

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031623\
 Data File : VU053230.D
 Acq On : 16 Mar 2023 16:42
 Operator : JC/MD
 Sample : 01930-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF4

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: VU053230.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	33	40	53	rBV	22378	36392	9.00%	1.157%
2	1.597	74	80	92	rVB	58565	66222	16.38%	2.106%
3	1.909	170	177	197	rVB	45115	61263	15.15%	1.948%
4	2.565	369	381	392	rBV	90411	146706	36.29%	4.665%
5	3.054	531	533	536	rBV	172	60	0.01%	0.002%
6	3.176	567	571	575	rVB3	390	326	0.08%	0.010%
7	3.890	790	793	796	rBV	226	112	0.03%	0.004%
8	3.912	797	800	802	rBV	193	91	0.02%	0.003%
9	4.137	867	870	875	rBV2	263	251	0.06%	0.008%
10	4.266	906	910	913	rVB2	223	142	0.04%	0.005%
11	4.385	945	947	953	rVB2	279	208	0.05%	0.007%
12	4.446	963	966	969	rBV	199	114	0.03%	0.004%
13	4.613	1008	1018	1046	rBV	37967	92470	22.87%	2.940%
14	4.896	1104	1106	1108	rBV	197	109	0.03%	0.003%
15	5.057	1141	1156	1180	rVB	75190	163477	40.44%	5.198%
16	5.214	1203	1205	1206	rBV	141	54	0.01%	0.002%
17	5.240	1212	1213	1218	rVB	234	126	0.03%	0.004%
18	5.269	1219	1222	1223	rBV	138	60	0.01%	0.002%
19	5.279	1223	1225	1227	rBV	302	158	0.04%	0.005%
20	5.459	1278	1281	1287	rVB	201	135	0.03%	0.004%
21	5.491	1288	1291	1292	rBV	189	90	0.02%	0.003%
22	5.719	1341	1362	1386	rBV2	148545	404255	100.00%	12.854%
23	5.909	1419	1421	1427	rBV	177	140	0.03%	0.004%
24	6.041	1460	1462	1465	rVB	286	185	0.05%	0.006%
25	6.079	1466	1474	1475	rBV	320	299	0.07%	0.010%
26	6.189	1502	1508	1510	rBV	194	224	0.06%	0.007%
27	6.243	1512	1525	1550	rVV	131399	244311	60.43%	7.769%
28	6.349	1555	1558	1560	rBV	253	153	0.04%	0.005%
29	6.536	1609	1616	1617	rBV4	1394	1319	0.33%	0.042%
30	6.571	1625	1627	1628	rVB	111	27	0.01%	0.001%
31	6.623	1640	1643	1648	rBV	196	127	0.03%	0.004%
32	6.684	1649	1662	1681	rBV	97033	184141	45.55%	5.855%
33	6.832	1703	1708	1711	rBV	238	283	0.07%	0.009%
34	6.867	1715	1719	1724	rVB	277	281	0.07%	0.009%
35	6.925	1736	1737	1738	rVB	113	22	0.01%	0.001%
36	6.951	1742	1745	1746	rBV	125	54	0.01%	0.002%

