

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100821\  
 Data File : VU045260.D  
 Acq On : 08 Oct 2021 18:38  
 Operator : SY/MD  
 Sample : M4024-21  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VHBLK001

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF Filtering: 5  
 Sampling : 1 Min Area: 0 % of largest Peak  
 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Title : VOC Analysis

Signal : TIC: VU045260.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	53	rBV	26784	47896	3.49%	0.475%
2	1.601	74	81	94	rVB	211152	230914	16.84%	2.289%
3	1.896	165	173	194	rVB	149534	205593	14.99%	2.038%
4	2.562	368	380	399	rBV	282618	474665	34.61%	4.706%
5	2.790	447	451	455	rBV3	259	261	0.02%	0.003%
6	2.954	496	502	503	rBV2	336	344	0.03%	0.003%
7	3.047	521	531	543	rVB2	6021	10736	0.78%	0.106%
8	3.192	570	576	580	rVB3	259	267	0.02%	0.003%
9	3.250	591	594	597	rBV	228	201	0.01%	0.002%
10	3.346	620	624	627	rBV	194	186	0.01%	0.002%
11	3.392	635	638	641	rBV2	195	161	0.01%	0.002%
12	3.536	680	683	687	rBV	248	270	0.02%	0.003%
13	3.739	744	746	751	rVB2	182	168	0.01%	0.002%
14	3.768	751	755	758	rBV2	203	234	0.02%	0.002%
15	3.845	775	779	782	rBV	216	216	0.02%	0.002%
16	4.083	848	853	859	rBV2	247	355	0.03%	0.004%
17	4.202	887	890	895	rBV2	162	173	0.01%	0.002%
18	4.269	907	911	915	rBV	229	215	0.02%	0.002%
19	4.324	922	928	933	rBV2	180	296	0.02%	0.003%
20	4.626	1007	1022	1052	rBV	155140	364649	26.59%	3.615%
21	5.067	1141	1159	1180	rBV	234463	518304	37.80%	5.139%
22	5.247	1212	1215	1219	rBV	225	185	0.01%	0.002%
23	5.289	1224	1228	1237	rVV3	695	1110	0.08%	0.011%
24	5.372	1252	1254	1258	rVB3	357	264	0.02%	0.003%
25	5.469	1282	1284	1287	rBV2	193	162	0.01%	0.002%
26	5.571	1309	1316	1320	rVB2	233	305	0.02%	0.003%
27	5.729	1340	1365	1385	rBV2	511589	1371337	100.00%	13.596%
28	6.044	1460	1463	1469	rVB2	361	410	0.03%	0.004%
29	6.115	1482	1485	1487	rBV2	261	173	0.01%	0.002%
30	6.253	1513	1528	1549	rBV	356693	663727	48.40%	6.581%
31	6.491	1599	1602	1606	rVV2	270	238	0.02%	0.002%
32	6.533	1606	1615	1627	rVB7	4824	9558	0.70%	0.095%
33	6.697	1651	1666	1686	rBV	324005	627196	45.74%	6.218%
34	6.797	1694	1697	1699	rBV2	563	380	0.03%	0.004%
35	6.813	1699	1702	1709	rVB5	1000	1172	0.09%	0.012%
36	6.851	1711	1714	1719	rVB2	332	267	0.02%	0.003%

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 ClientSampled :  
 VHBLK001

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

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Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Title : VOC Analysis

