

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031623\
 Data File : VU053231.D
 Acq On : 16 Mar 2023 17:05
 Operator : JC/MD
 Sample : 01930-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFG4

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: VU053231.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	51	rBV	18807	31185	5.22%	0.682%
2	1.597	73	80	91	rVB	82361	91480	15.31%	1.999%
3	1.912	170	178	195	rVB	64169	85979	14.39%	1.879%
4	2.565	369	381	396	rBV	125443	203951	34.13%	4.457%
5	2.957	500	503	504	rBV	268	115	0.02%	0.003%
6	3.346	622	624	625	rBV	272	121	0.02%	0.003%
7	3.575	692	695	698	rBV	190	136	0.02%	0.003%
8	3.964	813	816	821	rBV2	198	214	0.04%	0.005%
9	3.993	821	825	826	rBV	189	127	0.02%	0.003%
10	4.054	840	844	847	rVB2	195	140	0.02%	0.003%
11	4.147	870	873	876	rBV	330	288	0.05%	0.006%
12	4.186	882	885	887	rBV	207	100	0.02%	0.002%
13	4.237	898	901	902	rBV	150	89	0.01%	0.002%
14	4.314	924	925	926	rVB	97	19	0.00%	0.000%
15	4.427	957	960	964	rBV	168	96	0.02%	0.002%
16	4.485	975	978	983	rVB2	259	160	0.03%	0.003%
17	4.533	991	993	995	rBV	163	83	0.01%	0.002%
18	4.613	1006	1018	1043	rBV	45001	110458	18.48%	2.414%
19	4.887	1100	1103	1104	rBV	249	103	0.02%	0.002%
20	5.057	1140	1156	1179	rBV	111721	241294	40.37%	5.274%
21	5.253	1214	1217	1222	rVB	267	215	0.04%	0.005%
22	5.288	1223	1228	1229	rBV	262	227	0.04%	0.005%
23	5.446	1275	1277	1279	rBV	146	99	0.02%	0.002%
24	5.523	1299	1301	1304	rVB	273	112	0.02%	0.002%
25	5.568	1312	1315	1320	rBV	175	111	0.02%	0.002%
26	5.719	1341	1362	1386	rBV2	220424	597643	100.00%	13.062%
27	5.886	1411	1414	1418	rBV2	346	320	0.05%	0.007%
28	5.960	1435	1437	1439	rBV	198	103	0.02%	0.002%
29	6.050	1462	1465	1467	rBV	208	108	0.02%	0.002%
30	6.112	1481	1484	1488	rBV	213	112	0.02%	0.002%
31	6.173	1497	1503	1506	rBV	363	344	0.06%	0.008%
32	6.186	1506	1507	1509	rBV	130	42	0.01%	0.001%
33	6.243	1510	1525	1545	rBV	192261	358642	60.01%	7.838%
34	6.378	1564	1567	1571	rVB2	264	195	0.03%	0.004%
35	6.404	1571	1575	1576	rBV	146	89	0.01%	0.002%
36	6.478	1594	1598	1602	rBV2	227	160	0.03%	0.003%

