

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030666.D
 Acq On : 17 Aug 2022 17:35
 Operator : JC/MD
 Sample : VIBLK674
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VIBLK674

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\SFAMXML080422WMA.M

Title : VOC Analysis

Signal : TIC: VX030666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	42	rBV2	15965	38748	2.95%	0.442%
2	1.367	42	46	55	rVB	184270	184088	14.00%	2.099%
3	1.666	91	95	104	rVB	135850	161256	12.26%	1.839%
4	2.306	193	200	210	rBV	307633	482414	36.68%	5.501%
5	2.501	231	232	236	rVB3	601	540	0.04%	0.006%
6	2.562	238	242	245	rBV4	599	935	0.07%	0.011%
7	2.654	254	257	258	rBV3	685	691	0.05%	0.008%
8	2.672	258	260	264	rVV2	377	418	0.03%	0.005%
9	2.788	274	279	286	rVB4	3645	6792	0.52%	0.077%
10	2.946	296	305	313	rBV	17505	41818	3.18%	0.477%
11	3.135	334	336	338	rVV	463	425	0.03%	0.005%
12	3.270	354	358	360	rVB3	394	551	0.04%	0.006%
13	3.306	360	364	366	rBV2	545	610	0.05%	0.007%
14	3.331	366	368	371	rVB2	549	515	0.04%	0.006%
15	3.574	405	408	411	rBV2	629	531	0.04%	0.006%
16	3.757	435	438	439	rBV2	397	456	0.03%	0.005%
17	3.776	439	441	447	rVB	420	557	0.04%	0.006%
18	4.074	488	490	493	rBV2	461	491	0.04%	0.006%
19	4.336	530	533	534	rBV	387	357	0.03%	0.004%
20	4.373	537	539	541	rVB	507	382	0.03%	0.004%
21	4.397	541	543	545	rBV	383	489	0.04%	0.006%
22	4.464	545	554	566	rBV	112770	316399	24.05%	3.608%
23	4.885	621	623	627	rVB3	402	567	0.04%	0.006%
24	5.068	640	653	668	rBV	165062	515127	39.16%	5.874%
25	5.275	684	687	689	rBV3	383	352	0.03%	0.004%
26	5.385	703	705	713	rVB4	944	1969	0.15%	0.022%
27	5.562	729	734	741	rVV4	1623	4212	0.32%	0.048%
28	5.641	745	747	748	rBV	588	432	0.03%	0.005%
29	5.763	765	767	769	rBV2	432	417	0.03%	0.005%
30	5.812	773	775	777	rBV2	402	351	0.03%	0.004%
31	5.976	789	802	819	rBV2	454221	1315357	100.00%	15.000%
32	6.470	881	883	886	rBV3	391	365	0.03%	0.004%
33	6.769	922	932	947	rVV	163283	385477	29.31%	4.396%
34	6.952	960	962	968	rVB	418	693	0.05%	0.008%
35	7.007	968	971	973	rVB2	680	580	0.04%	0.007%
36	7.129	982	991	1002	rBV4	25726	65315	4.97%	0.745%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

