

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045210.D
 Acq On : 07 Oct 2021 14:30
 Operator : SY/MD
 Sample : M4025-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN4

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045210.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	54	rBV	39009	74017	5.79%	0.753%
2	1.601	74	81	94	rVB	184629	198797	15.55%	2.022%
3	1.893	164	172	185	rVB	134333	179463	14.04%	1.825%
4	2.562	367	380	400	rVV	259728	438725	34.32%	4.462%
5	2.777	435	447	460	rBV2	3854	7500	0.59%	0.076%
6	2.883	477	480	484	rBV2	233	270	0.02%	0.003%
7	3.054	523	533	536	rBV4	855	1293	0.10%	0.013%
8	3.134	553	558	560	rBV2	238	242	0.02%	0.002%
9	3.192	564	576	593	rVB2	4150	9583	0.75%	0.097%
10	3.404	637	642	647	rBV2	246	350	0.03%	0.004%
11	3.510	672	675	682	rVB	242	275	0.02%	0.003%
12	3.552	682	688	689	rBV2	198	219	0.02%	0.002%
13	3.745	746	748	753	rVB2	208	180	0.01%	0.002%
14	3.781	753	759	764	rBV2	238	367	0.03%	0.004%
15	3.935	805	807	812	rVB	208	180	0.01%	0.002%
16	3.970	812	818	820	rBV2	207	219	0.02%	0.002%
17	4.031	833	837	843	rVV2	220	250	0.02%	0.003%
18	4.137	866	870	875	rBV2	167	194	0.02%	0.002%
19	4.199	886	889	892	rBV	224	190	0.01%	0.002%
20	4.346	931	935	941	rBV	274	373	0.03%	0.004%
21	4.449	965	967	973	rBV2	164	179	0.01%	0.002%
22	4.507	978	985	986	rBV	242	232	0.02%	0.002%
23	4.629	1007	1023	1056	rBV	138640	356978	27.92%	3.631%
24	4.784	1069	1071	1077	rVB2	249	192	0.02%	0.002%
25	4.867	1094	1097	1099	rBV	270	194	0.02%	0.002%
26	4.925	1111	1115	1118	rVB2	220	222	0.02%	0.002%
27	4.957	1118	1125	1129	rBV2	194	334	0.03%	0.003%
28	5.067	1143	1159	1184	rBV	222332	488491	38.21%	4.968%
29	5.153	1184	1186	1189	rVB	321	196	0.02%	0.002%
30	5.215	1200	1205	1208	rBV2	252	199	0.02%	0.002%
31	5.250	1211	1216	1219	rVB	239	247	0.02%	0.003%
32	5.298	1219	1231	1236	rBV4	697	1545	0.12%	0.016%
33	5.382	1251	1257	1262	rVV	320	373	0.03%	0.004%
34	5.427	1267	1271	1277	rBV	245	239	0.02%	0.002%
35	5.729	1342	1365	1396	rBV2	473530	1278403	100.00%	13.002%
36	5.996	1445	1448	1453	rBV	227	192	0.02%	0.002%

