

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053275.D
 Acq On : 17 Mar 2023 18:24
 Operator : JC/MD
 Sample : 01930-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF8

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\SFAMULM031523WMA.M
 Title : VOC Analysis

Signal : TIC: VU053275.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	32	39	53	rBV	16003	27924	4.60%	0.622%
2	1.597	73	80	98	rVB	83385	93304	15.36%	2.080%
3	1.909	169	177	196	rBV	65798	89614	14.75%	1.998%
4	2.562	369	380	395	rBV	123359	198028	32.60%	4.414%
5	3.183	567	573	575	rBV	203	233	0.04%	0.005%
6	3.212	579	582	584	rBV	186	121	0.02%	0.003%
7	3.372	630	632	633	rBV	168	77	0.01%	0.002%
8	3.401	638	641	645	rBV	221	169	0.03%	0.004%
9	3.540	681	684	692	rBV2	240	259	0.04%	0.006%
10	3.575	692	695	697	rBV	193	109	0.02%	0.002%
11	3.697	730	733	736	rBV	197	124	0.02%	0.003%
12	3.996	824	826	827	rBV	128	54	0.01%	0.001%
13	4.073	848	850	856	rVB	206	132	0.02%	0.003%
14	4.128	865	867	873	rVB	261	143	0.02%	0.003%
15	4.234	897	900	901	rBV	147	83	0.01%	0.002%
16	4.298	918	920	931	rVB	232	199	0.03%	0.004%
17	4.433	961	962	965	rVB	143	55	0.01%	0.001%
18	4.466	970	972	978	rVV2	142	106	0.02%	0.002%
19	4.539	992	995	997	rBV2	211	134	0.02%	0.003%
20	4.568	1002	1004	1006	rBV	184	105	0.02%	0.002%
21	4.613	1007	1018	1047	rVV	46818	110130	18.13%	2.455%
22	4.887	1100	1103	1105	rBV2	254	152	0.03%	0.003%
23	4.900	1105	1107	1114	rVB2	224	231	0.04%	0.005%
24	5.057	1141	1156	1181	rBV2	109636	242878	39.99%	5.414%
25	5.221	1204	1207	1209	rBV	193	106	0.02%	0.002%
26	5.285	1226	1227	1230	rBV	197	92	0.02%	0.002%
27	5.330	1238	1241	1244	rVB2	139	103	0.02%	0.002%
28	5.385	1254	1258	1259	rBV	245	204	0.03%	0.005%
29	5.510	1295	1297	1298	rBV	141	57	0.01%	0.001%
30	5.549	1307	1309	1313	rBV	126	57	0.01%	0.001%
31	5.568	1313	1315	1317	rBV2	117	65	0.01%	0.001%
32	5.719	1341	1362	1381	rBV2	226858	607392	100.00%	13.539%
33	5.967	1436	1439	1441	rVB2	154	92	0.02%	0.002%
34	6.047	1460	1464	1468	rBV	190	147	0.02%	0.003%
35	6.141	1490	1493	1497	rVB	190	131	0.02%	0.003%
36	6.244	1512	1525	1543	rBV	182949	339949	55.97%	7.578%

