

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053271.D
 Acq On : 17 Mar 2023 16:49
 Operator : JC/MD
 Sample : 01930-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFC0

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_U\Method\SFAMULM031523WMA.M

Title : VOC Analysis

Signal : TIC: VU053271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	32	39	56	rBV	25756	45437	7.72%	1.030%
2	1.597	73	80	98	rVB	83488	94168	16.00%	2.134%
3	1.909	170	177	190	rBV	61748	82886	14.08%	1.878%
4	2.562	369	380	395	rBV	121028	196037	33.30%	4.442%
5	3.093	542	545	547	rBV2	239	137	0.02%	0.003%
6	3.633	711	713	720	rVB2	328	304	0.05%	0.007%
7	3.684	726	729	731	rBV	280	162	0.03%	0.004%
8	4.044	839	841	842	rBV	137	42	0.01%	0.001%
9	4.350	933	936	939	rVB	257	132	0.02%	0.003%
10	4.613	1006	1018	1042	rBV	46090	109635	18.63%	2.484%
11	4.855	1091	1093	1096	rBV	173	96	0.02%	0.002%
12	5.057	1140	1156	1175	rBV	111487	242444	41.19%	5.493%
13	5.150	1183	1185	1188	rVB2	272	142	0.02%	0.003%
14	5.205	1199	1202	1208	rBV	227	189	0.03%	0.004%
15	5.250	1213	1216	1217	rBV	230	156	0.03%	0.004%
16	5.308	1233	1234	1236	rBV	116	45	0.01%	0.001%
17	5.372	1250	1254	1255	rBV	235	158	0.03%	0.004%
18	5.433	1271	1273	1275	rBV	155	65	0.01%	0.001%
19	5.514	1295	1298	1301	rVB	141	63	0.01%	0.001%
20	5.719	1341	1362	1369	rBV2	221877	588618	100.00%	13.337%
21	5.954	1433	1435	1437	rVB	152	43	0.01%	0.001%
22	5.980	1441	1443	1444	rBV	161	68	0.01%	0.002%
23	6.006	1448	1451	1453	rVV2	283	178	0.03%	0.004%
24	6.031	1456	1459	1464	rVB2	241	234	0.04%	0.005%
25	6.109	1478	1483	1485	rBV	293	236	0.04%	0.005%
26	6.147	1492	1495	1498	rBV	219	191	0.03%	0.004%
27	6.244	1511	1525	1546	rBV	176636	332243	56.44%	7.528%
28	6.411	1574	1577	1578	rBV	206	100	0.02%	0.002%
29	6.436	1584	1585	1587	rBV	140	34	0.01%	0.001%
30	6.520	1609	1611	1612	rBV	222	70	0.01%	0.002%
31	6.536	1614	1616	1620	rVB2	459	242	0.04%	0.005%
32	6.684	1649	1662	1681	rBV	141119	271792	46.17%	6.158%
33	6.787	1691	1694	1695	rBV	145	100	0.02%	0.002%
34	6.912	1731	1733	1735	rBV	127	69	0.01%	0.002%
35	7.028	1766	1769	1771	rBV	189	158	0.03%	0.004%
36	7.179	1811	1816	1828	rVB5	1040	1679	0.29%	0.038%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
 Title : VOC Analysis

