

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042492.D
 Acq On : 23 Jul 2024 23:26
 Operator : JC/MD
 Sample : VX0724WBL02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK692

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\SFAMXML070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	11	13	15	rVB2	375	264	0.04%	0.005%
2	1.239	22	25	33	rBV2	18057	25203	3.54%	0.472%
3	1.367	43	46	58	rVB	62974	82540	11.58%	1.546%
4	1.526	69	72	73	rBV	894	847	0.12%	0.016%
5	1.605	73	85	87	rVV7	5893	16249	2.28%	0.304%
6	1.648	88	92	102	rVB	52911	69262	9.72%	1.297%
7	1.873	125	129	133	rVB2	1149	1589	0.22%	0.030%
8	2.166	175	177	178	rVB	235	135	0.02%	0.003%
9	2.300	192	199	211	rBV	145524	233500	32.77%	4.373%
10	2.391	211	214	220	rVB2	871	1563	0.22%	0.029%
11	2.446	220	223	225	rBV2	200	331	0.05%	0.006%
12	2.507	229	233	241	rBV2	985	1699	0.24%	0.032%
13	2.568	241	243	249	rVB3	250	398	0.06%	0.007%
14	2.629	249	253	254	rBV2	141	146	0.02%	0.003%
15	2.654	254	257	260	rVB2	122	155	0.02%	0.003%
16	2.708	262	266	273	rVB3	432	897	0.13%	0.017%
17	2.782	273	278	287	rBV3	1841	3703	0.52%	0.069%
18	2.940	297	304	318	rVB	5404	13262	1.86%	0.248%
19	3.044	318	321	324	rBV2	170	231	0.03%	0.004%
20	3.099	324	330	333	rBV3	1036	2327	0.33%	0.044%
21	3.568	405	407	408	rVB	235	157	0.02%	0.003%
22	3.605	408	413	420	rBV3	594	1408	0.20%	0.026%
23	3.964	469	472	473	rBV	150	147	0.02%	0.003%
24	4.111	494	496	499	rVB2	165	196	0.03%	0.004%
25	4.464	545	554	571	rBV	51564	157104	22.05%	2.942%
26	5.056	640	651	670	rVV	90302	280262	39.33%	5.249%
27	5.391	698	706	711	rVV6	565	1393	0.20%	0.026%
28	5.464	711	718	726	rVV4	757	2045	0.29%	0.038%
29	5.677	746	753	754	rBV3	549	969	0.14%	0.018%
30	5.964	789	800	821	rBV2	240132	712559	100.00%	13.345%
31	6.287	849	853	859	rBV3	147	274	0.04%	0.005%
32	6.763	922	931	958	rBV	177139	426285	59.82%	7.983%
33	7.061	979	980	983	rBV2	151	155	0.02%	0.003%
34	7.128	983	991	1001	rBV4	7396	17641	2.48%	0.330%
35	7.202	1001	1003	1004	rBV	182	176	0.02%	0.003%
36	7.305	1012	1020	1038	rBV	141509	317791	44.60%	5.952%

