

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050718\
 Data File : VU023719.D
 Acq On : 07 May 2018 17:43
 Operator : MD/SY
 Sample : J2725-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 17 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\SOMULM050118WMA.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	0.683	27	29	32	rVB	368	126	0.01%	0.001%
2	0.805	61	67	74	rBV2	184	288	0.02%	0.002%
3	0.918	98	102	108	rVB2	127	146	0.01%	0.001%
4	0.957	108	114	118	rBV2	151	171	0.01%	0.001%
5	1.005	118	129	132	rBV	146	230	0.02%	0.002%
6	1.088	135	155	180	rBV	970009	1103654	89.17%	9.561%
7	1.182	180	184	194	rVV2	7598	8240	0.67%	0.071%
8	1.291	208	218	234	rBV	26854	81111	6.55%	0.703%
9	1.400	246	252	260	rBV	142017	144724	11.69%	1.254%
10	1.680	332	339	358	rVB	117844	148214	11.98%	1.284%
11	2.272	513	523	537	rBV	243309	368692	29.79%	3.194%
12	2.403	561	564	567	rBV	306	226	0.02%	0.002%
13	2.445	567	577	600	rVB2	10893	23766	1.92%	0.206%
14	2.551	606	610	611	rBV	147	113	0.01%	0.001%
15	2.622	625	632	645	rVB2	930	1467	0.12%	0.013%
16	2.702	653	657	663	rVB3	559	593	0.05%	0.005%
17	2.754	670	673	678	rBV2	190	182	0.01%	0.002%
18	2.838	692	699	700	rBV2	815	975	0.08%	0.008%
19	2.911	719	722	730	rVB2	132	155	0.01%	0.001%
20	2.960	734	737	739	rBV	262	184	0.01%	0.002%
21	2.992	742	747	752	rVB3	820	940	0.08%	0.008%
22	3.227	816	820	824	rBV2	163	162	0.01%	0.001%
23	3.384	865	869	873	rBV3	279	291	0.02%	0.003%
24	3.526	910	913	915	rBV	185	130	0.01%	0.001%
25	3.574	925	928	932	rBV	196	188	0.02%	0.002%
26	3.622	938	943	949	rBV	220	219	0.02%	0.002%
27	3.661	952	955	961	rVB2	139	127	0.01%	0.001%
28	3.799	995	998	1003	rBV2	189	203	0.02%	0.002%
29	3.844	1009	1012	1015	rVB	200	121	0.01%	0.001%
30	3.966	1044	1050	1056	rBV2	191	235	0.02%	0.002%
31	4.043	1070	1074	1079	rBV2	198	196	0.02%	0.002%
32	4.178	1102	1116	1143	rBV	124434	328963	26.58%	2.850%
33	4.374	1174	1177	1179	rBV2	381	227	0.02%	0.002%
34	4.394	1179	1183	1185	rVV3	325	241	0.02%	0.002%