37	7.232	1006	1008	1010	rBV2	399	420	0.03%	0.005%
38	7.311	1012	1021	1036	rBV	270891	589857	44.84%	6.727%
39	7.476	1047	1048	1049	rBV2	615	395	0.03%	0.005%
40	7.665	1076	1079	1082	rVB2	357	416	0.03%	0.005%
41	7.702	1082	1085	1089	rBV2	585	1020	0.08%	0.012%
42	7.933	1120	1123	1124	rBV2	1076	1081	0.08%	0.012%
43	7.994	1131	1133	1134	rBV	412	370	0.03%	0.004%
44	8.037	1138	1140	1143	rBV	525	499	0.04%	0.006%
45	8.147	1157	1158	1163	rVB2	558	563	0.04%	0.006%
46	8.250	1172	1175	1179	rBV3	807	1242	0.09%	0.014%
47	8.330	1181	1188	1198	rBV	180219	292373	22.23%	3.334%
48	8.488	1210	1214	1220	rBV3	1160	1637	0.12%	0.019%
49	8.555	1224	1225	1228	rBV	383	400	0.03%	0.005%
50	8.580	1228	1229	1234	rVB2	939	643	0.05%	0.007%
51	8.653	1234	1241	1251	rBV	685015	1054694	80.18%	12.028%
52	8.830	1266	1270	1271	rVB3	455	513	0.04%	0.006%
53	8.951	1284	1290	1299	rBV	128375	193815	14.73%	2.210%
54	9.061	1306	1308	1311	rVB2	548	394	0.03%	0.004%
55	9.116	1316	1317	1322	rBV2	552	557	0.04%	0.006%
56	9.275	1338	1343	1351	rVB3	38707	58131	4.42%	0.663%
57	9.384	1356	1361	1373	rBV	470189	694240	52.78%	7.917%
58	9.610	1395	1398	1400	rBV2	452	444	0.03%	0.005%
59	9.707	1409	1414	1419	rBV3	3575	5047	0.38%	0.058%
60	9.799	1428	1429	1432	rVB	627	460	0.03%	0.005%
61	9.823	1432	1433	1436	rBV	566	463	0.04%	0.005%
62	9.896	1443	1445	1447	rBV2	487	374	0.03%	0.004%
63	10.055	1466	1471	1484	rBV	320595	449970	34.21%	5.131%
64	10.311	1509	1513	1516	rBV3	458	779	0.06%	0.009%
65	10.354	1519	1520	1526	rVB3	486	461	0.04%	0.005%
66	10.640	1564	1567	1570	rBV3	355	484	0.04%	0.006%
67	10.780	1587	1590	1593	rBV3	720	866	0.07%	0.010%
68	10.878	1602	1606	1608	rBV2	423	664	0.05%	0.008%
69	10.902	1608	1610	1612	rVB	499	400	0.03%	0.005%
70	11.012	1626	1628	1630	rBV	540	411	0.03%	0.005%
71	11.152	1648	1651	1652	rBV	370	437	0.03%	0.005%
72	11.195	1652	1658	1670	rVB	465113	594019	45.16%	6.774%
73	11.481	1703	1705	1709	rBV2	462	530	0.04%	0.006%
74	11.561	1714	1718	1721	rVB2	463	773	0.06%	0.009%
75	11.603	1723	1725	1728	rBV	481	456	0.03%	0.005%
76	11.756	1748	1750	1752	rBV	697	681	0.05%	0.008%

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 Title : VOC Analysis

77	11.805	1755	1758	1761	rBV2	328	522	0.04%	0.006%
78	11.847	1764	1765	1768	rBV2	354	431	0.03%	0.005%
79	11.951	1779	1782	1783	rBV2	486	486	0.04%	0.006%
80	12.024	1789	1794	1800	rBV	330728	404908	30.78%	4.618%
81	12.158	1814	1816	1817	rBV2	515	401	0.03%	0.005%
82	12.176	1817	1819	1822	rVV2	329	358	0.03%	0.004%
83	12.323	1837	1843	1850	rBV	702314	871261	66.24%	9.936%
84	12.469	1865	1867	1871	rBV2	345	346	0.03%	0.004%
85	12.762	1911	1915	1918	rBV3	549	736	0.06%	0.008%
86	13.012	1954	1956	1958	rBV	424	483	0.04%	0.006%
87	13.073	1964	1966	1968	rBV2	528	563	0.04%	0.006%
88	13.115	1972	1973	1977	rVV2	797	678	0.05%	0.008%
89	13.292	1999	2002	2003	rBV2	384	514	0.04%	0.006%
90	13.310	2003	2005	2006	rVV2	742	533	0.04%	0.006%
91	13.475	2030	2032	2035	rVV	434	351	0.03%	0.004%
92	13.512	2037	2038	2041	rBV2	524	385	0.03%	0.004%
93	13.585	2048	2050	2053	rBV	502	538	0.04%	0.006%
94	13.792	2082	2084	2088	rVB	681	565	0.04%	0.006%
95	14.548	2206	2208	2210	rBV	516	439	0.03%	0.005%
96	14.871	2259	2261	2264	rBV2	739	596	0.05%	0.007%
97	14.902	2264	2266	2269	rBV5	698	807	0.06%	0.009%
98	15.249	2321	2323	2325	rBV	663	359	0.03%	0.004%
99	15.944	2436	2437	2438	rBV	781	385	0.03%	0.004%
100	16.310	2495	2497	2498	rBV	771	612	0.05%	0.007%

