

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045293.D
 Acq On : 12 Oct 2021 15:46
 Operator : SY/MD
 Sample : M4103-08ME
 Misc : 4.33g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AC2ME

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: VU045293.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	37495	62539	4.79%	0.640%
2	1.597	73	80	100	rVB	101015	135800	10.40%	1.390%
3	1.871	159	165	176	rBV	40077	52340	4.01%	0.536%
4	2.517	353	366	388	rBV	192896	346317	26.52%	3.545%
5	2.613	390	396	406	rVV	4791	8785	0.67%	0.090%
6	2.777	443	447	451	rBV	300	291	0.02%	0.003%
7	2.970	496	507	515	rVV3	2103	4174	0.32%	0.043%
8	3.028	515	525	543	rVB	7640	17693	1.36%	0.181%
9	3.186	562	574	582	rBV4	612	1255	0.10%	0.013%
10	3.530	677	681	685	rBV2	175	165	0.01%	0.002%
11	3.639	709	715	717	rBV2	223	253	0.02%	0.003%
12	3.658	717	721	726	rVB3	354	372	0.03%	0.004%
13	4.183	879	884	886	rBV2	216	234	0.02%	0.002%
14	4.292	914	918	921	rBV	216	217	0.02%	0.002%
15	4.353	933	937	942	rVV	156	165	0.01%	0.002%
16	4.575	998	1006	1009	rBV2	212	343	0.03%	0.004%
17	4.652	1014	1030	1074	rVV	109708	381223	29.20%	3.902%
18	5.067	1140	1159	1187	rVV	212384	505725	38.73%	5.177%
19	5.205	1199	1202	1209	rVB3	304	236	0.02%	0.002%
20	5.285	1222	1227	1229	rBV2	522	542	0.04%	0.006%
21	5.359	1248	1250	1252	rBV3	334	205	0.02%	0.002%
22	5.379	1252	1256	1259	rVB2	411	394	0.03%	0.004%
23	5.588	1317	1321	1328	rBV2	179	208	0.02%	0.002%
24	5.719	1341	1362	1387	rBV2	523034	1305706	100.00%	13.366%
25	5.986	1434	1445	1459	rBV5	4437	10660	0.82%	0.109%
26	6.115	1482	1485	1488	rBV2	265	222	0.02%	0.002%
27	6.250	1512	1527	1554	rBV	348058	701896	53.76%	7.185%
28	6.526	1605	1613	1625	rVB6	4145	7652	0.59%	0.078%
29	6.604	1626	1637	1651	rBV3	3485	8727	0.67%	0.089%
30	6.694	1651	1665	1683	rBV	291732	608379	46.59%	6.228%
31	7.041	1771	1773	1776	rVV	265	236	0.02%	0.002%
32	7.063	1778	1780	1789	rVB3	474	568	0.04%	0.006%
33	7.195	1810	1821	1828	rBV3	4108	8126	0.62%	0.083%
34	7.343	1865	1867	1872	rVB2	277	196	0.02%	0.002%
35	7.504	1914	1917	1919	rBV	334	196	0.02%	0.002%
36	7.571	1924	1938	1960	rVV	145532	286556	21.95%	2.933%

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Instrument :
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 ClientSampleId :
 C0AC2ME

