

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053617.D
 Acq On : 10 Apr 2023 16:02
 Operator : JC/MD
 Sample : 02251-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD2

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: VU053617.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	53	rBV	29956	54153	4.60%	0.704%
2	1.597	74	80	97	rVB	107029	123576	10.49%	1.607%
3	1.909	170	177	194	rVB	87594	122930	10.44%	1.599%
4	2.565	369	381	399	rVB	170952	274732	23.33%	3.573%
5	2.716	427	428	434	rVB	515	304	0.03%	0.004%
6	2.745	434	437	439	rBV3	532	306	0.03%	0.004%
7	2.961	502	504	507	rVV2	349	228	0.02%	0.003%
8	2.993	511	514	517	rVV	481	305	0.03%	0.004%
9	3.009	517	519	524	rVV	263	234	0.02%	0.003%
10	3.044	524	530	533	rVB3	571	539	0.05%	0.007%
11	3.064	533	536	540	rBV2	288	239	0.02%	0.003%
12	3.166	562	568	569	rBV3	595	495	0.04%	0.006%
13	3.456	655	658	661	rVV	221	201	0.02%	0.003%
14	3.671	720	725	728	rBV	188	195	0.02%	0.003%
15	3.710	733	737	742	rBV	200	227	0.02%	0.003%
16	3.835	772	776	778	rBV	267	205	0.02%	0.003%
17	3.948	809	811	817	rVB2	371	407	0.03%	0.005%
18	3.986	817	823	827	rBV2	293	337	0.03%	0.004%
19	4.137	867	870	872	rBV2	276	207	0.02%	0.003%
20	4.176	879	882	885	rBV	466	309	0.03%	0.004%
