

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053618.D
 Acq On : 10 Apr 2023 16:26
 Operator : JC/MD
 Sample : 02251-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD3

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053618.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	53	rBV	35285	63409	7.91%	0.952%
2	1.597	74	80	99	rVB	109199	126421	15.77%	1.897%
3	1.909	170	177	196	rVB	86993	122935	15.34%	1.845%
4	2.565	369	381	394	rBV	161175	263785	32.91%	3.959%
5	2.752	432	439	445	rBV5	1744	2607	0.33%	0.039%
6	3.047	524	531	535	rBV3	649	774	0.10%	0.012%
7	3.276	598	602	604	rBV2	219	212	0.03%	0.003%
8	3.369	628	631	636	rVB2	348	288	0.04%	0.004%
9	3.417	644	646	648	rBV	330	162	0.02%	0.002%
10	3.536	681	683	685	rBV	249	134	0.02%	0.002%
11	3.665	717	723	725	rBV	260	263	0.03%	0.004%
12	3.713	732	738	739	rBV	203	192	0.02%	0.003%
13	3.861	779	784	787	rBV	382	332	0.04%	0.005%
14	3.948	802	811	815	rVB2	264	361	0.05%	0.005%
15	4.083	848	853	855	rBV2	295	311	0.04%	0.005%
16	4.166	876	879	882	rBV	261	173	0.02%	0.003%
17	4.189	883	886	889	rVB2	305	189	0.02%	0.003%
18	4.263	907	909	913	rBV	215	180	0.02%	0.003%
19	4.359	935	939	941	rBV2	304	189	0.02%	0.003%
20	4.465	968	972	975	rBV	317	143	0.02%	0.002%
21	4.613	1006	1018	1049	rBV	69250	165372	20.63%	2.482%
22	4.983	1130	1133	1136	rBV2	248	204	0.03%	0.003%
23	5.057	1141	1156	1176	rBV	151206	327542	40.86%	4.916%
24	5.321	1234	1238	1239	rBV	313	175	0.02%	0.003%
25	5.353	1246	1248	1252	rBV2	218	179	0.02%	0.003%
26	5.417	1262	1268	1270	rBV2	231	245	0.03%	0.004%
27	5.523	1289	1301	1315	rVB3	5976	12584	1.57%	0.189%
28	5.594	1315	1323	1329	rBV2	267	368	0.05%	0.006%
29	5.623	1329	1332	1336	rVB2	291	245	0.03%	0.004%
30	5.719	1340	1362	1374	rBV2	290253	801624	100.00%	12.031%
31	6.025	1454	1457	1461	rBV2	322	344	0.04%	0.005%
32	6.243	1511	1525	1543	rBV	234973	447161	55.78%	6.711%
33	6.526	1607	1613	1620	rVB4	1808	2410	0.30%	0.036%
34	6.565	1623	1625	1628	rBV2	210	150	0.02%	0.002%
35	6.613	1637	1640	1643	rBV2	226	174	0.02%	0.003%
36	6.684	1648	1662	1682	rBV	180476	353991	44.16%	5.313%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	6.780	1690	1692	1694	rBV2	427	215	0.03%	0.003%
38	6.851	1710	1714	1716	rBV2	247	198	0.02%	0.003%
39	6.957	1743	1747	1751	rBV2	454	314	0.04%	0.005%
40	7.067	1778	1781	1785	rVB2	197	172	0.02%	0.003%
41	7.182	1811	1817	1821	rBV2	1092	1128	0.14%	0.017%
42	7.375	1871	1877	1880	rBV2	311	256	0.03%	0.004%
43	7.407	1884	1887	1889	rBV	244	140	0.02%	0.002%
44	7.462	1900	1904	1907	rVB2	197	155	0.02%	0.002%
45	7.559	1922	1934	1959	rBV2	101726	180456	22.51%	2.708%
46	7.671	1966	1969	1970	rBV2	357	196	0.02%	0.003%
47	7.690	1970	1975	1980	rVB2	863	867	0.11%	0.013%
48	7.893	2025	2038	2063	rBV	372429	647248	80.74%	9.714%
49	8.099	2097	2102	2106	rVB2	329	247	0.03%	0.004%
50	8.128	2106	2111	2113	rBV2	255	211	0.03%	0.003%
51	8.176	2113	2126	2147	rBV2	71700	122720	15.31%	1.842%
52	8.272	2154	2156	2163	rVB2	456	382	0.05%	0.006%
53	8.398	2192	2195	2199	rVB	248	178	0.02%	0.003%
54	8.417	2199	2201	2204	rBV	194	133	0.02%	0.002%
55	8.465	2209	2216	2219	rBV4	682	863	0.11%	0.013%
56	8.549	2234	2242	2249	rVB6	1629	2215	0.28%	0.033%
57	8.626	2254	2266	2296	rBV	201561	371034	46.29%	5.569%
58	8.777	2309	2313	2316	rBV2	627	539	0.07%	0.008%
59	8.973	2368	2374	2376	rBV2	217	223	0.03%	0.003%
60	9.009	2381	2385	2390	rBV2	288	260	0.03%	0.004%
61	9.092	2407	2411	2416	rVB	223	168	0.02%	0.003%
62	9.179	2435	2438	2442	rBV2	160	154	0.02%	0.002%
63	9.221	2449	2451	2455	rBV	215	144	0.02%	0.002%
64	9.414	2495	2511	2517	rBV	331686	567258	70.76%	8.514%
65	9.642	2579	2582	2585	rBV2	324	265	0.03%	0.004%
66	9.687	2593	2596	2600	rBV2	267	227	0.03%	0.003%
67	9.886	2654	2658	2661	rBV2	238	210	0.03%	0.003%
68	9.967	2679	2683	2686	rBV2	304	252	0.03%	0.004%
69	10.140	2733	2737	2742	rBV	298	229	0.03%	0.003%
70	10.169	2743	2746	2749	rBV	351	210	0.03%	0.003%
71	10.298	2783	2786	2790	rVB	273	154	0.02%	0.002%
72	10.481	2838	2843	2847	rBV	170	168	0.02%	0.003%
73	10.661	2894	2899	2904	rBV	202	246	0.03%	0.004%
74	10.687	2904	2907	2910	rVB	306	174	0.02%	0.003%
75	10.751	2912	2927	2945	rBV	272245	435827	54.37%	6.541%
76	10.967	2991	2994	2997	rBV	205	132	0.02%	0.002%

