

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053273.D
 Acq On : 17 Mar 2023 17:36
 Operator : JC/MD
 Sample : 01930-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFD5

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: VU053273.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	32	39	55	rBV	14135	25157	4.01%	0.550%
2	1.598	73	80	96	rVB	86436	97742	15.59%	2.135%
3	1.909	170	177	195	rVB	66073	89328	14.25%	1.951%
4	2.565	368	381	395	rBV	124968	203294	32.42%	4.441%
5	2.710	424	426	432	rBV	215	116	0.02%	0.003%
6	2.745	432	437	444	rBV3	889	1370	0.22%	0.030%
7	2.868	473	475	479	rBV	246	167	0.03%	0.004%
8	3.176	569	571	580	rBV3	357	488	0.08%	0.011%
9	3.350	619	625	628	rBV3	656	652	0.10%	0.014%
10	3.417	644	646	649	rBV2	226	141	0.02%	0.003%
11	3.797	762	764	765	rBV2	171	78	0.01%	0.002%
12	3.839	774	777	782	rBV2	203	143	0.02%	0.003%
13	3.954	810	813	817	rBV	293	192	0.03%	0.004%
14	4.064	845	847	851	rVB	201	109	0.02%	0.002%
15	4.392	946	949	952	rVB	217	99	0.02%	0.002%
16	4.533	991	993	995	rVB	238	98	0.02%	0.002%
17	4.610	1006	1017	1050	rBV2	45507	121009	19.30%	2.643%
18	4.816	1076	1081	1084	rBV2	296	295	0.05%	0.006%
19	4.974	1128	1130	1131	rBV2	108	26	0.00%	0.001%
20	4.996	1133	1137	1139	rVB	279	170	0.03%	0.004%
21	5.057	1140	1156	1177	rBV	112883	252134	40.21%	5.508%
22	5.208	1201	1203	1205	rVB	139	56	0.01%	0.001%
23	5.234	1209	1211	1212	rBV	117	49	0.01%	0.001%
24	5.266	1219	1221	1225	rBV	185	114	0.02%	0.002%
25	5.347	1242	1246	1253	rBV	287	424	0.07%	0.009%
26	5.517	1295	1299	1301	rBV2	311	265	0.04%	0.006%
27	5.649	1339	1340	1341	rVB2	101	19	0.00%	0.000%
28	5.720	1341	1362	1385	rBV2	230564	627052	100.00%	13.698%
29	5.961	1436	1437	1438	rBV2	113	25	0.00%	0.001%
30	6.086	1472	1476	1482	rBV2	185	170	0.03%	0.004%
31	6.147	1490	1495	1497	rBV	326	254	0.04%	0.006%
32	6.163	1497	1500	1501	rVV	166	77	0.01%	0.002%
33	6.244	1511	1525	1549	rBV	183387	346220	55.21%	7.563%
34	6.411	1575	1577	1578	rVB	202	63	0.01%	0.001%
35	6.424	1578	1581	1585	rBV	326	221	0.04%	0.005%
36	6.607	1636	1638	1647	rVB2	221	176	0.03%	0.004%

