

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045193.D
 Acq On : 06 Oct 2021 18:12
 Operator : SY/MD
 Sample : M3974-10ME
 Misc : 5.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW8Z4ME

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: VU0451193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.456	29	36	52	rBV	94066	147841	10.42%	1.313%
2	1.598	72	80	97	rVB	162759	204968	14.45%	1.820%
3	1.848	152	158	162	rBV	90615	104796	7.39%	0.930%
4	2.524	355	368	385	rBV	270510	464026	32.71%	4.120%
5	2.739	430	435	437	rBV2	360	343	0.02%	0.003%
6	2.877	476	478	484	rBV2	161	176	0.01%	0.002%
7	2.967	496	506	516	rBV	2083	4174	0.29%	0.037%
8	3.032	516	526	539	rVB	4298	8762	0.62%	0.078%
9	3.180	563	572	591	rVB3	1719	3870	0.27%	0.034%
10	3.311	609	613	621	rVB2	180	197	0.01%	0.002%
11	3.350	621	625	629	rBV2	111	104	0.01%	0.001%
12	3.617	704	708	711	rBV2	117	115	0.01%	0.001%
13	3.662	719	722	725	rBV3	297	245	0.02%	0.002%
14	3.678	725	727	732	rVB2	270	147	0.01%	0.001%
15	3.713	732	738	743	rBV	241	361	0.03%	0.003%
16	3.765	749	754	756	rBV	148	176	0.01%	0.002%
17	4.022	828	834	841	rBV2	156	254	0.02%	0.002%
18	4.064	841	847	851	rVB2	135	137	0.01%	0.001%
19	4.253	903	906	909	rBV2	205	179	0.01%	0.002%
20	4.520	985	989	994	rBV	267	322	0.02%	0.003%
