

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045212.D
 Acq On : 07 Oct 2021 15:17
 Operator : SY/MD
 Sample : M4025-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN7

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: VU045212.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	26386	48811	0.75%	0.291%
2	1.597	74	80	100	rVB	178589	199778	3.07%	1.193%
3	1.893	164	172	188	rVB	131662	178054	2.74%	1.063%
4	2.568	367	382	412	rVB3	408505	818194	12.58%	4.885%
5	2.674	412	415	416	rBV2	308	186	0.00%	0.001%
6	2.787	446	450	457	rVB3	601	832	0.01%	0.005%
7	2.858	469	472	476	rVB2	239	223	0.00%	0.001%
8	2.880	476	479	481	rBV	224	163	0.00%	0.001%
9	2.951	498	501	502	rBV	461	277	0.00%	0.002%
10	2.999	514	516	521	rVB2	190	176	0.00%	0.001%
11	3.047	525	531	538	rVB4	1014	1544	0.02%	0.009%
12	3.121	547	554	559	rBV2	238	395	0.01%	0.002%
13	3.189	565	575	589	rVB2	2002	4357	0.07%	0.026%
14	3.356	617	627	636	rVB4	1319	2531	0.04%	0.015%
15	3.472	661	663	670	rVB2	272	319	0.00%	0.002%
16	3.874	773	788	800	rBV2	7674	17057	0.26%	0.102%
17	3.967	813	817	820	rVB2	246	177	0.00%	0.001%
18	4.057	841	845	849	rVB2	215	171	0.00%	0.001%
19	4.124	862	866	872	rBV	122	192	0.00%	0.001%
20	4.227	892	898	903	rVB2	184	228	0.00%	0.001%
21	4.327	924	929	931	rBV2	164	193	0.00%	0.001%