37	7.224	1828	1830	1833	rBV2	152	85	0.01%	0.002%
38	7.266	1840	1843	1844	rBV2	265	139	0.02%	0.003%
39	7.321	1857	1860	1862	rBV2	266	182	0.03%	0.004%
40	7.401	1883	1885	1889	rVB	158	57	0.01%	0.001%
41	7.427	1889	1893	1897	rBV2	186	134	0.02%	0.003%
42	7.562	1923	1935	1954	rBV	79611	136318	23.16%	3.089%
43	7.655	1963	1964	1966	rVB	128	48	0.01%	0.001%
44	7.687	1967	1974	1981	rBV3	1023	1171	0.20%	0.027%
45	7.893	2025	2038	2056	rBV	277960	470932	80.01%	10.671%
46	8.076	2092	2095	2096	rBV	168	69	0.01%	0.002%
47	8.176	2114	2126	2140	rBV	55151	91187	15.49%	2.066%
48	8.253	2147	2150	2152	rBV2	164	135	0.02%	0.003%
49	8.276	2155	2157	2161	rVB	240	141	0.02%	0.003%
50	8.337	2172	2176	2180	rBV2	356	422	0.07%	0.010%
51	8.359	2181	2183	2186	rVB	173	72	0.01%	0.002%
52	8.526	2234	2235	2238	rVB	171	53	0.01%	0.001%
53	8.546	2238	2241	2244	rBV	180	97	0.02%	0.002%
54	8.626	2254	2266	2296	rBV2	142114	267978	45.53%	6.072%
55	8.838	2330	2332	2336	rBV	286	220	0.04%	0.005%
56	8.877	2342	2344	2345	rBV	111	47	0.01%	0.001%
57	9.089	2408	2410	2412	rBV	177	90	0.02%	0.002%
58	9.102	2412	2414	2417	rVV	189	108	0.02%	0.002%
59	9.150	2427	2429	2432	rBV2	140	79	0.01%	0.002%
60	9.414	2497	2511	2532	rBV	241956	400816	68.09%	9.082%
61	9.565	2552	2558	2567	rBV	600	911	0.15%	0.021%
62	9.604	2567	2570	2573	rVB	191	120	0.02%	0.003%
63	9.838	2640	2643	2646	rBV	160	160	0.03%	0.004%
64	9.993	2688	2691	2692	rBV	162	94	0.02%	0.002%
65	10.028	2698	2702	2708	rVB	264	246	0.04%	0.006%
66	10.067	2711	2714	2716	rBV2	271	190	0.03%	0.004%
67	10.208	2756	2758	2762	rVB	183	70	0.01%	0.002%
68	10.224	2762	2763	2764	rBV	110	29	0.00%	0.001%
69	10.301	2784	2787	2790	rBV	231	172	0.03%	0.004%
70	10.382	2809	2812	2814	rBV	150	127	0.02%	0.003%
71	10.591	2874	2877	2880	rBV	203	102	0.02%	0.002%
72	10.751	2914	2927	2950	rBV	183633	292800	49.74%	6.634%
73	10.903	2972	2974	2978	rBV	159	87	0.01%	0.002%
74	11.092	3031	3033	3036	rBV	157	53	0.01%	0.001%
75	11.295	3094	3096	3098	rVB	164	85	0.01%	0.002%
76	11.462	3146	3148	3150	rVV	157	47	0.01%	0.001%

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Peak Location: TOP

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77	11.484	3153	3155	3157	rVB	148	56	0.01%	0.001%
78	11.552	3174	3176	3179	rBV	208	96	0.02%	0.002%
79	11.642	3202	3204	3206	rBV	171	62	0.01%	0.001%
80	11.693	3218	3220	3224	rVB	165	73	0.01%	0.002%
81	11.806	3243	3255	3277	rBV	239386	380513	64.65%	8.622%
82	12.189	3362	3374	3393	rBV	247834	395918	67.26%	8.971%
83	12.726	3539	3541	3543	rBV	130	56	0.01%	0.001%
84	12.806	3563	3566	3569	rBV2	203	136	0.02%	0.003%
85	12.964	3613	3615	3616	rBV2	170	56	0.01%	0.001%
86	13.005	3625	3628	3632	rVB	205	154	0.03%	0.003%
87	13.089	3651	3654	3656	rBV	175	126	0.02%	0.003%
88	13.591	3808	3810	3814	rVB	242	122	0.02%	0.003%
89	13.668	3830	3834	3838	rBV2	225	220	0.04%	0.005%
90	13.980	3929	3931	3935	rBV	184	110	0.02%	0.002%
91	14.182	3992	3994	3999	rVB	204	101	0.02%	0.002%
92	14.208	3999	4002	4009	rBV	180	137	0.02%	0.003%
93	14.574	4113	4116	4123	rBV2	252	278	0.05%	0.006%
94	14.697	4152	4154	4157	rVB	290	150	0.03%	0.003%
95	14.722	4157	4162	4165	rBV	335	344	0.06%	0.008%
96	14.758	4171	4173	4177	rVB	212	119	0.02%	0.003%
97	15.262	4327	4330	4333	rBV	371	316	0.05%	0.007%

