

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045289.D
 Acq On : 12 Oct 2021 14:11
 Operator : SY/MD
 Sample : M4103-04ME
 Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AB8ME

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: VU045289.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	34310	55007	4.15%	0.561%
2	1.597	73	80	101	rVB	105231	140649	10.61%	1.433%
3	1.871	159	165	180	rBV	42930	58044	4.38%	0.592%
4	2.520	354	367	387	rBV	197334	352427	26.59%	3.592%
5	2.610	389	395	409	rVB2	5194	10586	0.80%	0.108%
6	2.793	449	452	455	rBV	234	168	0.01%	0.002%
7	2.839	464	466	472	rVB2	145	156	0.01%	0.002%
8	2.964	493	505	516	rBV4	1601	3497	0.26%	0.036%
9	3.028	516	525	539	rVB3	3506	7873	0.59%	0.080%
10	3.147	560	562	565	rBV2	208	158	0.01%	0.002%
11	3.186	569	574	580	rVB3	600	702	0.05%	0.007%
12	3.221	580	585	586	rBV2	227	208	0.02%	0.002%
13	3.279	600	603	607	rVB2	223	205	0.02%	0.002%
14	3.437	645	652	656	rBV2	193	284	0.02%	0.003%
15	3.459	656	659	665	rVB	306	277	0.02%	0.003%
16	3.658	716	721	722	rBV	257	202	0.02%	0.002%
17	3.822	764	772	775	rBV2	225	259	0.02%	0.003%
18	3.906	793	798	801	rBV	222	283	0.02%	0.003%
19	3.986	820	823	826	rBV	223	164	0.01%	0.002%
20	4.485	974	978	984	rVV2	187	223	0.02%	0.002%
21	4.562	996	1002	1006	rBV2	269	367	0.03%	0.004%
22	4.649	1013	1029	1075	rBV	109257	370149	27.93%	3.772%
23	5.067	1141	1159	1184	rBV	213767	512554	38.67%	5.223%
24	5.211	1200	1204	1206	rVV2	290	188	0.01%	0.002%
25	5.289	1223	1228	1237	rVB2	625	1027	0.08%	0.010%
26	5.719	1342	1362	1392	rBV2	519792	1325418	100.00%	13.507%
27	5.986	1434	1445	1462	rBV5	4504	10963	0.83%	0.112%
28	6.118	1480	1486	1488	rBV	199	227	0.02%	0.002%
29	6.250	1512	1527	1552	rVV	351420	704608	53.16%	7.181%
30	6.340	1552	1555	1561	rVB	277	258	0.02%	0.003%
31	6.369	1561	1564	1567	rBV3	245	191	0.01%	0.002%
32	6.488	1598	1601	1604	rBV2	181	147	0.01%	0.001%
33	6.526	1604	1613	1624	rVV5	4121	7568	0.57%	0.077%
34	6.604	1626	1637	1650	rVV3	3757	8783	0.66%	0.090%
35	6.694	1650	1665	1690	rVB	296704	618531	46.67%	6.303%
36	6.806	1696	1700	1703	rBV3	487	460	0.03%	0.005%

