

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035138.D
 Acq On : 18 Apr 2023 21:29
 Operator : JC/MD
 Sample : 02397-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COML4

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: VX035138.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	24	28	42	rBV	60402	183690	9.03%	1.256%
2	1.368	42	46	59	rVB	256126	283830	13.95%	1.941%
3	1.672	91	96	112	rVB	174185	243652	11.98%	1.666%
4	2.306	194	200	211	rBV	454712	703936	34.60%	4.814%
5	2.697	263	264	267	rBV	372	327	0.02%	0.002%
6	2.739	269	271	272	rVB	340	214	0.01%	0.001%
7	2.758	272	274	275	rBV	245	240	0.01%	0.002%
8	2.788	275	279	285	rVB5	1033	1569	0.08%	0.011%
9	2.940	299	304	305	rBV3	489	774	0.04%	0.005%
10	3.093	324	329	331	rBV3	408	626	0.03%	0.004%
11	3.410	377	381	383	rBV	315	397	0.02%	0.003%
12	3.471	390	391	395	rVB2	248	226	0.01%	0.002%
13	3.544	402	403	407	rBV2	146	218	0.01%	0.001%
14	3.660	421	422	429	rVB	307	292	0.01%	0.002%
15	3.709	429	430	433	rBV	307	200	0.01%	0.001%
16	3.849	451	453	456	rBV3	261	243	0.01%	0.002%
17	3.934	466	467	470	rBV	312	210	0.01%	0.001%
18	4.007	477	479	483	rBV	182	222	0.01%	0.002%
19	4.099	492	494	498	rBV	342	411	0.02%	0.003%
20	4.300	524	527	528	rBV2	334	208	0.01%	0.001%