21	4.285	913	916	918	rBV	237	165	0.01%	0.002%
22	4.475	971	975	981	rBV	243	261	0.02%	0.003%
23	4.552	996	999	1002	rBV2	314	196	0.02%	0.003%
24	4.613	1006	1018	1042	rBV	71405	168774	14.33%	2.195%
25	4.986	1131	1134	1140	rBV2	307	365	0.03%	0.005%
26	5.057	1141	1156	1180	rBV	148382	331756	28.17%	4.315%
27	5.295	1226	1230	1232	rBV	467	280	0.02%	0.004%
28	5.388	1254	1259	1262	rBV2	305	305	0.03%	0.004%
29	5.446	1275	1277	1281	rBV2	173	168	0.01%	0.002%
30	5.510	1294	1297	1302	rVB2	195	187	0.02%	0.002%
31	5.549	1305	1309	1311	rBV2	221	206	0.02%	0.003%
32	5.594	1319	1323	1328	rVB2	264	223	0.02%	0.003%
33	5.629	1328	1334	1338	rBV2	300	334	0.03%	0.004%
34	5.719	1342	1362	1372	rBV2	301855	822689	69.86%	10.700%
35	5.973	1435	1441	1444	rVB3	302	278	0.02%	0.004%
36	6.063	1466	1469	1472	rVB2	457	272	0.02%	0.004%

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

37	6.105	1478	1482	1486	rVB2	331	248	0.02%	0.003%
38	6.128	1486	1489	1493	rVB	350	194	0.02%	0.003%
39	6.244	1511	1525	1546	rBV	306987	580664	49.31%	7.552%
40	6.465	1590	1594	1598	rVB2	430	314	0.03%	0.004%
41	6.491	1598	1602	1606	rBV	246	166	0.01%	0.002%
42	6.523	1606	1612	1613	rBV3	829	854	0.07%	0.011%
43	6.684	1649	1662	1688	rBV	189621	367740	31.23%	4.783%
