

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045214.D
 Acq On : 07 Oct 2021 16:05
 Operator : SY/MD
 Sample : M4025-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN9

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: VU045214.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	22437	41970	3.34%	0.436%
2	1.601	73	81	99	rVB	182971	195740	15.56%	2.032%
3	1.893	164	172	188	rVB	130396	176796	14.06%	1.836%
4	2.562	368	380	397	rBV	254214	426434	33.90%	4.428%
5	2.633	397	402	411	rVB2	3721	5702	0.45%	0.059%
6	2.787	439	450	461	rBV2	2904	5187	0.41%	0.054%
7	2.957	498	503	510	rBV3	350	489	0.04%	0.005%
8	3.047	525	531	544	rVB4	910	1458	0.12%	0.015%
9	3.105	544	549	551	rBV2	199	235	0.02%	0.002%
10	3.195	564	577	595	rVB4	7287	16943	1.35%	0.176%
11	3.269	595	600	603	rBV	156	175	0.01%	0.002%
12	3.485	662	667	672	rBV2	168	239	0.02%	0.002%
13	3.543	682	685	689	rBV	215	200	0.02%	0.002%
14	3.678	722	727	732	rVV2	170	234	0.02%	0.002%
15	3.919	798	802	804	rBV2	229	169	0.01%	0.002%
16	3.989	819	824	826	rBV	340	279	0.02%	0.003%
17	4.153	871	875	879	rBV2	203	199	0.02%	0.002%
18	4.198	881	889	891	rBV2	182	258	0.02%	0.003%
19	4.279	909	914	918	rVB2	193	176	0.01%	0.002%
20	4.305	918	922	924	rBV2	196	178	0.01%	0.002%
21	4.385	942	947	951	rBV2	277	333	0.03%	0.003%
22	4.629	1008	1023	1049	rBV	135104	323118	25.69%	3.355%
23	4.919	1110	1113	1116	rVV2	209	174	0.01%	0.002%
24	4.989	1126	1135	1140	rBV2	226	487	0.04%	0.005%
25	5.067	1143	1159	1183	rBV	220619	484174	38.49%	5.027%
26	5.150	1183	1185	1189	rVB2	296	218	0.02%	0.002%
27	5.208	1198	1203	1205	rBV2	304	255	0.02%	0.003%
28	5.292	1222	1229	1231	rBV2	513	696	0.06%	0.007%
29	5.366	1248	1252	1253	rBV2	291	196	0.02%	0.002%
30	5.494	1288	1292	1299	rBV	184	254	0.02%	0.003%
31	5.552	1306	1310	1315	rBV2	200	260	0.02%	0.003%
32	5.581	1315	1319	1324	rVB2	207	202	0.02%	0.002%
33	5.623	1329	1332	1339	rVB2	259	316	0.03%	0.003%
34	5.729	1343	1365	1391	rBV2	464659	1257762	100.00%	13.060%
35	5.977	1437	1442	1447	rBV4	516	550	0.04%	0.006%
36	6.038	1455	1461	1465	rBV2	203	298	0.02%	0.003%

