

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060920\
 Data File : VU038680.D
 Acq On : 08 Jun 2020 20:41
 Operator : SY/MD
 Sample : L2896-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW0N0

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 : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.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	1.501	43	50	68	rBV2	24407	63670	2.99%	0.378%
2	1.613	77	85	99	rVB	281865	306249	14.38%	1.817%
3	1.703	108	113	128	rVB	25939	36078	1.69%	0.214%
4	1.932	175	184	202	rVB	210930	271968	12.77%	1.614%
5	2.526	362	369	372	rBV4	1699	1923	0.09%	0.011%
6	2.594	377	390	405	rBV	472438	799412	37.55%	4.744%
7	2.822	447	461	477	rBV5	7456	22434	1.05%	0.133%
8	2.941	494	498	500	rBV	500	377	0.02%	0.002%
9	3.076	529	540	553	rBV6	3929	8661	0.41%	0.051%
10	3.166	566	568	574	rBV2	478	377	0.02%	0.002%
11	3.215	574	583	584	rBV5	1462	1812	0.09%	0.011%
12	3.292	601	607	609	rBV3	821	809	0.04%	0.005%
13	3.321	612	616	620	rVB2	422	323	0.02%	0.002%
14	3.369	628	631	633	rBV2	536	317	0.01%	0.002%
15	3.385	633	636	640	rVV3	590	576	0.03%	0.003%
16	3.462	656	660	662	rBV2	483	334	0.02%	0.002%
17	3.478	662	665	672	rVB2	549	478	0.02%	0.003%
18	3.787	757	761	767	rBV4	282	305	0.01%	0.002%
19	3.858	777	783	788	rBV2	1021	1179	0.06%	0.007%
20	4.070	845	849	855	rVB3	485	514	0.02%	0.003%
21	4.105	855	860	865	rBV2	383	469	0.02%	0.003%
22	4.169	876	880	883	rBV2	387	302	0.01%	0.002%
23	4.195	883	888	893	rVB3	320	301	0.01%	0.002%
24	4.369	936	942	946	rVB2	356	334	0.02%	0.002%
25	4.578	1004	1007	1009	rBV2	559	354	0.02%	0.002%
26	4.668	1018	1035	1073	rBV	227583	590529	27.74%	3.504%
27	4.938	1115	1119	1124	rVB3	431	385	0.02%	0.002%
28	4.999	1136	1138	1140	rVB2	610	283	0.01%	0.002%
29	5.102	1152	1170	1194	rBV	369054	807027	37.90%	4.789%
30	5.198	1198	1200	1206	rVB3	936	740	0.03%	0.004%
31	5.234	1206	1211	1217	rBV5	556	580	0.03%	0.003%
32	5.272	1221	1223	1227	rVB3	561	314	0.01%	0.002%
33	5.327	1230	1240	1252	rVB5	2099	3878	0.18%	0.023%
34	5.520	1296	1300	1304	rBV2	277	285	0.01%	0.002%

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Integration Parameters: LSCINT.P

