

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045291.D
 Acq On : 12 Oct 2021 14:58
 Operator : SY/MD
 Sample : M4103-06ME
 Misc : 4.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AC0ME

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: VU045291.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	50	rBV	33930	51386	3.89%	0.522%
2	1.597	73	80	101	rVB	104277	138415	10.49%	1.407%
3	1.871	159	165	177	rBV	42598	56028	4.25%	0.569%
4	2.520	354	367	387	rBV	194594	350407	26.56%	3.561%
5	2.732	429	433	434	rBV	225	162	0.01%	0.002%
6	2.970	499	507	515	rVV2	1787	3572	0.27%	0.036%
7	3.028	515	525	543	rVB3	5807	13066	0.99%	0.133%
8	3.170	562	569	570	rBV	449	407	0.03%	0.004%
9	3.182	570	573	577	rVB2	286	312	0.02%	0.003%
10	3.488	663	668	673	rBV2	200	312	0.02%	0.003%
11	3.533	678	682	686	rVB2	223	231	0.02%	0.002%
12	3.787	757	761	764	rBV2	221	230	0.02%	0.002%
13	3.877	783	789	792	rBV	194	270	0.02%	0.003%
14	4.128	864	867	871	rBV2	208	187	0.01%	0.002%
15	4.285	913	916	923	rVB2	158	162	0.01%	0.002%
16	4.440	961	964	969	rVB2	240	259	0.02%	0.003%
17	4.536	990	994	998	rBV	148	168	0.01%	0.002%
18	4.649	1012	1029	1072	rBV2	111819	382466	28.99%	3.887%
19	4.986	1131	1134	1140	rBV2	193	250	0.02%	0.003%
20	5.067	1140	1159	1186	rBV	214630	511162	38.74%	5.194%
21	5.289	1222	1228	1230	rBV3	458	501	0.04%	0.005%
22	5.427	1265	1271	1275	rBV2	213	299	0.02%	0.003%
23	5.719	1341	1362	1384	rBV2	526713	1319383	100.00%	13.407%
24	5.986	1434	1445	1457	rBV2	4311	9585	0.73%	0.097%
25	6.115	1482	1485	1487	rVV2	252	170	0.01%	0.002%
26	6.250	1511	1527	1554	rBV	346728	693599	52.57%	7.048%
27	6.530	1604	1614	1626	rVB6	4201	7987	0.61%	0.081%
28	6.610	1627	1639	1650	rBV5	3527	8854	0.67%	0.090%
29	6.694	1650	1665	1692	rVB	297650	618493	46.88%	6.285%
30	6.813	1695	1702	1705	rBV3	620	677	0.05%	0.007%
31	6.890	1723	1726	1729	rBV2	190	174	0.01%	0.002%
32	7.060	1769	1779	1782	rBV3	467	655	0.05%	0.007%
33	7.076	1782	1784	1790	rBV2	290	251	0.02%	0.003%
34	7.192	1811	1820	1829	rBV5	3818	8206	0.62%	0.083%
35	7.407	1882	1887	1888	rBV2	203	171	0.01%	0.002%
36	7.571	1924	1938	1959	rBV	150992	291161	22.07%	2.959%