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 Title : VOC Analysis

35	4.651	1246	1263	1290	rBV	198901	467595	37.78%	4.051%
36	4.854	1323	1326	1330	rBV	287	154	0.01%	0.001%
37	4.892	1330	1338	1346	rVB3	668	1392	0.11%	0.012%
38	5.030	1376	1381	1386	rBV2	162	182	0.01%	0.002%
39	5.220	1436	1440	1443	rVB2	192	154	0.01%	0.001%
40	5.345	1453	1479	1522	rBV2	407064	1237682	100.00%	10.722%
41	5.641	1569	1571	1574	rBV	148	114	0.01%	0.001%
42	5.725	1594	1597	1600	rBV	192	134	0.01%	0.001%
43	5.744	1600	1603	1605	rBV2	298	216	0.02%	0.002%
44	5.789	1613	1617	1622	rBV4	487	498	0.04%	0.004%
45	5.892	1633	1649	1686	rBV	438186	892000	72.07%	7.727%
46	6.159	1727	1732	1736	rBV3	1066	1196	0.10%	0.010%
47	6.336	1769	1787	1808	rBV	278189	561704	45.38%	4.866%
48	6.542	1849	1851	1857	rVB2	316	195	0.02%	0.002%
49	6.570	1857	1860	1863	rBV	170	128	0.01%	0.001%
50	6.702	1898	1901	1906	rVB2	176	149	0.01%	0.001%
51	6.731	1906	1910	1911	rBV	158	110	0.01%	0.001%
52	6.860	1943	1950	1953	rBV4	905	997	0.08%	0.009%
53	6.911	1962	1966	1971	rVB	106	110	0.01%	0.001%
54	7.233	2053	2066	2095	rBV	148755	269116	21.74%	2.331%
55	7.381	2108	2112	2113	rBV2	406	277	0.02%	0.002%
56	7.570	2157	2171	2188	rBV	561122	981788	79.32%	8.505%
57	7.853	2248	2259	2283	rBV	101773	173563	14.02%	1.504%
58	7.979	2295	2298	2303	rBV2	224	141	0.01%	0.001%
59	8.165	2353	2356	2357	rBV	286	163	0.01%	0.001%
60	8.181	2357	2361	2365	rVV2	685	550	0.04%	0.005%
61	8.236	2375	2378	2386	rVB2	320	256	0.02%	0.002%
62	8.313	2390	2402	2431	rBV	430992	733704	59.28%	6.356%
63	8.577	2481	2484	2488	rBB2	175	112	0.01%	0.001%
64	8.689	2513	2519	2524	rBV	229	288	0.02%	0.002%
65	9.049	2627	2631	2632	rBV	185	138	0.01%	0.001%
66	9.095	2632	2645	2673	rVV	642068	1068763	86.35%	9.258%
67	9.262	2689	2697	2705	rVB	1183	1838	0.15%	0.016%
68	9.342	2718	2722	2725	rBV2	284	202	0.02%	0.002%
69	9.384	2725	2735	2743	rBV3	3183	4758	0.38%	0.041%
70	9.448	2752	2755	2759	rVB2	425	304	0.02%	0.003%
71	9.660	2819	2821	2826	rVB	192	138	0.01%	0.001%

