

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053632.D
 Acq On : 11 Apr 2023 14:00
 Operator : JC/MD
 Sample : 02251-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD3

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	54	rBV	25782	48003	6.27%	0.734%
2	1.597	74	80	95	rVB	96303	113155	14.78%	1.730%
3	1.912	170	178	194	rVB	79665	110896	14.48%	1.695%
4	2.565	369	381	395	rBV	154375	249715	32.61%	3.818%
5	2.903	485	486	488	rBV	218	91	0.01%	0.001%
6	3.359	626	628	633	rBV	249	188	0.02%	0.003%
7	3.530	679	681	687	rVB2	228	153	0.02%	0.002%
8	3.658	719	721	722	rBV2	167	51	0.01%	0.001%
9	3.729	742	743	744	rBV	156	39	0.01%	0.001%
10	3.928	804	805	806	rBV	260	96	0.01%	0.001%
11	3.996	822	826	827	rBV	220	146	0.02%	0.002%
12	4.086	852	854	856	rBV	225	110	0.01%	0.002%
13	4.128	863	867	869	rBV	164	125	0.02%	0.002%
14	4.401	949	952	958	rBV2	310	312	0.04%	0.005%
15	4.504	982	984	986	rBV	196	113	0.01%	0.002%
16	4.546	991	997	1000	rBV	382	383	0.05%	0.006%
17	4.565	1000	1003	1006	rBV	210	128	0.02%	0.002%
18	4.610	1006	1017	1054	rBV	62329	154505	20.17%	2.362%
19	4.903	1104	1108	1109	rVV	228	116	0.02%	0.002%
20	4.922	1112	1114	1119	rVB2	259	205	0.03%	0.003%
21	5.054	1141	1155	1181	rBV2	142277	319010	41.65%	4.877%
22	5.269	1219	1222	1225	rBV	257	160	0.02%	0.002%
23	5.285	1225	1227	1228	rBV	186	56	0.01%	0.001%
24	5.340	1242	1244	1246	rBV	273	119	0.02%	0.002%