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

37	7.694	1968	1976	1990	rVB5	1777	3895	0.30%	0.040%
38	7.838	2017	2021	2023	rBV	184	139	0.01%	0.001%
39	7.899	2026	2040	2056	rBV	538280	986867	75.58%	10.102%
40	8.186	2114	2129	2151	rBV	97457	192588	14.75%	1.971%
41	8.356	2177	2182	2184	rBV3	763	746	0.06%	0.008%
42	8.462	2212	2215	2220	rBV2	363	394	0.03%	0.004%
43	8.481	2220	2221	2223	rVV	353	139	0.01%	0.001%
44	8.504	2226	2228	2232	rVB	262	165	0.01%	0.002%
45	8.652	2259	2274	2306	rBV	403531	800958	61.34%	8.199%
46	8.796	2315	2319	2322	rVB3	389	293	0.02%	0.003%
47	8.861	2335	2339	2347	rVB6	466	569	0.04%	0.006%
48	8.925	2351	2359	2367	rVB7	1539	2480	0.19%	0.025%
49	9.099	2410	2413	2415	rBV	194	157	0.01%	0.002%
50	9.124	2419	2421	2425	rVB2	263	198	0.02%	0.002%
51	9.366	2493	2496	2500	rBV2	205	185	0.01%	0.002%
52	9.427	2500	2515	2531	rBV	473394	858397	65.74%	8.787%
53	9.578	2556	2562	2570	rVB2	346	576	0.04%	0.006%
54	9.700	2593	2600	2609	rVB5	1372	2205	0.17%	0.023%
55	9.739	2609	2612	2614	rBV2	359	269	0.02%	0.003%
56	9.854	2643	2648	2651	rBV2	192	207	0.02%	0.002%
57	9.874	2651	2654	2658	rVB2	234	167	0.01%	0.002%
58	10.108	2721	2727	2732	rBV3	681	909	0.07%	0.009%
59	10.153	2736	2741	2746	rVB2	247	317	0.02%	0.003%
60	10.269	2772	2777	2782	rBV2	187	263	0.02%	0.003%
61	10.362	2803	2806	2808	rBV2	350	193	0.01%	0.002%
62	10.375	2808	2810	2813	rVV	269	163	0.01%	0.002%
63	10.394	2813	2816	2820	rVV2	599	482	0.04%	0.005%
64	10.523	2852	2856	2859	rVV2	396	321	0.02%	0.003%
65	10.539	2859	2861	2866	rVV2	403	334	0.03%	0.003%
66	10.562	2866	2868	2872	rVB2	264	169	0.01%	0.002%
67	10.610	2877	2883	2885	rBV2	193	208	0.02%	0.002%
68	10.671	2894	2902	2916	rVB4	2842	4684	0.36%	0.048%
69	10.764	2916	2931	2953	rBV	456020	741276	56.77%	7.588%
70	10.867	2959	2963	2967	rBV3	515	567	0.04%	0.006%
71	10.999	3001	3004	3005	rBV	243	158	0.01%	0.002%
72	11.118	3035	3041	3050	rVB6	1863	2605	0.20%	0.027%
73	11.205	3064	3068	3069	rBV	382	240	0.02%	0.002%
74	11.247	3074	3081	3087	rBV2	283	460	0.04%	0.005%
75	11.378	3118	3122	3127	rVB2	426	427	0.03%	0.004%
76	11.423	3128	3136	3139	rVV3	766	925	0.07%	0.009%

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 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AC2ME

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

77	11.462	3139	3148	3158	rVB4	2393	4240	0.32%	0.043%
78	11.504	3158	3161	3165	rVB	275	243	0.02%	0.002%
79	11.636	3199	3202	3205	rBV	218	172	0.01%	0.002%
80	11.661	3205	3210	3213	rBV	238	299	0.02%	0.003%
81	11.700	3214	3222	3228	rVV4	1220	1892	0.14%	0.019%
82	11.748	3234	3237	3240	rBV2	246	187	0.01%	0.002%
83	11.819	3246	3259	3280	rBV	498922	791208	60.60%	8.099%
84	11.976	3304	3308	3314	rVB2	2404	2527	0.19%	0.026%
85	12.076	3334	3339	3341	rBV3	637	494	0.04%	0.005%
86	12.198	3360	3377	3397	rBV	555064	888840	68.07%	9.099%
87	12.288	3403	3405	3409	rBV3	314	224	0.02%	0.002%
88	12.330	3412	3418	3425	rBV3	2148	2770	0.21%	0.028%
89	12.401	3436	3440	3442	rBV3	337	240	0.02%	0.002%
90	12.488	3463	3467	3473	rBV2	252	309	0.02%	0.003%
91	12.677	3523	3526	3534	rVB2	169	214	0.02%	0.002%
92	12.999	3620	3626	3629	rBV2	213	304	0.02%	0.003%
93	13.160	3667	3676	3686	rBV3	847	1659	0.13%	0.017%
94	13.436	3755	3762	3771	rBV5	1084	1538	0.12%	0.016%
95	13.819	3879	3881	3886	rBV2	224	185	0.01%	0.002%
96	14.099	3960	3968	3981	rBV2	1355	2188	0.17%	0.022%
97	14.192	3994	3997	4005	rVB2	1177	1276	0.10%	0.013%
98	14.455	4072	4079	4088	rVB4	1352	1687	0.13%	0.017%
99	14.841	4196	4199	4204	rBV3	355	423	0.03%	0.004%
100	15.217	4310	4316	4319	rBV3	703	800	0.06%	0.008%