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 Title : VOC Analysis

37	6.408	1574	1576	1578	rBV	131	54	0.01%	0.001%
38	6.607	1636	1638	1643	rBV	173	104	0.02%	0.002%
39	6.684	1649	1662	1686	rBV	143284	280536	46.19%	6.253%
40	6.790	1692	1695	1700	rVB2	290	296	0.05%	0.007%
41	6.826	1700	1706	1710	rBV	229	357	0.06%	0.008%
42	6.877	1720	1722	1723	rBV	140	61	0.01%	0.001%
43	7.070	1780	1782	1783	rBV	151	47	0.01%	0.001%
44	7.141	1803	1804	1808	rVB2	256	120	0.02%	0.003%
45	7.179	1809	1816	1817	rBV2	1047	866	0.14%	0.019%
46	7.250	1834	1838	1841	rBV2	182	111	0.02%	0.002%
47	7.279	1844	1847	1855	rBV2	166	177	0.03%	0.004%
48	7.414	1887	1889	1892	rBV	214	102	0.02%	0.002%
49	7.472	1906	1907	1909	rBV	117	67	0.01%	0.001%
50	7.485	1909	1911	1914	rVV2	253	152	0.03%	0.003%
51	7.504	1914	1917	1919	rVB2	233	127	0.02%	0.003%
52	7.562	1919	1935	1953	rBV	81955	142818	23.51%	3.184%
53	7.671	1966	1969	1970	rBV	141	57	0.01%	0.001%
54	7.690	1970	1975	1977	rBV3	603	629	0.10%	0.014%
55	7.784	2002	2004	2007	rBV	166	74	0.01%	0.002%
56	7.893	2026	2038	2057	rBV	281132	478925	78.85%	10.676%
57	8.047	2082	2086	2091	rBV3	318	317	0.05%	0.007%
58	8.176	2114	2126	2141	rBV2	55120	92086	15.16%	2.053%
59	8.292	2160	2162	2164	rBV	189	86	0.01%	0.002%
60	8.626	2256	2266	2291	rBV2	144594	265963	43.79%	5.929%
61	9.243	2454	2458	2461	rBV2	285	269	0.04%	0.006%
62	9.272	2463	2467	2471	rVB2	189	207	0.03%	0.005%
63	9.366	2493	2496	2498	rBV2	208	162	0.03%	0.004%
64	9.414	2498	2511	2532	rVV	252642	414394	68.23%	9.237%
65	9.639	2579	2581	2583	rBV	175	79	0.01%	0.002%
66	9.771	2620	2622	2626	rVB2	190	126	0.02%	0.003%
67	9.941	2673	2675	2677	rBV	156	60	0.01%	0.001%
68	10.089	2719	2721	2722	rBV	130	55	0.01%	0.001%
69	10.128	2730	2733	2735	rBV2	176	126	0.02%	0.003%
70	10.166	2743	2745	2747	rBV	167	68	0.01%	0.002%
71	10.224	2757	2763	2764	rBV	207	246	0.04%	0.005%
72	10.366	2804	2807	2808	rBV	155	74	0.01%	0.002%
73	10.391	2813	2815	2816	rBV	210	70	0.01%	0.002%
74	10.436	2826	2829	2832	rBV	175	103	0.02%	0.002%
75	10.571	2867	2871	2873	rBV2	251	206	0.03%	0.005%
76	10.620	2882	2886	2888	rBV	214	177	0.03%	0.004%

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 Title : VOC Analysis

77	10.710	2911	2914	2915	rBV	172	70	0.01%	0.002%
78	10.751	2915	2927	2948	rVV	185712	296762	48.86%	6.615%
79	11.205	3065	3068	3073	rBV2	241	167	0.03%	0.004%
80	11.404	3127	3130	3136	rBV	198	263	0.04%	0.006%
81	11.443	3141	3142	3145	rVB	156	55	0.01%	0.001%
82	11.539	3168	3172	3175	rBV	208	167	0.03%	0.004%
83	11.809	3243	3256	3277	rBV	245794	389991	64.21%	8.693%
84	11.919	3288	3290	3292	rVB	160	48	0.01%	0.001%
85	12.005	3315	3317	3319	rVB	178	70	0.01%	0.002%
86	12.025	3319	3323	3325	rBV2	207	183	0.03%	0.004%
87	12.079	3337	3340	3343	rBV	284	189	0.03%	0.004%
88	12.189	3361	3374	3392	rBV	250332	403098	66.37%	8.985%
89	12.333	3417	3419	3423	rBV	186	93	0.02%	0.002%
90	12.735	3541	3544	3546	rBV	151	82	0.01%	0.002%
91	12.989	3620	3623	3629	rVB2	214	176	0.03%	0.004%
92	13.266	3707	3709	3712	rBV2	188	118	0.02%	0.003%
93	13.632	3820	3823	3825	rBV	239	164	0.03%	0.004%
94	13.684	3836	3839	3843	rBV	212	138	0.02%	0.003%
95	13.848	3888	3890	3893	rVB	236	115	0.02%	0.003%
96	13.867	3894	3896	3900	rVB	346	202	0.03%	0.005%
97	14.365	4048	4051	4057	rBV	216	153	0.03%	0.003%
98	14.857	4201	4204	4209	rVB	265	187	0.03%	0.004%
99	14.886	4209	4213	4216	rBV2	227	191	0.03%	0.004%
100	15.652	4449	4451	4453	rBV	268	145	0.02%	0.003%

