

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045288.D
 Acq On : 12 Oct 2021 13:47
 Operator : SY/MD
 Sample : M4103-03ME
 Misc : 4.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AB7ME

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: VU045288.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	32	37	51	rVB	28822	41122	3.19%	0.421%
2	1.597	73	80	99	rVB	102470	131885	10.22%	1.349%
3	2.526	357	369	386	rBV	197690	346904	26.87%	3.549%
4	2.951	495	501	502	rBV	966	741	0.06%	0.008%
5	3.034	516	527	541	rVB	3730	7229	0.56%	0.074%
6	3.176	567	571	572	rBV	489	272	0.02%	0.003%
7	3.356	625	627	630	rVB	176	106	0.01%	0.001%
8	3.378	630	634	641	rVB	220	290	0.02%	0.003%
9	3.433	648	651	653	rBV2	142	97	0.01%	0.001%
10	3.456	656	658	662	rBV2	175	112	0.01%	0.001%
11	3.517	670	677	680	rBV2	189	275	0.02%	0.003%
12	3.600	696	703	706	rBV2	255	250	0.02%	0.003%
13	3.629	709	712	716	rVB	233	173	0.01%	0.002%
14	3.713	734	738	741	rBV	223	121	0.01%	0.001%
15	3.761	750	753	755	rBV	157	118	0.01%	0.001%
16	3.899	793	796	800	rBV2	162	154	0.01%	0.002%
17	3.967	813	817	820	rVB	225	178	0.01%	0.002%
18	3.999	820	827	832	rBV2	218	333	0.03%	0.003%
19	4.099	856	858	863	rVB2	216	178	0.01%	0.002%
20	4.150	871	874	877	rBV	128	121	0.01%	0.001%
21	4.208	889	892	895	rBV2	213	152	0.01%	0.002%
22	4.230	895	899	902	rBV	233	220	0.02%	0.002%
23	4.311	921	924	927	rVB2	175	113	0.01%	0.001%
24	4.337	930	932	937	rVB2	241	173	0.01%	0.002%
25	4.446	961	966	970	rBV	203	222	0.02%	0.002%
26	4.475	970	975	981	rVB2	210	252	0.02%	0.003%
27	4.507	981	985	991	rBV2	209	294	0.02%	0.003%
28	4.645	1012	1028	1070	rVV	113014	352053	27.27%	3.601%
29	4.964	1124	1127	1129	rBV2	246	139	0.01%	0.001%
30	5.066	1142	1159	1186	rVB	216714	502519	38.93%	5.141%
31	5.173	1190	1192	1193	rBV	242	99	0.01%	0.001%
32	5.205	1200	1202	1206	rVB2	217	141	0.01%	0.001%
33	5.256	1215	1218	1220	rBV	184	109	0.01%	0.001%
34	5.288	1222	1228	1229	rBV	518	474	0.04%	0.005%
35	5.385	1256	1258	1261	rVB	193	91	0.01%	0.001%
36	5.475	1280	1286	1289	rBV	174	250	0.02%	0.003%