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Integrator: RTE

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

37	6.948	1739	1744	1747	rBV2	195	211	0.02%	0.002%
38	6.980	1750	1754	1757	rBV	166	180	0.01%	0.002%
39	7.054	1771	1777	1778	rVV	398	318	0.02%	0.003%
40	7.195	1810	1821	1827	rBV6	3828	7559	0.57%	0.077%
41	7.571	1924	1938	1957	rBV	150361	291177	21.97%	2.967%
42	7.639	1957	1959	1966	rVB4	381	304	0.02%	0.003%
43	7.697	1969	1977	1978	rBV4	1586	1908	0.14%	0.019%
44	7.797	2002	2008	2012	rBV2	334	450	0.03%	0.005%
45	7.822	2012	2016	2021	rVB3	196	249	0.02%	0.003%
46	7.899	2026	2040	2056	rVV	554832	1009507	76.17%	10.288%
47	7.973	2057	2063	2089	rVB4	8643	22162	1.67%	0.226%
48	8.115	2103	2107	2111	rBV2	223	265	0.02%	0.003%
49	8.186	2117	2129	2148	rVV	97389	195074	14.72%	1.988%
50	8.308	2164	2167	2173	rBV3	231	299	0.02%	0.003%
51	8.353	2177	2181	2183	rVV2	603	538	0.04%	0.005%
52	8.366	2183	2185	2190	rVB2	590	408	0.03%	0.004%
53	8.481	2209	2221	2226	rBV2	542	1133	0.09%	0.012%
54	8.652	2258	2274	2308	rBV	400949	781435	58.96%	7.964%
55	8.925	2355	2359	2361	rBV2	591	377	0.03%	0.004%
56	8.973	2369	2374	2376	rBV2	183	208	0.02%	0.002%
57	9.423	2501	2514	2532	rVV	474738	858107	64.74%	8.745%
58	9.568	2556	2559	2563	rBV2	353	305	0.02%	0.003%
59	9.649	2581	2584	2586	rBV	207	158	0.01%	0.002%
60	9.700	2592	2600	2609	rVB4	1019	1771	0.13%	0.018%
61	10.112	2719	2728	2732	rBV3	533	788	0.06%	0.008%
62	10.131	2732	2734	2737	rVV	249	179	0.01%	0.002%
63	10.166	2742	2745	2748	rBV2	234	156	0.01%	0.002%
64	10.327	2790	2795	2796	rBV	166	162	0.01%	0.002%
65	10.443	2826	2831	2833	rBV2	216	232	0.02%	0.002%
66	10.539	2854	2861	2864	rVB3	540	604	0.05%	0.006%
67	10.671	2894	2902	2910	rVB4	2752	4045	0.31%	0.041%
68	10.764	2917	2931	2948	rBV	462527	738707	55.73%	7.528%
69	10.870	2961	2964	2967	rVB3	435	347	0.03%	0.004%
70	10.893	2967	2971	2973	rBV	284	222	0.02%	0.002%
71	10.931	2981	2983	2989	rVB2	497	331	0.02%	0.003%
72	10.970	2989	2995	2997	rBV	174	215	0.02%	0.002%
73	11.050	3016	3020	3022	rBV	172	169	0.01%	0.002%
74	11.118	3036	3041	3049	rVV4	925	1254	0.09%	0.013%
75	11.211	3066	3070	3075	rVB3	323	285	0.02%	0.003%
76	11.411	3130	3132	3135	rBV2	243	167	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M

Title : VOC Analysis

77	11.465	3140	3149	3160	rVB6	2127	3825	0.29%	0.039%
78	11.562	3175	3179	3182	rBV	231	237	0.02%	0.002%
79	11.581	3182	3185	3190	rVV2	486	472	0.04%	0.005%
80	11.648	3201	3206	3210	rBV2	277	308	0.02%	0.003%
81	11.697	3216	3221	3228	rVB4	1165	1624	0.12%	0.017%
82	11.755	3234	3239	3241	rBV2	335	315	0.02%	0.003%
83	11.819	3246	3259	3276	rBV	499813	790874	59.67%	8.060%
84	11.976	3304	3308	3315	rVB3	1921	2468	0.19%	0.025%
85	12.066	3333	3336	3339	rBV	264	234	0.02%	0.002%
86	12.198	3363	3377	3396	rBV	550265	889866	67.14%	9.069%
87	12.327	3413	3417	3418	rBV3	657	413	0.03%	0.004%
88	12.382	3430	3434	3435	rBV2	233	172	0.01%	0.002%
89	12.488	3463	3467	3469	rBV2	231	196	0.01%	0.002%
90	12.648	3512	3517	3522	rBV3	452	458	0.03%	0.005%
91	12.774	3551	3556	3559	rBV2	349	336	0.03%	0.003%
92	12.873	3584	3587	3592	rVB	248	213	0.02%	0.002%
93	12.983	3619	3621	3625	rBV2	205	157	0.01%	0.002%
94	13.144	3669	3671	3674	rBV	306	261	0.02%	0.003%
95	13.378	3739	3744	3746	rBV	281	279	0.02%	0.003%
96	14.092	3961	3966	3976	rVB2	2703	3778	0.29%	0.039%
97	14.192	3995	3997	4001	rBV2	275	214	0.02%	0.002%
98	14.571	4112	4115	4116	rBV	395	238	0.02%	0.002%
99	14.661	4140	4143	4146	rBV	320	303	0.02%	0.003%
100	14.877	4206	4210	4213	rBV2	524	510	0.04%	0.005%

