

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053276.D
 Acq On : 17 Mar 2023 18:48
 Operator : JC/MD
 Sample : 01930-20
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF9

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: VU053276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	32	39	55	rBV	14064	25768	4.23%	0.578%
2	1.597	73	80	99	rVB	82009	92445	15.16%	2.072%
3	1.909	170	177	193	rVB	63949	86578	14.20%	1.940%
4	2.562	369	380	396	rBV	126026	200663	32.91%	4.497%
5	3.395	635	639	641	rBV	220	177	0.03%	0.004%
6	3.642	715	716	717	rBV	134	36	0.01%	0.001%
7	3.796	760	764	769	rBV2	268	298	0.05%	0.007%
8	3.848	778	780	783	rBV2	228	180	0.03%	0.004%
9	3.951	810	812	816	rVB	206	102	0.02%	0.002%
10	4.002	826	828	831	rVB	220	102	0.02%	0.002%
11	4.051	841	843	845	rBV	199	66	0.01%	0.001%
12	4.096	855	857	858	rBV	150	49	0.01%	0.001%
13	4.176	879	882	884	rBV	225	132	0.02%	0.003%
14	4.366	938	941	942	rBV	202	137	0.02%	0.003%
15	4.613	1006	1018	1043	rBV2	46510	111703	18.32%	2.504%
16	4.912	1109	1111	1112	rBV2	134	57	0.01%	0.001%
17	4.941	1117	1120	1122	rBV2	209	134	0.02%	0.003%
18	5.057	1141	1156	1176	rBV	114688	245155	40.20%	5.495%
19	5.240	1211	1213	1219	rVB	346	270	0.04%	0.006%
20	5.266	1219	1221	1223	rBV	138	97	0.02%	0.002%
21	5.285	1223	1227	1235	rVB3	424	477	0.08%	0.011%
22	5.359	1247	1250	1253	rVB2	187	109	0.02%	0.002%
23	5.449	1276	1278	1280	rBV	165	94	0.02%	0.002%
24	5.475	1284	1286	1288	rVB	122	46	0.01%	0.001%
25	5.568	1313	1315	1316	rBV	143	67	0.01%	0.002%
26	5.719	1342	1362	1381	rBV2	224814	609780	100.00%	13.667%
27	5.854	1401	1404	1406	rVB2	314	178	0.03%	0.004%
28	5.973	1438	1441	1442	rBV	151	88	0.01%	0.002%
29	6.243	1512	1525	1543	rBV	177821	329479	54.03%	7.385%
30	6.472	1593	1596	1599	rVB	353	236	0.04%	0.005%
31	6.491	1599	1602	1603	rBV	183	115	0.02%	0.003%
32	6.513	1607	1609	1612	rVB	315	174	0.03%	0.004%
33	6.533	1612	1615	1619	rBV	440	332	0.05%	0.007%
34	6.584	1629	1631	1632	rBV	131	33	0.01%	0.001%
35	6.684	1649	1662	1680	rBV	144290	278070	45.60%	6.232%
36	6.800	1696	1698	1701	rBV2	191	131	0.02%	0.003%

