

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053282.D
 Acq On : 17 Mar 2023 21:34
 Operator : JC/MD
 Sample : 01930-23
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFG9

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: VU053282.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	53	rBV	27019	48306	7.91%	1.067%
2	1.597	74	80	95	rVB2	93129	107942	17.67%	2.384%
3	1.909	169	177	194	rBV	63467	87833	14.38%	1.940%
4	2.565	369	381	394	rBV	121324	194579	31.85%	4.298%
5	3.176	568	571	574	rBV2	366	258	0.04%	0.006%
6	3.372	627	632	638	rBV	226	249	0.04%	0.006%
7	3.613	703	707	717	rVB	274	295	0.05%	0.007%
8	4.183	881	884	886	rBV	304	232	0.04%	0.005%
9	4.324	926	928	929	rBV	127	35	0.01%	0.001%
10	4.523	988	990	992	rBV2	181	100	0.02%	0.002%
11	4.613	1007	1018	1049	rBV2	45650	111946	18.33%	2.473%
12	4.922	1111	1114	1121	rBV	196	205	0.03%	0.005%
13	5.057	1141	1156	1177	rBV	111950	243949	39.93%	5.389%
14	5.356	1246	1249	1251	rBV2	167	130	0.02%	0.003%
15	5.543	1304	1307	1311	rVB	196	105	0.02%	0.002%
16	5.633	1334	1335	1337	rBV	128	41	0.01%	0.001%
17	5.719	1341	1362	1384	rBV2	227110	610876	100.00%	13.494%
18	5.883	1412	1413	1423	rVB	284	280	0.05%	0.006%
19	5.925	1423	1426	1429	rBV	198	100	0.02%	0.002%
20	6.150	1492	1496	1500	rBV	282	227	0.04%	0.005%
21	6.170	1500	1502	1505	rVB	245	134	0.02%	0.003%
22	6.244	1512	1525	1545	rBV	181906	337883	55.31%	7.464%
23	6.401	1571	1574	1576	rVB2	166	92	0.02%	0.002%
24	6.462	1589	1593	1599	rVB2	182	143	0.02%	0.003%
25	6.507	1603	1607	1609	rBV	207	186	0.03%	0.004%
26	6.523	1609	1612	1615	rBV2	298	187	0.03%	0.004%
27	6.600	1634	1636	1639	rBV	138	106	0.02%	0.002%
28	6.639	1645	1648	1649	rBV2	136	80	0.01%	0.002%
29	6.684	1649	1662	1682	rVV	142699	276120	45.20%	6.099%
30	6.803	1696	1699	1704	rBV3	589	520	0.09%	0.011%
31	6.887	1723	1725	1726	rBV3	134	36	0.01%	0.001%
32	6.957	1744	1747	1750	rVB2	151	99	0.02%	0.002%
33	7.031	1767	1770	1771	rBV	167	107	0.02%	0.002%
34	7.105	1791	1793	1797	rVB2	247	156	0.03%	0.003%
35	7.173	1811	1814	1815	rBV	770	453	0.07%	0.010%
36	7.417	1888	1890	1893	rBV	222	127	0.02%	0.003%

