

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU032223\
 Data File : VU053350.D
 Acq On : 22 Mar 2023 14:23
 Operator : JC/MD
 Sample : 01961-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF7

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: VU053350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.498	41	49	65	rBV	5767	15950	3.91%	0.507%
2	1.598	74	80	97	rVB	55632	65096	15.95%	2.068%
3	1.913	171	178	191	rVB	47160	62200	15.24%	1.976%
4	2.565	370	381	397	rBV	85130	135874	33.29%	4.316%
5	2.794	448	452	456	rBV2	489	436	0.11%	0.014%
6	2.971	504	507	510	rBV	175	142	0.03%	0.005%
7	3.032	524	526	528	rBV	197	117	0.03%	0.004%
8	3.713	736	738	740	rBV	137	97	0.02%	0.003%
9	3.761	749	753	756	rBB	181	168	0.04%	0.005%
10	3.781	756	759	761	rBV	193	151	0.04%	0.005%
11	3.810	765	768	770	rBV	220	155	0.04%	0.005%
12	4.009	827	830	833	rBV	224	207	0.05%	0.007%
13	4.160	869	877	880	rBB	239	377	0.09%	0.012%
14	4.186	883	885	887	rBV	151	106	0.03%	0.003%
15	4.218	892	895	897	rBV	245	202	0.05%	0.006%
16	4.276	911	913	921	rVB	243	160	0.04%	0.005%
17	4.475	968	975	977	rBV	231	281	0.07%	0.009%
18	4.530	987	992	994	rBV	258	215	0.05%	0.007%
19	4.617	1009	1019	1041	rVV2	29105	72683	17.81%	2.309%
20	4.736	1054	1056	1059	rBV	293	123	0.03%	0.004%
21	4.823	1080	1083	1086	rBB	252	136	0.03%	0.004%
22	4.858	1091	1094	1098	rBV	223	185	0.05%	0.006%
23	4.880	1098	1101	1105	rVB	324	235	0.06%	0.007%
24	5.003	1136	1139	1142	rBV	217	223	0.05%	0.007%
25	5.057	1142	1156	1175	rVV2	75256	163849	40.15%	5.204%
26	5.369	1250	1253	1257	rBV	145	170	0.04%	0.005%
27	5.472	1283	1285	1291	rBB	188	215	0.05%	0.007%
28	5.501	1291	1294	1296	rBV	133	118	0.03%	0.004%
29	5.575	1314	1317	1319	rBV	145	128	0.03%	0.004%
30	5.585	1319	1320	1324	rVB	238	113	0.03%	0.004%
31	5.607	1324	1327	1330	rBB	157	135	0.03%	0.004%
32	5.636	1331	1336	1341	rBV	195	280	0.07%	0.009%
33	5.720	1341	1362	1387	rVV2	149861	408093	100.00%	12.962%
34	5.806	1387	1389	1392	rBV	169	142	0.03%	0.005%
35	5.864	1404	1407	1409	rBV2	206	139	0.03%	0.004%
36	5.906	1417	1420	1422	rBV	192	168	0.04%	0.005%