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 Title : VOC Analysis

37	6.838	1707	1710	1715	rBV	158	145	0.02%	0.003%
38	6.893	1725	1727	1728	rBV	122	33	0.01%	0.001%
39	7.182	1811	1817	1827	rBV4	1002	1566	0.26%	0.035%
40	7.259	1836	1841	1844	rBV	198	251	0.04%	0.006%
41	7.359	1869	1872	1875	rBV	171	138	0.02%	0.003%
42	7.456	1901	1902	1903	rVB	210	41	0.01%	0.001%
43	7.472	1904	1907	1910	rBV	161	161	0.03%	0.004%
44	7.494	1910	1914	1919	rVV2	191	163	0.03%	0.004%
45	7.562	1922	1935	1952	rBV	82312	141883	23.27%	3.180%
46	7.665	1962	1967	1969	rBV2	336	237	0.04%	0.005%
47	7.690	1969	1975	1979	rBV2	703	752	0.12%	0.017%
48	7.893	2024	2038	2061	rBV	285179	485833	79.67%	10.889%
49	8.057	2086	2089	2090	rBV	136	53	0.01%	0.001%
50	8.108	2103	2105	2107	rBV	136	58	0.01%	0.001%
51	8.176	2115	2126	2145	rBV	55941	93494	15.33%	2.095%
52	8.243	2145	2147	2149	rVB	263	125	0.02%	0.003%
53	8.365	2181	2185	2192	rVB2	302	247	0.04%	0.006%
54	8.571	2246	2249	2251	rBV	132	119	0.02%	0.003%
55	8.626	2255	2266	2296	rVV2	142754	265184	43.49%	5.944%
56	9.102	2412	2414	2416	rBV	151	81	0.01%	0.002%
57	9.118	2416	2419	2420	rBV	142	80	0.01%	0.002%
58	9.243	2457	2458	2463	rBV	144	90	0.01%	0.002%
59	9.414	2498	2511	2528	rBV	241073	399851	65.57%	8.962%
60	9.542	2546	2551	2555	rVB3	307	237	0.04%	0.005%
61	9.584	2562	2564	2566	rBV2	154	91	0.01%	0.002%
62	9.652	2582	2585	2588	rBV	246	190	0.03%	0.004%
63	9.709	2601	2603	2604	rBV	119	31	0.01%	0.001%
64	9.925	2667	2670	2674	rVB2	152	102	0.02%	0.002%
65	9.947	2674	2677	2681	rVB2	221	167	0.03%	0.004%
66	10.031	2701	2703	2706	rBB	126	63	0.01%	0.001%
67	10.330	2794	2796	2797	rBV	106	41	0.01%	0.001%
68	10.407	2818	2820	2824	rBV2	199	146	0.02%	0.003%
69	10.504	2848	2850	2855	rBV	266	172	0.03%	0.004%
70	10.561	2867	2868	2871	rVB	148	54	0.01%	0.001%
71	10.751	2914	2927	2943	rBV	188759	295731	48.50%	6.628%
72	11.018	3007	3010	3013	rBV2	154	99	0.02%	0.002%
73	11.063	3021	3024	3028	rBV2	224	162	0.03%	0.004%
74	11.124	3041	3043	3046	rVB	198	87	0.01%	0.002%
75	11.198	3064	3066	3068	rBV	131	53	0.01%	0.001%
76	11.250	3080	3082	3085	rBV	231	110	0.02%	0.002%

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Peak Location: TOP

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

77	11.494	3156	3158	3160	rBV	164	79	0.01%	0.002%
78	11.574	3180	3183	3187	rBV	249	297	0.05%	0.007%
79	11.806	3244	3255	3278	rBV	241045	382432	62.72%	8.571%
80	11.915	3286	3289	3293	rBV	211	176	0.03%	0.004%
81	12.063	3333	3335	3336	rBV	243	107	0.02%	0.002%
82	12.188	3362	3374	3390	rBV	253119	404437	66.33%	9.065%
83	12.571	3492	3493	3496	rBV	153	93	0.02%	0.002%
84	12.690	3527	3530	3531	rBV	139	60	0.01%	0.001%
85	12.803	3564	3565	3566	rBV	110	22	0.00%	0.000%
86	12.825	3570	3572	3573	rBV	175	54	0.01%	0.001%
87	12.915	3597	3600	3602	rVB2	199	111	0.02%	0.002%
88	12.941	3604	3608	3615	rVV2	303	300	0.05%	0.007%
89	13.124	3662	3665	3666	rBV2	166	89	0.01%	0.002%
90	14.040	3947	3950	3953	rBV	211	129	0.02%	0.003%
91	14.465	4080	4082	4085	rBV	253	161	0.03%	0.004%
92	14.661	4141	4143	4146	rVB2	277	137	0.02%	0.003%
93	14.722	4160	4162	4166	rBV	253	189	0.03%	0.004%
94	15.002	4246	4249	4252	rVB	215	99	0.02%	0.002%
95	15.458	4389	4391	4393	rBV	280	118	0.02%	0.003%
96	15.982	4551	4554	4559	rBV3	360	446	0.07%	0.010%
97	16.587	4740	4742	4748	rBV3	573	501	0.08%	0.011%