21	4.458	544	553	575	rBV	129237	396058	19.47%	2.709%
22	4.940	630	632	634	rBV2	379	419	0.02%	0.003%
23	5.056	637	651	668	rBV	252656	776741	38.18%	5.312%
24	5.367	701	702	703	rBV	397	265	0.01%	0.002%
25	5.440	712	714	717	rBV	345	217	0.01%	0.001%
26	5.537	727	730	731	rBV2	627	601	0.03%	0.004%
27	5.666	749	751	754	rBV2	283	330	0.02%	0.002%
28	5.842	778	780	783	rVB2	305	292	0.01%	0.002%
29	5.885	783	787	788	rBV2	215	284	0.01%	0.002%
30	5.970	788	801	816	rBV2	682378	2034629	100.00%	13.915%
31	6.330	857	860	861	rBV	297	210	0.01%	0.001%
32	6.464	879	882	883	rBV2	251	221	0.01%	0.002%
33	6.507	887	889	891	rBV2	205	228	0.01%	0.002%
34	6.525	891	892	894	rBV3	327	242	0.01%	0.002%
35	6.562	897	898	903	rVB2	667	527	0.03%	0.004%
36	6.604	903	905	908	rVB	322	322	0.02%	0.002%

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 Title : VOC Analysis

37	6.653	908	913	915	rBV3	332	530	0.03%	0.004%
38	6.763	921	931	949	rBV	479226	1153315	56.68%	7.887%
39	7.116	983	989	997	rVB3	3141	6916	0.34%	0.047%
40	7.177	997	999	1002	rBV2	281	363	0.02%	0.002%
41	7.305	1011	1020	1034	rBV	418183	914571	44.95%	6.255%
42	7.580	1062	1065	1068	rBV2	401	497	0.02%	0.003%
43	7.799	1099	1101	1105	rBV	144	222	0.01%	0.002%
44	7.939	1120	1124	1128	rBV3	1317	2475	0.12%	0.017%
