

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045252.D
 Acq On : 08 Oct 2021 15:29
 Operator : SY/MD
 Sample : M4023-05DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AJ2DL

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: VU045252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	31	39	60	rBV2	143484	263668	20.06%	2.451%
2	1.597	75	80	101	rVB	159738	189503	14.42%	1.762%
3	1.890	163	171	184	rVB	127562	171504	13.05%	1.594%
4	2.562	367	380	412	rVB2	256170	461690	35.13%	4.292%
5	2.784	438	449	461	rVB4	2299	4355	0.33%	0.040%
6	2.909	484	488	492	rBV2	183	153	0.01%	0.001%
7	2.957	495	503	505	rBV2	348	425	0.03%	0.004%
8	3.047	521	531	545	rVB3	4009	7635	0.58%	0.071%
9	3.189	559	575	593	rVB	6311	14474	1.10%	0.135%
10	3.350	618	625	634	rBV5	1318	2383	0.18%	0.022%
11	3.449	653	656	661	rBV	173	147	0.01%	0.001%
12	3.559	686	690	692	rBV2	205	184	0.01%	0.002%
13	3.601	698	703	705	rBV	188	178	0.01%	0.002%
14	3.716	737	739	744	rVB2	192	158	0.01%	0.001%
15	3.768	751	755	758	rBV	187	172	0.01%	0.002%
16	3.871	774	787	803	rBV	4719	10683	0.81%	0.099%
17	3.990	821	824	827	rBV2	143	140	0.01%	0.001%
18	4.067	845	848	854	rBV2	205	265	0.02%	0.002%
19	4.318	923	926	929	rBV2	219	192	0.01%	0.002%
20	4.385	941	947	950	rBV2	139	145	0.01%	0.001%
21	4.417	953	957	963	rBV	275	321	0.02%	0.003%
22	4.514	982	987	989	rBV	249	207	0.02%	0.002%
23	4.633	1008	1024	1027	rBV	160616	300144	22.83%	2.790%
24	4.816	1078	1081	1083	rBV2	173	145	0.01%	0.001%
25	4.880	1097	1101	1102	rBV	218	146	0.01%	0.001%
26	5.067	1142	1159	1178	rBV	233968	505788	38.48%	4.702%
27	5.321	1221	1238	1257	rBV	71621	162236	12.34%	1.508%
28	5.559	1308	1312	1317	rBV2	236	311	0.02%	0.003%
29	5.729	1343	1365	1392	rBV2	489307	1314404	100.00%	12.220%
30	5.948	1430	1433	1438	rBV3	198	229	0.02%	0.002%
31	6.031	1455	1459	1462	rBV2	338	313	0.02%	0.003%
32	6.076	1468	1473	1475	rBV2	190	212	0.02%	0.002%
33	6.086	1475	1476	1480	rVB2	320	173	0.01%	0.002%
34	6.108	1480	1483	1484	rBV2	392	186	0.01%	0.002%
35	6.253	1513	1528	1547	rBV	361712	680025	51.74%	6.322%
36	6.353	1557	1559	1565	rVB2	305	250	0.02%	0.002%