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 Title : VOC Analysis

37	6.112	1479	1484	1486	rBV4	343	256	0.02%	0.003%
38	6.169	1500	1502	1506	rVB3	259	177	0.01%	0.002%
39	6.253	1512	1528	1547	rBV	384096	712284	56.63%	7.396%
40	6.349	1555	1558	1562	rVB2	241	188	0.01%	0.002%
41	6.542	1606	1618	1631	rBV5	17841	35280	2.80%	0.366%
42	6.694	1651	1665	1687	rBV	297899	575717	45.77%	5.978%
43	6.803	1694	1699	1713	rVB4	1048	1659	0.13%	0.017%
44	6.880	1721	1723	1725	rBV4	377	219	0.02%	0.002%
45	7.002	1758	1761	1764	rBV2	232	205	0.02%	0.002%
46	7.050	1772	1776	1777	rBV2	224	164	0.01%	0.002%
47	7.182	1809	1817	1819	rBV3	983	1212	0.10%	0.013%
48	7.304	1851	1855	1863	rVB	253	411	0.03%	0.004%
49	7.343	1863	1867	1870	rBV	200	223	0.02%	0.002%
50	7.459	1899	1903	1905	rBV	210	178	0.01%	0.002%
51	7.568	1923	1937	1958	rBV	149573	257292	20.46%	2.672%
52	7.687	1971	1974	1981	rVB3	804	828	0.07%	0.009%
53	7.899	2026	2040	2055	rVV	570155	983612	78.20%	10.213%
54	7.970	2056	2062	2079	rVB	8912	15012	1.19%	0.156%
55	8.115	2104	2107	2115	rBV2	188	202	0.02%	0.002%
56	8.182	2115	2128	2148	rBV	105833	175322	13.94%	1.820%
57	8.407	2194	2198	2201	rBV	155	166	0.01%	0.002%
58	8.478	2215	2220	2225	rBV3	396	459	0.04%	0.005%
59	8.594	2247	2256	2257	rBV2	275	377	0.03%	0.004%
60	8.636	2257	2269	2300	rBV	403609	716468	56.96%	7.439%
61	8.915	2353	2356	2361	rVV	159	182	0.01%	0.002%
62	9.099	2408	2413	2420	rBV2	164	287	0.02%	0.003%
63	9.150	2426	2429	2433	rBV2	198	185	0.01%	0.002%
64	9.308	2471	2478	2481	rBV	187	276	0.02%	0.003%
65	9.420	2499	2513	2536	rBV	545789	896072	71.24%	9.304%
66	9.574	2555	2561	2565	rBV2	492	632	0.05%	0.007%
67	9.658	2582	2587	2589	rBV2	199	193	0.02%	0.002%
68	9.697	2592	2599	2606	rVV3	996	1413	0.11%	0.015%
69	9.761	2614	2619	2624	rBV2	237	335	0.03%	0.003%
70	10.012	2693	2697	2701	rBV2	267	238	0.02%	0.002%
71	10.057	2702	2711	2719	rVV4	2357	3525	0.28%	0.037%
72	10.099	2721	2724	2731	rVV2	373	503	0.04%	0.005%
73	10.301	2784	2787	2791	rBV2	221	241	0.02%	0.003%
74	10.375	2808	2810	2815	rBV2	237	251	0.02%	0.003%
75	10.420	2818	2824	2828	rBV2	238	297	0.02%	0.003%
76	10.459	2833	2836	2838	rBV2	229	180	0.01%	0.002%

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Peak Location: TOP

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 Title : VOC Analysis

77	10.674	2896	2903	2911	rVB5	926	1246	0.10%	0.013%
78	10.761	2917	2930	2948	rVB	411245	666562	53.00%	6.921%
79	10.902	2971	2974	2976	rVB2	270	184	0.01%	0.002%
80	11.208	3065	3069	3071	rBV3	260	179	0.01%	0.002%
81	11.349	3109	3113	3118	rVB2	201	248	0.02%	0.003%
82	11.449	3138	3144	3145	rBV	390	333	0.03%	0.003%
83	11.635	3194	3202	3210	rBV2	1942	2647	0.21%	0.027%
84	11.735	3230	3233	3239	rBV2	188	208	0.02%	0.002%
85	11.767	3239	3243	3245	rVV	243	197	0.02%	0.002%
86	11.816	3245	3258	3279	rVB	499918	790405	62.84%	8.207%
87	11.973	3304	3307	3312	rBV2	477	350	0.03%	0.004%
88	12.066	3332	3336	3339	rBV3	278	264	0.02%	0.003%
89	12.195	3363	3376	3397	rBV	526450	840588	66.83%	8.728%
90	12.465	3456	3460	3463	rBV	217	164	0.01%	0.002%
91	12.481	3463	3465	3472	rVB2	188	212	0.02%	0.002%
92	12.529	3475	3480	3483	rBV2	286	300	0.02%	0.003%
93	12.626	3506	3510	3515	rBV2	201	216	0.02%	0.002%
94	13.163	3675	3677	3680	rBV	225	194	0.02%	0.002%
95	13.272	3707	3711	3713	rBV	264	241	0.02%	0.003%
96	13.806	3874	3877	3879	rBV	248	197	0.02%	0.002%
97	13.954	3920	3923	3926	rBV2	230	205	0.02%	0.002%
98	14.430	4069	4071	4075	rVB	281	169	0.01%	0.002%
99	14.693	4150	4153	4156	rBV2	282	267	0.02%	0.003%
100	14.883	4206	4212	4213	rBV2	410	299	0.02%	0.003%