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

37	7.439	1038	1042	1047	rVB4	682	1246	0.17%	0.023%
38	7.555	1059	1061	1064	rVB	149	136	0.02%	0.003%
39	7.714	1085	1087	1089	rBV	125	157	0.02%	0.003%
40	7.829	1100	1106	1109	rBV3	355	666	0.09%	0.012%
41	7.951	1124	1126	1128	rBV2	395	485	0.07%	0.009%
42	8.159	1155	1160	1161	rBV2	171	261	0.04%	0.005%
43	8.329	1180	1188	1204	rBV	80016	140787	19.76%	2.637%
44	8.518	1216	1219	1221	rBV2	255	309	0.04%	0.006%
45	8.585	1226	1230	1233	rBV3	1092	1786	0.25%	0.033%
46	8.646	1234	1240	1250	rBV	356414	571284	80.17%	10.699%
47	8.951	1285	1290	1303	rBV	55943	89780	12.60%	1.681%
48	9.165	1320	1325	1329	rVB3	1059	1507	0.21%	0.028%
49	9.274	1339	1343	1349	rBV2	4013	6129	0.86%	0.115%
50	9.384	1356	1361	1380	rBV	218406	335317	47.06%	6.280%
51	9.518	1380	1383	1389	rVB4	802	1486	0.21%	0.028%
52	9.616	1395	1399	1404	rVB2	655	1038	0.15%	0.019%
53	9.701	1408	1413	1417	rBV	1144	1727	0.24%	0.032%
54	9.811	1427	1431	1433	rBV2	147	165	0.02%	0.003%
55	10.055	1465	1471	1488	rBV	349017	482093	67.66%	9.029%
56	10.201	1491	1495	1502	rVV	2325	3625	0.51%	0.068%
57	10.305	1508	1512	1518	rVV2	2138	3363	0.47%	0.063%
58	10.652	1563	1569	1575	rBV5	2421	5523	0.78%	0.103%
59	10.695	1575	1576	1579	rVB2	290	282	0.04%	0.005%
60	10.811	1590	1595	1597	rBV3	472	715	0.10%	0.013%
61	10.963	1616	1620	1627	rVB	2349	3015	0.42%	0.056%
62	11.024	1627	1630	1633	rBV	126	188	0.03%	0.004%
63	11.189	1652	1657	1665	rBV	273196	359229	50.41%	6.728%
64	11.311	1676	1677	1682	rVB2	175	231	0.03%	0.004%
65	11.457	1697	1701	1706	rVB	1840	2349	0.33%	0.044%
66	11.530	1710	1713	1715	rBV2	145	188	0.03%	0.004%
67	11.682	1735	1738	1741	rVB2	125	153	0.02%	0.003%
68	11.756	1746	1750	1756	rVV	2240	2486	0.35%	0.047%
69	11.975	1782	1786	1789	rBV2	2391	3240	0.45%	0.061%
70	12.024	1789	1794	1805	rVB	338422	430353	60.40%	8.060%
71	12.170	1816	1818	1819	rVV	303	151	0.02%	0.003%
72	12.316	1837	1842	1854	rBV	379234	493265	69.22%	9.238%
73	12.487	1867	1870	1871	rVB	281	219	0.03%	0.004%
74	12.548	1876	1880	1882	rBV2	117	163	0.02%	0.003%
75	12.762	1911	1915	1918	rVB2	487	617	0.09%	0.012%
76	12.804	1918	1922	1925	rBV2	153	208	0.03%	0.004%

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Integration Parameters: LSCINT.P

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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\SFAMXML070324WMA.M
 Title : VOC Analysis

77	12.944	1943	1945	1949	rBV2	405	385	0.05%	0.007%
78	13.115	1970	1973	1978	rVB2	2050	2600	0.36%	0.049%
79	13.353	2009	2012	2014	rBV	117	146	0.02%	0.003%
80	13.560	2044	2046	2047	rVB	200	142	0.02%	0.003%
81	13.591	2047	2051	2058	rBV2	2146	3162	0.44%	0.059%
82	13.682	2064	2066	2069	rBV2	132	194	0.03%	0.004%
83	13.780	2076	2082	2086	rBV	2364	3378	0.47%	0.063%
84	13.963	2108	2112	2119	rBV2	2183	3058	0.43%	0.057%
85	14.127	2135	2139	2143	rVB	1060	1489	0.21%	0.028%
86	14.469	2193	2195	2198	rVB2	228	232	0.03%	0.004%
87	14.706	2233	2234	2237	rVB	220	146	0.02%	0.003%
88	14.749	2237	2241	2242	rBV3	280	314	0.04%	0.006%
89	15.176	2304	2311	2312	rBV3	300	591	0.08%	0.011%
90	15.304	2330	2332	2333	rBV2	188	135	0.02%	0.003%
91	15.359	2339	2341	2342	rBV	321	217	0.03%	0.004%
92	15.389	2342	2346	2351	rVB3	1521	2349	0.33%	0.044%
93	15.554	2371	2373	2375	rBV3	240	156	0.02%	0.003%
94	15.578	2375	2377	2380	rBV3	222	297	0.04%	0.006%
95	15.773	2408	2409	2412	rVB3	428	332	0.05%	0.006%
96	15.798	2412	2413	2415	rBV	358	232	0.03%	0.004%
97	16.023	2448	2450	2453	rBV3	299	495	0.07%	0.009%
98	16.450	2518	2520	2521	rBV2	223	145	0.02%	0.003%
99	16.645	2550	2552	2554	rVB2	361	267	0.04%	0.005%
100	16.675	2554	2557	2560	rBV4	270	429	0.06%	0.008%

