

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050918\
 Data File : VU023759.D
 Acq On : 09 May 2018 14:19
 Operator : MD/SY
 Sample : J2746-04
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050818WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	0.661	16	22	26	rBV2	139	200	0.01%	0.002%
2	0.738	44	46	50	rVB	144	86	0.01%	0.001%
3	0.776	50	58	62	rBV2	167	256	0.02%	0.002%
4	0.799	62	65	70	rVB2	132	110	0.01%	0.001%
5	0.982	116	122	124	rBV2	121	133	0.01%	0.001%
6	1.088	147	155	180	rBV	1367453	1523424	100.00%	13.136%
7	1.182	181	184	190	rVB3	4991	5074	0.33%	0.044%
8	1.288	207	217	232	rBV	48985	133799	8.78%	1.154%
9	1.400	246	252	288	rVB	173133	241746	15.87%	2.085%
10	1.680	332	339	357	rVB	127969	160923	10.56%	1.388%
11	2.272	513	523	537	rBV	273984	414323	27.20%	3.573%
12	2.429	570	572	575	rBV2	436	363	0.02%	0.003%
13	2.583	616	620	624	rBV3	396	335	0.02%	0.003%
14	2.702	648	657	662	rBV3	677	872	0.06%	0.008%
15	2.773	676	679	682	rBV	224	155	0.01%	0.001%
16	2.841	691	700	710	rBV3	1891	3794	0.25%	0.033%
17	2.976	740	742	744	rBV	179	110	0.01%	0.001%
18	3.034	758	760	763	rBV	171	117	0.01%	0.001%
19	3.095	776	779	782	rBV	239	132	0.01%	0.001%
20	3.117	783	786	790	rVV	139	121	0.01%	0.001%
21	3.291	836	840	844	rBV2	226	266	0.02%	0.002%
22	3.384	866	869	875	rBV2	211	193	0.01%	0.002%
23	3.445	881	888	890	rBV2	218	268	0.02%	0.002%
24	3.487	898	901	904	rBV2	186	157	0.01%	0.001%
25	3.580	926	930	932	rBV	205	157	0.01%	0.001%
26	3.596	933	935	940	rVB	145	131	0.01%	0.001%
27	3.661	951	955	957	rBV2	141	114	0.01%	0.001%
28	3.673	957	959	963	rVV2	148	128	0.01%	0.001%
29	3.899	1021	1029	1032	rBV2	270	353	0.02%	0.003%
30	3.921	1032	1036	1037	rBV	99	74	0.00%	0.001%
31	4.024	1064	1068	1073	rBV2	103	116	0.01%	0.001%
32	4.079	1082	1085	1089	rVB2	165	148	0.01%	0.001%
33	4.098	1089	1091	1094	rVB2	279	155	0.01%	0.001%
34	4.117	1094	1097	1100	rBV	241	191	0.01%	0.002%

