

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053274.D
 Acq On : 17 Mar 2023 18:00
 Operator : JC/MD
 Sample : 01930-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF6

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: VU053274.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	32	39	61	rBV2	13709	27551	4.54%	0.613%
2	1.597	73	80	95	rVB	84024	94031	15.50%	2.092%
3	1.912	170	178	192	rVB	65060	87948	14.50%	1.957%
4	2.565	369	381	395	rBV	123512	198086	32.66%	4.408%
5	3.038	525	528	531	rVB2	329	203	0.03%	0.005%
6	3.147	559	562	568	rBV	271	190	0.03%	0.004%
7	3.176	568	571	579	rVB	282	225	0.04%	0.005%
8	3.343	621	623	626	rVB	165	75	0.01%	0.002%
9	3.819	769	771	775	rVB	222	116	0.02%	0.003%
10	3.877	787	789	793	rVB2	208	121	0.02%	0.003%
11	4.099	855	858	861	rBV2	199	170	0.03%	0.004%
12	4.147	870	873	875	rBV	164	104	0.02%	0.002%
13	4.366	938	941	944	rBV	129	65	0.01%	0.001%
14	4.613	1006	1018	1043	rBV	45437	110516	18.22%	2.459%
15	4.915	1110	1112	1114	rBV	152	53	0.01%	0.001%
16	5.057	1141	1156	1177	rBV2	111875	242941	40.05%	5.406%
17	5.192	1197	1198	1199	rBV2	214	42	0.01%	0.001%
18	5.221	1206	1207	1208	rVB2	122	24	0.00%	0.001%
19	5.263	1218	1220	1222	rBV	169	91	0.02%	0.002%
20	5.288	1227	1228	1231	rVB	206	85	0.01%	0.002%
21	5.395	1259	1261	1262	rBV	134	62	0.01%	0.001%
22	5.449	1277	1278	1280	rBV	114	49	0.01%	0.001%
23	5.719	1341	1362	1388	rBV2	224233	606521	100.00%	13.496%
24	5.864	1405	1407	1411	rVB	292	135	0.02%	0.003%
25	5.886	1411	1414	1418	rBV3	360	306	0.05%	0.007%
26	6.243	1511	1525	1543	rBV	183466	342117	56.41%	7.612%
27	6.417	1578	1579	1580	rBV	181	57	0.01%	0.001%
28	6.456	1586	1591	1593	rBV2	358	373	0.06%	0.008%
29	6.684	1648	1662	1681	rBV	144086	278576	45.93%	6.199%
30	6.809	1698	1701	1703	rBV2	254	202	0.03%	0.004%
31	6.909	1729	1732	1733	rBV	185	81	0.01%	0.002%
32	6.938	1739	1741	1744	rBV	138	67	0.01%	0.001%
33	7.134	1800	1802	1803	rBV	121	36	0.01%	0.001%
34	7.182	1810	1817	1824	rBV3	1095	1624	0.27%	0.036%
35	7.272	1843	1845	1848	rBV2	206	131	0.02%	0.003%
36	7.356	1870	1871	1873	rVB2	125	47	0.01%	0.001%

