

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031523\
 Data File : VU053202.D
 Acq On : 15 Mar 2023 15:53
 Operator : JC/MD
 Sample : 01929-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFC9

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: VU053202.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	32	40	61	rBV	128545	260875	61.62%	7.814%
2	2.568	370	382	399	rBV	93971	154017	36.38%	4.613%
3	2.781	445	448	450	rBV3	434	276	0.07%	0.008%
4	3.073	536	539	543	rBV	245	153	0.04%	0.005%
5	3.565	688	692	699	rVB	312	411	0.10%	0.012%
6	3.604	700	704	708	rBV	277	271	0.06%	0.008%
7	3.626	709	711	714	rBV2	176	135	0.03%	0.004%
8	3.668	722	724	726	rVB	208	66	0.02%	0.002%
9	3.716	735	739	744	rBV2	231	281	0.07%	0.008%
10	3.784	759	760	761	rBV2	112	32	0.01%	0.001%
11	3.861	780	784	790	rBV	318	358	0.08%	0.011%
12	4.108	856	861	862	rBV	339	281	0.07%	0.008%
13	4.154	872	875	879	rBV2	199	201	0.05%	0.006%
14	4.224	895	897	901	rBV	213	136	0.03%	0.004%
15	4.366	939	941	944	rVB	161	70	0.02%	0.002%
16	4.626	1010	1022	1044	rBV	25555	66325	15.67%	1.987%
17	4.989	1133	1135	1137	rBV	138	90	0.02%	0.003%
18	5.057	1141	1156	1186	rVV	78084	169681	40.08%	5.082%
19	5.186	1194	1196	1201	rVB	164	73	0.02%	0.002%
20	5.295	1227	1230	1231	rBV	148	65	0.02%	0.002%
21	5.346	1242	1246	1249	rBV2	365	327	0.08%	0.010%
22	5.411	1264	1266	1268	rBV	190	87	0.02%	0.003%
23	5.446	1274	1277	1280	rBV	199	91	0.02%	0.003%
24	5.591	1318	1322	1326	rBV2	209	164	0.04%	0.005%
25	5.645	1336	1339	1342	rBV2	151	87	0.02%	0.003%
26	5.719	1342	1362	1386	rBV3	156737	423358	100.00%	12.680%
27	5.858	1402	1405	1411	rBV2	331	407	0.10%	0.012%
28	6.006	1448	1451	1454	rVB	172	93	0.02%	0.003%
29	6.025	1454	1457	1459	rBV	218	131	0.03%	0.004%
30	6.150	1494	1496	1497	rBV	119	28	0.01%	0.001%
31	6.243	1512	1525	1554	rVB	131965	246559	58.24%	7.385%
32	6.452	1588	1590	1596	rBV2	179	177	0.04%	0.005%
33	6.504	1604	1606	1607	rBV	151	42	0.01%	0.001%
34	6.546	1617	1619	1621	rBV	155	95	0.02%	0.003%
35	6.687	1650	1663	1680	rBV	98673	189845	44.84%	5.686%
36	6.793	1694	1696	1699	rVB	219	88	0.02%	0.003%