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 Title : VOC Analysis

37	6.054	1462	1466	1468	rBV2	264	226	0.02%	0.002%
38	6.112	1480	1484	1485	rVV	343	233	0.02%	0.002%
39	6.121	1485	1487	1490	rVV2	427	292	0.02%	0.003%
40	6.253	1513	1528	1551	rBV	382293	716475	56.04%	7.287%
41	6.546	1605	1619	1631	rVB3	33283	62976	4.93%	0.640%
42	6.697	1649	1666	1686	rBV	299015	583763	45.66%	5.937%
43	6.800	1694	1698	1699	rBV2	513	338	0.03%	0.003%
44	6.883	1718	1724	1731	rBV2	142	254	0.02%	0.003%
45	7.186	1806	1818	1825	rBV4	1040	1798	0.14%	0.018%
46	7.314	1853	1858	1861	rBV2	173	188	0.01%	0.002%
47	7.359	1869	1872	1879	rVB2	192	184	0.01%	0.002%
48	7.568	1924	1937	1953	rBV	152790	262289	20.52%	2.668%
49	7.687	1968	1974	1982	rVB4	868	1135	0.09%	0.012%
50	7.903	2026	2041	2056	rVV	596383	1009326	78.95%	10.265%
51	7.973	2057	2063	2078	rVB	8585	13993	1.09%	0.142%
52	8.086	2095	2098	2104	rVB3	385	399	0.03%	0.004%
53	8.182	2116	2128	2145	rVV	109459	177869	13.91%	1.809%
54	8.468	2212	2217	2218	rBV2	464	306	0.02%	0.003%
55	8.565	2244	2247	2251	rBV2	191	227	0.02%	0.002%
56	8.636	2257	2269	2299	rBV	403368	718608	56.21%	7.309%
57	8.793	2314	2318	2324	rVB4	628	742	0.06%	0.008%
58	8.841	2330	2333	2339	rVB2	255	207	0.02%	0.002%
59	9.063	2399	2402	2406	rBV	255	221	0.02%	0.002%
60	9.118	2417	2419	2424	rBV2	213	183	0.01%	0.002%
61	9.420	2499	2513	2548	rVV	546491	897766	70.23%	9.131%
62	9.687	2593	2596	2597	rBV	439	226	0.02%	0.002%
63	9.790	2623	2628	2633	rBV2	260	279	0.02%	0.003%
64	9.893	2654	2660	2663	rBV2	247	316	0.02%	0.003%
65	9.960	2676	2681	2687	rBV2	204	277	0.02%	0.003%
66	10.063	2709	2713	2719	rBV2	264	298	0.02%	0.003%
67	10.105	2723	2726	2732	rVB2	432	437	0.03%	0.004%
68	10.156	2738	2742	2746	rBV	236	255	0.02%	0.003%
69	10.414	2817	2822	2826	rBV2	148	176	0.01%	0.002%
70	10.468	2833	2839	2842	rBV	169	215	0.02%	0.002%
71	10.674	2894	2903	2916	rBV6	1769	3483	0.27%	0.035%
72	10.761	2916	2930	2951	rVB	416285	676456	52.91%	6.880%
73	10.922	2977	2980	2986	rVB2	434	410	0.03%	0.004%
74	11.005	3002	3006	3011	rVB2	215	201	0.02%	0.002%
75	11.095	3030	3034	3037	rVV3	269	181	0.01%	0.002%
76	11.131	3039	3045	3049	rVV2	215	262	0.02%	0.003%

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Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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 Title : VOC Analysis

77	11.234	3072	3077	3082	rBV2	230	289	0.02%	0.003%
78	11.468	3141	3150	3158	rVV5	1092	1777	0.14%	0.018%
79	11.555	3172	3177	3180	rBV2	194	219	0.02%	0.002%
80	11.629	3196	3200	3209	rVB3	629	760	0.06%	0.008%
81	11.700	3216	3222	3226	rBV3	415	426	0.03%	0.004%
82	11.816	3245	3258	3278	rBV	508210	797832	62.41%	8.114%
83	11.912	3286	3288	3293	rVB	361	310	0.02%	0.003%
84	11.976	3306	3308	3314	rVB	742	412	0.03%	0.004%
85	12.195	3364	3376	3394	rBV	533024	851536	66.61%	8.660%
86	12.449	3452	3455	3460	rVV2	233	235	0.02%	0.002%
87	12.880	3586	3589	3592	rBV	248	186	0.01%	0.002%
88	12.899	3592	3595	3602	rVB3	710	651	0.05%	0.007%
89	12.999	3622	3626	3629	rBV2	293	257	0.02%	0.003%
90	13.111	3659	3661	3664	rBV2	216	179	0.01%	0.002%
91	13.208	3686	3691	3695	rBV2	225	259	0.02%	0.003%
92	13.234	3695	3699	3703	rBV	266	245	0.02%	0.002%
93	13.262	3705	3708	3712	rBV	207	220	0.02%	0.002%
94	13.488	3775	3778	3781	rBV2	271	261	0.02%	0.003%
95	13.668	3828	3834	3837	rBV2	299	324	0.03%	0.003%
96	14.404	4057	4063	4068	rBV2	307	380	0.03%	0.004%
97	14.471	4077	4084	4087	rBV2	288	437	0.03%	0.004%
98	14.790	4179	4183	4187	rVB3	392	290	0.02%	0.003%
99	14.819	4187	4192	4195	rBV2	347	364	0.03%	0.004%
100	14.860	4202	4205	4209	rBV2	273	246	0.02%	0.003%