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 Title : VOC Analysis

37	6.517	1608	1610	1611	rBV	274	128	0.02%	0.003%
38	6.536	1611	1616	1624	rVB4	1607	2388	0.40%	0.052%
39	6.600	1633	1636	1640	rVB2	166	122	0.02%	0.003%
40	6.684	1649	1662	1681	rBV	144875	273709	45.80%	5.982%
41	6.800	1694	1698	1700	rBV	340	275	0.05%	0.006%
42	6.980	1752	1754	1756	rBV	124	70	0.01%	0.002%
43	7.038	1771	1772	1774	rVB	130	46	0.01%	0.001%
44	7.108	1791	1794	1797	rBV	221	131	0.02%	0.003%
45	7.128	1797	1800	1804	rVB2	162	125	0.02%	0.003%
46	7.182	1811	1817	1821	rBV2	913	1034	0.17%	0.023%
47	7.330	1861	1863	1868	rVB	302	254	0.04%	0.006%
48	7.356	1868	1871	1872	rBV	208	140	0.02%	0.003%
49	7.465	1902	1905	1907	rBV	152	78	0.01%	0.002%
50	7.504	1915	1917	1920	rVB	167	75	0.01%	0.002%
51	7.558	1922	1934	1957	rBV2	80845	142459	23.84%	3.113%
52	7.755	1993	1995	1998	rBV	188	85	0.01%	0.002%
53	7.893	2023	2038	2054	rBV	278669	473234	79.18%	10.343%
54	8.115	2104	2107	2111	rVB	213	139	0.02%	0.003%
55	8.173	2114	2125	2143	rBV	54657	93261	15.60%	2.038%
56	8.449	2209	2211	2214	rVB	141	74	0.01%	0.002%
57	8.552	2241	2243	2244	rBV	171	54	0.01%	0.001%
58	8.626	2255	2266	2295	rBV2	138794	257855	43.15%	5.636%
59	8.870	2339	2342	2344	rBV	163	138	0.02%	0.003%
60	8.899	2345	2351	2355	rVB2	276	322	0.05%	0.007%
61	9.198	2442	2444	2446	rBV	195	88	0.01%	0.002%
62	9.214	2447	2449	2454	rVV	237	135	0.02%	0.003%
63	9.237	2454	2456	2462	rVB2	208	184	0.03%	0.004%
64	9.365	2494	2496	2498	rBV	193	100	0.02%	0.002%
65	9.410	2498	2510	2533	rVV	272767	444281	74.34%	9.710%
66	9.661	2586	2588	2591	rBV2	171	119	0.02%	0.003%
67	9.732	2609	2610	2611	rBV2	101	28	0.00%	0.001%
68	9.886	2657	2658	2659	rBV	116	44	0.01%	0.001%
69	9.931	2669	2672	2676	rVB	227	126	0.02%	0.003%
70	10.063	2710	2713	2718	rBV	208	158	0.03%	0.003%
71	10.320	2790	2793	2796	rVB	257	194	0.03%	0.004%
72	10.449	2829	2833	2836	rVB	208	155	0.03%	0.003%
73	10.481	2836	2843	2849	rBV3	780	1015	0.17%	0.022%
74	10.751	2914	2927	2947	rBV	183335	294596	49.29%	6.438%
75	10.912	2972	2977	2981	rBV	313	397	0.07%	0.009%
76	11.028	3010	3013	3015	rVB2	172	94	0.02%	0.002%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.089	3025	3032	3037	rBV2	579	646	0.11%	0.014%
78	11.359	3114	3116	3118	rBV	168	72	0.01%	0.002%
79	11.398	3126	3128	3130	rVB	178	52	0.01%	0.001%
80	11.414	3131	3133	3137	rVB	220	117	0.02%	0.003%
81	11.806	3242	3255	3275	rBV	283638	454731	76.09%	9.938%
82	11.928	3291	3293	3296	rVB2	252	146	0.02%	0.003%
83	11.989	3310	3312	3315	rBV	163	75	0.01%	0.002%
84	12.073	3331	3338	3339	rBV3	1152	1158	0.19%	0.025%
85	12.188	3362	3374	3390	rBV	250551	404219	67.64%	8.834%
86	12.478	3462	3464	3465	rBV	169	72	0.01%	0.002%
87	12.523	3473	3478	3479	rBV	241	163	0.03%	0.004%
88	12.896	3591	3594	3596	rBV	177	122	0.02%	0.003%
89	12.960	3612	3614	3616	rBV	204	90	0.02%	0.002%
90	13.012	3628	3630	3633	rBV	215	122	0.02%	0.003%
91	13.192	3685	3686	3690	rBV	130	65	0.01%	0.001%
92	13.243	3699	3702	3703	rBV2	223	145	0.02%	0.003%
93	13.362	3734	3739	3742	rBV2	180	190	0.03%	0.004%
94	13.677	3830	3837	3840	rBV2	226	271	0.05%	0.006%
95	14.086	3961	3964	3965	rBV	330	210	0.04%	0.005%
96	15.085	4272	4275	4279	rBV	368	302	0.05%	0.007%