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

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
 Title : VOC Analysis

35	5.555	1307	1311	1313	rBV2	590	416	0.02%	0.002%
36	5.600	1322	1325	1330	rBV3	381	347	0.02%	0.002%
37	5.758	1348	1374	1411	rBV2	790541	2129177	100.00%	12.635%
38	5.906	1418	1420	1425	rBV2	443	341	0.02%	0.002%
39	5.957	1433	1436	1438	rBV2	555	337	0.02%	0.002%
40	6.009	1448	1452	1457	rVB5	623	476	0.02%	0.003%
41	6.057	1464	1467	1468	rBV2	1010	471	0.02%	0.003%
42	6.134	1488	1491	1495	rBV4	664	670	0.03%	0.004%
43	6.202	1507	1512	1514	rBV2	325	322	0.02%	0.002%
44	6.279	1520	1536	1562	rBV	658331	1263970	59.36%	7.501%
45	6.562	1614	1624	1638	rBV	6532	17290	0.81%	0.103%
46	6.632	1644	1646	1651	rVB3	1523	1010	0.05%	0.006%
47	6.719	1658	1673	1691	rBV	465906	909694	42.73%	5.398%
48	6.912	1730	1733	1739	rBV2	582	544	0.03%	0.003%
49	7.047	1773	1775	1780	rVB2	758	533	0.03%	0.003%
50	7.073	1780	1783	1786	rBV2	437	324	0.02%	0.002%
51	7.169	1808	1813	1816	rBV2	258	305	0.01%	0.002%
52	7.211	1816	1826	1834	rVB3	1744	2775	0.13%	0.016%
53	7.475	1901	1908	1911	rBV	448	479	0.02%	0.003%
54	7.491	1911	1913	1918	rVB2	384	288	0.01%	0.002%
55	7.591	1930	1944	1963	rBV	273781	471670	22.15%	2.799%
56	7.700	1975	1978	1980	rBV3	918	555	0.03%	0.003%
57	7.771	1997	2000	2006	rVB3	930	661	0.03%	0.004%
58	7.816	2006	2014	2024	rBV3	3586	5778	0.27%	0.034%
59	7.922	2032	2047	2063	rBV	951222	1673151	78.58%	9.929%
60	8.121	2107	2109	2116	rVB5	734	573	0.03%	0.003%
61	8.201	2121	2134	2151	rBV	188719	319586	15.01%	1.896%
62	8.491	2214	2224	2234	rVB4	10435	18521	0.87%	0.110%
63	8.578	2244	2251	2256	rVB4	1125	1436	0.07%	0.009%
64	8.655	2256	2275	2310	rBV	721421	1290531	60.61%	7.658%
65	8.857	2336	2338	2343	rVB2	1149	670	0.03%	0.004%
66	9.436	2501	2518	2551	rVV	926064	1586014	74.49%	9.412%
67	9.587	2560	2565	2574	rVB6	1672	2417	0.11%	0.014%
68	9.706	2593	2602	2611	rBV6	3417	5229	0.25%	0.031%
69	10.121	2723	2731	2740	rBV6	2718	4384	0.21%	0.026%
70	10.205	2754	2757	2765	rVB2	441	482	0.02%	0.003%
71	10.388	2811	2814	2819	rBV2	454	320	0.02%	0.002%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
 Title : VOC Analysis

72	10.497	2842	2848	2855	rVB3	991	1319	0.06%	0.008%
73	10.770	2920	2933	2950	rBV	642703	1038853	48.79%	6.165%
74	10.902	2963	2974	2984	rBV2	9321	14751	0.69%	0.088%
75	10.973	2992	2996	3000	rBV	336	328	0.02%	0.002%
76	11.063	3021	3024	3027	rVB2	863	601	0.03%	0.004%
77	11.098	3030	3035	3041	rBV3	1109	1507	0.07%	0.009%
78	11.317	3100	3103	3106	rVB3	412	287	0.01%	0.002%
79	11.426	3134	3137	3142	rVB3	691	472	0.02%	0.003%
80	11.481	3148	3154	3161	rVB6	1788	2373	0.11%	0.014%
81	11.735	3229	3233	3234	rVV	506	388	0.02%	0.002%
82	11.758	3234	3240	3247	rVV4	3111	3670	0.17%	0.022%
83	11.822	3247	3260	3278	rVV	974088	1537358	72.20%	9.123%
84	11.899	3282	3284	3287	rVB2	525	287	0.01%	0.002%
85	11.967	3302	3305	3307	rBV2	498	300	0.01%	0.002%
86	12.031	3322	3325	3328	rBV2	503	314	0.01%	0.002%
87	12.082	3331	3341	3354	rBV4	7206	13946	0.65%	0.083%
88	12.204	3365	3379	3397	rVB	963242	1559574	73.25%	9.255%
89	12.587	3495	3498	3502	rBV	423	364	0.02%	0.002%
90	12.722	3535	3540	3544	rVB2	432	387	0.02%	0.002%
91	12.796	3557	3563	3564	rBV3	1400	1289	0.06%	0.008%
92	13.015	3626	3631	3638	rBV2	718	922	0.04%	0.005%
93	13.085	3650	3653	3655	rBV2	399	332	0.02%	0.002%
94	13.237	3691	3700	3708	rBV6	3313	5480	0.26%	0.033%
95	13.786	3869	3871	3876	rBV2	654	550	0.03%	0.003%
96	13.867	3889	3896	3904	rVB7	5026	7870	0.37%	0.047%
97	14.063	3954	3957	3960	rBV2	742	471	0.02%	0.003%
98	14.111	3965	3972	3984	rVB2	9410	14746	0.69%	0.088%
99	14.359	4042	4049	4055	rBV4	5354	6852	0.32%	0.041%
100	14.989	4243	4245	4248	rVB3	978	541	0.03%	0.003%