Sum of corrected areas: 8768913

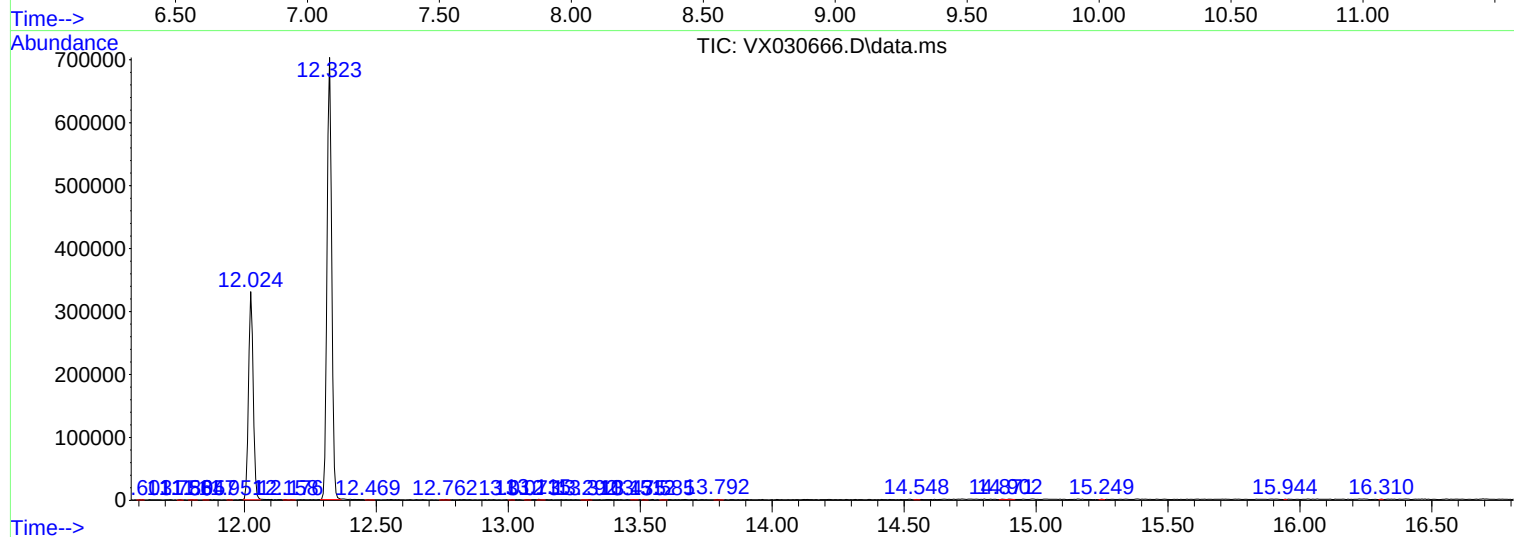
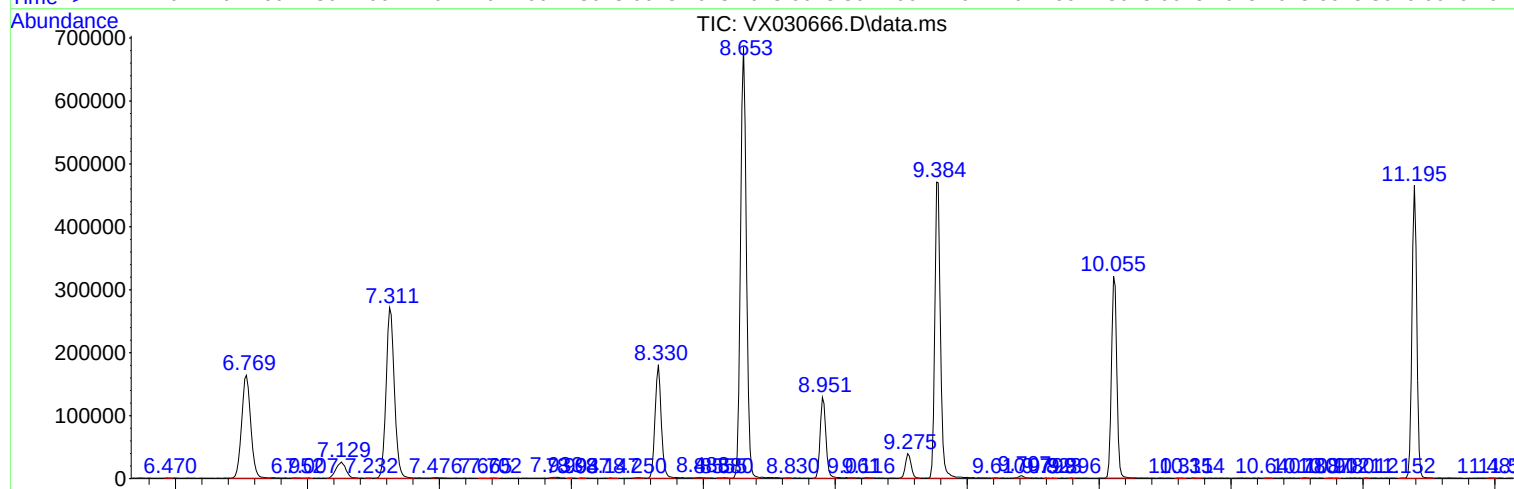
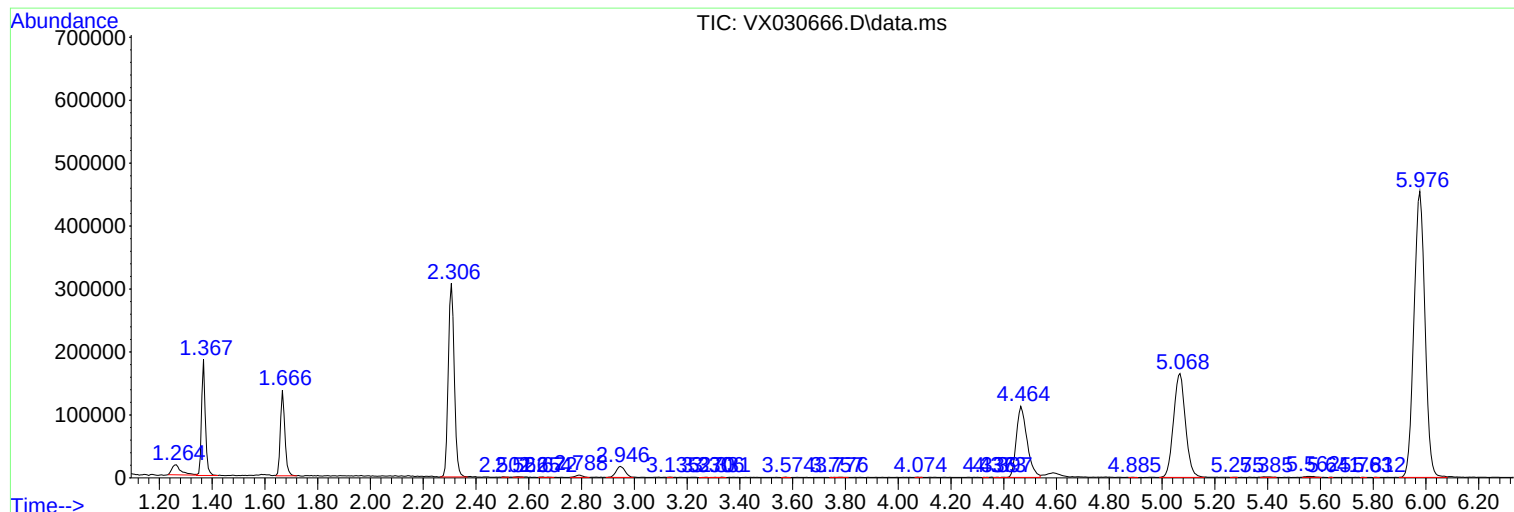
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
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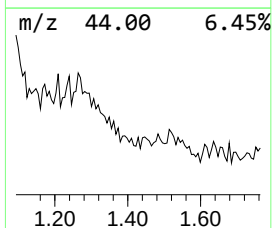