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

37	6.440	1582	1586	1590	rBV2	221	177	0.01%	0.002%
38	6.546	1603	1619	1645	rBV	268168	501505	38.15%	4.662%
39	6.694	1650	1665	1685	rBV	314896	609830	46.40%	5.670%
40	6.780	1690	1692	1695	rVV	375	233	0.02%	0.002%
41	6.809	1695	1701	1709	rVB5	992	1323	0.10%	0.012%
42	6.925	1732	1737	1743	rBV2	186	263	0.02%	0.002%
43	7.041	1769	1773	1774	rBV2	487	294	0.02%	0.003%
44	7.092	1784	1789	1791	rBV	244	220	0.02%	0.002%
45	7.131	1796	1801	1807	rBV2	255	278	0.02%	0.003%
46	7.186	1807	1818	1832	rVB4	3151	5646	0.43%	0.052%
47	7.243	1832	1836	1839	rBV	218	179	0.01%	0.002%
48	7.420	1889	1891	1896	rVB2	161	153	0.01%	0.001%
49	7.488	1907	1912	1918	rVB2	220	280	0.02%	0.003%
50	7.568	1923	1937	1962	rVB	169105	292822	22.28%	2.722%
51	7.690	1966	1975	1984	rVB4	1868	3178	0.24%	0.030%
52	7.813	2011	2013	2018	rBV2	178	174	0.01%	0.002%
53	7.854	2023	2026	2027	rBV	253	156	0.01%	0.001%
54	7.903	2027	2041	2056	rBV	588055	1003925	76.38%	9.333%
55	7.973	2056	2063	2073	rVB	8219	13394	1.02%	0.125%
56	8.182	2116	2128	2152	rBV	119274	196433	14.94%	1.826%
57	8.330	2171	2174	2179	rVB	186	180	0.01%	0.002%
58	8.407	2189	2198	2204	rVB4	1522	2252	0.17%	0.021%
59	8.472	2215	2218	2226	rVV3	323	480	0.04%	0.004%
60	8.591	2250	2255	2256	rBV2	156	140	0.01%	0.001%
61	8.639	2256	2270	2305	rBV	436646	781167	59.43%	7.262%
62	9.192	2438	2442	2445	rBV2	179	191	0.01%	0.002%
63	9.253	2458	2461	2464	rVB2	229	146	0.01%	0.001%
64	9.285	2464	2471	2474	rBV2	301	334	0.03%	0.003%
65	9.317	2479	2481	2486	rVB2	198	177	0.01%	0.002%
66	9.349	2486	2491	2495	rBV2	192	193	0.01%	0.002%
67	9.420	2500	2513	2540	rBV	519642	856228	65.14%	7.960%
68	9.575	2554	2561	2569	rVB4	763	1170	0.09%	0.011%
69	9.694	2590	2598	2608	rVV2	2712	4187	0.32%	0.039%
70	9.800	2625	2631	2636	rVB2	273	381	0.03%	0.004%
71	9.829	2636	2640	2642	rBV	169	138	0.01%	0.001%
72	9.899	2656	2662	2665	rVB2	215	181	0.01%	0.002%
73	9.919	2665	2668	2672	rVB2	245	181	0.01%	0.002%
74	10.041	2702	2706	2710	rBV	232	223	0.02%	0.002%
75	10.108	2721	2727	2731	rBV3	588	635	0.05%	0.006%
76	10.195	2748	2754	2758	rVB2	270	304	0.02%	0.003%

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 Title : VOC Analysis

77	10.340	2794	2799	2803	rBV2	207	228	0.02%	0.002%
78	10.478	2838	2842	2846	rBV2	472	460	0.03%	0.004%
79	10.674	2896	2903	2911	rBV3	2449	3282	0.25%	0.031%
80	10.761	2916	2930	2950	rBV	459507	732660	55.74%	6.811%
81	10.864	2960	2962	2966	rBV2	224	187	0.01%	0.002%
82	10.919	2974	2979	2982	rBV2	214	252	0.02%	0.002%
83	11.156	3051	3053	3055	rVB	315	152	0.01%	0.001%
84	11.176	3055	3059	3062	rBV2	241	225	0.02%	0.002%
85	11.259	3080	3085	3090	rVV2	184	245	0.02%	0.002%
86	11.391	3121	3126	3133	rBV2	201	269	0.02%	0.003%
87	11.462	3140	3148	3156	rBV4	1478	2586	0.20%	0.024%
88	11.513	3160	3164	3169	rBV	203	193	0.01%	0.002%
89	11.700	3215	3222	3232	rBV5	1077	1427	0.11%	0.013%
90	11.816	3246	3258	3277	rBV	479686	752055	57.22%	6.992%
91	11.941	3295	3297	3301	rBV2	578	488	0.04%	0.005%
92	11.976	3305	3308	3315	rVB4	1494	1689	0.13%	0.016%
93	12.195	3363	3376	3392	rBV	533657	876675	66.70%	8.150%
94	12.639	3510	3514	3516	rBV	215	190	0.01%	0.002%
95	12.677	3521	3526	3529	rBV2	205	238	0.02%	0.002%
96	13.166	3675	3678	3680	rVB	296	179	0.01%	0.002%
97	14.092	3956	3966	3978	rBV	5100	8547	0.65%	0.079%
98	14.629	4130	4133	4139	rVB2	504	393	0.03%	0.004%
99	15.237	4317	4322	4326	rBV4	568	603	0.05%	0.006%
100	15.362	4356	4361	4365	rBV3	485	532	0.04%	0.005%

