

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
 Data File : VU045271.D
 Acq On : 09 Oct 2021 18:36
 Operator : SY/MD
 Sample : M4138-04DL 100X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F3DL

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: VU045271.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	34	40	53	rBV	17717	32223	1.77%	0.254%
2	1.600	74	81	93	rVB	196792	208895	11.48%	1.647%
3	1.899	166	174	193	rVB	141368	191378	10.52%	1.509%
4	2.565	367	381	399	rBV	264615	442764	24.33%	3.491%
5	2.790	441	451	470	rBV4	1032	2555	0.14%	0.020%
6	2.861	471	473	480	rVB2	311	251	0.01%	0.002%
7	2.896	480	484	487	rBV3	270	213	0.01%	0.002%
8	2.928	491	494	495	rBV	292	175	0.01%	0.001%
9	3.009	515	519	522	rBV2	190	200	0.01%	0.002%
10	3.047	522	531	541	rVB3	2802	5069	0.28%	0.040%
11	3.192	565	576	587	rBV2	1762	3936	0.22%	0.031%
12	3.272	599	601	603	rBV	200	131	0.01%	0.001%
13	3.308	608	612	616	rBV	164	188	0.01%	0.001%
14	3.452	653	657	660	rBV	184	196	0.01%	0.002%
15	3.549	684	687	689	rBV	255	189	0.01%	0.001%
16	3.809	763	768	771	rVB2	167	164	0.01%	0.001%
17	3.851	778	781	782	rBV2	268	168	0.01%	0.001%
18	3.864	782	785	786	rBV2	366	218	0.01%	0.002%
19	3.941	806	809	816	rBV2	192	302	0.02%	0.002%
20	4.012	828	831	836	rVB2	224	215	0.01%	0.002%
21	4.124	861	866	869	rBV2	257	296	0.02%	0.002%
