

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045263.D
 Acq On : 08 Oct 2021 19:49
 Operator : SY/MD
 Sample : M4026-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 27 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: VU045263.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	54	rBV	24410	45703	3.38%	0.462%
2	1.600	74	81	96	rVB	208963	224525	16.61%	2.269%
3	1.890	163	171	186	rVB	147906	198463	14.69%	2.005%
4	2.562	367	380	404	rBV	277720	467496	34.59%	4.724%
5	2.758	436	441	445	rVV2	184	217	0.02%	0.002%
6	2.790	445	451	456	rVB2	475	647	0.05%	0.007%
7	2.835	459	465	466	rBV2	126	151	0.01%	0.002%
8	2.960	497	504	509	rBV2	414	571	0.04%	0.006%
9	3.044	521	530	541	rBV2	5373	9776	0.72%	0.099%
10	3.186	568	574	577	rBV2	445	581	0.04%	0.006%
11	3.263	594	598	603	rBV	150	146	0.01%	0.001%
12	3.488	665	668	673	rVB2	151	122	0.01%	0.001%
13	3.751	747	750	758	rVB2	178	180	0.01%	0.002%
14	3.803	761	766	769	rBV2	166	189	0.01%	0.002%
15	3.896	793	795	799	rVB	229	166	0.01%	0.002%
16	4.137	866	870	872	rBV	207	202	0.01%	0.002%
17	4.173	876	881	883	rBV2	185	195	0.01%	0.002%
18	4.237	897	901	903	rBV	162	125	0.01%	0.001%
19	4.337	929	932	941	rVB	300	401	0.03%	0.004%
20	4.378	941	945	949	rBV2	215	252	0.02%	0.003%
21	4.420	951	958	962	rVV2	142	207	0.02%	0.002%