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 Title : VOC Analysis

37	5.977	1440	1442	1444	rBV	193	119	0.03%	0.004%
38	6.012	1450	1453	1454	rBV	172	119	0.03%	0.004%
39	6.099	1477	1480	1487	rBB	206	286	0.07%	0.009%
40	6.134	1488	1491	1494	rBV	221	180	0.04%	0.006%
41	6.244	1512	1525	1544	rBV	132310	250654	61.42%	7.962%
42	6.340	1553	1555	1559	rVB2	312	198	0.05%	0.006%
43	6.388	1568	1570	1572	rBV	191	118	0.03%	0.004%
44	6.443	1584	1587	1589	rBV	115	85	0.02%	0.003%
45	6.498	1601	1604	1605	rBV	167	110	0.03%	0.003%
46	6.552	1616	1621	1630	rBV	237	454	0.11%	0.014%
47	6.604	1634	1637	1639	rBV	182	142	0.03%	0.005%
48	6.684	1649	1662	1682	rBV2	96098	187790	46.02%	5.965%
49	6.826	1703	1706	1708	rBV	123	110	0.03%	0.003%
50	6.967	1748	1750	1753	rBV	125	111	0.03%	0.004%
51	7.083	1781	1786	1789	rBV	214	253	0.06%	0.008%
52	7.157	1805	1809	1814	rBV	235	288	0.07%	0.009%
53	7.183	1814	1817	1818	rBV	218	92	0.02%	0.003%
54	7.257	1837	1840	1843	rBV	163	173	0.04%	0.005%
55	7.359	1870	1872	1874	rBV	138	96	0.02%	0.003%
56	7.562	1923	1935	1950	rBV	54967	93889	23.01%	2.982%
57	7.720	1981	1984	1991	rBB	189	279	0.07%	0.009%
58	7.787	2000	2005	2008	rBV	294	325	0.08%	0.010%
59	7.893	2024	2038	2057	rBV	191703	327451	80.24%	10.401%
60	8.035	2079	2082	2086	rVB	318	215	0.05%	0.007%
61	8.080	2093	2096	2099	rBB	149	124	0.03%	0.004%
62	8.102	2099	2103	2104	rBV	169	144	0.04%	0.005%
63	8.173	2116	2125	2141	rBV	37991	62876	15.41%	1.997%
64	8.289	2155	2161	2164	rBV	152	222	0.05%	0.007%
65	8.392	2188	2193	2194	rBV	168	137	0.03%	0.004%
66	8.562	2240	2246	2248	rBV	280	284	0.07%	0.009%
67	8.629	2256	2267	2289	rBV2	87505	166501	40.80%	5.289%
68	8.826	2320	2328	2333	rBB	243	364	0.09%	0.012%
69	8.855	2334	2337	2339	rBB	177	110	0.03%	0.003%
70	8.871	2340	2342	2345	rBV	142	121	0.03%	0.004%
71	9.051	2393	2398	2401	rBV	168	226	0.06%	0.007%
72	9.118	2417	2419	2422	rBV	180	142	0.03%	0.005%
73	9.324	2480	2483	2485	rBV	175	150	0.04%	0.005%
74	9.366	2491	2496	2498	rBV	272	249	0.06%	0.008%
75	9.411	2498	2510	2530	rVV	191936	319614	78.32%	10.152%
76	9.568	2555	2559	2562	rBV2	370	312	0.08%	0.010%

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Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	9.713	2602	2604	2605	rBV	135	75	0.02%	0.002%
78	9.941	2672	2675	2678	rBV	234	204	0.05%	0.006%
79	10.115	2724	2729	2735	rBV3	597	723	0.18%	0.023%
80	10.237	2765	2767	2769	rBV	178	122	0.03%	0.004%
81	10.289	2781	2783	2785	rBV	184	127	0.03%	0.004%
82	10.469	2836	2839	2841	rBV	138	87	0.02%	0.003%
83	10.546	2861	2863	2865	rBB	155	79	0.02%	0.003%
84	10.565	2866	2869	2871	rBV	175	118	0.03%	0.004%
85	10.752	2915	2927	2942	rBV	129455	205901	50.45%	6.540%
86	10.877	2962	2966	2969	rBV	230	239	0.06%	0.008%
87	11.006	3002	3006	3009	rBV	210	220	0.05%	0.007%
88	11.462	3145	3148	3150	rBV	151	131	0.03%	0.004%
89	11.665	3208	3211	3216	rBV	218	277	0.07%	0.009%
90	11.806	3243	3255	3277	rBV	197537	310816	76.16%	9.872%
91	11.906	3283	3286	3289	rBV2	162	146	0.04%	0.005%
92	12.189	3362	3374	3394	rBV	176121	283376	69.44%	9.001%
93	12.536	3477	3482	3485	rBV	236	279	0.07%	0.009%
94	12.835	3573	3575	3577	rVB	192	75	0.02%	0.002%
95	13.629	3819	3822	3824	rBV	183	134	0.03%	0.004%
96	15.076	4270	4272	4275	rBV2	175	106	0.03%	0.003%
97	15.243	4321	4324	4327	rBV2	316	222	0.05%	0.007%
98	15.382	4363	4367	4369	rBV2	280	205	0.05%	0.007%
99	15.443	4383	4386	4389	rBV2	254	187	0.05%	0.006%
100	15.739	4473	4478	4480	rBV2	229	271	0.07%	0.009%