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 Title : VOC Analysis

37	7.562	1923	1935	1952	rBV	78805	137147	22.45%	3.030%
38	7.665	1965	1967	1969	rBV	197	87	0.01%	0.002%
39	7.690	1969	1975	1977	rBV3	712	798	0.13%	0.018%
40	7.764	1997	1998	1999	rBV3	109	41	0.01%	0.001%
41	7.816	2012	2014	2018	rBV	256	211	0.03%	0.005%
42	7.893	2024	2038	2059	rBV	286117	482313	78.95%	10.654%
43	8.047	2082	2086	2087	rBV	205	145	0.02%	0.003%
44	8.079	2092	2096	2101	rBV2	281	277	0.05%	0.006%
45	8.176	2114	2126	2143	rBV	53870	91245	14.94%	2.016%
46	8.343	2175	2178	2180	rBV	202	148	0.02%	0.003%
47	8.362	2181	2184	2188	rVV	182	152	0.02%	0.003%
48	8.411	2197	2199	2202	rVB	150	60	0.01%	0.001%
49	8.481	2218	2221	2225	rBV	201	140	0.02%	0.003%
50	8.626	2255	2266	2295	rBV2	144571	261672	42.84%	5.780%
51	8.841	2331	2333	2340	rBV2	161	121	0.02%	0.003%
52	9.034	2387	2393	2397	rBV	251	325	0.05%	0.007%
53	9.105	2410	2415	2418	rBV	211	258	0.04%	0.006%
54	9.128	2419	2422	2426	rVB	260	210	0.03%	0.005%
55	9.179	2437	2438	2441	rVB	111	24	0.00%	0.001%
56	9.198	2441	2444	2447	rVB	347	233	0.04%	0.005%
57	9.221	2448	2451	2453	rBV	182	149	0.02%	0.003%
58	9.327	2482	2484	2488	rVB2	190	136	0.02%	0.003%
59	9.414	2498	2511	2528	rBV	255794	411563	67.37%	9.091%
60	9.568	2555	2559	2560	rBV	215	138	0.02%	0.003%
61	9.677	2589	2593	2596	rBV2	244	222	0.04%	0.005%
62	9.710	2599	2603	2606	rBV	392	344	0.06%	0.008%
63	9.787	2625	2627	2628	rBV	120	27	0.00%	0.001%
64	10.038	2702	2705	2709	rBV	293	265	0.04%	0.006%
65	10.124	2730	2732	2734	rBV	151	43	0.01%	0.001%
66	10.182	2746	2750	2751	rBV	211	137	0.02%	0.003%
67	10.263	2772	2775	2779	rBV2	226	166	0.03%	0.004%
68	10.584	2874	2875	2876	rBV2	155	41	0.01%	0.001%
69	10.629	2881	2889	2894	rBV	224	434	0.07%	0.010%
70	10.658	2895	2898	2900	rBV	158	98	0.02%	0.002%
71	10.700	2908	2911	2915	rBV	221	145	0.02%	0.003%
72	10.751	2915	2927	2946	rVV	187680	296350	48.51%	6.546%
73	10.841	2953	2955	2962	rVB	240	147	0.02%	0.003%
74	10.870	2962	2964	2965	rBV	108	28	0.00%	0.001%
75	11.050	3018	3020	3022	rBV	159	75	0.01%	0.002%
76	11.150	3049	3051	3053	rBV	142	104	0.02%	0.002%

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

77	11.163	3053	3055	3056	rVV	204	79	0.01%	0.002%
78	11.185	3060	3062	3064	rVB	200	94	0.02%	0.002%
79	11.279	3087	3091	3093	rBV	272	265	0.04%	0.006%
80	11.642	3202	3204	3206	rBV	200	94	0.02%	0.002%
81	11.809	3244	3256	3277	rBV	248755	391927	64.16%	8.658%
82	12.073	3336	3338	3339	rBV	308	113	0.02%	0.002%
83	12.189	3362	3374	3391	rBV	250999	404178	66.16%	8.928%
84	12.546	3482	3485	3491	rVB2	281	182	0.03%	0.004%
85	12.922	3597	3602	3606	rBV2	500	569	0.09%	0.013%
86	13.394	3747	3749	3753	rVB	291	146	0.02%	0.003%
87	13.542	3792	3795	3798	rVB2	259	179	0.03%	0.004%
88	13.677	3834	3837	3839	rBV	173	106	0.02%	0.002%
89	13.845	3884	3889	3893	rVB2	634	632	0.10%	0.014%
90	13.918	3910	3912	3916	rVB	228	97	0.02%	0.002%
91	14.089	3953	3965	3978	rBV	7881	12624	2.07%	0.279%
92	14.359	4046	4049	4051	rBV	173	120	0.02%	0.003%
93	14.607	4123	4126	4130	rBV	194	129	0.02%	0.003%
94	14.648	4137	4139	4141	rBV	264	138	0.02%	0.003%
95	15.015	4251	4253	4255	rBV	218	70	0.01%	0.002%
96	15.169	4299	4301	4304	rBV	356	188	0.03%	0.004%
97	17.098	4894	4901	4911	rBV5	2611	4701	0.77%	0.104%

