

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061020\
 Data File : VU038739.D
 Acq On : 09 Jun 2020 21:43
 Operator : SY/MD
 Sample : L2897-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW0H7

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	1.492	40	47	62	rBV	37961	82920	4.17%	0.518%
2	1.614	78	85	99	rVB	226937	249671	12.55%	1.560%
3	1.929	175	183	196	rVB	179516	231215	11.62%	1.445%
4	2.446	340	344	347	rBV6	963	776	0.04%	0.005%
5	2.514	361	365	366	rBV2	1264	841	0.04%	0.005%
6	2.591	377	389	405	rBV	414061	680676	34.21%	4.254%
7	2.713	424	427	429	rBV	792	535	0.03%	0.003%
8	2.803	449	455	456	rBV3	863	748	0.04%	0.005%
9	2.916	487	490	494	rBV2	342	325	0.02%	0.002%
10	2.987	509	512	516	rVB2	430	320	0.02%	0.002%
11	3.102	546	548	551	rBV	585	367	0.02%	0.002%
12	3.151	561	563	566	rVB	530	267	0.01%	0.002%
13	3.180	566	572	575	rBV2	504	559	0.03%	0.003%
14	3.209	575	581	585	rBV3	1153	1156	0.06%	0.007%
15	3.250	592	594	597	rVB	461	262	0.01%	0.002%
16	3.276	598	602	605	rVB	524	386	0.02%	0.002%
17	3.299	605	609	617	rBV4	401	558	0.03%	0.003%
18	3.385	628	636	638	rBV3	727	793	0.04%	0.005%
19	3.443	651	654	659	rVB2	701	667	0.03%	0.004%
20	3.472	659	663	664	rBV2	515	323	0.02%	0.002%
21	3.556	686	689	695	rVB2	528	612	0.03%	0.004%
22	3.598	695	702	707	rBV2	483	792	0.04%	0.005%
23	3.636	709	714	716	rVB2	552	489	0.02%	0.003%
24	3.665	716	723	725	rBV	299	299	0.02%	0.002%
25	3.745	746	748	752	rVB	475	284	0.01%	0.002%
26	3.845	775	779	785	rBV2	215	268	0.01%	0.002%
27	3.890	789	793	798	rVV2	349	339	0.02%	0.002%
28	4.022	831	834	838	rBV	496	349	0.02%	0.002%
29	4.308	920	923	929	rVB2	463	381	0.02%	0.002%
30	4.443	961	965	969	rVV3	381	468	0.02%	0.003%
31	4.662	1016	1033	1061	rBV	221802	589747	29.64%	3.686%
32	4.877	1096	1100	1102	rBV2	456	290	0.01%	0.002%
33	4.996	1132	1137	1142	rVB3	605	543	0.03%	0.003%
34	5.099	1151	1169	1188	rBV	356599	782350	39.32%	4.890%

