

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035172.D
 Acq On : 19 Apr 2023 16:15
 Operator : JC/MD
 Sample : 02397-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM5

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: VX035172.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	16	rVB2	6786	6547	0.36%	0.048%
2	1.258	24	28	42	rBV	70434	188457	10.47%	1.388%
3	1.367	43	46	58	rVB	202795	229376	12.74%	1.690%
4	1.672	92	96	106	rBV	155559	195747	10.87%	1.442%
5	2.306	194	200	210	rBV	379923	603498	33.52%	4.446%
6	2.514	230	234	239	rVV2	724	1181	0.07%	0.009%
7	2.764	273	275	276	rBV	429	231	0.01%	0.002%
8	2.898	295	297	300	rBV	337	345	0.02%	0.003%
9	3.300	361	363	364	rBV	318	235	0.01%	0.002%
10	3.440	384	386	390	rVB2	528	498	0.03%	0.004%
11	3.501	393	396	398	rBV2	216	256	0.01%	0.002%
12	3.690	425	427	429	rBV	208	237	0.01%	0.002%
13	3.721	430	432	433	rVV2	341	209	0.01%	0.002%
14	3.739	433	435	439	rVV	213	202	0.01%	0.001%
15	3.946	466	469	471	rVV2	313	345	0.02%	0.003%
16	3.971	471	473	474	rVV2	340	261	0.01%	0.002%
17	4.019	476	481	484	rVV3	558	967	0.05%	0.007%
18	4.050	484	486	488	rVB	435	295	0.02%	0.002%
19	4.160	501	504	505	rBV3	205	226	0.01%	0.002%
20	4.251	514	519	520	rBV	735	804	0.04%	0.006%
21	4.458	544	553	573	rBV	114377	356174	19.78%	2.624%
22	4.714	593	595	597	rBV2	392	247	0.01%	0.002%
23	5.056	639	651	669	rBV	222851	685914	38.10%	5.053%
24	5.391	699	706	708	rBV3	1343	2421	0.13%	0.018%
25	5.458	714	717	720	rBV2	222	295	0.02%	0.002%
26	5.556	726	733	743	rVB2	3675	9017	0.50%	0.066%
27	5.659	748	750	752	rBV	343	241	0.01%	0.002%
28	5.769	765	768	769	rBV	258	262	0.01%	0.002%
29	5.818	773	776	777	rBV2	240	240	0.01%	0.002%
30	5.970	788	801	824	rBV2	603527	1800492	100.00%	13.264%
31	6.342	860	862	864	rVB	282	198	0.01%	0.001%
32	6.446	878	879	886	rVB3	316	501	0.03%	0.004%
33	6.531	892	893	896	rBV2	344	327	0.02%	0.002%
34	6.763	921	931	949	rBV	466580	1122206	62.33%	8.267%
35	7.068	979	981	983	rVB2	340	200	0.01%	0.001%
36	7.110	983	988	996	rVB4	2361	5225	0.29%	0.038%