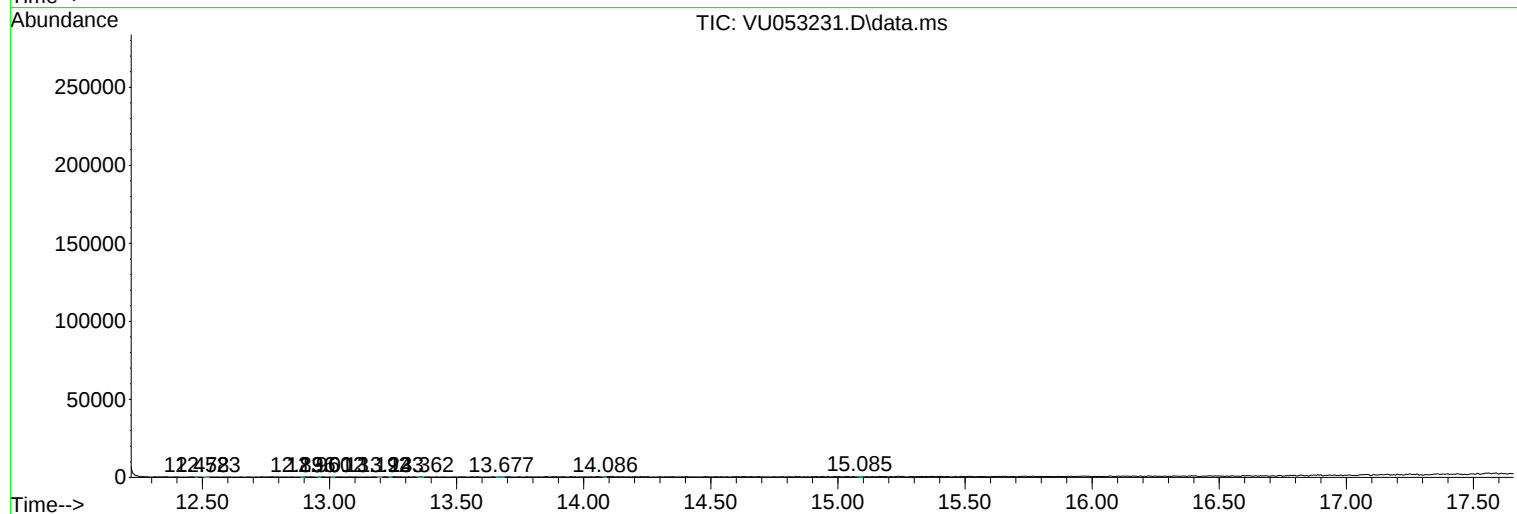
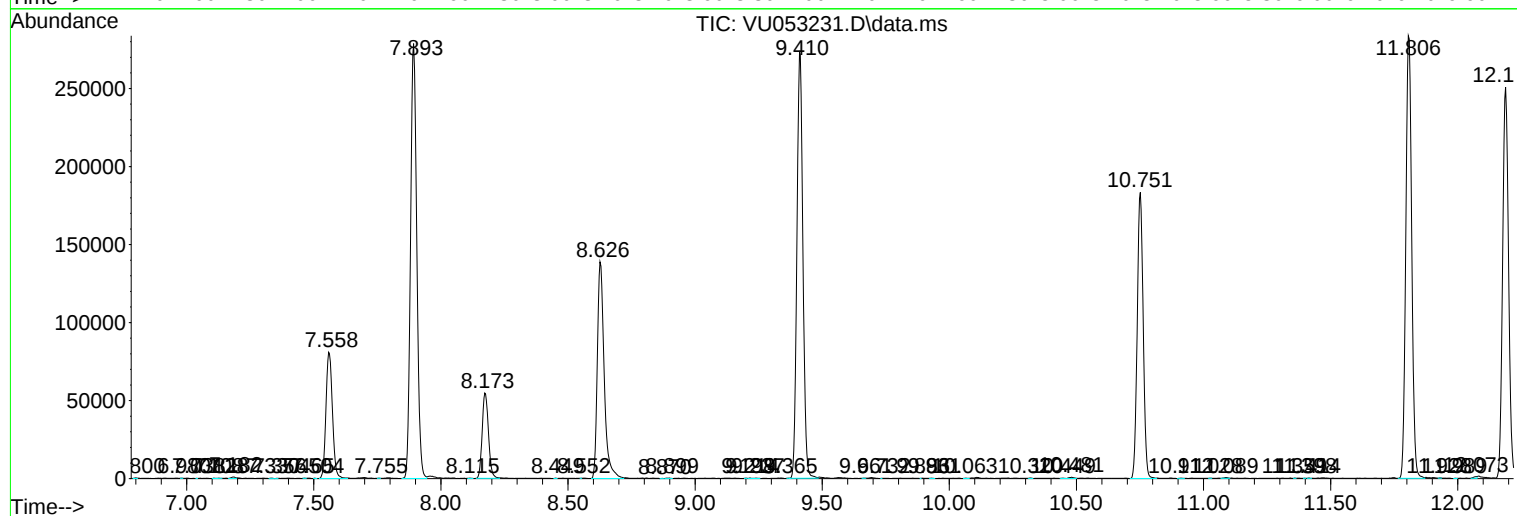
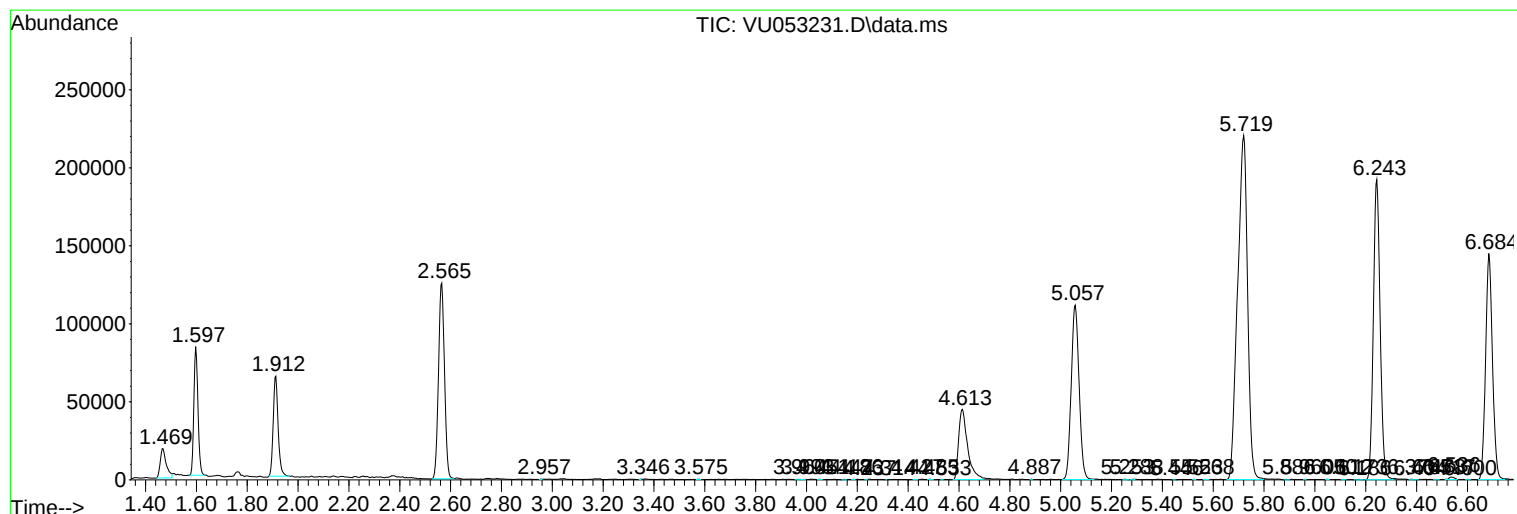
Sum of corrected areas: 4575538