37	6.880	1719	1723	1728	rBV2	301	292	0.02%	0.003%
38	6.954	1741	1746	1751	rBV2	202	334	0.02%	0.003%
39	6.977	1751	1753	1758	rVV2	203	204	0.01%	0.002%
40	7.051	1769	1776	1787	rVV3	636	1175	0.09%	0.012%
41	7.153	1801	1808	1810	rBV2	271	366	0.03%	0.004%
42	7.182	1810	1817	1826	rVV3	891	1433	0.10%	0.014%
43	7.327	1857	1862	1866	rVB2	258	276	0.02%	0.003%
44	7.359	1866	1872	1875	rBV2	231	318	0.02%	0.003%
45	7.459	1900	1903	1907	rVB	217	196	0.01%	0.002%
46	7.488	1907	1912	1916	rBV2	147	198	0.01%	0.002%
47	7.568	1924	1937	1954	rBV	174213	301747	22.00%	2.992%
48	7.687	1972	1974	1976	rBV2	349	199	0.01%	0.002%
49	7.739	1985	1990	1994	rBV2	212	273	0.02%	0.003%
50	7.845	2020	2023	2027	rBV2	217	219	0.02%	0.002%
51	7.903	2027	2041	2055	rBV	612128	1052555	76.75%	10.436%
52	7.970	2057	2062	2074	rVB3	8236	13554	0.99%	0.134%
53	8.060	2089	2090	2095	rBV	197	197	0.01%	0.002%
54	8.086	2095	2098	2107	rVB3	395	482	0.04%	0.005%
55	8.182	2116	2128	2146	rBV	122870	202706	14.78%	2.010%
56	8.382	2186	2190	2193	rBV2	300	253	0.02%	0.003%
57	8.636	2256	2269	2307	rBV	448707	790447	57.64%	7.837%
58	8.829	2327	2329	2334	rVB	270	254	0.02%	0.003%
59	9.034	2389	2393	2397	rBV2	172	173	0.01%	0.002%
60	9.147	2422	2428	2432	rBV2	179	254	0.02%	0.003%
61	9.288	2466	2472	2475	rBV2	195	239	0.02%	0.002%
62	9.369	2494	2497	2499	rBV2	228	184	0.01%	0.002%
63	9.420	2499	2513	2547	rVB	514402	836330	60.99%	8.292%
64	9.568	2553	2559	2561	rBV2	489	509	0.04%	0.005%
65	9.581	2561	2563	2569	rVB2	465	405	0.03%	0.004%
66	9.694	2590	2598	2608	rVB2	2076	2906	0.21%	0.029%
67	9.825	2636	2639	2642	rBV2	193	157	0.01%	0.002%
68	9.909	2661	2665	2667	rBV2	257	244	0.02%	0.002%
69	9.967	2679	2683	2687	rBV	253	308	0.02%	0.003%
70	10.021	2697	2700	2704	rVB	215	193	0.01%	0.002%
71	10.050	2704	2709	2711	rBV	251	264	0.02%	0.003%
72	10.102	2722	2725	2733	rVV3	328	382	0.03%	0.004%
73	10.185	2745	2751	2753	rBV	209	256	0.02%	0.003%
74	10.337	2795	2798	2801	rVB2	221	166	0.01%	0.002%
75	10.356	2801	2804	2807	rBV2	316	214	0.02%	0.002%
76	10.494	2844	2847	2851	rVB2	194	160	0.01%	0.002%

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 Title : VOC Analysis

77	10.636	2886	2891	2895	rBV	368	381	0.03%	0.004%
78	10.674	2895	2903	2912	rVB2	3603	5159	0.38%	0.051%
79	10.761	2917	2930	2951	rVB	440083	714253	52.08%	7.082%
80	10.841	2951	2955	2958	rBV2	719	595	0.04%	0.006%
81	10.867	2958	2963	2967	rBV4	661	723	0.05%	0.007%
82	11.208	3065	3069	3073	rVB2	377	327	0.02%	0.003%
83	11.462	3138	3148	3158	rVB4	2179	3877	0.28%	0.038%
84	11.645	3202	3205	3211	rBV2	153	184	0.01%	0.002%
85	11.697	3215	3221	3230	rVB4	1420	1833	0.13%	0.018%
86	11.816	3245	3258	3277	rBV	468995	728781	53.14%	7.226%
87	11.919	3286	3290	3292	rBV3	428	379	0.03%	0.004%
88	11.944	3292	3298	3300	rVV3	1172	1436	0.10%	0.014%
89	11.973	3303	3307	3316	rVB3	2611	3215	0.23%	0.032%
90	12.124	3351	3354	3358	rBV	250	213	0.02%	0.002%
91	12.195	3361	3376	3394	rBV	541692	878539	64.06%	8.710%
92	12.327	3414	3417	3418	rBV	798	369	0.03%	0.004%
93	12.632	3509	3512	3514	rBV	237	191	0.01%	0.002%
94	13.060	3640	3645	3648	rBV2	194	209	0.02%	0.002%
95	13.237	3696	3700	3703	rBV2	232	246	0.02%	0.002%
96	14.092	3963	3966	3969	rVB3	360	282	0.02%	0.003%
97	14.584	4115	4119	4124	rBB3	324	374	0.03%	0.004%
98	14.664	4140	4144	4147	rBV3	296	238	0.02%	0.002%
99	14.861	4201	4205	4210	rBV3	360	454	0.03%	0.005%
100	15.970	4548	4550	4555	rBV2	389	243	0.02%	0.002%