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

37	5.552	1304	1310	1311	rBV2	153	152	0.01%	0.002%
38	5.645	1334	1339	1342	rBV2	177	175	0.01%	0.002%
39	5.719	1342	1362	1385	rBV2	504247	1290820	100.00%	13.205%
40	5.896	1415	1417	1420	rVB	332	167	0.01%	0.002%
41	5.922	1422	1425	1428	rBV2	236	186	0.01%	0.002%
42	5.983	1434	1444	1459	rBV4	4180	9472	0.73%	0.097%
43	6.089	1472	1477	1478	rBV	139	123	0.01%	0.001%
44	6.118	1480	1486	1491	rVB3	302	414	0.03%	0.004%
45	6.140	1491	1493	1495	rBV	132	94	0.01%	0.001%
46	6.250	1507	1527	1549	rBV	357753	703726	54.52%	7.199%
47	6.356	1558	1560	1563	rVB	251	134	0.01%	0.001%
48	6.468	1592	1595	1600	rBV2	185	208	0.02%	0.002%
49	6.529	1604	1614	1624	rVB4	3998	7227	0.56%	0.074%
50	6.610	1628	1639	1650	rBV4	3690	8316	0.64%	0.085%
51	6.693	1650	1665	1683	rBV	295392	604276	46.81%	6.181%
52	6.809	1698	1701	1708	rVB4	733	701	0.05%	0.007%
53	6.896	1725	1728	1732	rBV	203	225	0.02%	0.002%
54	6.922	1733	1736	1739	rVV2	221	150	0.01%	0.002%
55	6.960	1743	1748	1750	rBV	163	200	0.02%	0.002%
56	7.054	1769	1777	1781	rBV	646	861	0.07%	0.009%
57	7.144	1802	1805	1807	rBV	165	104	0.01%	0.001%
58	7.189	1811	1819	1827	rBV3	4199	7534	0.58%	0.077%
59	7.275	1843	1846	1849	rBV	133	127	0.01%	0.001%
60	7.320	1855	1860	1861	rBV	209	140	0.01%	0.001%
61	7.430	1891	1894	1895	rBV	158	97	0.01%	0.001%
62	7.465	1901	1905	1907	rBV	183	167	0.01%	0.002%
63	7.488	1910	1912	1917	rBV2	155	134	0.01%	0.001%
64	7.571	1924	1938	1966	rVB	157101	293507	22.74%	3.002%
65	7.693	1968	1976	1988	rBV4	1685	3322	0.26%	0.034%
66	7.793	2003	2007	2008	rBV	173	115	0.01%	0.001%
67	7.902	2022	2041	2056	rBV	568984	1009386	78.20%	10.326%
68	8.185	2117	2129	2150	rBV	103791	199828	15.48%	2.044%
69	8.433	2200	2206	2208	rBV	124	123	0.01%	0.001%
70	8.449	2208	2211	2213	rBV2	132	96	0.01%	0.001%
71	8.468	2213	2217	2222	rBV3	366	486	0.04%	0.005%
72	8.652	2259	2274	2304	rBV	403821	766685	59.40%	7.843%
73	8.928	2353	2360	2366	rVB4	1039	1404	0.11%	0.014%
74	9.098	2410	2413	2415	rBV2	205	138	0.01%	0.001%
75	9.195	2439	2443	2445	rBV2	150	123	0.01%	0.001%
76	9.288	2469	2472	2475	rVB2	227	160	0.01%	0.002%

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Integrator: RTE

Smoothing : OFF

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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

77	9.369	2493	2497	2500	rBV	222	235	0.02%	0.002%
78	9.426	2500	2515	2537	rVV	508995	897083	69.50%	9.177%
79	9.539	2547	2550	2553	rBV2	162	134	0.01%	0.001%
80	9.738	2609	2612	2614	rBV	175	120	0.01%	0.001%
81	9.848	2642	2646	2650	rBV2	171	166	0.01%	0.002%
82	9.880	2653	2656	2663	rBV2	225	260	0.02%	0.003%
83	10.108	2723	2727	2736	rVB4	595	1011	0.08%	0.010%
84	10.147	2736	2739	2741	rBV	194	132	0.01%	0.001%
85	10.674	2895	2903	2912	rVB3	3692	5569	0.43%	0.057%
86	10.713	2913	2915	2919	rBV2	176	132	0.01%	0.001%
87	10.767	2919	2932	2950	rBV	464274	751703	58.23%	7.690%
88	11.092	3029	3033	3035	rBV3	631	560	0.04%	0.006%
89	11.375	3118	3121	3123	rBV	287	152	0.01%	0.002%
90	11.391	3123	3126	3130	rBV	352	353	0.03%	0.004%
91	11.465	3141	3149	3160	rVB6	3162	5752	0.45%	0.059%
92	11.700	3215	3222	3233	rBV4	1933	3140	0.24%	0.032%
93	11.819	3247	3259	3277	rBV	541102	847406	65.65%	8.669%
94	12.201	3360	3378	3397	rBV	583114	943330	73.08%	9.650%
95	12.336	3414	3420	3428	rVB4	2486	3607	0.28%	0.037%
96	12.378	3428	3433	3435	rBV2	261	251	0.02%	0.003%
97	12.404	3435	3441	3449	rVV5	964	1118	0.09%	0.011%
98	13.851	3885	3891	3898	rVB4	1589	2123	0.16%	0.022%
99	14.092	3960	3966	3978	rVB2	5343	8475	0.66%	0.087%
100	14.336	4036	4042	4050	rBV5	2519	3500	0.27%	0.036%