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 Title : VOC Analysis

37	7.420	1889	1891	1892	rBV2	137	61	0.01%	0.001%
38	7.481	1908	1910	1913	rVB2	207	108	0.02%	0.002%
39	7.504	1913	1917	1919	rBV2	254	175	0.03%	0.004%
40	7.562	1923	1935	1950	rBV2	81089	141428	23.32%	3.147%
41	7.690	1970	1975	1982	rBV3	814	1029	0.17%	0.023%
42	7.796	2006	2008	2010	rBV	165	95	0.02%	0.002%
43	7.809	2010	2012	2015	rVB	201	75	0.01%	0.002%
44	7.825	2015	2017	2020	rBV	136	96	0.02%	0.002%
45	7.893	2025	2038	2061	rBV	276992	480173	79.17%	10.684%
46	8.063	2087	2091	2092	rBV	213	164	0.03%	0.004%
47	8.176	2115	2126	2146	rVB	55253	92554	15.26%	2.059%
48	8.247	2146	2148	2151	rVB2	295	176	0.03%	0.004%
49	8.301	2164	2165	2166	rBV2	139	43	0.01%	0.001%
50	8.375	2186	2188	2190	rBV2	152	78	0.01%	0.002%
51	8.446	2209	2210	2211	rVB2	117	23	0.00%	0.001%
52	8.472	2216	2218	2222	rVB	168	85	0.01%	0.002%
53	8.539	2237	2239	2245	rVB2	249	212	0.03%	0.005%
54	8.626	2255	2266	2294	rBV2	136226	258282	42.58%	5.747%
55	8.774	2309	2312	2315	rBV2	284	197	0.03%	0.004%
56	8.812	2321	2324	2326	rBV2	285	158	0.03%	0.004%
57	8.902	2350	2352	2357	rVB	207	157	0.03%	0.003%
58	8.989	2375	2379	2381	rBV2	189	130	0.02%	0.003%
59	9.028	2388	2391	2396	rVB2	193	148	0.02%	0.003%
60	9.160	2429	2432	2439	rBV	211	200	0.03%	0.004%
61	9.275	2466	2468	2472	rBV	171	81	0.01%	0.002%
62	9.311	2477	2479	2481	rBB	270	137	0.02%	0.003%
63	9.340	2481	2488	2495	rBV2	382	642	0.11%	0.014%
64	9.414	2498	2511	2525	rBV	252876	417906	68.90%	9.299%
65	9.533	2545	2548	2551	rVB	261	163	0.03%	0.004%
66	9.565	2555	2558	2560	rVV	143	64	0.01%	0.001%
67	9.748	2612	2615	2617	rBV	188	79	0.01%	0.002%
68	9.799	2628	2631	2632	rBV	137	60	0.01%	0.001%
69	9.841	2641	2644	2646	rBV	214	101	0.02%	0.002%
70	9.899	2660	2662	2665	rBV	143	130	0.02%	0.003%
71	9.947	2671	2677	2680	rBV	273	386	0.06%	0.009%
72	10.385	2811	2813	2815	rVB	216	74	0.01%	0.002%
73	10.597	2877	2879	2881	rBV	153	66	0.01%	0.001%
74	10.751	2915	2927	2945	rBV	185774	294607	48.57%	6.555%
75	10.925	2978	2981	2989	rVB	296	221	0.04%	0.005%
76	11.079	3025	3029	3032	rBV	196	159	0.03%	0.004%

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77	11.166	3054	3056	3059	rBV2	131	85	0.01%	0.002%
78	11.224	3071	3074	3077	rBV2	202	144	0.02%	0.003%
79	11.404	3125	3130	3132	rBV	290	280	0.05%	0.006%
80	11.806	3244	3255	3275	rBV	248347	399573	65.88%	8.891%
81	12.127	3351	3355	3357	rBV	197	157	0.03%	0.003%
82	12.188	3362	3374	3395	rBV	253386	408650	67.38%	9.093%
83	12.301	3406	3409	3412	rVB	326	188	0.03%	0.004%
84	12.500	3468	3471	3474	rBV	243	120	0.02%	0.003%
85	12.893	3590	3593	3596	rBV2	208	162	0.03%	0.004%
86	13.208	3689	3691	3694	rBV	183	88	0.01%	0.002%
87	13.327	3725	3728	3731	rBV	262	159	0.03%	0.004%
88	13.809	3875	3878	3879	rBV2	151	88	0.01%	0.002%
89	13.989	3932	3934	3935	rBV2	185	67	0.01%	0.001%
90	14.918	4221	4223	4225	rBV	174	54	0.01%	0.001%
91	14.931	4225	4227	4232	rVV	297	155	0.03%	0.003%
92	15.127	4284	4288	4293	rBV3	513	521	0.09%	0.012%

