

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053261.D
 Acq On : 17 Mar 2023 12:52
 Operator : JC/MD
 Sample : 01929-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF1

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: VU053261.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	31	39	61	rBV	83056	154282	22.76%	2.961%
2	1.597	74	80	94	rVB2	158837	196512	28.99%	3.771%
3	1.909	170	177	191	rVB	73647	97335	14.36%	1.868%
4	2.562	369	380	393	rBV	142916	233208	34.40%	4.476%
5	3.729	741	743	746	rVB2	184	124	0.02%	0.002%
6	3.845	777	779	783	rBV	246	183	0.03%	0.004%
7	3.941	807	809	811	rBV	154	82	0.01%	0.002%
8	4.199	886	889	894	rVB	206	119	0.02%	0.002%
9	4.613	1006	1018	1026	rBV2	54070	120530	17.78%	2.313%
10	4.938	1116	1119	1122	rBV2	168	136	0.02%	0.003%
11	4.973	1127	1130	1132	rBV	175	131	0.02%	0.003%
12	5.057	1139	1156	1180	rVB	125713	272183	40.15%	5.224%
13	5.166	1187	1190	1193	rBV	188	148	0.02%	0.003%
14	5.292	1225	1229	1232	rVB3	264	170	0.03%	0.003%
15	5.363	1248	1251	1255	rVB2	318	277	0.04%	0.005%
16	5.388	1256	1259	1260	rBV	194	131	0.02%	0.003%
17	5.401	1260	1263	1267	rVV	286	215	0.03%	0.004%
18	5.424	1268	1270	1273	rVB2	193	122	0.02%	0.002%
19	5.488	1287	1290	1297	rVB2	232	250	0.04%	0.005%
20	5.600	1319	1325	1326	rBV	224	228	0.03%	0.004%
21	5.719	1341	1362	1384	rBV2	253988	677946	100.00%	13.011%
22	5.928	1423	1427	1428	rBV	158	107	0.02%	0.002%
23	5.967	1438	1439	1443	rVB2	279	133	0.02%	0.003%
24	5.986	1443	1445	1451	rVB	170	72	0.01%	0.001%
25	6.041	1458	1462	1464	rBV	175	126	0.02%	0.002%
26	6.057	1465	1467	1470	rBV	320	144	0.02%	0.003%
27	6.073	1470	1472	1475	rBV	121	94	0.01%	0.002%
28	6.150	1492	1496	1499	rBV2	244	178	0.03%	0.003%
29	6.170	1499	1502	1503	rBV	190	84	0.01%	0.002%
30	6.244	1512	1525	1543	rBV	193131	360703	53.21%	6.923%
31	6.372	1560	1565	1572	rBV2	225	343	0.05%	0.007%
32	6.481	1596	1599	1602	rVB2	162	91	0.01%	0.002%
33	6.504	1603	1606	1607	rBV	211	98	0.01%	0.002%
34	6.539	1607	1617	1627	rVB4	5687	9960	1.47%	0.191%
35	6.684	1648	1662	1680	rBV	158880	305850	45.11%	5.870%
36	6.787	1691	1694	1696	rBV2	232	171	0.03%	0.003%