21	4.646	1007	1028	1071	rBV	117512	372380	26.25%	3.306%
22	4.874	1096	1099	1100	rBV	232	144	0.01%	0.001%
23	4.913	1107	1111	1115	rBV2	200	200	0.01%	0.002%
24	5.064	1141	1158	1189	rBV	232047	540803	38.12%	4.802%
25	5.202	1197	1201	1205	rVB2	416	435	0.03%	0.004%
26	5.298	1221	1231	1237	rVB4	671	1197	0.08%	0.011%
27	5.421	1264	1269	1271	rBV	188	211	0.01%	0.002%
28	5.501	1288	1294	1301	rVB	251	336	0.02%	0.003%
29	5.533	1301	1304	1308	rBV	195	195	0.01%	0.002%
30	5.565	1311	1314	1317	rVB2	213	161	0.01%	0.001%
31	5.588	1317	1321	1323	rBV2	209	198	0.01%	0.002%
32	5.646	1336	1339	1341	rBV2	173	148	0.01%	0.001%
33	5.720	1341	1362	1382	rBV2	565364	1418543	100.00%	12.595%
34	5.871	1406	1409	1410	rBV2	172	100	0.01%	0.001%
35	5.983	1433	1444	1460	rBV3	8400	20266	1.43%	0.180%
36	6.073	1468	1472	1476	rBV2	116	113	0.01%	0.001%

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 Title : VOC Analysis

37	6.122	1477	1487	1490	rVV2	409	502	0.04%	0.004%
38	6.250	1510	1527	1550	rBV	420853	831201	58.60%	7.380%
39	6.456	1588	1591	1594	rBV	247	229	0.02%	0.002%
40	6.533	1606	1615	1625	rVB8	6234	12567	0.89%	0.112%
41	6.604	1625	1637	1650	rBV2	4117	8820	0.62%	0.078%
42	6.694	1650	1665	1688	rVB	316954	643295	45.35%	5.712%
43	6.803	1695	1699	1700	rBV3	729	461	0.03%	0.004%
