.007%
17	3.581	406	409	412	rBV2	338	411	0.03%	0.003%
18	3.617	412	415	416	rVV	396	357	0.02%	0.003%
19	3.660	420	422	423	rVV	480	359	0.02%	0.003%
20	4.117	496	497	501	rVB2	265	266	0.02%	0.002%
21	4.343	533	534	537	rBV	278	313	0.02%	0.003%
22	4.379	539	540	543	rBV2	215	288	0.02%	0.002%
23	4.458	545	553	572	rBV	89486	273488	18.78%	2.298%
24	4.824	609	613	617	rBV3	275	423	0.03%	0.004%
25	4.891	623	624	626	rBV2	259	234	0.02%	0.002%
26	5.056	640	651	670	rBV	179397	552259	37.93%	4.641%
27	5.373	700	703	704	rBV	475	411	0.03%	0.003%
28	5.556	727	733	743	rVB4	1870	4378	0.30%	0.037%
29	5.659	748	750	753	rVB2	279	270	0.02%	0.002%
30	5.970	787	801	818	rBV2	491623	1455903	100.00%	12.234%
31	6.324	851	859	866	rBV3	3410	9052	0.62%	0.076%
32	6.409	869	873	875	rVB2	234	286	0.02%	0.002%
33	6.495	885	887	889	rVB	415	253	0.02%	0.002%
34	6.550	893	896	899	rBV2	564	642	0.04%	0.005%
35	6.647	909	912	915	rBV2	266	248	0.02%	0.002%
36	6.763	921	931	948	rBV	484468	1170148	80.37%	9.833%

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 Title : VOC Analysis

37	6.909	953	955	956	rVB2	675	384	0.03%	0.003%
38	6.982	965	967	969	rBV2	312	331	0.02%	0.003%
39	7.110	983	988	990	rBV5	922	1569	0.11%	0.013%
40	7.196	1001	1002	1008	rBV2	346	572	0.04%	0.005%
41	7.306	1011	1020	1037	rBV	297374	650695	44.69%	5.468%
42	7.482	1046	1049	1053	rBV4	740	1015	0.07%	0.009%
43	7.665	1075	1079	1081	rBV2	210	304	0.02%	0.003%
44	7.946	1123	1125	1132	rVB3	627	871	0.06%	0.007%
45	8.135	1154	1156	1160	rVB	273	318	0.02%	0.003%
46	8.220	1168	1170	1172	rBV	328	238	0.02%	0.002%
47	8.324	1181	1187	1203	rBV	164073	270572	18.58%	2.274%
48	8.494	1213	1215	1222	rVB4	509	1002	0.07%	0.008%
49	8.647	1234	1240	1259	rBV	759067	1198408	82.31%	10.070%
50	8.952	1284	1290	1303	rBV	109589	167047	11.47%	1.404%
51	9.141	1320	1321	1326	rVB2	445	395	0.03%	0.003%
52	9.202	1329	1331	1334	rBV2	210	259	0.02%	0.002%
53	9.281	1339	1344	1347	rVB2	1006	1719	0.12%	0.014%
54	9.384	1356	1361	1376	rBV	418734	604366	41.51%	5.078%
55	9.677	1408	1409	1412	rVB2	519	313	0.02%	0.003%
56	10.055	1465	1471	1482	rBV	930599	1313012	90.19%	11.033%
57	10.299	1509	1511	1513	rBV2	431	480	0.03%	0.004%
58	10.384	1524	1525	1527	rBV2	321	248	0.02%	0.002%
59	10.537	1548	1550	1552	rBV	352	241	0.02%	0.002%
60	10.640	1565	1567	1571	rBV3	363	413	0.03%	0.003%
61	10.707	1577	1578	1580	rVB2	487	254	0.02%	0.002%
62	10.781	1587	1590	1591	rBV2	286	266	0.02%	0.002%
63	10.902	1609	1610	1614	rVB2	281	274	0.02%	0.002%
64	10.945	1614	1617	1619	rBV2	203	266	0.02%	0.002%
65	10.976	1619	1622	1623	rVV2	300	301	0.02%	0.003%
66	11.116	1644	1645	1648	rVB	346	281	0.02%	0.002%
67	11.189	1652	1657	1666	rBV	470574	620115	42.59%	5.211%
68	11.305	1673	1676	1681	rBV5	847	1312	0.09%	0.011%
69	11.384	1687	1689	1691	rBV	308	346	0.02%	0.003%
70	11.451	1698	1700	1705	rVB3	418	529	0.04%	0.004%
71	11.494	1705	1707	1709	rBV	237	230	0.02%	0.002%
72	11.555	1714	1717	1720	rBV2	295	368	0.03%	0.003%
73	11.707	1740	1742	1746	rBV2	339	337	0.02%	0.003%
74	11.750	1747	1749	1751	rBV2	477	444	0.03%	0.004%
75	11.969	1783	1785	1788	rBV3	575	491	0.03%	0.004%
76	12.024	1788	1794	1805	rBV	902928	1185852	81.45%	9.965%