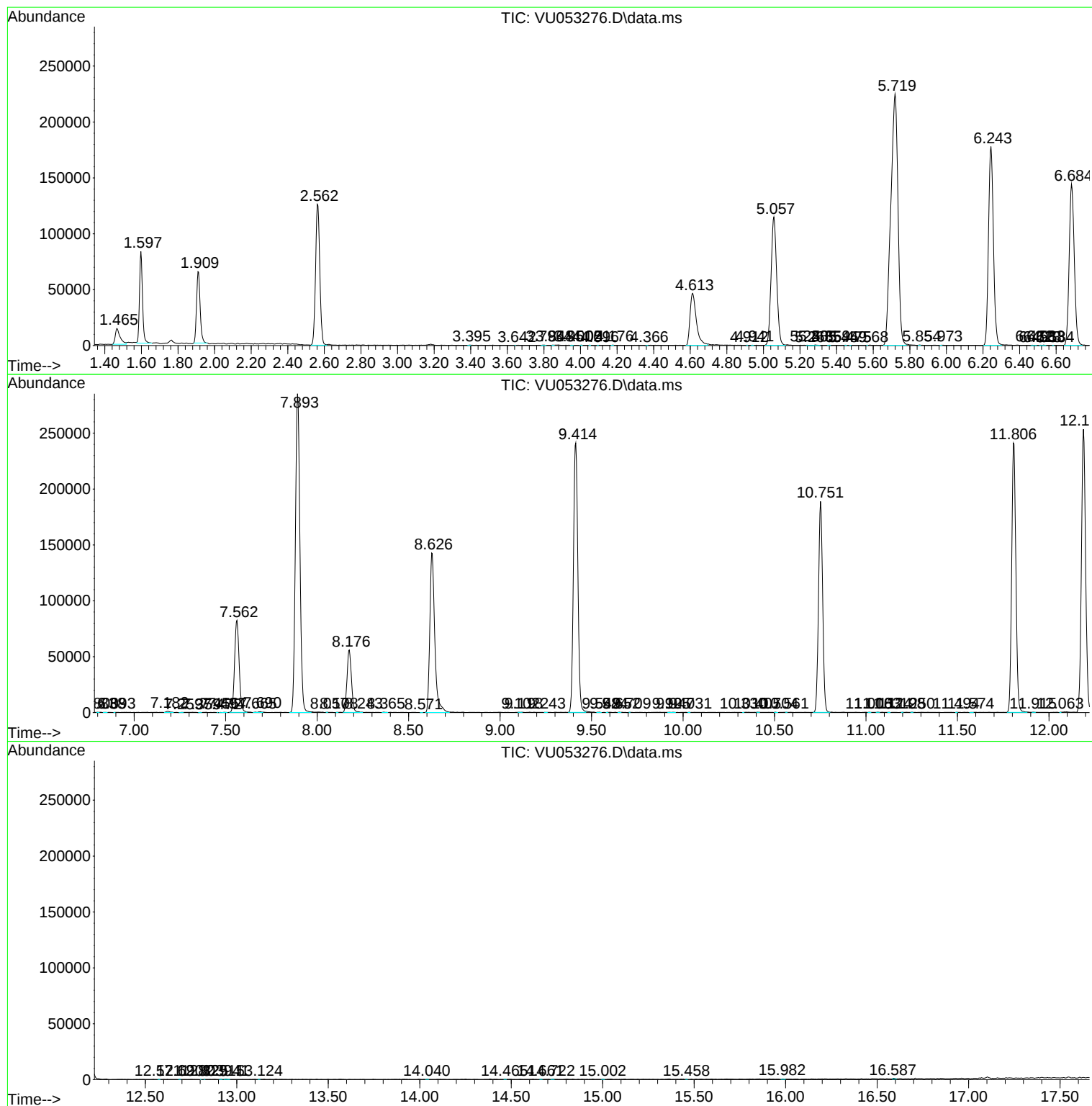
Sum of corrected areas: 4461716

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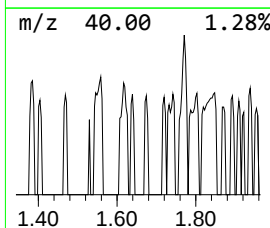
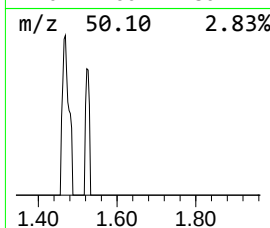
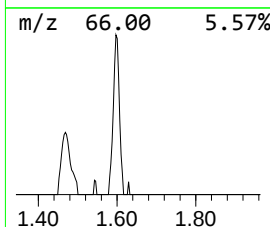
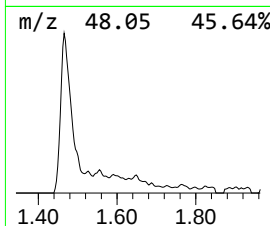
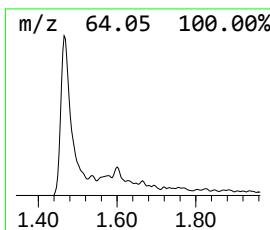
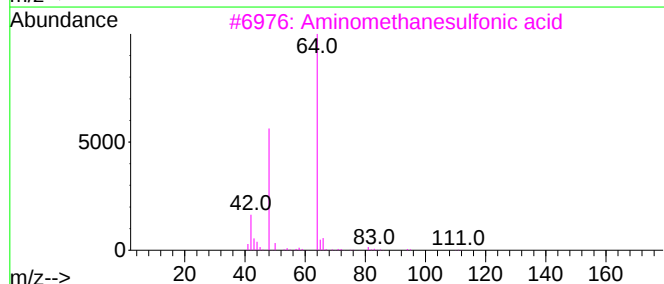
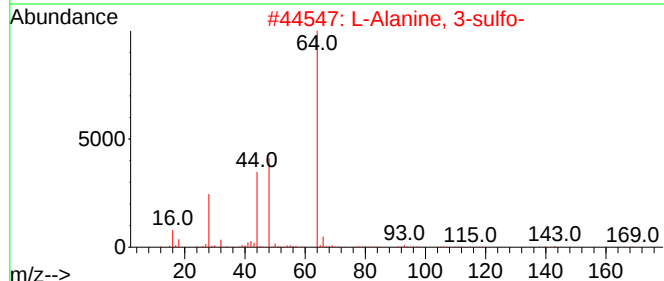