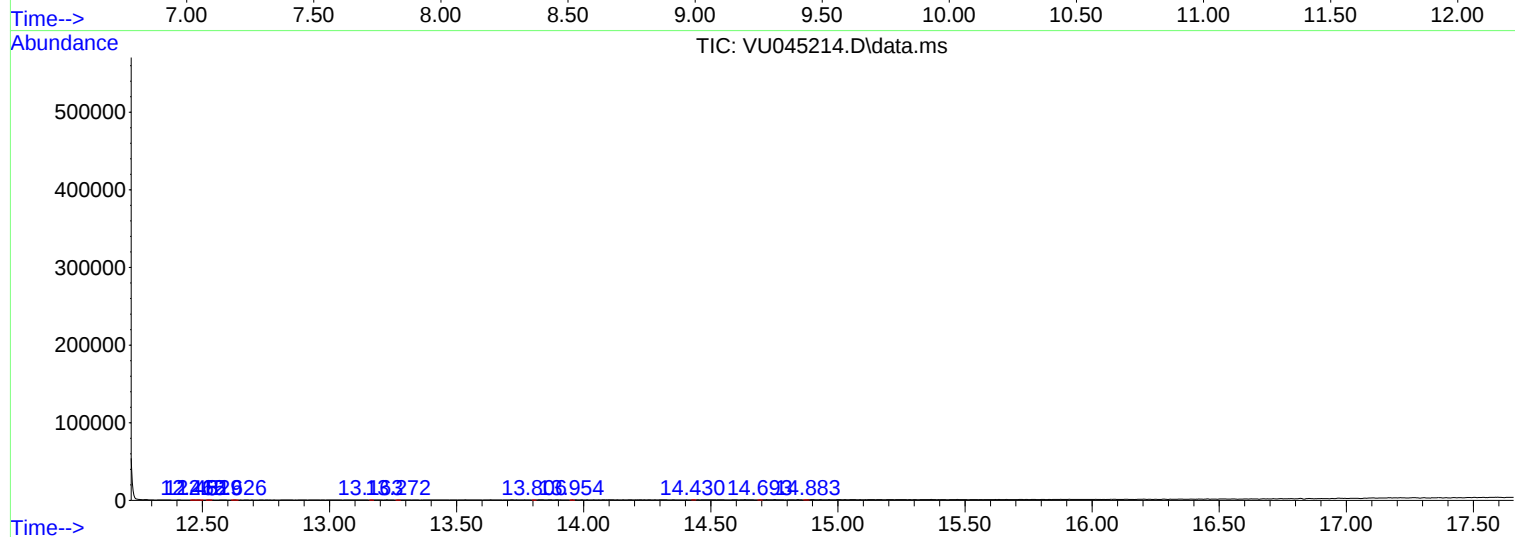
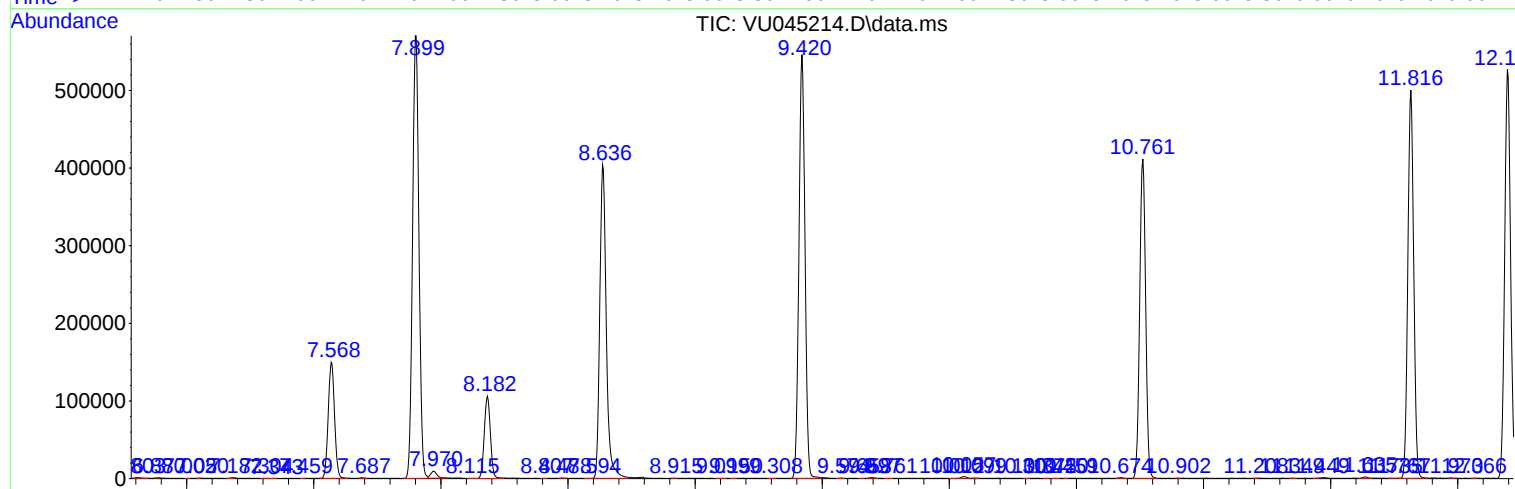