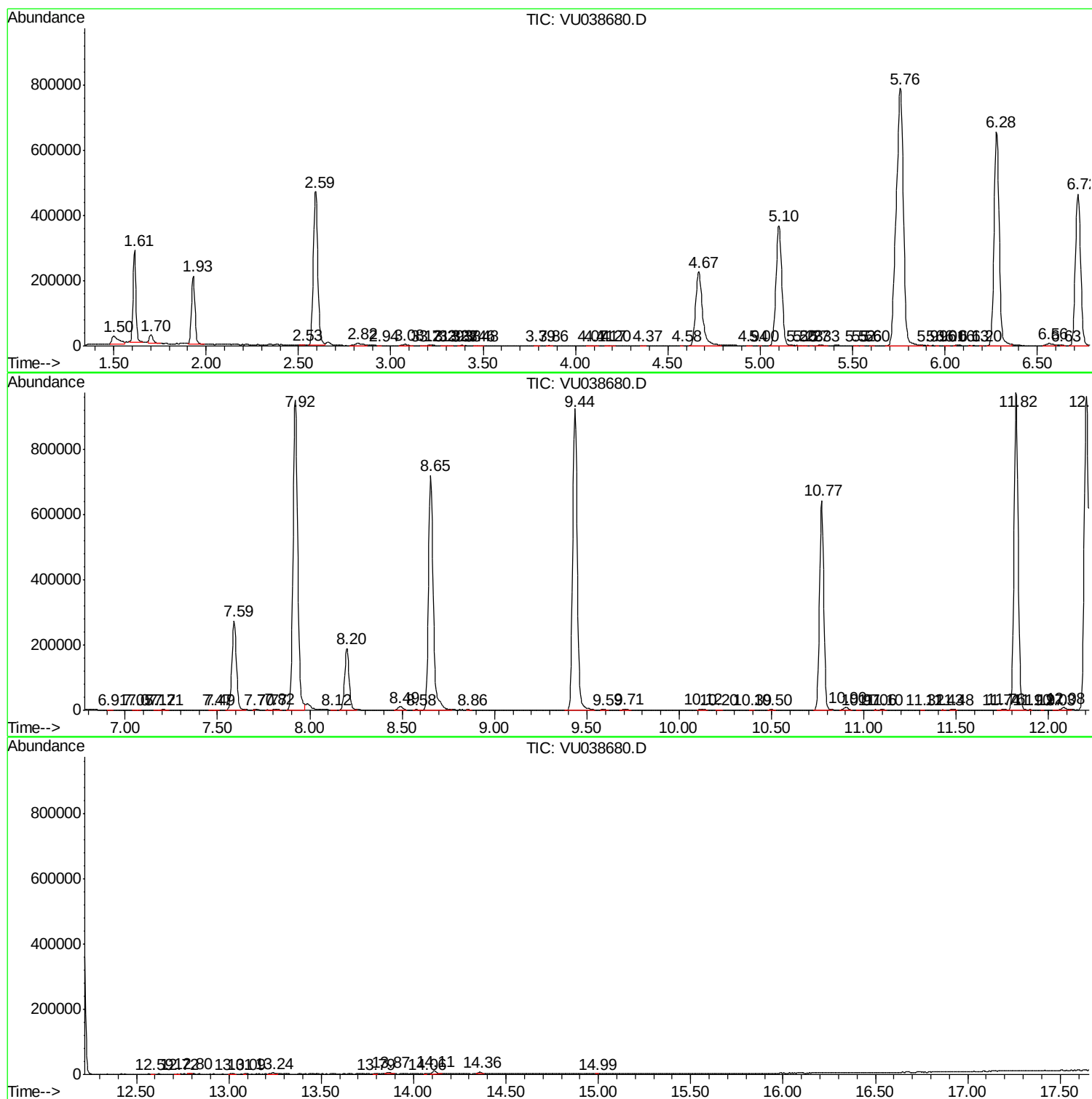
Sum of corrected areas: 16851456

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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



