

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU032123\
 Data File : VU053320.D
 Acq On : 21 Mar 2023 13:40
 Operator : JC/MD
 Sample : 01980-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYGA9

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: VU053320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	34	43	68	rBV	45633	114384	24.02%	3.149%
2	1.597	74	80	95	rVB	69032	81028	17.02%	2.230%
3	1.912	171	178	193	rVB	59948	79149	16.62%	2.179%
4	2.565	369	381	396	rVB	100179	160948	33.80%	4.430%
5	2.633	396	402	412	rBV2	472	1063	0.22%	0.029%
6	3.192	573	576	580	rVB	386	217	0.05%	0.006%
7	3.623	707	710	715	rBV	173	148	0.03%	0.004%
8	3.665	721	723	725	rVB	154	59	0.01%	0.002%
9	3.835	770	776	782	rBV	271	449	0.09%	0.012%
10	4.022	830	834	837	rBV	224	248	0.05%	0.007%
11	4.157	872	876	879	rBV	181	211	0.04%	0.006%
12	4.356	936	938	939	rBV	126	69	0.01%	0.002%
13	4.620	1009	1020	1045	rBV	33023	84246	17.69%	2.319%
14	4.813	1078	1080	1082	rBV	190	91	0.02%	0.003%
15	4.858	1092	1094	1095	rBV	135	75	0.02%	0.002%
16	4.909	1106	1110	1113	rBV	226	255	0.05%	0.007%
17	4.941	1118	1120	1122	rBV	171	67	0.01%	0.002%
18	5.057	1138	1156	1177	rBV	88314	192015	40.32%	5.286%
19	5.189	1194	1197	1199	rBV	176	156	0.03%	0.004%
20	5.346	1244	1246	1248	rBB	126	68	0.01%	0.002%
21	5.372	1248	1254	1255	rBV	164	185	0.04%	0.005%
22	5.407	1263	1265	1267	rBV	159	105	0.02%	0.003%
23	5.501	1290	1294	1296	rBV	167	139	0.03%	0.004%
24	5.533	1302	1304	1305	rBV	119	64	0.01%	0.002%
25	5.578	1316	1318	1320	rBV	164	115	0.02%	0.003%
26	5.719	1341	1362	1388	rBV2	174352	476202	100.00%	13.108%
27	5.854	1401	1404	1406	rBV2	283	217	0.05%	0.006%
28	5.970	1437	1440	1443	rBV	168	154	0.03%	0.004%
29	5.986	1443	1445	1447	rVV	147	52	0.01%	0.001%
30	6.034	1456	1460	1464	rBV	358	310	0.07%	0.009%
31	6.163	1498	1500	1501	rBV	128	69	0.01%	0.002%
32	6.243	1512	1525	1542	rBV	148718	280555	58.92%	7.723%
33	6.385	1566	1569	1572	rBV	194	182	0.04%	0.005%
34	6.443	1582	1587	1588	rBV	211	197	0.04%	0.005%
35	6.475	1594	1597	1600	rBV	159	128	0.03%	0.004%
36	6.629	1642	1645	1647	rBV	189	161	0.03%	0.004%