22	4.189	881	886	889	rBV2	152	174	0.01%	0.001%
23	4.253	903	906	909	rVV2	157	135	0.01%	0.001%
24	4.276	909	913	916	rVV2	260	199	0.01%	0.002%
25	4.295	916	919	923	rVB2	169	163	0.01%	0.001%
26	4.321	923	927	931	rBV2	218	262	0.01%	0.002%
27	4.343	931	934	940	rVB2	179	163	0.01%	0.001%
28	4.395	947	950	954	rBV	154	130	0.01%	0.001%
29	4.626	1008	1022	1049	rBV	147858	348145	19.13%	2.745%
30	4.993	1129	1136	1143	rVV4	1400	2599	0.14%	0.020%
31	5.067	1143	1159	1183	rVB	223529	490185	26.94%	3.865%
32	5.208	1199	1203	1207	rBV2	507	598	0.03%	0.005%
33	5.298	1222	1231	1238	rBV4	645	1185	0.07%	0.009%
34	5.491	1288	1291	1295	rBV2	260	247	0.01%	0.002%
35	5.729	1343	1365	1395	rBV2	477241	1290008	70.88%	10.171%
36	6.076	1466	1473	1479	rBV3	295	486	0.03%	0.004%

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Integrator: RTE

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Peak separation: 5

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

37	6.112	1479	1484	1485	rBV2	345	271	0.01%	0.002%
38	6.253	1513	1528	1548	rBV	336816	633873	34.83%	4.998%
39	6.462	1590	1593	1595	rBV	207	174	0.01%	0.001%
40	6.533	1607	1615	1622	rVV3	1695	2700	0.15%	0.021%
41	6.697	1651	1666	1696	rBV	301084	586897	32.25%	4.628%
42	6.803	1696	1699	1701	rBV2	255	190	0.01%	0.001%
43	6.874	1717	1721	1724	rVB2	278	168	0.01%	0.001%