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 Title : VOC Analysis

35	4.178	1100	1116	1158	rBV	121851	325400	21.36%	2.806%
36	4.323	1159	1161	1168	rVB3	624	675	0.04%	0.006%
37	4.474	1201	1208	1215	rVB3	257	497	0.03%	0.004%
38	4.506	1215	1218	1221	rBV	296	239	0.02%	0.002%
39	4.538	1225	1228	1229	rBV	262	170	0.01%	0.001%
40	4.651	1245	1263	1292	rBV	204092	479809	31.50%	4.137%
41	4.860	1324	1328	1331	rBV2	264	246	0.02%	0.002%
42	4.886	1331	1336	1339	rBV3	549	660	0.04%	0.006%
43	4.960	1356	1359	1363	rVB	187	146	0.01%	0.001%
44	4.979	1363	1365	1366	rBV	179	80	0.01%	0.001%
45	4.989	1366	1368	1370	rVV	147	68	0.00%	0.001%
46	5.053	1386	1388	1392	rVB	100	64	0.00%	0.001%
47	5.088	1395	1399	1402	rBV	263	220	0.01%	0.002%
48	5.239	1438	1446	1453	rVB	322	499	0.03%	0.004%
49	5.342	1453	1478	1522	rBV2	423847	1283745	84.27%	11.070%
50	5.638	1564	1570	1575	rVB2	242	339	0.02%	0.003%
51	5.677	1575	1582	1586	rBV2	272	354	0.02%	0.003%
52	5.715	1591	1594	1602	rVB2	157	185	0.01%	0.002%
53	5.754	1602	1606	1610	rBV2	284	275	0.02%	0.002%
54	5.799	1617	1620	1624	rVB	151	126	0.01%	0.001%
55	5.889	1633	1648	1678	rBV	382936	771413	50.64%	6.652%
56	6.178	1733	1738	1739	rBV3	1068	805	0.05%	0.007%
57	6.252	1760	1761	1764	rVB	167	63	0.00%	0.001%
58	6.268	1764	1766	1769	rBV	174	83	0.01%	0.001%
59	6.336	1769	1787	1808	rBV	282494	577185	37.89%	4.977%
60	6.516	1840	1843	1848	rVB2	119	119	0.01%	0.001%
61	6.541	1848	1851	1855	rVB2	126	90	0.01%	0.001%
62	6.648	1879	1884	1886	rBV	196	219	0.01%	0.002%
63	6.747	1911	1915	1921	rVB2	206	260	0.02%	0.002%
64	6.857	1944	1949	1951	rBV	361	344	0.02%	0.003%
65	6.937	1971	1974	1977	rBV	108	79	0.01%	0.001%
66	6.956	1977	1980	1982	rBV	126	67	0.00%	0.001%
67	6.972	1982	1985	1987	rBV	102	70	0.00%	0.001%
68	7.120	2028	2031	2033	rBV	124	90	0.01%	0.001%
69	7.149	2036	2040	2049	rVB2	606	721	0.05%	0.006%
70	7.233	2049	2066	2084	rBV	151921	274588	18.02%	2.368%
71	7.339	2097	2099	2102	rVB	204	69	0.00%	0.001%

