

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045254.D
 Acq On : 08 Oct 2021 16:17
 Operator : SY/MD
 Sample : M4070-06DL 50X
 Misc : 5.41g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7D7DL

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: VU045254.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	61	rBV	47806	92825	7.01%	0.795%
2	1.601	74	81	105	rVB	143425	163618	12.36%	1.401%
3	1.890	163	171	186	rVB	115844	156881	11.85%	1.343%
4	2.562	367	380	401	rVV	212087	361749	27.32%	3.097%
5	2.636	401	403	409	rVV4	1023	968	0.07%	0.008%
6	2.662	409	411	415	rVB3	301	186	0.01%	0.002%
7	2.787	446	450	454	rBV3	465	492	0.04%	0.004%
8	2.951	495	501	502	rBV2	434	395	0.03%	0.003%
9	3.048	520	531	545	rVB3	6410	12162	0.92%	0.104%
10	3.125	551	555	561	rBV2	216	195	0.01%	0.002%
11	3.186	572	574	577	rBV	236	125	0.01%	0.001%
12	3.282	600	604	606	rBV	172	140	0.01%	0.001%
13	3.375	629	633	636	rVB2	237	160	0.01%	0.001%
14	3.427	642	649	659	rBV2	303	614	0.05%	0.005%
15	3.684	720	729	732	rBV2	185	335	0.03%	0.003%
16	4.067	846	848	855	rVB2	206	208	0.02%	0.002%
17	4.138	864	870	872	rBV2	141	149	0.01%	0.001%
18	4.256	903	907	915	rBV2	487	658	0.05%	0.006%
19	4.629	1007	1023	1058	rBV	144675	340641	25.72%	2.917%
20	5.067	1141	1159	1184	rBV	214983	469054	35.42%	4.016%
21	5.292	1223	1229	1240	rVB3	650	1190	0.09%	0.010%
22	5.372	1247	1254	1256	rBV3	329	283	0.02%	0.002%
23	5.501	1291	1294	1297	rBV	194	161	0.01%	0.001%
24	5.649	1337	1340	1343	rBV	214	190	0.01%	0.002%
25	5.729	1343	1365	1385	rBV2	453734	1221209	92.22%	10.457%
26	6.080	1470	1474	1478	rBV	266	269	0.02%	0.002%
27	6.115	1478	1485	1488	rBV3	288	382	0.03%	0.003%
28	6.253	1513	1528	1547	rBV	359209	671257	50.69%	5.748%
29	6.533	1603	1615	1626	rBV7	4453	8545	0.65%	0.073%
30	6.607	1635	1638	1640	rBV	236	125	0.01%	0.001%
31	6.694	1651	1665	1684	rBV	294583	570692	43.10%	4.887%
32	6.858	1712	1716	1720	rVV	199	176	0.01%	0.002%
33	6.880	1720	1723	1729	rVB2	199	243	0.02%	0.002%
34	6.999	1755	1760	1763	rBV	152	186	0.01%	0.002%
35	7.044	1769	1774	1777	rBV3	596	642	0.05%	0.005%
36	7.128	1797	1800	1804	rBV	197	188	0.01%	0.002%

