

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
 Data File : VV033842.D
 Acq On : 24 Jan 2024 09:53
 Operator : SY/MD
 Sample : VV0124WBL01
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK223

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033842.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	32	39	51	rBV	28479	33693	4.36%	0.557%
2	1.282	68	75	93	rBV	99197	111720	14.46%	1.846%
3	1.532	145	153	169	rVB	87699	108287	14.01%	1.790%
4	2.060	307	317	338	rVB	183330	270960	35.06%	4.478%
5	2.185	352	356	362	rBV2	595	565	0.07%	0.009%
6	2.243	368	374	381	rBV2	533	757	0.10%	0.013%
7	2.426	420	431	434	rBV2	299	365	0.05%	0.006%
8	2.449	434	438	444	rVV	433	464	0.06%	0.008%
9	2.561	465	473	481	rVB3	689	1246	0.16%	0.021%
10	2.854	554	564	567	rBV2	290	508	0.07%	0.008%
11	2.995	605	608	615	rVV2	182	202	0.03%	0.003%
12	3.162	655	660	663	rBV	256	265	0.03%	0.004%
13	3.217	674	677	680	rBV2	145	126	0.02%	0.002%
14	3.343	712	716	718	rBV2	144	134	0.02%	0.002%
15	3.516	766	770	771	rBV	325	172	0.02%	0.003%
16	3.529	771	774	780	rVB2	282	270	0.03%	0.004%
17	3.564	780	785	789	rBV2	225	262	0.03%	0.004%
18	3.619	799	802	805	rVB	164	133	0.02%	0.002%
19	3.638	805	808	811	rVB	236	178	0.02%	0.003%
20	3.664	811	816	820	rBV2	303	357	0.05%	0.006%
21	3.722	830	834	838	rVB2	143	129	0.02%	0.002%
22	3.783	844	853	891	rBV2	51291	141082	18.26%	2.332%
23	4.249	982	998	1031	rBV	117534	303820	39.31%	5.021%
24	4.471	1064	1067	1068	rBV	192	121	0.02%	0.002%
25	4.484	1068	1071	1076	rVB2	264	238	0.03%	0.004%
26	4.510	1077	1079	1084	rBV2	260	174	0.02%	0.003%