45	8.031	1135	1139	1140	rBV2	427	361	0.02%	0.002%
46	8.165	1159	1161	1162	rVB2	353	221	0.01%	0.002%
47	8.324	1181	1187	1197	rBV	248481	413670	20.33%	2.829%
48	8.647	1233	1240	1263	rBV	1067156	1661807	81.68%	11.365%
49	8.952	1284	1290	1309	rVB	174990	264806	13.01%	1.811%
50	9.275	1339	1343	1348	rVV3	2488	4251	0.21%	0.029%
51	9.384	1356	1361	1373	rBV	609899	852345	41.89%	5.829%
52	9.896	1443	1445	1448	rBV4	258	308	0.02%	0.002%
53	9.957	1453	1455	1457	rBV2	325	295	0.01%	0.002%
54	10.055	1465	1471	1487	rBV	940284	1285153	63.16%	8.789%
55	10.311	1510	1513	1515	rBV2	621	608	0.03%	0.004%
56	10.366	1520	1522	1524	rVB	443	366	0.02%	0.003%
57	10.390	1524	1526	1528	rBV2	422	406	0.02%	0.003%
58	10.451	1534	1536	1540	rVV	509	356	0.02%	0.002%
59	10.482	1540	1541	1543	rVV2	310	213	0.01%	0.001%
60	10.567	1553	1555	1558	rBV2	332	286	0.01%	0.002%
61	10.640	1566	1567	1570	rBV	257	242	0.01%	0.002%
62	10.805	1591	1594	1595	rBV	224	231	0.01%	0.002%
63	10.927	1612	1614	1616	rVV	351	236	0.01%	0.002%
64	10.963	1618	1620	1624	rVB	554	324	0.02%	0.002%
65	11.128	1643	1647	1649	rBV2	222	276	0.01%	0.002%
66	11.189	1652	1657	1670	rVV	691005	885522	43.52%	6.056%
67	11.317	1674	1678	1680	rVB2	756	868	0.04%	0.006%