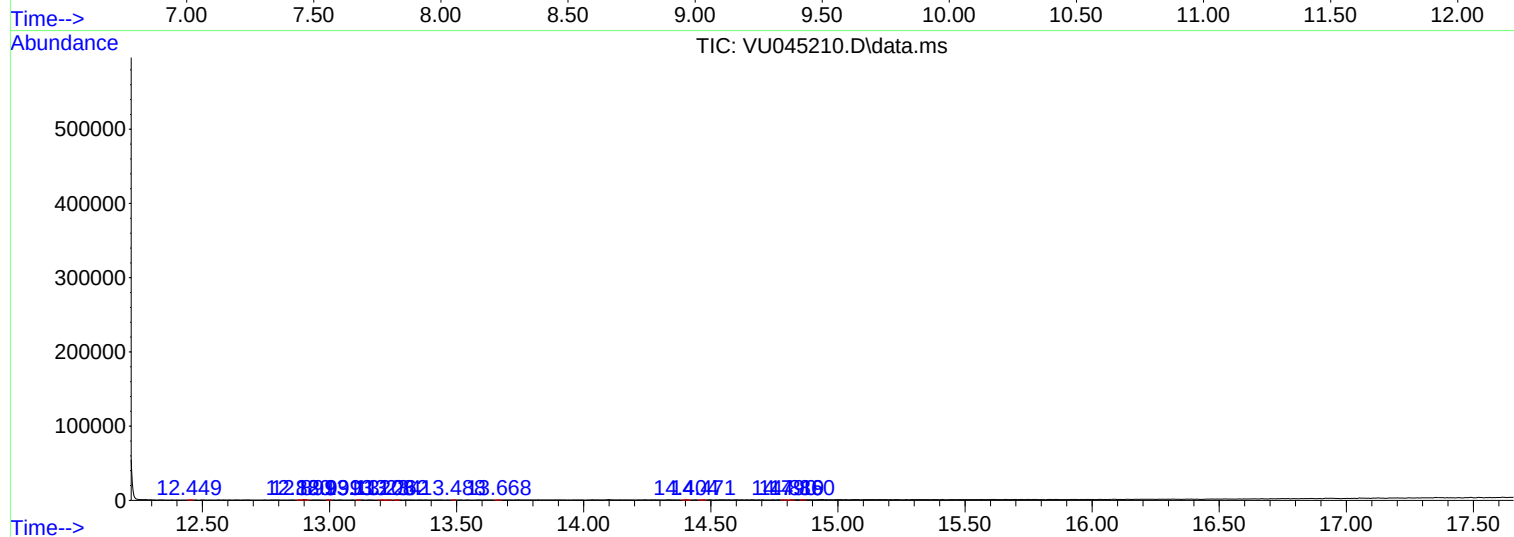
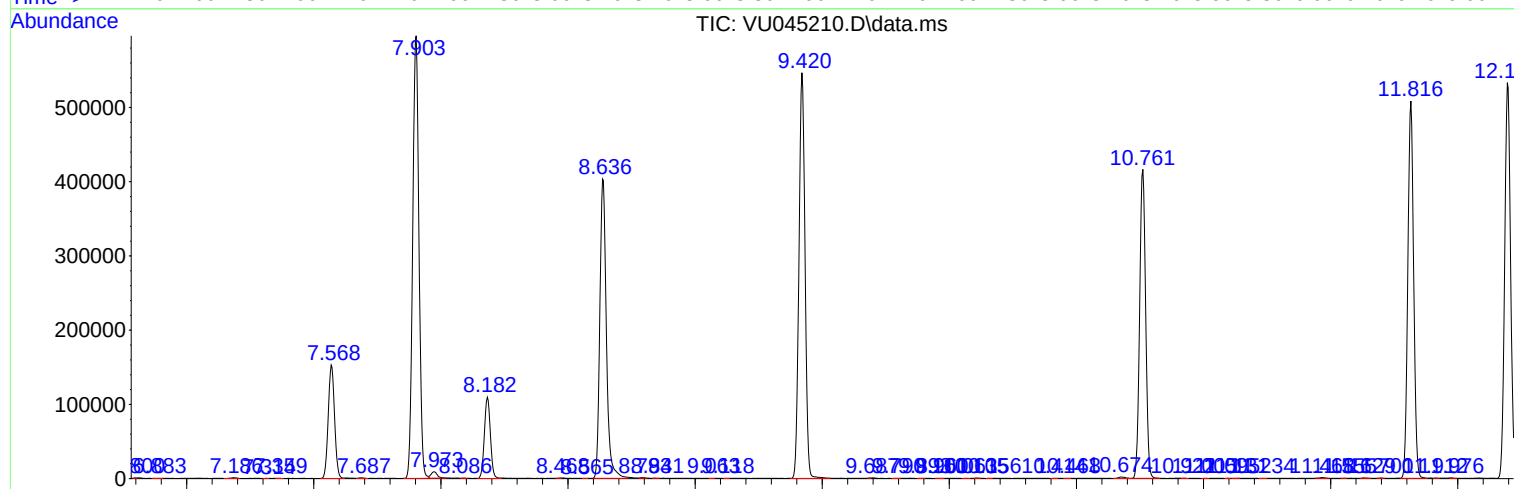