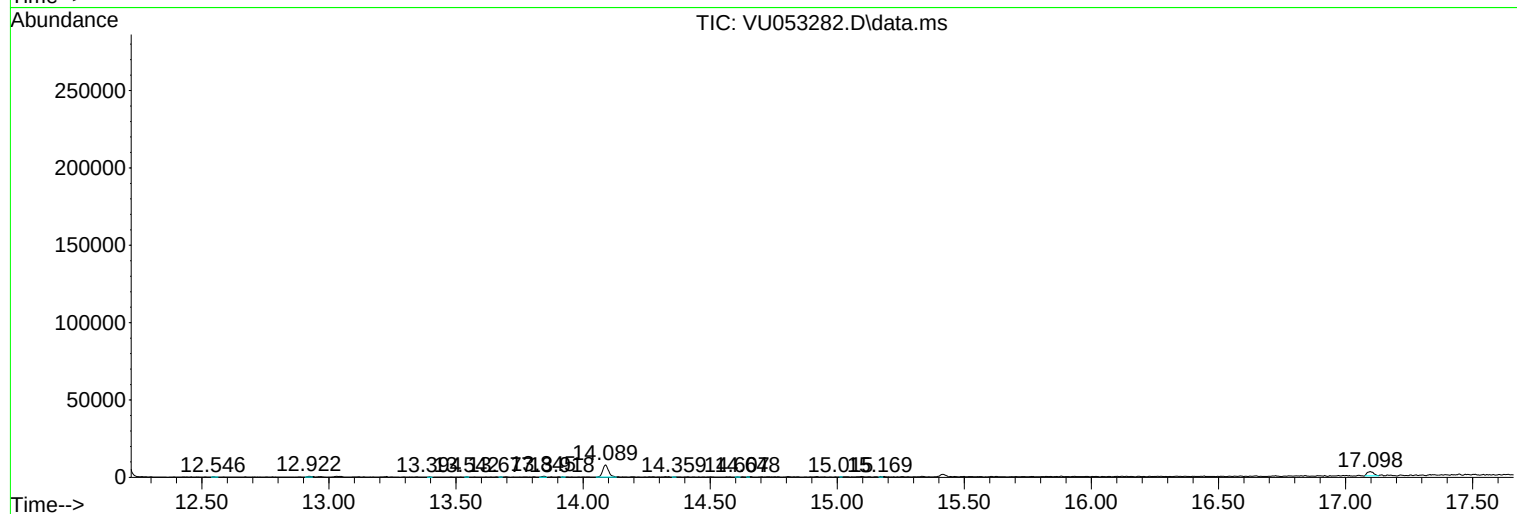
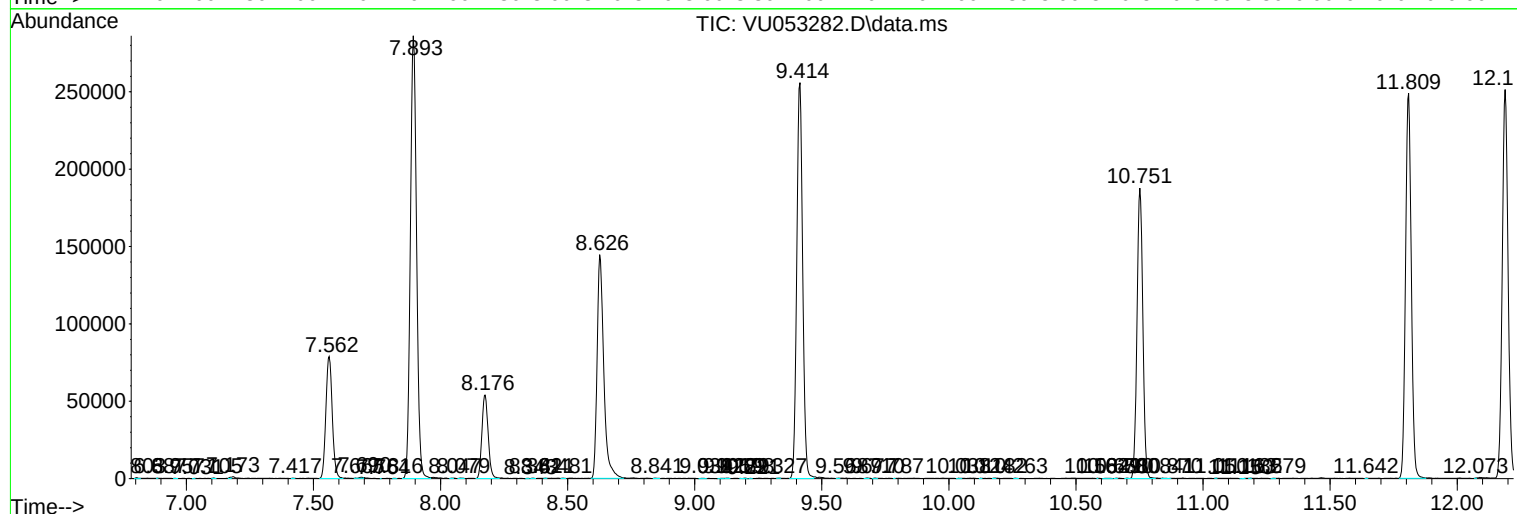
