

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035174.D
 Acq On : 19 Apr 2023 17:01
 Operator : JC/MD
 Sample : 02333-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMG6

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: VX035174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.251	23	27	43	rBV	219180	430887	31.57%	3.933%
2	1.367	43	46	58	rVB	163660	187991	13.77%	1.716%
3	1.672	92	96	105	rBV	120950	151923	11.13%	1.387%
4	2.306	194	200	211	rBV	303829	480005	35.17%	4.381%
5	2.507	231	233	238	rVB2	651	891	0.07%	0.008%
6	2.702	264	265	268	rBV2	413	339	0.02%	0.003%
7	2.794	276	280	284	rVV4	1033	1783	0.13%	0.016%
8	2.824	284	285	288	rVB	449	188	0.01%	0.002%
9	3.105	329	331	332	rVB	372	169	0.01%	0.002%
10	3.141	335	337	340	rBV3	242	262	0.02%	0.002%
11	3.257	353	356	359	rBV2	339	417	0.03%	0.004%
12	3.342	368	370	372	rVB	300	161	0.01%	0.001%
13	3.373	372	375	377	rVB2	178	189	0.01%	0.002%
14	3.403	377	380	383	rVB2	300	428	0.03%	0.004%
15	3.458	386	389	392	rVB2	254	292	0.02%	0.003%
16	3.489	392	394	396	rBV2	180	150	0.01%	0.001%
17	3.513	396	398	400	rBV2	239	233	0.02%	0.002%
18	3.580	406	409	412	rBV2	187	221	0.02%	0.002%
19	3.629	414	417	418	rVB2	257	195	0.01%	0.002%
20	3.672	423	424	427	rVB2	302	261	0.02%	0.002%