44	7.041	1767	1773	1776	rBV2	566	627	0.03%	0.005%
45	7.105	1789	1793	1796	rVB	214	182	0.01%	0.001%
46	7.176	1809	1815	1816	rVV3	810	709	0.04%	0.006%
47	7.185	1816	1818	1825	rVB3	1088	1099	0.06%	0.009%
48	7.349	1866	1869	1872	rBV2	262	190	0.01%	0.001%
49	7.436	1893	1896	1902	rVB2	162	147	0.01%	0.001%
50	7.568	1924	1937	1953	rBV	148148	255426	14.04%	2.014%
51	7.684	1967	1973	1983	rVB3	638	1207	0.07%	0.010%
52	7.748	1986	1993	1999	rVV2	128	227	0.01%	0.002%
53	7.800	2000	2009	2016	rVB3	1381	1942	0.11%	0.015%
54	7.902	2027	2041	2053	rBV	569646	985917	54.18%	7.774%
55	7.973	2053	2063	2082	rVB	139862	236765	13.01%	1.867%
56	8.182	2117	2128	2142	rBV	104185	170130	9.35%	1.341%
57	8.298	2162	2164	2167	rVB	344	145	0.01%	0.001%
58	8.346	2176	2179	2181	rBV	257	193	0.01%	0.002%
59	8.475	2215	2219	2226	rVB2	267	285	0.02%	0.002%
60	8.517	2227	2232	2234	rBV2	133	134	0.01%	0.001%
61	8.636	2256	2269	2301	rBV	426861	751956	41.32%	5.929%
62	9.095	2408	2412	2413	rBV	213	169	0.01%	0.001%
63	9.420	2499	2513	2532	rBV	488689	793328	43.59%	6.255%
64	9.574	2548	2561	2579	rBV	372315	586681	32.24%	4.626%
65	9.693	2585	2598	2627	rVB	1126449	1819874	100.00%	14.349%
66	10.012	2694	2697	2701	rBV2	233	206	0.01%	0.002%
67	10.102	2713	2725	2746	rBV	326252	523222	28.75%	4.126%
68	10.349	2799	2802	2806	rBV2	217	200	0.01%	0.002%