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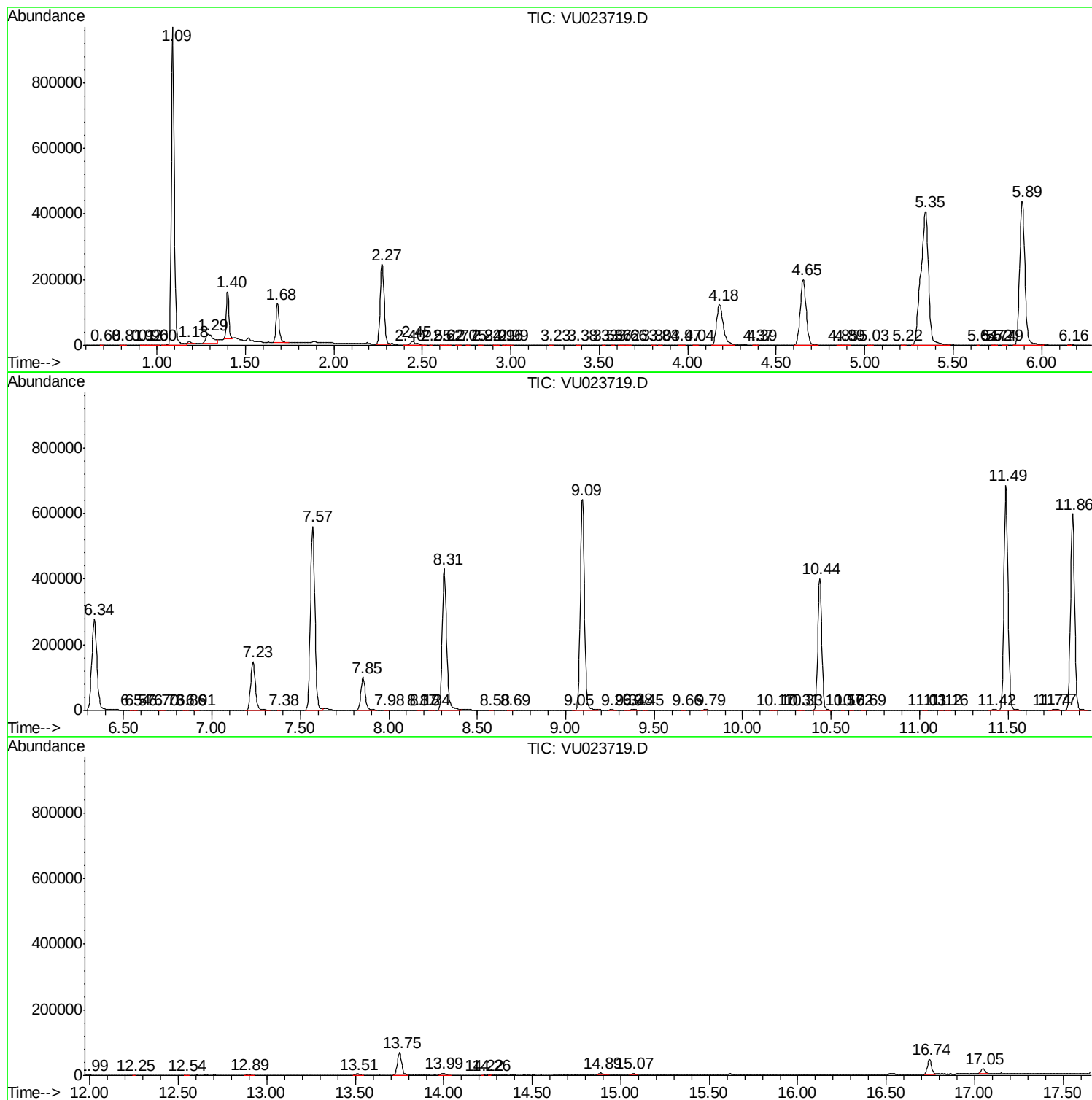
72	9.792	2853	2862	2864	rBV5	1117	1561	0.13%	0.014%
73	10.172	2973	2980	2986	rBV3	694	880	0.07%	0.008%
74	10.313	3021	3024	3027	rBV	192	125	0.01%	0.001%
75	10.332	3027	3030	3034	rVV2	204	140	0.01%	0.001%
76	10.435	3049	3062	3082	rBV	401293	635014	51.31%	5.501%
77	10.567	3099	3103	3104	rBV2	204	138	0.01%	0.001%
78	10.615	3115	3118	3121	rBV2	332	237	0.02%	0.002%
79	10.689	3136	3141	3143	rBV2	378	379	0.03%	0.003%
80	11.027	3243	3246	3251	rBV	185	183	0.01%	0.002%
81	11.120	3272	3275	3278	rVB3	334	240	0.02%	0.002%
82	11.156	3282	3286	3292	rVB3	576	664	0.05%	0.006%
83	11.422	3359	3369	3377	rVB7	1474	2657	0.21%	0.023%
84	11.487	3377	3389	3413	rBV	685600	1084481	87.62%	9.395%
85	11.737	3463	3467	3468	rBV	265	215	0.02%	0.002%
86	11.770	3469	3477	3486	rVB5	1986	3160	0.26%	0.027%
87	11.863	3493	3506	3532	rBV	598851	953586	77.05%	8.261%
88	11.985	3537	3544	3555	rVB4	1559	2456	0.20%	0.021%
89	12.249	3624	3626	3628	rBV	301	124	0.01%	0.001%
90	12.538	3714	3716	3724	rBV4	366	411	0.03%	0.004%
91	12.892	3819	3826	3837	rBV3	2962	3877	0.31%	0.034%
92	13.509	4011	4018	4028	rVB3	3954	5995	0.48%	0.052%
93	13.750	4082	4093	4108	rBV	68855	113570	9.18%	0.984%
94	13.991	4161	4168	4183	rVB4	4484	7709	0.62%	0.067%
95	14.216	4235	4238	4240	rBV	374	310	0.03%	0.003%
96	14.258	4249	4251	4254	rBV3	394	267	0.02%	0.002%
97	14.885	4440	4446	4460	rVB3	5742	9787	0.79%	0.085%
98	15.069	4496	4503	4512	rBV	4201	6010	0.49%	0.052%
99	16.744	5015	5024	5035	rBV	45412	71636	5.79%	0.621%
100	17.046	5112	5118	5127	rVB2	14315	21585	1.74%	0.187%

Sum of corrected areas: 11543706

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Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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



