

Data Path : W:\HPCHEM1\MSVOA U\Data\VU050818\
 Data File : VU023747.D
 Acq On : 08 May 2018 20:03
 Operator : MD/SY
 Sample : J2746-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 24 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	0.641	10	16	19	rVB	167	164	0.01%	0.001%
2	0.793	60	63	68	rBB2	119	111	0.00%	0.001%
3	0.867	83	86	88	rVV	208	119	0.01%	0.001%
4	0.992	119	125	132	rBV2	176	272	0.01%	0.002%
5	1.059	137	146	147	rBV	1220	1272	0.05%	0.009%
6	1.088	147	155	174	rBV	344128	396564	16.73%	2.682%
7	1.182	180	184	193	rBV3	6927	7491	0.32%	0.051%
8	1.281	206	215	229	rBV	178205	419490	17.70%	2.837%
9	1.397	246	251	300	rVB2	235356	474284	20.01%	3.208%
10	1.680	333	339	359	rVB	145494	190854	8.05%	1.291%
11	1.886	397	403	414	rVB	53557	74445	3.14%	0.504%
12	2.272	512	523	536	rBV	303753	457560	19.31%	3.095%
13	2.448	568	578	596	rBV3	10627	20052	0.85%	0.136%
14	2.612	624	629	632	rBV3	811	838	0.04%	0.006%
15	2.706	650	658	664	rBV4	1351	2209	0.09%	0.015%
16	2.837	688	699	712	rVB	4100	8102	0.34%	0.055%
17	2.928	724	727	735	rBV3	357	274	0.01%	0.002%
18	2.979	740	743	744	rBV	537	310	0.01%	0.002%
19	3.037	758	761	763	rBV2	439	329	0.01%	0.002%
20	3.387	866	870	876	rVB2	390	440	0.02%	0.003%
21	3.686	957	963	967	rBV2	181	202	0.01%	0.001%
22	3.821	1001	1005	1010	rBV2	198	204	0.01%	0.001%
23	3.963	1045	1049	1050	rBV	157	109	0.00%	0.001%
24	3.989	1054	1057	1062	rBV2	121	109	0.00%	0.001%
25	4.178	1100	1116	1161	rVV	132978	391596	16.52%	2.649%
26	4.374	1175	1177	1179	rVB2	484	210	0.01%	0.001%
27	4.558	1232	1234	1239	rVB3	314	257	0.01%	0.002%
28	4.651	1245	1263	1291	rVV	213226	503679	21.25%	3.407%
29	4.850	1323	1325	1330	rVB2	338	142	0.01%	0.001%
30	4.879	1330	1334	1336	rBV3	569	459	0.02%	0.003%
31	4.921	1344	1347	1351	rVB	195	134	0.01%	0.001%
32	4.979	1363	1365	1368	rBV	278	244	0.01%	0.002%
33	5.136	1406	1414	1423	rVV4	1036	2077	0.09%	0.014%
34	5.175	1423	1426	1430	rVB2	177	138	0.01%	0.001%