27	4.622	1110	1114	1118	rBV2	323	357	0.05%	0.006%
28	4.696	1133	1137	1142	rBV2	190	176	0.02%	0.003%
29	4.719	1142	1144	1148	rBV	137	113	0.01%	0.002%
30	4.741	1148	1151	1152	rBV	219	143	0.02%	0.002%
31	4.841	1180	1182	1188	rVB	160	119	0.02%	0.002%
32	4.876	1189	1193	1198	rBV2	129	155	0.02%	0.003%
33	4.957	1202	1218	1253	rBV2	290835	772803	100.00%	12.772%
34	5.111	1262	1266	1268	rBV3	315	253	0.03%	0.004%
35	5.166	1278	1283	1285	rBV2	312	321	0.04%	0.005%
36	5.243	1304	1307	1315	rVB4	372	411	0.05%	0.007%

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 Title : VOC Analysis

37	5.291	1320	1322	1326	rVB2	292	180	0.02%	0.003%
38	5.314	1326	1329	1331	rBV3	219	118	0.02%	0.002%
39	5.352	1339	1341	1344	rVB	258	126	0.02%	0.002%
40	5.371	1344	1347	1351	rBV3	321	263	0.03%	0.004%
41	5.458	1370	1374	1377	rBV	108	127	0.02%	0.002%
42	5.532	1386	1397	1432	rBV	251991	517731	66.99%	8.556%
43	5.831	1482	1490	1506	rBV6	2184	4780	0.62%	0.079%
44	5.989	1524	1539	1570	rBV	169097	348347	45.08%	5.757%
45	6.153	1586	1590	1596	rVB5	620	606	0.08%	0.010%
46	6.175	1596	1597	1601	rVB2	297	174	0.02%	0.003%
47	6.198	1601	1604	1607	rBV3	208	154	0.02%	0.003%
48	6.220	1609	1611	1616	rBV	274	224	0.03%	0.004%
49	6.432	1672	1677	1680	rBV	273	226	0.03%	0.004%
50	6.686	1750	1756	1760	rBV2	165	273	0.04%	0.005%
51	6.741	1765	1773	1779	rBV	330	436	0.06%	0.007%
52	6.770	1779	1782	1784	rBV2	172	126	0.02%	0.002%
53	6.850	1805	1807	1813	rBV2	143	142	0.02%	0.002%
54	6.912	1816	1826	1859	rBV	92696	176402	22.83%	2.915%