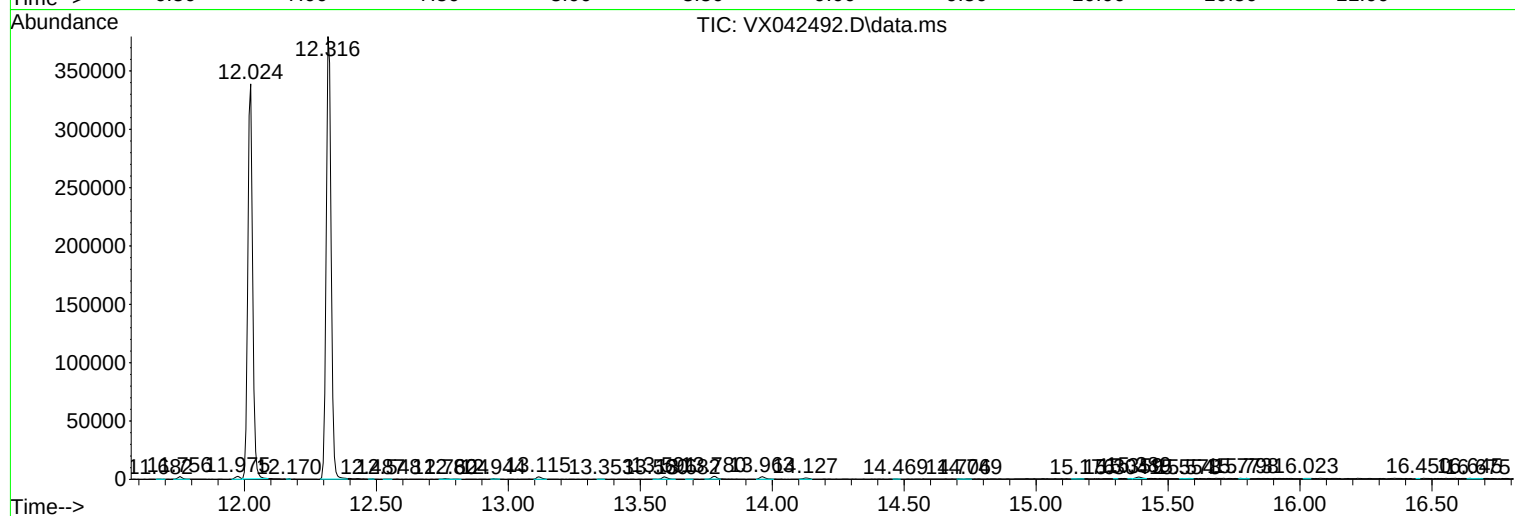
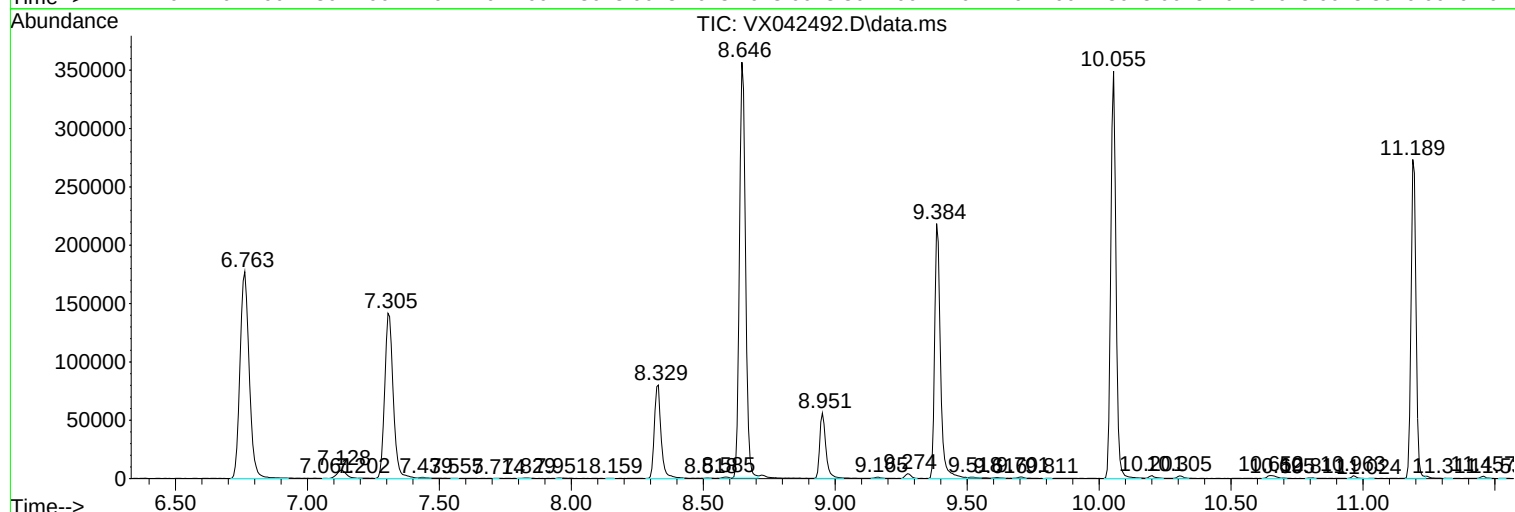
