

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045241.D
 Acq On : 08 Oct 2021 11:07
 Operator : SY/MD
 Sample : M4023-02 1000X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AH7

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: VU045241.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	53	rBV	19958	39887	2.00%	0.289%
2	1.601	73	81	93	rBV	242558	263469	13.19%	1.910%
3	1.887	162	170	187	rVB	166772	229923	11.51%	1.667%
4	2.485	354	356	360	rVB2	470	275	0.01%	0.002%
5	2.562	364	380	406	rVV2	366032	670287	33.56%	4.860%
6	2.784	445	449	460	rVB2	457	702	0.04%	0.005%
7	3.047	517	531	550	rVV	59684	115959	5.81%	0.841%
8	3.183	570	573	575	rBV2	231	163	0.01%	0.001%
9	3.231	581	588	594	rVB2	173	244	0.01%	0.002%
10	3.295	605	608	611	rBV	200	189	0.01%	0.001%
11	3.398	636	640	644	rBV	176	180	0.01%	0.001%
12	3.552	685	688	690	rBV	197	162	0.01%	0.001%
13	3.642	711	716	721	rBV2	241	317	0.02%	0.002%
14	3.729	740	743	746	rVB	234	166	0.01%	0.001%
15	3.761	748	753	755	rBV2	222	179	0.01%	0.001%
16	3.871	776	787	801	rVV2	2061	4482	0.22%	0.032%
17	4.549	995	998	1006	rVB2	285	414	0.02%	0.003%
18	4.629	1006	1023	1061	rBV2	166736	520237	26.05%	3.772%
19	4.928	1112	1116	1120	rBV	210	181	0.01%	0.001%
20	4.948	1120	1122	1127	rVB3	236	204	0.01%	0.001%