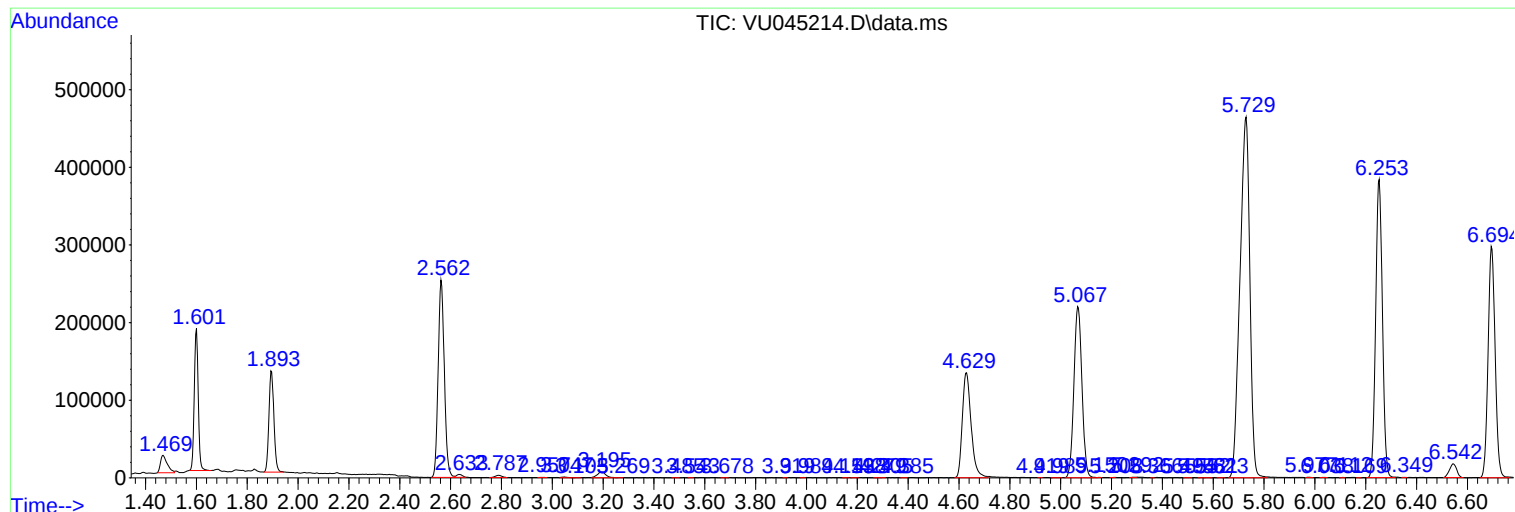
Sum of corrected areas: 9630950