21	3.702	427	429	430	rBV	214	160	0.01%	0.001%
22	3.818	444	448	449	rBV2	156	192	0.01%	0.002%
23	3.836	449	451	452	rVB	406	226	0.02%	0.002%
24	3.861	452	455	459	rBV2	299	614	0.04%	0.006%
25	4.111	494	496	499	rBV2	261	309	0.02%	0.003%
26	4.147	501	502	504	rVB	302	197	0.01%	0.002%
27	4.172	504	506	510	rBV2	244	361	0.03%	0.003%
28	4.306	525	528	531	rBV2	264	328	0.02%	0.003%
29	4.367	534	538	539	rBV2	435	427	0.03%	0.004%
30	4.464	545	554	577	rBV2	77078	241180	17.67%	2.201%
31	4.885	620	623	626	rBV3	329	309	0.02%	0.003%
32	5.056	639	651	666	rBV	180885	522870	38.31%	4.772%
33	5.464	715	718	721	rBV	290	336	0.02%	0.003%
34	5.549	725	732	733	rBV3	1423	2228	0.16%	0.020%
35	5.623	743	744	746	rVB	413	175	0.01%	0.002%
36	5.690	753	755	757	rVB	250	191	0.01%	0.002%

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 Title : VOC Analysis

37	5.781	767	770	772	rBV2	267	281	0.02%	0.003%
38	5.970	789	801	819	rBV2	456762	1364767	100.00%	12.456%
39	6.196	837	838	840	rVV	368	157	0.01%	0.001%
40	6.232	843	844	846	rVB	287	166	0.01%	0.002%
41	6.324	855	859	862	rVB2	327	349	0.03%	0.003%
42	6.403	870	872	873	rVB	384	194	0.01%	0.002%
43	6.464	880	882	884	rBV2	280	179	0.01%	0.002%
44	6.537	890	894	896	rBV2	400	525	0.04%	0.005%
