

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030223\
 Data File : VU053181.D
 Acq On : 02 Mar 2023 12:38
 Operator : JC/MD
 Sample : 01745-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COLF3

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\SFAMULM021423WMA.M
 Title : VOC Analysis

Signal : TIC: VU053181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.257	45	52	69	rVB	57571	68948	8.17%	1.080%
2	1.498	118	127	151	rBV3	11856	46046	5.46%	0.721%
3	1.598	152	158	175	rVB	95399	112777	13.36%	1.766%
4	1.913	249	256	269	rVB	83761	110229	13.06%	1.727%
5	2.566	448	459	474	rBV	160328	260035	30.81%	4.073%
6	3.235	664	667	670	rBV	218	169	0.02%	0.003%
7	3.321	691	694	696	rVB2	180	98	0.01%	0.002%
8	3.338	696	699	703	rVB2	218	173	0.02%	0.003%
9	3.974	896	897	898	rBV2	121	34	0.00%	0.001%
10	4.202	965	968	971	rVB	184	138	0.02%	0.002%
11	4.254	982	984	988	rBV2	198	134	0.02%	0.002%
12	4.276	988	991	993	rBV	200	144	0.02%	0.002%
13	4.624	1086	1099	1130	rBV	56784	149001	17.66%	2.334%
14	4.913	1186	1189	1194	rVB	244	207	0.02%	0.003%
15	4.974	1204	1208	1210	rBV2	285	267	0.03%	0.004%
16	5.058	1218	1234	1255	rBV	158108	345031	40.89%	5.404%
17	5.370	1327	1331	1332	rBV	473	358	0.04%	0.006%
18	5.453	1355	1357	1361	rVB2	204	128	0.02%	0.002%
19	5.720	1420	1440	1463	rBV2	309040	843859	100.00%	13.217%
20	5.952	1507	1512	1516	rBV3	372	379	0.04%	0.006%
21	5.977	1516	1520	1524	rVV2	193	184	0.02%	0.003%
22	6.038	1534	1539	1541	rBV2	380	349	0.04%	0.005%
23	6.071	1547	1549	1554	rVB2	427	320	0.04%	0.005%
24	6.122	1557	1565	1569	rVV3	340	477	0.06%	0.007%
25	6.244	1589	1603	1629	rBV	244887	464335	55.03%	7.273%
26	6.685	1726	1740	1762	rBV	200304	389830	46.20%	6.106%
27	6.797	1773	1775	1780	rBV2	332	282	0.03%	0.004%
28	6.862	1792	1795	1798	rBV2	191	155	0.02%	0.002%
29	6.926	1813	1815	1819	rBV	175	110	0.01%	0.002%
30	6.971	1827	1829	1831	rBV2	133	67	0.01%	0.001%
31	7.077	1860	1862	1863	rBV2	131	52	0.01%	0.001%
32	7.135	1878	1880	1882	rBV	318	180	0.02%	0.003%
33	7.186	1888	1896	1898	rBV3	1186	1480	0.18%	0.023%
34	7.267	1917	1921	1926	rVB2	358	465	0.06%	0.007%
35	7.312	1926	1935	1937	rBV	230	379	0.04%	0.006%
36	7.559	2000	2012	2038	rBV	118280	207625	24.60%	3.252%