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 Title : VOC Analysis

35	5.257	1216	1218	1229	rVB4	622	863	0.04%	0.005%
36	5.321	1229	1238	1249	rBV8	1808	3826	0.19%	0.024%
37	5.475	1281	1286	1288	rBV3	363	273	0.01%	0.002%
38	5.552	1306	1310	1314	rBV3	554	398	0.02%	0.002%
39	5.643	1333	1338	1341	rBV2	313	290	0.01%	0.002%
40	5.761	1351	1375	1403	rBV2	725228	1989508	100.00%	12.434%
41	6.279	1520	1536	1575	rBV	647032	1261665	63.42%	7.885%
42	6.459	1589	1592	1595	rBV2	547	430	0.02%	0.003%
43	6.562	1614	1624	1635	rBV5	7274	17961	0.90%	0.112%
44	6.720	1658	1673	1697	rBV	452708	872918	43.88%	5.456%
45	6.829	1705	1707	1708	rBV2	963	441	0.02%	0.003%
46	6.893	1726	1727	1731	rBV2	429	333	0.02%	0.002%
47	7.060	1776	1779	1784	rBV2	267	297	0.01%	0.002%
48	7.122	1793	1798	1805	rBV	536	692	0.03%	0.004%
49	7.186	1816	1818	1819	rBV	824	382	0.02%	0.002%
50	7.202	1819	1823	1833	rVB4	1502	2417	0.12%	0.015%
51	7.321	1856	1860	1865	rBV	233	251	0.01%	0.002%
52	7.588	1930	1943	1960	rBV	250815	439746	22.10%	2.748%
53	7.707	1973	1980	1986	rVB3	1496	2458	0.12%	0.015%
54	7.749	1986	1993	1996	rBV2	483	580	0.03%	0.004%
55	7.922	2030	2047	2086	rBV	858650	1560956	78.46%	9.756%
56	8.138	2111	2114	2120	rVB3	286	267	0.01%	0.002%
57	8.199	2120	2133	2153	rBV	177483	299072	15.03%	1.869%
58	8.437	2204	2207	2211	rVB2	658	387	0.02%	0.002%
59	8.488	2213	2223	2233	rVB4	2368	4383	0.22%	0.027%
60	8.575	2244	2250	2258	rVB4	1800	2463	0.12%	0.015%
61	8.652	2258	2274	2305	rBV	690048	1229346	61.79%	7.683%
62	8.938	2360	2363	2365	rBV2	613	360	0.02%	0.002%
63	9.173	2428	2436	2440	rBV3	583	885	0.04%	0.006%
64	9.433	2503	2517	2557	rBV	928954	1597650	80.30%	9.985%
65	9.588	2557	2565	2572	rBV4	2064	3184	0.16%	0.020%
66	9.655	2581	2586	2591	rBV3	382	418	0.02%	0.003%
67	9.710	2598	2603	2610	rVB3	756	1010	0.05%	0.006%
68	9.765	2618	2620	2625	rVB	456	377	0.02%	0.002%
69	9.790	2625	2628	2634	rBV2	379	460	0.02%	0.003%
70	9.819	2634	2637	2641	rBV2	353	261	0.01%	0.002%
71	10.057	2707	2711	2715	rBV2	254	267	0.01%	0.002%

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 Title : VOC Analysis

72	10.121	2726	2731	2736	rBV3	764	1075	0.05%	0.007%
73	10.176	2745	2748	2752	rVB2	393	275	0.01%	0.002%
74	10.424	2821	2825	2830	rBV2	386	492	0.02%	0.003%
75	10.655	2894	2897	2899	rBV2	471	280	0.01%	0.002%
76	10.703	2909	2912	2916	rVB2	684	438	0.02%	0.003%
77	10.771	2916	2933	2955	rBV	633372	1021639	51.35%	6.385%
78	10.861	2955	2961	2964	rBV2	464	540	0.03%	0.003%
79	10.900	2969	2973	2974	rBV3	1102	674	0.03%	0.004%
80	11.092	3031	3033	3039	rVB2	371	302	0.02%	0.002%
81	11.121	3039	3042	3045	rBV2	511	296	0.01%	0.002%
82	11.472	3147	3151	3152	rBV	634	415	0.02%	0.003%
83	11.546	3172	3174	3178	rVB	453	284	0.01%	0.002%
84	11.581	3178	3185	3188	rBV2	562	707	0.04%	0.004%
85	11.729	3227	3231	3233	rBV2	464	360	0.02%	0.002%
86	11.822	3246	3260	3280	rBV	963324	1522023	76.50%	9.513%
87	12.080	3330	3340	3355	rBV3	5370	10395	0.52%	0.065%
88	12.202	3365	3378	3393	rBV	936754	1507153	75.76%	9.420%
89	12.298	3406	3408	3412	rVB3	649	391	0.02%	0.002%
90	12.385	3433	3435	3439	rBV2	319	255	0.01%	0.002%
91	12.591	3497	3499	3507	rVB2	687	540	0.03%	0.003%
92	12.777	3554	3557	3559	rBV2	708	500	0.03%	0.003%
93	12.871	3583	3586	3588	rBV	358	250	0.01%	0.002%
94	12.925	3600	3603	3607	rVB	615	428	0.02%	0.003%
95	13.044	3637	3640	3643	rBV2	463	403	0.02%	0.003%
96	13.424	3755	3758	3760	rBV2	700	409	0.02%	0.003%
97	13.555	3796	3799	3801	rBV3	656	394	0.02%	0.002%
98	13.922	3912	3913	3916	rBV2	527	338	0.02%	0.002%
99	14.063	3955	3957	3961	rBV2	528	362	0.02%	0.002%
100	15.256	4326	4328	4329	rBV	726	292	0.01%	0.002%

