

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053265.D
 Acq On : 17 Mar 2023 14:26
 Operator : JC/MD
 Sample : 01929-15 20X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFE8

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: VU053265.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	33	40	52	rBV	16467	27906	3.28%	0.472%
2	1.600	73	81	102	rVB2	296936	358113	42.05%	6.062%
3	1.909	169	177	197	rVB	73420	100360	11.78%	1.699%
4	2.565	369	381	396	rVB	141674	230420	27.06%	3.901%
5	2.867	472	475	478	rBV2	267	185	0.02%	0.003%
6	3.044	521	530	539	rVB3	1836	3185	0.37%	0.054%
7	3.179	562	572	591	rVV4	1622	3992	0.47%	0.068%
8	3.250	592	594	596	rVV	218	106	0.01%	0.002%
9	3.263	596	598	600	rVB	201	66	0.01%	0.001%
10	3.346	616	624	634	rVB5	1224	2396	0.28%	0.041%
11	3.385	634	636	641	rBV	167	79	0.01%	0.001%
12	3.661	719	722	725	rVB	213	100	0.01%	0.002%
13	3.735	743	745	747	rBV	135	55	0.01%	0.001%
14	3.758	750	752	754	rBV	171	73	0.01%	0.001%
15	3.832	772	775	778	rBV	219	138	0.02%	0.002%
16	3.861	781	784	786	rBV	206	128	0.02%	0.002%
17	4.002	826	828	830	rBV	164	99	0.01%	0.002%
18	4.031	835	837	838	rBV	147	42	0.00%	0.001%
19	4.131	865	868	873	rVB2	290	215	0.03%	0.004%
20	4.224	895	897	900	rVB	251	116	0.01%	0.002%