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 Title : VOC Analysis

37	6.867	1714	1719	1722	rBV2	238	224	0.03%	0.004%
38	7.018	1764	1766	1768	rBV	158	65	0.01%	0.001%
39	7.076	1775	1784	1786	rBV	252	383	0.06%	0.007%
40	7.102	1790	1792	1795	rVB	169	80	0.01%	0.002%
41	7.253	1837	1839	1843	rVB	179	93	0.01%	0.002%
42	7.433	1889	1895	1896	rBV	170	191	0.03%	0.004%
43	7.559	1923	1934	1949	rBV	88122	155779	22.98%	2.990%
44	7.694	1969	1976	1983	rBV3	824	1018	0.15%	0.020%
45	7.893	2025	2038	2055	rBV	311048	537294	79.25%	10.312%
46	8.057	2087	2089	2093	rVB	166	64	0.01%	0.001%
47	8.099	2099	2102	2103	rBV	162	79	0.01%	0.002%
48	8.131	2110	2112	2115	rBB	153	63	0.01%	0.001%
49	8.173	2115	2125	2140	rBV	62233	102845	15.17%	1.974%
50	8.301	2162	2165	2168	rBV2	165	145	0.02%	0.003%
51	8.356	2180	2182	2185	rVB	164	85	0.01%	0.002%
52	8.459	2208	2214	2216	rBV2	296	333	0.05%	0.006%
53	8.501	2224	2227	2228	rBV2	247	128	0.02%	0.002%
54	8.626	2255	2266	2296	rBV2	177114	323914	47.78%	6.217%
55	8.941	2360	2364	2370	rVB2	237	193	0.03%	0.004%
56	9.067	2401	2403	2407	rBV	199	103	0.02%	0.002%
57	9.208	2445	2447	2448	rBV	153	74	0.01%	0.001%
58	9.247	2457	2459	2463	rVB	192	85	0.01%	0.002%
59	9.266	2463	2465	2473	rVB	171	141	0.02%	0.003%
60	9.414	2498	2511	2529	rBV	263621	435222	64.20%	8.353%
61	9.568	2557	2559	2561	rVB	149	62	0.01%	0.001%
62	9.584	2561	2564	2566	rBV	190	104	0.02%	0.002%
63	9.649	2582	2584	2586	rVB	272	110	0.02%	0.002%
64	9.671	2587	2591	2592	rBV	168	119	0.02%	0.002%
65	9.687	2593	2596	2600	rVV2	206	171	0.03%	0.003%
66	9.755	2615	2617	2621	rVB	161	56	0.01%	0.001%
67	9.800	2629	2631	2636	rVB	144	55	0.01%	0.001%
68	9.832	2640	2641	2644	rVB	243	98	0.01%	0.002%
69	9.848	2645	2646	2647	rBV	106	40	0.01%	0.001%
70	9.867	2649	2652	2654	rBV	162	141	0.02%	0.003%
71	10.028	2700	2702	2705	rVB	165	53	0.01%	0.001%
72	10.321	2791	2793	2794	rBV	130	55	0.01%	0.001%
73	10.459	2834	2836	2838	rBV	141	61	0.01%	0.001%
74	10.629	2886	2889	2890	rBV	214	99	0.01%	0.002%
75	10.751	2914	2927	2946	rBV	211641	338526	49.93%	6.497%
76	11.012	3005	3008	3010	rVB2	175	100	0.01%	0.002%

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77	11.121	3039	3042	3045	rVB2	391	247	0.04%	0.005%
78	11.137	3045	3047	3050	rBV	179	82	0.01%	0.002%
79	11.182	3058	3061	3062	rBV	163	76	0.01%	0.001%
80	11.353	3113	3114	3115	rBV	110	25	0.00%	0.000%
81	11.510	3161	3163	3164	rBV	148	43	0.01%	0.001%
82	11.681	3213	3216	3218	rBV	132	88	0.01%	0.002%
83	11.809	3244	3256	3277	rBV	263432	422631	62.34%	8.111%
84	11.947	3297	3299	3304	rVB	269	136	0.02%	0.003%
85	11.970	3304	3306	3308	rBV	150	64	0.01%	0.001%
86	12.073	3330	3338	3340	rBV2	1393	1437	0.21%	0.028%
87	12.189	3362	3374	3393	rVB	285412	452564	66.76%	8.686%
88	12.510	3472	3474	3475	rBV	178	54	0.01%	0.001%
89	12.902	3593	3596	3598	rBV2	203	131	0.02%	0.003%
90	12.973	3614	3618	3623	rVB2	242	251	0.04%	0.005%
91	13.044	3636	3640	3643	rBV2	245	240	0.04%	0.005%
92	13.095	3653	3656	3659	rBV2	203	189	0.03%	0.004%
93	13.189	3682	3685	3686	rBV2	191	97	0.01%	0.002%
94	13.246	3698	3703	3705	rBV	192	163	0.02%	0.003%
95	13.484	3775	3777	3782	rVB2	260	200	0.03%	0.004%
96	13.835	3885	3886	3887	rBV2	209	68	0.01%	0.001%
97	14.050	3951	3953	3958	rBV2	225	168	0.02%	0.003%
98	14.880	4209	4211	4213	rBV	222	137	0.02%	0.003%
99	15.687	4457	4462	4466	rBV	397	506	0.07%	0.010%

