

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053267.D
 Acq On : 17 Mar 2023 15:14
 Operator : JC/MD
 Sample : 01930-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFB3

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: VU053267.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	57	rBV	23315	40103	7.13%	0.940%
2	1.597	74	80	93	rVB	69331	77033	13.70%	1.805%
3	1.912	169	178	192	rVB	56956	77930	13.86%	1.826%
4	2.565	369	381	394	rVB	112024	180647	32.12%	4.232%
5	2.986	508	512	517	rBV	233	275	0.05%	0.006%
6	3.041	526	529	531	rVV2	253	139	0.02%	0.003%
7	3.054	531	533	536	rVB	144	41	0.01%	0.001%
8	3.604	703	704	707	rBV	121	40	0.01%	0.001%
9	3.642	713	716	718	rBV2	197	130	0.02%	0.003%
10	3.845	775	779	782	rBV2	240	194	0.03%	0.005%
11	3.874	786	788	791	rVB	152	63	0.01%	0.001%
12	3.986	820	823	826	rBV	343	279	0.05%	0.007%
13	4.047	837	842	849	rBV2	218	244	0.04%	0.006%
14	4.144	868	872	874	rBV	229	159	0.03%	0.004%
15	4.169	878	880	882	rBV	172	95	0.02%	0.002%
16	4.266	905	910	914	rBV2	246	320	0.06%	0.007%
17	4.613	1007	1018	1046	rBV	41302	101283	18.01%	2.373%
18	4.925	1112	1115	1116	rBV	179	85	0.02%	0.002%
19	4.989	1131	1135	1140	rVB2	263	249	0.04%	0.006%
20	5.057	1140	1156	1180	rBV2	105071	228412	40.61%	5.351%
21	5.330	1236	1241	1244	rBV2	241	190	0.03%	0.004%
22	5.456	1279	1280	1281	rBV2	117	34	0.01%	0.001%
23	5.507	1294	1296	1299	rBV	139	43	0.01%	0.001%
24	5.571	1313	1316	1319	rBV	245	145	0.03%	0.003%
25	5.719	1341	1362	1388	rBV2	208748	562399	100.00%	13.176%
26	5.919	1421	1424	1427	rBV2	241	142	0.03%	0.003%
27	5.983	1440	1444	1447	rBV2	324	338	0.06%	0.008%
28	6.073	1470	1472	1473	rBV2	158	47	0.01%	0.001%
29	6.124	1486	1488	1489	rBV2	141	56	0.01%	0.001%
30	6.243	1511	1525	1543	rBV	190067	354857	63.10%	8.314%
31	6.568	1623	1626	1627	rBV	153	74	0.01%	0.002%
32	6.684	1648	1662	1683	rBV	133966	258473	45.96%	6.056%
33	6.803	1696	1699	1702	rBV	283	212	0.04%	0.005%
34	6.854	1713	1715	1718	rBV2	128	71	0.01%	0.002%
35	6.912	1730	1733	1734	rBV2	151	70	0.01%	0.002%
36	7.044	1772	1774	1776	rBV	144	42	0.01%	0.001%