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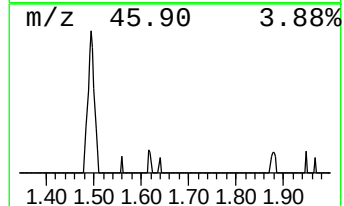
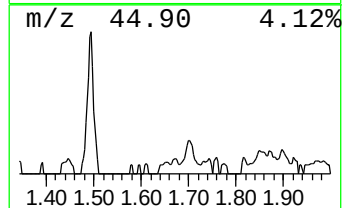
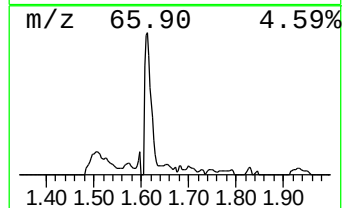
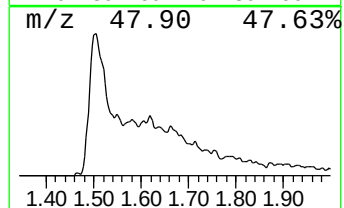
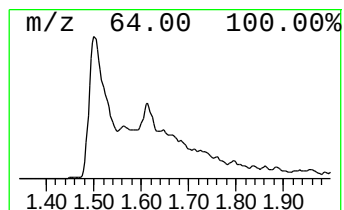
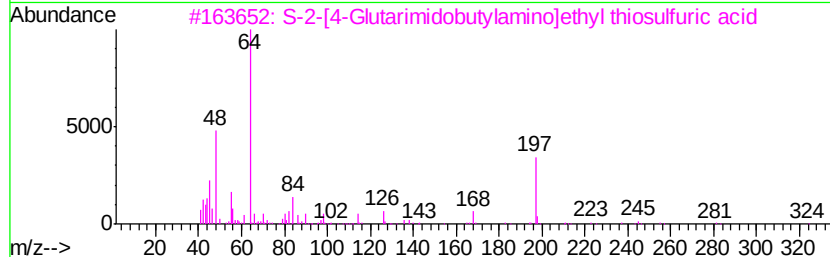
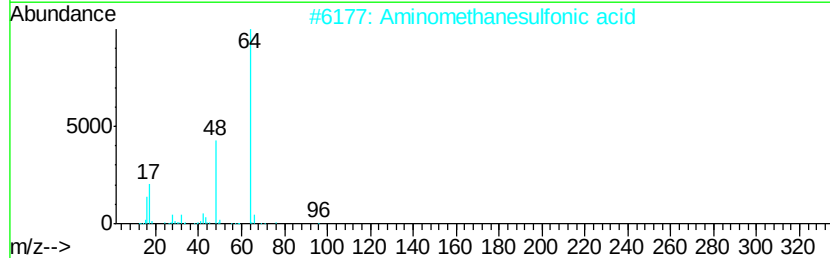
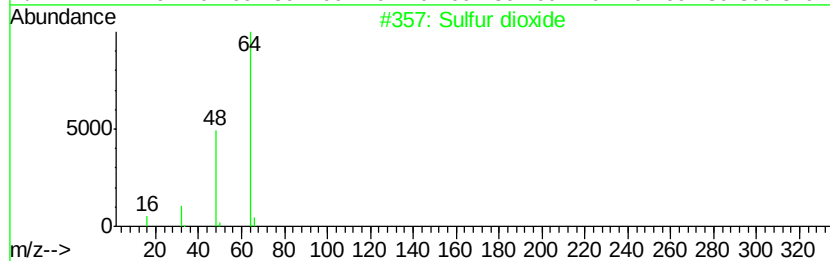
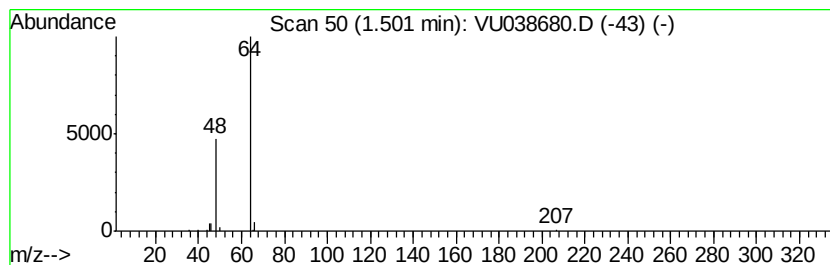
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	2.52 ug/L	63670	1,4-Difluorobenzene	6.28
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		S-2-[4-Glutarimidobutylamino]eth...	324 C11H20N2O5S2	031701-78-7 9
4		L-Alanine, 3-sulfo-	169 C3H7NO5S	000498-40-8 9
5		2,4,6-Triamino-5-pyrimidinyl hyd...	221 C4H7N5O4S	071552-23-3 9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.50	2.5	ug/L	63670	1	6.28	1263970	50.0