

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045290.D
 Acq On : 12 Oct 2021 14:35
 Operator : SY/MD
 Sample : M4103-05ME
 Misc : 4.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AB9ME

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: VU045290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	30	37	51	rBV	38456	62055	4.67%	0.616%
2	1.597	73	80	99	rVB	103534	136348	10.27%	1.354%
3	1.871	159	165	179	rBV	44275	58289	4.39%	0.579%
4	2.520	354	367	388	rBV	196583	352049	26.51%	3.496%
5	2.613	389	396	411	rVB2	5371	12363	0.93%	0.123%
6	2.742	432	436	437	rBV	417	330	0.02%	0.003%
7	2.967	498	506	507	rBV2	1682	1921	0.14%	0.019%
8	3.031	515	526	542	rVB3	5065	11518	0.87%	0.114%
9	3.186	565	574	581	rVB4	532	965	0.07%	0.010%
10	3.288	600	606	609	rVB2	244	272	0.02%	0.003%
11	3.494	662	670	673	rBV2	244	359	0.03%	0.004%
12	3.600	700	703	709	rBV2	190	268	0.02%	0.003%
13	4.224	889	897	900	rBV2	227	329	0.02%	0.003%
14	4.649	1012	1029	1078	rBV2	115619	383017	28.84%	3.804%
15	5.067	1140	1159	1186	rBV	216297	514379	38.73%	5.108%
16	5.288	1218	1228	1230	rBV2	446	654	0.05%	0.006%
17	5.356	1246	1249	1251	rBV2	714	500	0.04%	0.005%
18	5.446	1276	1277	1288	rVB2	447	289	0.02%	0.003%
19	5.719	1341	1362	1386	rBV2	525487	1327973	100.00%	13.188%