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 ClientSampleId :
 COACOME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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	rVB4	1718	3767	0.29%	0.038%
38	7.899	2025	2040	2056	rBV	552570	1000892	75.86%	10.171%
39	7.977	2057	2064	2087	rVB5	8152	22134	1.68%	0.225%
40	8.185	2117	2129	2145	rBV	97450	195224	14.80%	1.984%
41	8.308	2166	2167	2171	rVB	265	161	0.01%	0.002%
42	8.349	2177	2180	2183	rVV2	562	486	0.04%	0.005%
43	8.366	2183	2185	2191	rVB2	644	445	0.03%	0.005%
44	8.391	2191	2193	2201	rBV2	210	169	0.01%	0.002%
45	8.652	2258	2274	2308	rBV	410926	809308	61.34%	8.224%
46	8.861	2337	2339	2346	rVB2	190	168	0.01%	0.002%
47	8.899	2347	2351	2356	rVB2	222	216	0.02%	0.002%
48	9.066	2400	2403	2407	rVB2	278	207	0.02%	0.002%
49	9.092	2407	2411	2416	rBV2	287	373	0.03%	0.004%
50	9.202	2441	2445	2448	rBV2	169	189	0.01%	0.002%
51	9.423	2500	2514	2537	rBV	469726	855110	64.81%	8.689%
52	9.575	2555	2561	2566	rBV2	459	549	0.04%	0.006%
53	9.703	2593	2601	2611	rVB4	1149	1829	0.14%	0.019%
54	9.819	2633	2637	2642	rBV2	198	165	0.01%	0.002%
55	10.009	2693	2696	2699	rBV	178	162	0.01%	0.002%
56	10.105	2719	2726	2737	rBV3	527	941	0.07%	0.010%
57	10.359	2802	2805	2809	rBV2	181	162	0.01%	0.002%
58	10.410	2815	2821	2826	rBV2	176	232	0.02%	0.002%
59	10.533	2855	2859	2863	rBV2	516	453	0.03%	0.005%
60	10.607	2877	2882	2887	rBV2	261	355	0.03%	0.004%
61	10.674	2895	2903	2911	rVB2	3442	4750	0.36%	0.048%
62	10.764	2918	2931	2948	rBV	467347	753655	57.12%	7.659%
63	10.870	2959	2964	2966	rBV2	616	586	0.04%	0.006%
64	11.115	3035	3040	3050	rBV4	1527	2345	0.18%	0.024%
65	11.211	3067	3070	3075	rVB2	402	337	0.03%	0.003%
66	11.385	3119	3124	3127	rBV2	289	269	0.02%	0.003%
67	11.417	3131	3134	3137	rVV3	476	352	0.03%	0.004%
68	11.459	3139	3147	3160	rVB6	2347	4654	0.35%	0.047%
69	11.510	3160	3163	3167	rBV	193	174	0.01%	0.002%
70	11.552	3172	3176	3179	rBV	157	168	0.01%	0.002%
71	11.581	3181	3185	3187	rBV2	297	223	0.02%	0.002%
72	11.703	3214	3223	3230	rBB3	1308	2051	0.16%	0.021%
73	11.819	3246	3259	3281	rBV	509405	785420	59.53%	7.981%
74	11.896	3281	3283	3286	rVV3	326	192	0.01%	0.002%
75	11.922	3286	3291	3293	rVV2	845	720	0.05%	0.007%
76	11.947	3294	3299	3303	rVV4	1472	2039	0.15%	0.021%

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 ClientSampleId :
 C0AC0ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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

77	11.976	3305	3308	3317	rVB3	2451	2799	0.21%	0.028%
78	12.060	3329	3334	3337	rBV	417	394	0.03%	0.004%
79	12.198	3361	3377	3397	rBV	556255	900640	68.26%	9.152%
80	12.333	3412	3419	3429	rVB4	1975	2946	0.22%	0.030%
81	12.407	3437	3442	3448	rVB3	598	746	0.06%	0.008%
82	12.623	3504	3509	3511	rBV	380	307	0.02%	0.003%
83	12.719	3535	3539	3541	rBV	213	207	0.02%	0.002%
84	12.928	3601	3604	3606	rBV	279	164	0.01%	0.002%
85	13.063	3644	3646	3650	rVB2	239	167	0.01%	0.002%
86	13.089	3652	3654	3659	rVB2	283	171	0.01%	0.002%
87	13.150	3670	3673	3675	rBV2	309	163	0.01%	0.002%
88	13.221	3692	3695	3698	rBV2	248	192	0.01%	0.002%
89	13.436	3757	3762	3766	rBV3	1131	1047	0.08%	0.011%
90	13.742	3854	3857	3862	rVB2	309	194	0.01%	0.002%
91	13.844	3886	3889	3893	rBV3	421	367	0.03%	0.004%
92	14.095	3958	3967	3977	rBV	1386	2194	0.17%	0.022%
93	14.156	3983	3986	3989	rBV2	252	227	0.02%	0.002%
94	14.340	4037	4043	4049	rBV3	541	810	0.06%	0.008%
95	14.455	4074	4079	4084	rBV4	1004	959	0.07%	0.010%
96	14.584	4109	4119	4127	rBV3	1017	2313	0.18%	0.024%
97	14.655	4137	4141	4143	rBV2	347	258	0.02%	0.003%
98	15.227	4316	4319	4321	rBV2	582	412	0.03%	0.004%
99	15.407	4371	4375	4383	rVB4	905	1076	0.08%	0.011%
100	16.291	4648	4650	4657	rVB4	931	735	0.06%	0.007%