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 Title : VOC Analysis

37	7.147	1804	1806	1811	rVB	157	56	0.01%	0.001%
38	7.179	1811	1816	1830	rVB4	979	1631	0.29%	0.038%
39	7.240	1832	1835	1837	rBV	126	76	0.01%	0.002%
40	7.317	1855	1859	1862	rBV	300	283	0.05%	0.007%
41	7.562	1924	1935	1953	rBV	74806	130833	23.26%	3.065%
42	7.690	1969	1975	1980	rBV2	575	760	0.14%	0.018%
43	7.742	1989	1991	1993	rBV2	152	88	0.02%	0.002%
44	7.893	2026	2038	2056	rBV	255994	438624	77.99%	10.276%
45	8.176	2115	2126	2143	rBV	51343	84730	15.07%	1.985%
46	8.385	2188	2191	2196	rVB2	324	303	0.05%	0.007%
47	8.420	2197	2202	2206	rBV	304	369	0.07%	0.009%
48	8.626	2255	2266	2294	rBV2	125286	237360	42.20%	5.561%
49	8.873	2340	2343	2344	rBV	177	123	0.02%	0.003%
50	8.960	2367	2370	2373	rBV	245	125	0.02%	0.003%
51	9.041	2391	2395	2399	rBV2	151	120	0.02%	0.003%
52	9.140	2425	2426	2429	rVB	142	50	0.01%	0.001%
53	9.208	2443	2447	2452	rBV	305	208	0.04%	0.005%
54	9.340	2486	2488	2491	rVB	200	94	0.02%	0.002%
55	9.414	2498	2511	2533	rBV	255865	423762	75.35%	9.928%
56	9.536	2548	2549	2552	rBV	129	67	0.01%	0.002%
57	9.864	2648	2651	2653	rBV	210	113	0.02%	0.003%
58	9.928	2668	2671	2674	rBV	182	134	0.02%	0.003%
59	10.089	2719	2721	2722	rBV	118	52	0.01%	0.001%
60	10.259	2772	2774	2779	rBV	164	63	0.01%	0.001%
61	10.333	2795	2797	2800	rVB	148	62	0.01%	0.001%
62	10.359	2803	2805	2807	rBV	123	51	0.01%	0.001%
63	10.751	2916	2927	2946	rVB	173127	274786	48.86%	6.438%
64	10.819	2946	2948	2949	rBV	151	65	0.01%	0.002%
65	11.079	3027	3029	3032	rVB	178	74	0.01%	0.002%
66	11.362	3114	3117	3119	rBV	154	79	0.01%	0.002%
67	11.725	3227	3230	3233	rBV2	210	149	0.03%	0.003%
68	11.806	3244	3255	3277	rBV	257171	407090	72.38%	9.537%
69	11.912	3286	3288	3289	rBV	181	84	0.01%	0.002%
70	11.999	3312	3315	3317	rBV	224	143	0.03%	0.003%
71	12.188	3362	3374	3392	rBV	232593	378808	67.36%	8.875%
72	12.352	3422	3425	3426	rBV	258	134	0.02%	0.003%
73	12.764	3550	3553	3559	rVB3	378	311	0.06%	0.007%
74	13.053	3640	3643	3649	rBV	213	133	0.02%	0.003%
75	13.179	3679	3682	3687	rBV2	239	176	0.03%	0.004%
76	13.243	3698	3702	3705	rBV2	387	296	0.05%	0.007%

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77	13.417	3753	3756	3758	rBV	192	129	0.02%	0.003%
78	13.478	3772	3775	3778	rBV	289	179	0.03%	0.004%
79	13.616	3815	3818	3819	rBV2	158	91	0.02%	0.002%
80	14.198	3997	3999	4001	rBV	180	89	0.02%	0.002%
81	14.523	4097	4100	4104	rBV	232	163	0.03%	0.004%
82	15.651	4448	4451	4454	rBV	366	312	0.06%	0.007%