45	6.616	905	907	908	rBV	212	164	0.01%	0.001%
46	6.763	921	931	951	rBV	456860	1093595	80.13%	9.981%
47	7.110	984	988	991	rBV4	784	1241	0.09%	0.011%
48	7.305	1011	1020	1034	rBV	274214	612758	44.90%	5.593%
49	7.665	1076	1079	1082	rBV2	340	483	0.04%	0.004%
50	7.848	1106	1109	1111	rBV	238	336	0.02%	0.003%
51	7.921	1119	1121	1123	rBV	303	362	0.03%	0.003%
52	8.171	1158	1162	1163	rBV2	261	255	0.02%	0.002%
53	8.244	1171	1174	1175	rBV2	288	281	0.02%	0.003%
54	8.323	1181	1187	1201	rBV	136291	229214	16.80%	2.092%
55	8.646	1233	1240	1252	rBV	698710	1114866	81.69%	10.175%
56	8.951	1284	1290	1300	rBV	95791	141342	10.36%	1.290%
57	9.274	1340	1343	1347	rBV3	1749	2172	0.16%	0.020%
58	9.384	1356	1361	1383	rBV	367546	532949	39.05%	4.864%
59	9.811	1429	1431	1434	rBV	295	221	0.02%	0.002%
60	10.055	1465	1471	1487	rBV	913321	1234432	90.45%	11.267%
61	10.396	1525	1527	1528	rVB2	345	200	0.01%	0.002%
62	10.408	1528	1529	1533	rBV2	226	274	0.02%	0.003%
63	10.445	1533	1535	1536	rBV	268	169	0.01%	0.002%
64	10.585	1556	1558	1559	rBV	271	152	0.01%	0.001%
65	10.719	1578	1580	1582	rBV	402	302	0.02%	0.003%
66	10.933	1614	1615	1617	rBV	185	163	0.01%	0.001%
67	11.061	1634	1636	1638	rVB	284	150	0.01%	0.001%