20	5.986	1434	1445	1462	rBV4	4672	11789	0.89%	0.117%
21	6.121	1485	1487	1492	rVB3	334	272	0.02%	0.003%
22	6.250	1512	1527	1553	rBV	351904	710149	53.48%	7.052%
23	6.526	1604	1613	1623	rVB5	3951	7094	0.53%	0.070%
24	6.693	1650	1665	1681	rBV	298664	620992	46.76%	6.167%
25	6.809	1697	1701	1709	rBV2	620	870	0.07%	0.009%
26	7.192	1810	1820	1830	rBV5	3986	8840	0.67%	0.088%
27	7.501	1907	1916	1923	rVB4	526	764	0.06%	0.008%
28	7.571	1923	1938	1956	rBV	152698	293296	22.09%	2.913%
29	7.693	1968	1976	1985	rBV4	1822	3498	0.26%	0.035%
30	7.902	2018	2041	2056	rVV	557394	1022573	77.00%	10.155%
31	7.973	2056	2063	2089	rVB4	8900	24396	1.84%	0.242%
32	8.189	2116	2130	2144	rBV2	99368	196071	14.76%	1.947%
33	8.362	2176	2184	2191	rBV6	1280	2163	0.16%	0.021%
34	8.475	2214	2219	2225	rBV2	457	712	0.05%	0.007%
35	8.652	2259	2274	2304	rBV	418582	813917	61.29%	8.083%
36	8.864	2333	2340	2349	rVB3	1485	2397	0.18%	0.024%

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

37	8.928	2349	2360	2371	rBV4	4969	8619	0.65%	0.086%
38	9.121	2412	2420	2427	rBV3	914	1351	0.10%	0.013%
39	9.214	2447	2449	2453	rVB	439	288	0.02%	0.003%
40	9.333	2484	2486	2493	rVB2	375	313	0.02%	0.003%
41	9.423	2500	2514	2535	rBV	482442	877056	66.04%	8.710%
42	9.578	2554	2562	2566	rBV3	670	872	0.07%	0.009%
43	9.703	2590	2601	2609	rBV4	3073	4911	0.37%	0.049%
