

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045102.D
 Acq On : 04 Oct 2021 17:31
 Operator : SY/MD
 Sample : M3996-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A42

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: VU045102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	35	47	54	rBV	66661	158342	14.24%	1.653%
2	1.601	76	81	92	rVB	124770	138623	12.46%	1.448%
3	1.909	171	177	197	rVB	108741	156623	14.08%	1.635%
4	2.568	370	382	400	rBV	209895	347912	31.28%	3.633%
5	2.687	412	419	426	rBV4	1298	1961	0.18%	0.020%
6	2.803	443	455	462	rBV2	2482	5400	0.49%	0.056%
7	3.192	566	576	592	rVB2	9292	20557	1.85%	0.215%
8	3.359	614	628	647	rVB	53090	105646	9.50%	1.103%
9	3.758	749	752	756	rVB2	268	229	0.02%	0.002%
10	3.784	756	760	762	rBV2	218	188	0.02%	0.002%
11	3.854	777	782	790	rVB3	798	1195	0.11%	0.012%
12	4.015	827	832	835	rVB2	230	243	0.02%	0.003%
13	4.034	835	838	841	rBV	223	175	0.02%	0.002%
14	4.089	851	855	858	rBV	216	220	0.02%	0.002%
15	4.195	884	888	891	rBV	197	175	0.02%	0.002%
16	4.526	988	991	993	rBV	221	168	0.02%	0.002%
17	4.571	1001	1005	1006	rVV	568	390	0.04%	0.004%
18	4.626	1007	1022	1061	rVV	148807	412228	37.07%	4.304%
19	5.070	1143	1160	1185	rBV	198964	438461	39.43%	4.578%
20	5.215	1201	1205	1209	rBV2	441	351	0.03%	0.004%
21	5.282	1222	1226	1228	rBV3	439	312	0.03%	0.003%
22	5.375	1250	1255	1256	rBV2	251	192	0.02%	0.002%
23	5.530	1297	1303	1308	rBV2	152	216	0.02%	0.002%
24	5.591	1317	1322	1330	rBV2	212	385	0.03%	0.004%
25	5.645	1336	1339	1343	rVB2	222	167	0.02%	0.002%