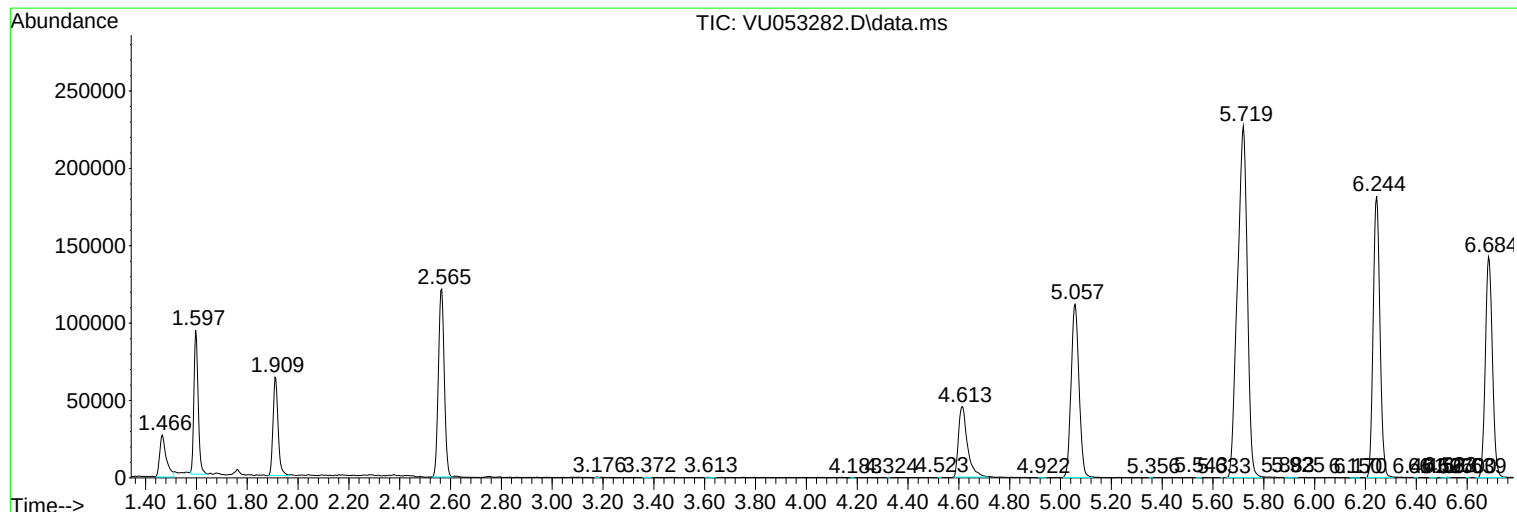
Sum of corrected areas: 4526967