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 Title : VOC Analysis

37	7.179	1809	1816	1826	rBV5	2379	4405	0.33%	0.038%
38	7.317	1856	1859	1865	rVB2	146	136	0.01%	0.001%
39	7.382	1876	1879	1885	rBV2	166	183	0.01%	0.002%
40	7.472	1903	1907	1910	rBV	204	198	0.01%	0.002%
41	7.568	1924	1937	1955	rBV	157021	268253	20.26%	2.297%
42	7.687	1966	1974	1987	rVB3	1749	2710	0.20%	0.023%
43	7.903	2027	2041	2054	rBV	551778	938873	70.90%	8.039%
44	7.973	2054	2063	2077	rVB	50720	85609	6.47%	0.733%
45	8.182	2115	2128	2145	rBV	109702	180229	13.61%	1.543%
46	8.465	2214	2216	2221	rBV2	143	155	0.01%	0.001%
47	8.636	2253	2269	2302	rBV	416212	740969	55.96%	6.345%
48	8.880	2344	2345	2350	rVB	326	167	0.01%	0.001%
49	8.922	2350	2358	2362	rBV2	290	480	0.04%	0.004%
50	8.960	2366	2370	2373	rBV2	217	195	0.01%	0.002%
51	9.150	2425	2429	2433	rBV2	185	183	0.01%	0.002%
52	9.420	2499	2513	2532	rBV	531715	845895	63.88%	7.243%
53	9.575	2548	2561	2581	rBV	249650	399181	30.15%	3.418%
54	9.697	2585	2599	2631	rVB	815040	1324191	100.00%	11.338%
55	9.848	2641	2646	2649	rBV3	257	224	0.02%	0.002%
56	10.105	2713	2726	2745	rBV	263496	420798	31.78%	3.603%
57	10.488	2835	2845	2855	rVB	6798	9769	0.74%	0.084%
58	10.674	2896	2903	2910	rVB2	2520	3243	0.24%	0.028%
59	10.761	2917	2930	2948	rBV	426091	682083	51.51%	5.840%
60	10.867	2960	2963	2964	rBV	509	312	0.02%	0.003%
61	10.912	2968	2977	2984	rVB2	1915	2886	0.22%	0.025%
62	11.002	2995	3005	3022	rBV	8357	15284	1.15%	0.131%
63	11.092	3022	3033	3038	rBV2	4068	5781	0.44%	0.049%
64	11.237	3076	3078	3081	rVB2	253	124	0.01%	0.001%
65	11.256	3081	3084	3087	rBV	167	134	0.01%	0.001%
66	11.295	3087	3096	3104	rBV2	3249	4349	0.33%	0.037%
67	11.420	3131	3135	3140	rBB4	584	394	0.03%	0.003%
68	11.472	3140	3151	3163	rBB	13628	20875	1.58%	0.179%
69	11.536	3168	3171	3173	rBV2	192	134	0.01%	0.001%
70	11.578	3180	3184	3188	rVB2	311	301	0.02%	0.003%
71	11.632	3198	3201	3203	rBV	165	122	0.01%	0.001%
72	11.700	3213	3222	3227	rVV3	1156	1428	0.11%	0.012%
73	11.816	3245	3258	3275	rBV	489437	768746	58.05%	6.582%
74	11.899	3277	3284	3293	rVB2	5278	7573	0.57%	0.065%
75	11.980	3303	3309	3319	rVB2	2111	2583	0.20%	0.022%
76	12.095	3340	3345	3353	rVB2	1505	1733	0.13%	0.015%

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 Title : VOC Analysis

77	12.140	3356	3359	3360	rBV	216	140	0.01%	0.001%
78	12.198	3360	3377	3396	rBV	521266	846477	63.92%	7.248%
79	12.333	3412	3419	3429	rBV6	1747	2729	0.21%	0.023%
80	12.410	3440	3443	3445	rBV	329	207	0.02%	0.002%
81	12.507	3471	3473	3476	rBV2	191	138	0.01%	0.001%
82	12.581	3491	3496	3499	rBV2	242	273	0.02%	0.002%
83	12.681	3523	3527	3530	rBV	230	228	0.02%	0.002%
84	12.857	3578	3582	3584	rBV	234	192	0.01%	0.002%
85	13.263	3703	3708	3711	rBV2	301	314	0.02%	0.003%
86	13.333	3726	3730	3737	rBB2	208	240	0.02%	0.002%
87	13.436	3755	3762	3766	rBV4	1047	1364	0.10%	0.012%
88	13.552	3795	3798	3800	rBV2	222	159	0.01%	0.001%
89	13.587	3805	3809	3810	rBV	263	196	0.01%	0.002%
90	13.883	3896	3901	3904	rBV2	237	285	0.02%	0.002%
91	13.951	3918	3922	3926	rBV2	197	231	0.02%	0.002%
92	14.092	3959	3966	3978	rBV3	1767	2647	0.20%	0.023%
93	14.443	4071	4075	4076	rBV	463	311	0.02%	0.003%
94	14.578	4112	4117	4121	rBV3	513	665	0.05%	0.006%
95	14.713	4156	4159	4167	rBV3	271	355	0.03%	0.003%
96	14.832	4192	4196	4200	rBV3	384	414	0.03%	0.004%
97	14.870	4205	4208	4210	rBV3	305	214	0.02%	0.002%
98	15.153	4293	4296	4299	rBV	277	247	0.02%	0.002%
99	15.234	4314	4321	4329	rVB5	996	1645	0.12%	0.014%
100	15.414	4371	4377	4384	rBV4	771	982	0.07%	0.008%