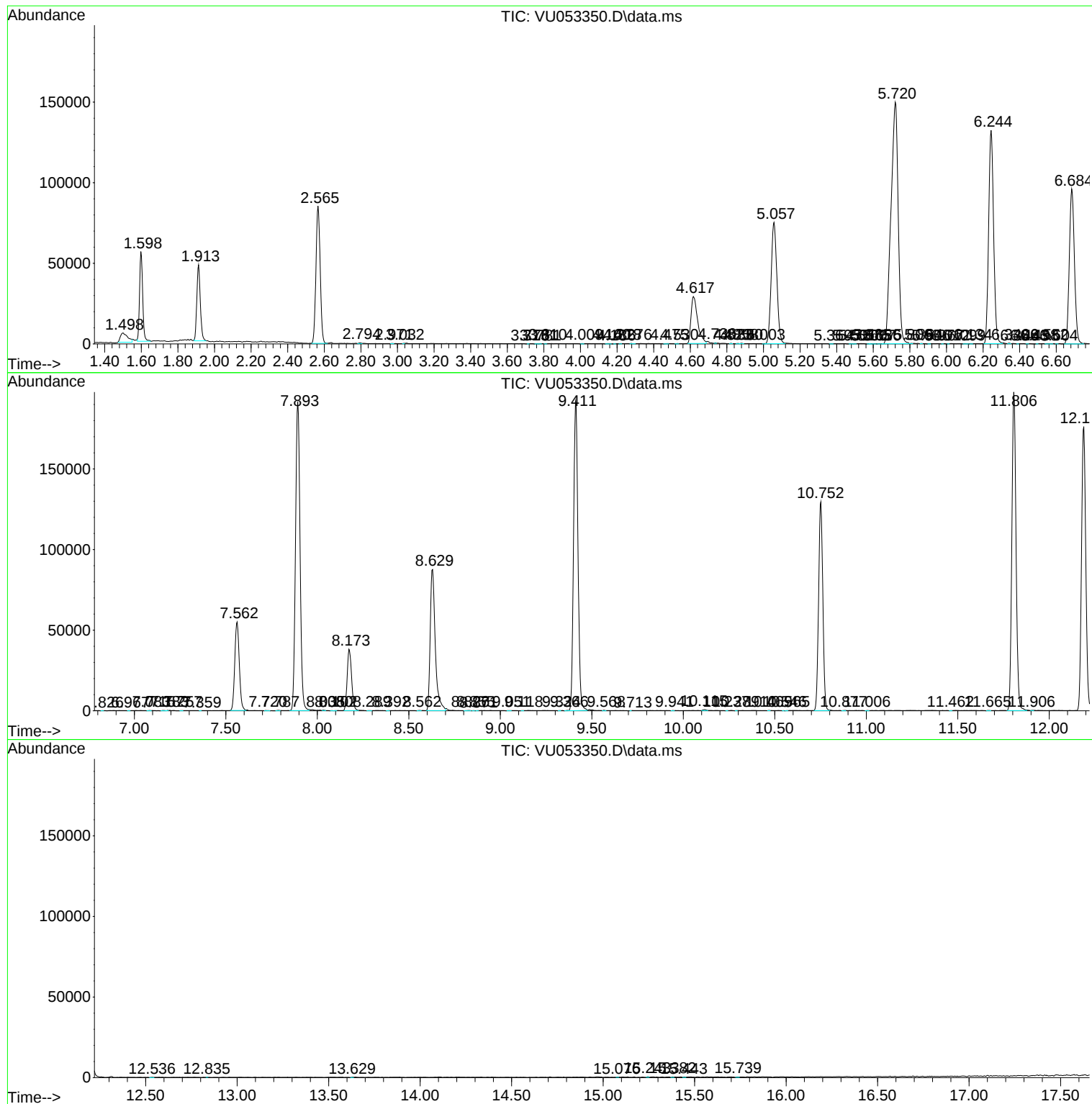
Sum of corrected areas: 3148302

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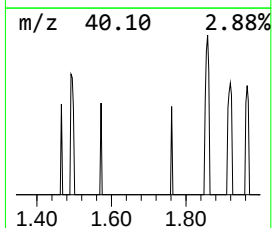
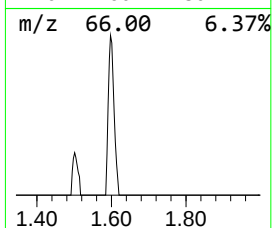
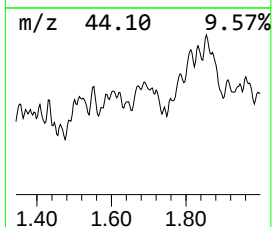
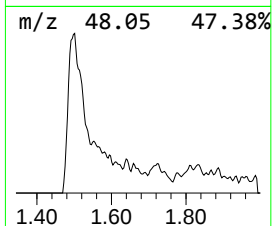
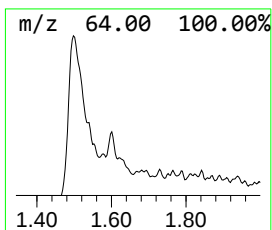
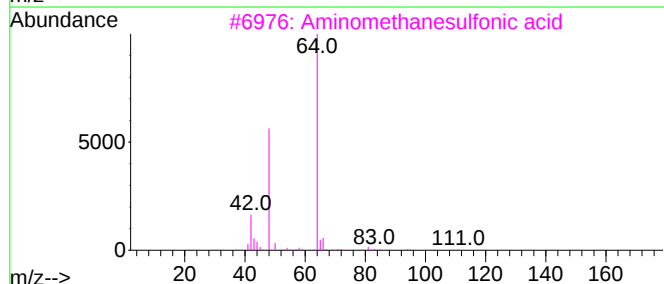