22	4.366	934	941	945	rVB2	206	300	0.00%	0.002%
23	4.417	951	957	958	rBV2	186	193	0.00%	0.001%
24	4.468	966	973	977	rBV	234	310	0.00%	0.002%
25	4.632	1008	1024	1026	rBV	142358	246420	3.79%	1.471%
26	4.812	1077	1080	1085	rBV3	262	250	0.00%	0.001%
27	4.954	1121	1124	1130	rVB2	331	270	0.00%	0.002%
28	4.986	1130	1134	1137	rBV2	174	169	0.00%	0.001%
29	5.066	1142	1159	1183	rVV	224003	491639	7.56%	2.935%
30	5.163	1186	1189	1195	rVB3	266	234	0.00%	0.001%
31	5.321	1221	1238	1257	rVV	115535	260441	4.00%	1.555%
32	5.449	1271	1278	1280	rBV2	161	224	0.00%	0.001%
33	5.558	1306	1312	1317	rVB2	213	322	0.00%	0.002%
34	5.729	1342	1365	1397	rBV2	472199	1271834	19.56%	7.593%
35	6.012	1450	1453	1456	rBV2	164	161	0.00%	0.001%
36	6.121	1481	1487	1491	rVV3	459	538	0.01%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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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

37	6.147	1491	1495	1502	rVB2	292	402	0.01%	0.002%
38	6.253	1513	1528	1546	rBV	381468	718259	11.04%	4.288%
39	6.465	1591	1594	1597	rBV2	237	201	0.00%	0.001%
40	6.546	1602	1619	1651	rBV	3511079	6503618	100.00%	38.827%
41	6.693	1653	1665	1691	rVB	300181	590497	9.08%	3.525%
42	6.986	1753	1756	1760	rVB	258	202	0.00%	0.001%
43	7.050	1768	1776	1783	rVB2	720	1057	0.02%	0.006%