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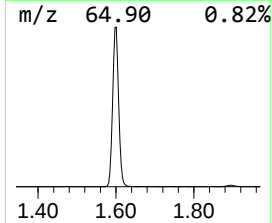
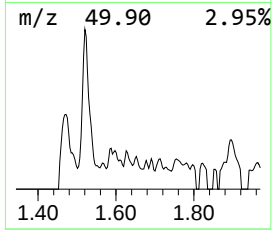
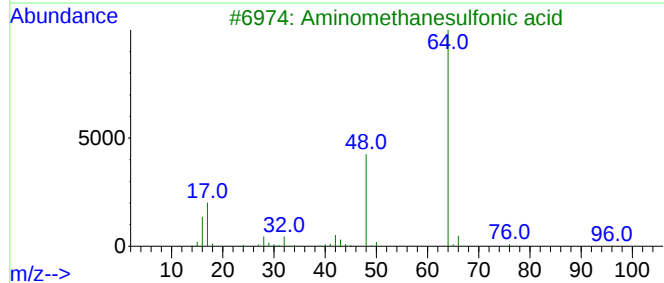
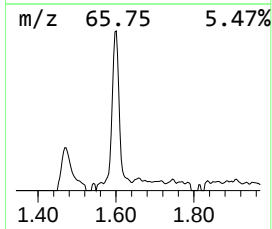
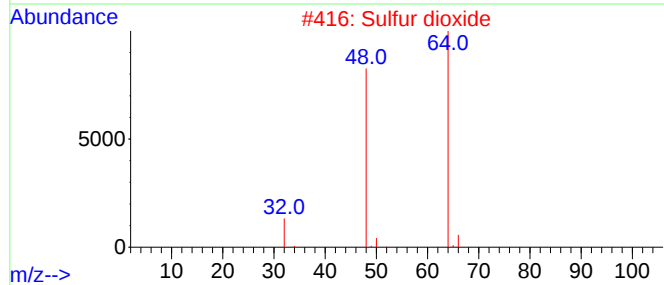
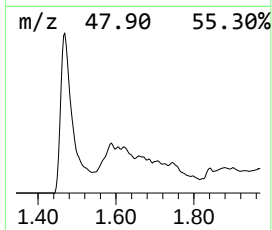
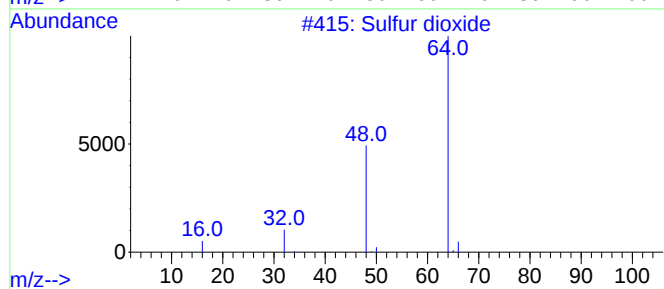
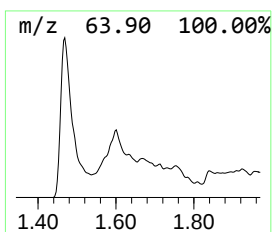
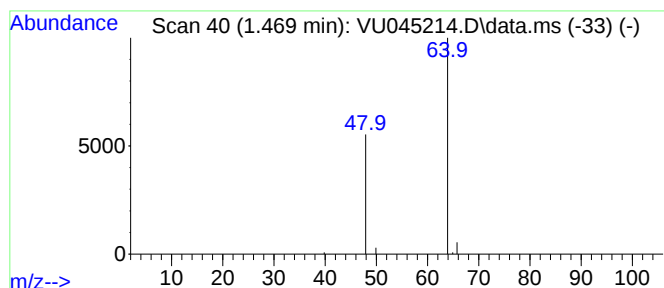
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	2.95 ug/L	41970	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.0	ug/L	41970	1	6.253	712284	50.0