68	11.427	1694	1696	1698	rVB	294	208	0.01%	0.001%
69	11.451	1698	1700	1702	rBV2	282	323	0.02%	0.002%
70	11.475	1702	1704	1706	rVB	441	300	0.01%	0.002%
71	11.713	1740	1743	1745	rBV3	801	770	0.04%	0.005%
72	11.975	1782	1786	1788	rBV3	868	1092	0.05%	0.007%
73	12.018	1788	1793	1806	rVV	888632	1173606	57.68%	8.026%
74	12.219	1822	1826	1834	rVB3	5338	8400	0.41%	0.057%
75	12.317	1837	1842	1858	rVV	1019650	1334117	65.57%	9.124%
76	12.579	1882	1885	1887	rBV2	317	342	0.02%	0.002%

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

77	12.762	1912	1915	1920	rVV3	455	580	0.03%	0.004%
78	12.841	1927	1928	1931	rBV2	408	292	0.01%	0.002%
79	12.981	1948	1951	1952	rBV2	259	283	0.01%	0.002%
80	13.073	1964	1966	1967	rBV	363	232	0.01%	0.002%
81	13.115	1970	1973	1979	rVB2	873	1163	0.06%	0.008%
82	13.262	1995	1997	2002	rVB2	483	415	0.02%	0.003%
83	13.304	2002	2004	2006	rVB	320	223	0.01%	0.002%
84	13.347	2009	2011	2014	rVB2	319	383	0.02%	0.003%
85	13.384	2014	2017	2018	rBV	272	254	0.01%	0.002%
86	13.432	2024	2025	2027	rBV	291	239	0.01%	0.002%
87	13.591	2047	2051	2057	rBV3	2115	3042	0.15%	0.021%
88	13.670	2062	2064	2066	rBV2	227	260	0.01%	0.002%
89	13.725	2071	2073	2075	rVV	344	253	0.01%	0.002%
90	13.792	2079	2084	2088	rBV3	581	1129	0.06%	0.008%