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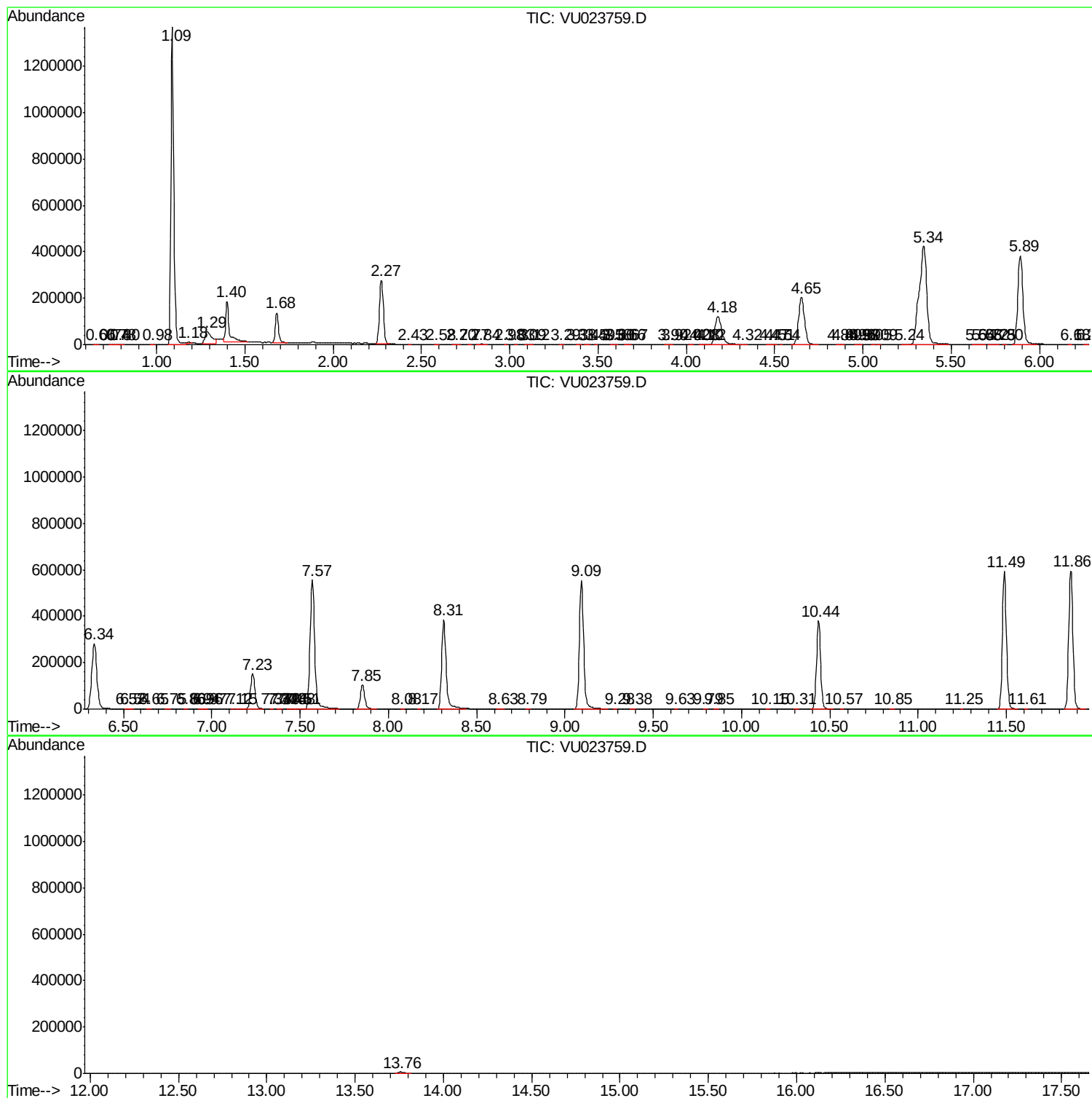
72	7.374	2108	2110	2113	rBV2	194	108	0.01%	0.001%
73	7.394	2113	2116	2118	rBV3	395	223	0.01%	0.002%
74	7.429	2126	2127	2133	rVB2	204	111	0.01%	0.001%
75	7.455	2133	2135	2139	rVB2	186	89	0.01%	0.001%
76	7.477	2139	2142	2145	rVB2	121	71	0.00%	0.001%
77	7.509	2147	2152	2157	rBV2	629	828	0.05%	0.007%
78	7.570	2157	2171	2218	rBV	555782	1027284	67.43%	8.858%
79	7.853	2248	2259	2284	rBV	102930	178133	11.69%	1.536%
80	8.078	2326	2329	2332	rBV	182	112	0.01%	0.001%
81	8.172	2355	2358	2360	rBV2	328	238	0.02%	0.002%
82	8.313	2390	2402	2441	rBV	385967	684341	44.92%	5.901%
83	8.628	2495	2500	2508	rVB3	566	719	0.05%	0.006%
84	8.789	2546	2550	2554	rBV	244	196	0.01%	0.002%
85	9.094	2632	2645	2690	rVV	554662	956741	62.80%	8.250%
86	9.284	2701	2704	2707	rBV	192	156	0.01%	0.001%
87	9.384	2730	2735	2740	rVB2	368	451	0.03%	0.004%
88	9.628	2808	2811	2814	rBV	176	138	0.01%	0.001%
89	9.789	2859	2861	2866	rVB	306	155	0.01%	0.001%
90	9.850	2877	2880	2886	rBV2	163	186	0.01%	0.002%
91	10.149	2969	2973	2976	rBV2	278	238	0.02%	0.002%
92	10.307	3019	3022	3027	rBV2	172	158	0.01%	0.001%
93	10.435	3049	3062	3087	rVB	380756	618289	40.59%	5.332%
94	10.570	3100	3104	3106	rBV2	268	257	0.02%	0.002%
95	10.847	3187	3190	3196	rBV	231	209	0.01%	0.002%
96	11.249	3312	3315	3316	rBV	219	125	0.01%	0.001%
97	11.487	3377	3389	3412	rBV	593109	941908	61.83%	8.122%
98	11.609	3424	3427	3431	rVB2	355	221	0.01%	0.002%
99	11.863	3494	3506	3532	rBV	593671	964817	63.33%	8.320%
100	13.757	4086	4095	4113	rBV3	5564	11817	0.78%	0.102%

Sum of corrected areas: 11596905

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Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050818WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