22	4.629	1007	1023	1051	rBV	150837	352812	26.11%	3.565%
23	4.899	1103	1107	1110	rVV2	205	170	0.01%	0.002%
24	5.067	1142	1159	1181	rBV	233489	512187	37.90%	5.176%
25	5.185	1193	1196	1199	rVV	220	180	0.01%	0.002%
26	5.208	1199	1203	1208	rVB2	334	252	0.02%	0.003%
27	5.256	1214	1218	1221	rBV	165	178	0.01%	0.002%
28	5.433	1270	1273	1279	rVB2	146	135	0.01%	0.001%
29	5.501	1288	1294	1301	rBV2	129	189	0.01%	0.002%
30	5.610	1325	1328	1333	rVB2	205	208	0.02%	0.002%
31	5.636	1333	1336	1340	rBV2	148	141	0.01%	0.001%
32	5.729	1340	1365	1385	rBV2	505122	1351385	100.00%	13.656%
33	5.948	1430	1433	1437	rBV2	229	209	0.02%	0.002%
34	6.012	1449	1453	1458	rBV2	243	308	0.02%	0.003%
35	6.038	1458	1461	1463	rBV2	206	180	0.01%	0.002%
36	6.066	1468	1470	1474	rVB2	247	209	0.02%	0.002%

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 Title : VOC Analysis

37	6.118	1481	1486	1493	rVB2	352	379	0.03%	0.004%
38	6.253	1513	1528	1549	rBV	344412	643217	47.60%	6.500%
39	6.465	1589	1594	1599	rVB3	294	328	0.02%	0.003%
40	6.533	1606	1615	1625	rVB4	4195	7945	0.59%	0.080%
41	6.693	1651	1665	1695	rVB	318911	617278	45.68%	6.238%
42	6.809	1695	1701	1711	rVB5	613	1113	0.08%	0.011%
43	6.944	1740	1743	1747	rVB	205	153	0.01%	0.002%
44	6.970	1747	1751	1755	rBV	119	125	0.01%	0.001%