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

37	6.684	1648	1662	1683	rBV	147641	286500	45.69%	6.259%
38	6.851	1711	1714	1715	rBV	197	139	0.02%	0.003%
39	6.916	1732	1734	1736	rBV	136	33	0.01%	0.001%
40	7.186	1812	1818	1826	rBV3	972	1291	0.21%	0.028%
41	7.301	1848	1854	1856	rBV	182	234	0.04%	0.005%
42	7.375	1873	1877	1880	rBV	246	249	0.04%	0.005%
43	7.408	1884	1887	1891	rBV	177	193	0.03%	0.004%
44	7.504	1913	1917	1920	rBV	195	211	0.03%	0.005%
45	7.520	1920	1922	1923	rVV	220	120	0.02%	0.003%
46	7.562	1923	1935	1953	rVV	81964	143457	22.88%	3.134%
47	7.684	1969	1973	1974	rBV	557	334	0.05%	0.007%
48	7.742	1989	1991	1992	rBV	155	72	0.01%	0.002%
49	7.771	1997	2000	2006	rVB	310	306	0.05%	0.007%
50	7.800	2007	2009	2010	rBV	149	82	0.01%	0.002%
51	7.826	2015	2017	2019	rBV	166	110	0.02%	0.002%
52	7.848	2023	2024	2025	rBV	113	24	0.00%	0.001%
53	7.893	2025	2038	2056	rBV	291258	492988	78.62%	10.770%
54	8.051	2084	2087	2091	rVB	232	145	0.02%	0.003%
55	8.176	2115	2126	2149	rVB	55899	95300	15.20%	2.082%
56	8.269	2153	2155	2156	rBV	229	100	0.02%	0.002%
57	8.414	2197	2200	2201	rBV	158	111	0.02%	0.002%
58	8.626	2254	2266	2297	rBV2	139914	261277	41.67%	5.708%
59	8.809	2322	2323	2324	rBV2	174	61	0.01%	0.001%
60	8.989	2375	2379	2382	rBV	184	222	0.04%	0.005%
61	9.035	2390	2393	2396	rBV2	177	107	0.02%	0.002%
62	9.160	2431	2432	2433	rBB2	96	19	0.00%	0.000%
63	9.321	2479	2482	2485	rBB	258	141	0.02%	0.003%
64	9.411	2496	2510	2528	rBV	253899	416833	66.48%	9.106%
65	9.607	2569	2571	2579	rVB	220	175	0.03%	0.004%
66	9.697	2596	2599	2602	rVB	165	78	0.01%	0.002%
67	9.957	2672	2680	2682	rBV	263	388	0.06%	0.008%
68	10.031	2700	2703	2705	rVB	249	150	0.02%	0.003%
69	10.096	2721	2723	2728	rVB2	232	167	0.03%	0.004%
70	10.224	2760	2763	2765	rBV	211	170	0.03%	0.004%
71	10.346	2799	2801	2803	rBV2	186	107	0.02%	0.002%
72	10.555	2864	2866	2867	rBB	135	30	0.00%	0.001%
73	10.665	2897	2900	2902	rBV	178	115	0.02%	0.003%
74	10.751	2915	2927	2943	rBV	191374	301114	48.02%	6.578%
75	10.928	2980	2982	2985	rVB	192	96	0.02%	0.002%
76	11.584	3182	3186	3188	rBV	342	268	0.04%	0.006%

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 Title : VOC Analysis

77	11.607	3191	3193	3197	rVB	237	137	0.02%	0.003%
78	11.716	3224	3227	3231	rVB2	201	121	0.02%	0.003%
79	11.809	3244	3256	3280	rBV	245992	391473	62.43%	8.552%
80	11.957	3299	3302	3304	rBV	168	76	0.01%	0.002%
81	12.076	3337	3339	3340	rBV2	247	99	0.02%	0.002%
82	12.189	3362	3374	3390	rBV	252785	412106	65.72%	9.003%
83	12.385	3432	3435	3439	rBV	184	154	0.02%	0.003%
84	12.452	3453	3456	3462	rBV	205	140	0.02%	0.003%
85	12.755	3548	3550	3553	rVB	178	78	0.01%	0.002%
86	12.832	3572	3574	3578	rBV	167	87	0.01%	0.002%
87	13.124	3664	3665	3668	rBV	123	51	0.01%	0.001%
88	13.436	3759	3762	3763	rBV	205	94	0.01%	0.002%
89	14.047	3950	3952	3956	rBV	161	99	0.02%	0.002%
90	14.121	3971	3975	3978	rBV2	286	199	0.03%	0.004%
91	14.484	4086	4088	4092	rVB	242	100	0.02%	0.002%
92	14.581	4116	4118	4120	rBV	182	73	0.01%	0.002%
93	14.755	4169	4172	4173	rBV	205	113	0.02%	0.002%
94	15.201	4309	4311	4314	rVB2	401	219	0.03%	0.005%
95	15.311	4343	4345	4347	rBV2	271	190	0.03%	0.004%
96	16.963	4856	4859	4861	rBV2	692	496	0.08%	0.011%