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

35	5.342	1454	1478	1531	rBV2	447718	1343601	56.70%	9.088%
36	5.619	1562	1564	1567	rVB	212	135	0.01%	0.001%
37	5.638	1567	1570	1573	rBV2	193	176	0.01%	0.001%
38	5.654	1573	1575	1578	rVV2	254	202	0.01%	0.001%
39	5.686	1582	1585	1588	rBV2	275	188	0.01%	0.001%
40	5.754	1603	1606	1612	rVB3	314	374	0.02%	0.003%
41	5.802	1617	1621	1626	rVB	260	224	0.01%	0.002%
42	5.889	1631	1648	1686	rBV	390685	799146	33.72%	5.405%
43	6.191	1726	1742	1773	rBV	1216604	2369751	100.00%	16.028%
44	6.336	1774	1787	1818	rVB	295630	610648	25.77%	4.130%
45	6.529	1844	1847	1851	rBV2	185	135	0.01%	0.001%
46	6.654	1882	1886	1891	rBV2	149	138	0.01%	0.001%
47	6.741	1907	1913	1915	rBV	105	112	0.00%	0.001%
48	6.870	1947	1953	1955	rBV2	251	295	0.01%	0.002%
49	6.960	1977	1981	1985	rBV2	194	198	0.01%	0.001%
50	7.233	2052	2066	2095	rBV	164002	291743	12.31%	1.973%
51	7.394	2113	2116	2126	rVB5	838	883	0.04%	0.006%
52	7.445	2126	2132	2134	rBV	233	193	0.01%	0.001%
53	7.474	2138	2141	2146	rVB2	266	182	0.01%	0.001%
54	7.570	2156	2171	2190	rBV	605951	1074298	45.33%	7.266%
55	7.812	2243	2246	2247	rBV2	267	172	0.01%	0.001%
56	7.853	2247	2259	2281	rVV	109142	186330	7.86%	1.260%
57	8.017	2306	2310	2312	rBV2	206	156	0.01%	0.001%
58	8.075	2323	2328	2335	rBV5	1097	1437	0.06%	0.010%
59	8.178	2352	2360	2364	rBV2	854	1155	0.05%	0.008%
60	8.230	2364	2376	2391	rVV	329647	572792	24.17%	3.874%
61	8.313	2392	2402	2439	rVB	440478	757864	31.98%	5.126%
62	8.622	2494	2498	2500	rBV2	280	224	0.01%	0.002%
63	8.776	2542	2546	2548	rBV2	452	279	0.01%	0.002%
64	8.850	2566	2569	2573	rVB2	179	151	0.01%	0.001%
65	8.879	2573	2578	2581	rBV2	203	226	0.01%	0.002%
66	8.914	2586	2589	2591	rBV	156	108	0.00%	0.001%
67	8.953	2598	2601	2604	rVB2	198	127	0.01%	0.001%
68	9.094	2631	2645	2686	rBV	576140	967371	40.82%	6.543%
69	9.262	2692	2697	2704	rVB2	998	1453	0.06%	0.010%
70	9.307	2704	2711	2717	rBV3	439	624	0.03%	0.004%
71	9.381	2728	2734	2743	rVB3	1765	2713	0.11%	0.018%