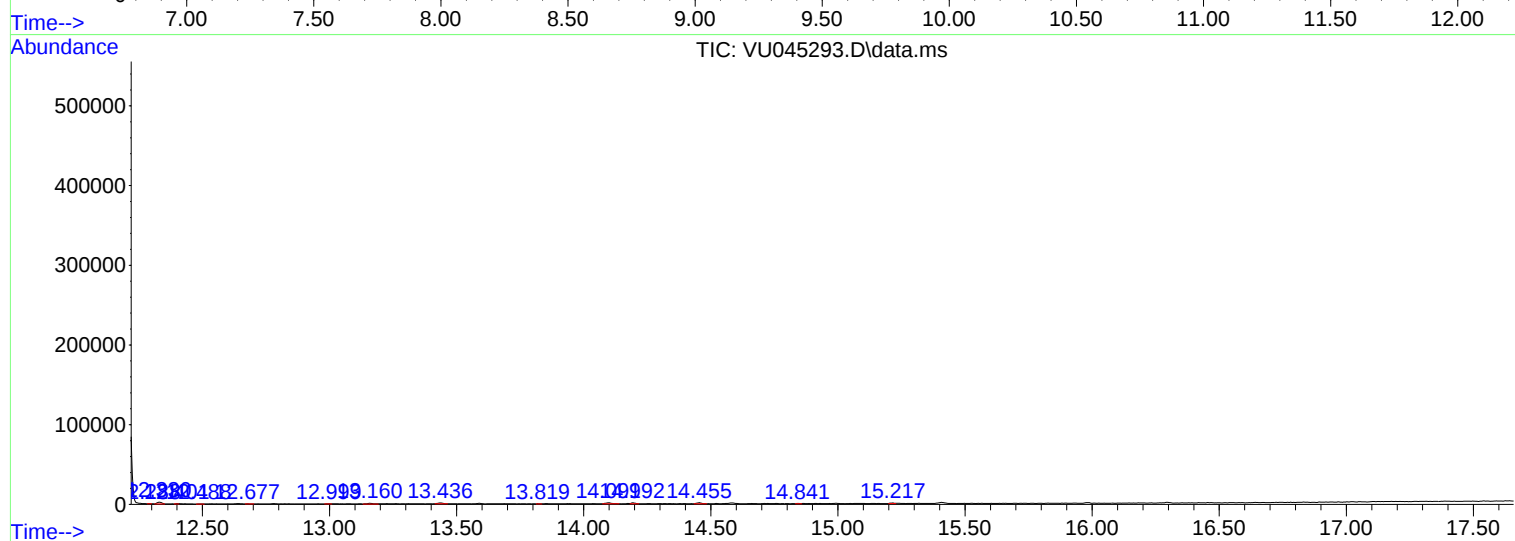
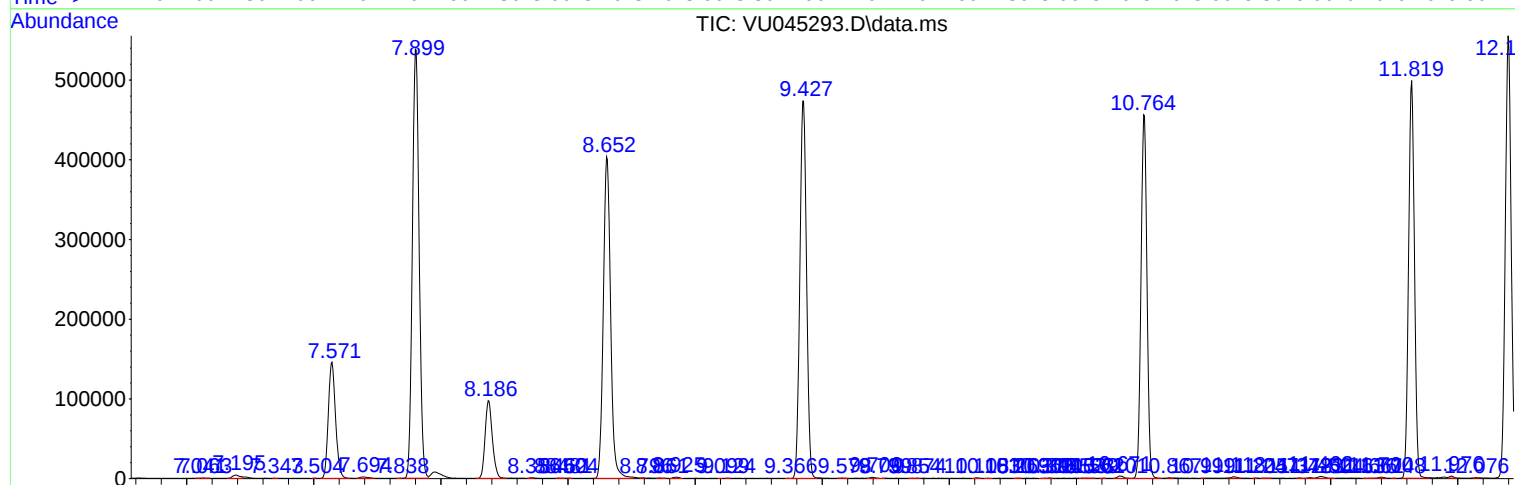