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 Title : VOC Analysis

37	6.684	1649	1662	1680	rVV2	108645	210477	44.20%	5.794%
38	6.822	1703	1705	1709	rVB2	290	208	0.04%	0.006%
39	6.848	1710	1713	1717	rBV	144	172	0.04%	0.005%
40	6.883	1721	1724	1725	rBV	150	61	0.01%	0.002%
41	6.915	1733	1734	1736	rBB	115	41	0.01%	0.001%
42	6.938	1739	1741	1742	rBV	170	91	0.02%	0.003%
43	7.028	1767	1769	1771	rBV	162	110	0.02%	0.003%
44	7.121	1794	1798	1800	rBB	176	114	0.02%	0.003%
45	7.176	1810	1815	1818	rBV	202	244	0.05%	0.007%
46	7.195	1818	1821	1824	rVB	150	92	0.02%	0.003%
47	7.391	1880	1882	1883	rBV	111	60	0.01%	0.002%
48	7.501	1914	1916	1918	rBV	157	106	0.02%	0.003%
49	7.562	1923	1935	1954	rVV	62663	107642	22.60%	2.963%
50	7.687	1972	1974	1975	rVB	130	31	0.01%	0.001%
51	7.706	1977	1980	1983	rVB	214	103	0.02%	0.003%
52	7.761	1993	1997	1999	rBV	153	128	0.03%	0.004%
53	7.796	2004	2008	2009	rBV	241	144	0.03%	0.004%
54	7.835	2018	2020	2021	rBV	108	41	0.01%	0.001%
55	7.893	2025	2038	2055	rBV	216577	372428	78.21%	10.252%
56	8.086	2094	2098	2100	rBV	186	141	0.03%	0.004%
57	8.176	2114	2126	2143	rBV	42930	71656	15.05%	1.972%
58	8.369	2185	2186	2188	rVB	229	65	0.01%	0.002%
59	8.385	2188	2191	2194	rBV	182	178	0.04%	0.005%
60	8.533	2236	2237	2240	rVB	235	108	0.02%	0.003%
61	8.629	2256	2267	2296	rBV3	96071	187253	39.32%	5.154%
62	8.877	2342	2344	2345	rBV	136	65	0.01%	0.002%
63	8.993	2378	2380	2381	rBV	125	67	0.01%	0.002%
64	9.095	2409	2412	2415	rBV	234	193	0.04%	0.005%
65	9.218	2448	2450	2453	rBV	168	135	0.03%	0.004%
66	9.411	2498	2510	2530	rBV	206605	344574	72.36%	9.485%
67	9.539	2547	2550	2554	rBV	218	148	0.03%	0.004%
68	9.565	2555	2558	2561	rVV	172	111	0.02%	0.003%
69	9.648	2581	2584	2586	rBV	163	136	0.03%	0.004%
70	9.851	2645	2647	2649	rVB	177	73	0.02%	0.002%
71	9.954	2676	2679	2683	rVV	251	176	0.04%	0.005%
72	9.999	2687	2693	2697	rBV	175	254	0.05%	0.007%
73	10.086	2716	2720	2721	rBV	174	147	0.03%	0.004%
74	10.118	2721	2730	2737	rVV3	1496	2127	0.45%	0.059%
75	10.192	2750	2753	2755	rBV	155	135	0.03%	0.004%
76	10.266	2773	2776	2778	rBV	145	120	0.03%	0.003%

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77	10.455	2833	2835	2838	rBB	191	123	0.03%	0.003%
78	10.481	2839	2843	2845	rBV	180	147	0.03%	0.004%
79	10.751	2915	2927	2946	rBV	145361	225986	47.46%	6.221%
80	10.861	2957	2961	2965	rBV	296	325	0.07%	0.009%
81	11.015	3004	3009	3011	rBV	165	202	0.04%	0.006%
82	11.057	3017	3022	3026	rBV	273	277	0.06%	0.008%
83	11.118	3038	3041	3043	rBV	158	134	0.03%	0.004%
84	11.259	3082	3085	3088	rBV	132	79	0.02%	0.002%
85	11.349	3104	3113	3115	rBV	198	353	0.07%	0.010%
86	11.497	3153	3159	3162	rBV	210	281	0.06%	0.008%
87	11.806	3244	3255	3280	rBV	203926	321055	67.42%	8.838%
88	11.957	3300	3302	3305	rVB	163	51	0.01%	0.001%
89	12.092	3341	3344	3348	rBV	177	155	0.03%	0.004%
90	12.189	3362	3374	3394	rBV	191689	308203	64.72%	8.484%
91	12.295	3404	3407	3408	rBV	285	169	0.04%	0.005%
92	12.690	3527	3530	3531	rBV	140	62	0.01%	0.002%
93	13.851	3887	3891	3893	rBV	179	158	0.03%	0.004%
94	14.089	3962	3965	3966	rBV	279	177	0.04%	0.005%
95	14.330	4037	4040	4042	rBV	181	95	0.02%	0.003%
96	14.880	4207	4211	4215	rBV2	293	292	0.06%	0.008%
97	15.028	4254	4257	4259	rBV2	247	159	0.03%	0.004%
98	15.182	4302	4305	4307	rBV	164	75	0.02%	0.002%
99	15.549	4416	4419	4422	rBV2	228	174	0.04%	0.005%
100	15.896	4525	4527	4528	rBV	397	192	0.04%	0.005%