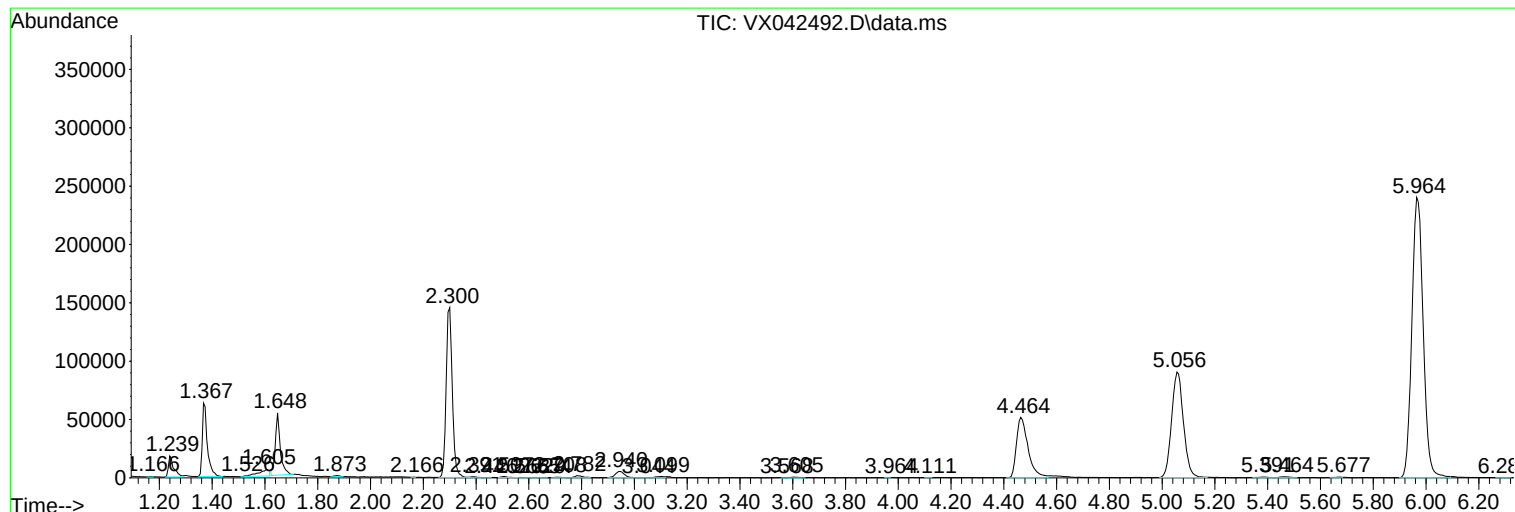
Sum of corrected areas: 5339676