26	5.729	1343	1365	1397	rBV2	402510	1112125	100.00%	11.613%
27	6.112	1480	1484	1489	rVB2	366	388	0.03%	0.004%
28	6.253	1512	1528	1552	rBV	343681	649303	58.38%	6.780%
29	6.369	1562	1564	1567	rVB2	494	273	0.02%	0.003%
30	6.395	1570	1572	1580	rVB2	511	556	0.05%	0.006%
31	6.546	1606	1619	1629	rBV4	7143	13077	1.18%	0.137%
32	6.694	1651	1665	1690	rBV	268313	520827	46.83%	5.438%
33	6.912	1728	1733	1739	rBV2	245	339	0.03%	0.004%
34	6.941	1739	1742	1747	rVB	274	268	0.02%	0.003%
35	6.970	1747	1751	1754	rBV2	203	181	0.02%	0.002%
36	7.041	1769	1773	1774	rBV2	303	231	0.02%	0.002%

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 Title : VOC Analysis

37	7.185	1808	1818	1828	rBV4	2465	4050	0.36%	0.042%
38	7.317	1853	1859	1861	rBV2	195	196	0.02%	0.002%
39	7.378	1874	1878	1882	rBV	201	205	0.02%	0.002%
40	7.427	1887	1893	1896	rBV2	167	177	0.02%	0.002%
41	7.507	1913	1918	1922	rVB	309	333	0.03%	0.003%
42	7.568	1922	1937	1954	rBV	144552	252525	22.71%	2.637%
43	7.690	1967	1975	1984	rVB2	1666	2549	0.23%	0.027%
44	7.790	2003	2006	2014	rVB2	217	239	0.02%	0.002%
45	7.903	2027	2041	2055	rBV	472607	811346	72.95%	8.472%
46	7.973	2056	2063	2078	rVB	12602	21838	1.96%	0.228%
47	8.182	2116	2128	2144	rBV	102569	167960	15.10%	1.754%
48	8.427	2201	2204	2208	rBV3	312	278	0.02%	0.003%
49	8.478	2216	2220	2228	rVB3	865	1064	0.10%	0.011%
50	8.555	2231	2244	2257	rBV	298099	505881	45.49%	5.282%
51	8.636	2257	2269	2296	rVV	441569	751081	67.54%	7.843%
52	8.822	2325	2327	2332	rVB	210	164	0.01%	0.002%
53	9.050	2394	2398	2404	rBV	185	197	0.02%	0.002%
54	9.195	2432	2443	2446	rBV	213	433	0.04%	0.005%