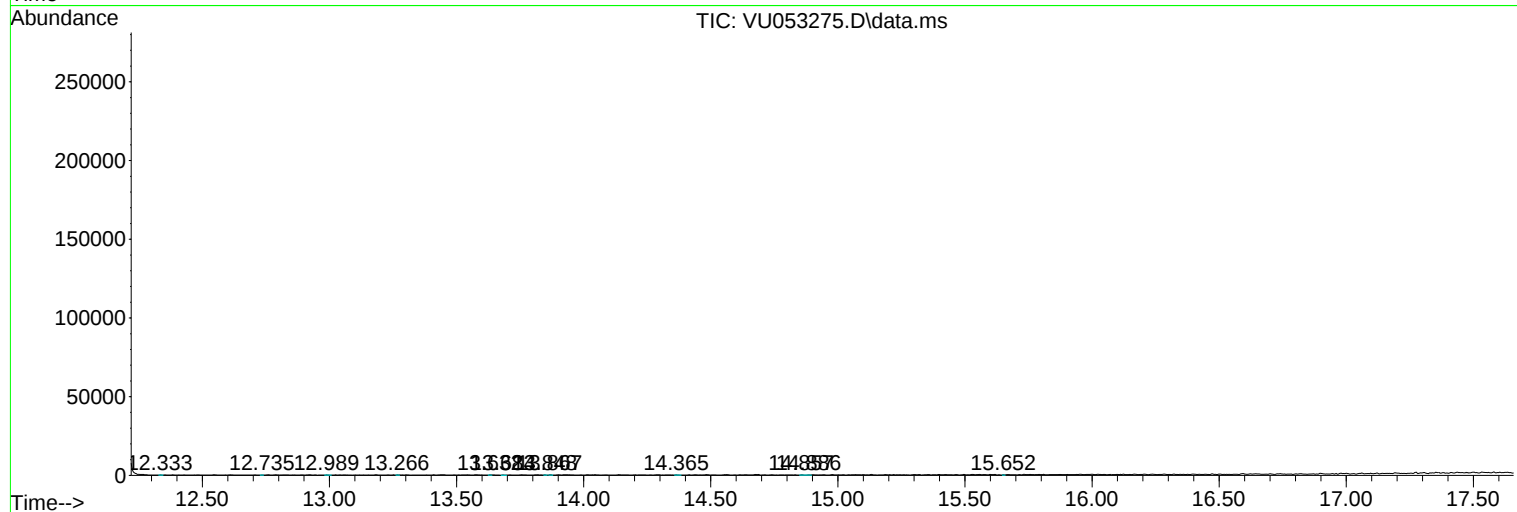
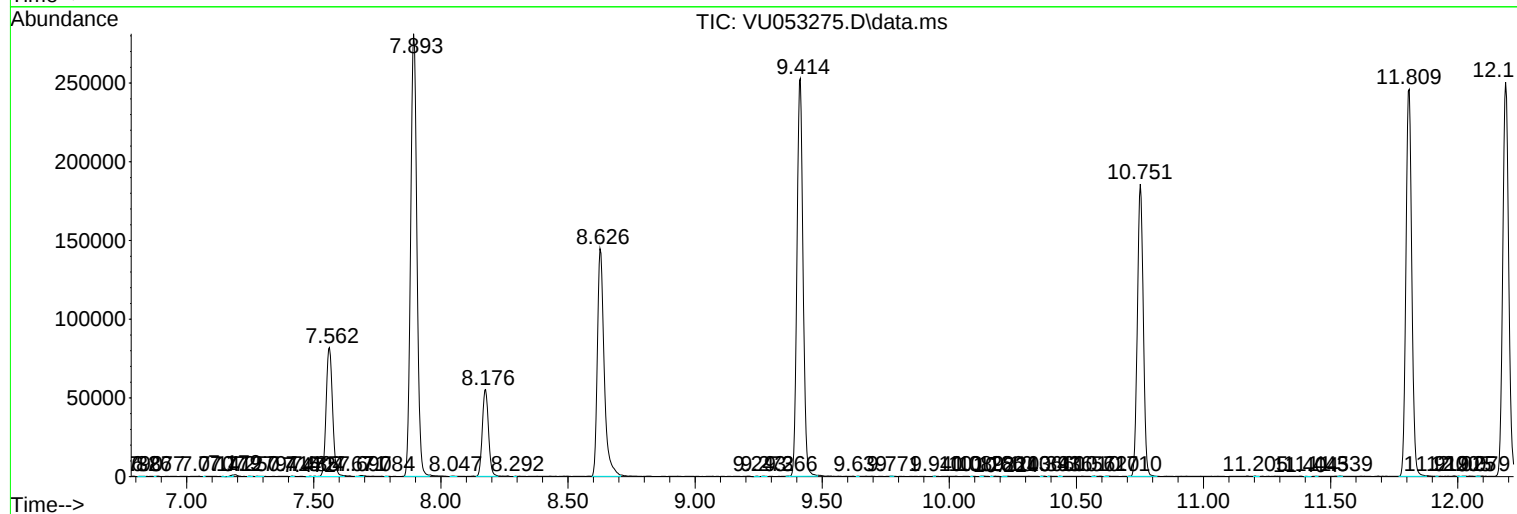