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 Title : VOC Analysis

37	7.208	1000	1004	1006	rBV	283	348	0.02%	0.003%
38	7.305	1011	1020	1036	rBV	368963	809213	44.94%	5.961%
39	7.598	1067	1068	1071	rBV2	410	336	0.02%	0.002%
40	7.629	1071	1073	1074	rVB	632	295	0.02%	0.002%
41	7.683	1079	1082	1084	rBV2	278	258	0.01%	0.002%
42	7.885	1111	1115	1117	rBV	343	523	0.03%	0.004%
43	7.946	1120	1125	1130	rBV4	1300	2940	0.16%	0.022%
44	8.122	1152	1154	1157	rBV	373	382	0.02%	0.003%
45	8.324	1181	1187	1203	rBV	217993	364984	20.27%	2.689%
46	8.494	1212	1215	1217	rBV3	758	1133	0.06%	0.008%
47	8.573	1224	1228	1234	rBV	11288	19907	1.11%	0.147%
48	8.647	1234	1240	1256	rVB	913605	1450036	80.54%	10.682%
49	8.951	1284	1290	1301	rBV	151643	226619	12.59%	1.669%
50	9.177	1326	1327	1329	rVB2	417	232	0.01%	0.002%
51	9.201	1329	1331	1334	rVB2	282	222	0.01%	0.002%
52	9.268	1340	1342	1343	rBV	534	316	0.02%	0.002%
53	9.323	1349	1351	1353	rVB	438	229	0.01%	0.002%
54	9.384	1356	1361	1375	rBV	553623	782521	43.46%	5.765%
55	9.896	1441	1445	1448	rBV3	408	722	0.04%	0.005%
56	10.055	1465	1471	1494	rBV	948657	1282607	71.24%	9.449%
57	10.311	1509	1513	1516	rBV3	713	945	0.05%	0.007%
58	10.402	1525	1528	1530	rBV2	411	441	0.02%	0.003%
59	10.457	1535	1537	1539	rVV2	324	239	0.01%	0.002%
60	10.646	1566	1568	1571	rBV2	370	449	0.02%	0.003%
61	10.762	1586	1587	1590	rVV	317	276	0.02%	0.002%
62	10.793	1590	1592	1594	rVB	374	364	0.02%	0.003%
63	10.939	1615	1616	1619	rBV2	278	330	0.02%	0.002%
64	11.061	1634	1636	1637	rBV	497	339	0.02%	0.002%
65	11.189	1652	1657	1670	rVB	621057	798006	44.32%	5.879%
66	11.280	1670	1672	1673	rBV2	496	274	0.02%	0.002%
67	11.378	1687	1688	1691	rBV	270	244	0.01%	0.002%
68	11.549	1714	1716	1718	rBV2	225	212	0.01%	0.002%
69	11.591	1722	1723	1726	rBV	328	226	0.01%	0.002%
70	11.622	1726	1728	1730	rBV2	290	248	0.01%	0.002%
71	11.707	1740	1742	1746	rVB3	714	808	0.04%	0.006%
72	11.762	1746	1751	1753	rBV2	318	554	0.03%	0.004%
73	11.866	1766	1768	1769	rVB2	362	215	0.01%	0.002%
74	11.890	1769	1772	1773	rVB	381	271	0.02%	0.002%
75	11.920	1775	1777	1779	rVB2	306	239	0.01%	0.002%
76	11.969	1779	1785	1789	rBV	22135	29835	1.66%	0.220%

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Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMXLM041823WMA.M
 Title : VOC Analysis

77	12.024	1789	1794	1806	rVB	906321	1203579	66.85%	8.867%
78	12.219	1822	1826	1831	rBV4	4103	6821	0.38%	0.050%
79	12.317	1837	1842	1856	rVB	906139	1232711	68.47%	9.081%
80	12.475	1866	1868	1870	rBV2	391	356	0.02%	0.003%
81	12.762	1913	1915	1920	rVB3	773	927	0.05%	0.007%
82	12.798	1920	1921	1923	rBV2	285	205	0.01%	0.002%
83	12.865	1927	1932	1933	rBV2	614	625	0.03%	0.005%
84	12.951	1945	1946	1949	rVB2	605	437	0.02%	0.003%
85	12.981	1949	1951	1954	rBV2	427	508	0.03%	0.004%
86	13.048	1960	1962	1963	rBV2	315	258	0.01%	0.002%
87	13.115	1970	1973	1978	rVB5	831	1023	0.06%	0.008%
88	13.262	1995	1997	2000	rBV2	351	395	0.02%	0.003%
89	13.317	2004	2006	2007	rBV	367	209	0.01%	0.002%
90	13.585	2045	2050	2059	rBV	90243	115702	6.43%	0.852%
91	13.835	2089	2091	2094	rVB2	340	262	0.01%	0.002%
92	13.877	2094	2098	2101	rBV2	493	551	0.03%	0.004%
93	13.963	2108	2112	2119	rVB	9680	11771	0.65%	0.087%
94	14.085	2129	2132	2136	rBV2	333	493	0.03%	0.004%
95	14.219	2153	2154	2156	rBV2	555	339	0.02%	0.002%
96	14.280	2161	2164	2167	rBV3	377	586	0.03%	0.004%
97	14.737	2237	2239	2240	rVB2	535	274	0.02%	0.002%
98	14.975	2276	2278	2280	rBV2	600	441	0.02%	0.003%
99	15.249	2320	2323	2327	rVB4	2562	3282	0.18%	0.024%
100	15.487	2360	2362	2363	rBV2	511	296	0.02%	0.002%