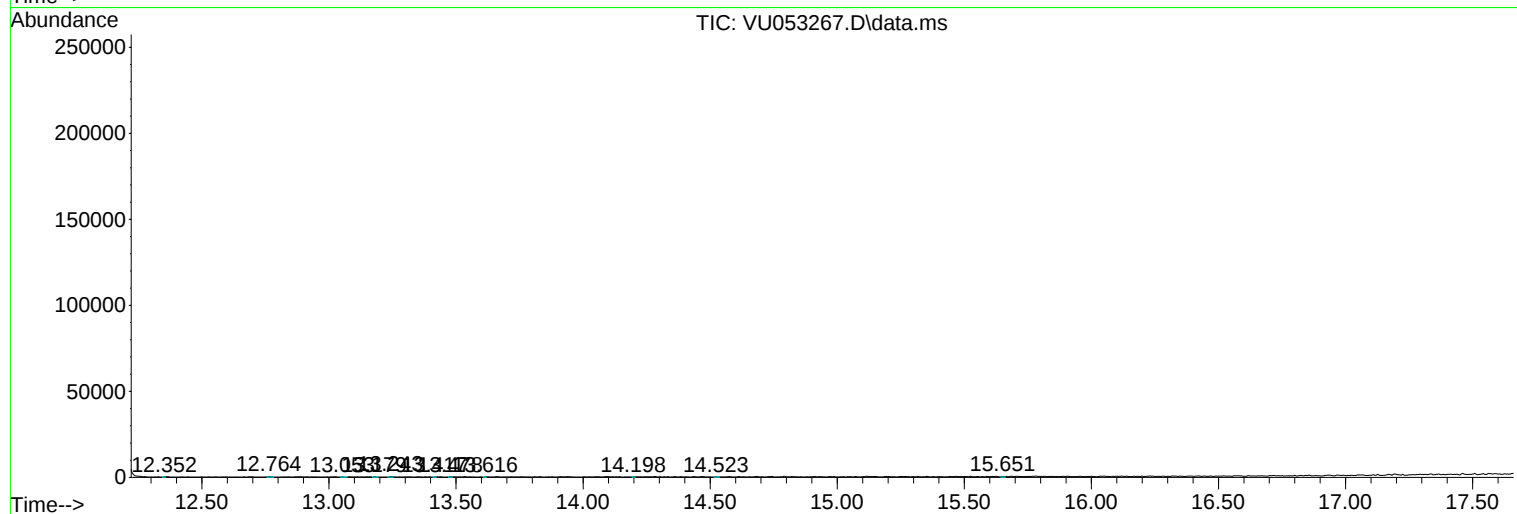
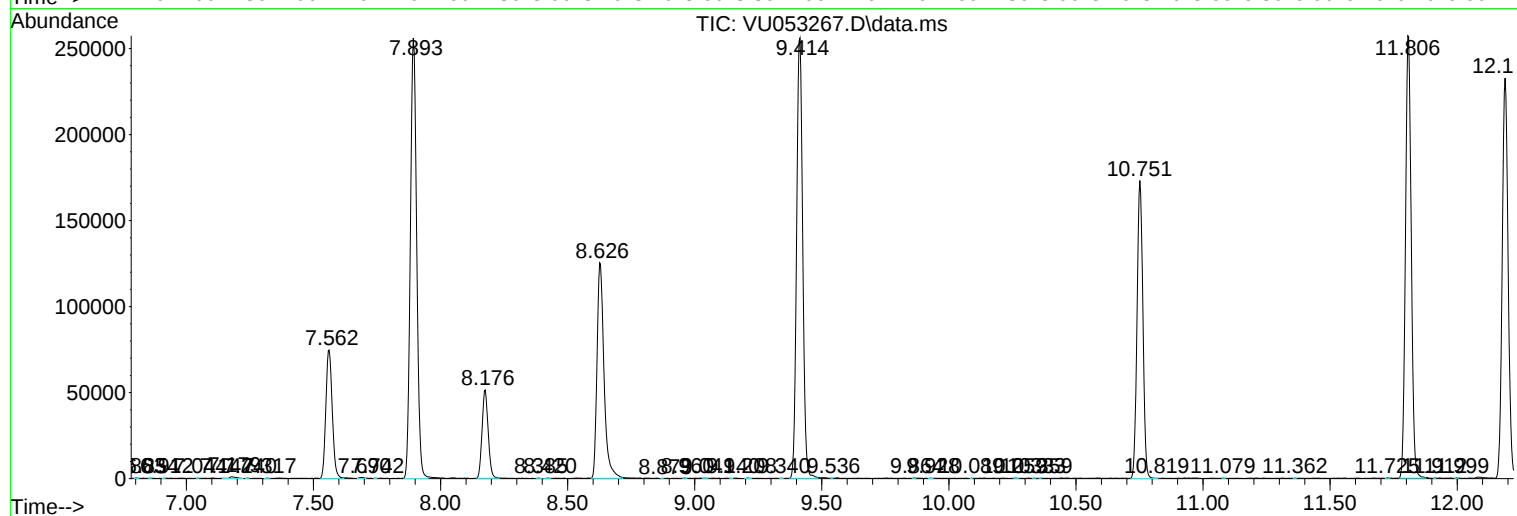
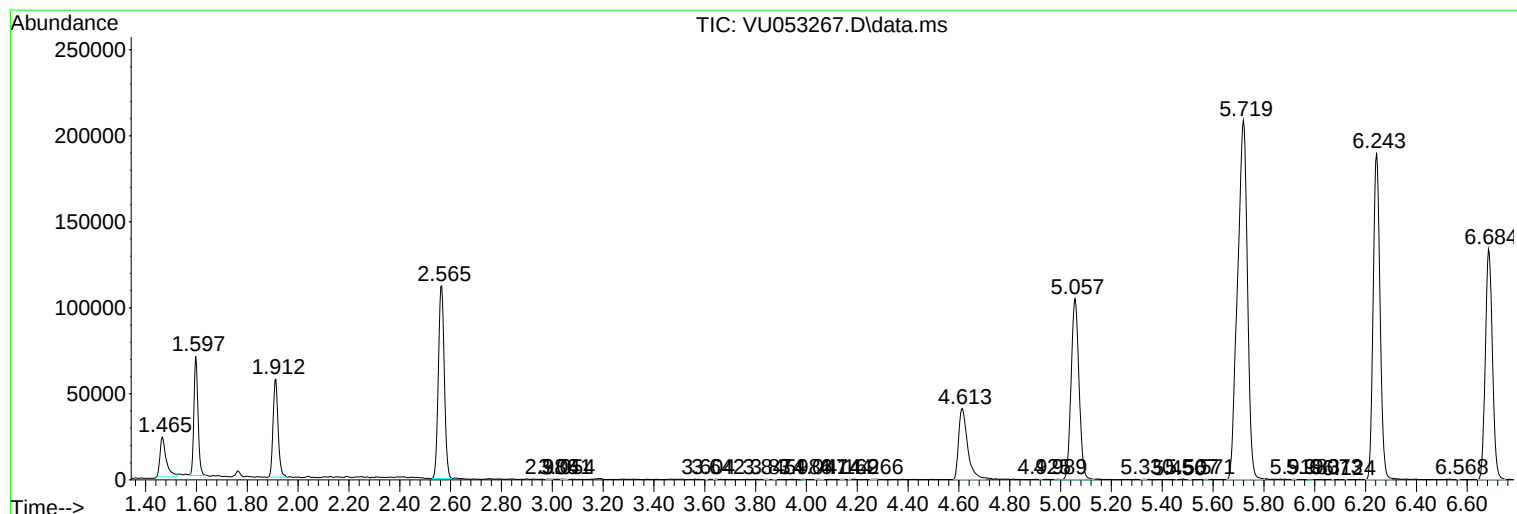
Sum of corrected areas: 4268342