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 Title : VOC Analysis

37	6.813	1699	1702	1705	rBV2	277	195	0.05%	0.006%
38	6.896	1725	1728	1731	rVB	244	170	0.04%	0.005%
39	6.925	1735	1737	1740	rVV	177	63	0.01%	0.002%
40	7.166	1808	1812	1813	rBV	197	146	0.03%	0.004%
41	7.321	1859	1860	1864	rVB	263	122	0.03%	0.004%
42	7.343	1864	1867	1868	rBV	278	156	0.04%	0.005%
43	7.562	1922	1935	1957	rBV	59155	102404	24.19%	3.067%
44	7.787	2003	2005	2007	rBV2	160	89	0.02%	0.003%
45	7.838	2019	2021	2024	rVB	157	88	0.02%	0.003%
46	7.893	2025	2038	2057	rBV	195957	342710	80.95%	10.265%
47	8.047	2085	2086	2087	rBV	238	71	0.02%	0.002%
48	8.073	2092	2094	2098	rVB2	172	125	0.03%	0.004%
49	8.176	2114	2126	2145	rBV	39989	66362	15.68%	1.988%
50	8.337	2173	2176	2177	rBV	226	149	0.04%	0.004%
51	8.378	2187	2189	2193	rVB2	237	147	0.03%	0.004%
52	8.407	2195	2198	2199	rBV2	157	76	0.02%	0.002%
53	8.629	2257	2267	2294	rBV4	81961	162694	38.43%	4.873%
54	8.784	2313	2315	2318	rVB	277	117	0.03%	0.004%
55	9.050	2396	2398	2401	rBV	190	124	0.03%	0.004%
56	9.073	2402	2405	2410	rVB	209	135	0.03%	0.004%
57	9.414	2497	2511	2530	rBV	188217	310739	73.40%	9.307%
58	9.648	2581	2584	2586	rBV	199	105	0.02%	0.003%
59	9.677	2590	2593	2595	rBV2	192	126	0.03%	0.004%
60	9.857	2646	2649	2651	rBV	181	130	0.03%	0.004%
61	10.063	2711	2713	2716	rBV	222	139	0.03%	0.004%
62	10.102	2722	2725	2729	rBV3	270	213	0.05%	0.006%
63	10.121	2729	2731	2734	rVB	252	104	0.02%	0.003%
64	10.140	2734	2737	2739	rBV2	262	175	0.04%	0.005%
65	10.156	2739	2742	2743	rBV2	142	68	0.02%	0.002%
66	10.372	2806	2809	2812	rVB	270	185	0.04%	0.006%
67	10.462	2834	2837	2840	rBV	191	133	0.03%	0.004%
68	10.517	2853	2854	2855	rBV	101	20	0.00%	0.001%
69	10.751	2914	2927	2945	rBV	123542	197658	46.69%	5.920%
70	10.828	2949	2951	2952	rBV	140	42	0.01%	0.001%
71	10.883	2966	2968	2972	rBV2	333	175	0.04%	0.005%
72	10.973	2995	2996	3000	rVB	157	62	0.01%	0.002%
73	10.999	3001	3004	3006	rBV	200	101	0.02%	0.003%
74	11.054	3020	3021	3022	rBV	161	32	0.01%	0.001%
75	11.147	3049	3050	3051	rBV	142	46	0.01%	0.001%
76	11.250	3081	3082	3085	rVB	139	46	0.01%	0.001%

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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

77	11.468	3147	3150	3152	rBV2	457	286	0.07%	0.009%
78	11.600	3188	3191	3195	rBV	249	189	0.04%	0.006%
79	11.729	3226	3231	3233	rBV2	236	202	0.05%	0.006%
80	11.806	3244	3255	3272	rBV	206091	330999	78.18%	9.914%
81	12.073	3330	3338	3349	rBV7	2229	4757	1.12%	0.142%
82	12.189	3362	3374	3395	rBV	182352	298693	70.55%	8.946%
83	12.697	3529	3532	3534	rBV	268	139	0.03%	0.004%
84	12.751	3547	3549	3550	rBV	312	140	0.03%	0.004%
85	12.909	3593	3598	3601	rBV2	321	276	0.07%	0.008%
86	13.362	3736	3739	3742	rBV2	235	156	0.04%	0.005%
87	13.581	3805	3807	3808	rBV	195	65	0.02%	0.002%
88	13.632	3821	3823	3824	rBV	199	73	0.02%	0.002%
89	13.729	3850	3853	3855	rBV	254	166	0.04%	0.005%
90	13.877	3896	3899	3902	rBV	270	190	0.04%	0.006%
91	14.533	4101	4103	4106	rBV	211	105	0.02%	0.003%
92	15.005	4246	4250	4255	rBV2	452	499	0.12%	0.015%