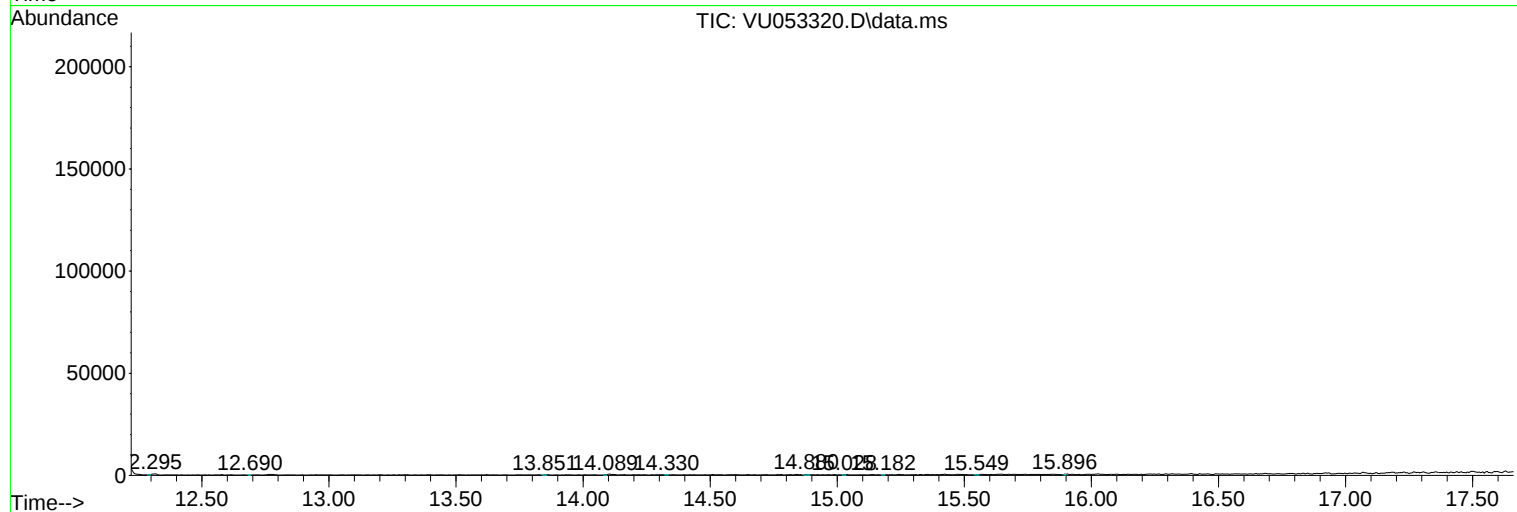
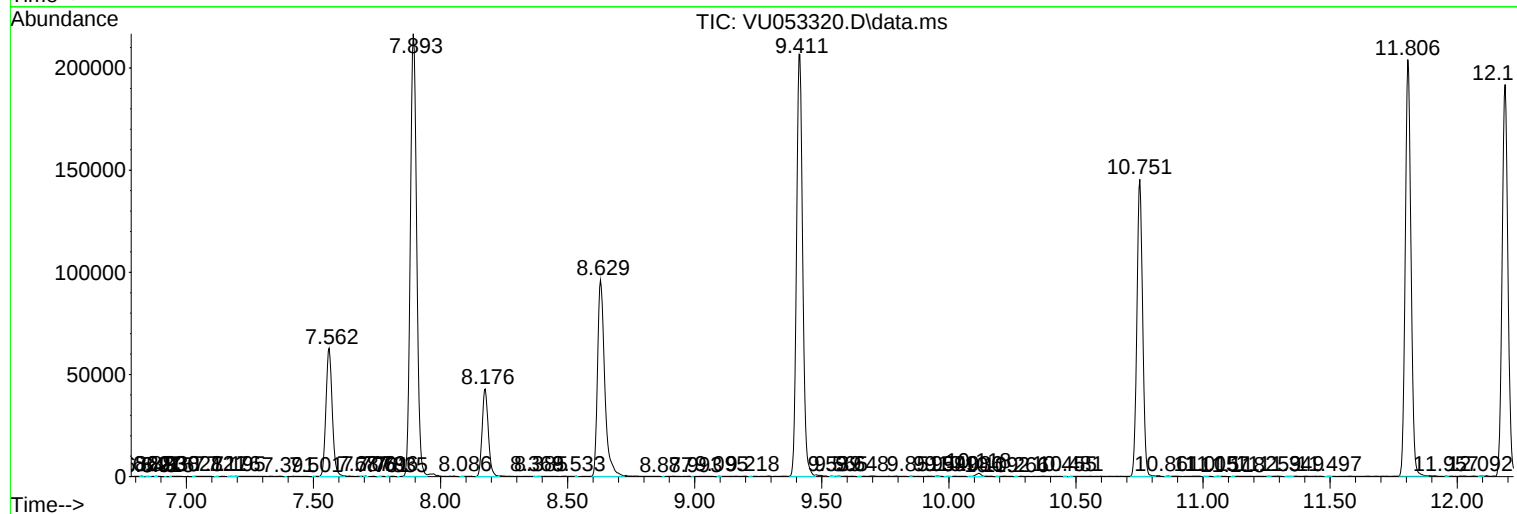
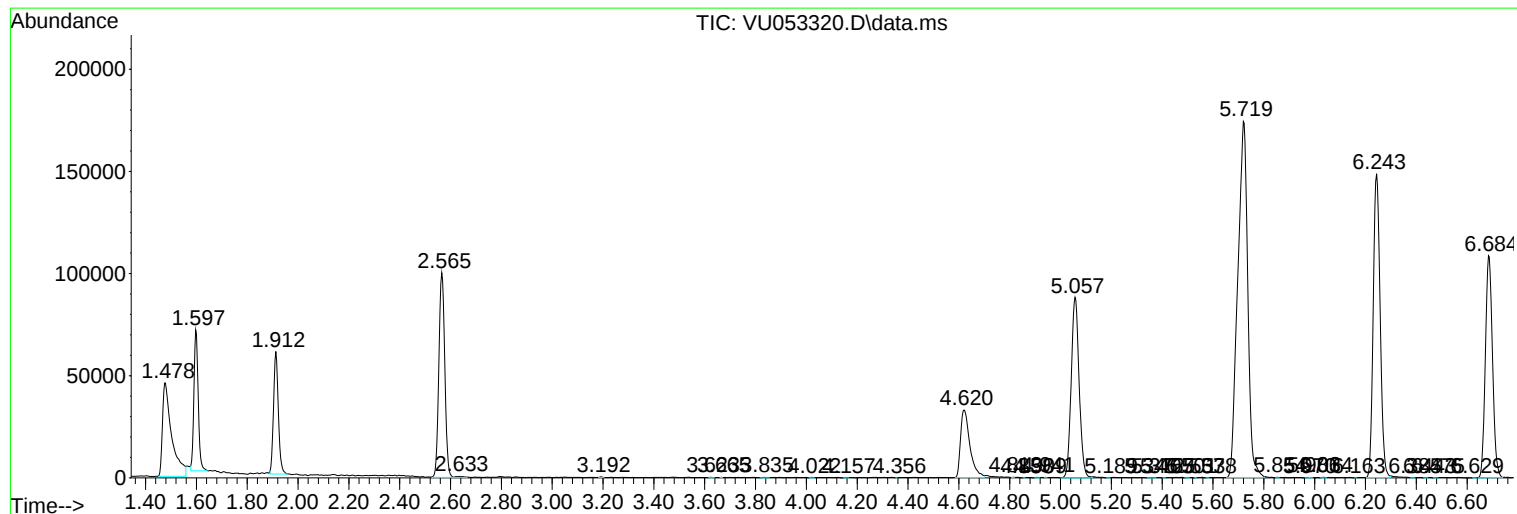
Sum of corrected areas: 3632860