55	9.420	2499	2513	2538	rBV	487819	801888	72.10%	8.373%
56	9.571	2552	2560	2570	rBV3	2509	3742	0.34%	0.039%
57	9.645	2579	2583	2586	rBV2	167	173	0.02%	0.002%
58	9.700	2591	2600	2607	rBV3	3064	4605	0.41%	0.048%
59	9.777	2617	2624	2632	rVB	2690	3860	0.35%	0.040%
60	10.047	2706	2708	2713	rVB	237	207	0.02%	0.002%
61	10.108	2713	2727	2733	rBV2	1708	2621	0.24%	0.027%
62	10.153	2736	2741	2745	rVB2	345	354	0.03%	0.004%
63	10.195	2745	2754	2757	rBV2	251	435	0.04%	0.005%
64	10.320	2788	2793	2796	rBV2	175	180	0.02%	0.002%
65	10.378	2807	2811	2816	rVB2	291	338	0.03%	0.004%
66	10.410	2816	2821	2823	rBV2	222	238	0.02%	0.002%
67	10.491	2843	2846	2850	rVB3	305	183	0.02%	0.002%
68	10.529	2851	2858	2860	rBV2	2152	2453	0.22%	0.026%
69	10.616	2881	2885	2889	rBV	246	195	0.02%	0.002%
70	10.677	2897	2904	2910	rBV4	1652	2091	0.19%	0.022%
71	10.761	2917	2930	2950	rBV	396256	636601	57.24%	6.647%
72	10.899	2968	2973	2976	rBV3	411	433	0.04%	0.005%
73	11.089	3028	3032	3036	rBV3	435	423	0.04%	0.004%
74	11.291	3092	3095	3100	rVB2	300	256	0.02%	0.003%
75	11.372	3112	3120	3124	rBV2	292	464	0.04%	0.005%
76	11.468	3142	3150	3159	rVB6	2275	3694	0.33%	0.039%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.529	3163	3169	3173	rBV2	347	399	0.04%	0.004%
78	11.594	3185	3189	3193	rBV2	185	208	0.02%	0.002%
79	11.687	3214	3218	3219	rBV	326	199	0.02%	0.002%
80	11.700	3219	3222	3227	rVB2	830	738	0.07%	0.008%
81	11.725	3227	3230	3234	rBV2	265	210	0.02%	0.002%
82	11.748	3234	3237	3240	rBV	199	188	0.02%	0.002%
83	11.816	3245	3258	3275	rBV	463163	736379	66.21%	7.689%