44	7.082	1783	1786	1790	rBV2	172	172	0.00%	0.001%
45	7.105	1790	1793	1796	rVV2	264	212	0.00%	0.001%
46	7.185	1810	1818	1827	rVB4	1034	1714	0.03%	0.010%
47	7.266	1840	1843	1846	rVB	240	158	0.00%	0.001%
48	7.568	1925	1937	1959	rBV	153771	265304	4.08%	1.584%
49	7.693	1964	1976	1982	rBV2	725	1093	0.02%	0.007%
50	7.767	1995	1999	2006	rVB2	179	188	0.00%	0.001%
51	7.845	2015	2023	2027	rVB	235	229	0.00%	0.001%
52	7.902	2027	2041	2056	rBV	586249	994037	15.28%	5.934%
53	7.973	2056	2063	2074	rVB	8531	14135	0.22%	0.084%
54	8.082	2094	2097	2102	rVB2	345	235	0.00%	0.001%
55	8.182	2116	2128	2142	rBV	108840	176516	2.71%	1.054%
56	8.269	2152	2155	2158	rBV2	299	199	0.00%	0.001%
57	8.404	2189	2197	2207	rVB2	4711	7266	0.11%	0.043%
58	8.478	2211	2220	2230	rBV2	1368	2150	0.03%	0.013%
59	8.558	2237	2245	2252	rBV6	681	849	0.01%	0.005%
60	8.635	2255	2269	2300	rBV	407339	713028	10.96%	4.257%
61	9.070	2399	2404	2408	rBV	178	156	0.00%	0.001%
62	9.144	2424	2427	2430	rBV2	209	163	0.00%	0.001%
63	9.320	2479	2482	2486	rVB2	260	206	0.00%	0.001%
64	9.420	2500	2513	2535	rBV	554319	892267	13.72%	5.327%
65	9.536	2543	2549	2557	rVB4	2080	2884	0.04%	0.017%
66	9.578	2557	2562	2565	rBV	288	246	0.00%	0.001%
67	9.690	2592	2597	2606	rVB3	725	1172	0.02%	0.007%