21	4.980	1127	1132	1136	rBV2	243	264	0.01%	0.002%
22	5.067	1141	1159	1188	rBV	263419	577686	28.92%	4.189%
23	5.202	1199	1201	1205	rVB2	314	194	0.01%	0.001%
24	5.221	1205	1207	1212	rBV2	339	273	0.01%	0.002%
25	5.317	1221	1237	1260	rBV	114241	256098	12.82%	1.857%
26	5.729	1343	1365	1400	rBV2	573634	1534447	76.82%	11.126%
27	6.038	1456	1461	1468	rBV3	493	706	0.04%	0.005%
28	6.253	1513	1528	1548	rBV	372120	692184	34.65%	5.019%
29	6.324	1548	1550	1554	rVB2	454	286	0.01%	0.002%
30	6.546	1604	1619	1651	rBV	1084681	1997383	100.00%	14.482%
31	6.694	1651	1665	1684	rVB	361157	696275	34.86%	5.048%
32	6.806	1696	1700	1707	rVB6	957	1254	0.06%	0.009%
33	6.899	1726	1729	1731	rVB2	296	169	0.01%	0.001%
34	6.919	1731	1735	1740	rBV2	186	215	0.01%	0.002%
35	7.002	1755	1761	1764	rBV2	231	295	0.01%	0.002%
36	7.047	1769	1775	1785	rVB3	562	906	0.05%	0.007%

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 Title : VOC Analysis

37	7.179	1809	1816	1826	rBV5	1163	1830	0.09%	0.013%
38	7.353	1868	1870	1874	rBV	211	204	0.01%	0.001%
39	7.568	1923	1937	1958	rBV	201319	346663	17.36%	2.513%
40	7.687	1968	1974	1980	rBV4	864	1312	0.07%	0.010%
41	7.793	2002	2007	2014	rBV2	344	537	0.03%	0.004%
42	7.903	2026	2041	2055	rBV	695485	1189043	59.53%	8.621%