21	4.247	902	904	907	rVV2	170	91	0.01%	0.002%
22	4.276	910	913	916	rBV2	178	102	0.01%	0.002%
23	4.292	916	918	920	rBV	154	65	0.01%	0.001%
24	4.382	944	946	951	rBV	220	137	0.02%	0.002%
25	4.658	1006	1032	1063	rBV2	327778	851620	100.00%	14.416%
26	4.822	1080	1083	1087	rBV3	512	386	0.05%	0.007%
27	4.874	1098	1099	1100	rBV3	128	37	0.00%	0.001%
28	5.057	1141	1156	1177	rBV	125814	267636	31.43%	4.530%
29	5.462	1280	1282	1285	rVB	201	69	0.01%	0.001%
30	5.488	1288	1290	1293	rBV	181	132	0.02%	0.002%
31	5.591	1321	1322	1326	rVB	294	173	0.02%	0.003%
32	5.626	1327	1333	1337	rBV	180	310	0.04%	0.005%
33	5.719	1341	1362	1385	rVV2	249665	674374	79.19%	11.416%
34	5.993	1445	1447	1450	rVB	196	85	0.01%	0.001%
35	6.050	1463	1465	1470	rBV	212	124	0.01%	0.002%
36	6.102	1478	1481	1482	rBV	147	67	0.01%	0.001%

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 Title : VOC Analysis

37	6.115	1483	1485	1489	rVV2	359	186	0.02%	0.003%
38	6.140	1491	1493	1497	rVB	243	128	0.02%	0.002%
39	6.160	1497	1499	1502	rBV	250	102	0.01%	0.002%
40	6.243	1512	1525	1546	rBV	197195	369259	43.36%	6.251%
41	6.491	1598	1602	1606	rBV2	247	188	0.02%	0.003%
42	6.684	1649	1662	1681	rBV	159151	306214	35.96%	5.184%
43	6.938	1739	1741	1744	rBV	148	104	0.01%	0.002%
44	7.182	1811	1817	1822	rBV4	1319	1749	0.21%	0.030%