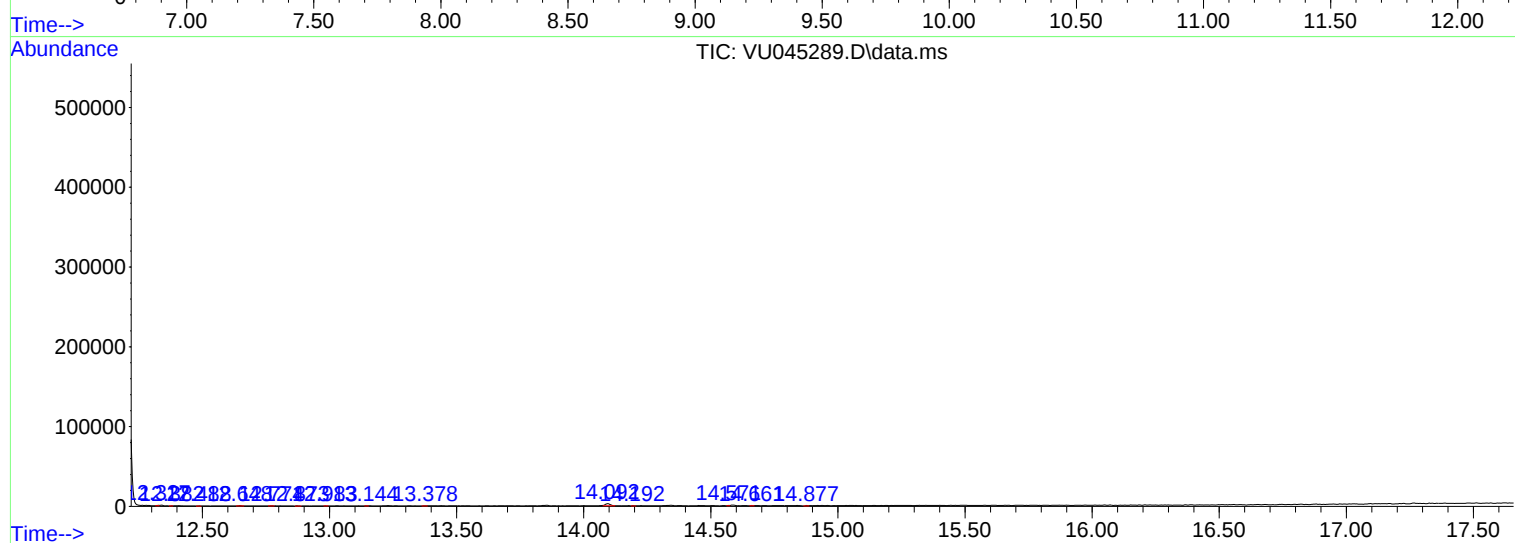
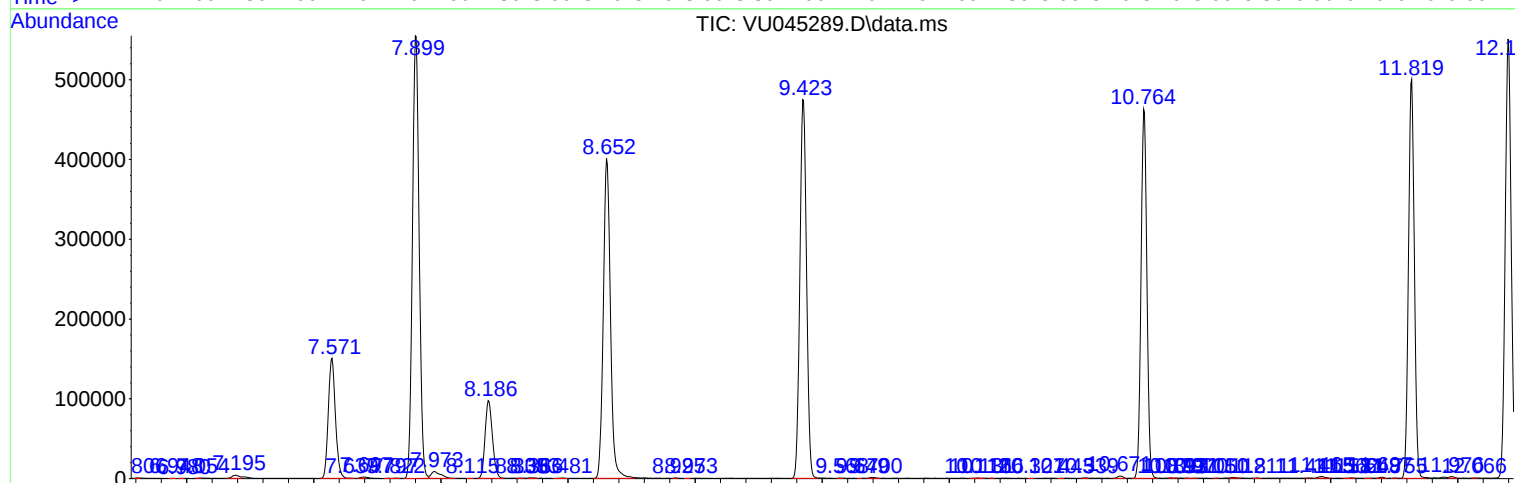