91	13.835	2088	2091	2094	rVB2	343	409	0.02%	0.003%
92	13.963	2109	2112	2116	rVB3	910	1328	0.07%	0.009%
93	14.060	2126	2128	2129	rBV	417	366	0.02%	0.003%
94	14.371	2176	2179	2180	rBV2	290	287	0.01%	0.002%
95	14.518	2201	2203	2204	rBV2	297	247	0.01%	0.002%
96	14.676	2228	2229	2232	rVB	528	350	0.02%	0.002%
97	14.700	2232	2233	2235	rBV2	506	392	0.02%	0.003%
98	14.774	2243	2245	2248	rVB2	781	812	0.04%	0.006%
99	15.249	2319	2323	2329	rBV4	3045	4580	0.23%	0.031%
100	15.712	2398	2399	2400	rBV	812	419	0.02%	0.003%

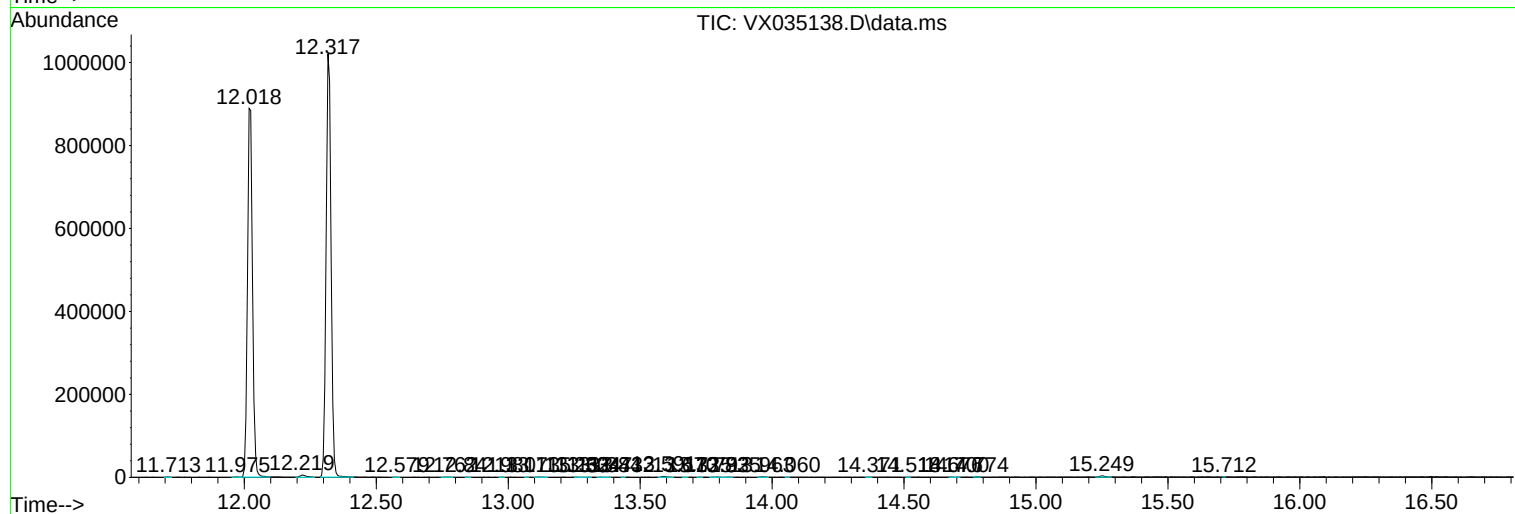
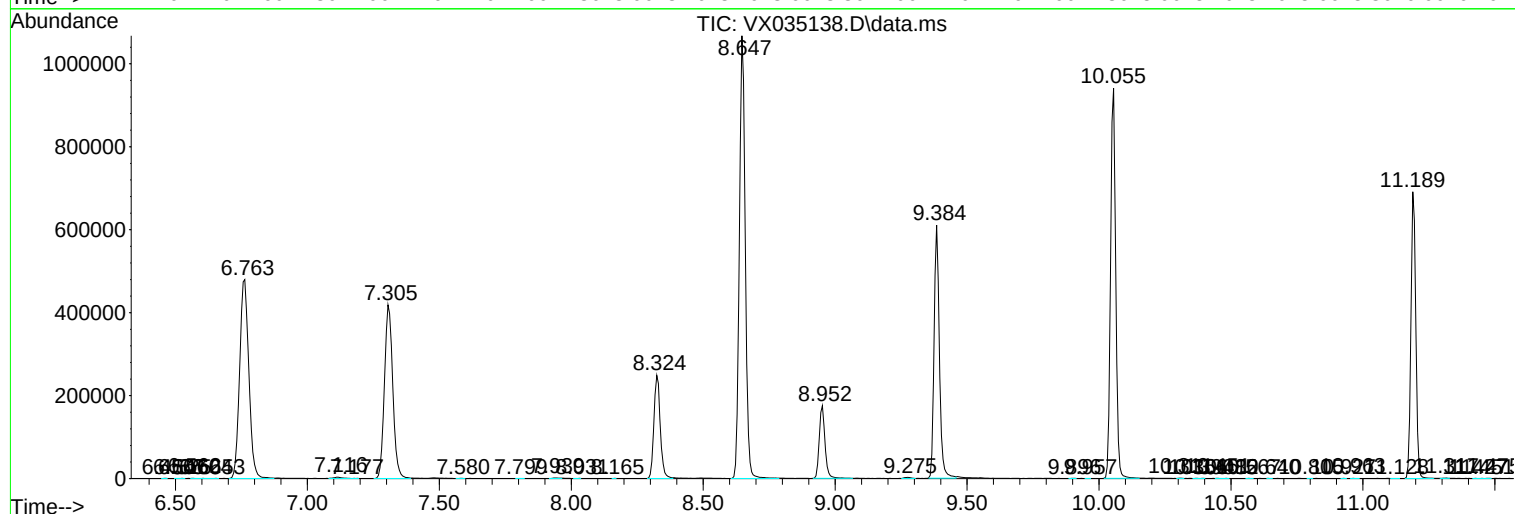
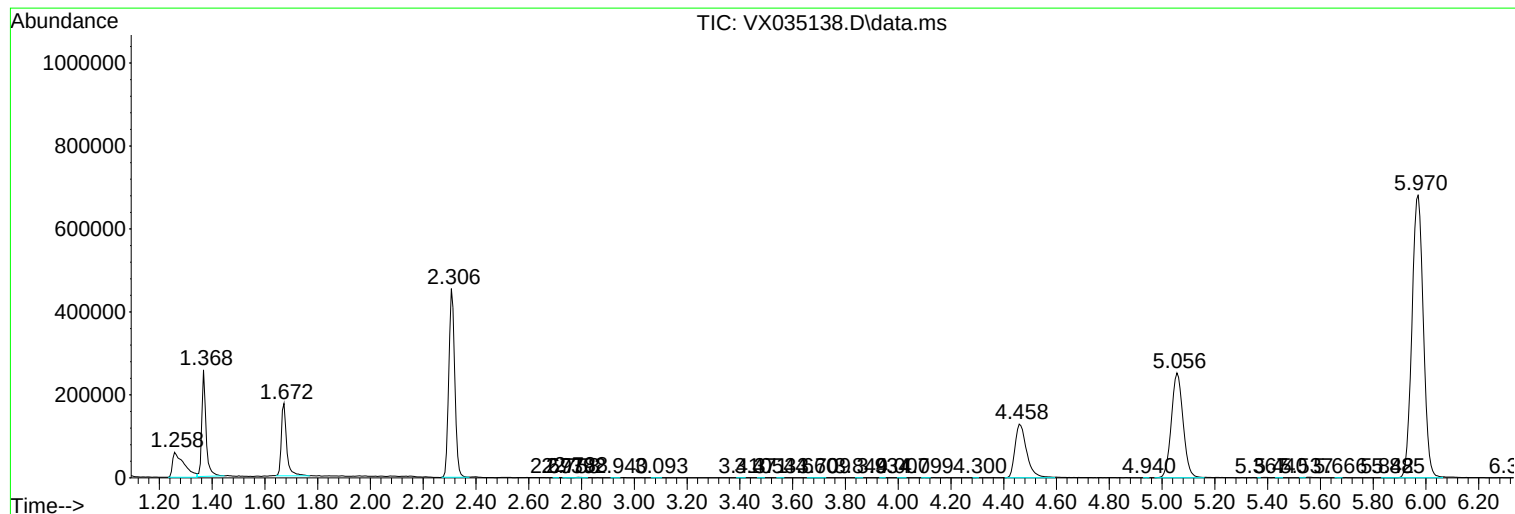
Sum of corrected areas: 14622207

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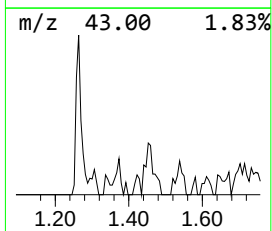
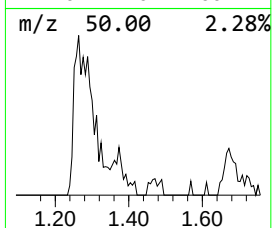
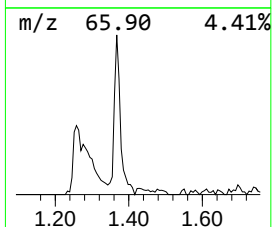
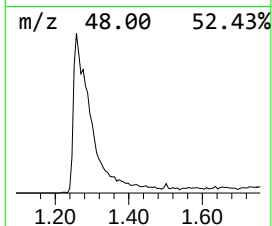
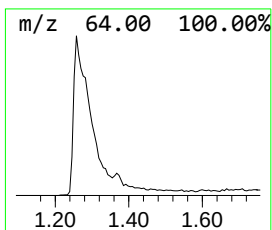
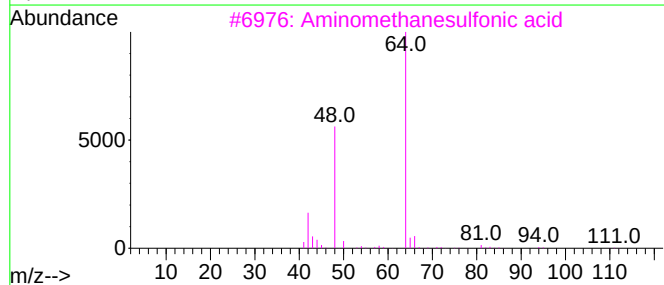
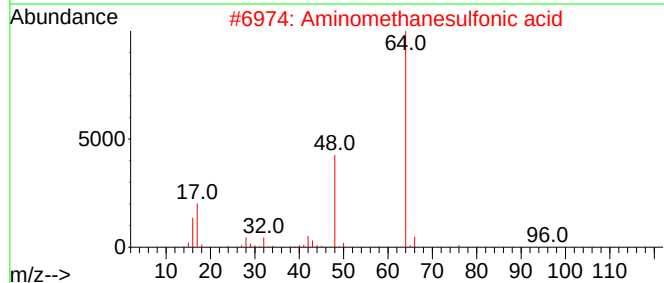
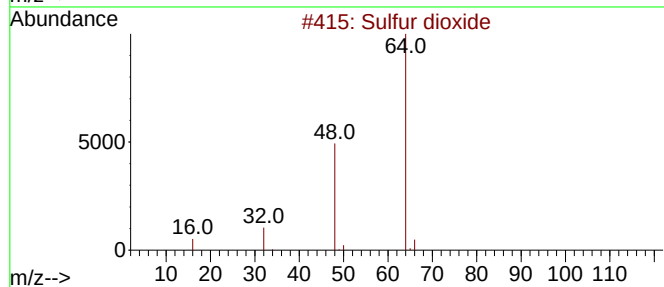
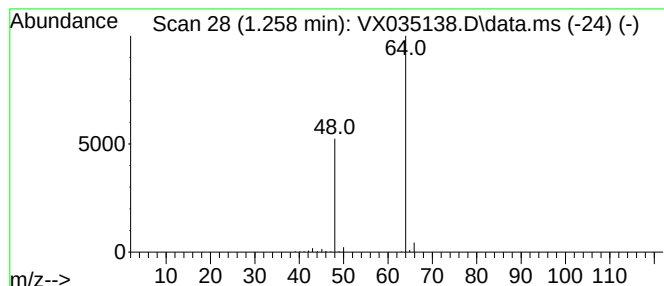
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	7.96 ug/L	183690	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	8.0	ug/L	183690	1	6.763	1153320	50.0