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Stop Thrs : 0

Peak Location: TOP

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
 Title : VOC Analysis

77	12.195	1821	1822	1823	rBV	413	292	0.02%	0.002%
78	12.219	1823	1826	1832	rVB3	2563	3785	0.26%	0.032%
79	12.317	1837	1842	1853	rBV	735543	953461	65.49%	8.012%
80	12.451	1862	1864	1867	rVB2	627	435	0.03%	0.004%
81	12.622	1889	1892	1894	rVB2	344	315	0.02%	0.003%
82	12.640	1894	1895	1897	rBV	295	279	0.02%	0.002%
83	12.890	1934	1936	1939	rVB2	307	279	0.02%	0.002%
84	12.951	1945	1946	1948	rBV	482	304	0.02%	0.003%
85	13.085	1967	1968	1971	rBV	371	248	0.02%	0.002%
86	13.122	1971	1974	1977	rVV	297	283	0.02%	0.002%
87	13.146	1977	1978	1981	rVB	315	245	0.02%	0.002%
88	13.183	1981	1984	1986	rBV2	273	293	0.02%	0.002%
89	13.439	2025	2026	2029	rVB2	387	285	0.02%	0.002%
90	13.591	2048	2051	2052	rBV2	470	483	0.03%	0.004%
91	13.676	2063	2065	2067	rBV2	403	373	0.03%	0.003%
92	13.786	2080	2083	2085	rBV2	575	614	0.04%	0.005%
93	13.908	2101	2103	2104	rBV	393	257	0.02%	0.002%
94	13.938	2104	2108	2110	rVB3	289	422	0.03%	0.004%
95	13.963	2110	2112	2116	rBV2	436	455	0.03%	0.004%
96	14.036	2121	2124	2126	rBV	388	472	0.03%	0.004%
97	14.115	2136	2137	2139	rBV	516	336	0.02%	0.003%
98	14.365	2176	2178	2180	rBV2	514	386	0.03%	0.003%
99	14.536	2202	2206	2207	rBV2	317	306	0.02%	0.003%
100	14.865	2258	2260	2264	rBV3	546	597	0.04%	0.005%