44	6.887	1721	1725	1729	rVB2	301	300	0.02%	0.003%
45	6.922	1729	1736	1738	rBV	393	477	0.03%	0.004%
46	6.983	1752	1755	1761	rBV2	154	155	0.01%	0.001%
47	7.044	1768	1774	1775	rBV2	259	217	0.02%	0.002%
48	7.125	1796	1799	1801	rBV	155	126	0.01%	0.001%
49	7.192	1811	1820	1825	rBV4	1616	2862	0.20%	0.025%
50	7.305	1852	1855	1859	rBV2	267	266	0.02%	0.002%
51	7.369	1872	1875	1881	rVB2	152	123	0.01%	0.001%
52	7.462	1901	1904	1907	rBV	143	141	0.01%	0.001%
53	7.568	1923	1937	1957	rBV	176427	328733	23.17%	2.919%
54	7.694	1970	1976	1980	rBV3	671	667	0.05%	0.006%
55	7.793	2005	2007	2011	rBV	183	133	0.01%	0.001%
56	7.900	2025	2040	2056	rBV	642290	1150489	81.10%	10.215%
57	7.974	2056	2063	2080	rVB3	8972	18151	1.28%	0.161%
58	8.060	2088	2090	2093	rVB2	173	94	0.01%	0.001%
59	8.186	2116	2129	2148	rBV	117287	221830	15.64%	1.970%
60	8.269	2153	2155	2159	rBV2	206	119	0.01%	0.001%
61	8.289	2159	2161	2165	rBV2	260	188	0.01%	0.002%
62	8.363	2182	2184	2188	rBV2	375	163	0.01%	0.001%
63	8.449	2208	2211	2214	rVB2	184	124	0.01%	0.001%
64	8.555	2240	2244	2247	rBV	552	392	0.03%	0.003%
65	8.652	2259	2274	2299	rBV	436613	815358	57.48%	7.240%
66	8.887	2343	2347	2349	rBV2	271	187	0.01%	0.002%
67	8.925	2357	2359	2361	rBV2	289	142	0.01%	0.001%
68	9.057	2398	2400	2403	rBV2	134	95	0.01%	0.001%