45	7.247	1832	1837	1839	rBV	304	279	0.03%	0.005%
46	7.279	1844	1847	1849	rVV	155	80	0.01%	0.001%
47	7.359	1871	1872	1873	rBV	120	34	0.00%	0.001%
48	7.382	1877	1879	1881	rBV	143	57	0.01%	0.001%
49	7.433	1888	1895	1899	rBV	232	380	0.04%	0.006%
50	7.562	1923	1935	1957	rBV2	90036	154700	18.17%	2.619%
51	7.681	1969	1972	1973	rBV2	712	343	0.04%	0.006%
52	7.806	2009	2011	2016	rVB2	213	179	0.02%	0.003%
53	7.893	2024	2038	2057	rBV	311220	536232	62.97%	9.077%
54	8.057	2086	2089	2096	rBV3	315	325	0.04%	0.006%
55	8.176	2113	2126	2140	rBV	60155	101781	11.95%	1.723%
56	8.533	2233	2237	2240	rBV	202	183	0.02%	0.003%
57	8.626	2255	2266	2295	rBV2	152330	274777	32.27%	4.651%
58	8.780	2311	2314	2315	rBV	169	73	0.01%	0.001%
59	8.935	2360	2362	2365	rBB	167	106	0.01%	0.002%
60	8.960	2365	2370	2371	rBV	130	143	0.02%	0.002%
61	9.128	2419	2422	2425	rBV	180	126	0.01%	0.002%
62	9.160	2430	2432	2434	rBV	155	110	0.01%	0.002%
63	9.173	2434	2436	2438	rVB2	152	80	0.01%	0.001%
64	9.185	2438	2440	2442	rBV2	178	85	0.01%	0.001%
65	9.214	2446	2449	2451	rBV	165	100	0.01%	0.002%
66	9.253	2458	2461	2466	rVB	271	180	0.02%	0.003%
67	9.275	2466	2468	2471	rBV	210	111	0.01%	0.002%
68	9.333	2484	2486	2491	rVB	149	62	0.01%	0.001%
69	9.414	2498	2511	2525	rBV	262321	437070	51.32%	7.399%