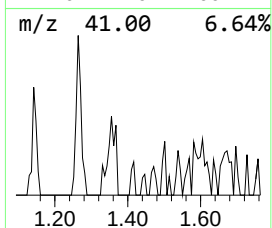
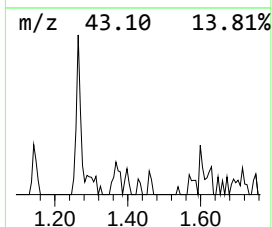
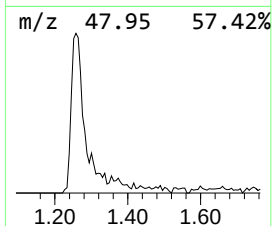
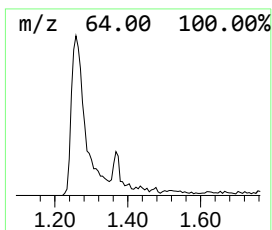
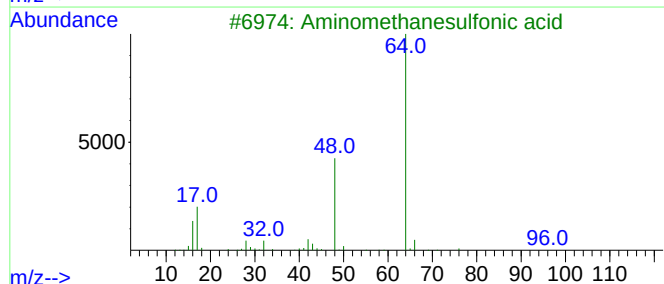
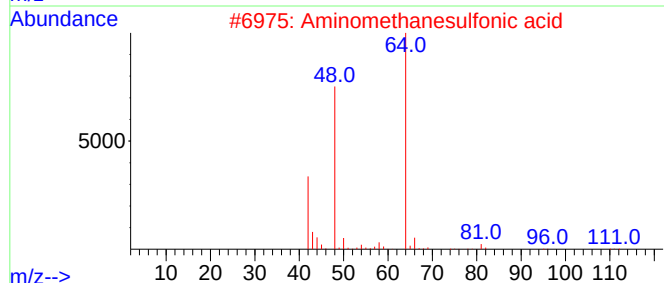
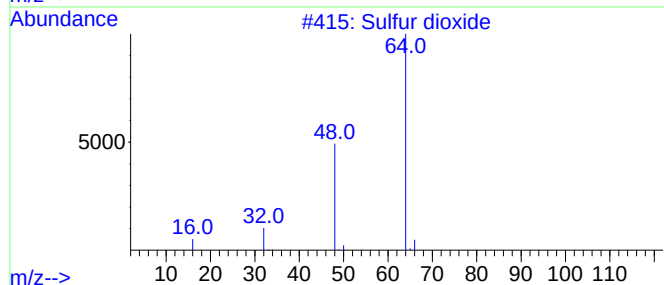
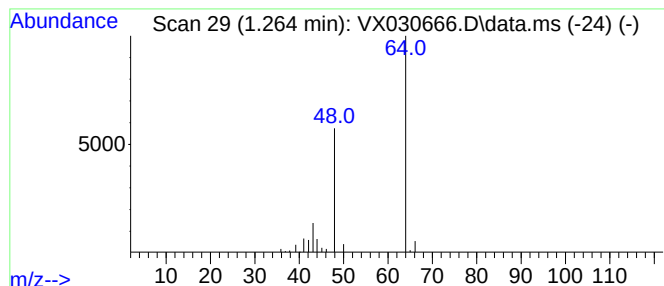
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.03 ug/L	38748	1,4-Difluorobenzene	6.769

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	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			Sulfur dioxide	64	O2S	007446-09-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.264	5.0	ug/L	38748	1	6.769	385477	50.0