55	7.075	1875	1877	1881	rBV2	220	146	0.02%	0.002%
56	7.140	1892	1897	1899	rBV2	489	431	0.06%	0.007%
57	7.243	1917	1929	1959	rBV	350896	622573	80.56%	10.289%
58	7.497	2006	2008	2012	rVB3	181	129	0.02%	0.002%
59	7.555	2017	2026	2059	rBV	62999	114601	14.83%	1.894%
60	7.883	2123	2128	2131	rVB2	370	358	0.05%	0.006%
61	7.902	2131	2134	2135	rBV	215	146	0.02%	0.002%
62	8.024	2162	2172	2218	rBV	175268	349023	45.16%	5.768%
63	8.667	2369	2372	2374	rBV	181	149	0.02%	0.002%
64	8.741	2392	2395	2398	rBV	189	147	0.02%	0.002%
65	8.783	2398	2408	2433	rBV	381308	621158	80.38%	10.266%
66	9.664	2679	2682	2687	rBV	142	111	0.01%	0.002%
67	9.770	2711	2715	2720	rBV2	138	159	0.02%	0.003%
68	9.879	2745	2749	2753	rBV2	253	246	0.03%	0.004%
69	10.153	2822	2834	2855	rBV	216678	339808	43.97%	5.616%
70	10.329	2886	2889	2890	rBV	195	117	0.02%	0.002%
71	10.487	2935	2938	2943	rBV3	233	270	0.03%	0.004%
72	10.538	2951	2954	2960	rBV2	190	158	0.02%	0.003%
73	10.612	2973	2977	2978	rBV	161	127	0.02%	0.002%
74	10.776	3023	3028	3031	rBV2	126	134	0.02%	0.002%
75	10.863	3051	3055	3060	rBV	250	313	0.04%	0.005%
76	11.124	3133	3136	3137	rBV	204	119	0.02%	0.002%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.185	3144	3155	3178	rBV	392526	612131	79.21%	10.117%
78	11.410	3222	3225	3231	rVB2	124	126	0.02%	0.002%
79	11.500	3250	3253	3256	rBV2	159	131	0.02%	0.002%
80	11.558	3260	3271	3295	rBV	354281	563991	72.98%	9.321%
81	11.738	3325	3327	3330	rBV	214	154	0.02%	0.003%
82	11.905	3376	3379	3383	rVB	177	126	0.02%	0.002%
83	12.271	3490	3493	3496	rBV2	154	120	0.02%	0.002%