69	9.366	2492	2496	2498	rBV2	195	135	0.01%	0.001%
70	9.424	2500	2514	2534	rVV	593687	1037901	73.17%	9.216%
71	9.572	2554	2560	2564	rBV2	265	339	0.02%	0.003%
72	9.607	2569	2571	2575	rVB2	198	121	0.01%	0.001%
73	9.700	2591	2600	2608	rBV2	1380	2062	0.15%	0.018%
74	9.948	2674	2677	2681	rBV	222	210	0.01%	0.002%
75	9.967	2681	2683	2688	rVB	234	203	0.01%	0.002%
76	9.993	2688	2691	2694	rBV2	270	215	0.02%	0.002%

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 Title : VOC Analysis

77	10.131	2732	2734	2739	rBV2	210	175	0.01%	0.002%
78	10.170	2743	2746	2748	rBV2	253	128	0.01%	0.001%
79	10.215	2756	2760	2762	rBV2	329	237	0.02%	0.002%
80	10.231	2764	2765	2768	rBV	383	230	0.02%	0.002%
81	10.350	2793	2802	2809	rBV5	634	1162	0.08%	0.010%
82	10.391	2813	2815	2818	rVB2	338	187	0.01%	0.002%
83	10.433	2826	2828	2831	rVB2	323	202	0.01%	0.002%
84	10.459	2831	2836	2840	rBV3	463	479	0.03%	0.004%
85	10.526	2854	2857	2859	rBV3	836	634	0.04%	0.006%
86	10.597	2876	2879	2880	rBV	271	125	0.01%	0.001%
87	10.623	2884	2887	2888	rBV	282	156	0.01%	0.001%
88	10.674	2894	2903	2913	rVB2	7479	11258	0.79%	0.100%
89	10.713	2913	2915	2917	rBV	208	109	0.01%	0.001%
90	10.764	2917	2931	2948	rBV	475974	767958	54.14%	6.819%
91	10.925	2978	2981	2990	rVB3	1569	1792	0.13%	0.016%