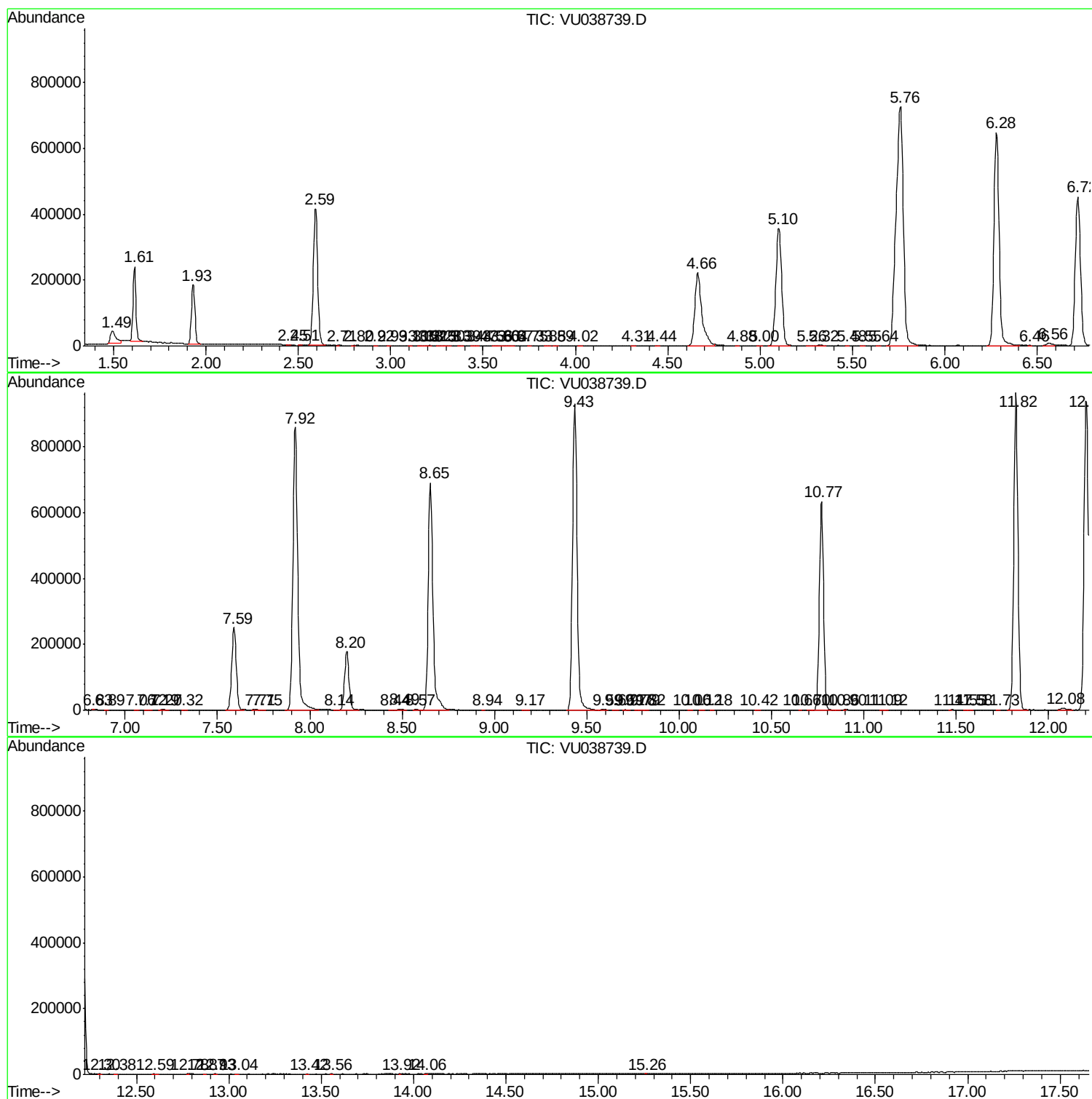
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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