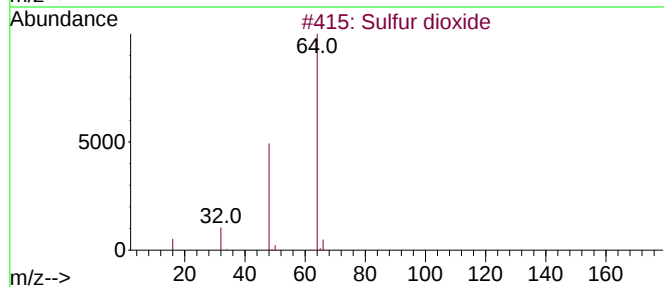
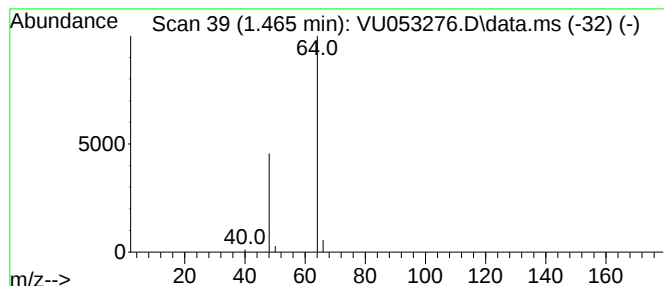
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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.
1.465	3.91 ug/L	25768	1,4-Difluorobenzene	6.243

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			Sulfur dioxide	64	O2S	007446-09-5	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	1.465	3.9	ug/L	25768	1	6.243	329479	50.0