44	9.967	2677	2683	2687	rBV2	297	368	0.03%	0.004%
45	10.015	2694	2698	2704	rBV3	611	712	0.05%	0.007%
46	10.044	2704	2707	2712	rVB3	431	353	0.03%	0.004%
47	10.066	2712	2714	2719	rBV3	401	357	0.03%	0.004%
48	10.111	2719	2728	2734	rVB4	1762	2593	0.20%	0.026%
49	10.160	2740	2743	2748	rVB	264	269	0.02%	0.003%
50	10.253	2763	2772	2777	rBV5	1106	1659	0.12%	0.016%
51	10.356	2799	2804	2810	rBV3	1010	1267	0.10%	0.013%
52	10.397	2810	2817	2826	rVV4	1512	1943	0.15%	0.019%
53	10.491	2839	2846	2852	rBV2	503	793	0.06%	0.008%
54	10.533	2855	2859	2863	rVV2	663	634	0.05%	0.006%
55	10.561	2863	2868	2876	rVB2	739	1182	0.09%	0.012%
56	10.626	2884	2888	2891	rBV3	661	567	0.04%	0.006%
57	10.674	2895	2903	2911	rVV4	3430	5735	0.43%	0.057%
58	10.764	2918	2931	2953	rBV	468097	756151	56.94%	7.509%
59	10.867	2958	2963	2968	rBV2	464	595	0.04%	0.006%
60	11.005	3000	3006	3009	rBV2	787	691	0.05%	0.007%
61	11.118	3028	3041	3052	rBV4	3743	7632	0.57%	0.076%
62	11.205	3065	3068	3074	rVB3	412	378	0.03%	0.004%
63	11.311	3090	3101	3106	rBV5	711	1309	0.10%	0.013%
64	11.420	3128	3135	3141	rBV4	3013	3977	0.30%	0.039%
65	11.465	3141	3149	3163	rVB5	4160	7639	0.58%	0.076%
66	11.581	3179	3185	3192	rVB5	1028	1246	0.09%	0.012%
67	11.645	3202	3205	3209	rVB4	758	634	0.05%	0.006%