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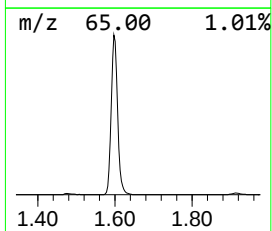
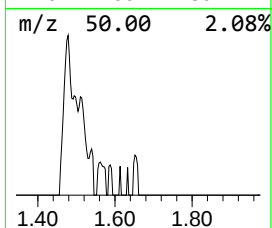
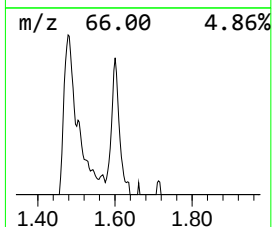
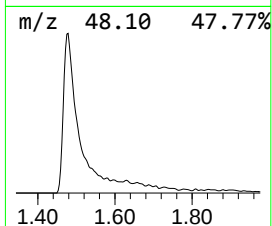
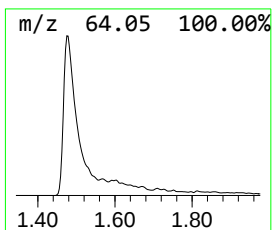
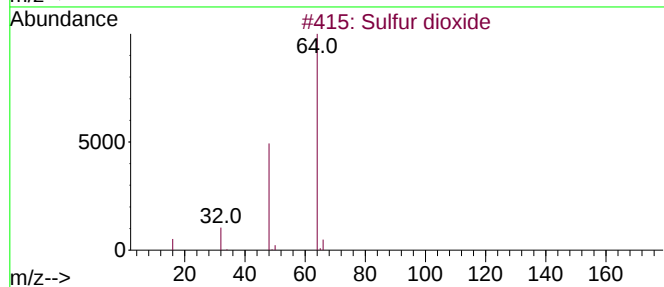
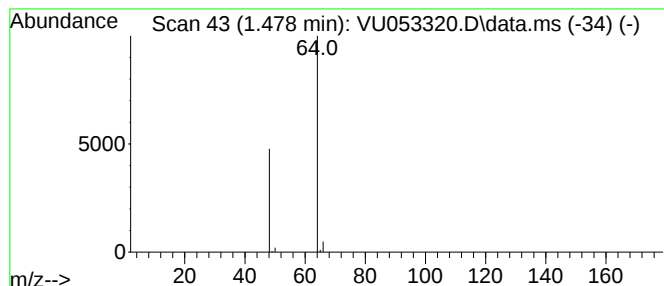
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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.
1.478	20.39 ug/L	114384	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.478	20.4	ug/L	114384	1	6.243	280555	50.0