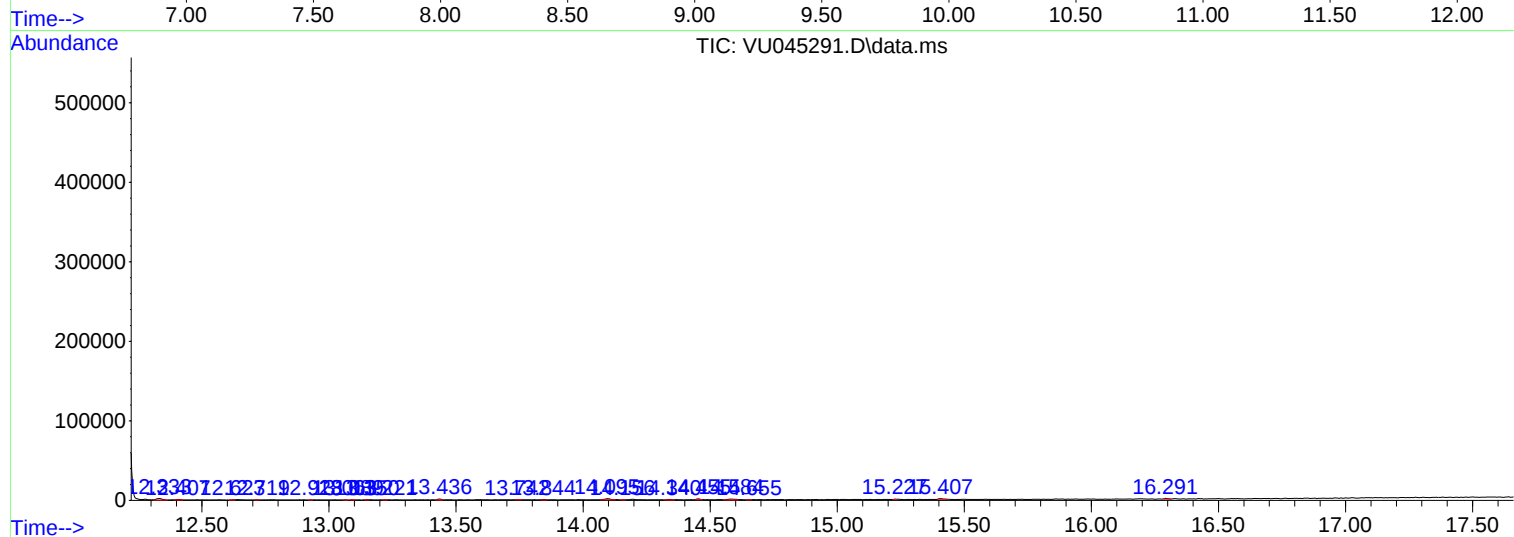
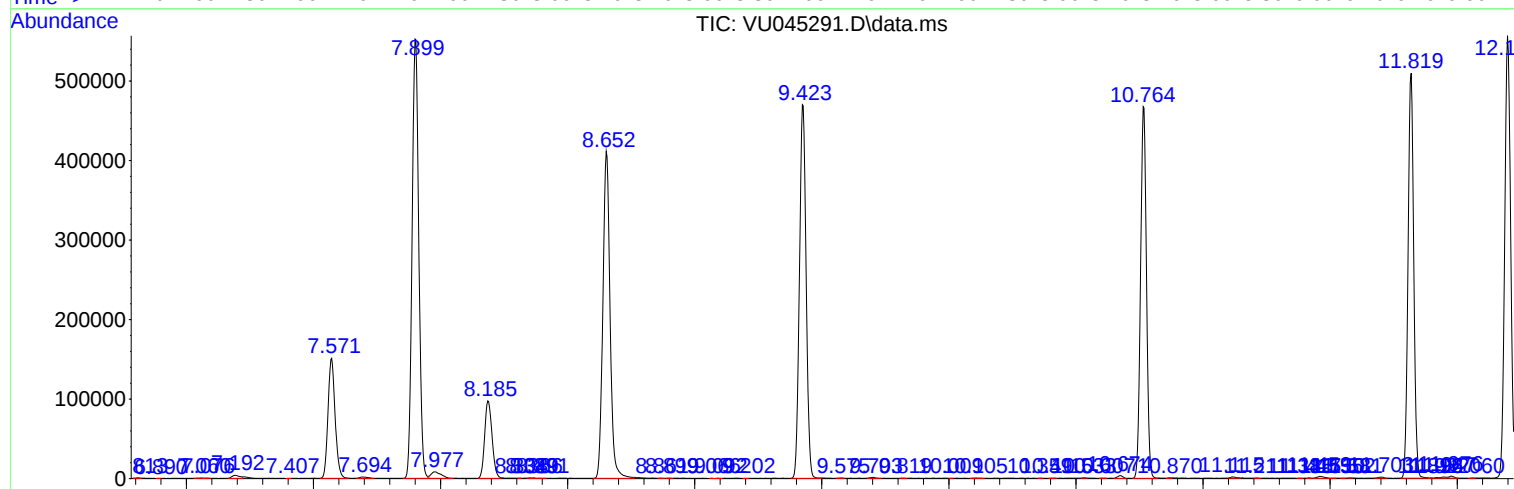