43	7.973	2056	2063	2077	rVB	11921	19957	1.00%	0.145%
44	8.105	2101	2104	2109	rVB2	221	166	0.01%	0.001%
45	8.182	2115	2128	2143	rBV	142728	232613	11.65%	1.687%
46	8.372	2180	2187	2191	rBV2	172	202	0.01%	0.001%
47	8.404	2191	2197	2204	rBV2	1763	2287	0.11%	0.017%
48	8.558	2241	2245	2248	rBV2	415	367	0.02%	0.003%
49	8.639	2256	2270	2303	rBV	488384	864219	43.27%	6.266%
50	8.864	2336	2340	2343	rVB2	241	189	0.01%	0.001%
51	9.169	2426	2435	2437	rBV2	210	295	0.01%	0.002%
52	9.420	2500	2513	2536	rBV	536954	865337	43.32%	6.274%
53	9.533	2546	2548	2553	rVB	282	195	0.01%	0.001%
54	9.571	2553	2560	2569	rVB2	3308	4555	0.23%	0.033%
55	9.697	2588	2599	2610	rVB	14658	22568	1.13%	0.164%
56	9.999	2688	2693	2695	rBV	224	263	0.01%	0.002%
57	10.105	2717	2726	2735	rVV2	7699	11564	0.58%	0.084%
58	10.137	2735	2736	2743	rVB	231	203	0.01%	0.001%
59	10.179	2746	2749	2754	rBV2	142	175	0.01%	0.001%
60	10.491	2842	2846	2849	rBV	324	328	0.02%	0.002%
61	10.555	2862	2866	2869	rVB2	183	169	0.01%	0.001%
62	10.629	2884	2889	2892	rBV2	224	240	0.01%	0.002%
63	10.674	2895	2903	2911	rVB	4192	5965	0.30%	0.043%
64	10.761	2917	2930	2949	rBV	505265	803704	40.24%	5.827%
65	10.835	2949	2953	2956	rVB2	405	343	0.02%	0.002%
66	10.870	2956	2964	2965	rBV3	762	847	0.04%	0.006%
67	11.005	3003	3006	3011	rVV2	264	280	0.01%	0.002%