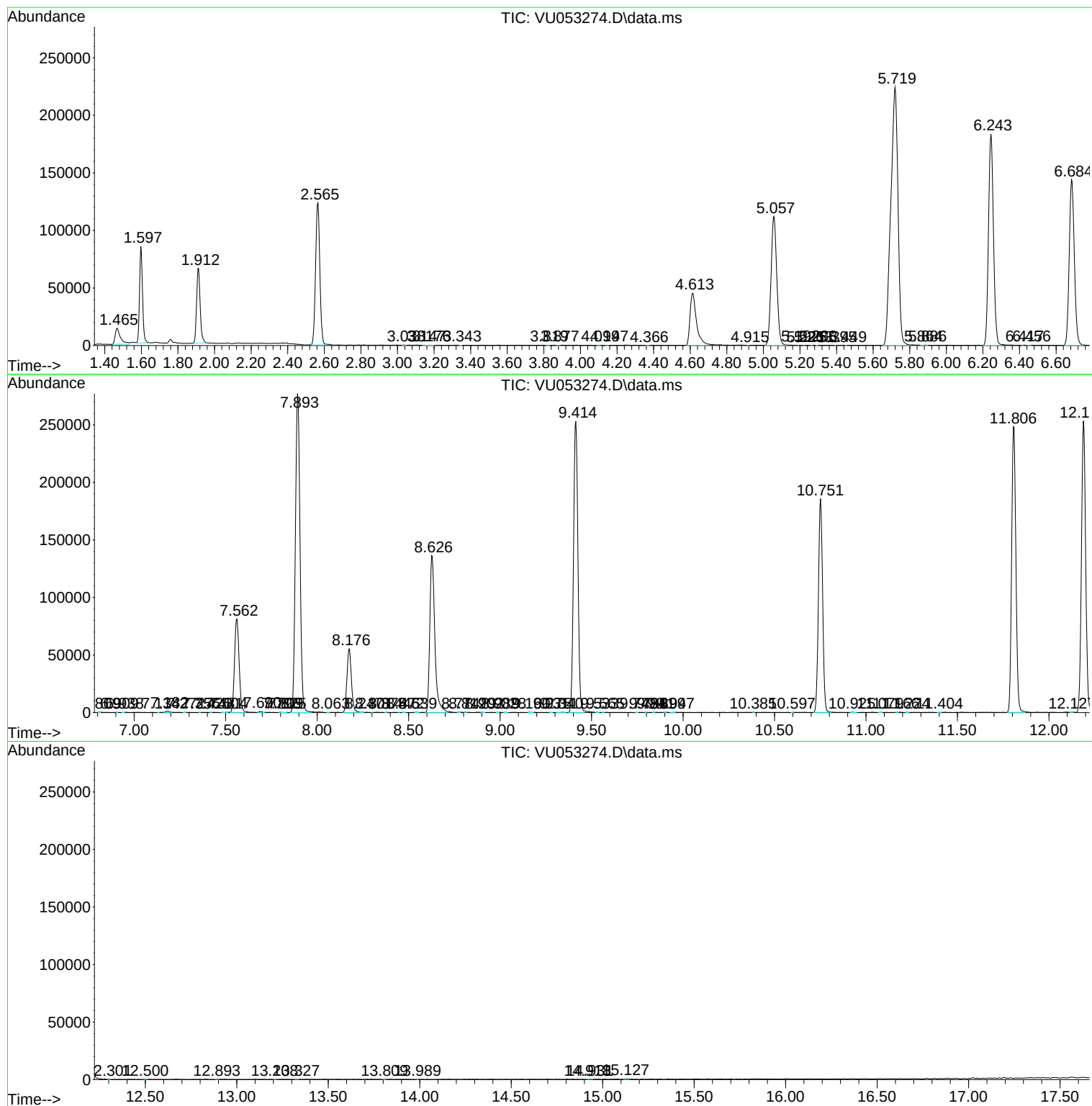
Sum of corrected areas: 4494235

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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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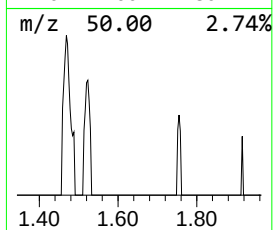
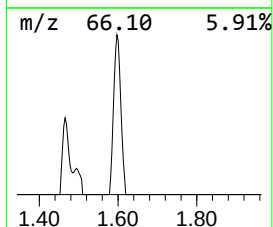
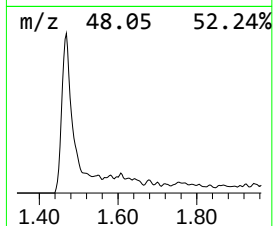
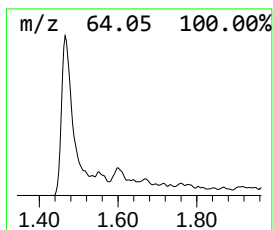