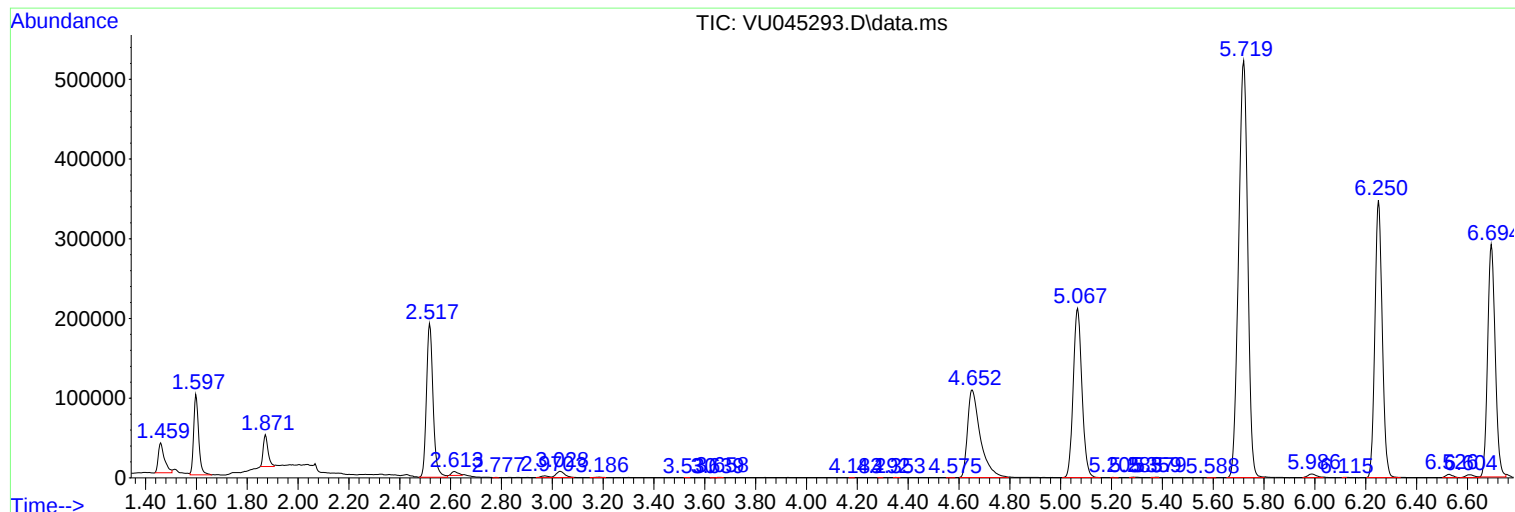
Sum of corrected areas: 9768810