45	7.054	1773	1777	1781	rVB3	427	367	0.03%	0.004%
46	7.156	1807	1809	1811	rVV	248	165	0.01%	0.002%
47	7.185	1811	1818	1827	rVB3	1238	1967	0.15%	0.020%
48	7.295	1849	1852	1858	rVB2	216	240	0.02%	0.002%
49	7.330	1858	1863	1864	rBV	148	128	0.01%	0.001%
50	7.346	1865	1868	1874	rVB2	193	197	0.01%	0.002%
51	7.404	1880	1886	1890	rBV2	205	279	0.02%	0.003%
52	7.427	1890	1893	1895	rBV	211	168	0.01%	0.002%
53	7.568	1923	1937	1960	rBV	170146	297045	21.98%	3.002%
54	7.690	1968	1975	1982	rBV3	851	1184	0.09%	0.012%
55	7.902	2026	2041	2056	rVV	610356	1034756	76.57%	10.456%
56	7.973	2056	2063	2074	rVB	8716	14467	1.07%	0.146%
57	8.182	2116	2128	2148	rBV	122498	198569	14.69%	2.007%
58	8.523	2230	2234	2238	rVB	181	170	0.01%	0.002%
59	8.545	2238	2241	2244	rBV	230	204	0.02%	0.002%
60	8.578	2248	2251	2257	rBV	133	145	0.01%	0.001%
61	8.639	2257	2270	2305	rBV	437963	784030	58.02%	7.923%
62	8.935	2359	2362	2370	rVB2	134	149	0.01%	0.002%
63	9.082	2406	2408	2412	rVB	209	132	0.01%	0.001%
64	9.420	2499	2513	2534	rBV	497774	806118	59.65%	8.146%
65	9.574	2555	2561	2566	rVV2	320	412	0.03%	0.004%
66	9.693	2592	2598	2608	rBV3	1468	2262	0.17%	0.023%
67	9.790	2621	2628	2631	rBV2	231	335	0.02%	0.003%
68	9.979	2681	2687	2690	rBV2	176	222	0.02%	0.002%
69	10.105	2722	2726	2730	rBV3	628	698	0.05%	0.007%
