

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053636.D
 Acq On : 11 Apr 2023 15:37
 Operator : JC/MD
 Sample : 02251-12DL 50X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD0DL

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: VU053636.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	32	39	60	rBV	33226	62810	7.87%	0.934%
2	1.597	74	80	98	rVB	99600	117735	14.75%	1.751%
3	1.909	169	177	204	rVB	83923	122216	15.31%	1.818%
4	2.565	369	381	394	rBV	156488	253852	31.80%	3.775%
5	2.752	436	439	443	rBV2	697	625	0.08%	0.009%
6	3.041	517	529	550	rVB2	23304	45142	5.66%	0.671%
7	3.176	569	571	574	rVB	286	174	0.02%	0.003%
8	3.202	577	579	584	rVB	212	111	0.01%	0.002%
9	3.263	595	598	603	rVB2	331	200	0.03%	0.003%
10	3.346	621	624	628	rBV3	797	690	0.09%	0.010%
11	3.440	651	653	656	rBV	196	81	0.01%	0.001%
12	3.581	693	697	701	rBV2	352	264	0.03%	0.004%
13	3.645	715	717	719	rBV2	180	101	0.01%	0.002%
14	3.797	761	764	765	rBV2	149	64	0.01%	0.001%
15	3.806	765	767	770	rVV	227	117	0.01%	0.002%
16	3.838	775	777	782	rVV	202	132	0.02%	0.002%
17	3.877	786	789	797	rVV2	407	317	0.04%	0.005%
18	3.909	797	799	805	rVB	361	178	0.02%	0.003%
19	4.031	835	837	841	rVB	205	103	0.01%	0.002%
20	4.057	842	845	848	rBV	274	149	0.02%	0.002%
21	4.076	848	851	855	rBV2	251	216	0.03%	0.003%
22	4.173	878	881	884	rBV2	226	186	0.02%	0.003%
23	4.301	917	921	924	rBV2	334	274	0.03%	0.004%
24	4.356	935	938	941	rBV	138	86	0.01%	0.001%
25	4.514	984	987	989	rBV	224	128	0.02%	0.002%
26	4.613	1005	1018	1049	rBV	69001	168550	21.12%	2.507%
27	5.057	1141	1156	1176	rBV2	149316	327772	41.06%	4.874%
28	5.311	1232	1235	1238	rBV2	191	161	0.02%	0.002%
29	5.366	1248	1252	1253	rBV2	222	155	0.02%	0.002%
30	5.504	1292	1295	1296	rBV	353	190	0.02%	0.003%
31	5.591	1316	1322	1327	rBV2	309	329	0.04%	0.005%
32	5.616	1328	1330	1333	rVB	309	152	0.02%	0.002%
33	5.633	1333	1335	1336	rBV	225	109	0.01%	0.002%
34	5.649	1337	1340	1341	rBV	131	66	0.01%	0.001%
35	5.719	1341	1362	1370	rBV2	289427	784102	98.23%	11.661%
36	5.989	1442	1446	1447	rBV	258	139	0.02%	0.002%