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

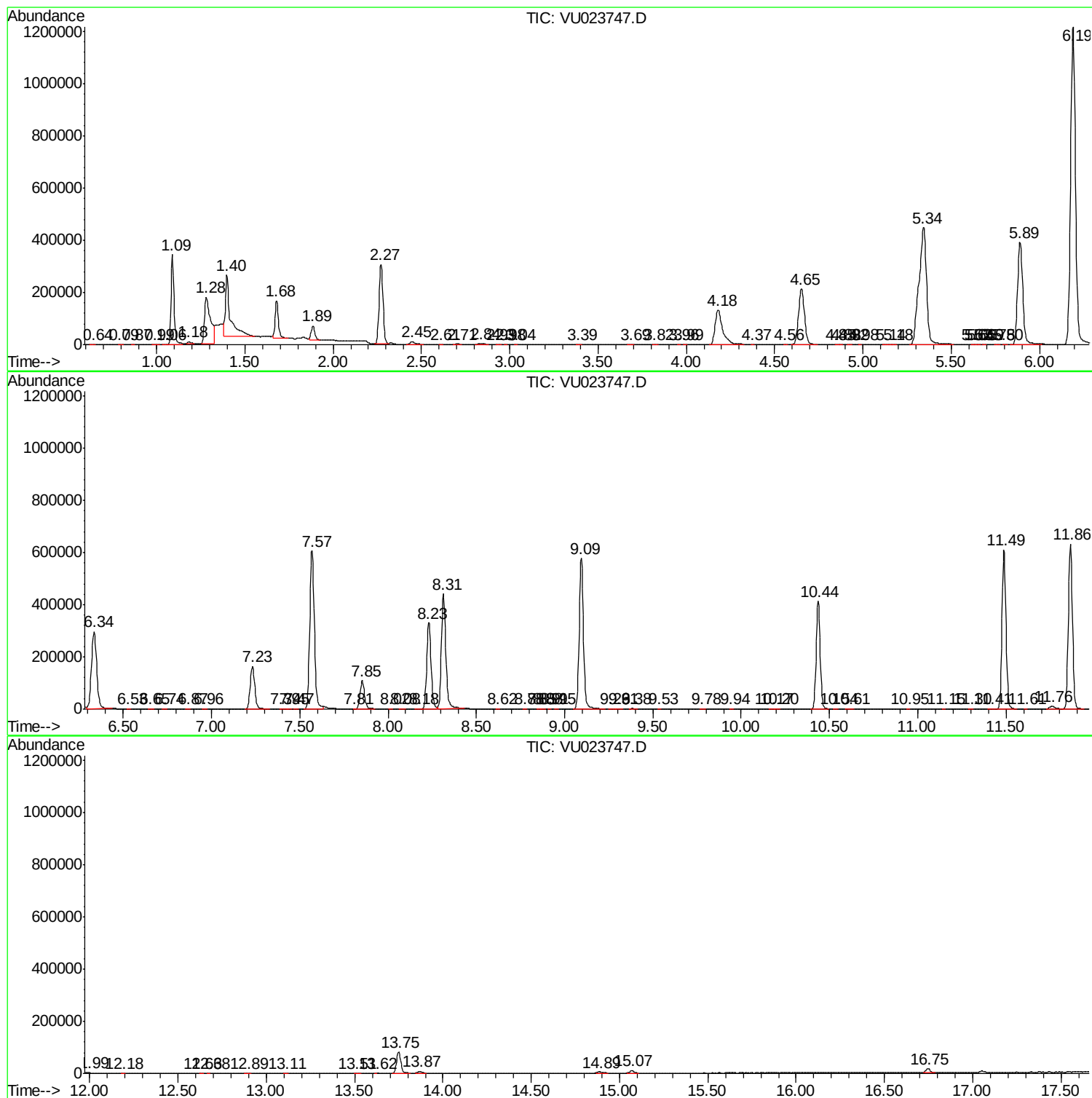
72	9.535	2779	2782	2785	rBV2	204	146	0.01%	0.001%
73	9.779	2854	2858	2863	rBV4	517	658	0.03%	0.004%
74	9.940	2906	2908	2913	rVB2	154	113	0.00%	0.001%
75	10.175	2975	2981	2985	rVV3	385	416	0.02%	0.003%
76	10.204	2985	2990	2994	rVB2	206	243	0.01%	0.002%
77	10.435	3049	3062	3080	rBV	412281	653677	27.58%	4.421%
78	10.541	3089	3095	3097	rBV2	210	230	0.01%	0.002%
79	10.612	3109	3117	3124	rVB4	612	986	0.04%	0.007%
80	10.947	3218	3221	3223	rBV	383	278	0.01%	0.002%
81	11.149	3281	3284	3285	rBV3	444	288	0.01%	0.002%
82	11.297	3327	3330	3334	rBV	262	239	0.01%	0.002%
83	11.413	3360	3366	3375	rVB5	864	1500	0.06%	0.010%
84	11.487	3377	3389	3412	rBV	610984	952954	40.21%	6.446%
85	11.609	3424	3427	3429	rBV2	300	197	0.01%	0.001%
86	11.760	3464	3474	3493	rBV4	10168	22077	0.93%	0.149%
87	11.863	3494	3506	3529	rVB	631816	1007164	42.50%	6.812%
88	11.988	3538	3545	3555	rVB3	3203	5237	0.22%	0.035%
89	12.184	3603	3606	3610	rBV	269	235	0.01%	0.002%
90	12.628	3742	3744	3748	rBV2	332	204	0.01%	0.001%
91	12.676	3754	3759	3760	rBV3	741	662	0.03%	0.004%
92	12.892	3821	3826	3832	rBB3	790	855	0.04%	0.006%
93	13.107	3890	3893	3897	rVB	404	281	0.01%	0.002%
94	13.506	4014	4017	4025	rBV2	683	966	0.04%	0.007%
95	13.618	4050	4052	4053	rBV	546	261	0.01%	0.002%
96	13.747	4081	4092	4112	rBV	82450	137034	5.78%	0.927%
97	13.869	4123	4130	4140	rVB	6399	8789	0.37%	0.059%
98	14.885	4441	4446	4461	rVB4	4780	8786	0.37%	0.059%
99	15.069	4495	4503	4514	rVB	9685	14949	0.63%	0.101%
100	16.747	5017	5025	5037	rVB4	14994	24799	1.05%	0.168%

Sum of corrected areas: 14784768

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ALS Vial : 24 Sample Multiplier: 1