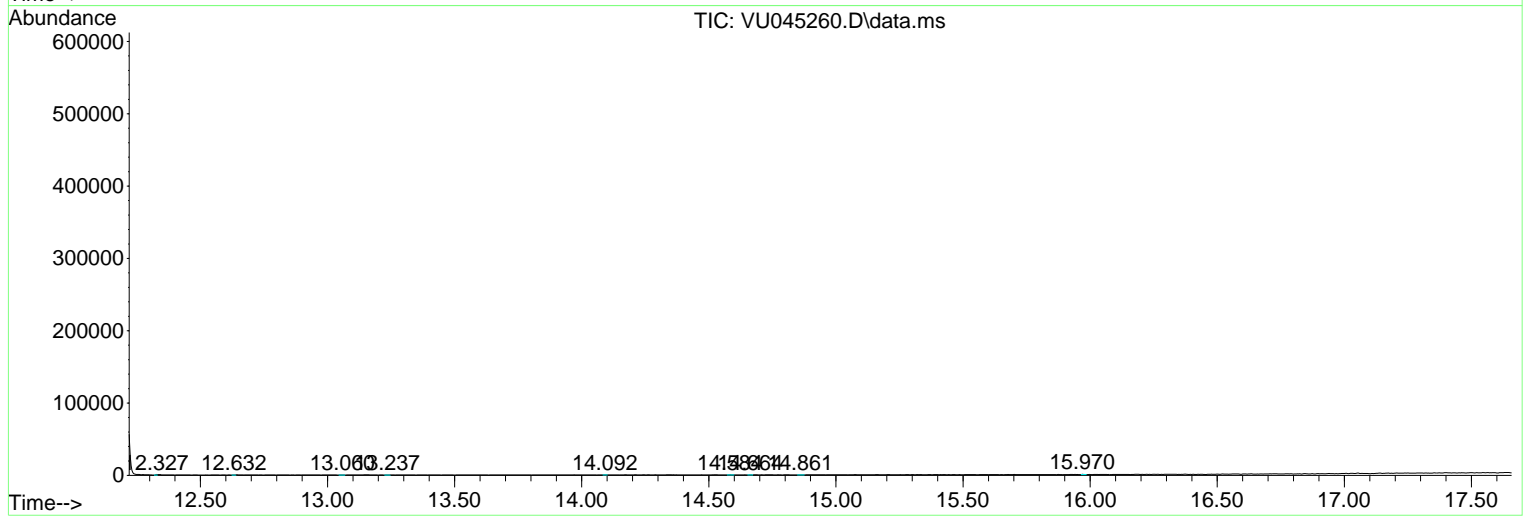
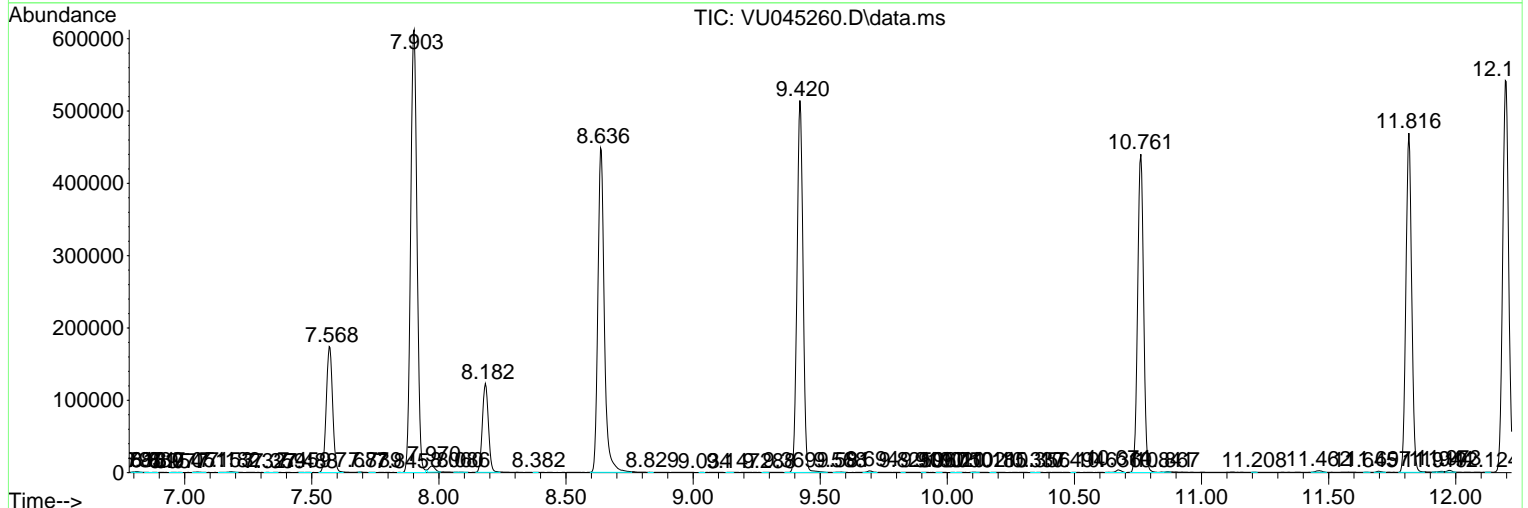