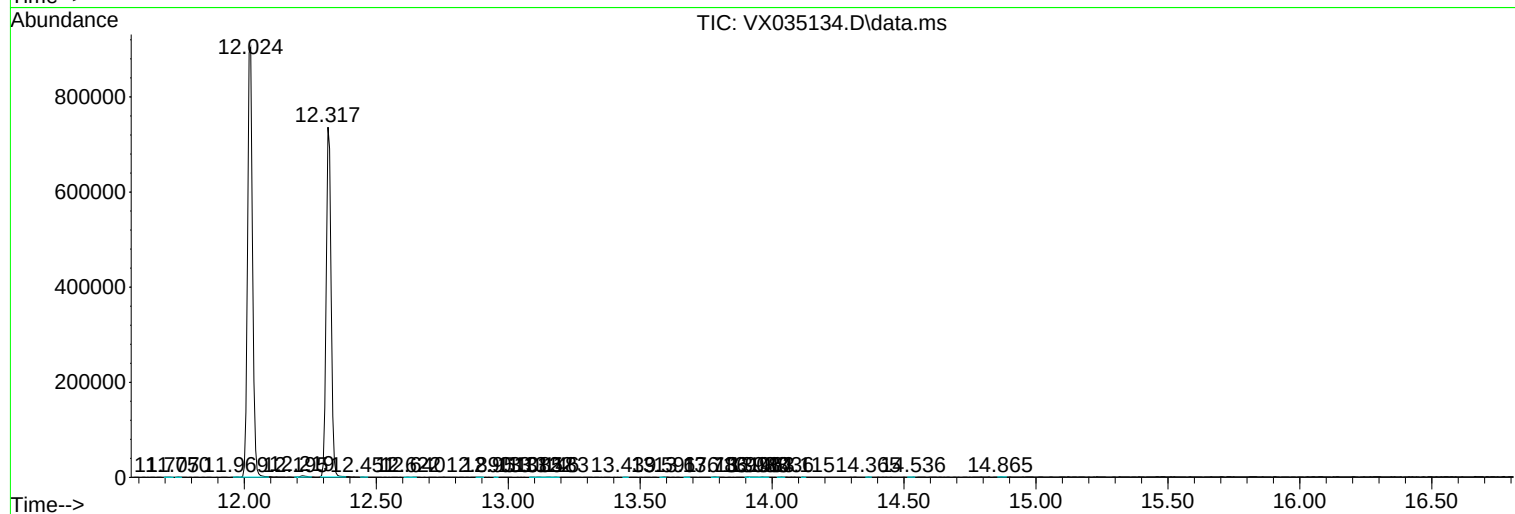
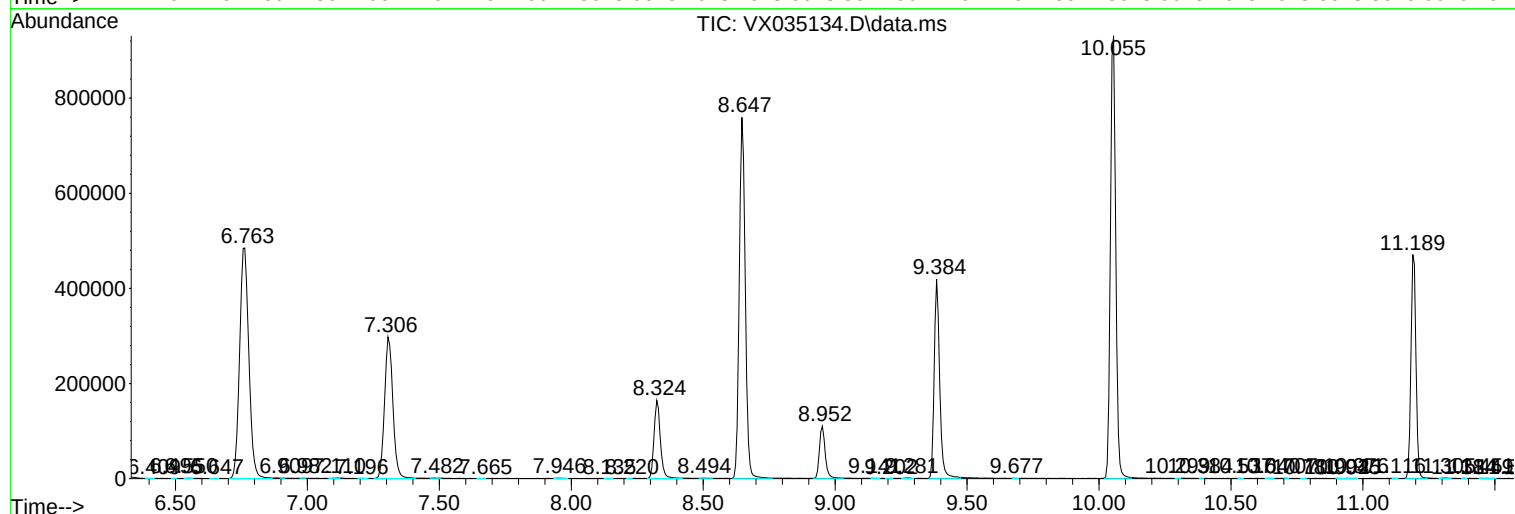
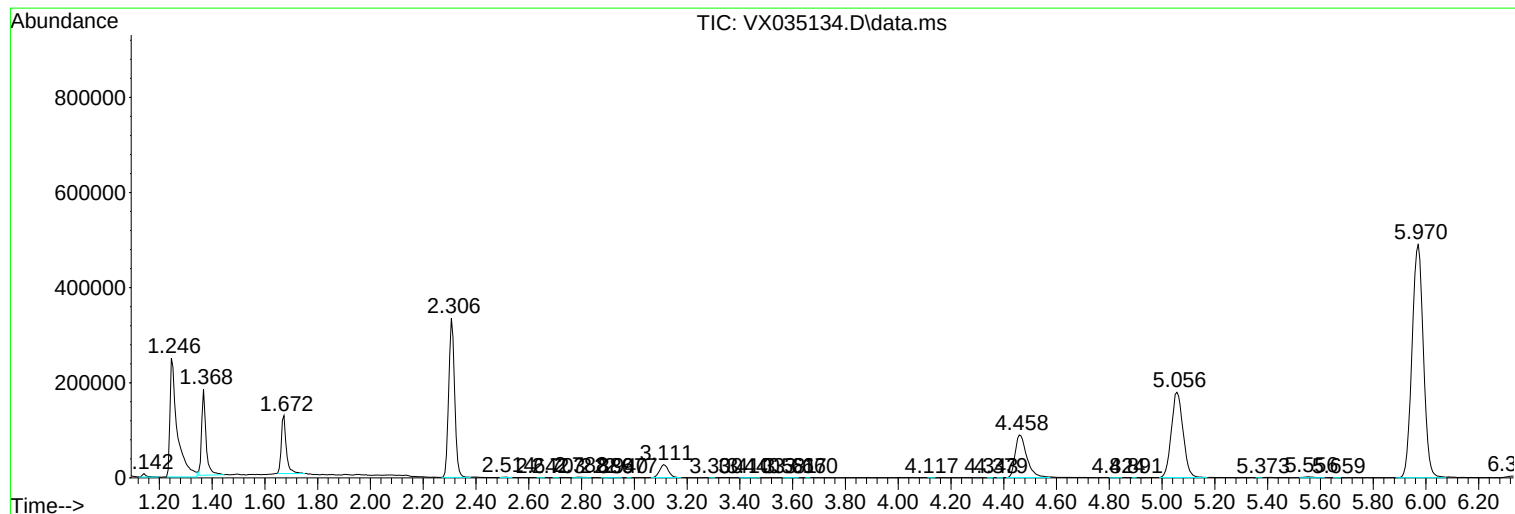
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