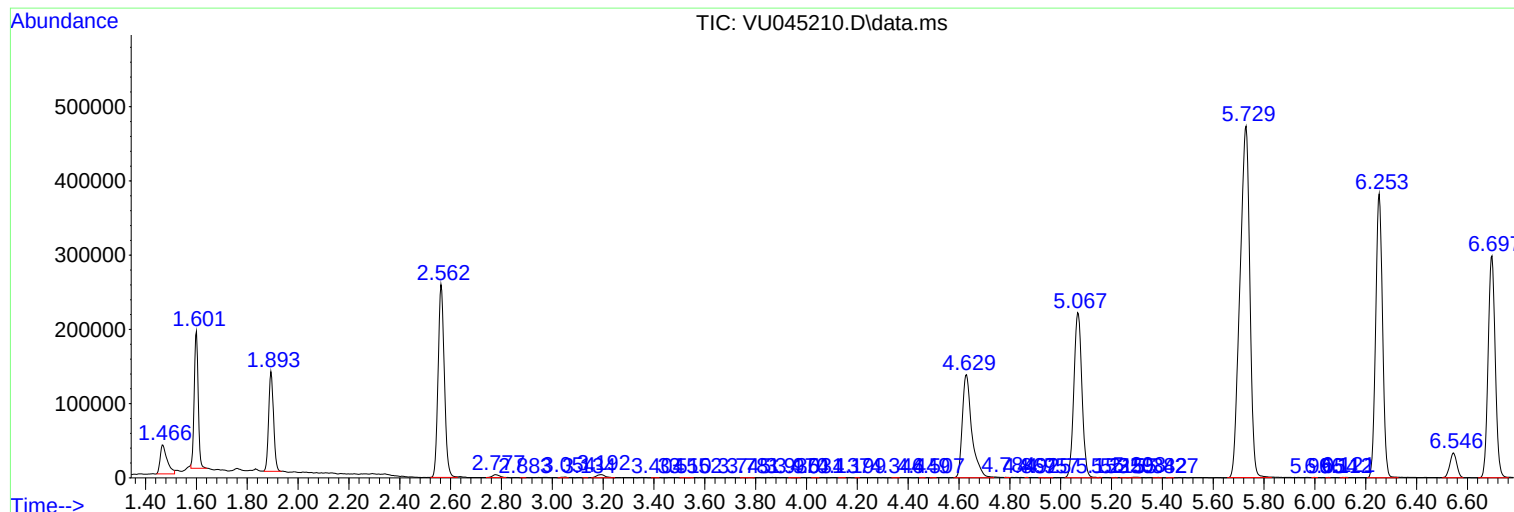
Sum of corrected areas: 9832468