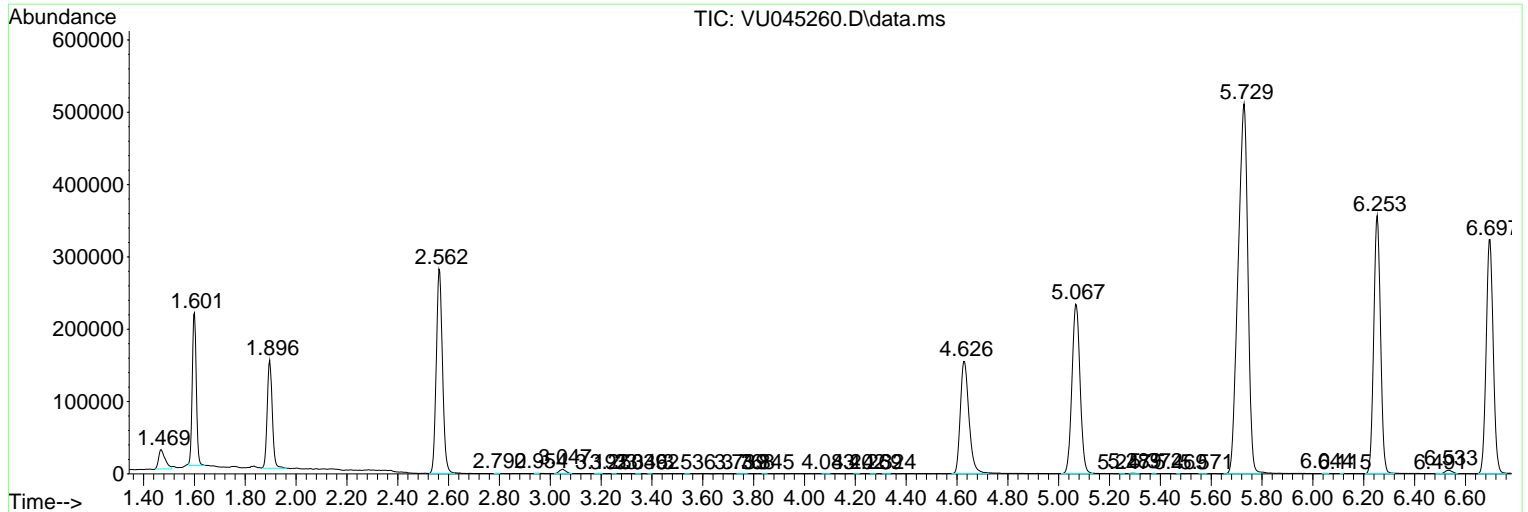
Sum of corrected areas: 10086111