Sum of corrected areas: 13574266

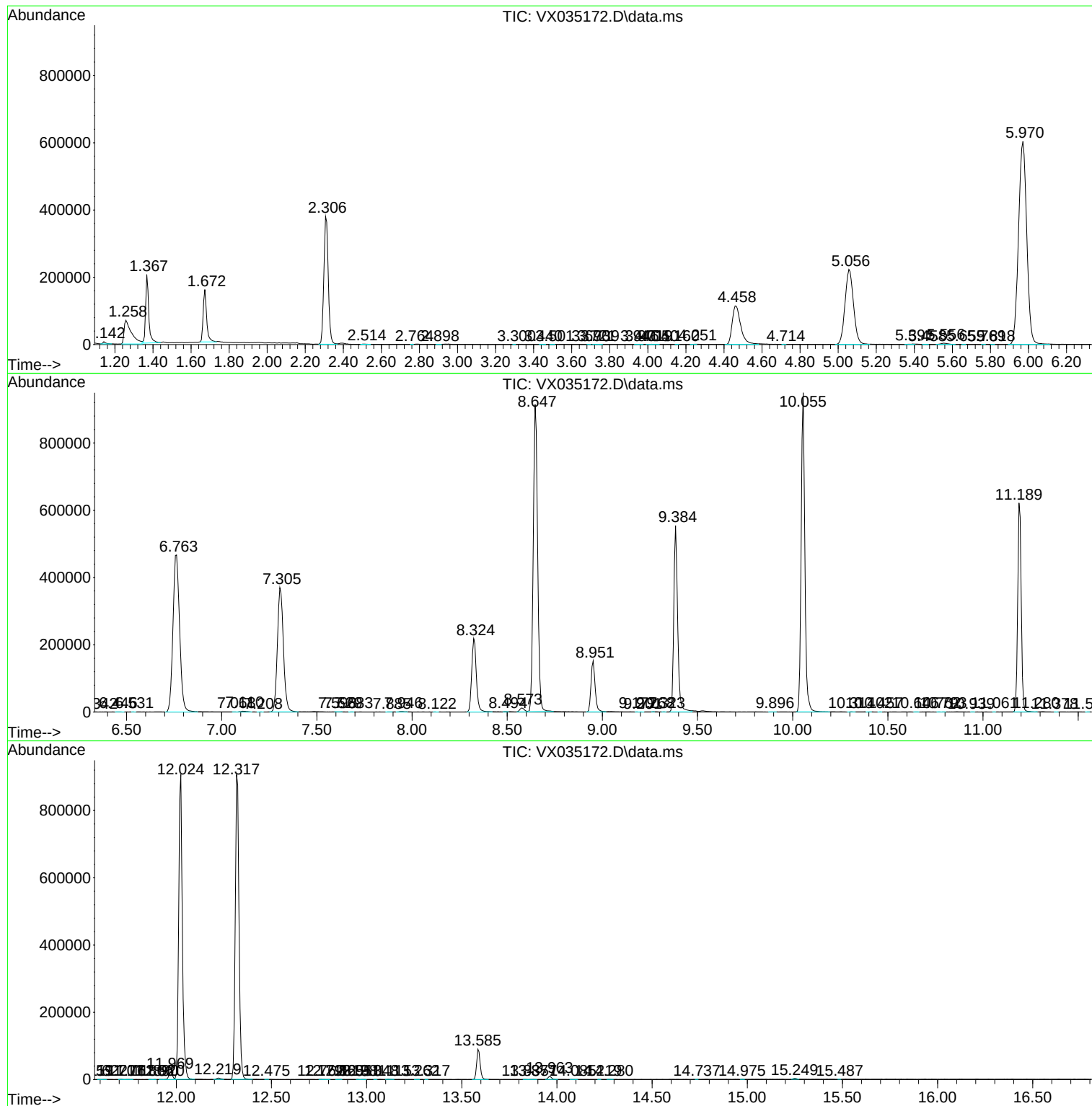
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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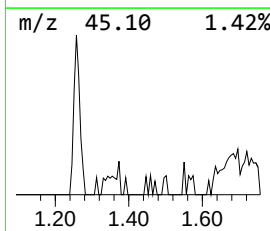
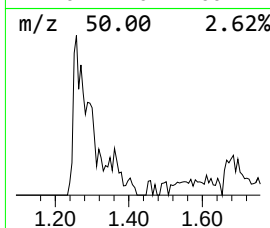
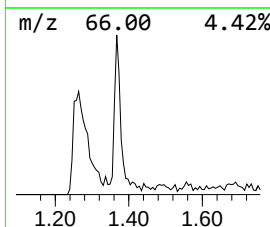
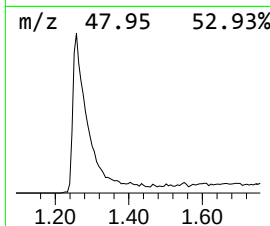
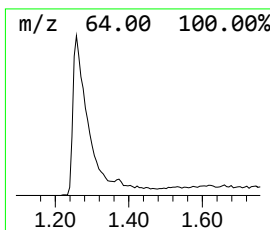