92	10.999	2995	3004	3005	rBV4	973	1145	0.08%	0.010%
93	11.121	3031	3042	3049	rBV9	2929	6434	0.45%	0.057%
94	11.459	3140	3147	3159	rVB4	6272	10461	0.74%	0.093%
95	11.700	3217	3222	3231	rVB6	4750	6820	0.48%	0.061%
96	11.816	3245	3258	3273	rBV	646409	1017770	71.75%	9.037%
97	11.909	3285	3287	3289	rBV3	780	404	0.03%	0.004%
98	12.198	3363	3377	3391	rVB	640667	1017443	71.72%	9.034%
99	12.330	3412	3418	3425	rBV6	3241	4431	0.31%	0.039%
100	15.980	4548	4553	4567	rVB	25698	36357	2.56%	0.323%

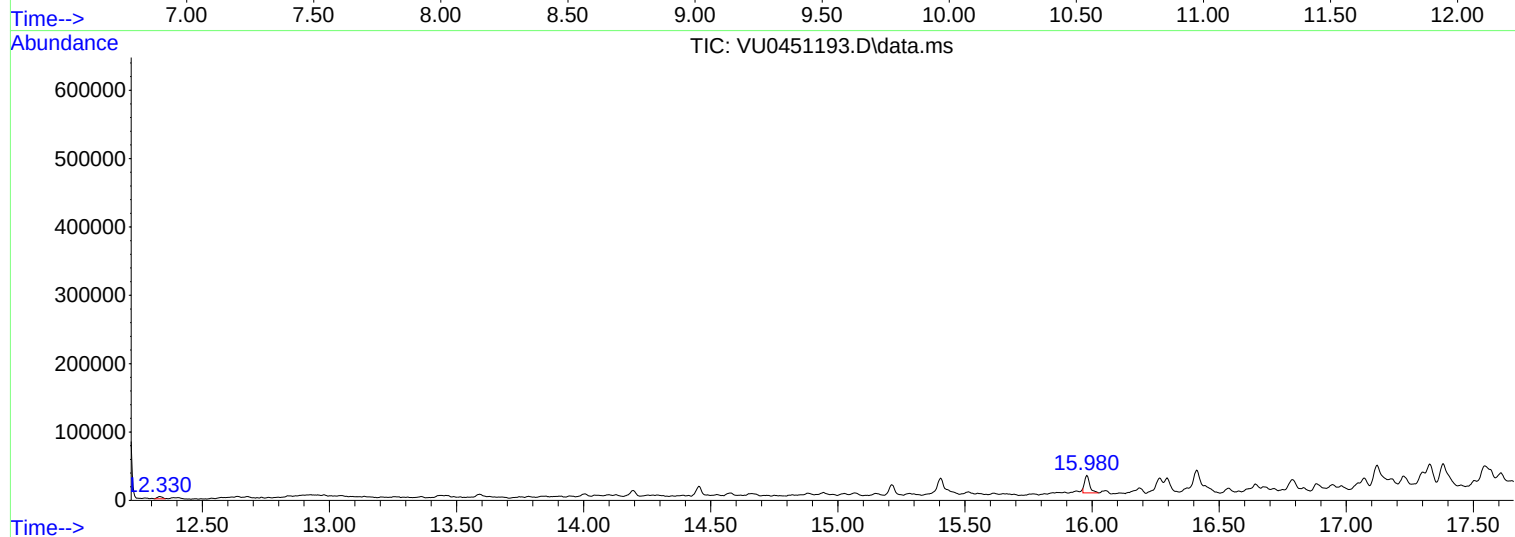
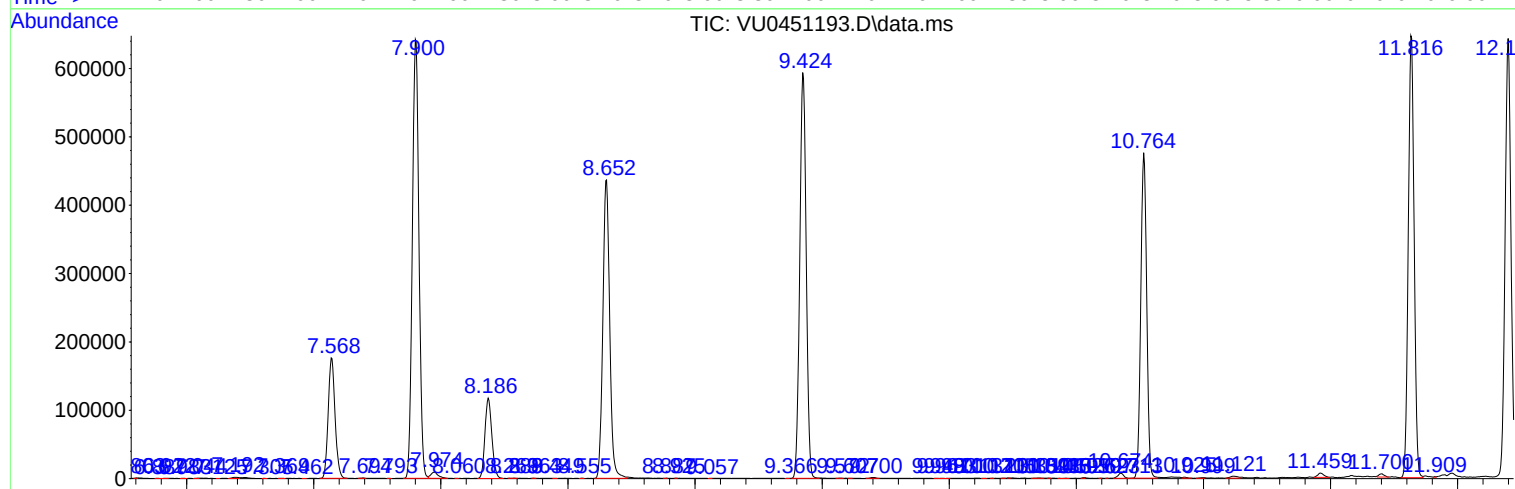
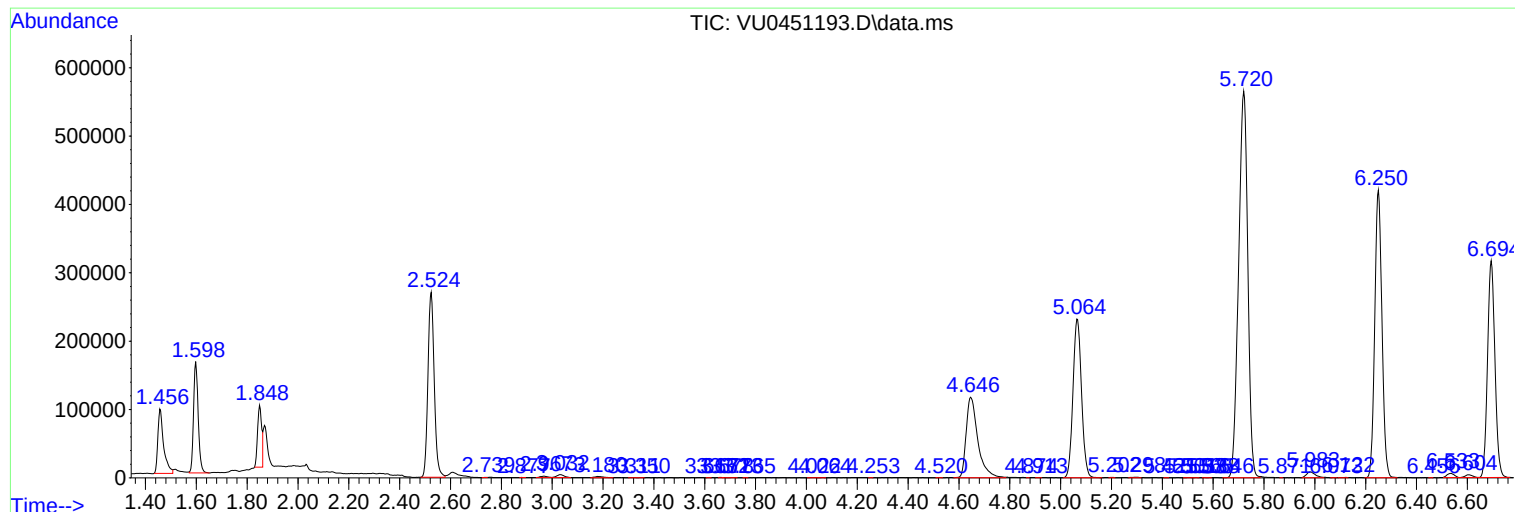
Sum of corrected areas: 11262513

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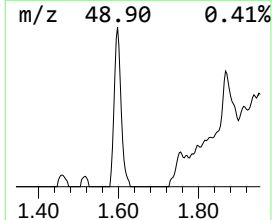
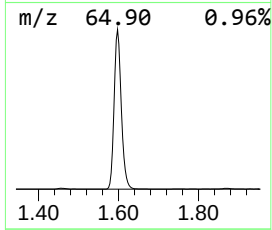
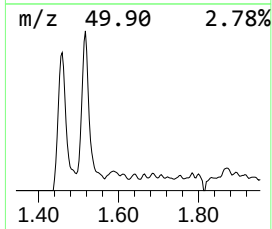
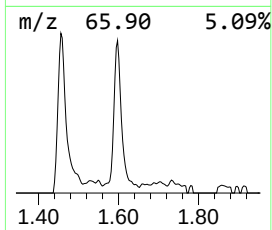
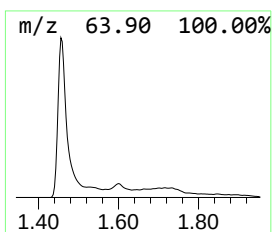
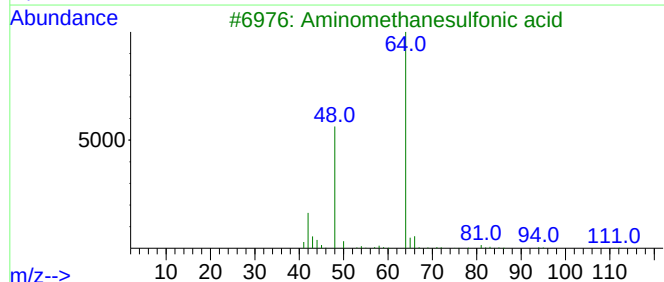
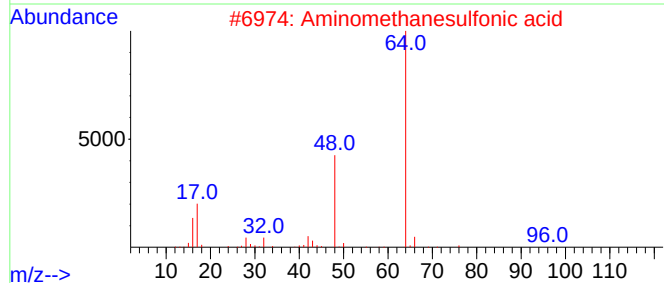
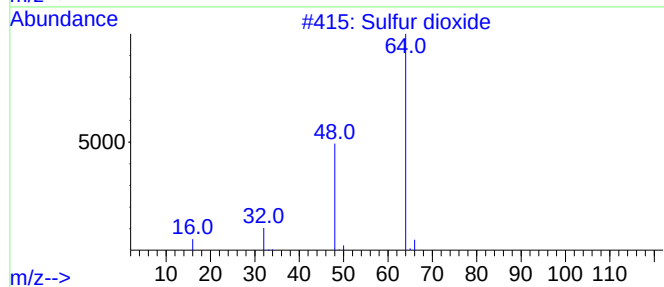
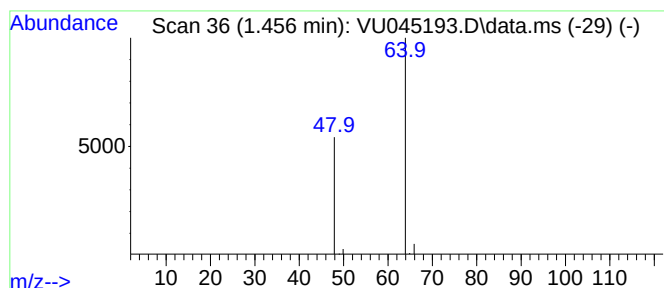
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.456	8.89 ug/L	147841	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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	1.456	8.9	ug/L	147841	1	6.250	831201	50.0