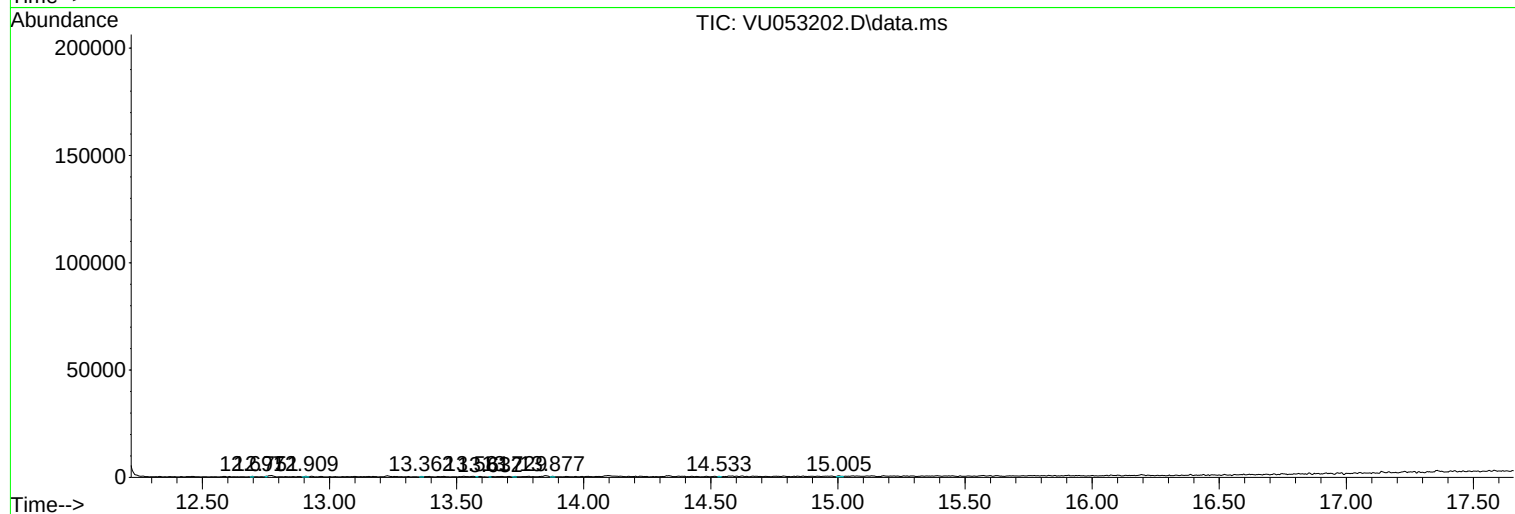
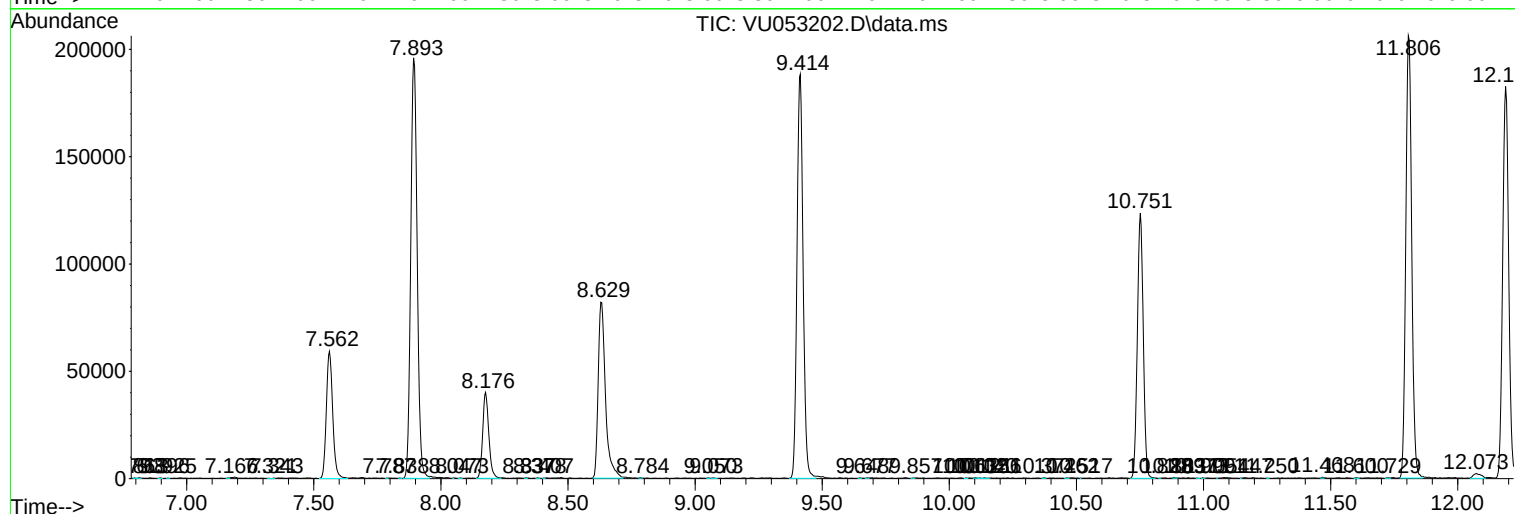