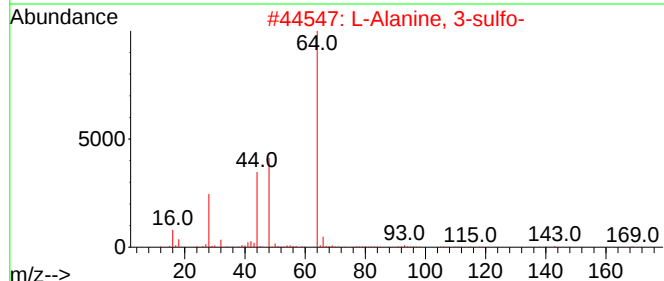
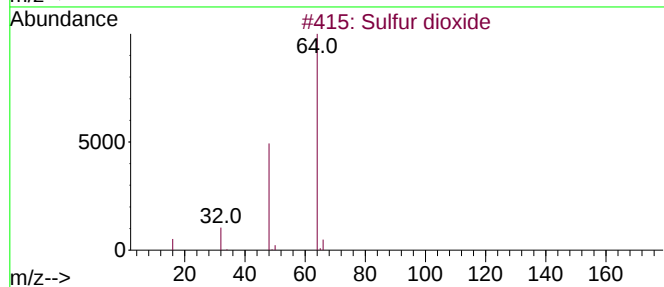
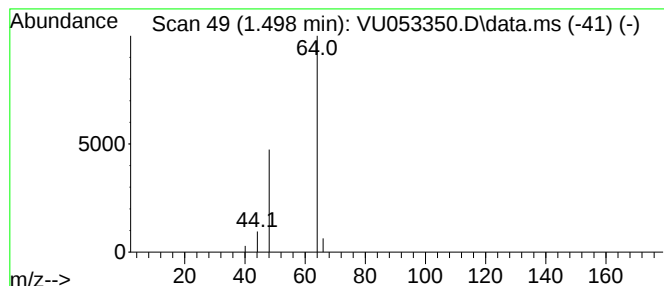
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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.
1.498	3.18 ug/L	15950	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.498	3.2	ug/L	15950	1	6.244	250654	50.0