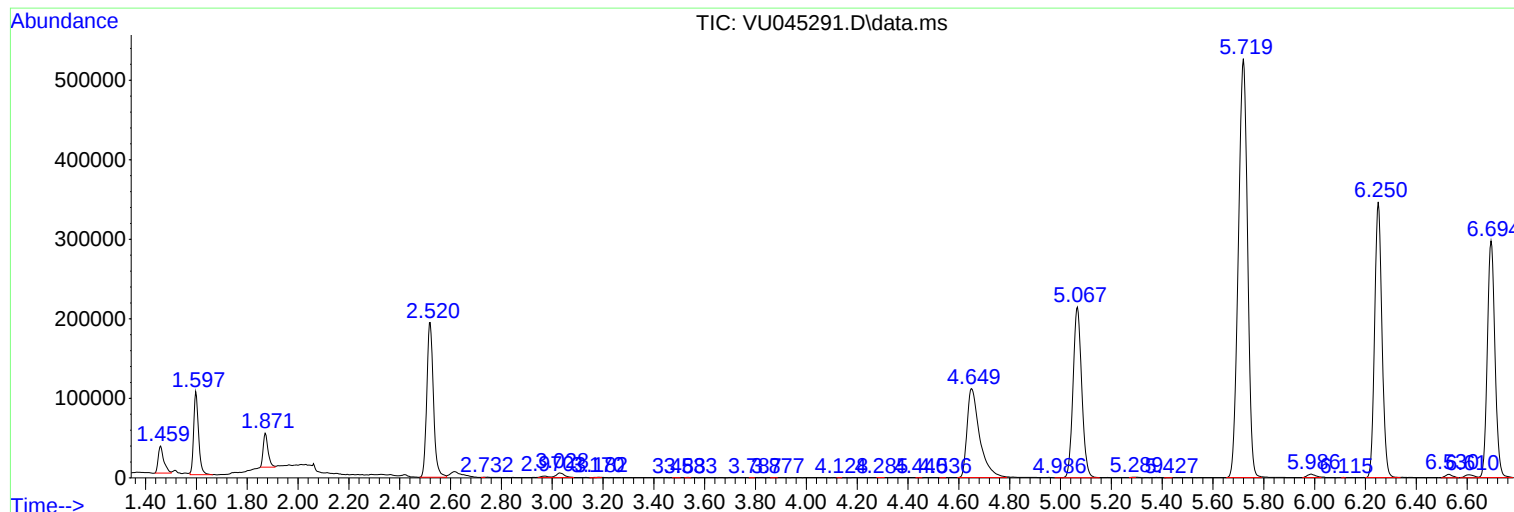
Sum of corrected areas: 9840738