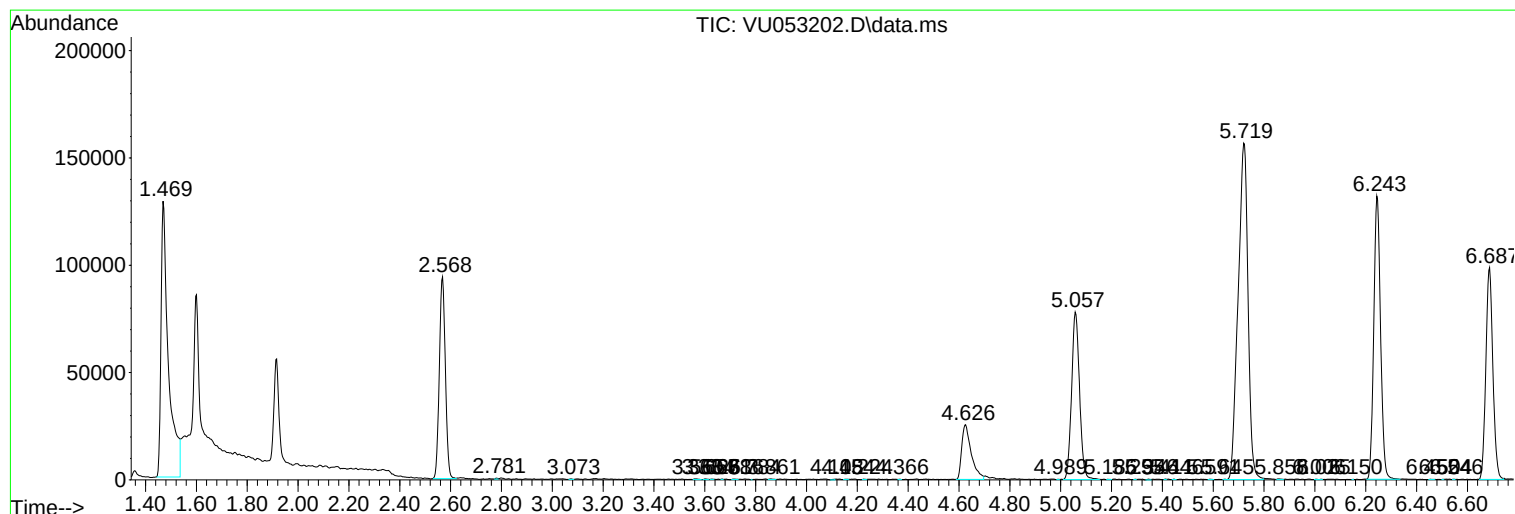
Sum of corrected areas: 3338753