68	11.700	3209	3222	3235	rBV7	2541	4957	0.37%	0.049%
69	11.748	3235	3237	3242	rVB3	891	617	0.05%	0.006%
70	11.819	3247	3259	3272	rBV	519782	813917	61.29%	8.083%
71	11.944	3295	3298	3303	rBV5	777	948	0.07%	0.009%
72	11.976	3304	3308	3315	rVB3	2325	2573	0.19%	0.026%
73	12.198	3361	3377	3395	rBV	573082	919492	69.24%	9.131%
74	12.330	3411	3418	3429	rVB2	5824	8380	0.63%	0.083%
75	12.401	3431	3440	3450	rVB8	1246	2573	0.19%	0.026%
76	12.475	3457	3463	3466	rBV3	782	732	0.06%	0.007%

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Title : VOC Analysis

77	12.532	3476	3481	3482	rBV2	983	853	0.06%	0.008%
78	12.584	3494	3497	3500	rBV2	351	302	0.02%	0.003%
79	12.639	3510	3514	3516	rBV3	708	489	0.04%	0.005%
80	12.841	3575	3577	3579	rVB	557	261	0.02%	0.003%
81	12.934	3602	3606	3610	rBV2	549	702	0.05%	0.007%
82	13.012	3627	3630	3633	rVB3	396	265	0.02%	0.003%
83	13.047	3633	3641	3646	rBV4	1001	1479	0.11%	0.015%
84	13.095	3653	3656	3663	rVB2	369	410	0.03%	0.004%
85	13.143	3663	3671	3673	rBV4	1004	1150	0.09%	0.011%
86	13.224	3694	3696	3701	rVB	445	294	0.02%	0.003%
87	13.433	3755	3761	3770	rBV3	3437	4920	0.37%	0.049%
88	13.590	3802	3810	3817	rBV4	2027	2935	0.22%	0.029%
89	13.854	3886	3892	3899	rVB4	538	785	0.06%	0.008%
90	14.002	3936	3938	3941	rVB	563	307	0.02%	0.003%