25	5.446	1275	1277	1280	rVB	234	93	0.01%	0.001%
26	5.517	1289	1299	1300	rBV2	4815	5457	0.71%	0.083%
27	5.581	1316	1319	1320	rBV2	159	71	0.01%	0.001%
28	5.719	1342	1362	1386	rBV3	275124	765845	100.00%	11.708%
29	6.015	1451	1454	1457	rBV	269	185	0.02%	0.003%
30	6.076	1471	1473	1476	rBV	208	109	0.01%	0.002%
31	6.108	1481	1483	1485	rBV	203	86	0.01%	0.001%
32	6.243	1512	1525	1547	rBV	292619	556994	72.73%	8.515%
33	6.523	1604	1612	1620	rBV6	1870	3097	0.40%	0.047%
34	6.687	1649	1663	1687	rBV	176222	346354	45.23%	5.295%
35	6.835	1706	1709	1713	rVB2	327	259	0.03%	0.004%
36	6.951	1743	1745	1747	rBB	137	53	0.01%	0.001%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.121	1797	1798	1799	rBV	139	36	0.00%	0.001%
38	7.182	1809	1817	1818	rBV2	1228	1175	0.15%	0.018%
39	7.304	1853	1855	1858	rBV	172	92	0.01%	0.001%
40	7.478	1908	1909	1910	rBV	141	27	0.00%	0.000%
41	7.558	1923	1934	1951	rBV	96362	170616	22.28%	2.608%
42	7.690	1966	1975	1980	rBV3	1027	1505	0.20%	0.023%
43	7.812	2011	2013	2018	rVB	218	114	0.01%	0.002%
44	7.893	2025	2038	2069	rBV	356602	623650	81.43%	9.534%
45	8.176	2114	2126	2142	rBV	67235	114869	15.00%	1.756%
46	8.462	2213	2215	2219	rBV3	586	546	0.07%	0.008%
47	8.552	2236	2243	2251	rVB3	1276	1871	0.24%	0.029%
48	8.626	2255	2266	2292	rBV	185066	345252	45.08%	5.278%
49	8.870	2340	2342	2344	rBV	202	74	0.01%	0.001%