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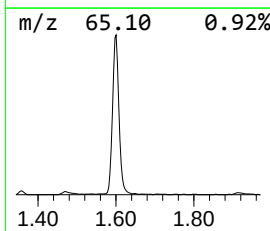
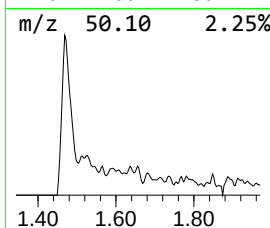
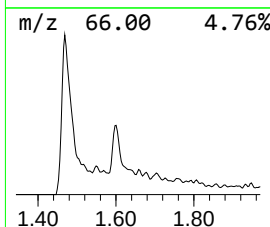
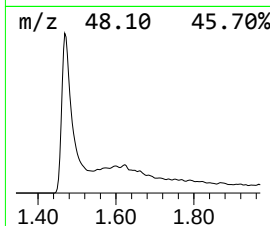
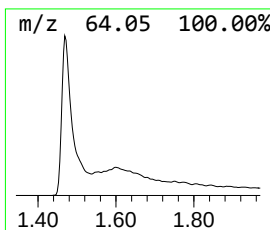
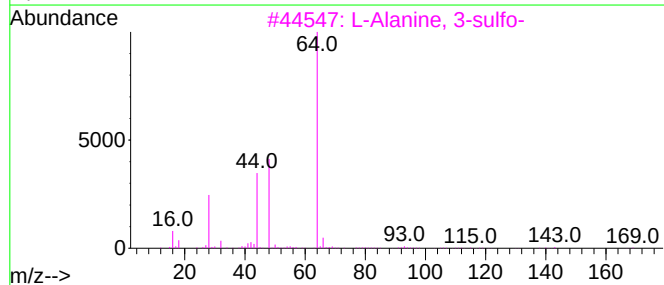
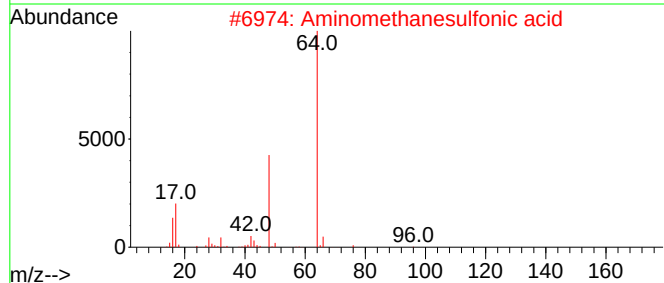
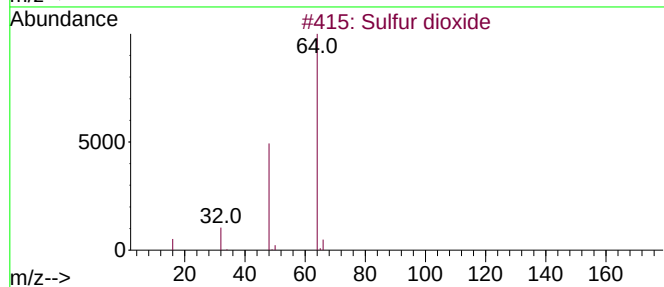
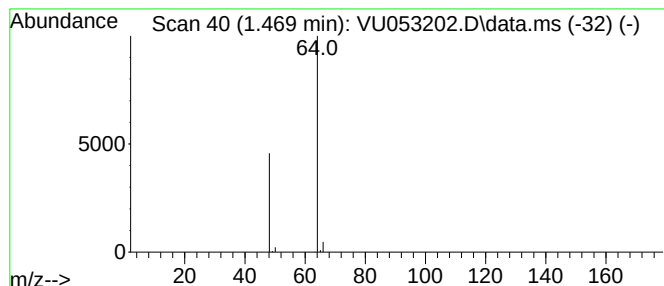
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	52.90 ug/L	260875	1,4-Difluorobenzene	6.247

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			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	1.469	52.9	ug/L	260875	1	6.247	246559	50.0