44	6.838	1707	1710	1713	rBV2	349	214	0.02%	0.003%
45	7.144	1802	1805	1808	rBV	189	171	0.01%	0.002%
46	7.189	1811	1819	1825	rBV5	1116	1802	0.15%	0.023%
47	7.260	1838	1841	1844	rBV	244	177	0.02%	0.002%
48	7.562	1921	1935	1952	rBV	104638	186904	15.87%	2.431%
49	7.681	1970	1972	1973	rBV	409	215	0.02%	0.003%
50	7.787	2000	2005	2012	rVB3	281	404	0.03%	0.005%
51	7.893	2025	2038	2060	rBV	388172	667579	56.69%	8.683%
52	8.176	2115	2126	2145	rBV	74323	124864	10.60%	1.624%
53	8.288	2158	2161	2163	rBV	279	214	0.02%	0.003%
54	8.343	2175	2178	2185	rVB2	320	252	0.02%	0.003%
55	8.433	2202	2206	2209	rBV	279	236	0.02%	0.003%
56	8.452	2209	2212	2216	rBV2	577	623	0.05%	0.008%
57	8.626	2255	2266	2294	rBV	209670	389386	33.07%	5.064%
58	8.841	2330	2333	2334	rBV	295	174	0.01%	0.002%
59	8.915	2353	2356	2360	rVB	274	181	0.02%	0.002%
60	9.079	2404	2407	2412	rVB	273	255	0.02%	0.003%
61	9.105	2412	2415	2416	rBV2	417	194	0.02%	0.003%
62	9.259	2460	2463	2465	rBV	267	164	0.01%	0.002%
63	9.321	2479	2482	2486	rVB	236	196	0.02%	0.003%
64	9.414	2497	2511	2516	rBV	428292	735583	62.46%	9.567%
65	9.568	2555	2559	2563	rVB4	678	578	0.05%	0.008%
66	9.613	2571	2573	2577	rBV2	478	273	0.02%	0.004%
67	9.658	2585	2587	2593	rVB	310	174	0.01%	0.002%