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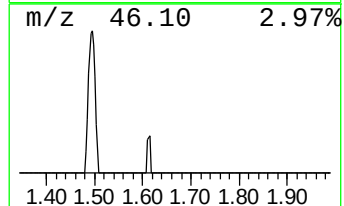
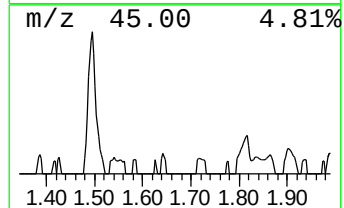
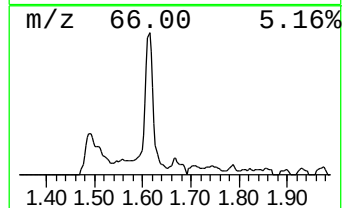
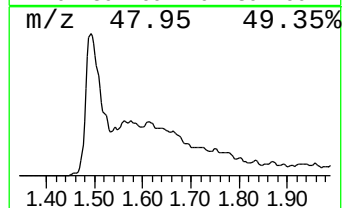
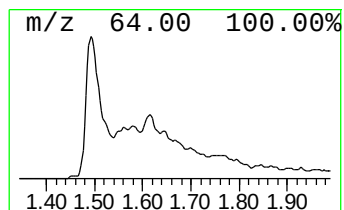
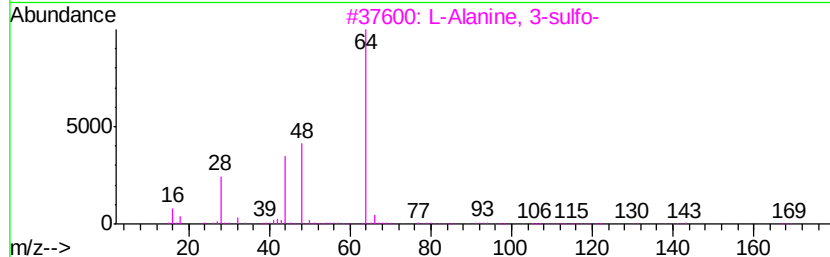
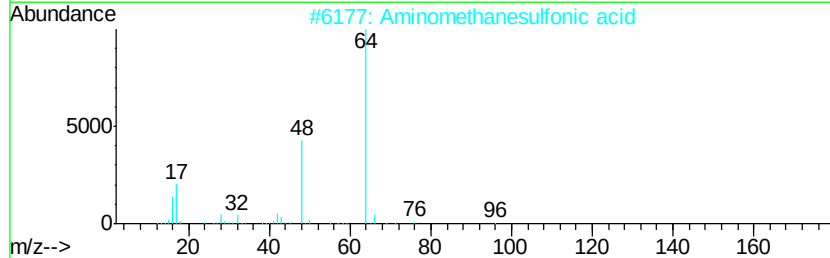
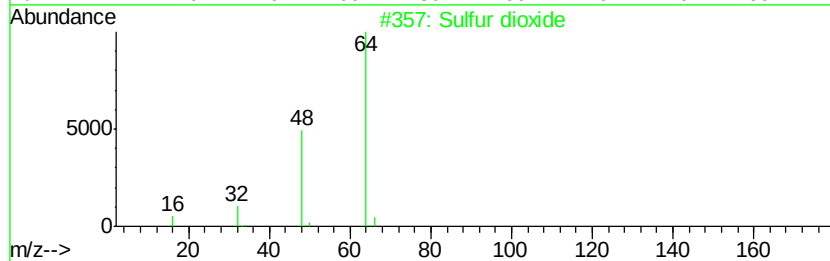
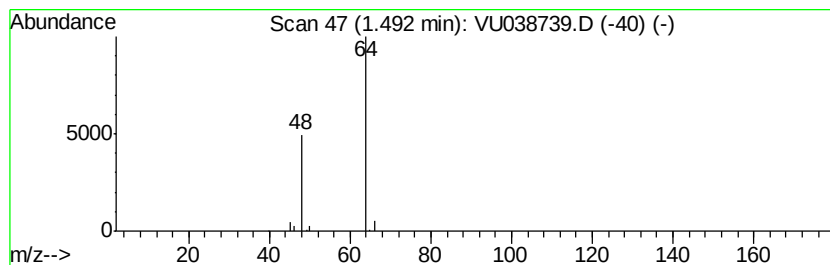
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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.
1.49	3.29 ug/L	82920	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 74
3		L-Alanine, 3-sulfo-	169 C3H7NO5S	000498-40-8 9
4		Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9 9
5		Ethene, 1,2-difluoro-	64 C2H2F2	001691-13-0 5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.49	3.3	ug/L	82920	1	6.28	1261670	50.0