68	9.915	2663	2667	2672	rBV2	233	304	0.00%	0.002%
69	10.176	2743	2748	2752	rBV2	182	208	0.00%	0.001%
70	10.507	2847	2851	2855	rVV	223	233	0.00%	0.001%
71	10.603	2878	2881	2885	rBV2	158	158	0.00%	0.001%
72	10.674	2895	2903	2910	rVV4	1732	2114	0.03%	0.013%
73	10.761	2916	2930	2951	rVB	413863	668385	10.28%	3.990%
74	10.841	2951	2955	2959	rBV	247	272	0.00%	0.002%
75	10.899	2966	2973	2979	rBV4	775	959	0.01%	0.006%
76	11.012	3005	3008	3012	rVB	360	272	0.00%	0.002%

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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
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77	11.034	3012	3015	3017	rBV	219	161	0.00%	0.001%
78	11.160	3049	3054	3057	rBV	417	455	0.01%	0.003%
79	11.359	3110	3116	3120	rBV2	263	316	0.00%	0.002%
80	11.462	3140	3148	3149	rBV2	1097	1038	0.02%	0.006%
81	11.584	3182	3186	3190	rBV2	348	346	0.01%	0.002%
82	11.632	3195	3201	3209	rVV2	760	934	0.01%	0.006%
83	11.703	3216	3223	3227	rVB	580	673	0.01%	0.004%
84	11.815	3245	3258	3280	rBV	498211	790775	12.16%	4.721%
85	11.973	3302	3307	3316	rVB2	907	963	0.01%	0.006%
86	12.066	3332	3336	3338	rBV2	173	164	0.00%	0.001%
87	12.105	3345	3348	3351	rBV	197	164	0.00%	0.001%
88	12.195	3363	3376	3395	rBV	523544	841930	12.95%	5.026%
89	12.423	3444	3447	3454	rBV2	153	159	0.00%	0.001%