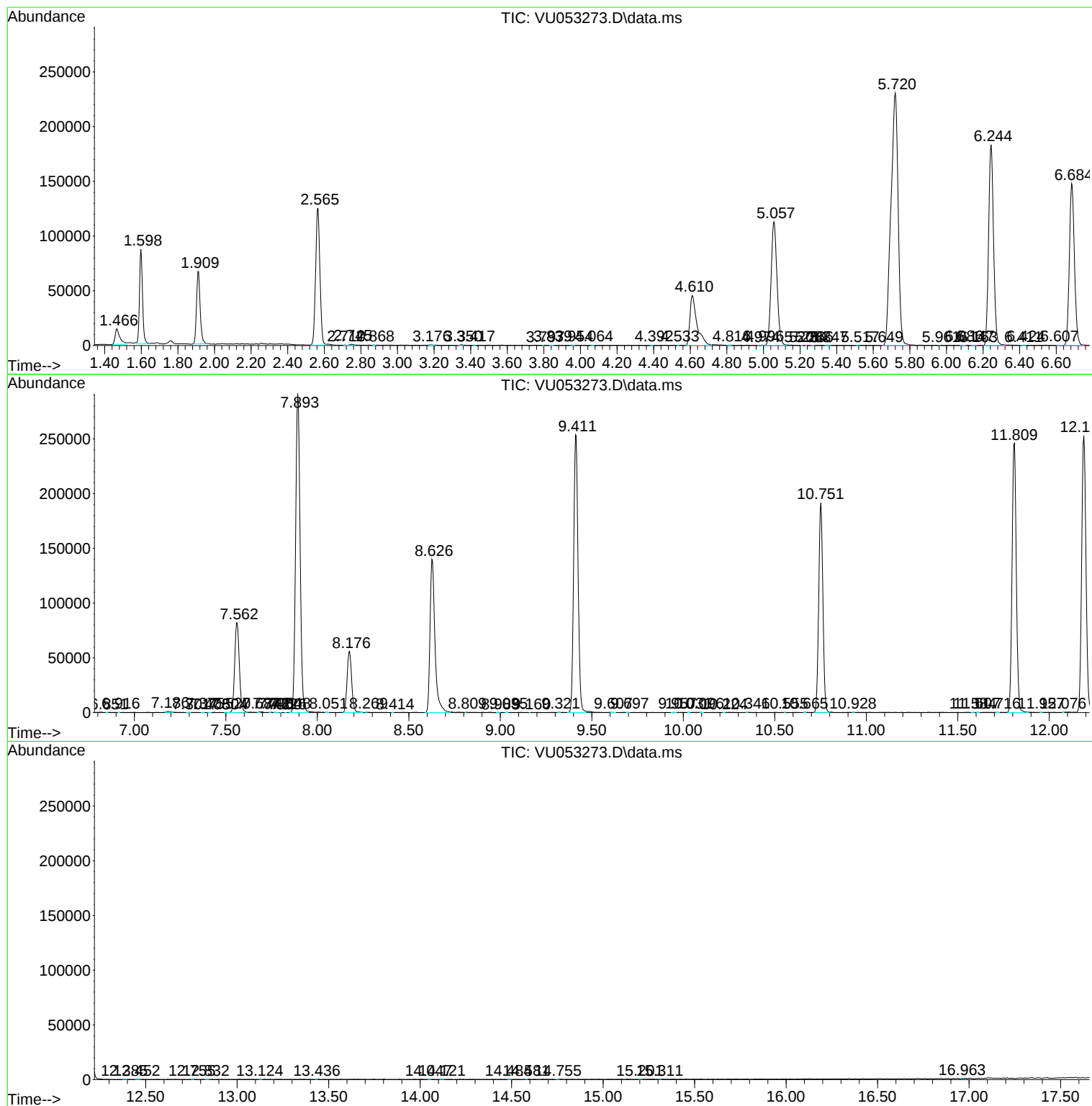
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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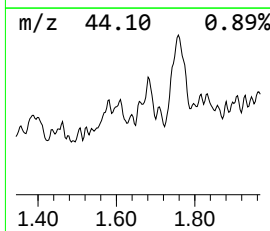
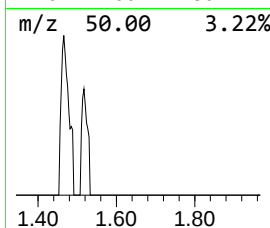
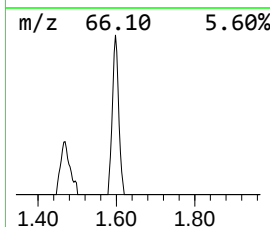
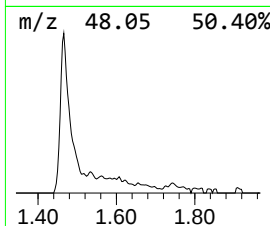
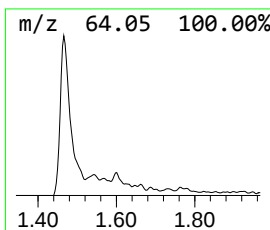
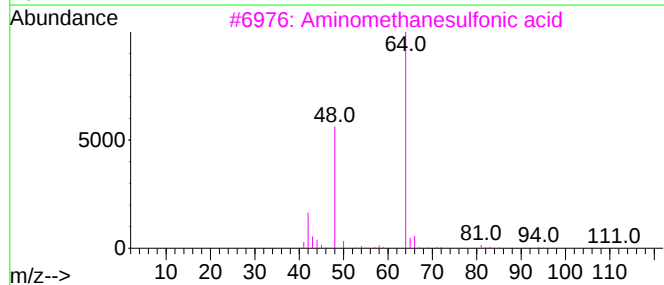