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 Title : VOC Analysis

37	6.976	1752	1753	1754	rBV	127	34	0.01%	0.001%
38	7.025	1766	1768	1769	rBV	129	34	0.01%	0.001%
39	7.150	1805	1807	1811	rBV	218	135	0.03%	0.004%
40	7.253	1836	1839	1840	rBV	139	99	0.02%	0.003%
41	7.259	1840	1841	1842	rVV	108	31	0.01%	0.001%
42	7.314	1857	1858	1859	rVB	103	20	0.00%	0.001%
43	7.356	1868	1871	1874	rBV2	230	177	0.04%	0.006%
44	7.523	1920	1923	1924	rBV2	161	78	0.02%	0.002%
45	7.562	1924	1935	1953	rVB	53460	94258	23.32%	2.997%
46	7.636	1954	1958	1963	rBV2	267	306	0.08%	0.010%
47	7.671	1967	1969	1970	rBV2	172	75	0.02%	0.002%
48	7.751	1992	1994	1996	rBV	181	65	0.02%	0.002%
49	7.790	2004	2006	2009	rVB	245	109	0.03%	0.003%
50	7.893	2025	2038	2056	rBV	188818	320983	79.40%	10.207%
51	8.008	2072	2074	2077	rVB	317	194	0.05%	0.006%
52	8.076	2093	2095	2099	rBV2	252	132	0.03%	0.004%
53	8.176	2115	2126	2139	rBV	36175	60087	14.86%	1.911%
54	8.330	2171	2174	2177	rBV2	241	175	0.04%	0.006%
55	8.510	2228	2230	2236	rVB	213	151	0.04%	0.005%
56	8.629	2255	2267	2295	rBV2	108263	203888	50.44%	6.483%
57	8.774	2309	2312	2315	rBV2	337	227	0.06%	0.007%
58	8.790	2315	2317	2321	rVB2	316	210	0.05%	0.007%
59	8.828	2326	2329	2331	rBV	195	123	0.03%	0.004%
60	8.909	2350	2354	2356	rBV	198	186	0.05%	0.006%
61	8.986	2376	2378	2379	rBV	155	48	0.01%	0.002%
62	9.089	2407	2410	2412	rBV	173	97	0.02%	0.003%
63	9.137	2421	2425	2428	rBV2	181	170	0.04%	0.005%
64	9.198	2440	2444	2447	rBV	199	162	0.04%	0.005%
65	9.307	2476	2478	2481	rBB	151	101	0.02%	0.003%
66	9.330	2481	2485	2488	rBV	326	273	0.07%	0.009%
67	9.372	2494	2498	2499	rBV	221	152	0.04%	0.005%
68	9.414	2499	2511	2535	rVV	177040	294853	72.94%	9.376%
69	9.561	2553	2557	2561	rVB2	211	215	0.05%	0.007%
70	9.635	2578	2580	2583	rBV2	200	118	0.03%	0.004%
71	9.774	2620	2623	2629	rBV	139	155	0.04%	0.005%
72	9.848	2644	2646	2647	rBV	118	30	0.01%	0.001%
73	9.951	2675	2678	2681	rVB2	239	154	0.04%	0.005%
74	9.979	2685	2687	2693	rBV	203	158	0.04%	0.005%
75	10.024	2698	2701	2702	rBV	144	68	0.02%	0.002%
76	10.115	2727	2729	2733	rVB	222	107	0.03%	0.003%

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77	10.221	2760	2762	2764	rBV	157	47	0.01%	0.001%
78	10.279	2778	2780	2782	rBV	211	121	0.03%	0.004%
79	10.369	2806	2808	2812	rVB2	173	94	0.02%	0.003%
80	10.446	2829	2832	2835	rBV2	174	161	0.04%	0.005%
81	10.626	2886	2888	2891	rBV	150	97	0.02%	0.003%
82	10.751	2916	2927	2947	rVB	132261	207242	51.27%	6.590%
83	10.896	2969	2972	2973	rBV2	270	153	0.04%	0.005%
84	11.230	3073	3076	3081	rBV	262	238	0.06%	0.008%
85	11.343	3106	3111	3113	rBV2	235	204	0.05%	0.006%
86	11.806	3243	3255	3274	rBV	181731	293128	72.51%	9.321%
87	11.934	3293	3295	3299	rBV	189	83	0.02%	0.003%
88	12.073	3335	3338	3341	rBV2	626	461	0.11%	0.015%
89	12.188	3362	3374	3393	rBV	159663	257772	63.76%	8.197%
90	12.288	3404	3405	3409	rVB	243	136	0.03%	0.004%
91	12.420	3443	3446	3449	rBV2	228	166	0.04%	0.005%
92	12.729	3540	3542	3545	rBV	202	84	0.02%	0.003%
93	13.182	3680	3683	3686	rBV2	224	181	0.04%	0.006%
94	13.487	3773	3778	3782	rBV	303	276	0.07%	0.009%
95	13.995	3930	3936	3939	rBV2	258	322	0.08%	0.010%
96	14.259	4016	4018	4021	rBV	184	90	0.02%	0.003%
97	14.413	4064	4066	4069	rBV	154	56	0.01%	0.002%
98	14.989	4243	4245	4247	rBV	213	118	0.03%	0.004%
99	15.082	4271	4274	4276	rBV	304	221	0.05%	0.007%
100	15.227	4315	4319	4324	rBV2	451	408	0.10%	0.013%