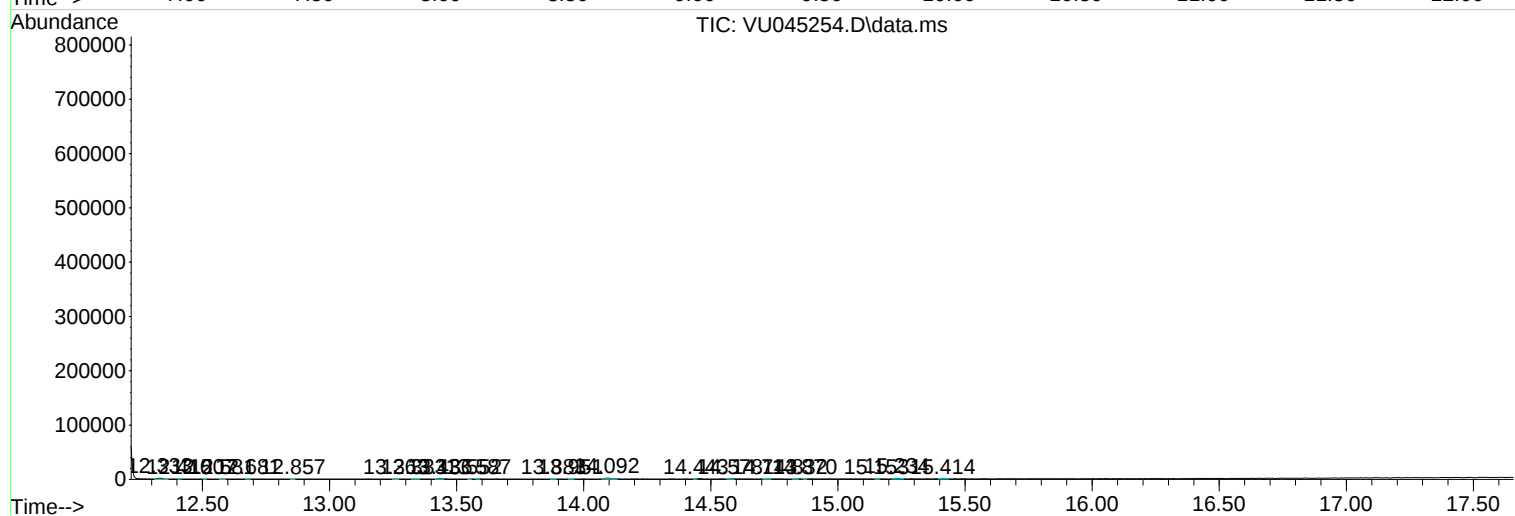
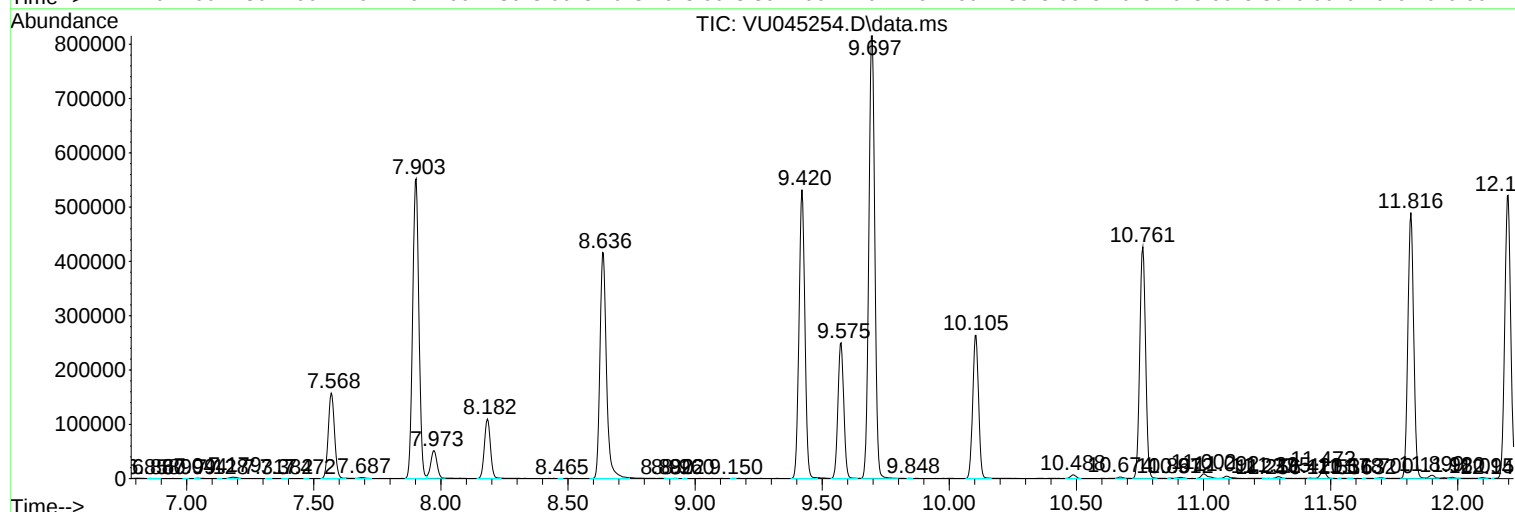