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Peak Location: TOP

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77	11.054	3019	3021	3025	rBV2	200	140	0.02%	0.002%
78	11.144	3046	3049	3052	rBV	243	159	0.02%	0.002%
79	11.359	3114	3116	3120	rBV2	287	189	0.02%	0.003%
80	11.433	3136	3139	3144	rBV2	270	238	0.03%	0.004%
81	11.459	3144	3147	3148	rBV2	219	148	0.02%	0.002%
82	11.591	3186	3188	3193	rVB	405	198	0.02%	0.003%
83	11.616	3194	3196	3199	rVB	249	150	0.02%	0.002%
84	11.642	3199	3204	3206	rBV	203	133	0.02%	0.002%
85	11.745	3224	3236	3244	rBV2	14862	21956	2.74%	0.330%
86	11.809	3244	3256	3282	rVV2	360119	770527	96.12%	11.564%
87	11.941	3295	3297	3305	rVB4	631	481	0.06%	0.007%
88	12.012	3317	3319	3322	rBV	274	146	0.02%	0.002%
89	12.189	3361	3374	3396	rBV2	399440	765067	95.44%	11.482%
90	12.333	3415	3419	3420	rBV	366	230	0.03%	0.003%
91	12.687	3526	3529	3532	rVB2	330	186	0.02%	0.003%
92	12.767	3549	3554	3557	rBV	464	374	0.05%	0.006%
93	12.935	3603	3606	3612	rVB	323	239	0.03%	0.004%
94	12.970	3612	3617	3621	rBV	381	449	0.06%	0.007%
95	13.455	3766	3768	3769	rVB2	482	132	0.02%	0.002%
96	13.533	3789	3792	3793	rBV2	316	186	0.02%	0.003%
97	13.767	3862	3865	3871	rVB	387	284	0.04%	0.004%
98	13.838	3876	3887	3900	rBV	31506	50612	6.31%	0.760%
99	14.327	4030	4039	4051	rBV4	11921	18496	2.31%	0.278%
100	14.867	4204	4207	4209	rBV2	455	267	0.03%	0.004%