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 Title : VOC Analysis

37	6.044	1459	1463	1468	rVB2	331	292	0.04%	0.004%
38	6.243	1512	1525	1543	rBV	275296	526843	66.00%	7.835%
39	6.449	1585	1589	1591	rBV	269	203	0.03%	0.003%
40	6.497	1601	1604	1606	rBV2	297	237	0.03%	0.004%
41	6.639	1647	1648	1649	rBB	73	34	0.00%	0.001%
42	6.684	1649	1662	1682	rVV	183262	355105	44.49%	5.281%
43	6.867	1717	1719	1725	rVB	359	317	0.04%	0.005%
44	6.896	1725	1728	1730	rBV	186	146	0.02%	0.002%
45	6.912	1731	1733	1735	rVB	185	68	0.01%	0.001%
46	6.999	1757	1760	1766	rVB	350	257	0.03%	0.004%
47	7.028	1767	1769	1772	rVB	183	80	0.01%	0.001%
48	7.076	1782	1784	1785	rBV	149	47	0.01%	0.001%
49	7.189	1813	1819	1823	rVB3	939	1083	0.14%	0.016%
50	7.562	1922	1935	1955	rBV	102900	180318	22.59%	2.682%
51	7.764	1996	1998	2001	rVB	160	52	0.01%	0.001%
52	7.790	2004	2006	2011	rVB3	659	453	0.06%	0.007%
53	7.893	2025	2038	2058	rBV	366396	638928	80.04%	9.502%
54	8.079	2093	2096	2101	rBV	370	294	0.04%	0.004%
55	8.105	2101	2104	2110	rVB2	189	225	0.03%	0.003%
56	8.176	2115	2126	2142	rBV	68907	117947	14.78%	1.754%
57	8.269	2152	2155	2159	rBV2	203	215	0.03%	0.003%
58	8.417	2198	2201	2203	rBV	255	209	0.03%	0.003%
59	8.462	2207	2215	2224	rVV2	589	959	0.12%	0.014%
60	8.552	2236	2243	2247	rBV3	632	743	0.09%	0.011%
61	8.626	2255	2266	2293	rBV	201719	373439	46.78%	5.554%
62	8.800	2318	2320	2328	rVB2	318	285	0.04%	0.004%
63	8.857	2336	2338	2340	rBV	330	175	0.02%	0.003%
64	8.886	2345	2347	2348	rBV	161	52	0.01%	0.001%
65	9.169	2432	2435	2437	rBV	139	76	0.01%	0.001%
66	9.189	2439	2441	2444	rVB	281	117	0.01%	0.002%
67	9.237	2454	2456	2457	rVB	265	85	0.01%	0.001%
68	9.250	2457	2460	2464	rVB2	221	146	0.02%	0.002%
69	9.266	2464	2465	2468	rBV2	318	155	0.02%	0.002%
70	9.414	2498	2511	2515	rBV	404357	639610	80.13%	9.512%
71	9.648	2582	2584	2588	rVB	142	78	0.01%	0.001%
72	9.671	2588	2591	2592	rBV	354	181	0.02%	0.003%
73	9.681	2592	2594	2595	rBV	355	144	0.02%	0.002%
74	9.835	2635	2642	2645	rBV2	272	294	0.04%	0.004%
75	10.224	2761	2763	2766	rBV	255	113	0.01%	0.002%
76	10.372	2807	2809	2810	rBV	226	101	0.01%	0.002%

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77	10.700	2909	2911	2913	rBV	239	101	0.01%	0.002%
78	10.751	2914	2927	2945	rVV	270723	439723	55.09%	6.539%
79	11.404	3127	3130	3132	rBV	315	213	0.03%	0.003%
80	11.745	3228	3236	3244	rVB5	3921	5303	0.66%	0.079%
81	11.809	3244	3256	3277	rBV2	437758	798238	100.00%	11.871%
82	12.189	3361	3374	3394	rBV2	409004	746936	93.57%	11.108%
83	12.613	3502	3506	3509	rBV	279	229	0.03%	0.003%
84	12.632	3509	3512	3513	rBV	196	106	0.01%	0.002%
85	12.883	3589	3590	3597	rVB2	362	264	0.03%	0.004%
86	12.970	3614	3617	3621	rBV	314	218	0.03%	0.003%
87	13.021	3631	3633	3634	rBV	174	53	0.01%	0.001%
88	13.192	3682	3686	3689	rBV	366	361	0.05%	0.005%
89	13.819	3877	3881	3883	rBV	411	296	0.04%	0.004%
90	13.848	3884	3890	3901	rVB7	2834	4566	0.57%	0.068%