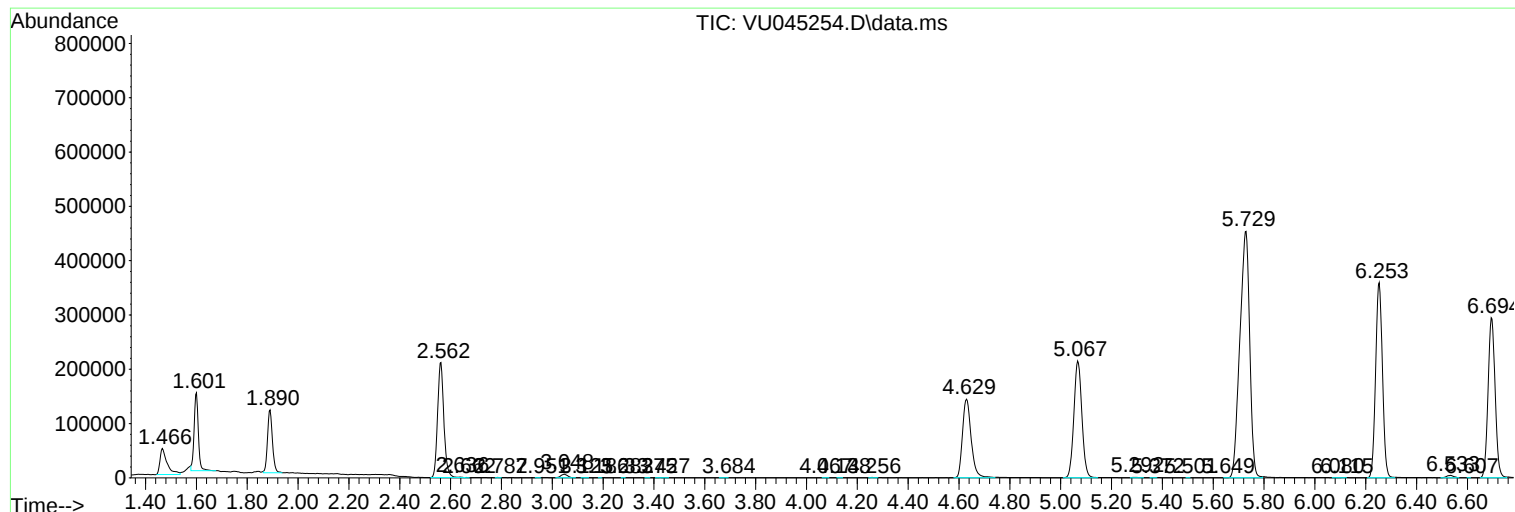
Sum of corrected areas: 11678834