70	10.230	2762	2765	2769	rBV	169	140	0.01%	0.001%
71	10.253	2769	2772	2775	rBV2	166	139	0.01%	0.001%
72	10.311	2783	2790	2793	rBV2	233	288	0.02%	0.003%
73	10.417	2817	2823	2824	rBV	261	256	0.02%	0.003%
74	10.565	2865	2869	2872	rBV	172	139	0.01%	0.001%
75	10.674	2894	2903	2911	rVB4	3477	4837	0.36%	0.049%
76	10.761	2917	2930	2950	rBV	450086	711852	52.68%	7.193%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M

Title : VOC Analysis

77	10.870	2956	2964	2969	rBV4	843	1340	0.10%	0.014%
78	10.893	2969	2971	2978	rVB4	406	399	0.03%	0.004%
79	11.034	3012	3015	3018	rVB2	205	124	0.01%	0.001%
80	11.124	3034	3043	3047	rBV4	682	787	0.06%	0.008%
81	11.208	3065	3069	3073	rBV3	272	247	0.02%	0.002%
82	11.462	3138	3148	3158	rVB4	2449	4043	0.30%	0.041%
83	11.507	3158	3162	3164	rBV	290	255	0.02%	0.003%
84	11.584	3180	3186	3190	rBV2	416	457	0.03%	0.005%
85	11.668	3206	3212	3215	rBV2	283	347	0.03%	0.004%
86	11.700	3215	3222	3229	rBV4	1390	2115	0.16%	0.021%
87	11.815	3245	3258	3279	rBV	452198	703569	52.06%	7.110%
88	11.922	3287	3291	3293	rBV	296	262	0.02%	0.003%
89	11.947	3293	3299	3301	rVV3	969	1202	0.09%	0.012%
90	11.976	3303	3308	3318	rVB4	2594	3529	0.26%	0.036%
91	12.063	3332	3335	3338	rBV2	294	287	0.02%	0.003%
92	12.195	3358	3376	3398	rBV	537351	872491	64.56%	8.817%