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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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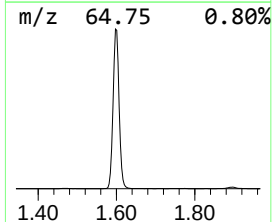
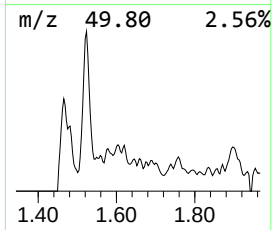
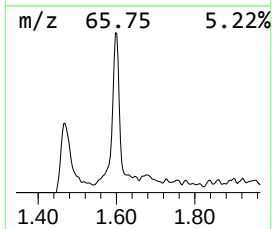
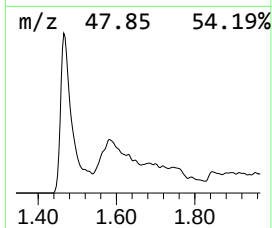
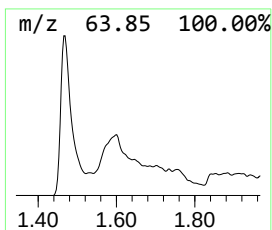
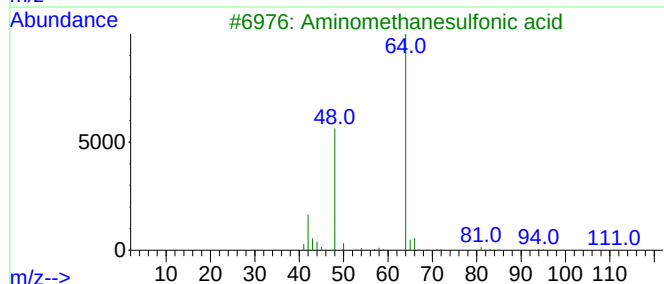
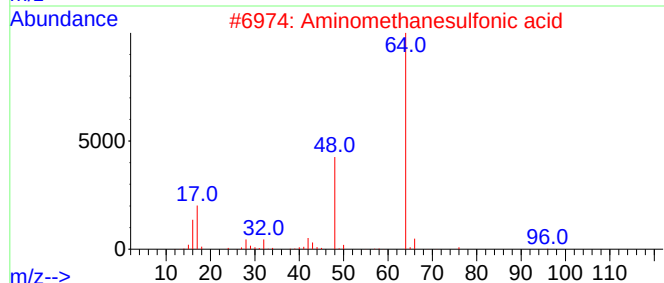
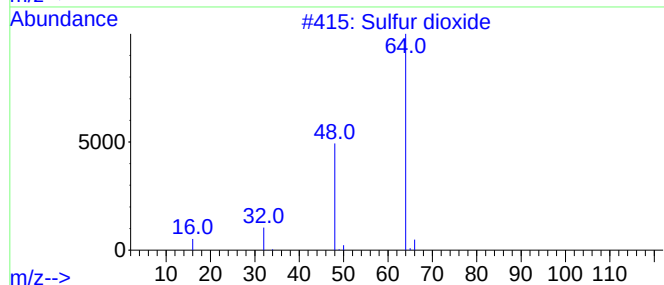
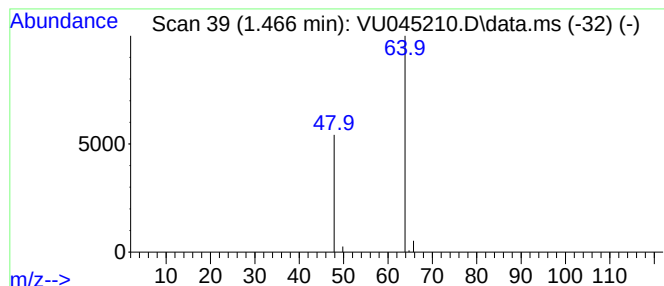
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	5.17 ug/L	74017	1,4-Difluorobenzene	6.253

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	5.2	ug/L	74017	1	6.253	716475	50.0