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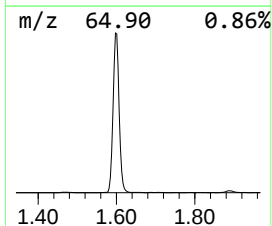
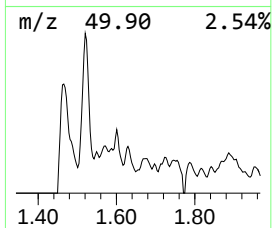
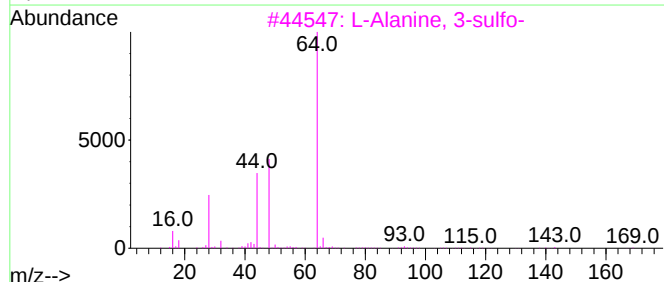
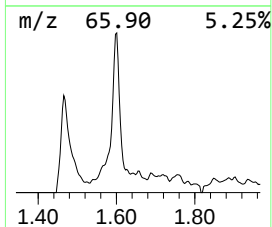
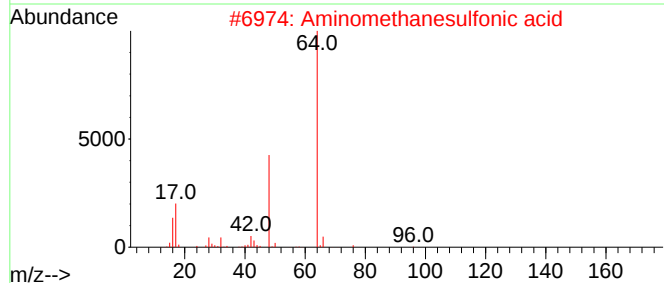
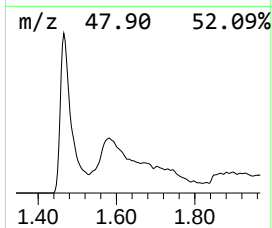
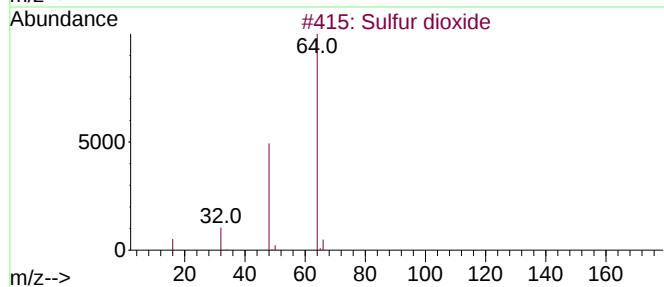
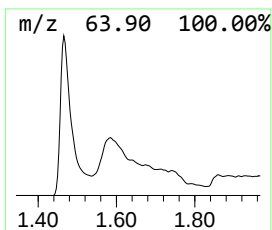
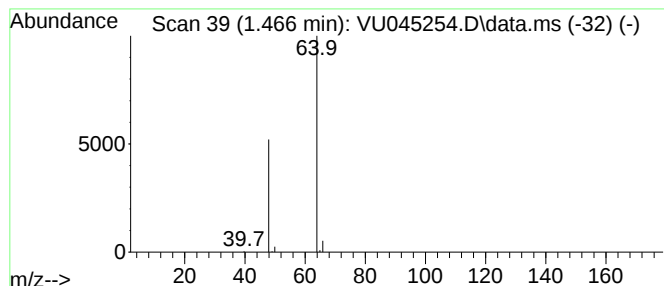
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.466	6.91 ug/L	92825	1,4-Difluorobenzene	6.253

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	6.9	ug/L	92825	1	6.253	671257	50.0