50	8.960	2368	2370	2374	rVB	254	127	0.02%	0.002%
51	9.005	2382	2384	2387	rVB	160	51	0.01%	0.001%
52	9.144	2425	2427	2428	rBV	153	74	0.01%	0.001%
53	9.214	2447	2449	2456	rVB	199	124	0.02%	0.002%
54	9.246	2456	2459	2460	rBV	205	122	0.02%	0.002%
55	9.353	2490	2492	2494	rBV	196	98	0.01%	0.001%
56	9.414	2498	2511	2535	rBV	402972	687319	89.75%	10.508%
57	9.549	2550	2553	2556	rBV2	475	370	0.05%	0.006%
58	9.610	2570	2572	2577	rVB	232	133	0.02%	0.002%
59	9.658	2585	2587	2590	rBV2	171	112	0.01%	0.002%
60	9.729	2606	2609	2610	rBV	264	151	0.02%	0.002%
61	9.983	2685	2688	2693	rBV	161	149	0.02%	0.002%
62	10.102	2723	2725	2728	rBV	208	161	0.02%	0.002%
63	10.214	2757	2760	2762	rBV	254	156	0.02%	0.002%
64	10.285	2780	2782	2783	rBV	226	113	0.01%	0.002%
65	10.475	2840	2841	2845	rBV2	364	208	0.03%	0.003%
66	10.639	2890	2892	2896	rVB2	480	285	0.04%	0.004%
67	10.751	2915	2927	2948	rVB	260442	425244	55.53%	6.501%
68	10.832	2949	2952	2956	rVB2	451	277	0.04%	0.004%
69	10.938	2982	2985	2988	rBV	205	139	0.02%	0.002%
70	11.507	3159	3162	3165	rBB	285	152	0.02%	0.002%
71	11.745	3227	3236	3244	rBV2	7102	10518	1.37%	0.161%
72	11.809	3244	3256	3278	rBV	446532	753769	98.42%	11.523%
73	11.944	3296	3298	3301	rBV	265	124	0.02%	0.002%
74	12.008	3317	3318	3320	rBV	392	106	0.01%	0.002%
75	12.188	3362	3374	3396	rBV	381833	678316	88.57%	10.370%