91	14.040	3949	3950	3958	rVB5	665	703	0.05%	0.007%
92	14.092	3958	3966	3974	rBV2	4712	6683	0.50%	0.066%
93	14.195	3990	3998	4008	rVB3	3036	4490	0.34%	0.045%
94	14.336	4037	4042	4048	rBV2	649	919	0.07%	0.009%
95	14.375	4048	4054	4057	rBV2	302	384	0.03%	0.004%
96	14.455	4071	4079	4087	rBV2	2763	3599	0.27%	0.036%
97	14.748	4166	4170	4172	rBV2	306	272	0.02%	0.003%
98	15.082	4270	4274	4280	rVB4	582	465	0.04%	0.005%
99	15.224	4310	4318	4328	rVB5	1313	2617	0.20%	0.026%
100	15.410	4368	4376	4387	rBV4	2698	4695	0.35%	0.047%

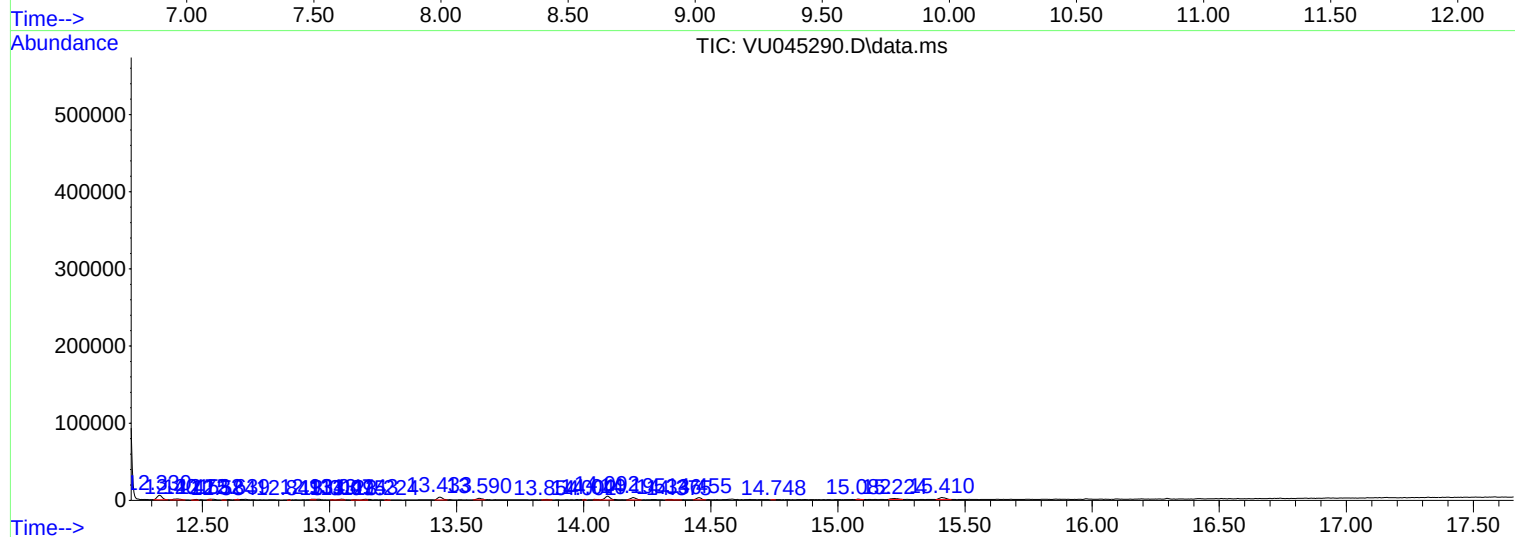
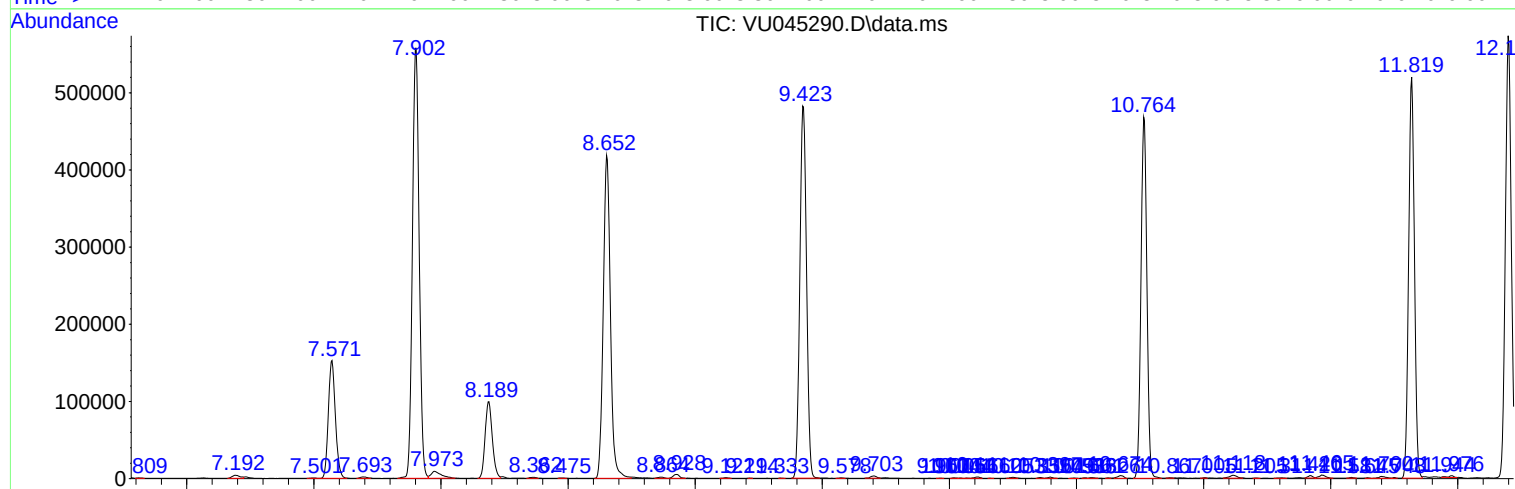
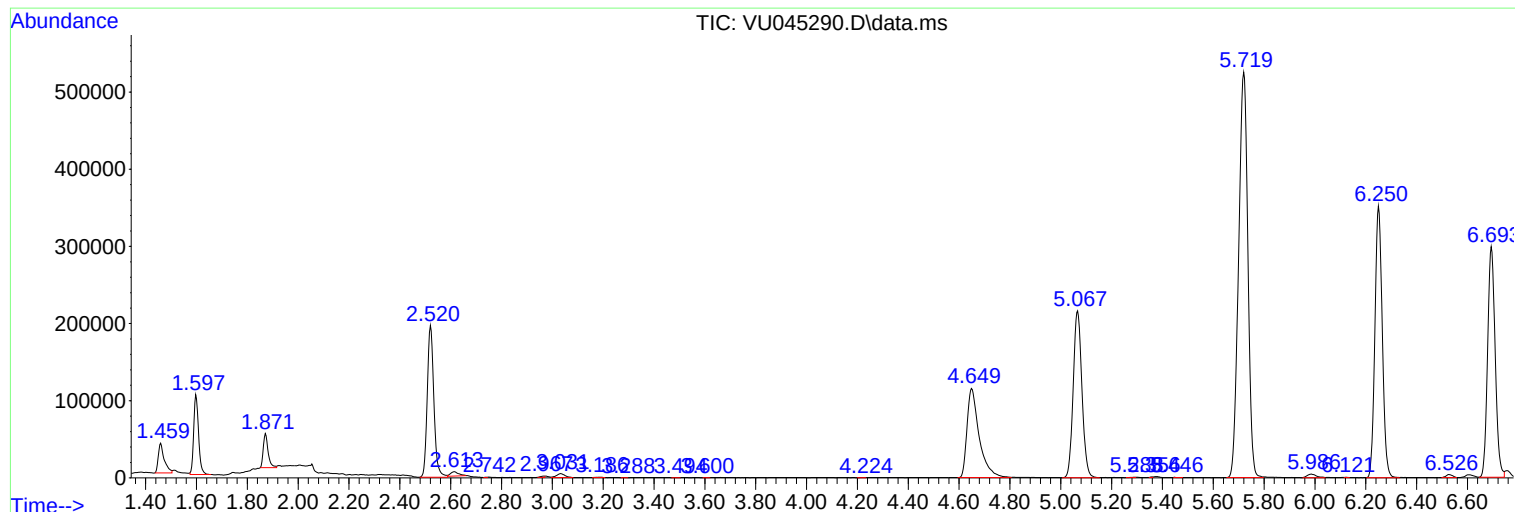
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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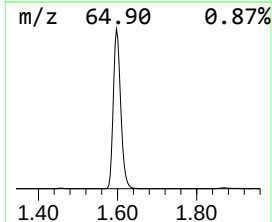
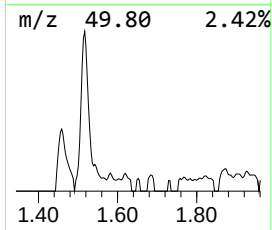
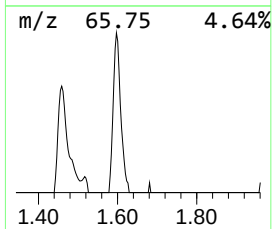
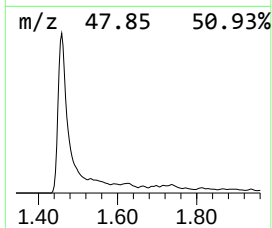
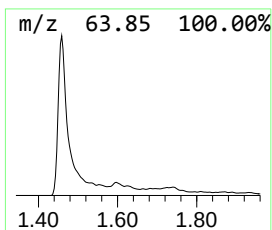
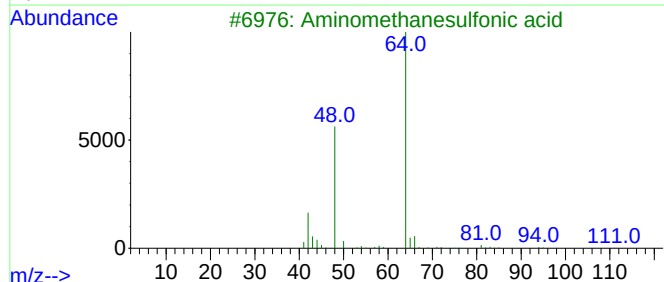
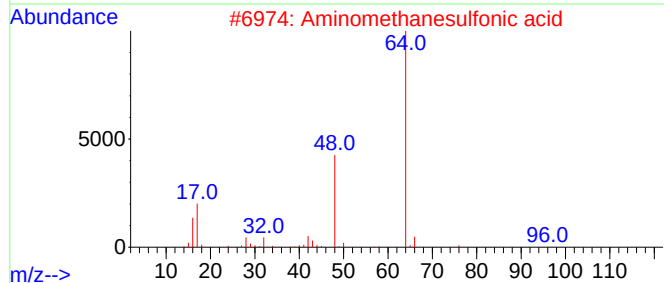
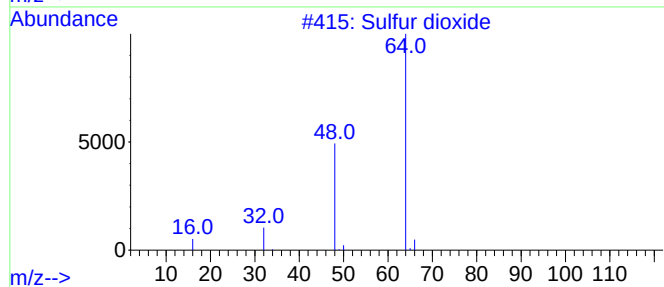
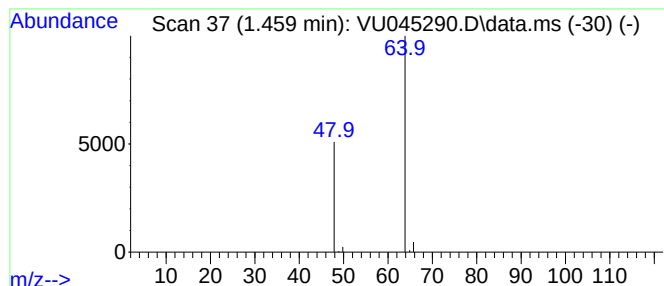
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.459	4.37 ug/L	62055	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	4.4	ug/L	62055	1	6.250	710149	50.0