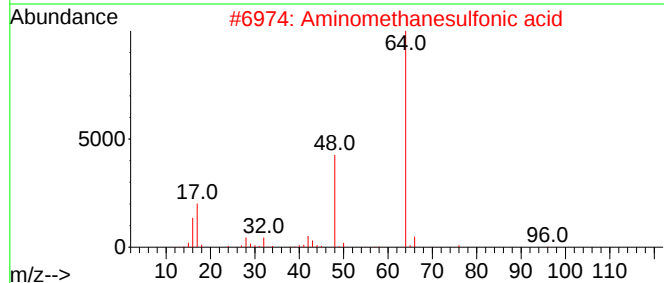
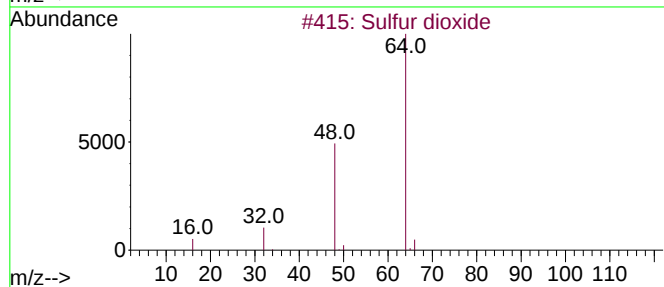
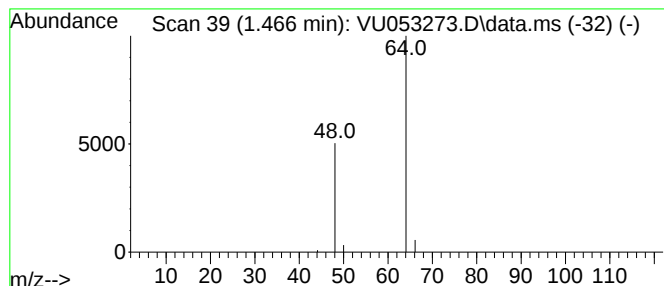
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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.
1.466	3.63 ug/L	25157	1,4-Difluorobenzene	6.244

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 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	1.466	3.6	ug/L	25157	1	6.244	346220	50.0