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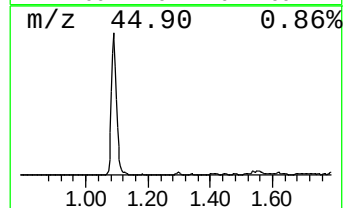
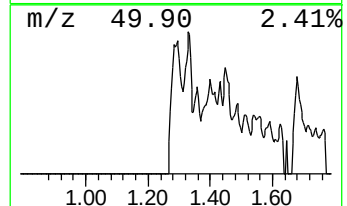
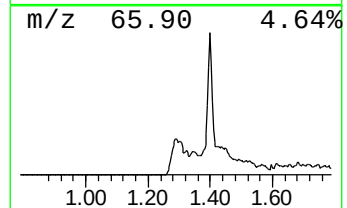
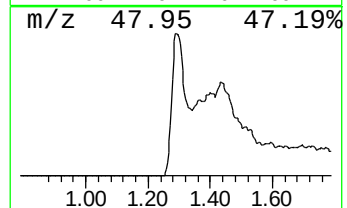
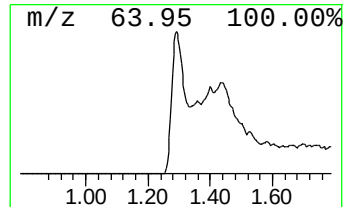
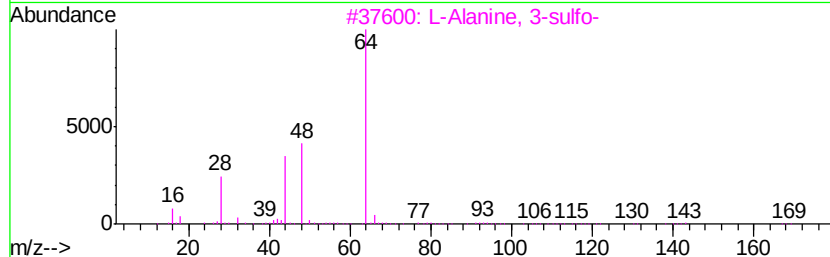
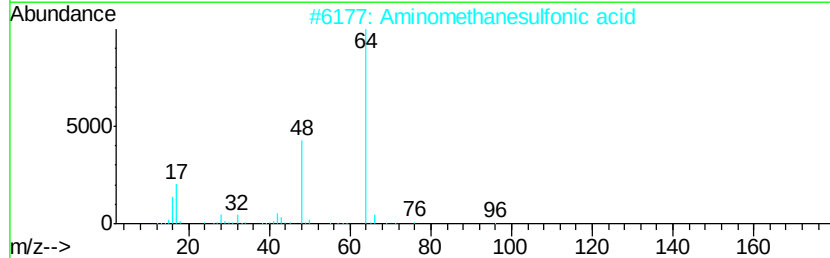
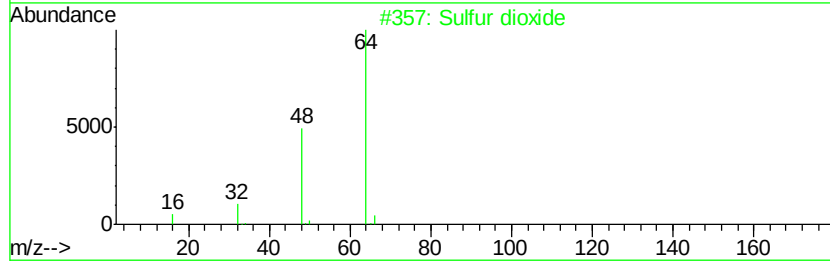
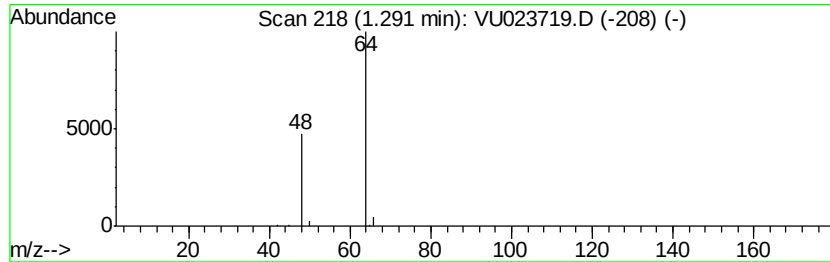
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.29	4.55 ug/L	81111	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.29	4.5	ug/L	81111	1	5.89	892000	50.0