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ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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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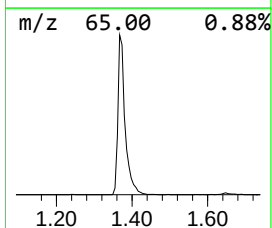
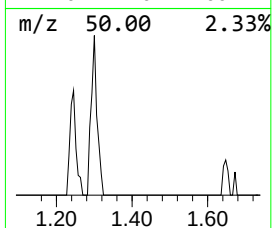
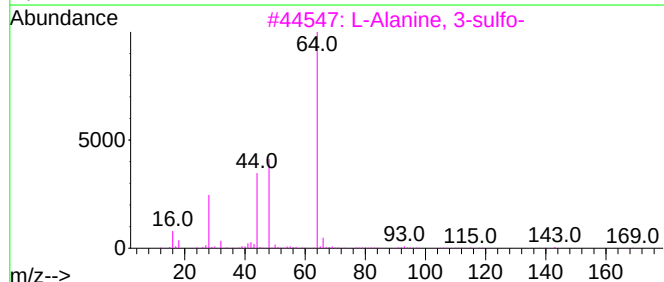
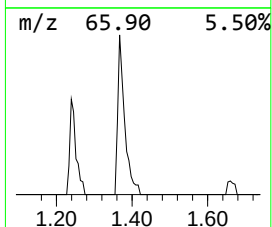
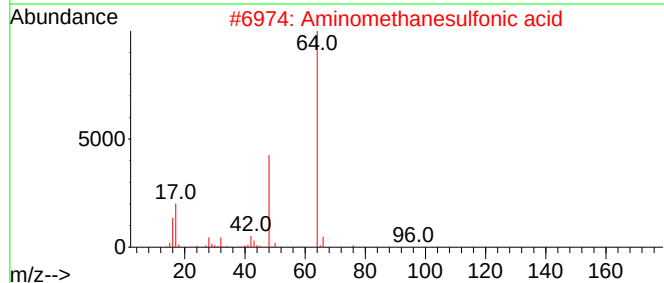
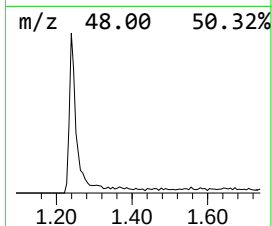
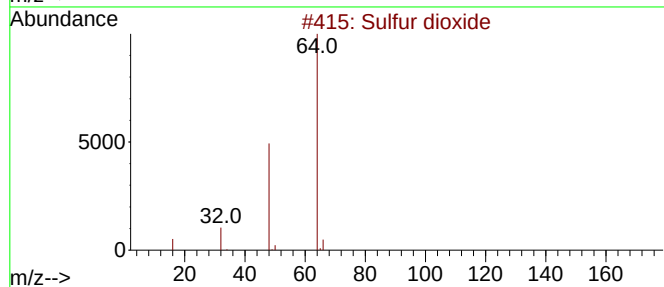
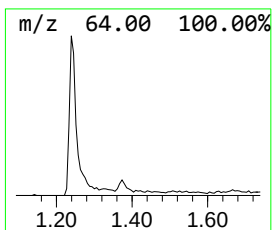
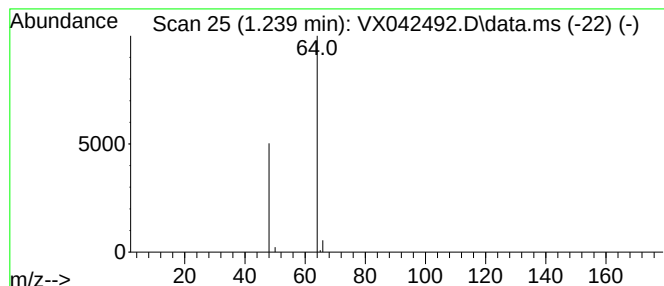
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.239	2.96 ug/L	25203	1,4-Difluorobenzene	6.763

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	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	3.0	ug/L	25203	1	6.763	426285	50.0