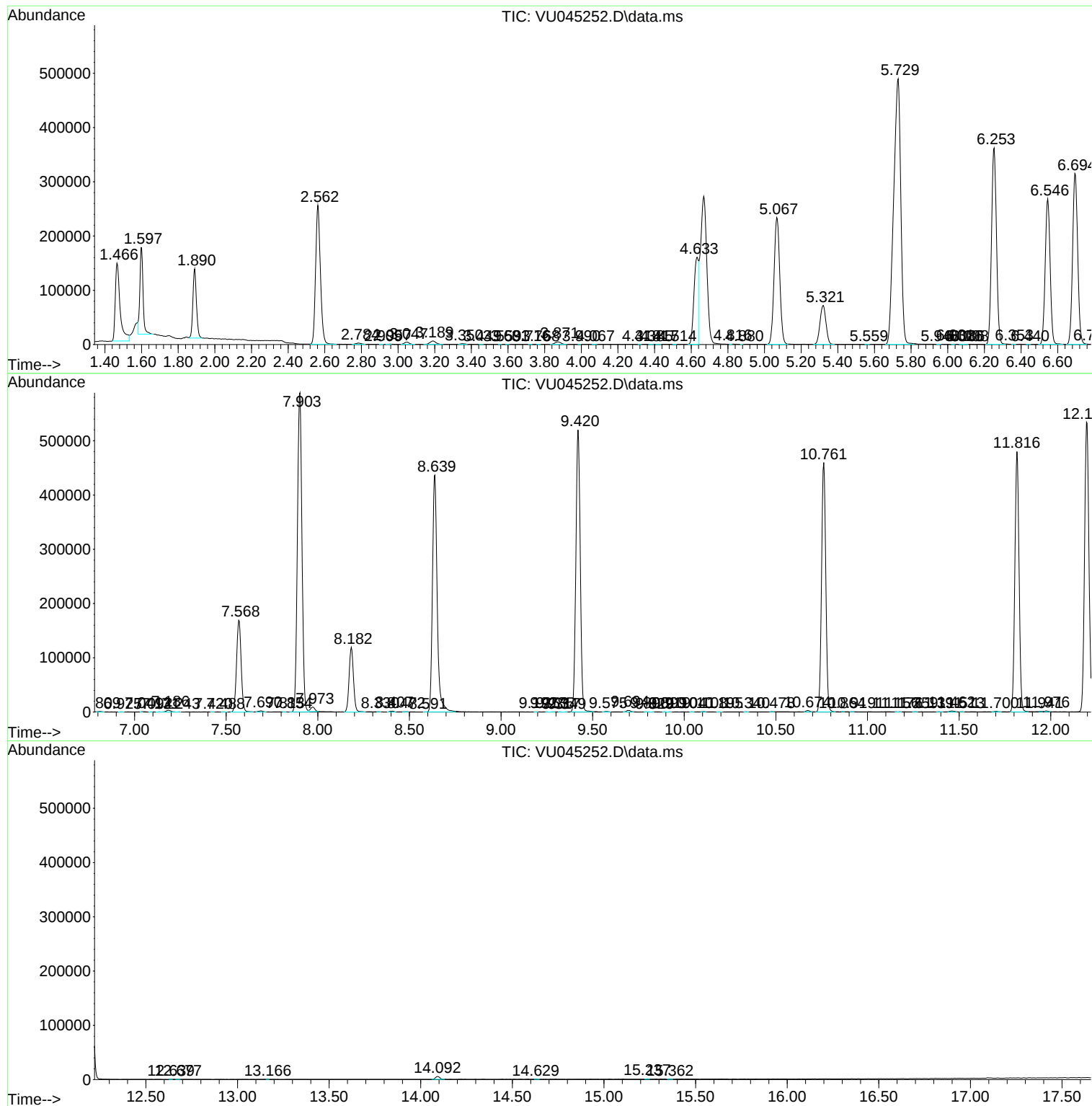
Sum of corrected areas: 10756250

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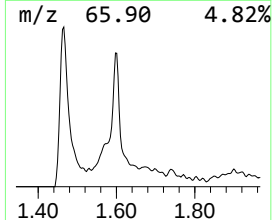
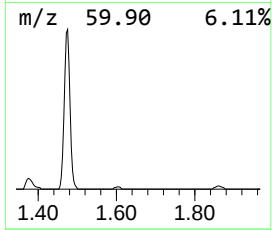
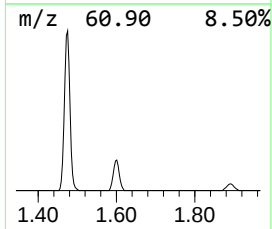
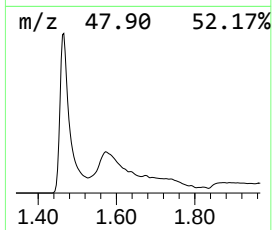
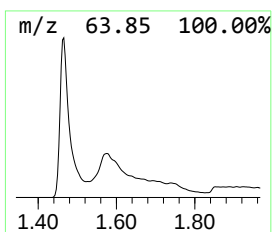