69	10.488	2836	2845	2854	rBV2	7355	10490	0.58%	0.083%
70	10.677	2897	2904	2912	rVB4	1470	2125	0.12%	0.017%
71	10.761	2917	2930	2948	rVV	421533	675256	37.10%	5.324%
72	10.909	2968	2976	2985	rVB3	2288	3389	0.19%	0.027%
73	11.002	2996	3005	3023	rVB	7847	15934	0.88%	0.126%
74	11.092	3023	3033	3043	rBV	3952	5662	0.31%	0.045%
75	11.150	3048	3051	3057	rBV2	207	231	0.01%	0.002%
76	11.240	3075	3079	3083	rVB2	231	225	0.01%	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
 Title : VOC Analysis

77	11.298	3087	3097	3107	rVB	3530	5184	0.28%	0.041%
78	11.365	3114	3118	3122	rBV2	183	176	0.01%	0.001%
79	11.471	3141	3151	3162	rVB	14567	22129	1.22%	0.174%
80	11.700	3218	3222	3229	rVB2	610	583	0.03%	0.005%
81	11.748	3234	3237	3241	rVB	531	389	0.02%	0.003%
82	11.815	3245	3258	3275	rVV	445489	707492	38.88%	5.578%
83	11.899	3277	3284	3293	rVB3	5038	7182	0.39%	0.057%
84	11.944	3293	3298	3301	rBV2	493	499	0.03%	0.004%
85	11.979	3302	3309	3316	rVB3	947	1211	0.07%	0.010%
86	12.063	3326	3335	3338	rBV4	817	1199	0.07%	0.009%
87	12.098	3342	3346	3353	rVB4	1852	2221	0.12%	0.018%
88	12.195	3363	3376	3396	rBV	520207	831996	45.72%	6.560%
89	12.484	3462	3466	3467	rBV2	444	243	0.01%	0.002%
90	12.748	3545	3548	3554	rBV2	259	321	0.02%	0.003%
91	12.938	3604	3607	3614	rBV	191	248	0.01%	0.002%
92	13.131	3664	3667	3670	rVB	267	164	0.01%	0.001%