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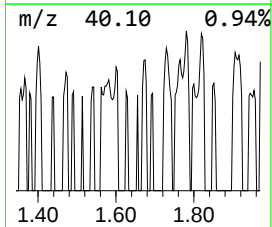
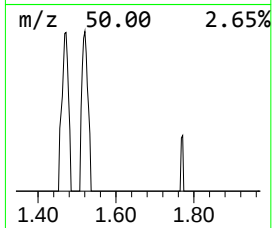
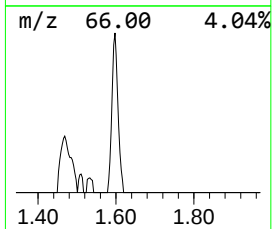
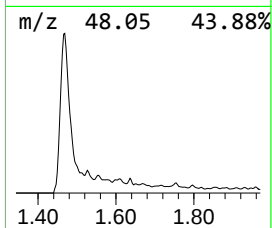
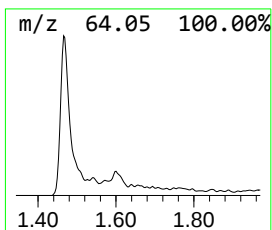
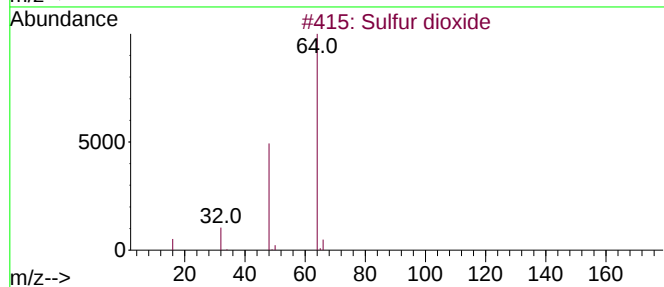
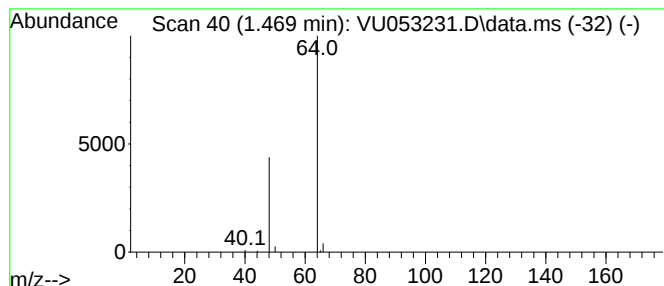
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	4.35 ug/L	31185	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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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Quant Title : VOC Analysis

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	4.3	ug/L	31185	1	6.243	358642	50.0