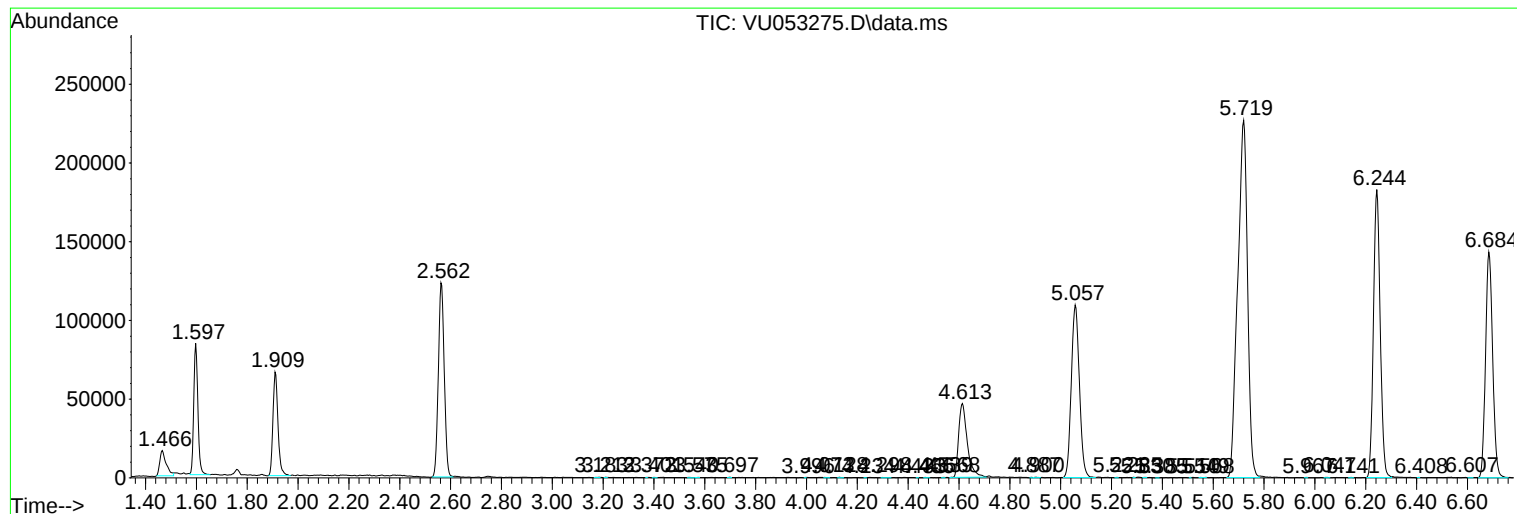
Sum of corrected areas: 4486140