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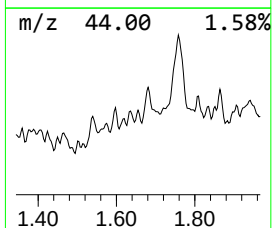
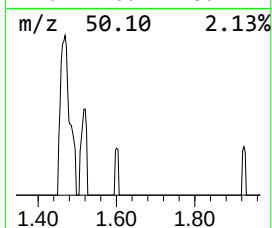
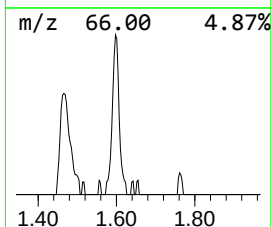
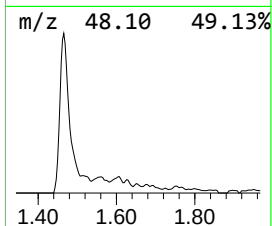
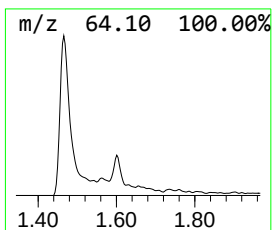
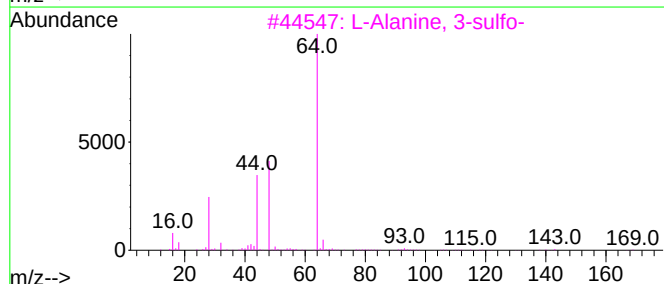
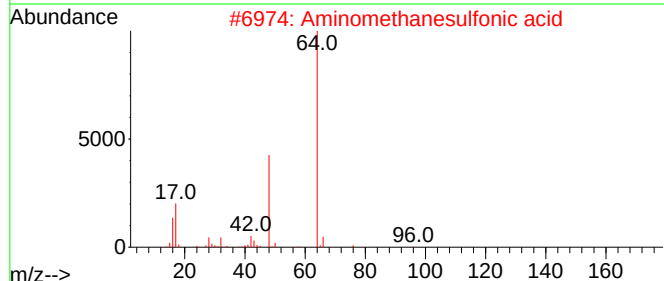
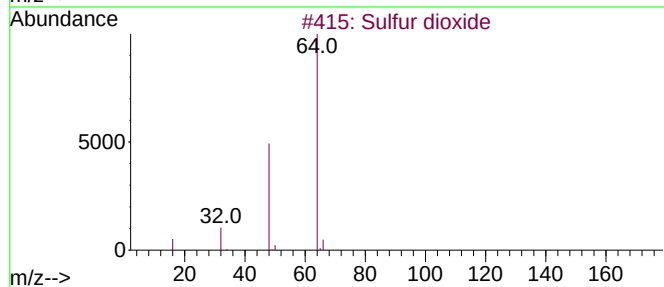
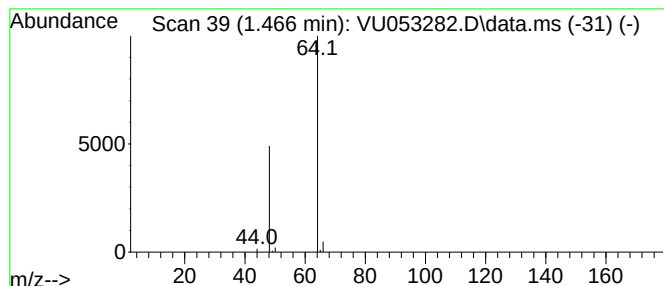
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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	7.15 ug/L	48306	1,4-Difluorobenzene	6.244

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	7.2	ug/L	48306	1	6.244	337883	50.0