68	9.690	2593	2597	2598	rBV2	416	267	0.02%	0.003%
69	9.874	2652	2654	2660	rVB	340	229	0.02%	0.003%
70	9.909	2661	2665	2670	rBV	214	218	0.02%	0.003%
71	10.044	2705	2707	2713	rVB2	229	189	0.02%	0.002%
72	10.288	2776	2783	2786	rBV	294	317	0.03%	0.004%
73	10.394	2813	2816	2822	rVB2	219	181	0.02%	0.002%
74	10.475	2838	2841	2848	rVB3	446	418	0.04%	0.005%
75	10.751	2915	2927	2944	rBV	276730	445383	37.82%	5.793%
76	11.054	3017	3021	3028	rBV3	352	378	0.03%	0.005%

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 Title : VOC Analysis

77	11.439	3137	3141	3143	rBV2	216	176	0.01%	0.002%
78	11.475	3149	3152	3156	rBV2	446	398	0.03%	0.005%
79	11.549	3171	3175	3178	rBV2	259	238	0.02%	0.003%
80	11.681	3213	3216	3220	rBV	264	208	0.02%	0.003%
81	11.742	3225	3235	3244	rBV2	36365	54873	4.66%	0.714%
82	11.809	3244	3256	3282	rVB2	473895	1177615	100.00%	15.316%
83	11.941	3293	3297	3306	rVB3	571	733	0.06%	0.010%
84	12.060	3332	3334	3337	rBV	518	404	0.03%	0.005%
85	12.192	3362	3375	3396	rBV3	441064	973399	82.66%	12.660%
86	12.369	3427	3430	3435	rBV3	534	378	0.03%	0.005%
87	12.529	3476	3480	3482	rBV2	269	185	0.02%	0.002%
88	12.600	3500	3502	3506	rBV	263	169	0.01%	0.002%
89	12.774	3551	3556	3559	rBV	235	252	0.02%	0.003%
90	12.864	3581	3584	3588	rBV	280	213	0.02%	0.003%