93	12.333	3414	3419	3426	rVB4	723	842	0.06%	0.009%
94	12.577	3492	3495	3498	rBV2	194	144	0.01%	0.001%
95	12.642	3510	3515	3521	rVB2	432	576	0.04%	0.006%
96	12.815	3567	3569	3572	rVB2	239	124	0.01%	0.001%
97	12.838	3572	3576	3578	rBV2	198	199	0.01%	0.002%
98	12.902	3591	3596	3598	rBV	226	257	0.02%	0.003%
99	13.137	3666	3669	3670	rBV	329	153	0.01%	0.002%
100	14.577	4111	4117	4123	rBV4	411	636	0.05%	0.006%

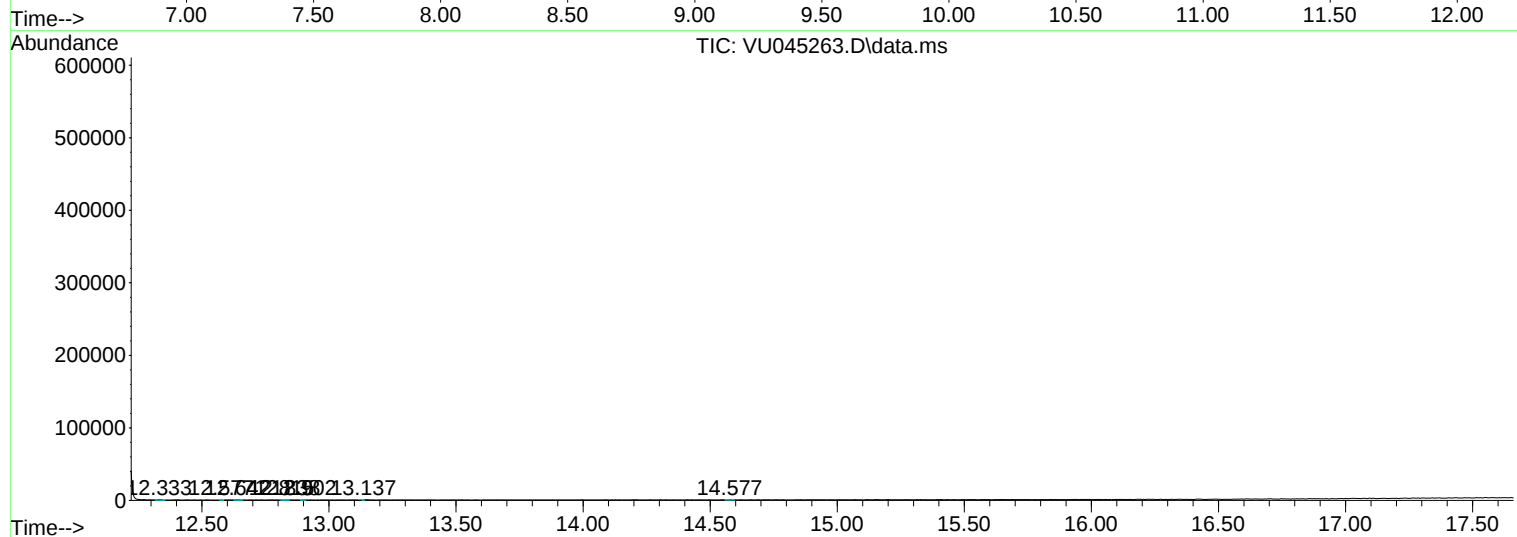
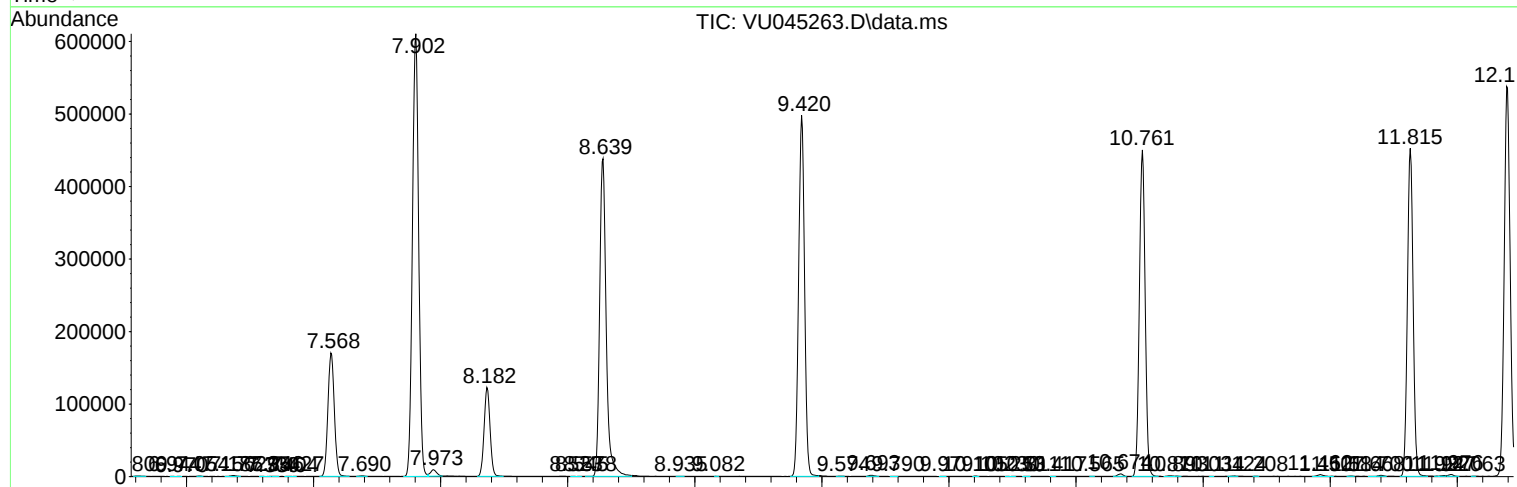
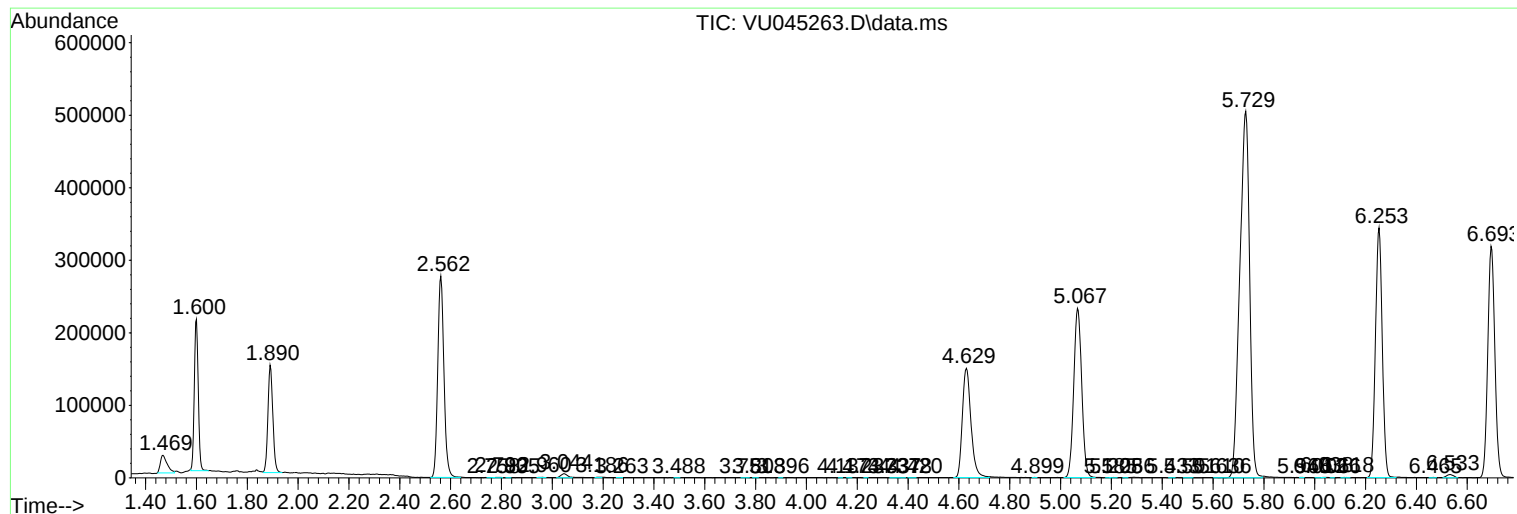
Sum of corrected areas: 9896041

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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



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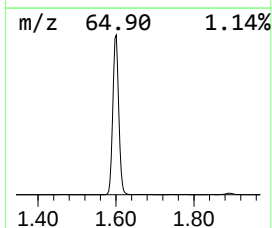
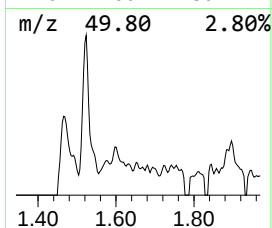
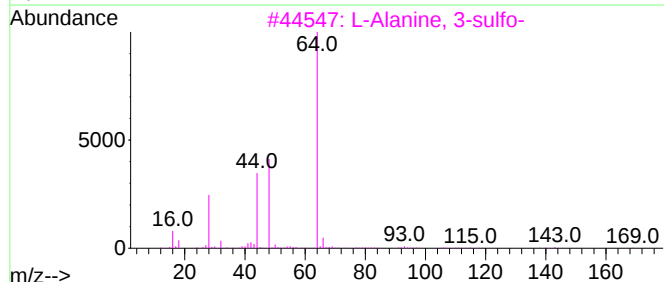
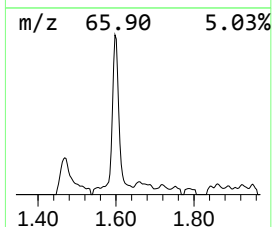
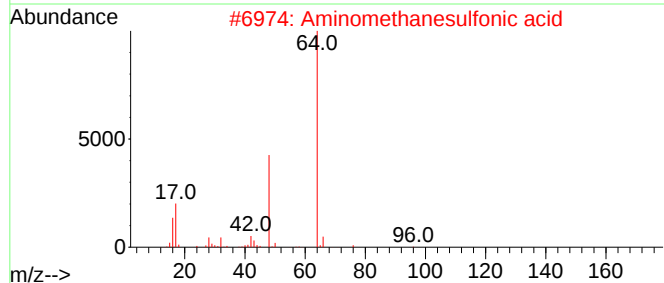
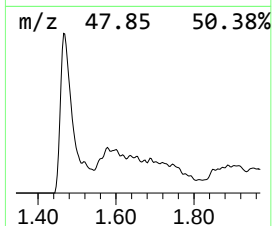
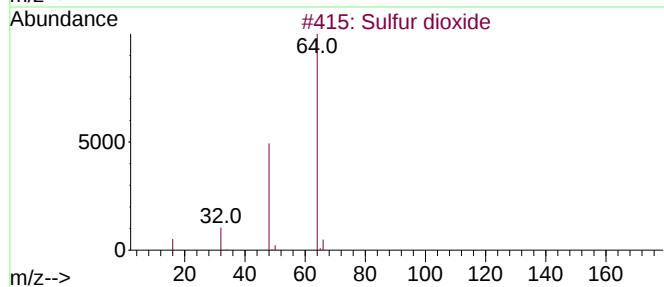
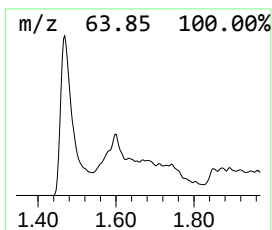
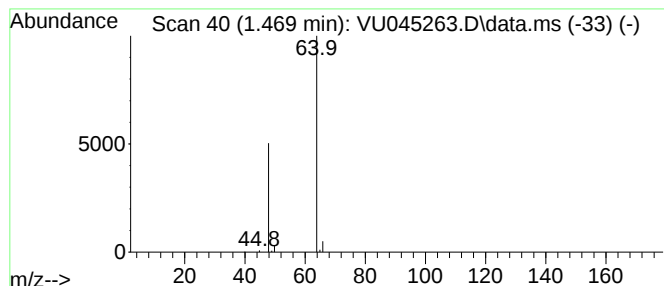
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.55 ug/L	45703	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.5	ug/L	45703	1	6.253	643217	50.0