84	12.587	3587	3591	3592	rBV	473	300	0.04%	0.005%
85	12.635	3602	3606	3609	rBV	184	167	0.02%	0.003%
86	13.207	3777	3784	3791	rVV2	1824	2192	0.28%	0.036%
87	13.445	3849	3858	3873	rBV2	7944	13091	1.69%	0.216%
88	13.525	3880	3883	3888	rVB3	311	211	0.03%	0.003%
89	13.686	3926	3933	3942	rVB3	2568	3342	0.43%	0.055%
90	13.837	3978	3980	3985	rVB	247	135	0.02%	0.002%
91	13.976	4020	4023	4028	rBV3	380	352	0.05%	0.006%
92	14.095	4053	4060	4063	rBV2	317	440	0.06%	0.007%
93	14.130	4068	4071	4074	rBV	238	214	0.03%	0.004%
94	14.259	4107	4111	4114	rBV3	257	245	0.03%	0.004%
95	14.278	4114	4117	4119	rBV2	211	145	0.02%	0.002%
96	14.413	4154	4159	4161	rBV3	301	289	0.04%	0.005%
97	14.532	4193	4196	4198	rVB2	256	133	0.02%	0.002%
98	15.033	4349	4352	4355	rBV3	338	262	0.03%	0.004%
99	15.355	4450	4452	4454	rBV	363	193	0.02%	0.003%
100	15.480	4488	4491	4494	rVB3	492	357	0.05%	0.006%

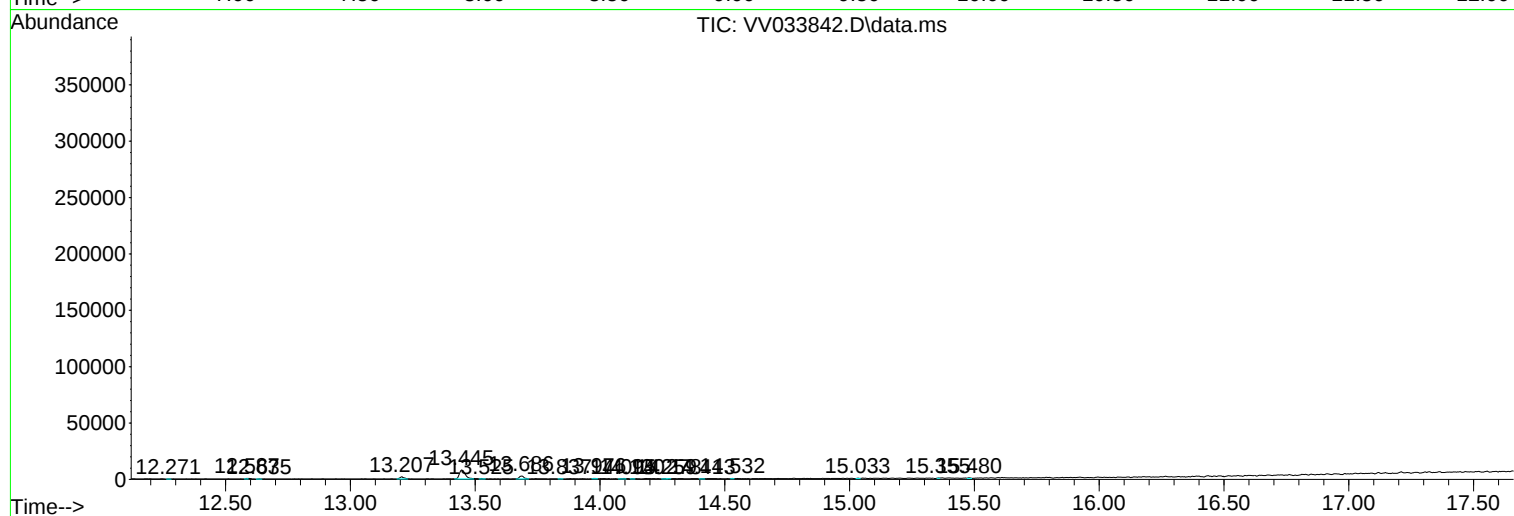
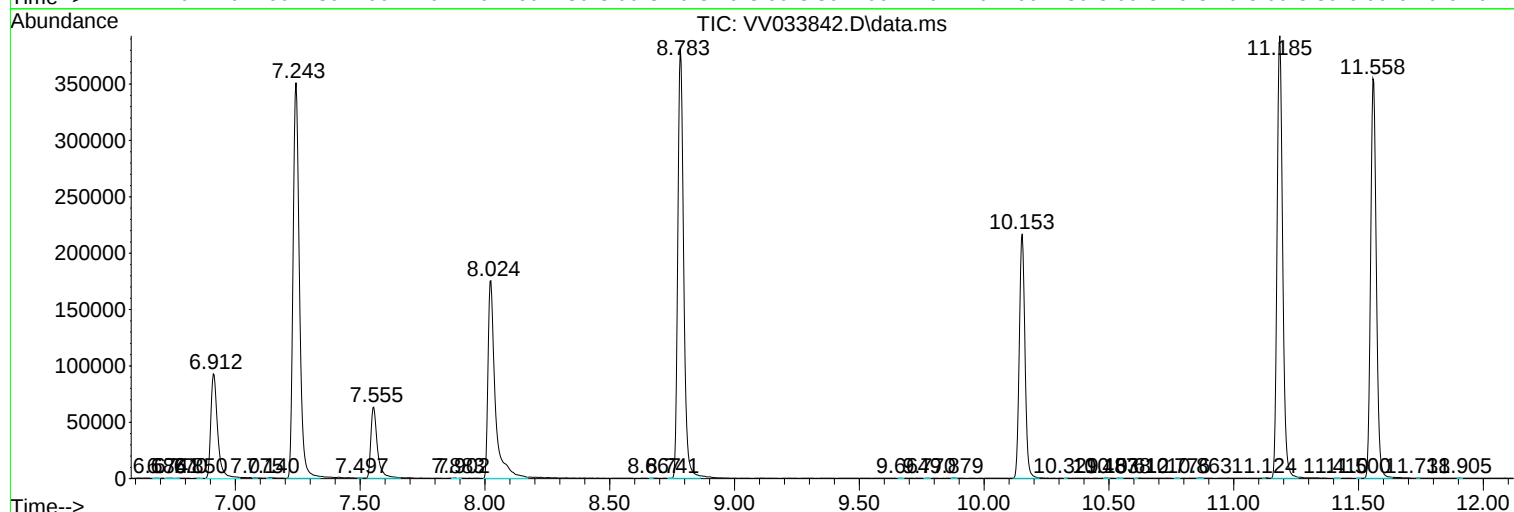
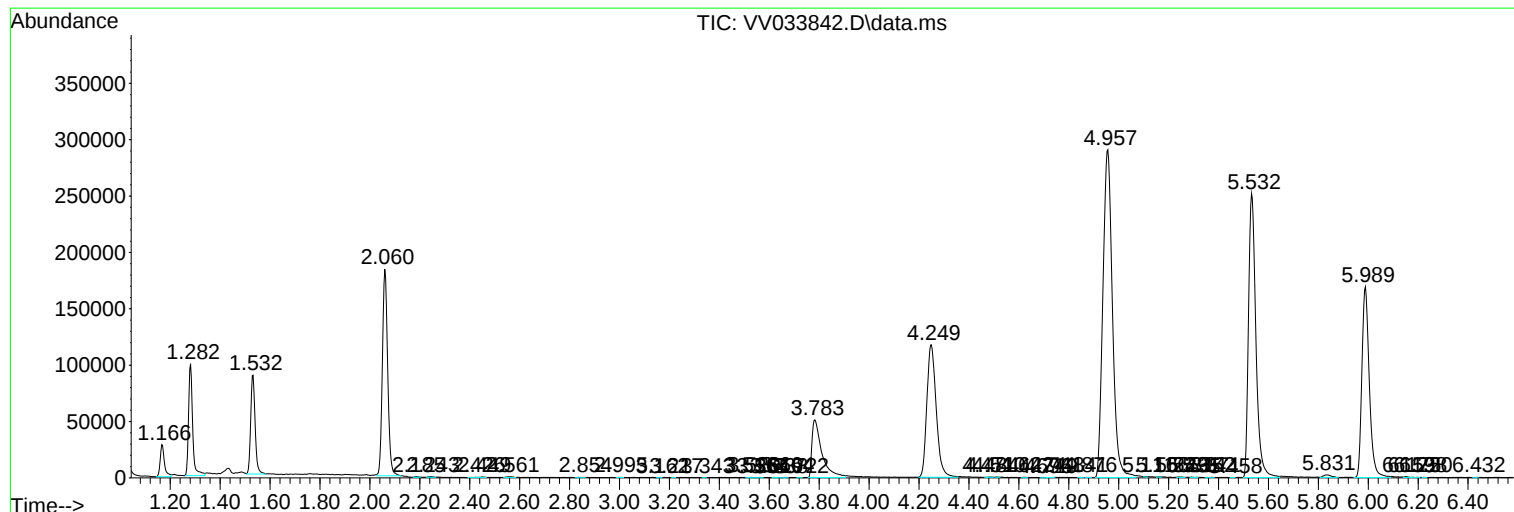
Sum of corrected areas: 6050784

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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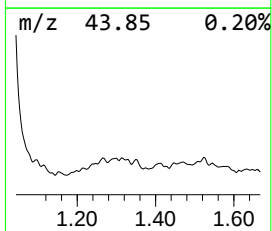
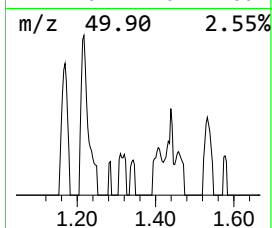
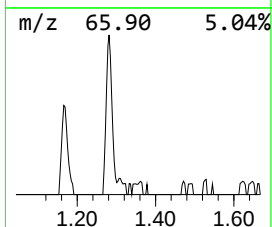
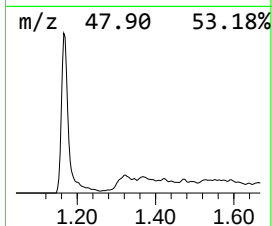
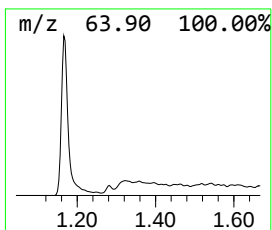
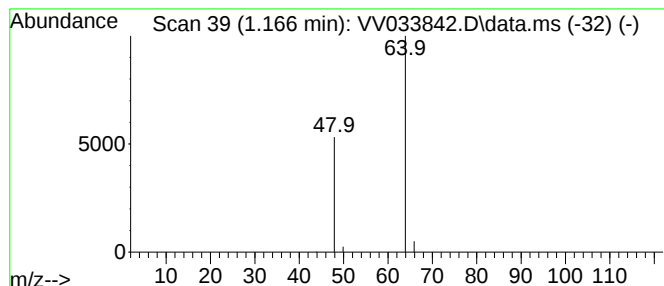
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
1.166	3.25 ug/L	33693	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	3.3	ug/L	33693	1	5.532	517731	50.0