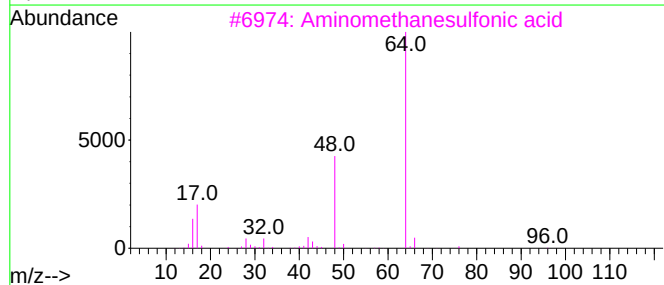
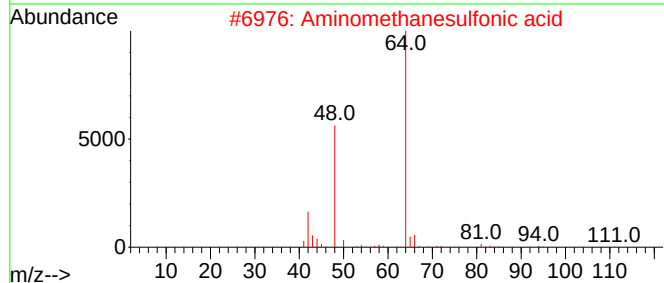
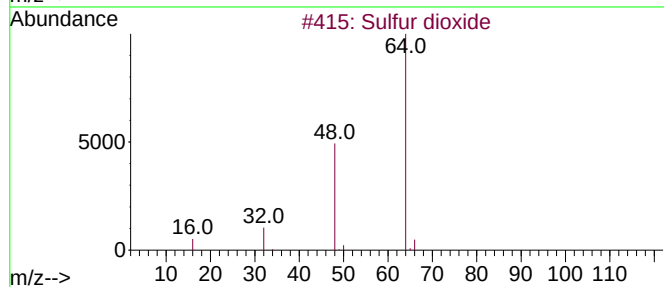
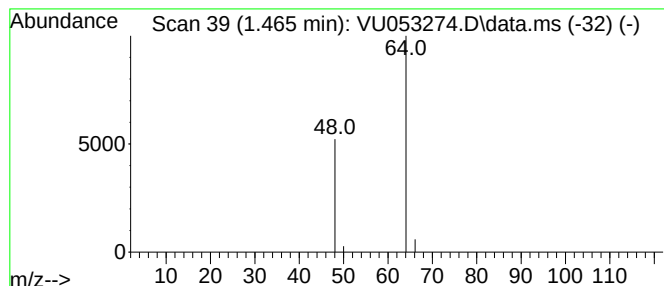
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Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	4.03 ug/L	27551	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	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	1.465	4.0	ug/L	27551	1	6.243	342117	50.0