91	13.127	3662	3666	3669	rBV	311	249	0.02%	0.003%
92	13.436	3760	3762	3767	rVB	310	202	0.02%	0.003%
93	13.462	3767	3770	3777	rBV2	480	429	0.04%	0.006%
94	13.754	3858	3861	3863	rBV	332	196	0.02%	0.003%
95	13.838	3878	3887	3902	rVB2	32342	50775	4.31%	0.660%
96	13.896	3902	3905	3908	rVB3	574	404	0.03%	0.005%
97	14.092	3963	3966	3972	rBB2	545	459	0.04%	0.006%
98	14.169	3988	3990	3993	rBV2	305	166	0.01%	0.002%
99	14.259	4015	4018	4019	rBV2	297	194	0.02%	0.003%
100	14.327	4031	4039	4052	rBV4	7486	11254	0.96%	0.146%

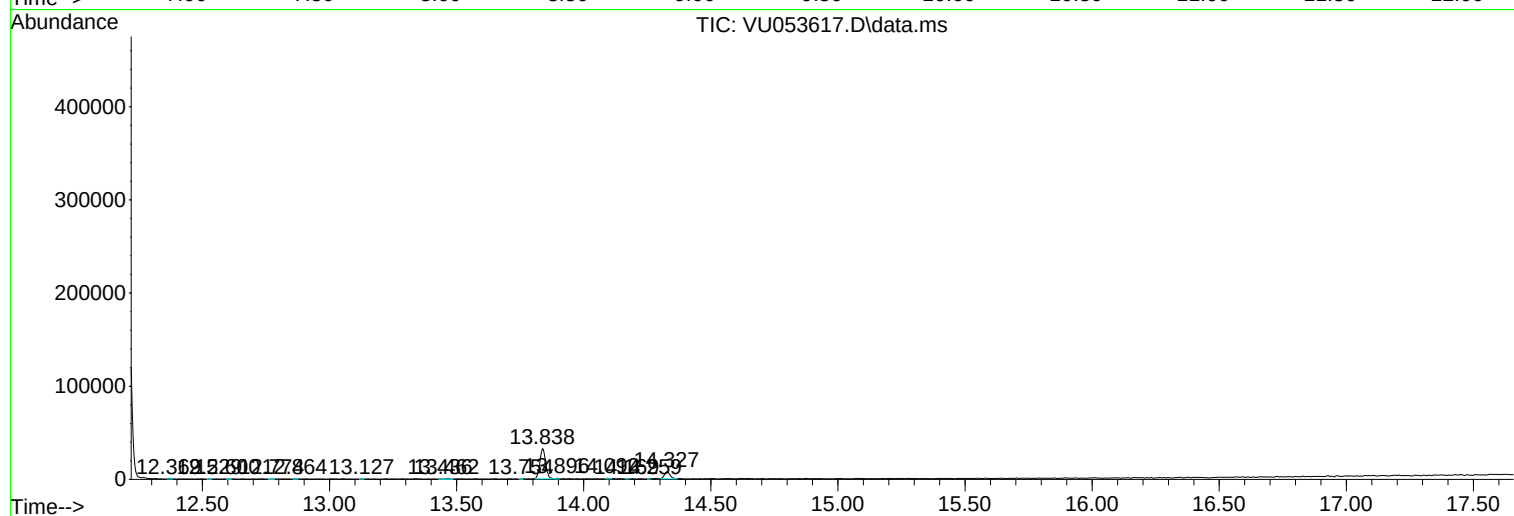
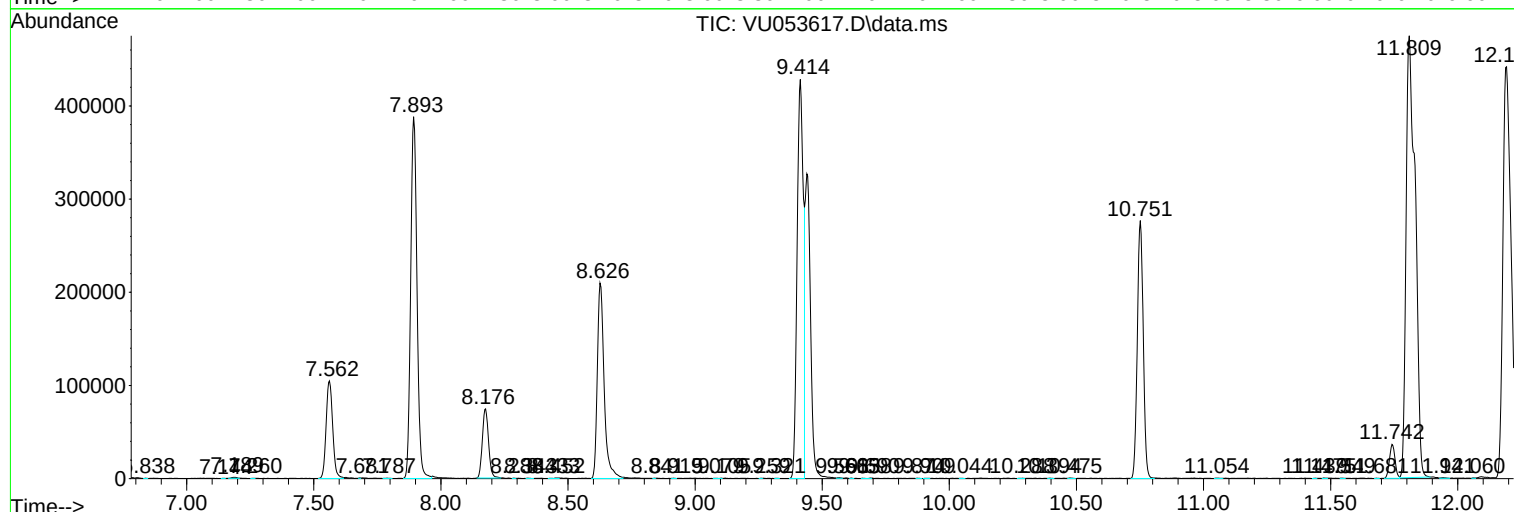
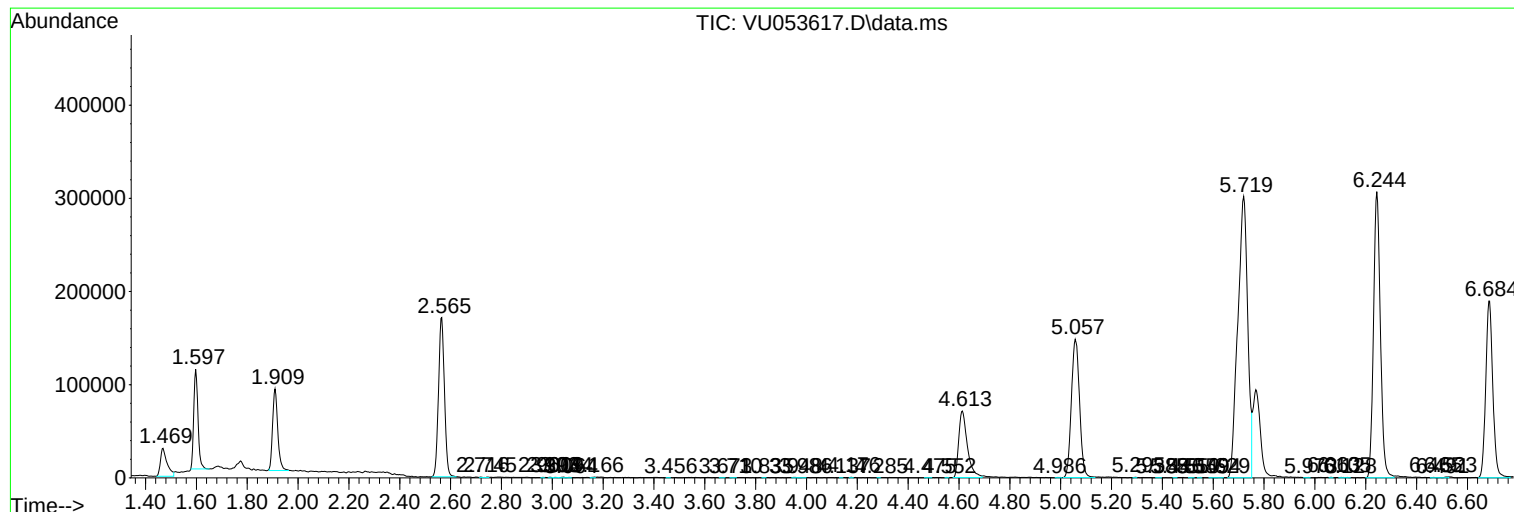
Sum of corrected areas: 7688730

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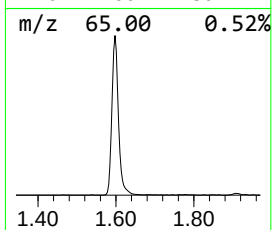
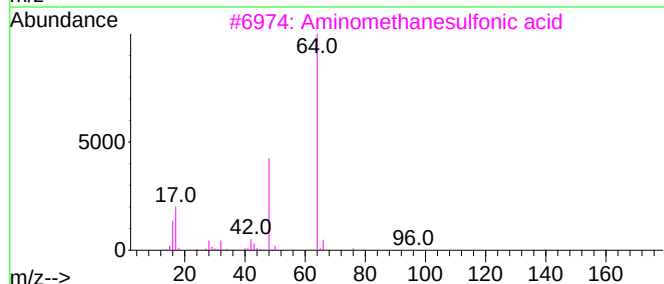
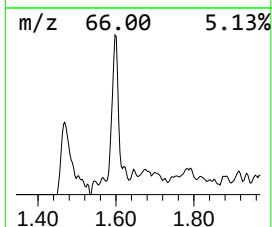
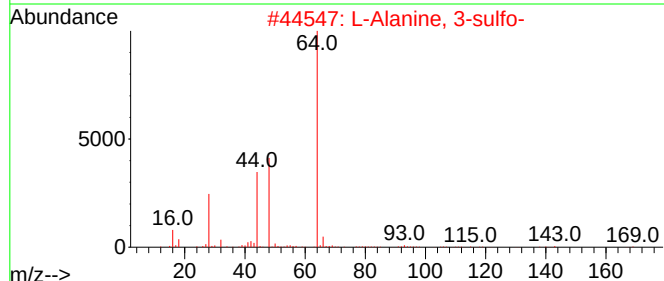
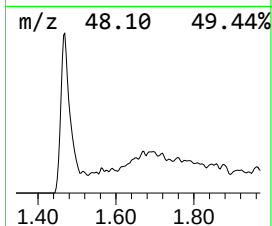
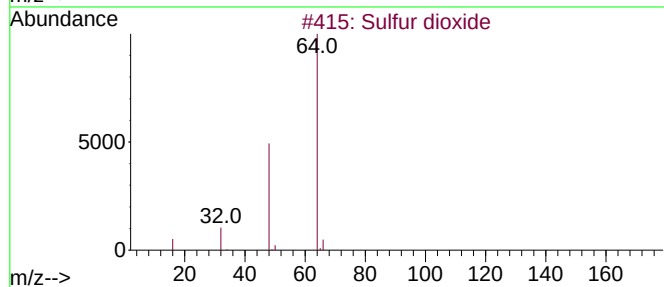
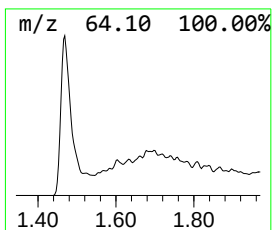
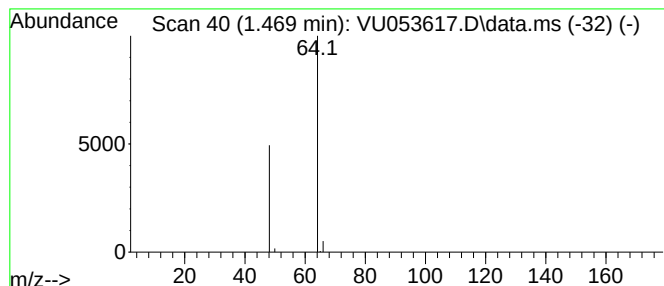
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	4.66 ug/L	54153	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.469	4.7	ug/L	54153	1	6.244	580664	50.0