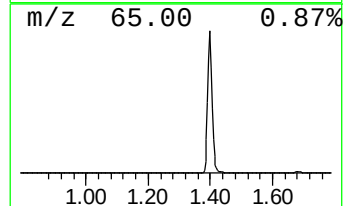
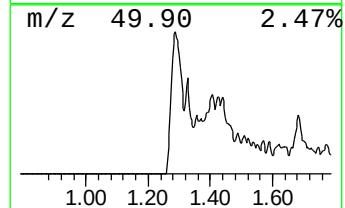
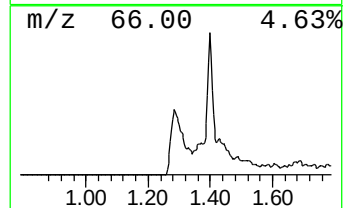
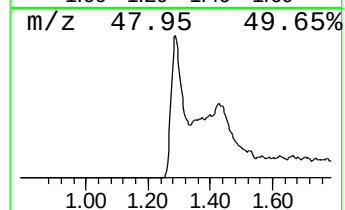
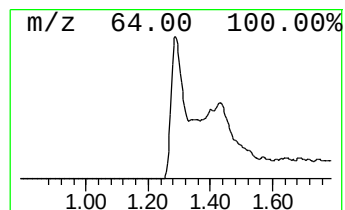
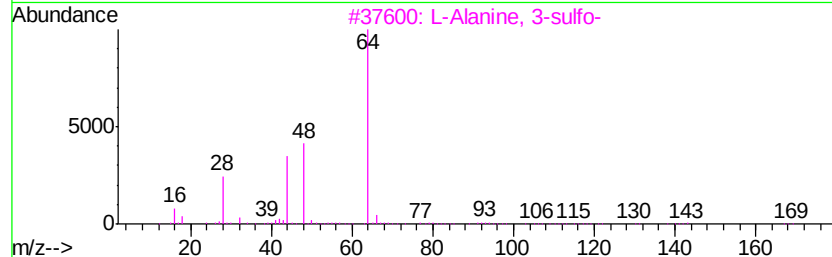
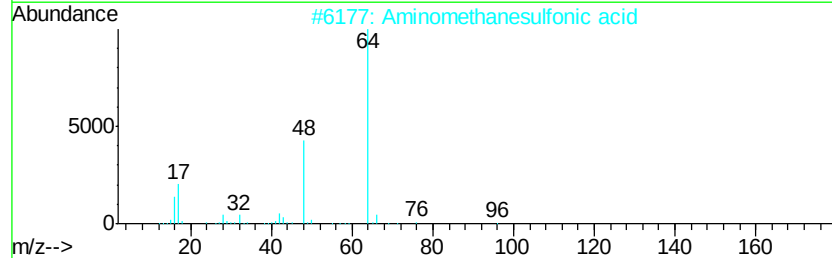
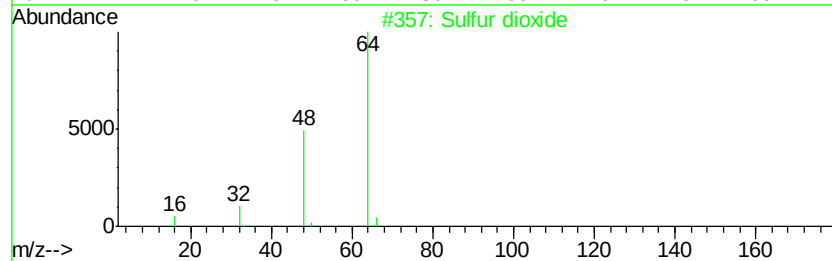
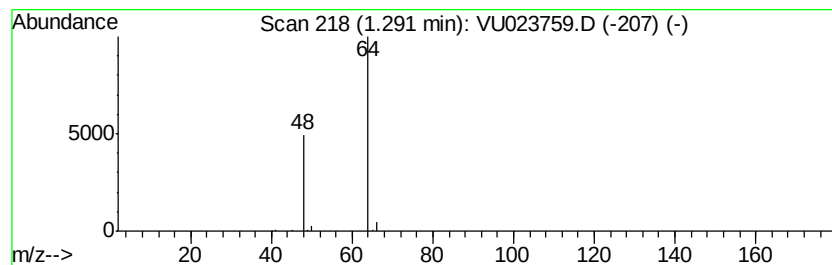
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.29	8.67 ug/L	133799	1,4-Difluorobenzene	5.89
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	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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.29	8.7	ug/L	133799	1	5.89	771413	50.0