70	9.603	2568	2570	2572	rBV	122	58	0.01%	0.001%
71	9.697	2595	2599	2601	rBV	170	164	0.02%	0.003%
72	9.713	2601	2604	2606	rVV	179	106	0.01%	0.002%
73	9.783	2622	2626	2629	rBV	322	282	0.03%	0.005%
74	9.935	2670	2673	2675	rBV	149	94	0.01%	0.002%
75	9.951	2675	2678	2681	rVV2	195	144	0.02%	0.002%
76	10.324	2791	2794	2800	rVB2	169	160	0.02%	0.003%

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 Title : VOC Analysis

77	10.468	2838	2839	2842	rVB	130	37	0.00%	0.001%
78	10.488	2842	2845	2849	rBV2	164	99	0.01%	0.002%
79	10.539	2859	2861	2864	rVB	149	46	0.01%	0.001%
80	10.623	2883	2887	2889	rBV	166	102	0.01%	0.002%
81	10.645	2892	2894	2896	rBV	172	71	0.01%	0.001%
82	10.693	2907	2909	2910	rBV	194	66	0.01%	0.001%
83	10.751	2914	2927	2948	rVV	200989	320906	37.68%	5.432%
84	10.973	2993	2996	3000	rBV2	284	233	0.03%	0.004%
85	11.217	3070	3072	3075	rBV	240	163	0.02%	0.003%
86	11.272	3085	3089	3092	rBV2	226	195	0.02%	0.003%
87	11.623	3195	3198	3202	rVB2	209	168	0.02%	0.003%
88	11.661	3208	3210	3213	rBV	192	87	0.01%	0.001%
89	11.806	3243	3255	3279	rBV	267613	424107	49.80%	7.179%
90	11.938	3293	3296	3297	rBV	120	70	0.01%	0.001%
91	12.188	3361	3374	3397	rBV	283182	449995	52.84%	7.617%
92	12.896	3592	3594	3597	rBV	143	46	0.01%	0.001%