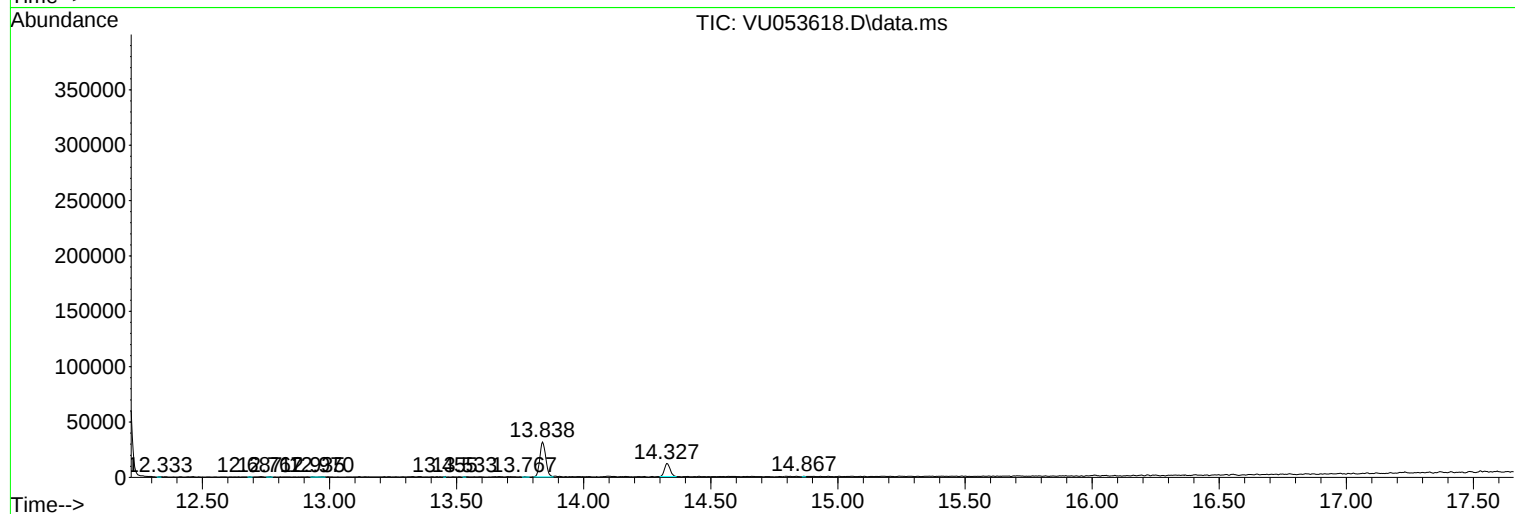
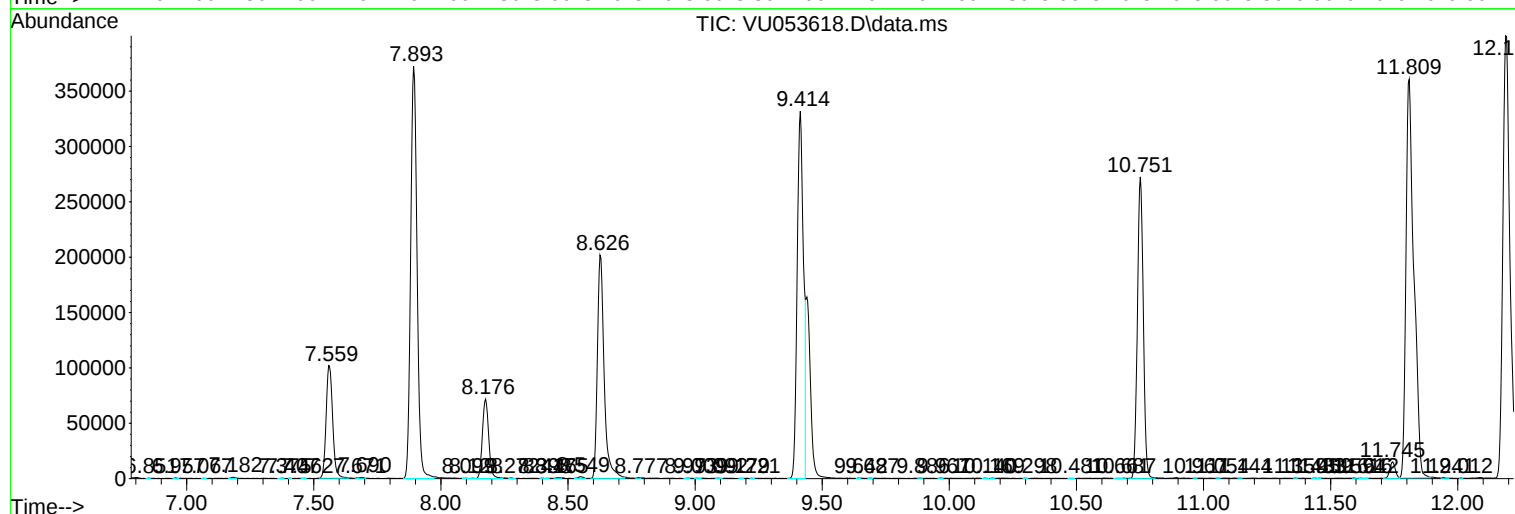
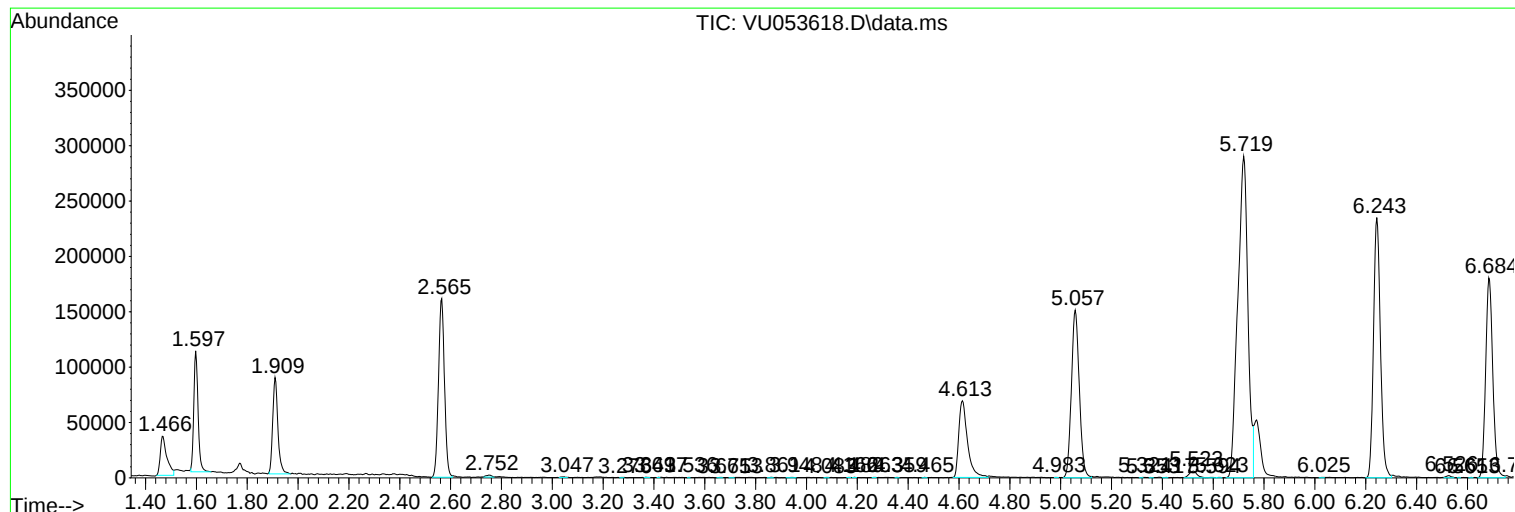
Sum of corrected areas: 6662983