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AC2ME

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 :
MSVOA_U
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C0AC2ME

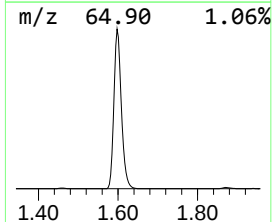
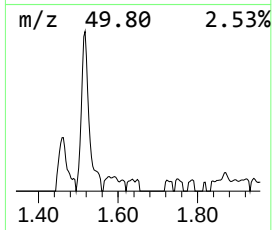
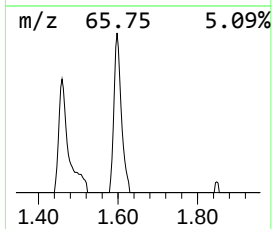
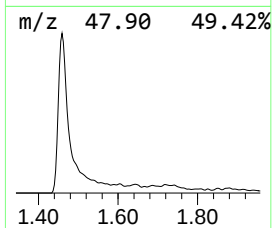
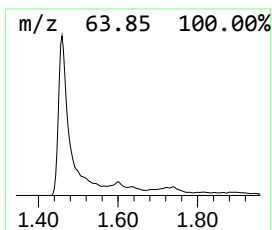
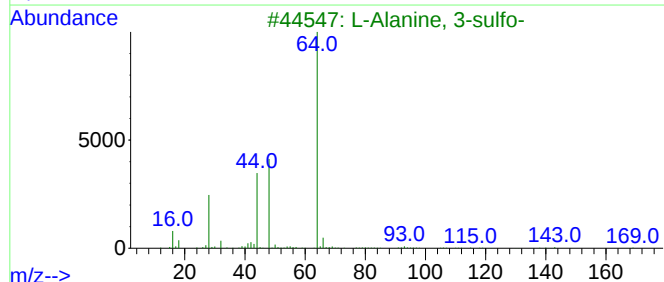
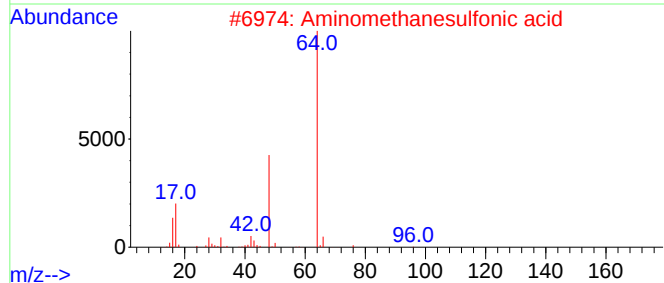
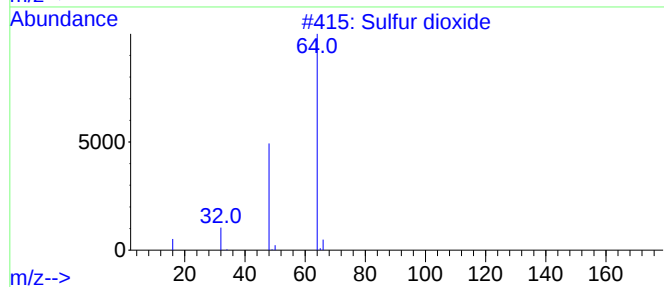
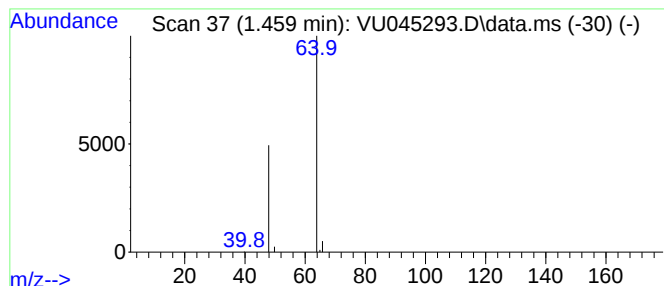
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	4.46 ug/L	62539	1,4-Difluorobenzene	6.250

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	4.5	ug/L	62539	1	6.250	701896	50.0