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 VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P



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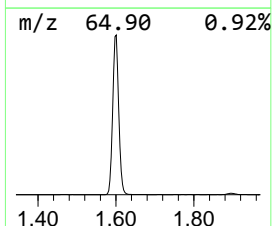
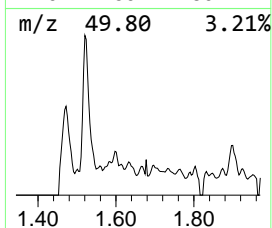
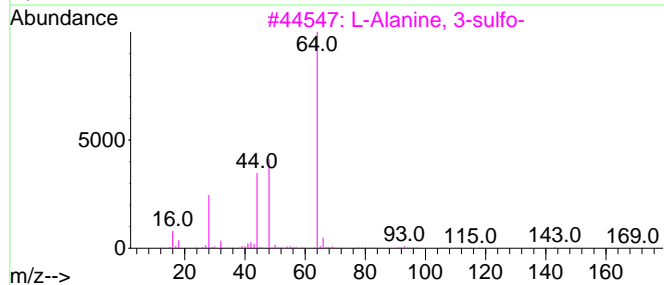
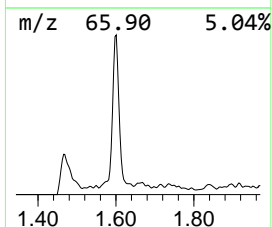
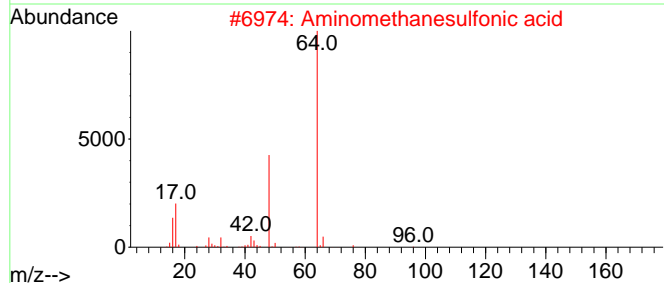
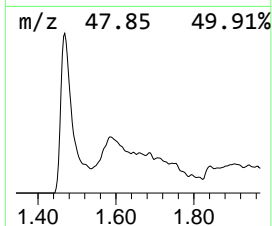
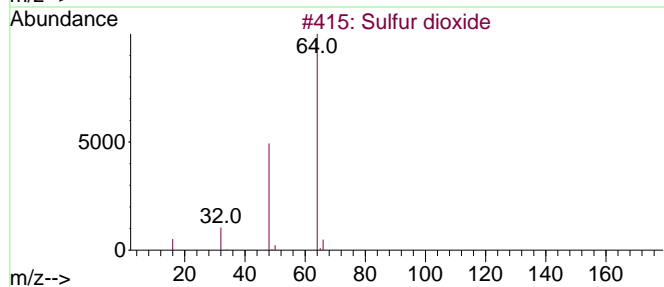
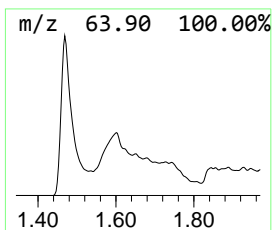
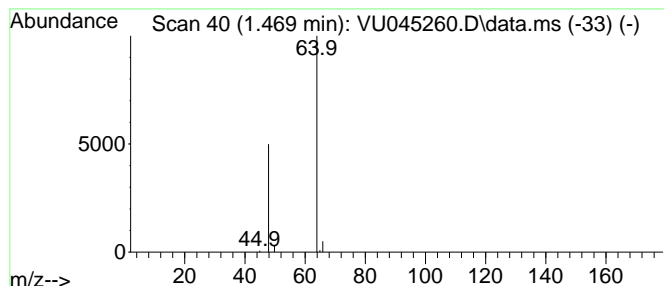
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
 Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	3.61 ug/L	47896	1,4-Difluorobenzene	6.253

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		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	1.469	3.6	ug/L	47896	1	6.253	663727	50.0