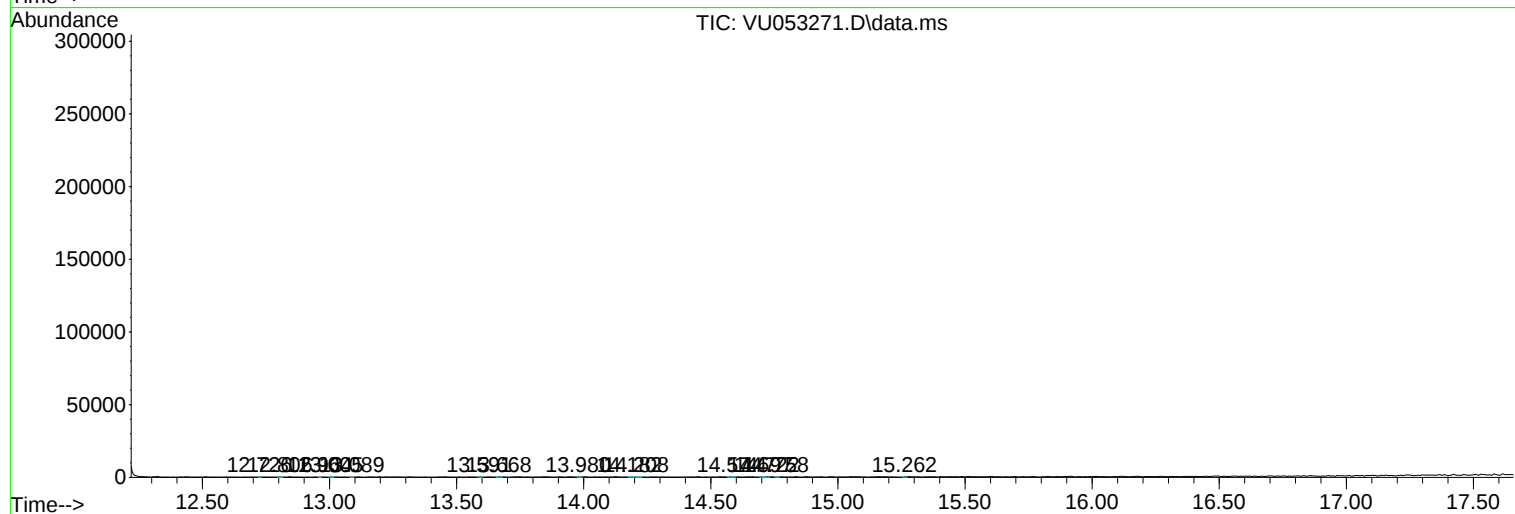
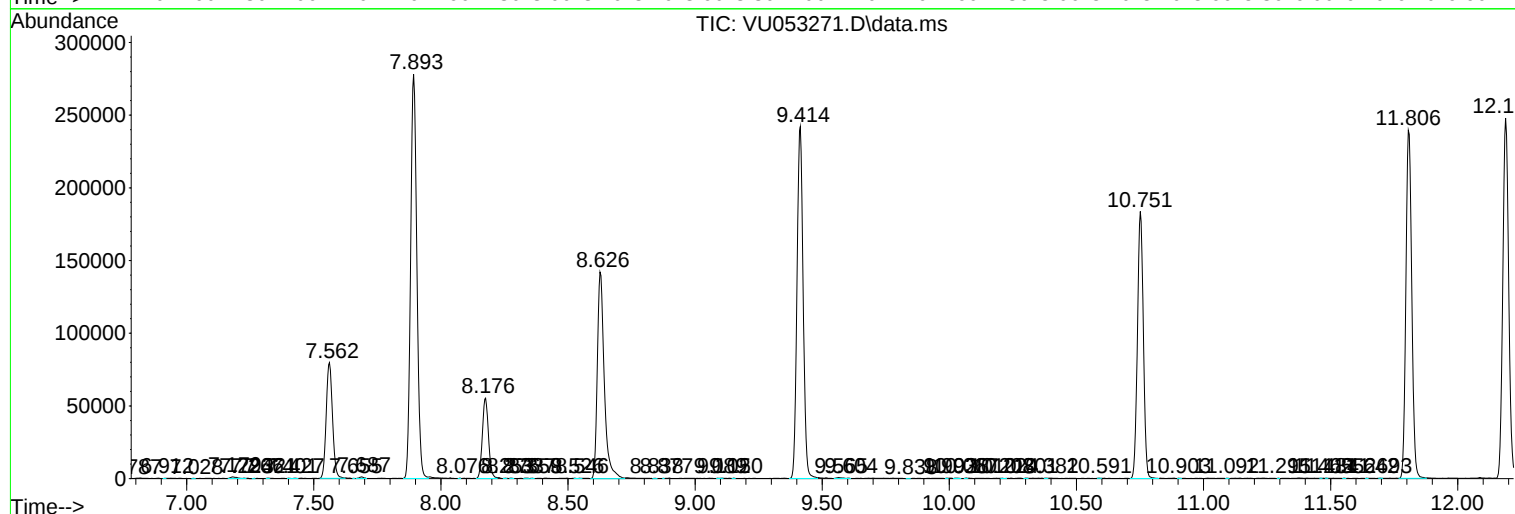
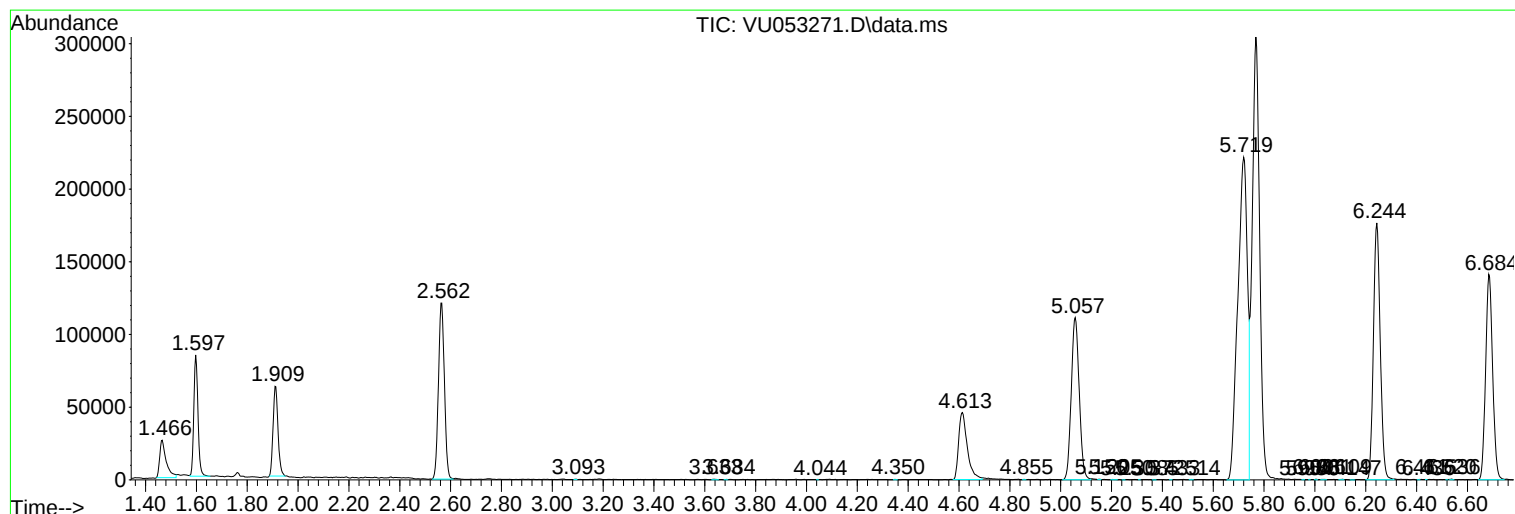
Sum of corrected areas: 4413369