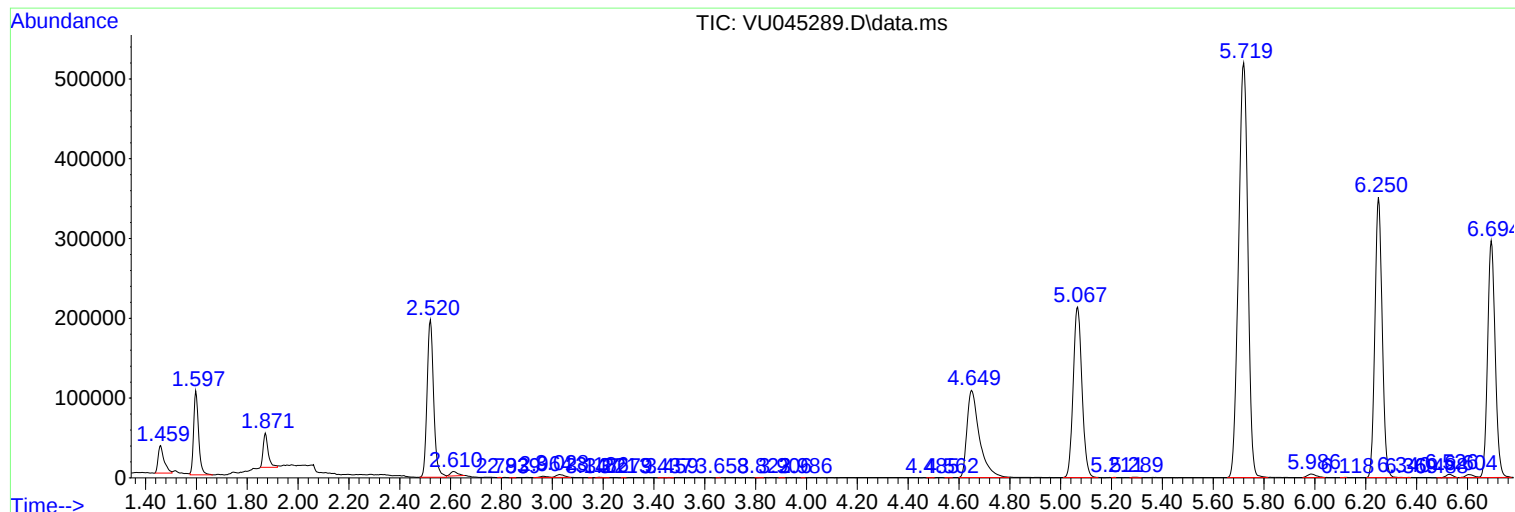
Sum of corrected areas: 9812528