68	11.118	3037	3041	3043	rBV3	853	796	0.04%	0.006%
69	11.201	3065	3067	3073	rVB2	273	261	0.01%	0.002%
70	11.401	3122	3129	3132	rBV	183	225	0.01%	0.002%
71	11.420	3133	3135	3138	rVB2	334	178	0.01%	0.001%
72	11.462	3138	3148	3158	rBV4	3425	5290	0.26%	0.038%
73	11.581	3182	3185	3197	rVB2	657	750	0.04%	0.005%
74	11.697	3214	3221	3229	rVB3	1947	2593	0.13%	0.019%
75	11.735	3229	3233	3236	rBV	343	354	0.02%	0.003%
76	11.751	3236	3238	3244	rVB3	481	251	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M

Title : VOC Analysis

77	11.816	3245	3258	3277	rBV	493381	774671	38.78%	5.617%
78	11.935	3291	3295	3296	rBV3	1145	727	0.04%	0.005%
79	11.976	3303	3308	3317	rVB3	3080	3978	0.20%	0.029%
80	12.195	3359	3376	3398	rBV	616043	1007507	50.44%	7.305%
81	12.333	3414	3419	3425	rVB4	1116	1272	0.06%	0.009%
82	12.414	3441	3444	3448	rVB2	379	241	0.01%	0.002%
83	12.571	3489	3493	3496	rBV2	213	178	0.01%	0.001%
84	12.719	3535	3539	3544	rBV2	192	270	0.01%	0.002%
85	12.925	3599	3603	3605	rBV2	195	171	0.01%	0.001%
86	13.227	3693	3697	3700	rBV2	434	441	0.02%	0.003%
87	13.513	3782	3786	3790	rBV2	191	230	0.01%	0.002%
88	13.539	3791	3794	3798	rVB2	327	250	0.01%	0.002%
89	13.771	3863	3866	3869	rBV2	183	164	0.01%	0.001%
90	13.848	3884	3890	3896	rBV2	734	905	0.05%	0.007%