84	11.934	3292	3295	3298	rBV3	497	424	0.04%	0.004%
85	11.973	3303	3307	3316	rVB5	938	1073	0.10%	0.011%
86	12.195	3362	3376	3394	rBV	465894	754640	67.86%	7.880%
87	12.423	3444	3447	3451	rBV	228	208	0.02%	0.002%
88	12.471	3458	3462	3466	rBV	279	264	0.02%	0.003%
89	12.597	3498	3501	3505	rBV	246	189	0.02%	0.002%
90	12.774	3552	3556	3558	rBV2	316	218	0.02%	0.002%
91	12.832	3568	3574	3577	rBV2	183	249	0.02%	0.003%
92	12.873	3583	3587	3590	rBV2	199	189	0.02%	0.002%
93	12.960	3608	3614	3615	rBV2	485	425	0.04%	0.004%
94	13.397	3747	3750	3754	rBV	194	196	0.02%	0.002%
95	13.896	3901	3905	3908	rBV2	272	283	0.03%	0.003%
96	14.092	3958	3966	3976	rBV3	2195	3502	0.31%	0.037%
97	14.275	4019	4023	4030	rBV3	395	374	0.03%	0.004%
98	14.449	4074	4077	4080	rBV	319	241	0.02%	0.003%
99	14.584	4115	4119	4122	rBV2	374	327	0.03%	0.003%
100	15.420	4372	4379	4386	rBV5	1051	1703	0.15%	0.018%

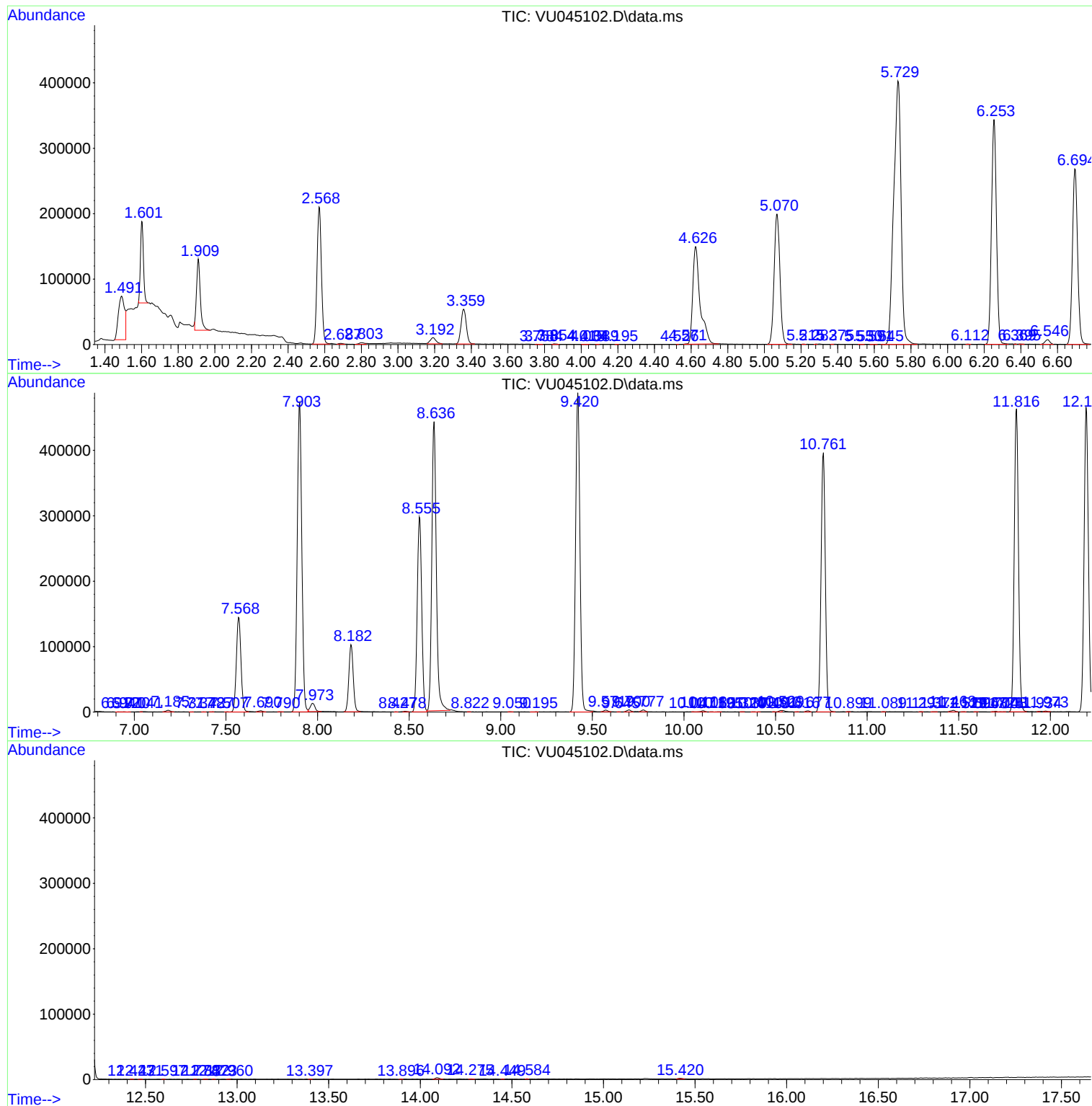
Sum of corrected areas: 9576703

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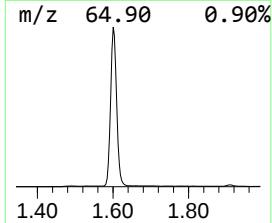
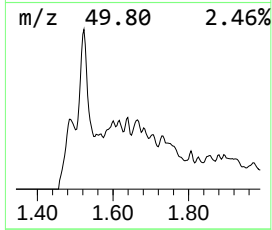
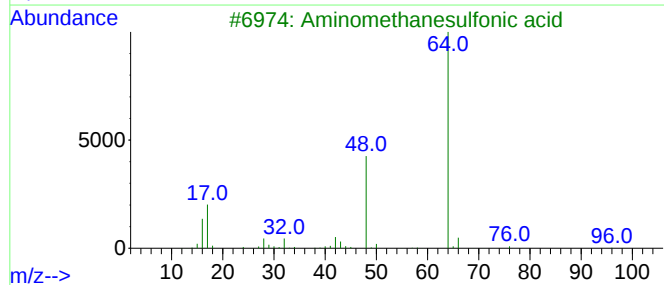
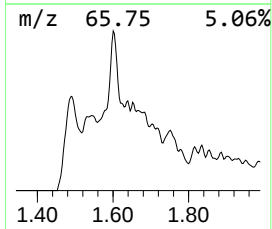
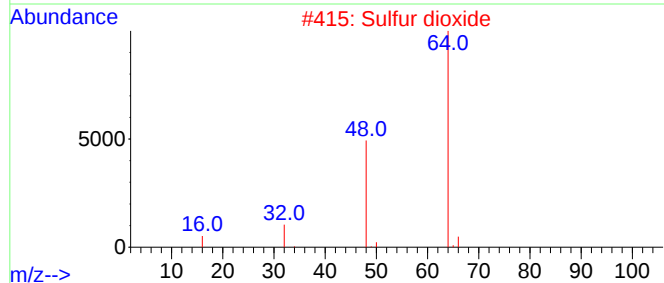
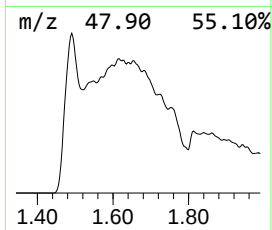
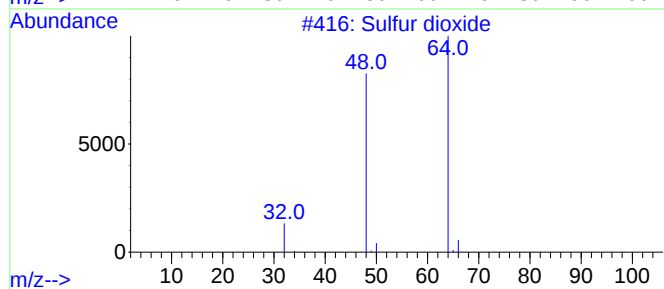
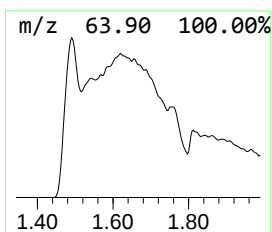
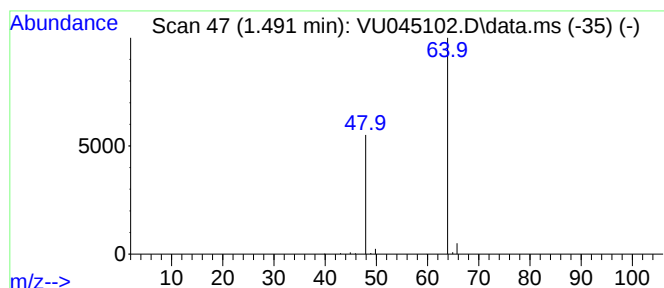
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.491	12.19 ug/L	158342	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.491	12.2	ug/L	158342	1	6.253	649303	50.0