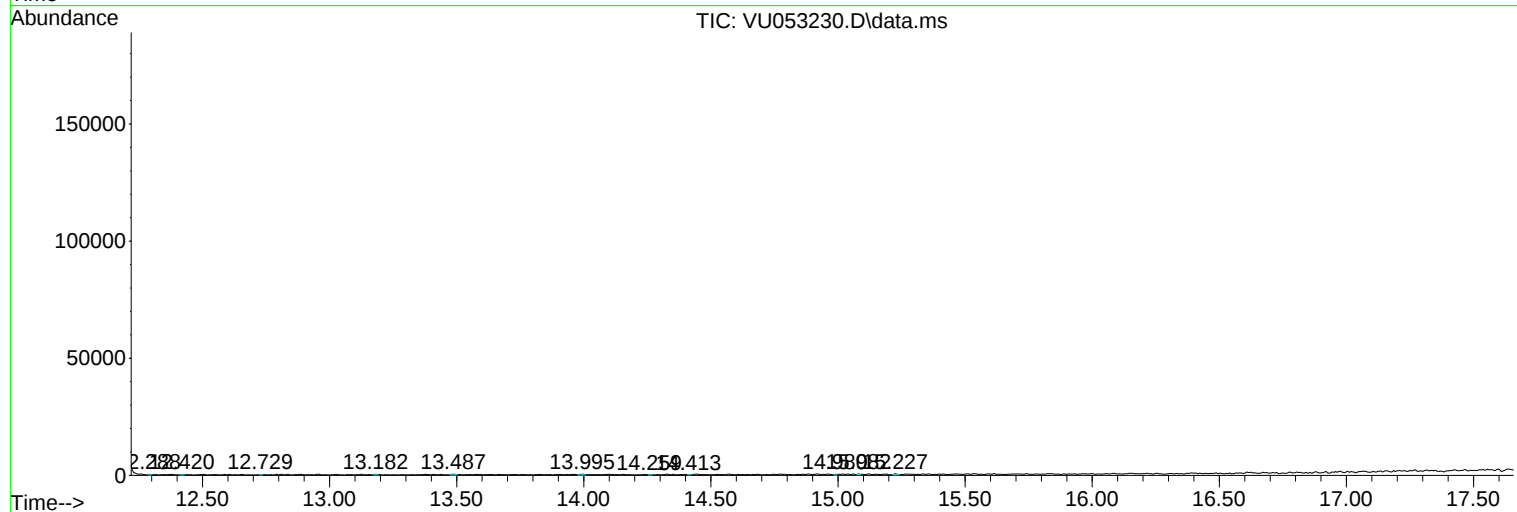
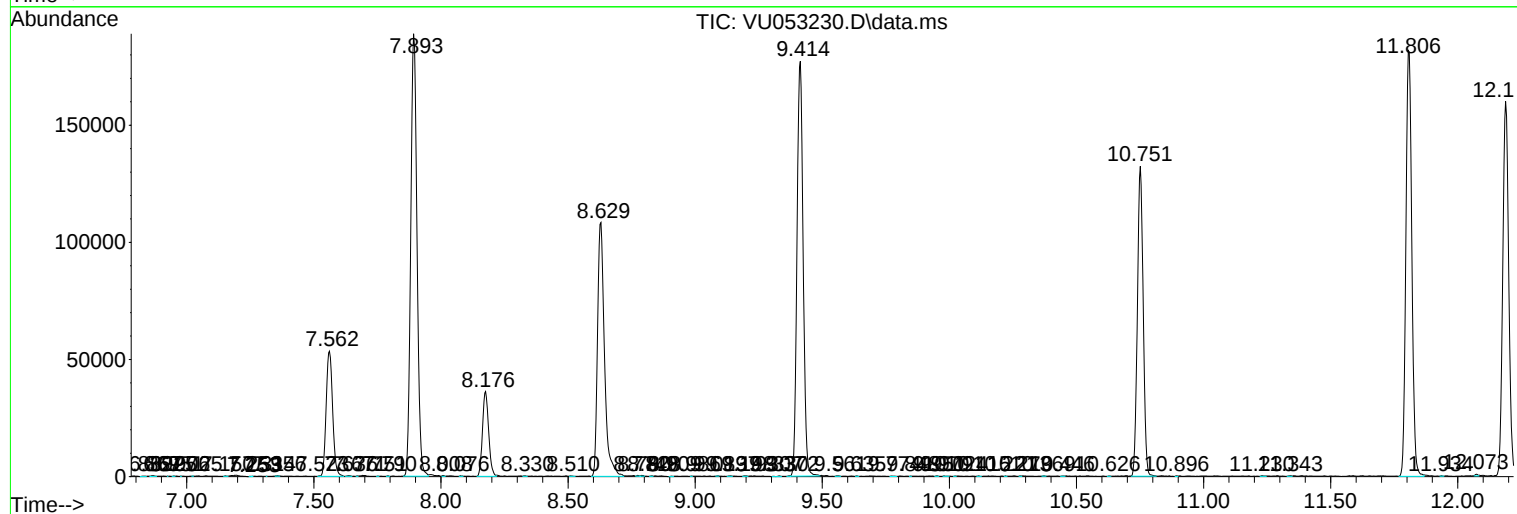
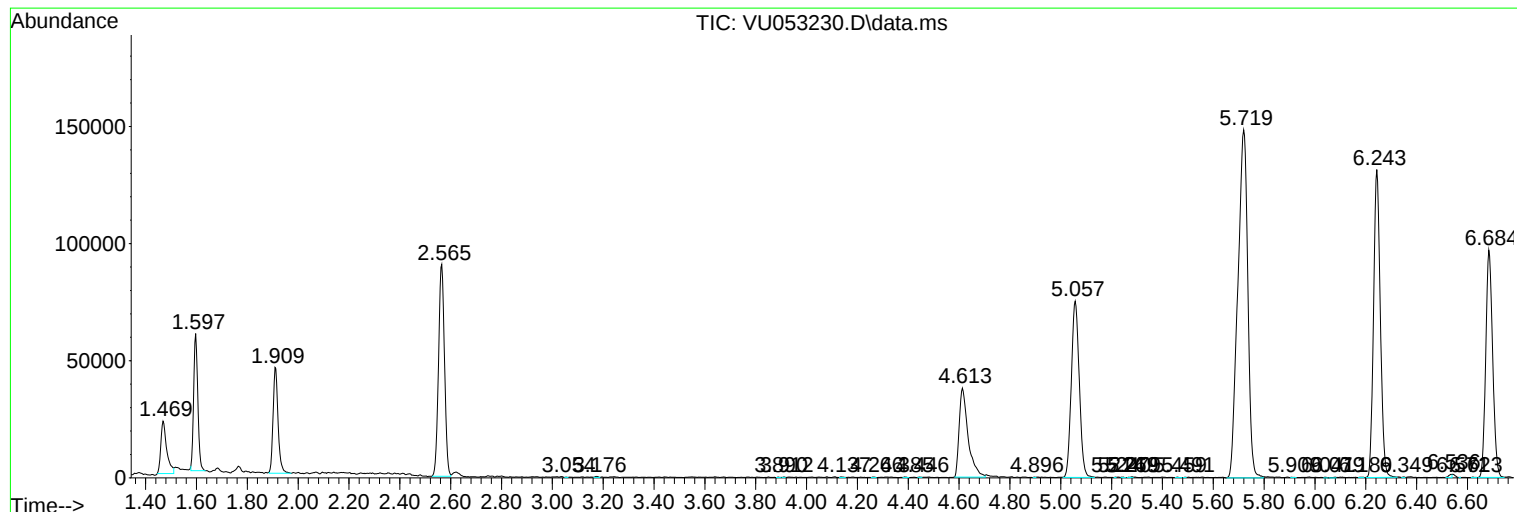
Sum of corrected areas: 3144884