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 Title : VOC Analysis

37	7.894	2103	2116	2146	rBV	401963	694203	82.27%	10.873%
38	8.054	2162	2166	2168	rBV	342	302	0.04%	0.005%
39	8.173	2192	2203	2222	rBV	78883	136557	16.18%	2.139%
40	8.321	2247	2249	2253	rBV2	166	130	0.02%	0.002%
41	8.341	2253	2255	2260	rVB2	286	236	0.03%	0.004%
42	8.366	2260	2263	2264	rBV2	258	146	0.02%	0.002%
43	8.572	2325	2327	2332	rVB2	230	143	0.02%	0.002%
44	8.630	2333	2345	2372	rVV2	181687	348100	41.25%	5.452%
45	8.816	2400	2403	2406	rBV2	217	178	0.02%	0.003%
46	8.935	2436	2440	2443	rVB	293	197	0.02%	0.003%
47	9.016	2462	2465	2467	rVB	238	109	0.01%	0.002%
48	9.090	2485	2488	2491	rVB	250	142	0.02%	0.002%
49	9.141	2502	2504	2506	rVB	144	57	0.01%	0.001%
50	9.160	2508	2510	2513	rBV	226	134	0.02%	0.002%
51	9.263	2539	2542	2544	rBV	184	103	0.01%	0.002%
52	9.308	2553	2556	2560	rVB2	181	130	0.02%	0.002%
53	9.337	2562	2565	2569	rVB2	236	152	0.02%	0.002%
54	9.411	2575	2588	2611	rBV	345618	578748	68.58%	9.065%
55	9.591	2641	2644	2648	rBV2	327	288	0.03%	0.005%
56	9.929	2746	2749	2752	rBV	222	159	0.02%	0.002%
57	10.482	2919	2921	2923	rBV	182	82	0.01%	0.001%
58	10.749	2993	3004	3025	rBV	256951	413924	49.05%	6.483%
59	10.855	3035	3037	3038	rBV	153	42	0.00%	0.001%
60	10.874	3041	3043	3045	rBV2	233	125	0.01%	0.002%
61	11.051	3096	3098	3099	rBV	194	104	0.01%	0.002%
62	11.746	3310	3314	3315	rBV	310	164	0.02%	0.003%
63	11.807	3321	3333	3358	rBV	371378	591758	70.13%	9.269%
64	12.064	3406	3413	3430	rBV5	3823	9397	1.11%	0.147%
65	12.189	3439	3452	3474	rBV	367051	603495	71.52%	9.453%
66	12.315	3489	3491	3495	rBV2	271	171	0.02%	0.003%
67	12.659	3595	3598	3600	rBV	247	140	0.02%	0.002%
68	12.887	3667	3669	3672	rBV	402	196	0.02%	0.003%
69	14.321	4113	4115	4117	rBV2	366	227	0.03%	0.004%