90	12.600	3496	3502	3504	rBV2	198	253	0.00%	0.002%
91	12.651	3513	3518	3524	rVB3	312	389	0.01%	0.002%
92	12.767	3550	3554	3561	rBV3	272	383	0.01%	0.002%
93	12.896	3591	3594	3597	rBV2	288	267	0.00%	0.002%
94	13.089	3651	3654	3657	rBV	189	157	0.00%	0.001%
95	13.864	3891	3895	3900	rBV2	245	340	0.01%	0.002%
96	14.098	3964	3968	3974	rBV2	519	684	0.01%	0.004%
97	14.558	4108	4111	4115	rBV2	296	189	0.00%	0.001%
98	14.786	4180	4182	4186	rBV3	280	229	0.00%	0.001%
99	15.191	4304	4308	4309	rBV	387	288	0.00%	0.002%
100	15.693	4461	4464	4466	rBV3	359	262	0.00%	0.002%

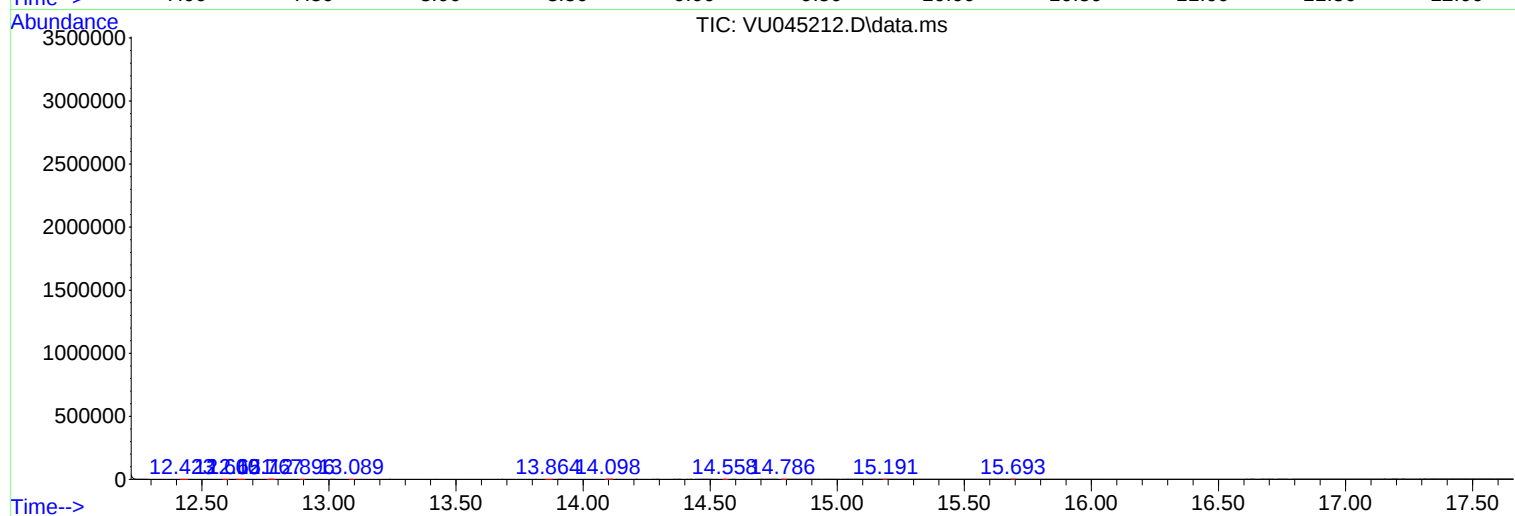
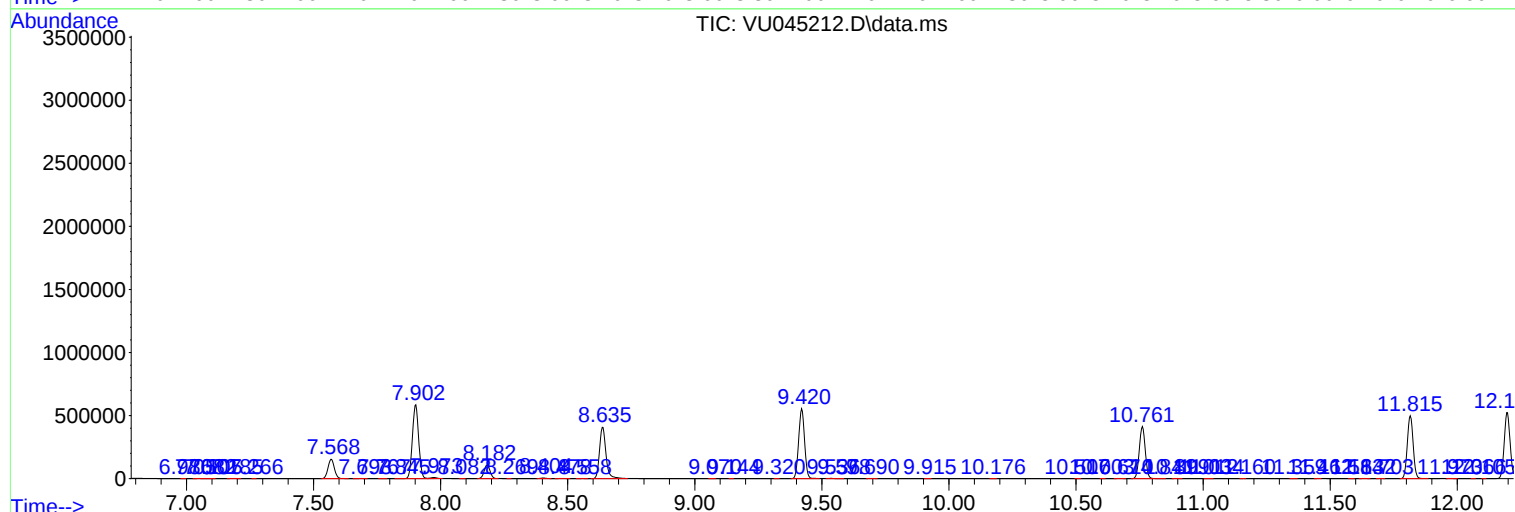
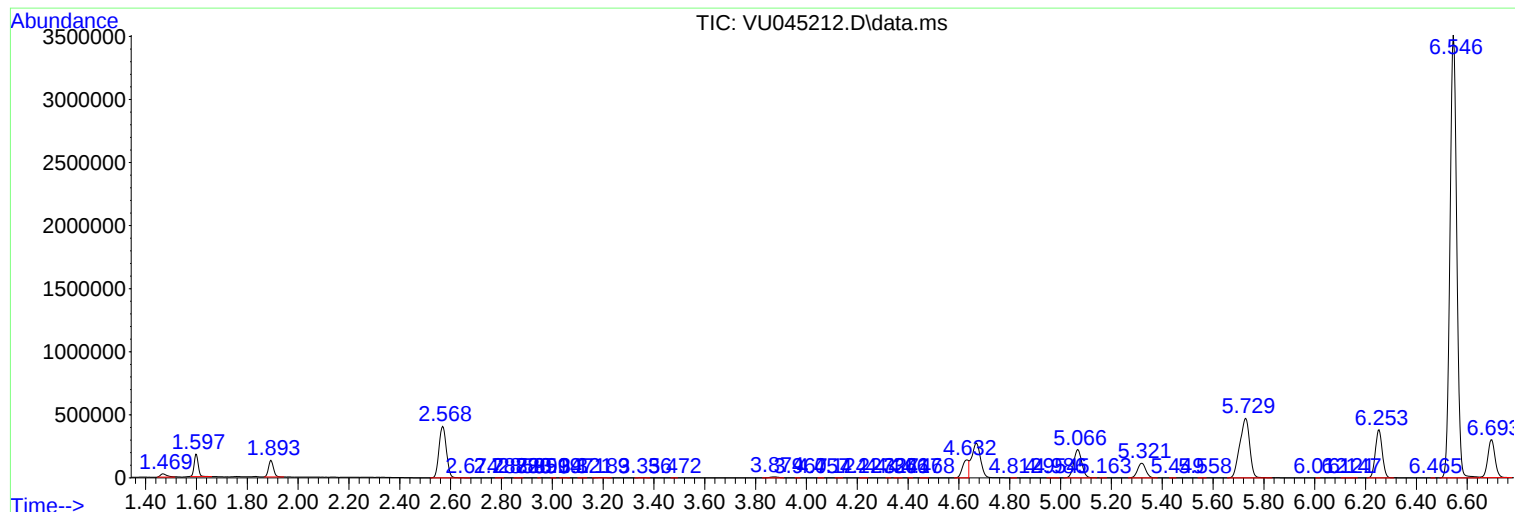
Sum of corrected areas: 16750402

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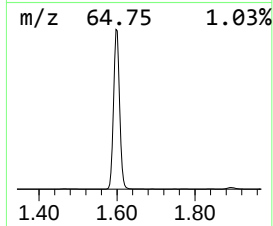
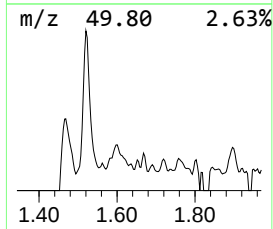
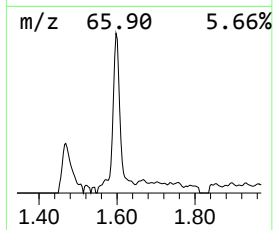
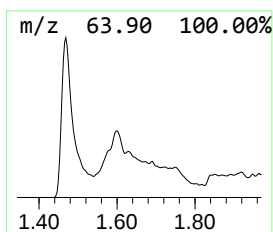
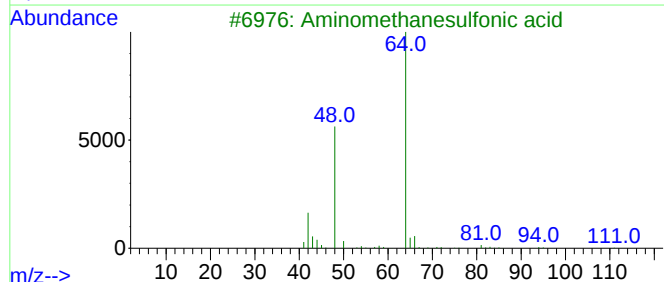
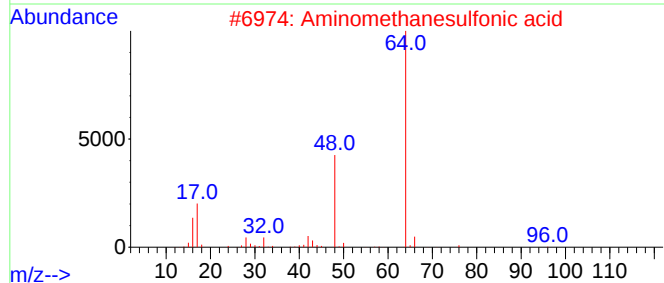
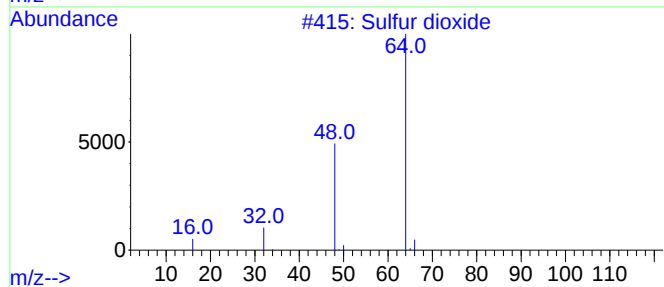
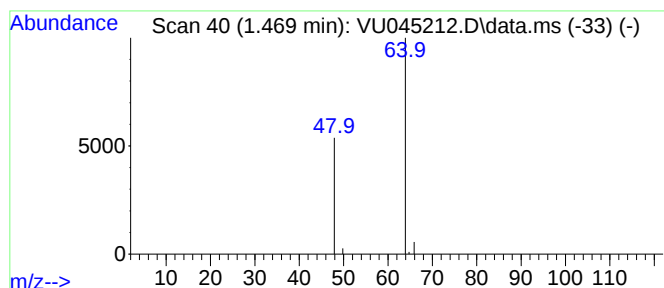
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.40 ug/L	48811	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.4	ug/L	48811	1	6.253	718259	50.0