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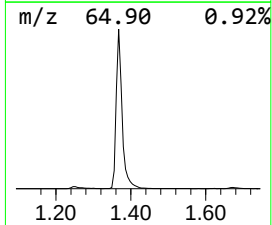
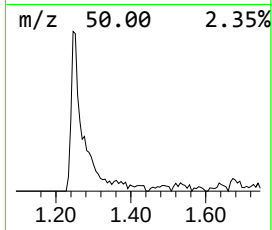
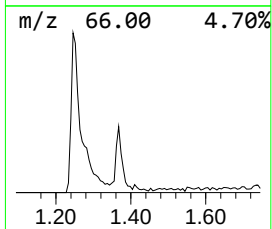
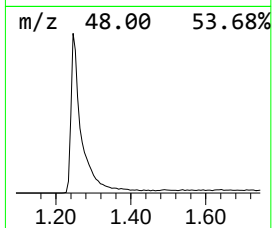
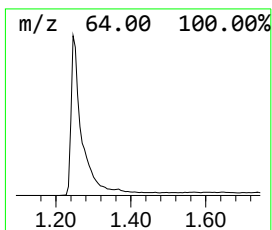
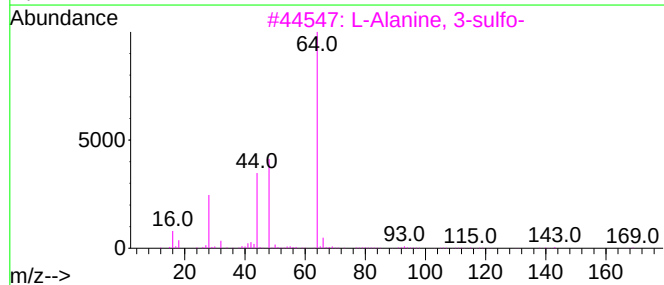
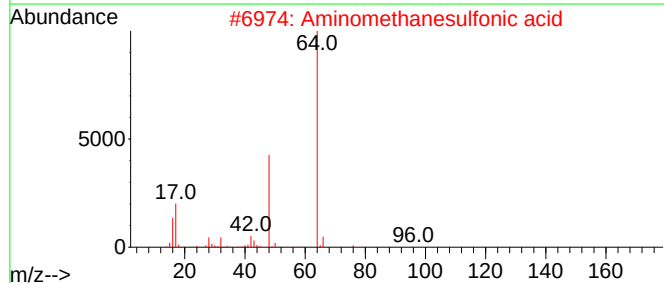
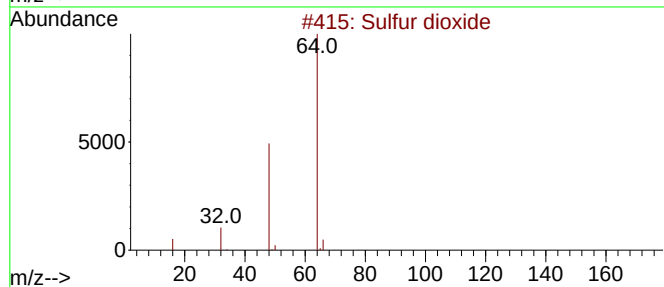
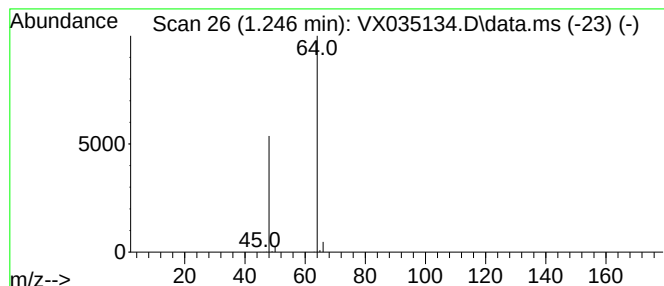
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	20.42 ug/L	477965	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.246	20.4	ug/L	477965	1	6.763	1170150	50.0