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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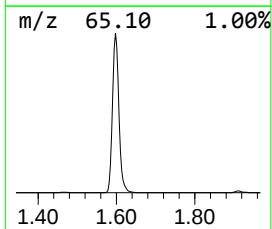
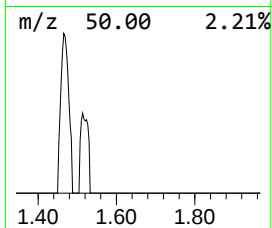
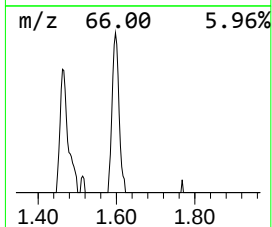
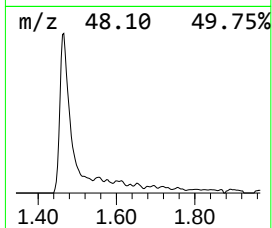
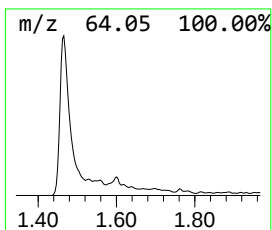
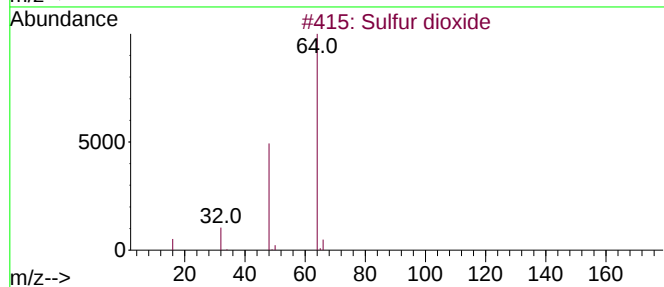
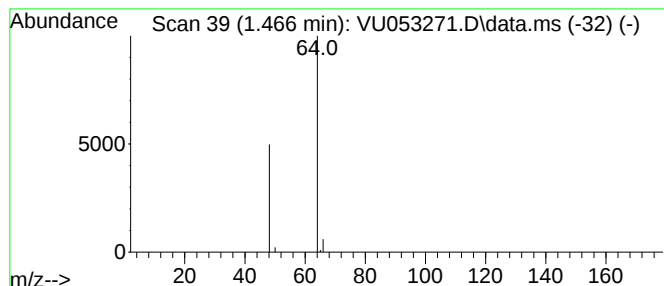
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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.
1.466	6.84 ug/L	45437	1,4-Difluorobenzene	6.244

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	5



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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	1.466	6.8	ug/L	45437	1	6.244	332243	50.0