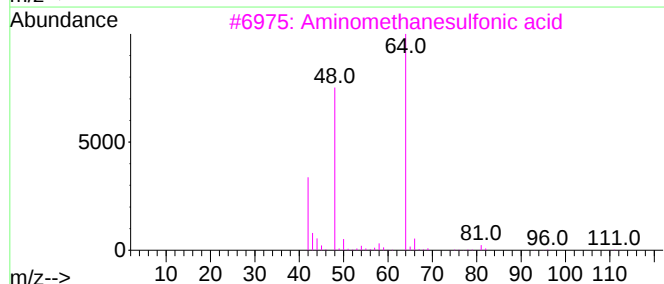
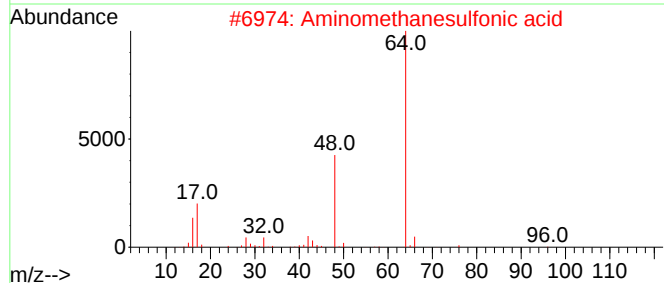
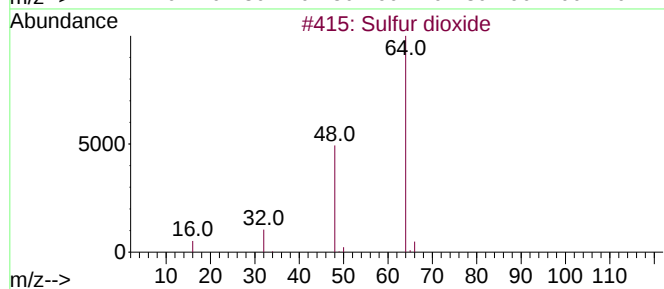
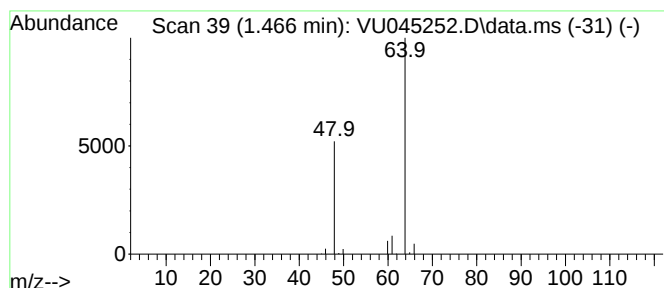
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.466	19.39 ug/L	263668	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	19.4	ug/L	263668	1	6.253	680025	50.0