93	13.150	3670	3673	3675	rBV3	264	190	0.01%	0.001%
94	13.288	3713	3716	3722	rBV2	213	288	0.02%	0.002%
95	13.780	3866	3869	3873	rBV2	174	156	0.01%	0.001%
96	13.848	3884	3890	3893	rBV4	814	889	0.05%	0.007%
97	14.095	3957	3967	3973	rBV2	3828	5698	0.31%	0.045%
98	14.330	4036	4040	4041	rBV	747	516	0.03%	0.004%
99	14.385	4054	4057	4062	rBV2	357	314	0.02%	0.002%
100	14.581	4114	4118	4122	rBV2	458	375	0.02%	0.003%

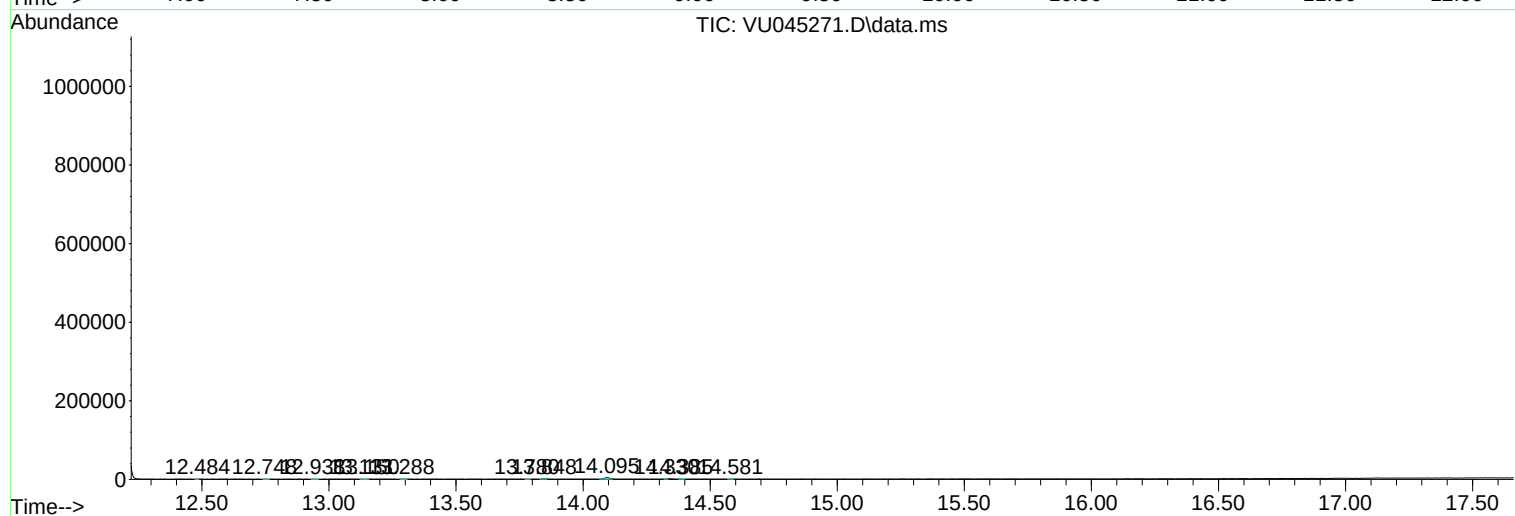
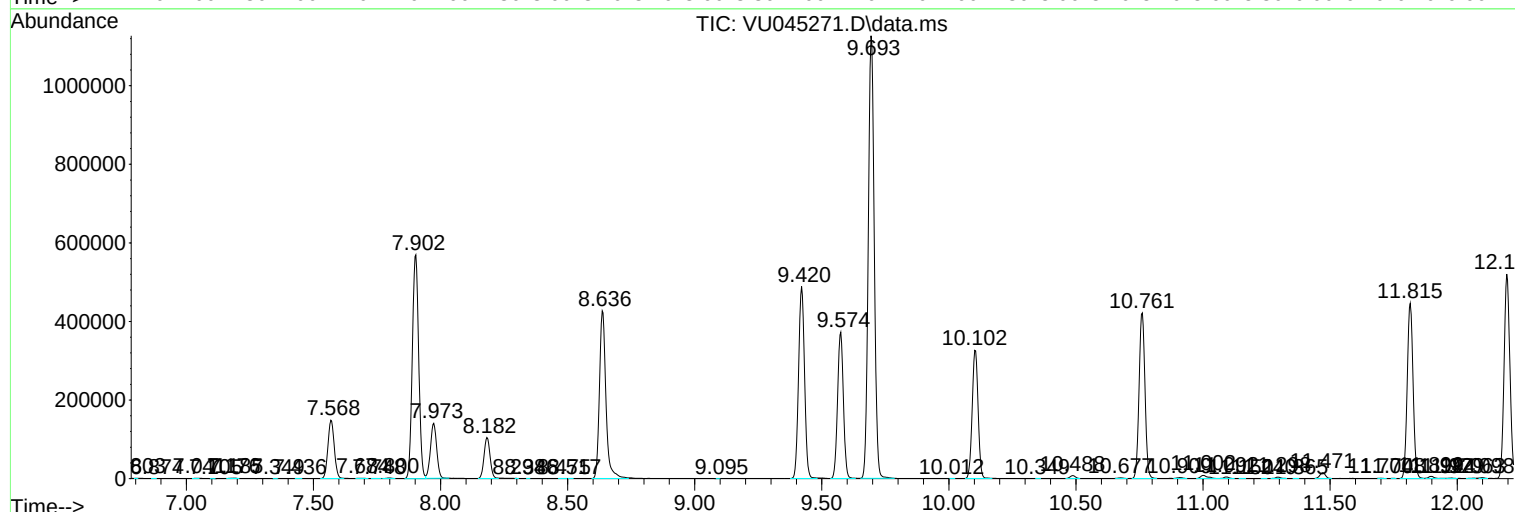
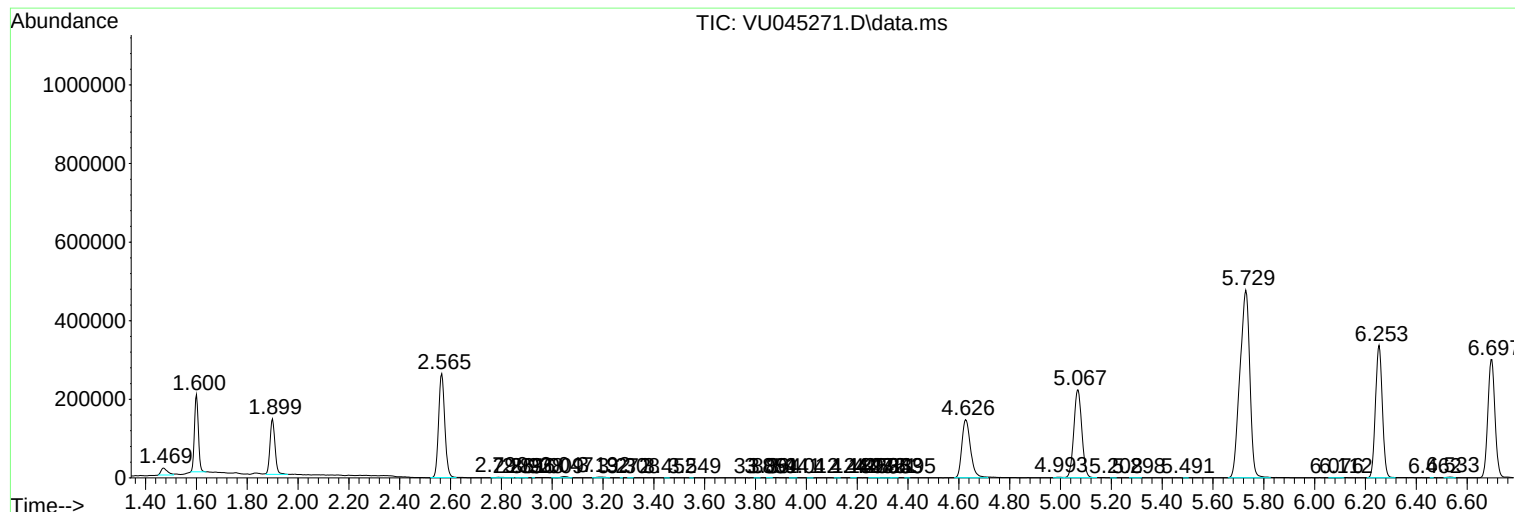
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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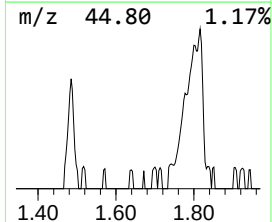
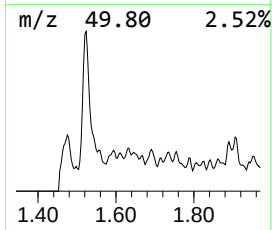
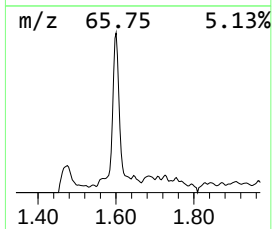
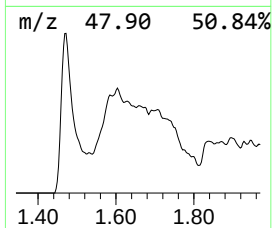
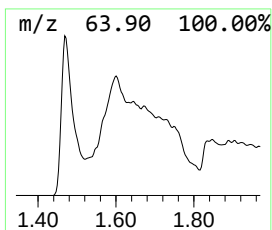
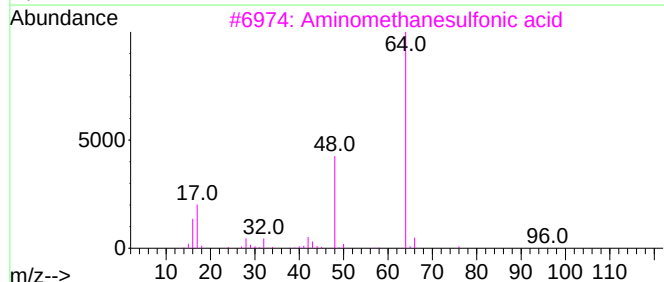
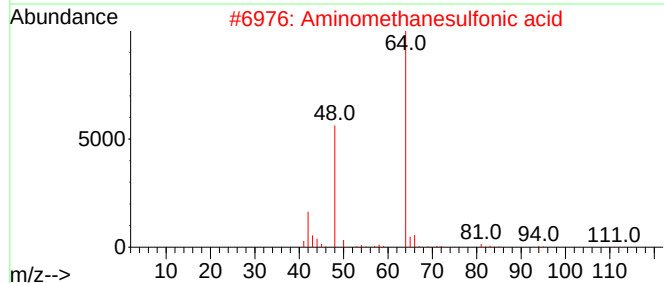
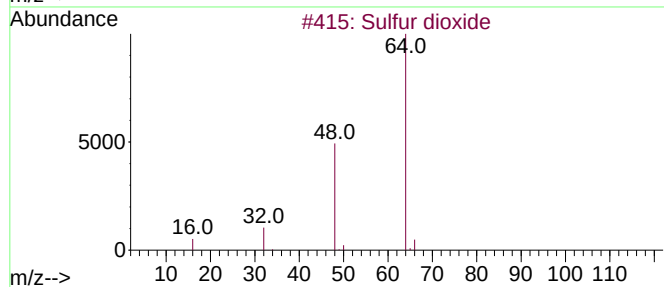
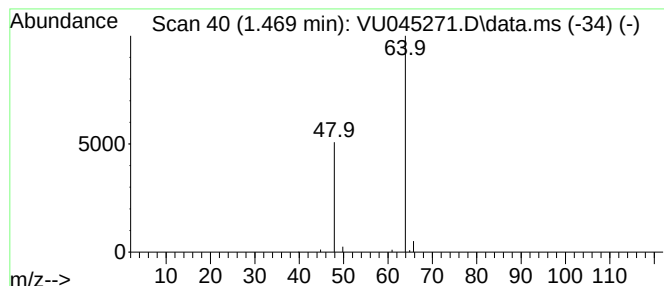
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	2.54 ug/L	32223	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	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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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	2.5	ug/L	32223	1	6.253	633873	50.0