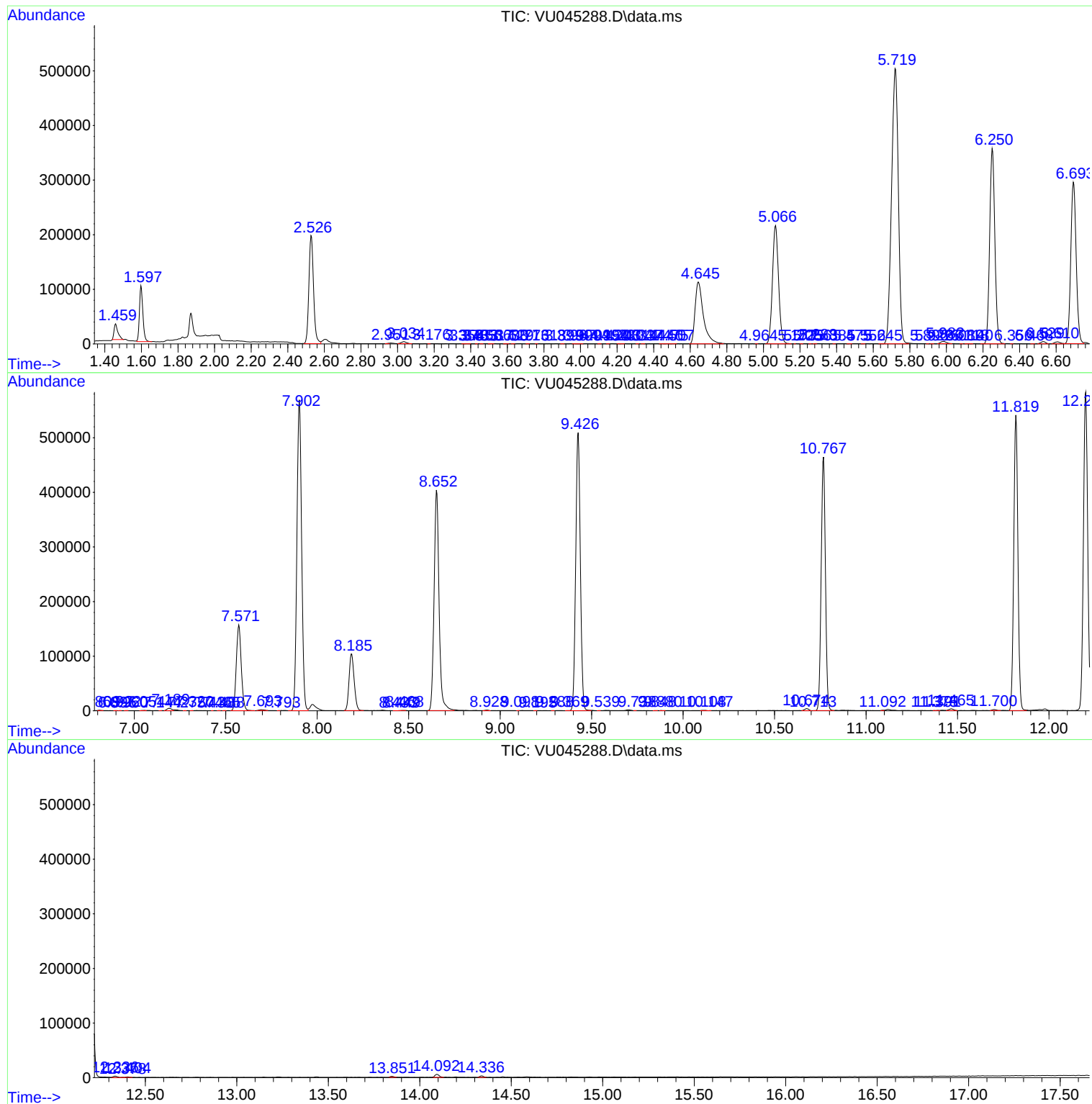
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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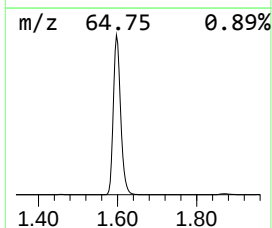
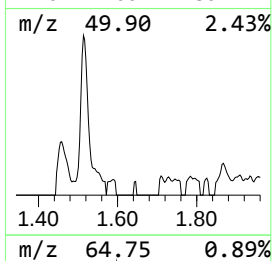
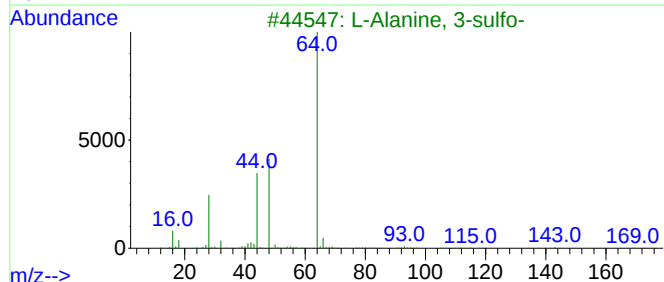
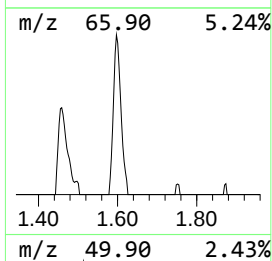
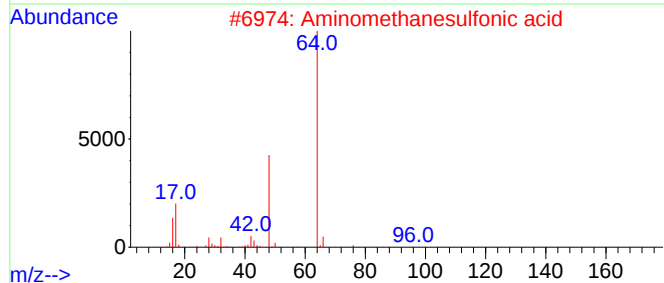
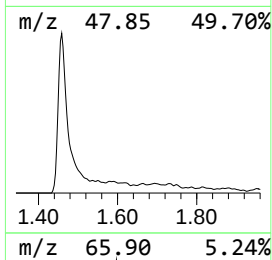