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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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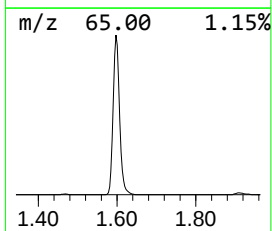
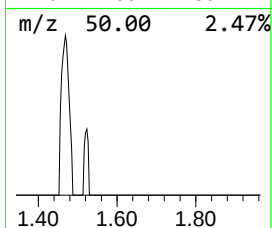
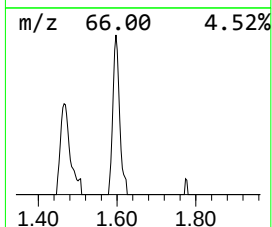
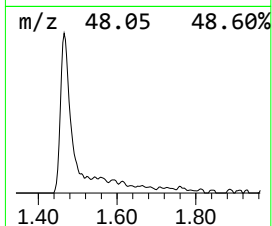
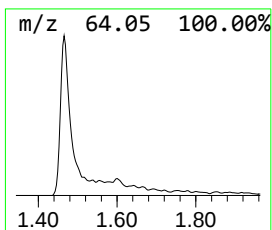
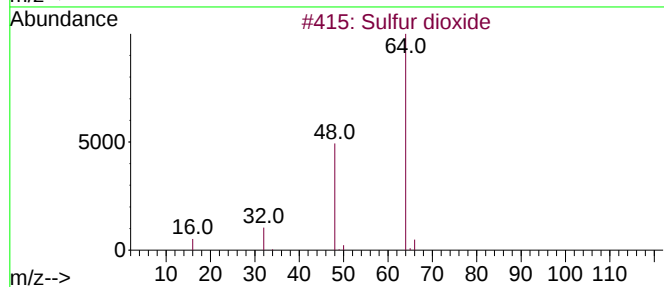
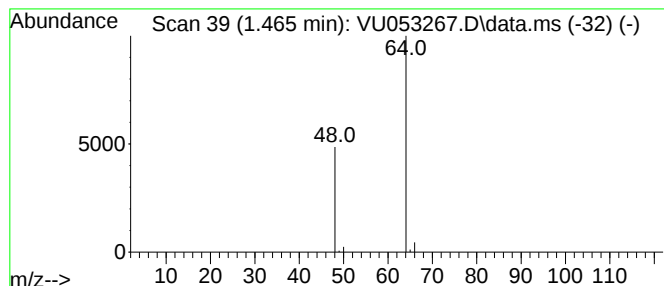
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Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	5.65 ug/L	40103	1,4-Difluorobenzene	6.243

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



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.465	5.7	ug/L	40103	1	6.243	354857	50.0