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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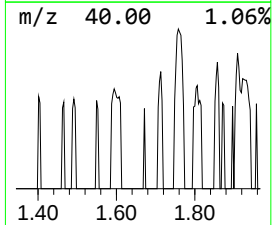
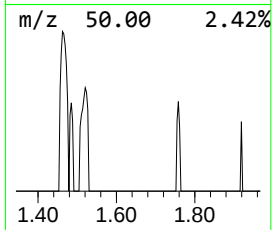
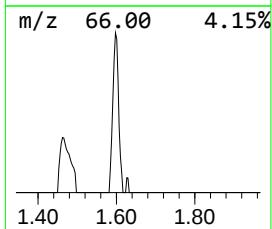
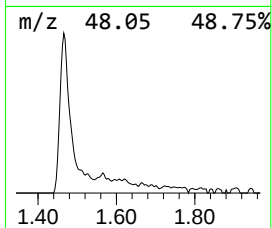
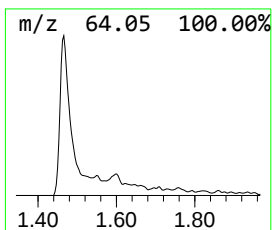
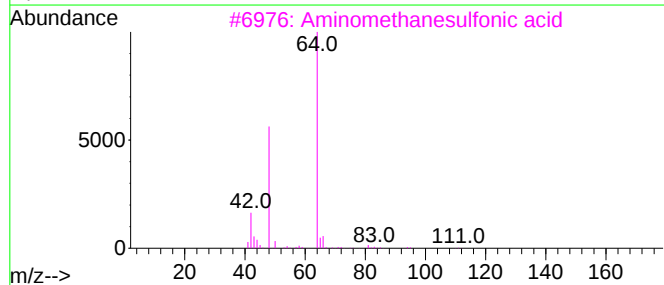
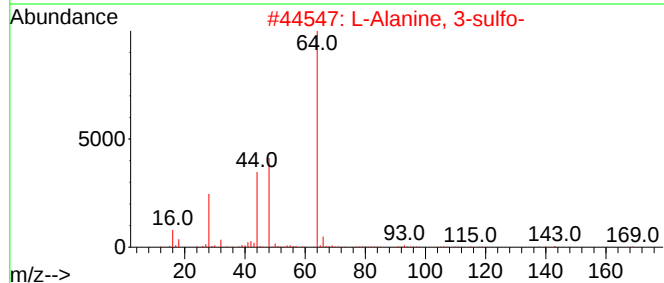
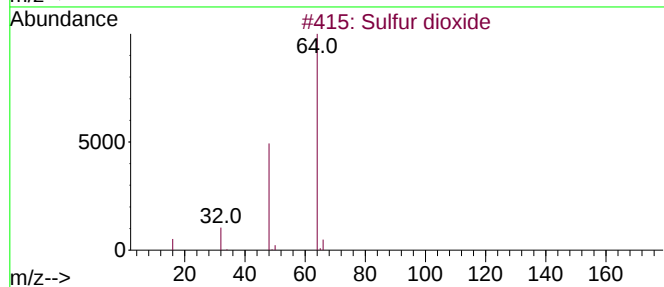
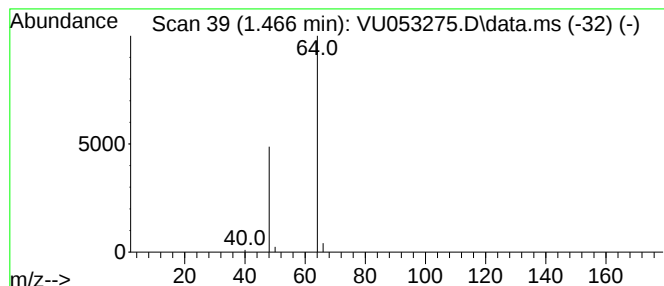
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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	4.11 ug/L	27924	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.466	4.1	ug/L	27924	1	6.244	339949	50.0