91	13.951	3919	3922	3926	rBV	163	172	0.01%	0.001%
92	14.095	3957	3967	3979	rBV	2844	4191	0.21%	0.030%
93	14.298	4026	4030	4033	rBV2	310	300	0.02%	0.002%
94	14.336	4036	4042	4049	rVV3	1163	1313	0.07%	0.010%
95	14.423	4066	4069	4071	rBV	194	171	0.01%	0.001%
96	14.513	4094	4097	4102	rVV3	273	282	0.01%	0.002%
97	14.587	4117	4120	4123	rVB	387	242	0.01%	0.002%
98	14.709	4153	4158	4161	rBV2	269	273	0.01%	0.002%
99	14.835	4194	4197	4199	rBV2	314	206	0.01%	0.001%
100	16.677	4767	4770	4771	rBV	573	324	0.02%	0.002%

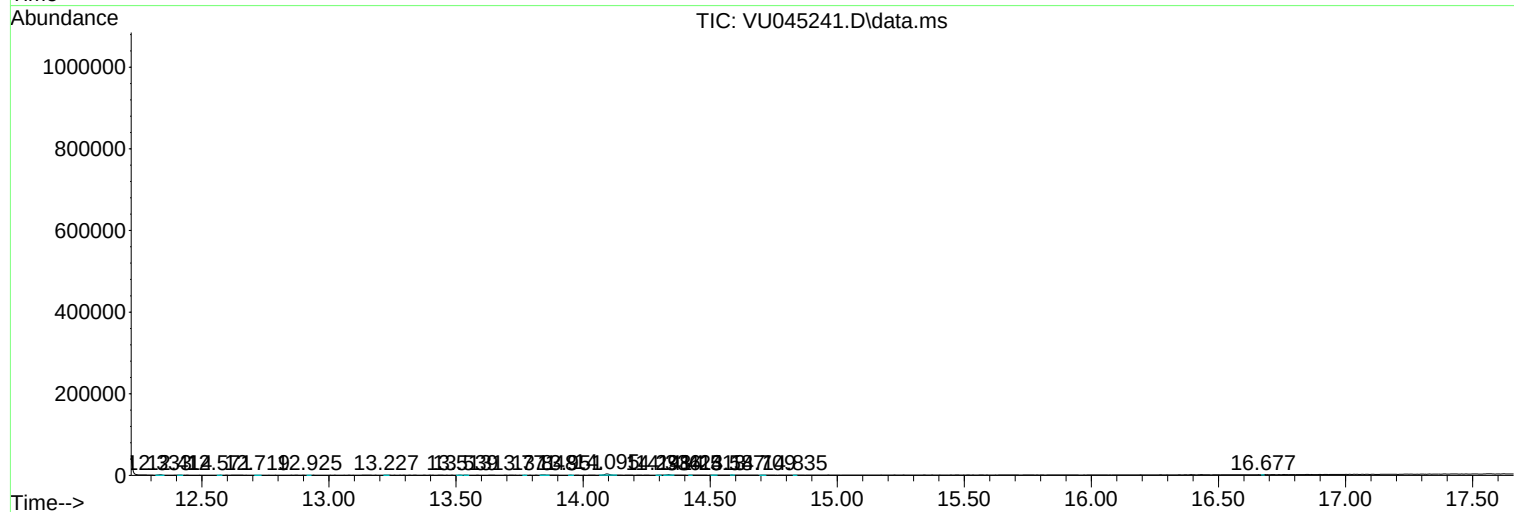
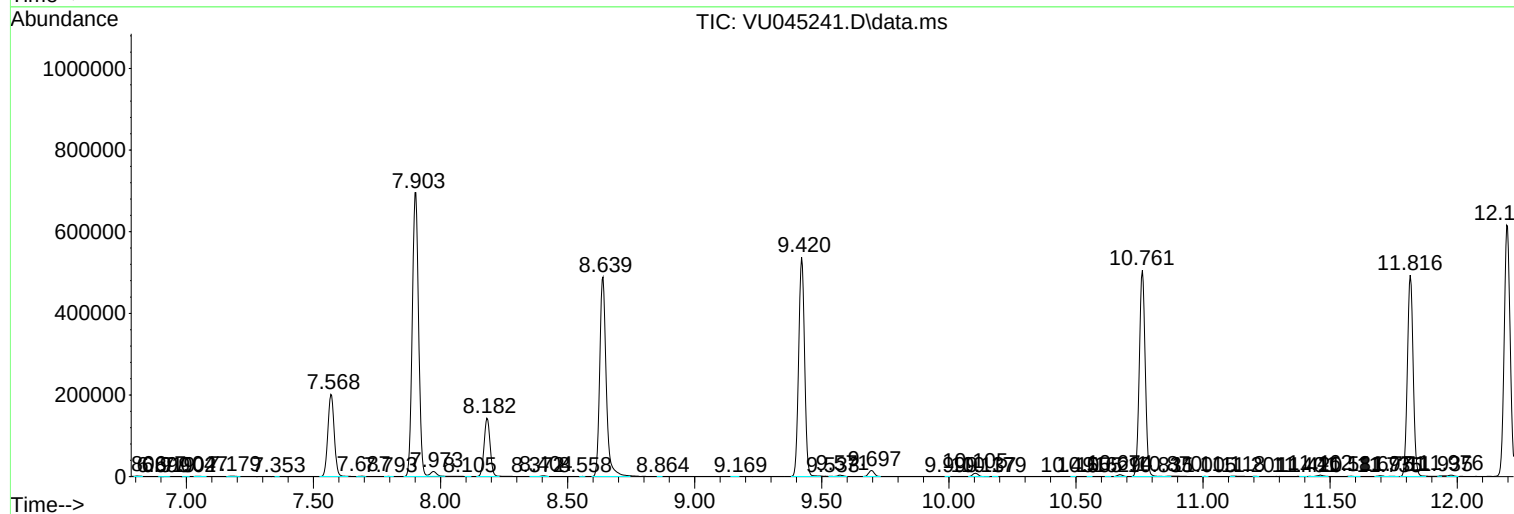
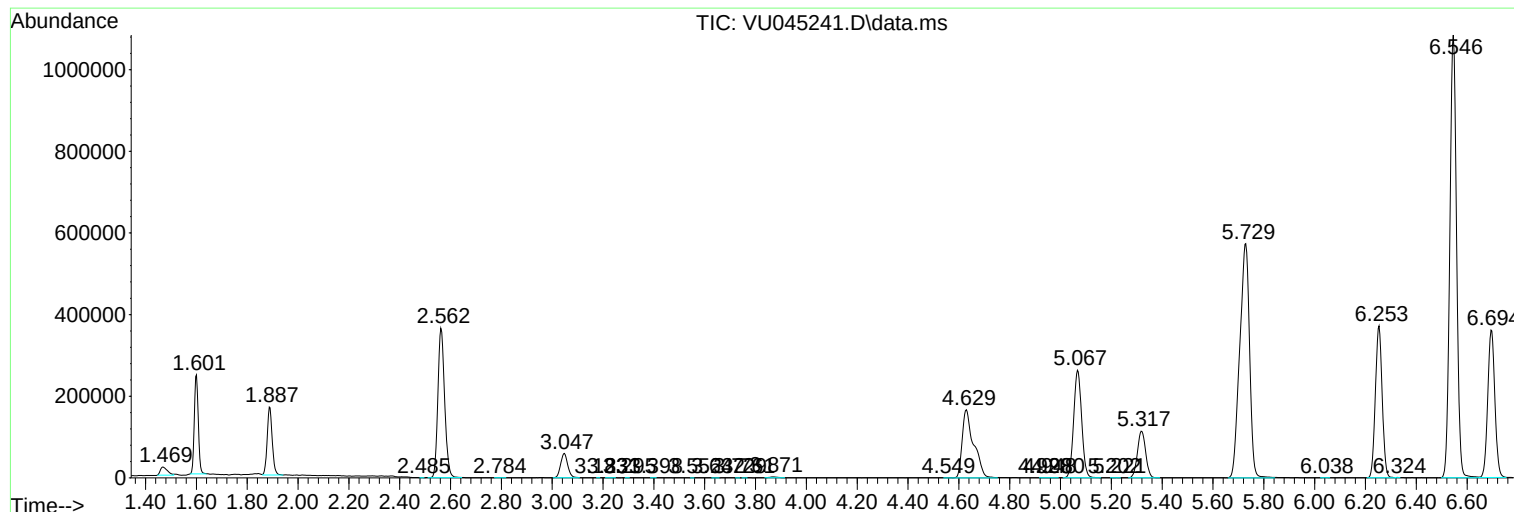
Sum of corrected areas: 13792052

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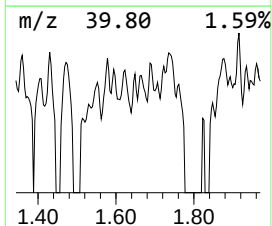
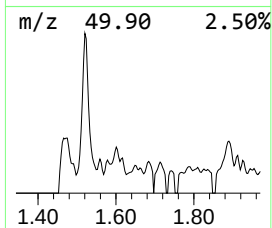
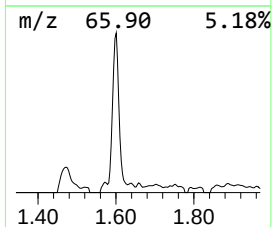
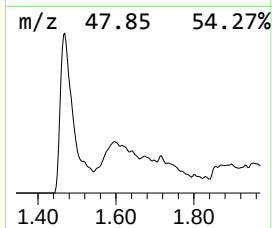
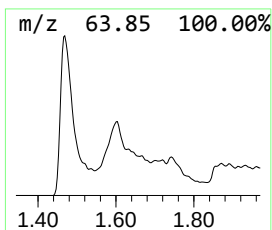
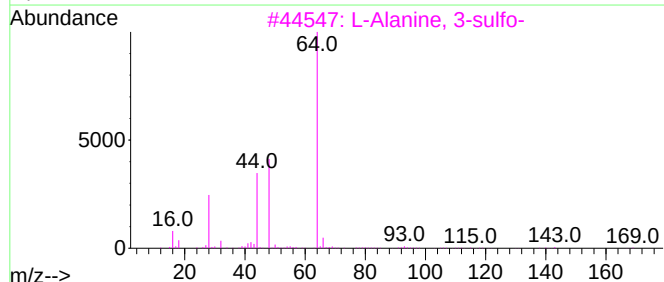
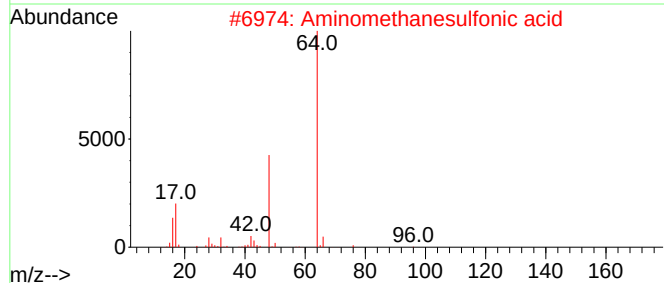
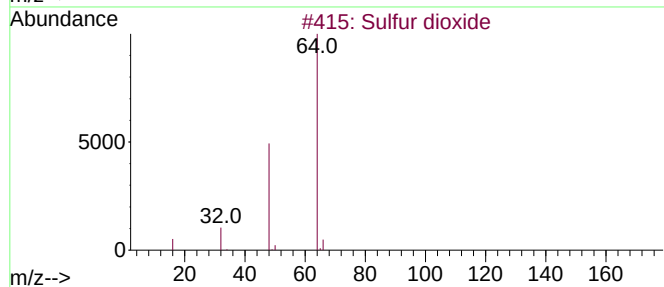
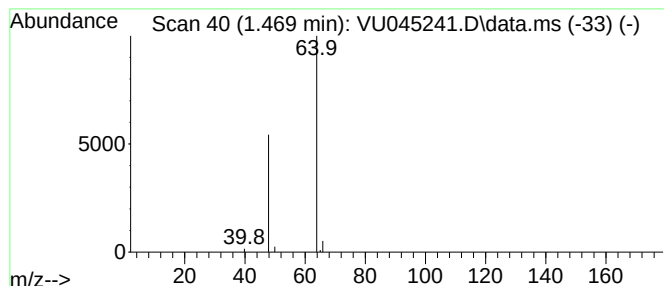
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	2.88 ug/L	39887	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.469	2.9	ug/L	39887	1	6.253	692184	50.0