93	12.941	3605	3608	3612	rVB	263	162	0.02%	0.003%
94	13.269	3707	3710	3713	rBV2	234	159	0.02%	0.003%
95	13.542	3792	3795	3797	rBV	216	137	0.02%	0.002%
96	14.005	3936	3939	3941	rBV2	178	130	0.02%	0.002%
97	14.102	3966	3969	3971	rBV2	308	191	0.02%	0.003%
98	14.430	4068	4071	4074	rBV	242	173	0.02%	0.003%
99	14.603	4122	4125	4128	rBV	276	171	0.02%	0.003%
100	15.102	4278	4280	4285	rVB	310	201	0.02%	0.003%

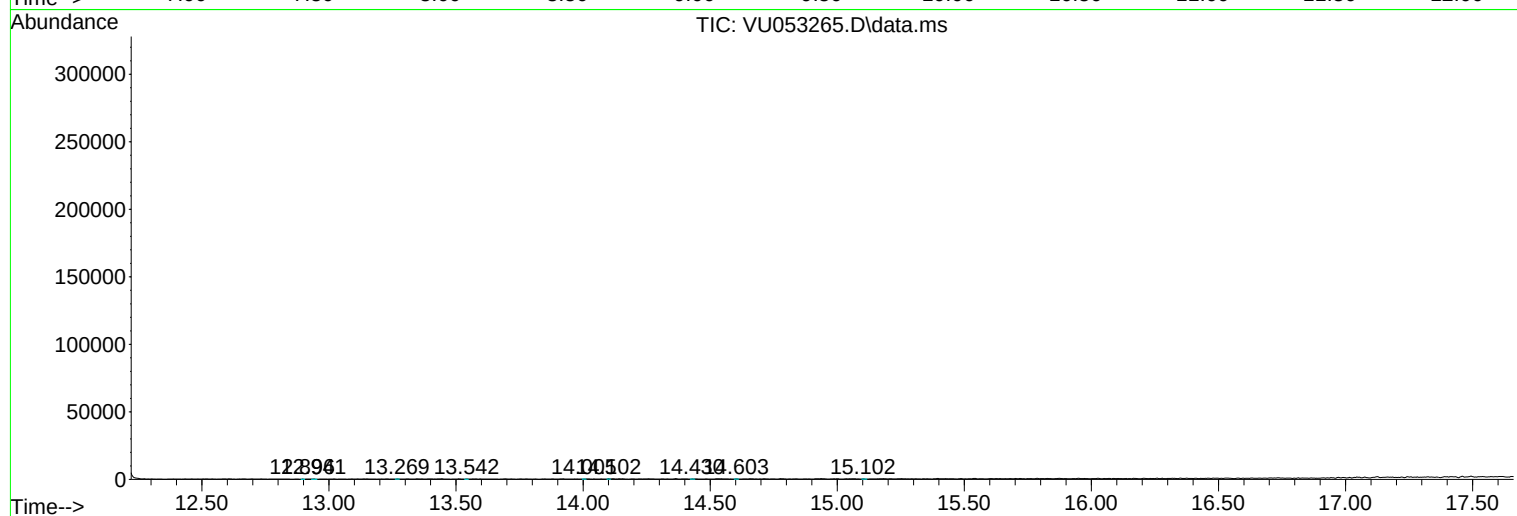
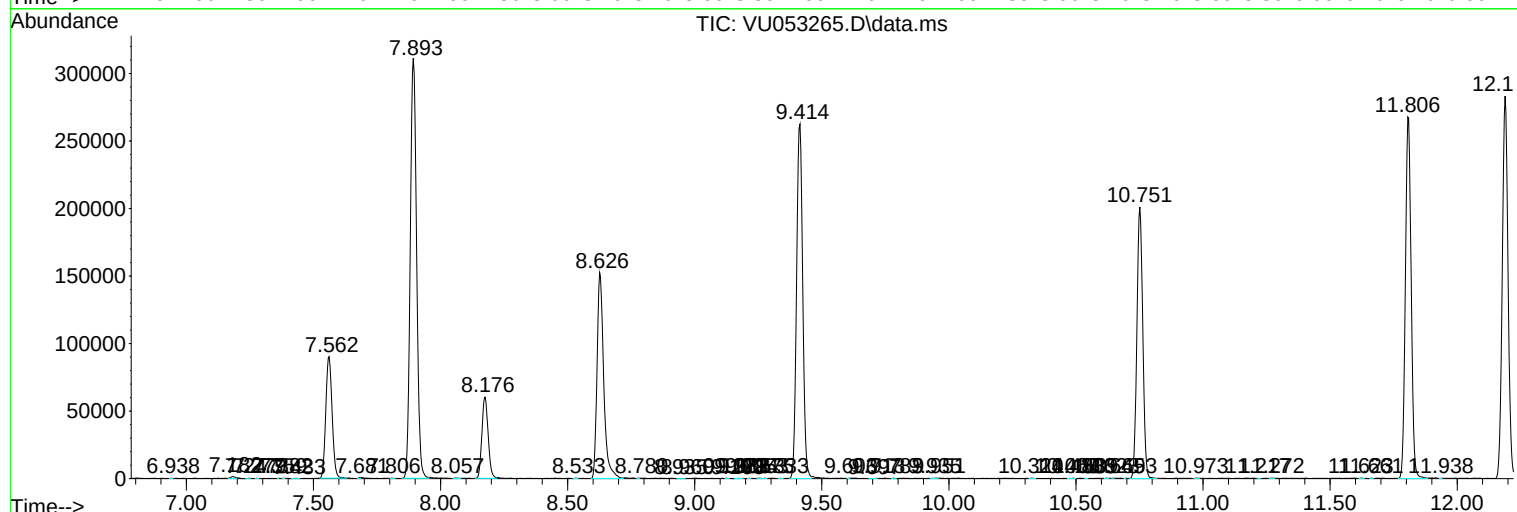
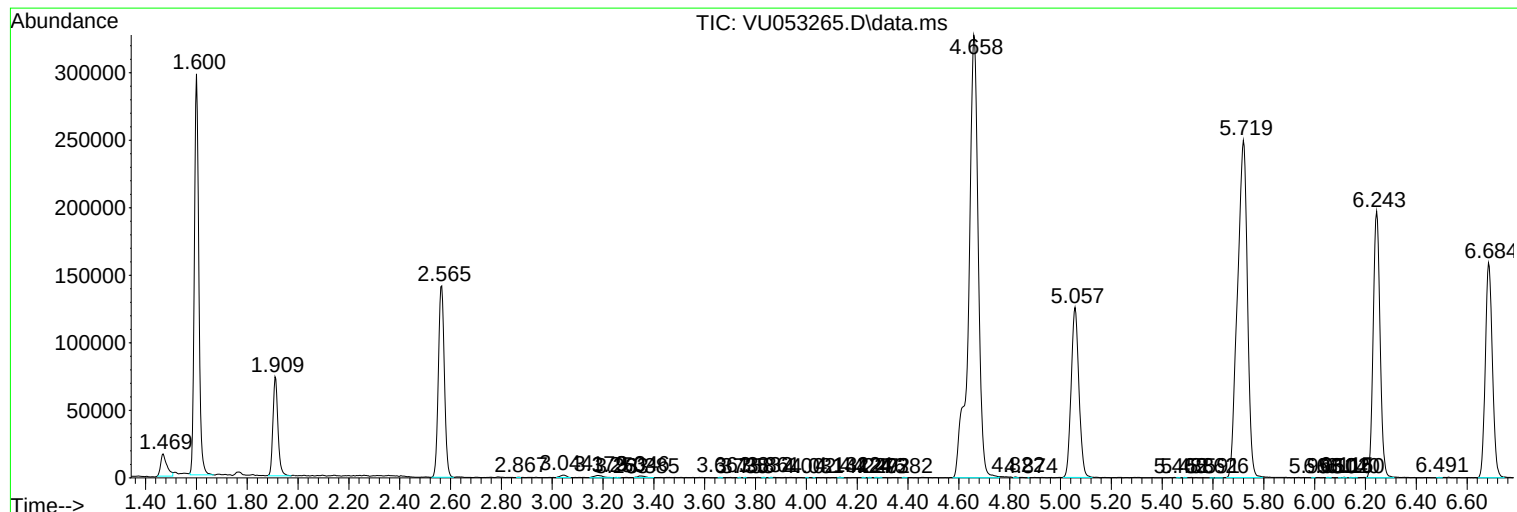
Sum of corrected areas: 5907431

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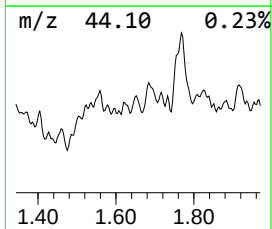
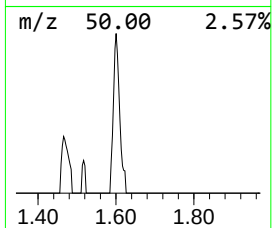
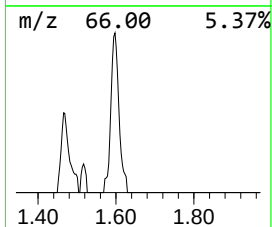
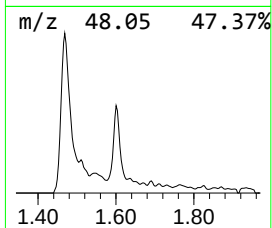
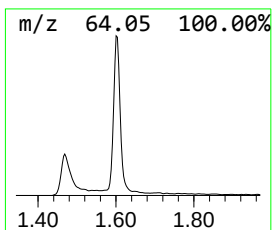
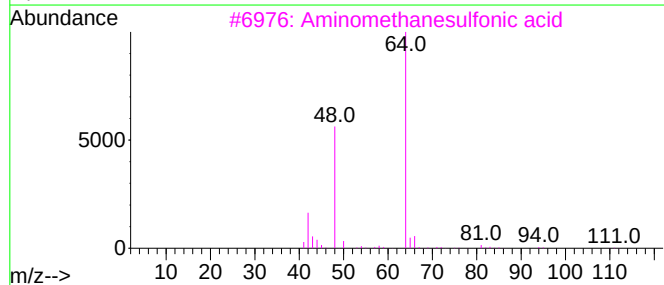
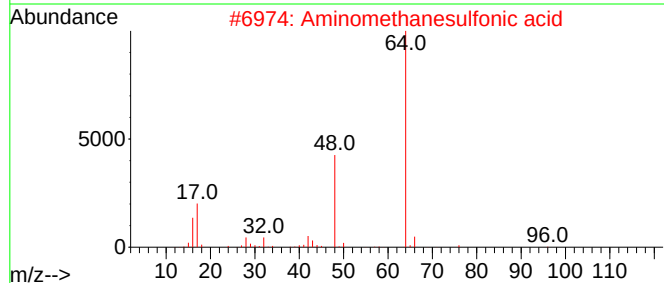
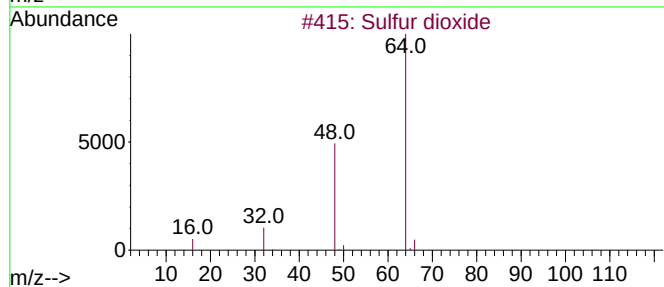
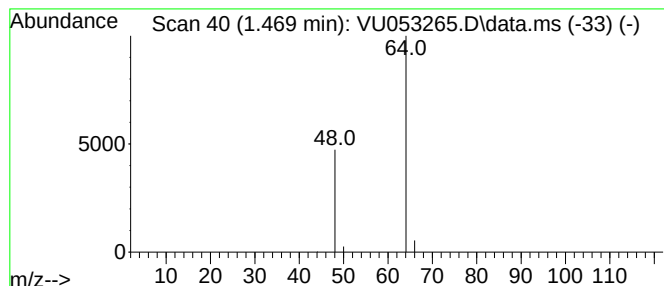
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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	3.78 ug/L	27906	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 Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.8	ug/L	27906	1	6.243	369259	50.0