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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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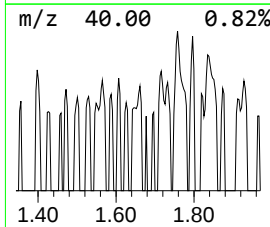
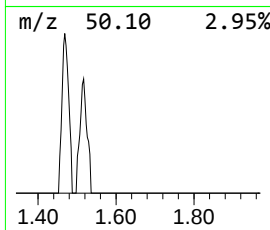
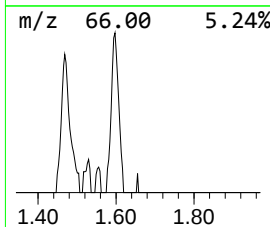
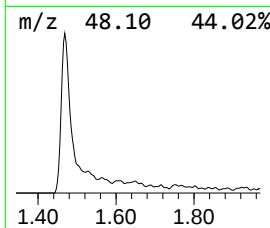
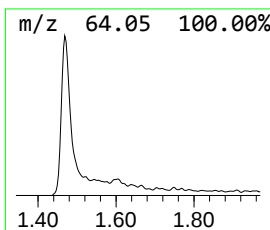
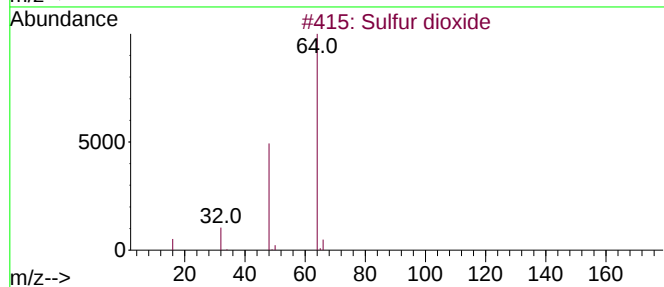
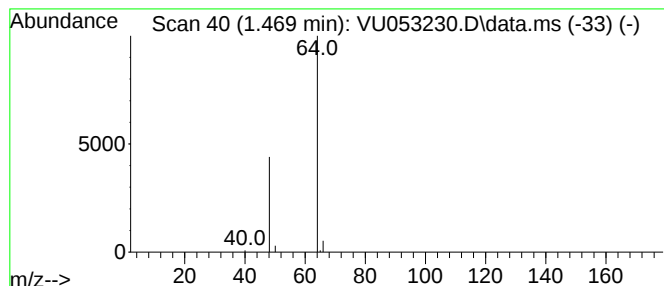
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	7.45 ug/L	36392	1,4-Difluorobenzene	6.243

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	4



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	7.5	ug/L	36392	1	6.243	244311	50.0