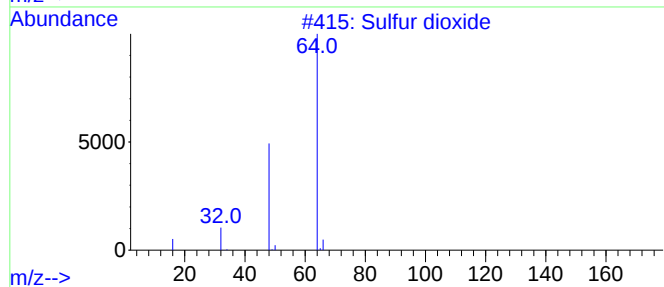
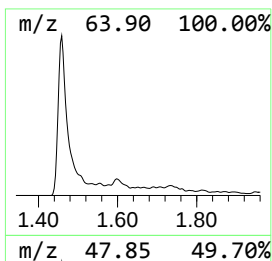
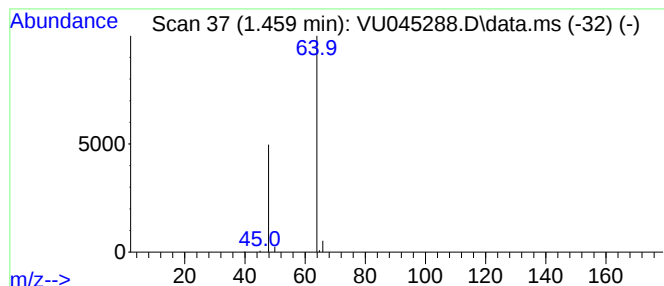
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.459	2.92 ug/L	41122	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			Sulfur dioxide	64	O2S	007446-09-5	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	2.9	ug/L	41122	1	6.250	703726	50.0