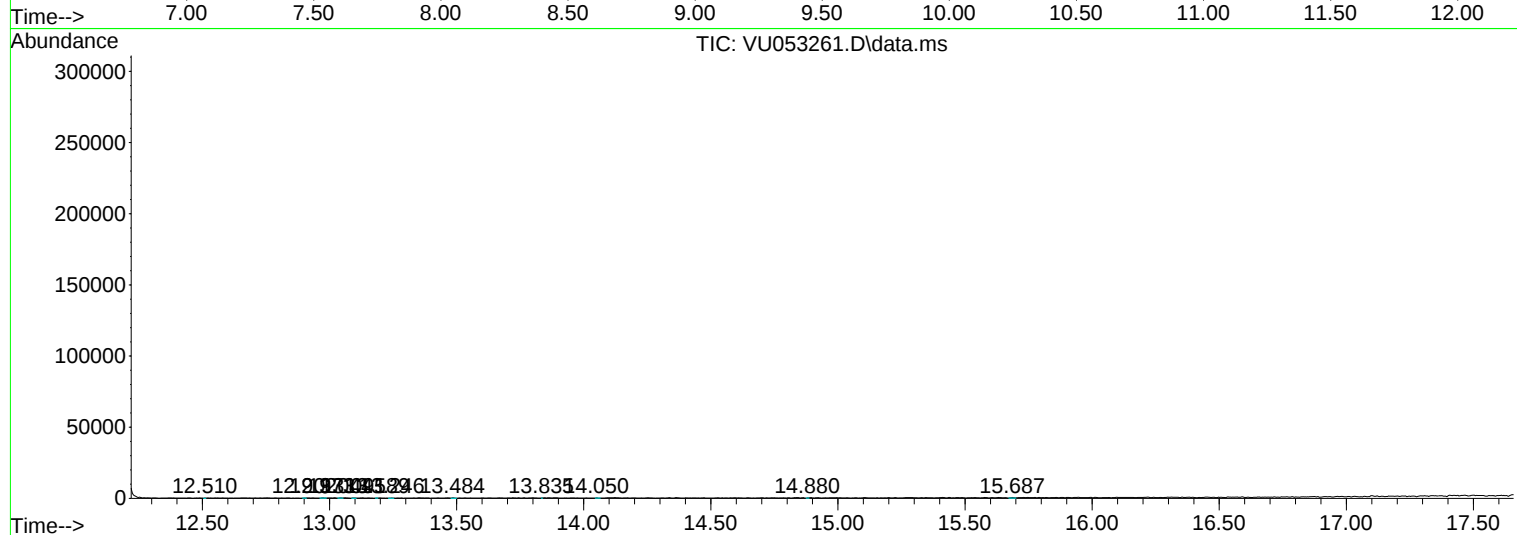
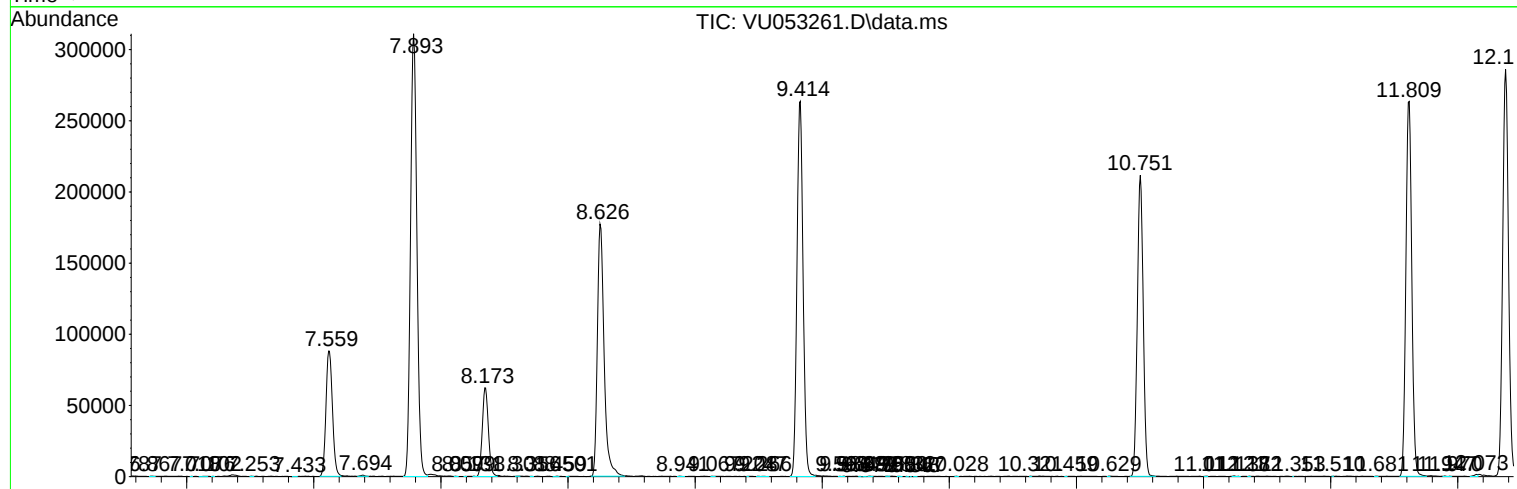
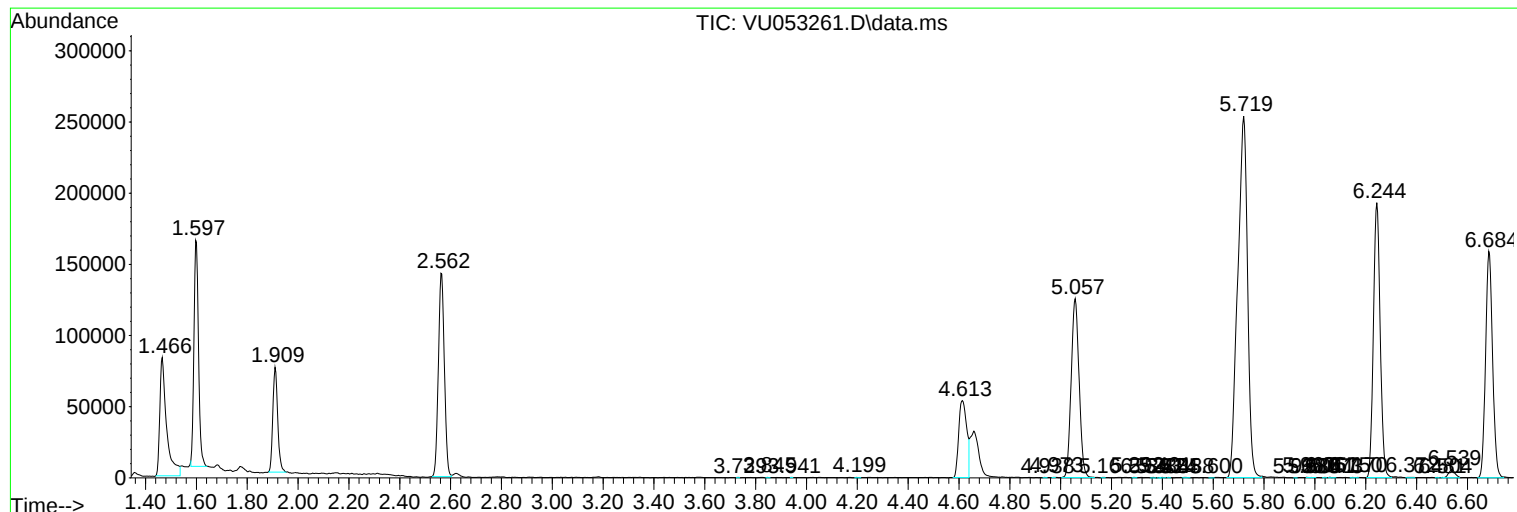
Sum of corrected areas: 5210514