68	11.085	1638	1640	1642	rBV2	214	207	0.02%	0.002%
69	11.189	1652	1657	1668	rBV	440709	574323	42.08%	5.242%
70	11.317	1675	1678	1681	rVB3	705	1002	0.07%	0.009%
71	11.414	1692	1694	1696	rBV	268	258	0.02%	0.002%
72	11.554	1716	1717	1718	rBV	296	150	0.01%	0.001%
73	11.646	1728	1732	1733	rBV2	234	356	0.03%	0.003%
74	11.676	1736	1737	1740	rVV2	317	249	0.02%	0.002%
75	11.713	1740	1743	1744	rVV2	335	339	0.02%	0.003%
76	11.750	1747	1749	1753	rVB2	263	248	0.02%	0.002%

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77	11.926	1777	1778	1780	rBV	409	263	0.02%	0.002%
78	11.969	1782	1785	1788	rBV3	1384	1819	0.13%	0.017%
79	12.024	1788	1794	1805	rVV	850339	1104202	80.91%	10.078%
80	12.219	1822	1826	1835	rBV5	3794	6755	0.49%	0.062%
81	12.316	1837	1842	1851	rBV	682811	887943	65.06%	8.104%
82	12.542	1878	1879	1881	rBV	420	175	0.01%	0.002%
83	12.627	1891	1893	1895	rBV2	347	407	0.03%	0.004%
84	12.719	1906	1908	1911	rVV	233	202	0.01%	0.002%
85	12.871	1930	1933	1934	rBV3	341	350	0.03%	0.003%
86	12.963	1946	1948	1951	rBV2	313	396	0.03%	0.004%
87	13.085	1967	1968	1971	rBV	221	242	0.02%	0.002%
88	13.146	1976	1978	1983	rVB2	342	381	0.03%	0.003%
89	13.188	1983	1985	1986	rBV	355	173	0.01%	0.002%
90	13.292	2000	2002	2003	rBV	253	170	0.01%	0.002%