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AC0ME

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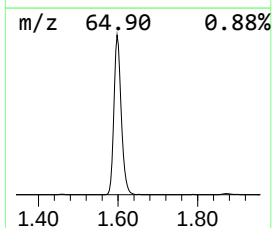
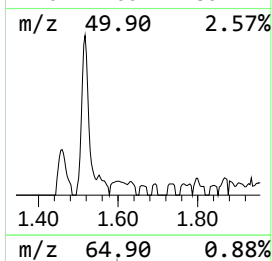
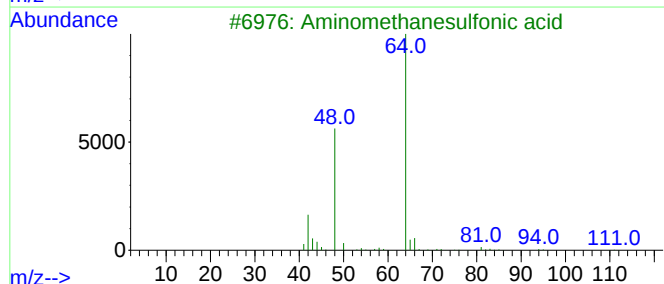
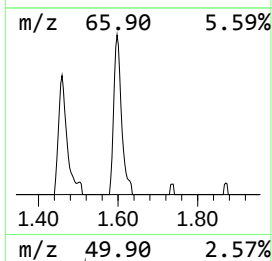
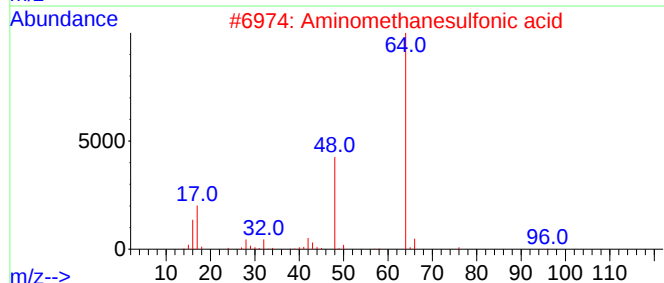
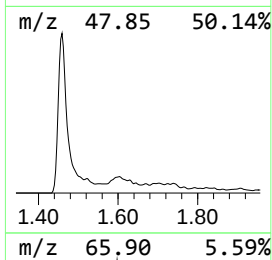
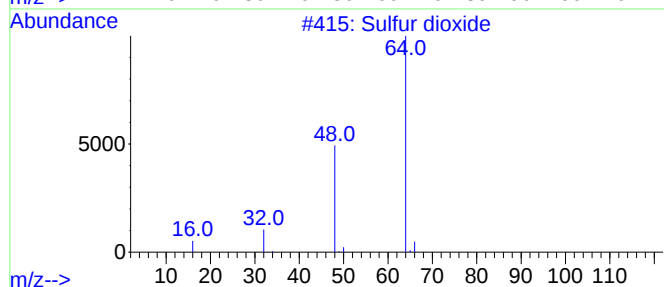
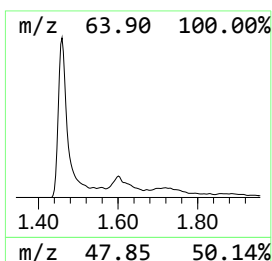
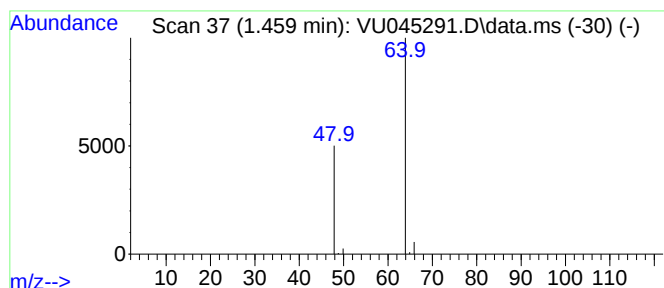
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.70 ug/L	51386	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			Sulfur dioxide	64	O2S	007446-09-5	4



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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	3.7	ug/L	51386	1	6.250	693599	50.0