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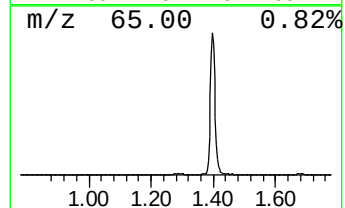
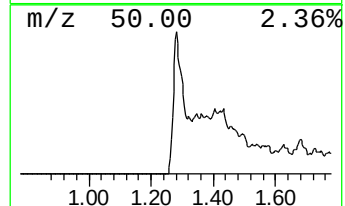
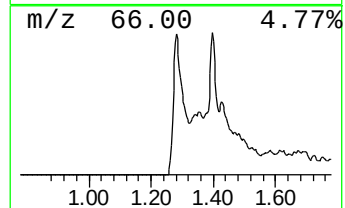
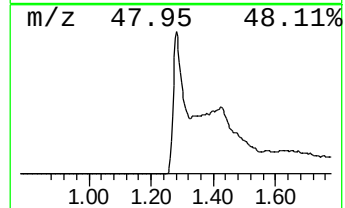
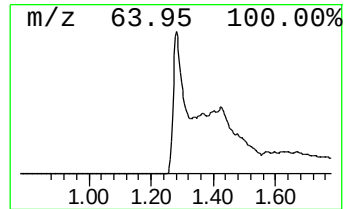
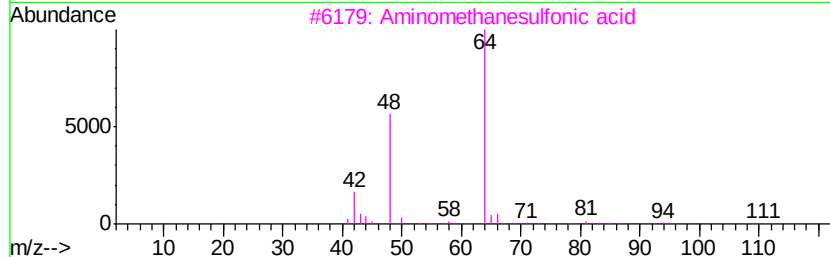
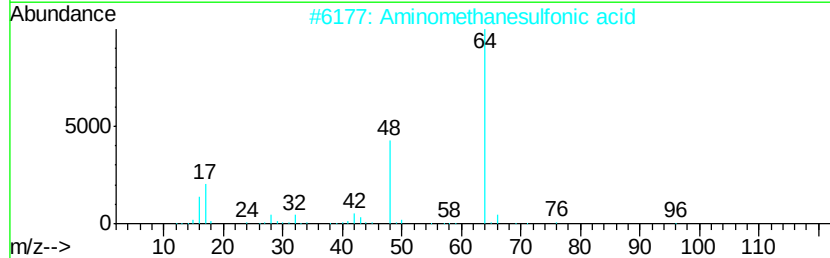
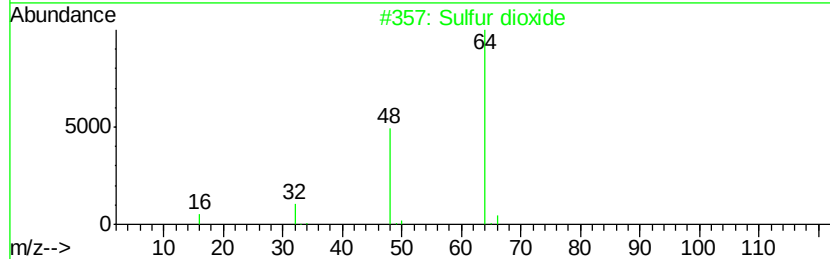
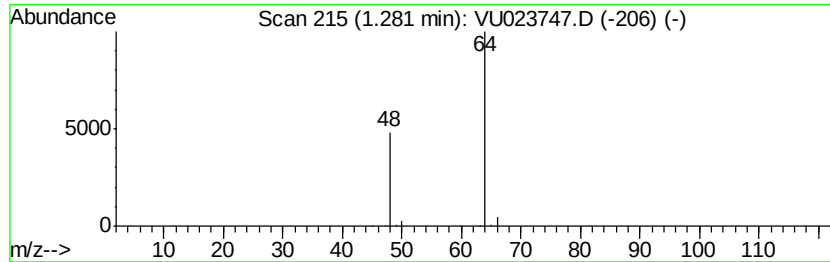
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050818WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	26.25 ug/L	419490	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		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	1.28	26.3	ug/L	419490	1	5.89	799146	50.0