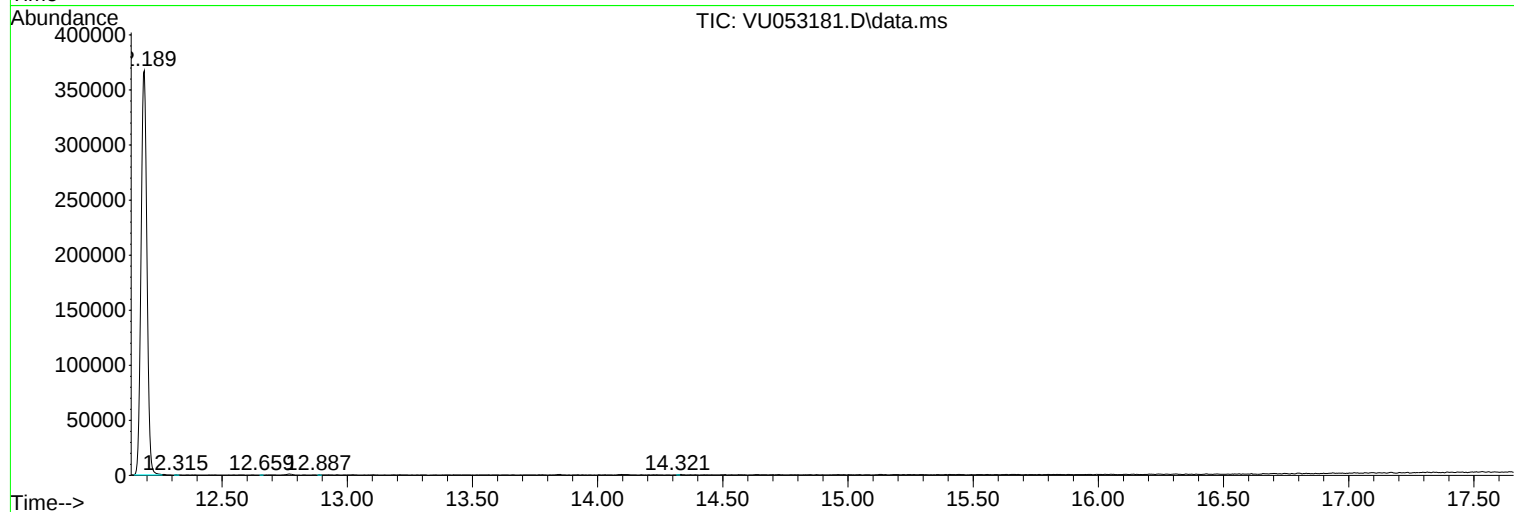
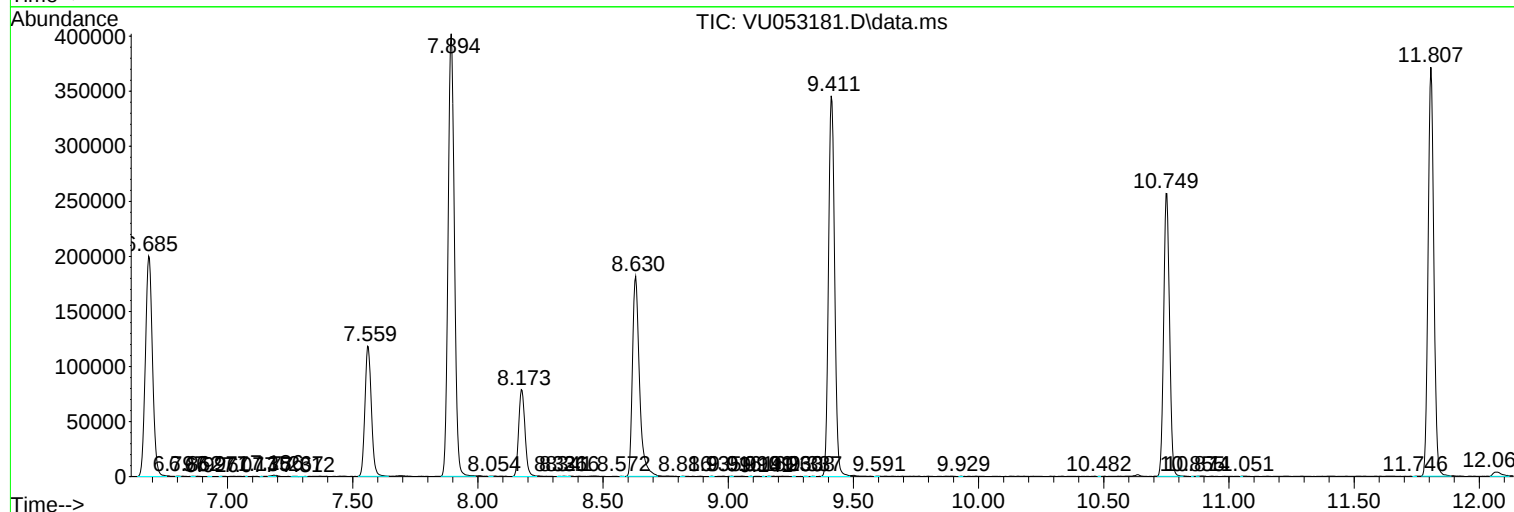
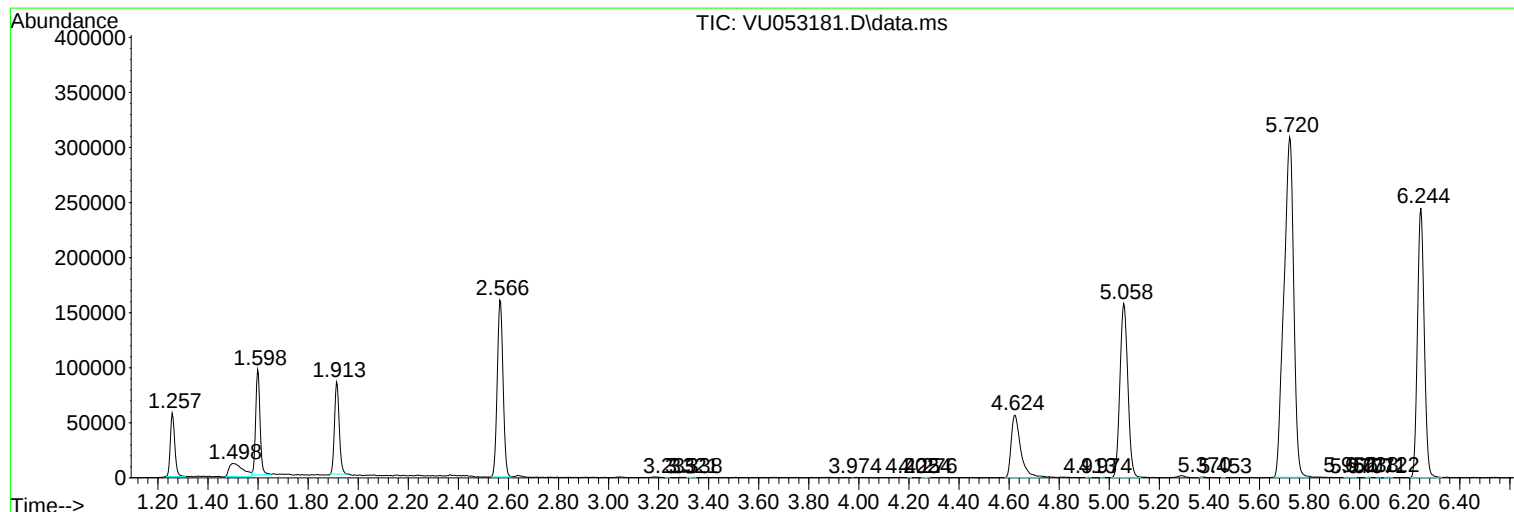
Sum of corrected areas: 6384484