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ALS Vial : 8 Sample Multiplier: 1

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



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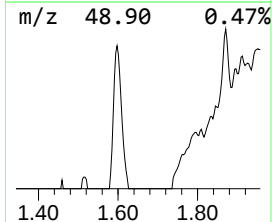
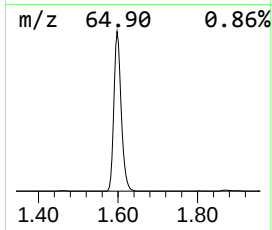
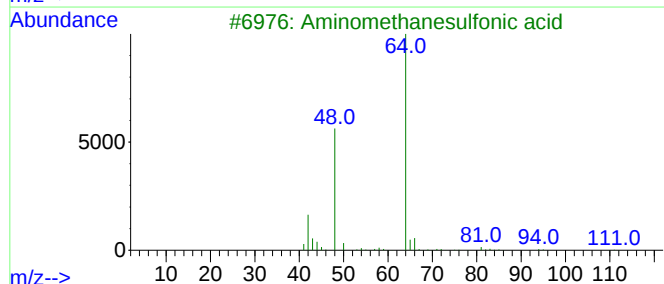
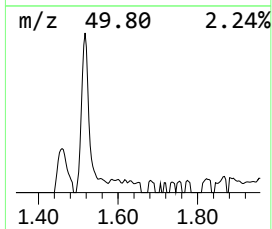
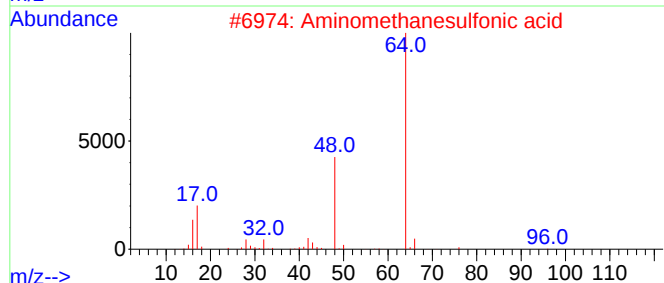
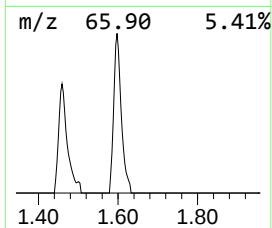
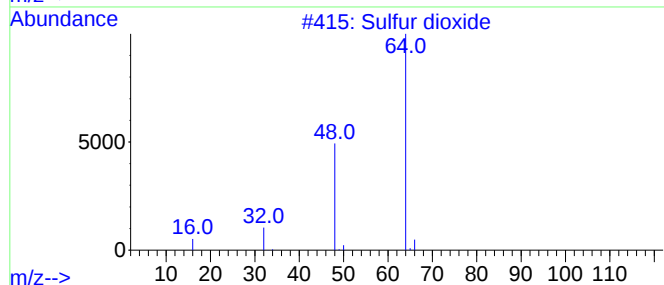
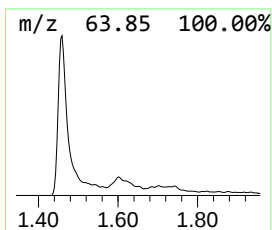
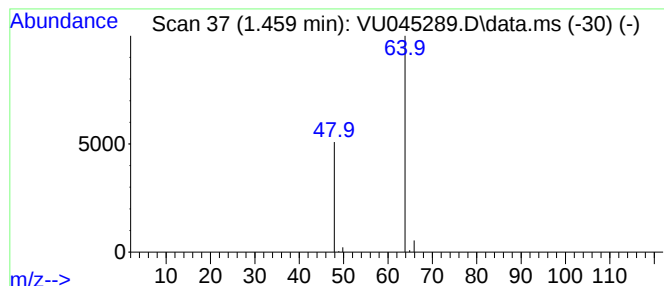
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.90 ug/L	55007	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 Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	3.9	ug/L	55007	1	6.250	704608	50.0