76	12.520	3474	3477	3478	rBV	249	146	0.02%	0.002%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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Title : VOC Analysis

77	12.915	3597	3600	3606	rBV	392	254	0.03%	0.004%
78	13.069	3646	3648	3649	rBV	343	79	0.01%	0.001%
79	13.111	3658	3661	3671	rBV	416	401	0.05%	0.006%
80	13.343	3730	3733	3734	rBV	344	171	0.02%	0.003%
81	13.465	3769	3771	3772	rBV	361	139	0.02%	0.002%
82	13.838	3879	3887	3901	rVV3	18825	28777	3.76%	0.440%
83	13.905	3905	3908	3914	rBV	440	324	0.04%	0.005%
84	14.330	4032	4040	4051	rVB3	10445	15744	2.06%	0.241%
85	14.616	4127	4129	4131	rBV	376	243	0.03%	0.004%
86	14.921	4222	4224	4225	rBV	411	197	0.03%	0.003%

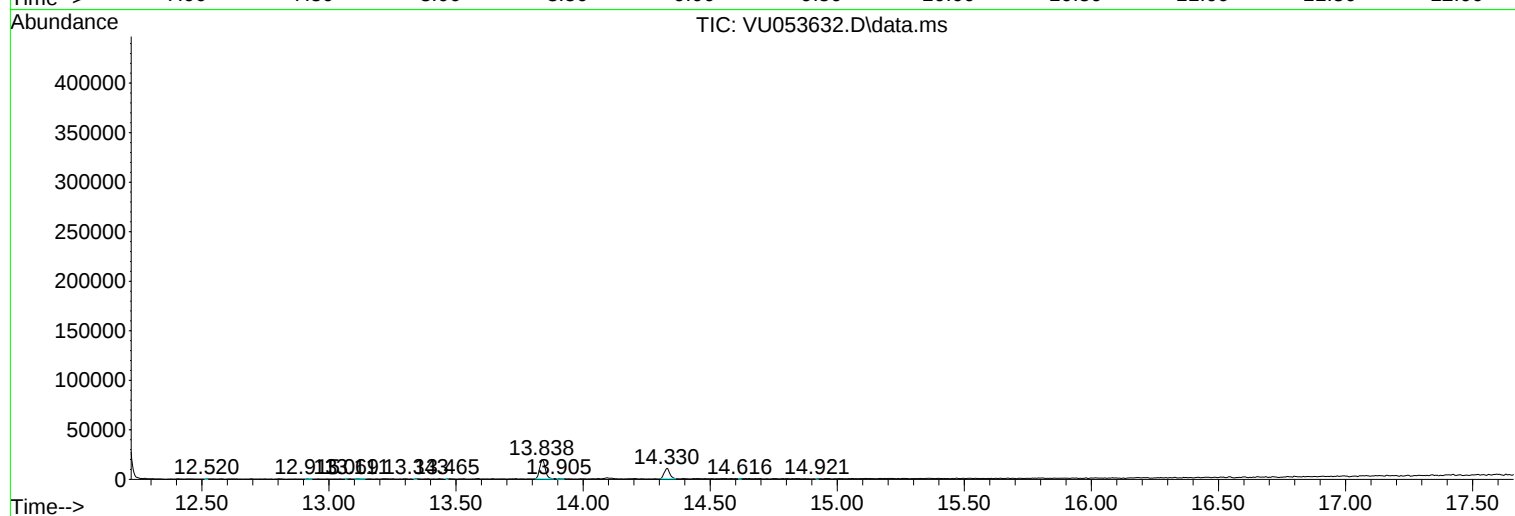
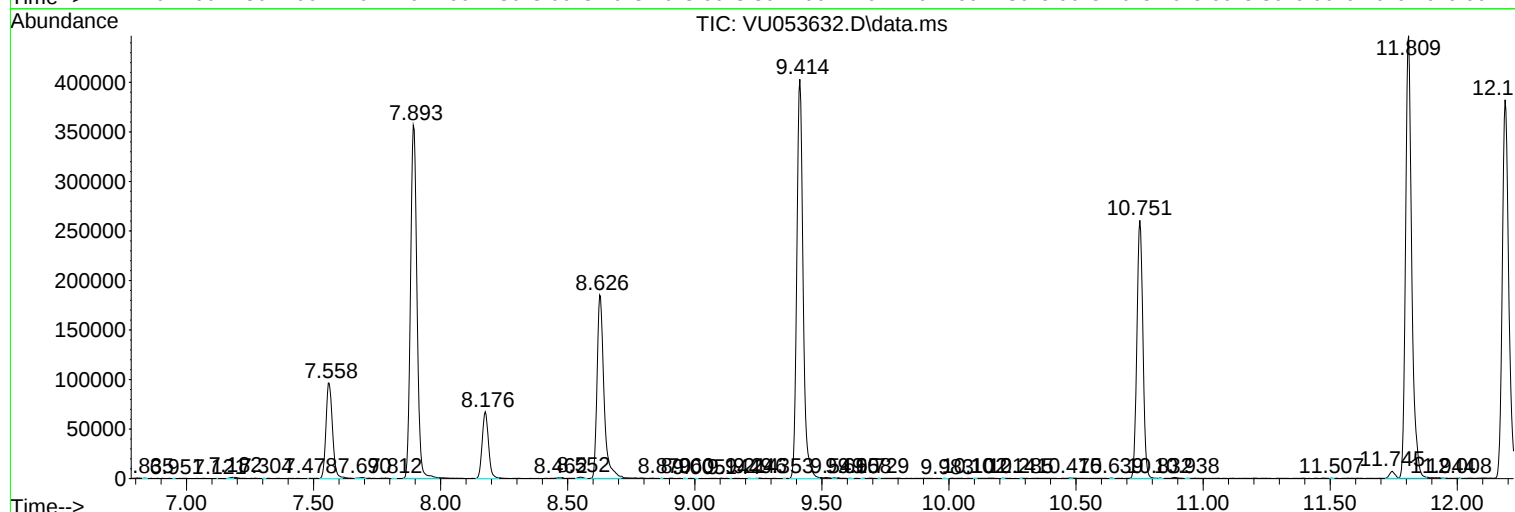
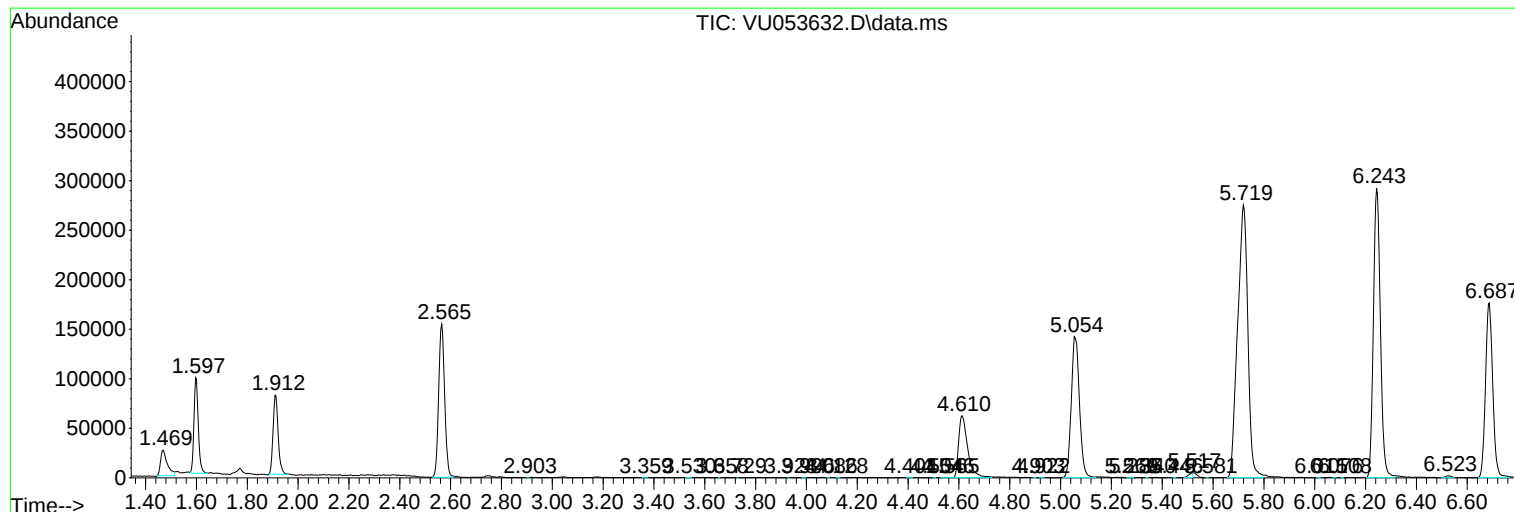
Sum of corrected areas: 6541178

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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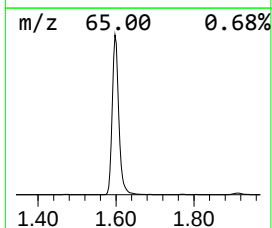
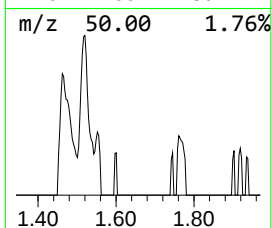
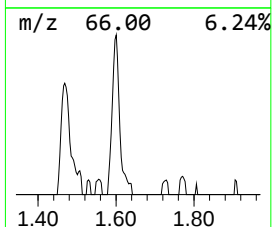
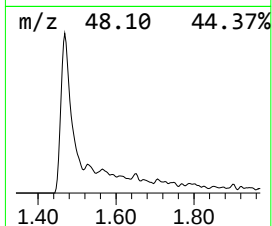
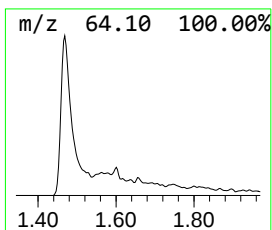
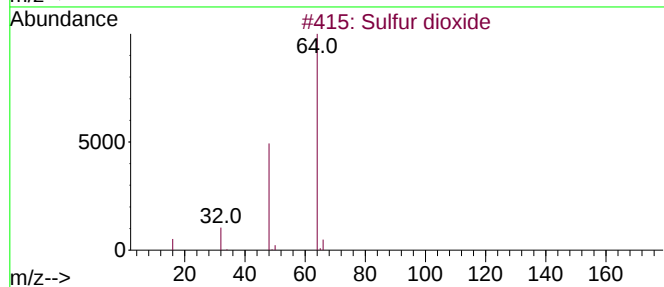
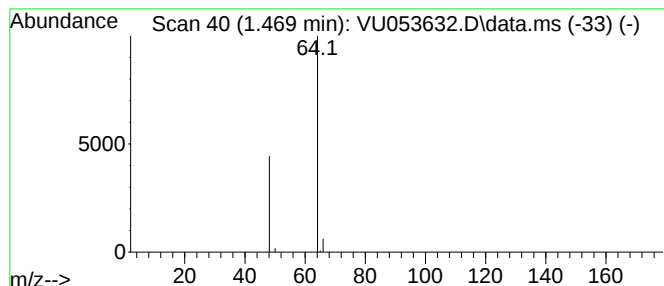
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	4.31 ug/L	48003	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	4.3	ug/L	48003	1	6.243	556994	50.0