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021423WMA.M
Quant Title : VOC Analysis

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



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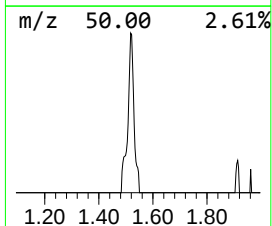
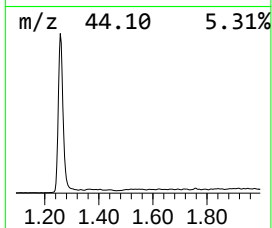
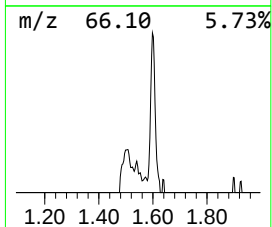
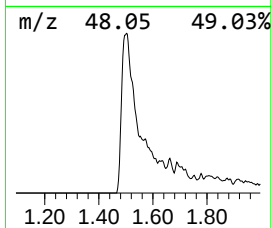
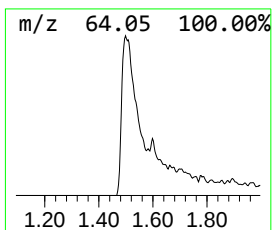
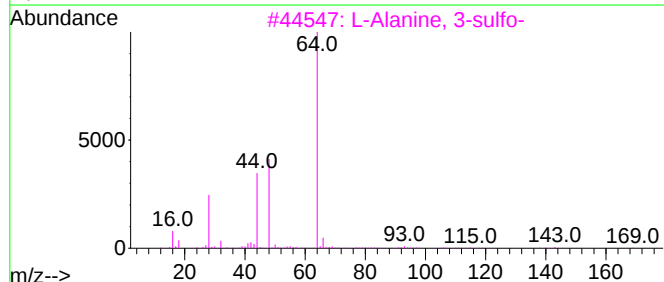
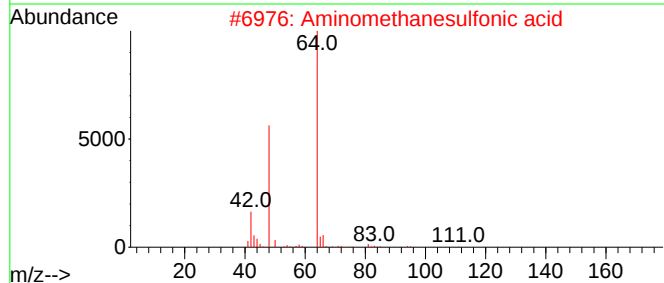
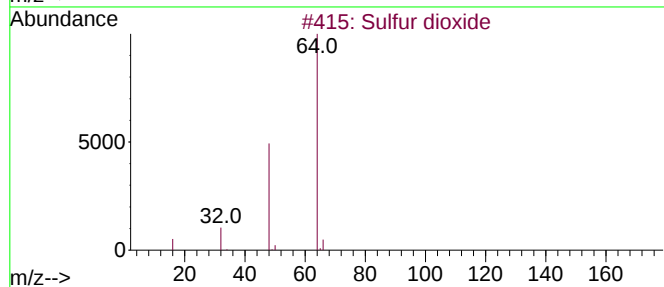
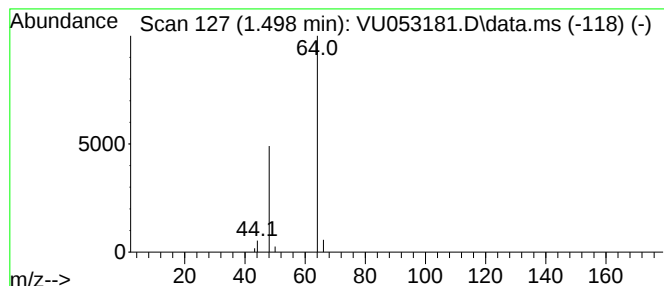
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021423WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.498	4.96 ug/L	46046	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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Quant Title : VOC Analysis

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	1.498	5.0	ug/L	46046	1	6.244	464335	50.0