91	13.359	2011	2013	2018	rBV2	373	444	0.03%	0.004%
92	13.463	2028	2030	2033	rVB2	246	168	0.01%	0.002%
93	13.591	2047	2051	2056	rBV2	7621	9923	0.73%	0.091%
94	13.700	2066	2069	2070	rBV2	308	285	0.02%	0.003%
95	13.719	2070	2072	2075	rBV2	206	242	0.02%	0.002%
96	13.963	2108	2112	2116	rVB4	1604	2209	0.16%	0.020%
97	14.170	2143	2146	2150	rBV2	444	608	0.04%	0.006%
98	14.688	2229	2231	2234	rBV2	504	582	0.04%	0.005%
99	15.249	2321	2323	2326	rBV2	883	1062	0.08%	0.010%
100	15.468	2357	2359	2360	rVB2	804	465	0.03%	0.004%

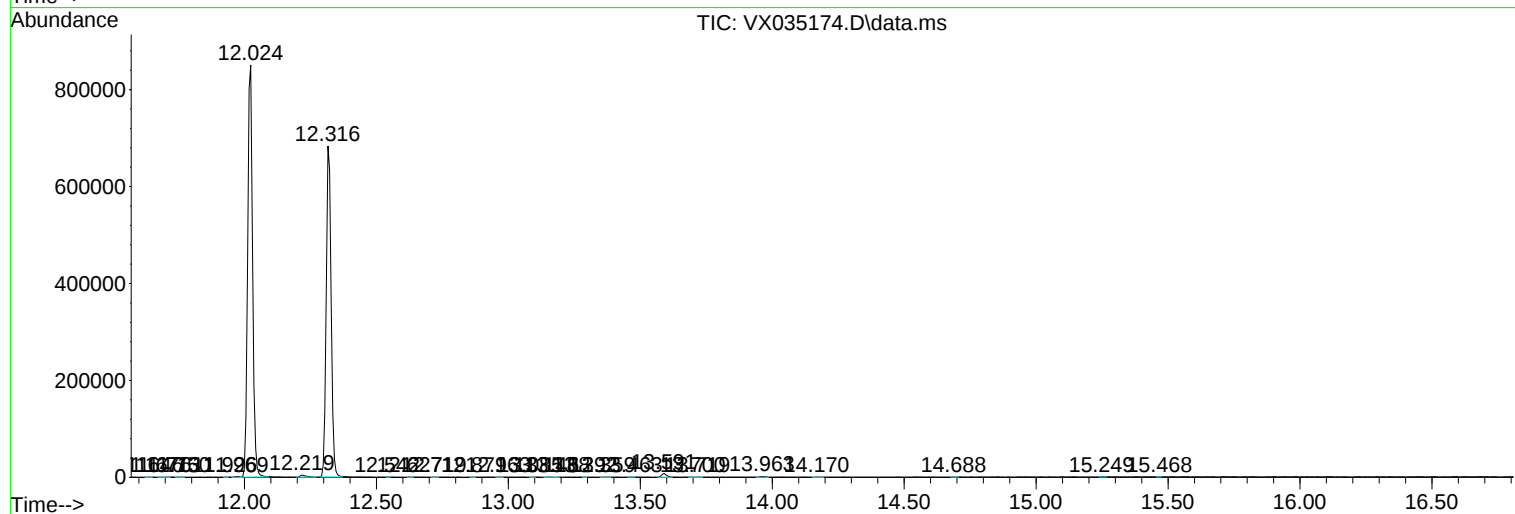
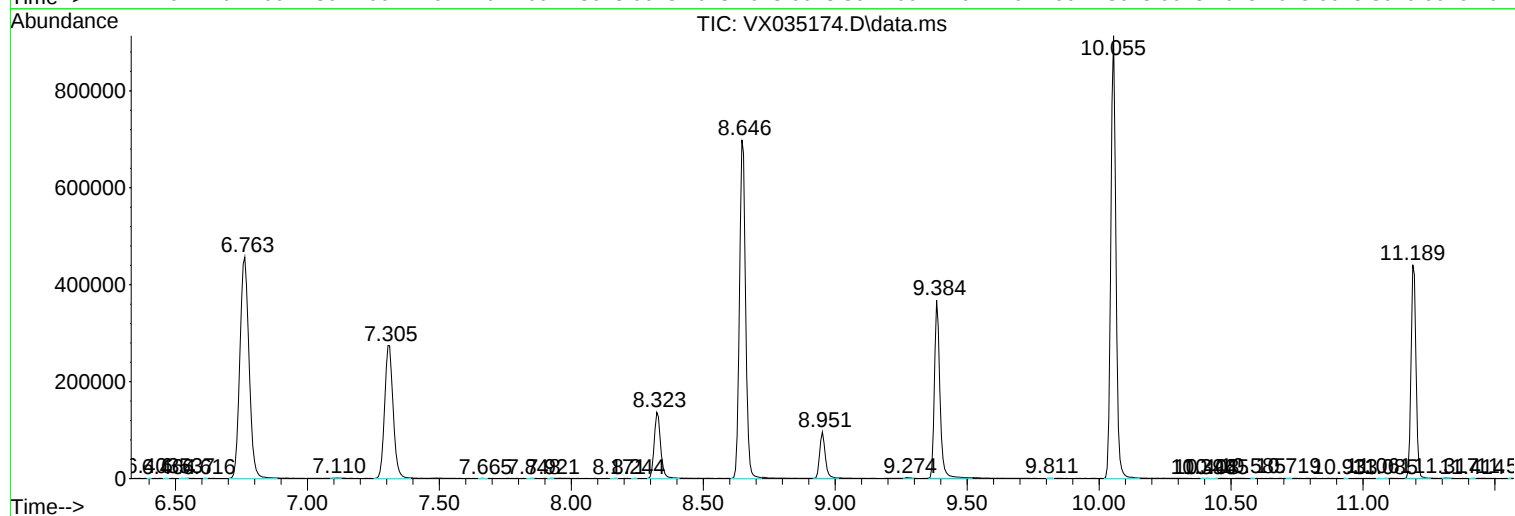
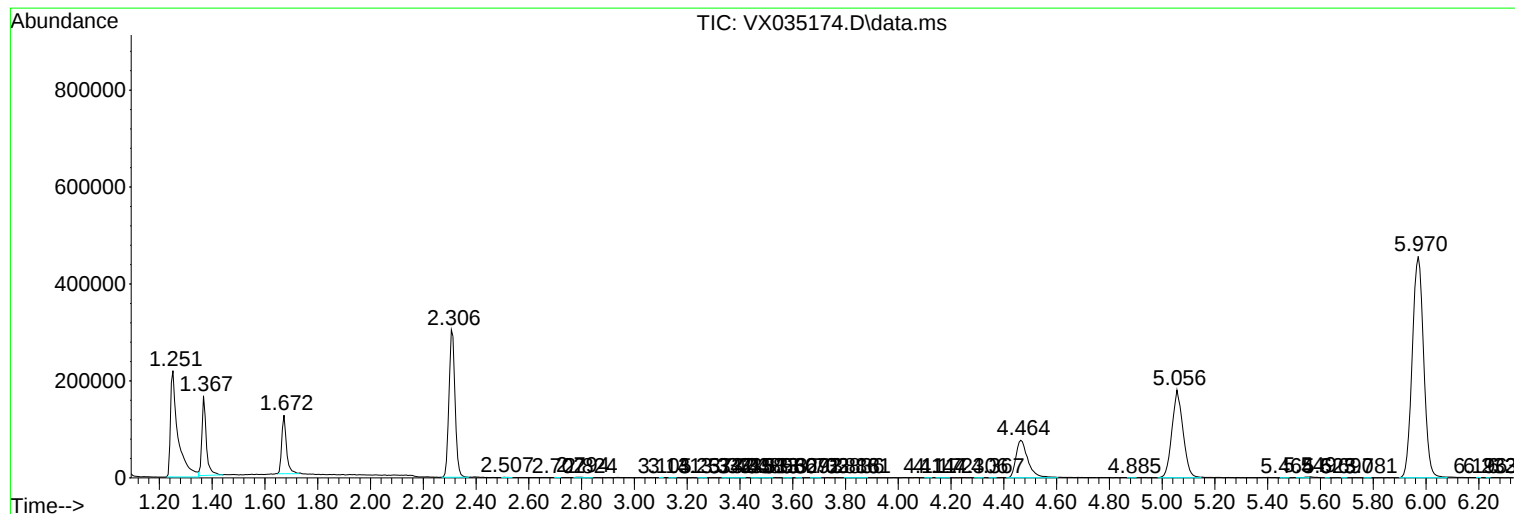
Sum of corrected areas: 10956385

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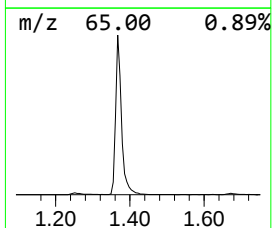
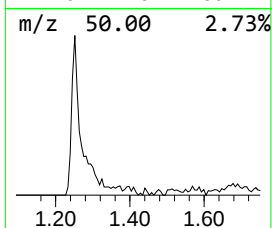
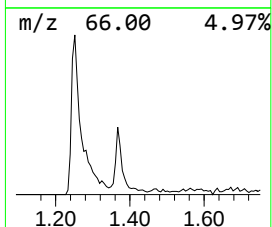
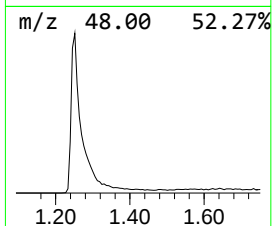
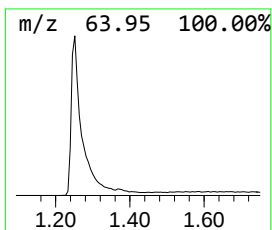
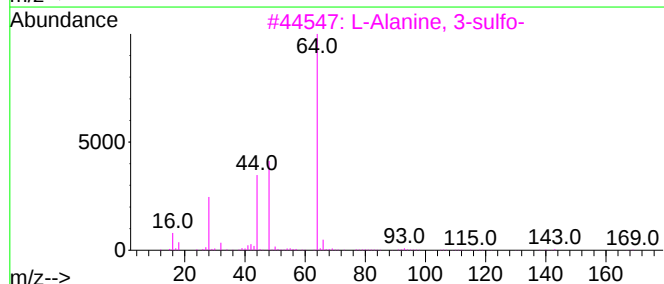
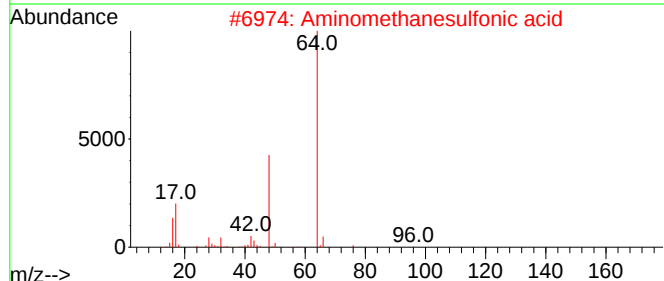
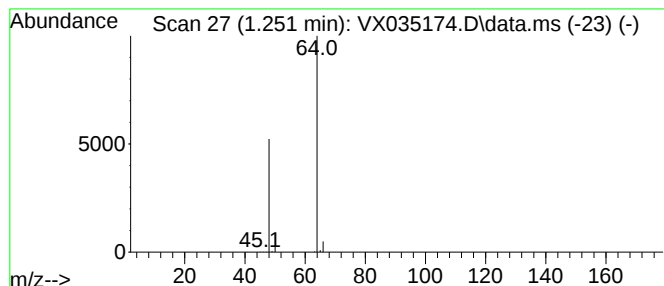
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.251	19.70 ug/L	430887	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	1.251	19.7	ug/L	430887	1	6.763	1093600	50.0