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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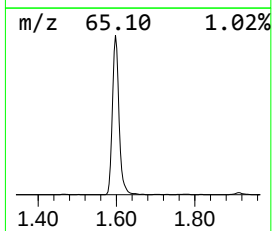
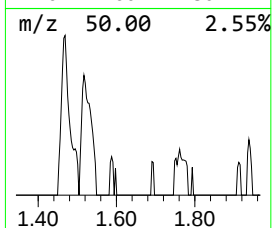
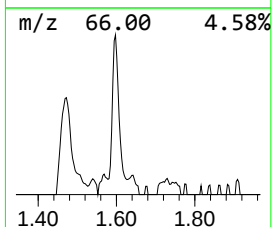
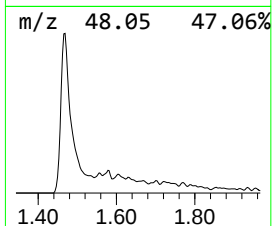
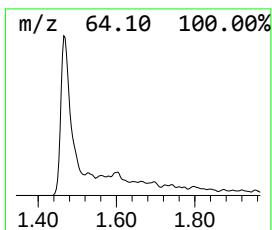
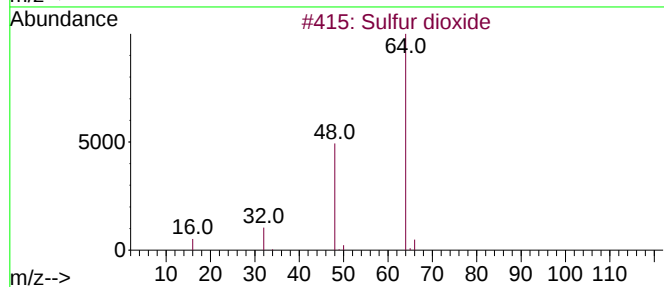
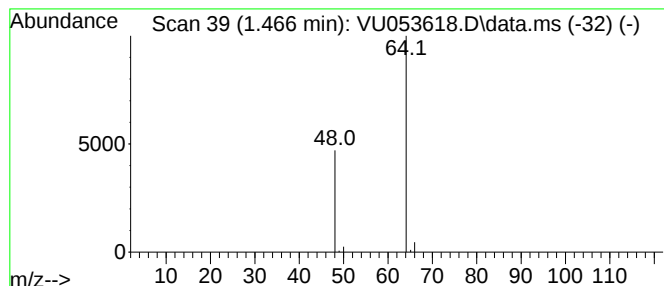
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	7.09 ug/L	63409	1,4-Difluorobenzene	6.243

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	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	7.1	ug/L	63409	1	6.243	447161	50.0