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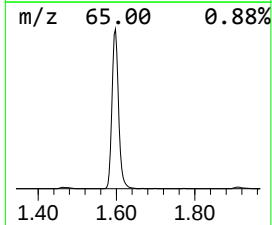
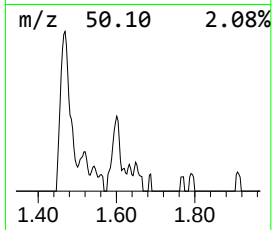
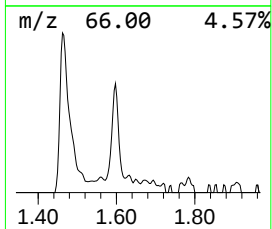
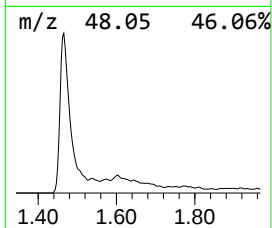
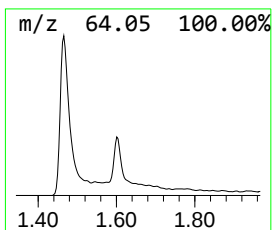
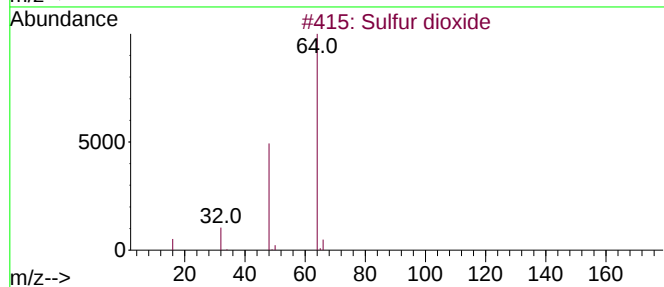
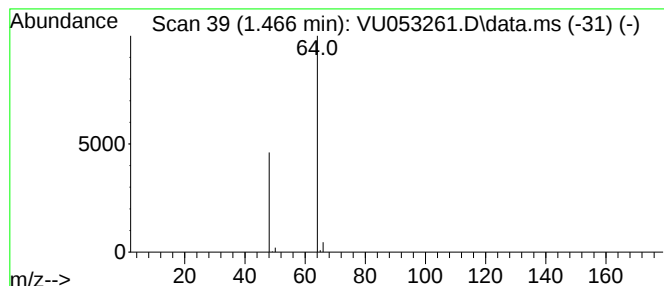
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	21.39 ug/L	154282	1,4-Difluorobenzene	6.244

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			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	21.4	ug/L	154282	1	6.244	360703	50.0