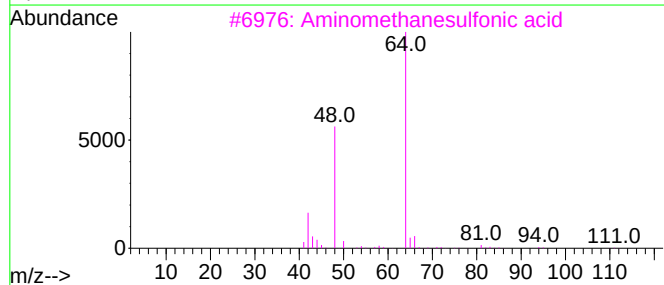
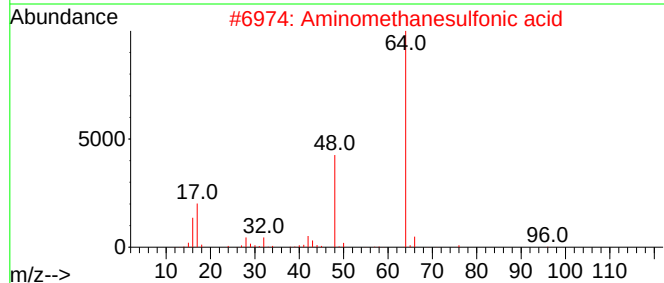
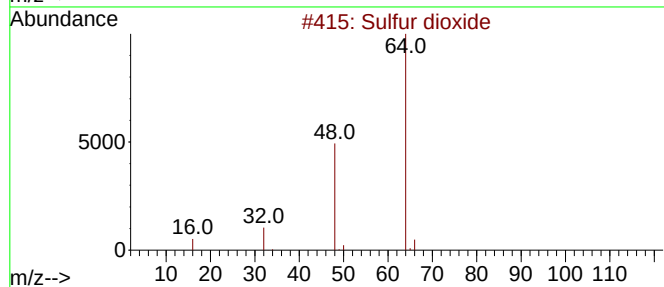
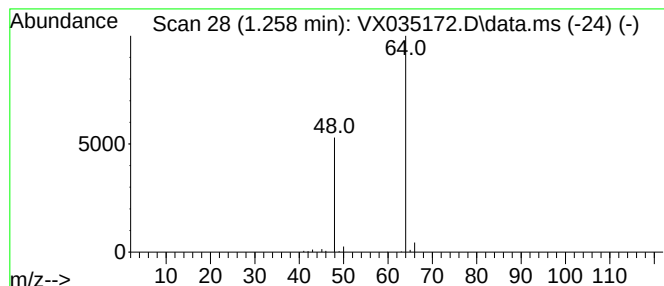
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	8.40 ug/L	188457	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			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	1.258	8.4	ug/L	188457	1	6.763	1122210	50.0