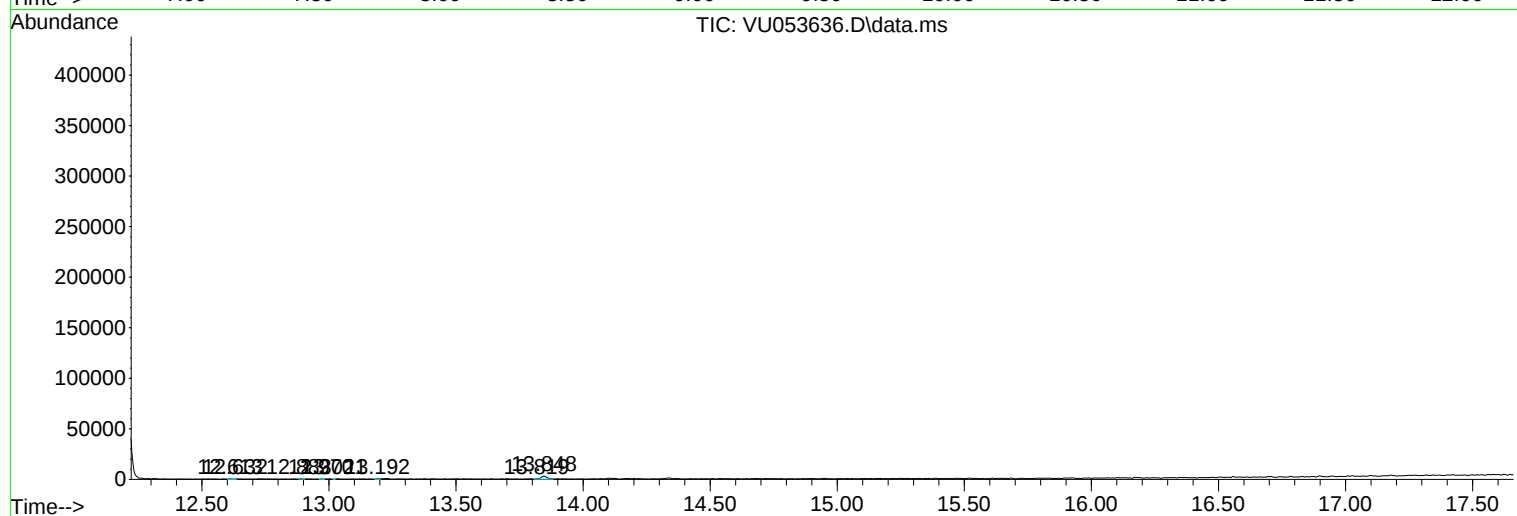
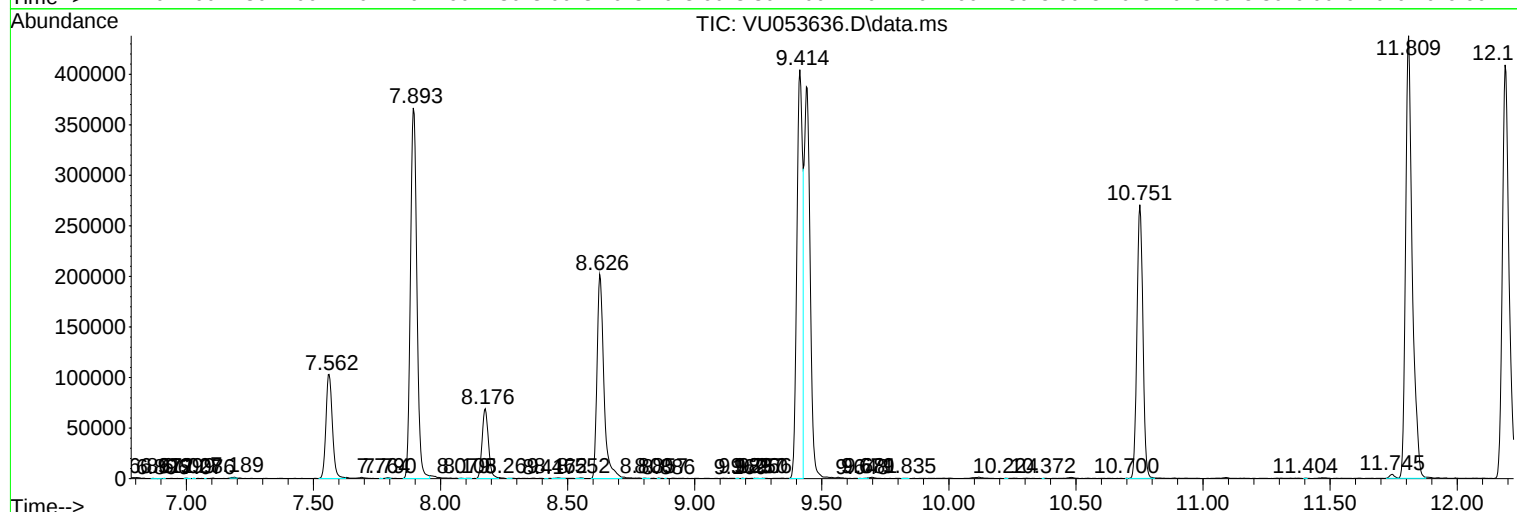
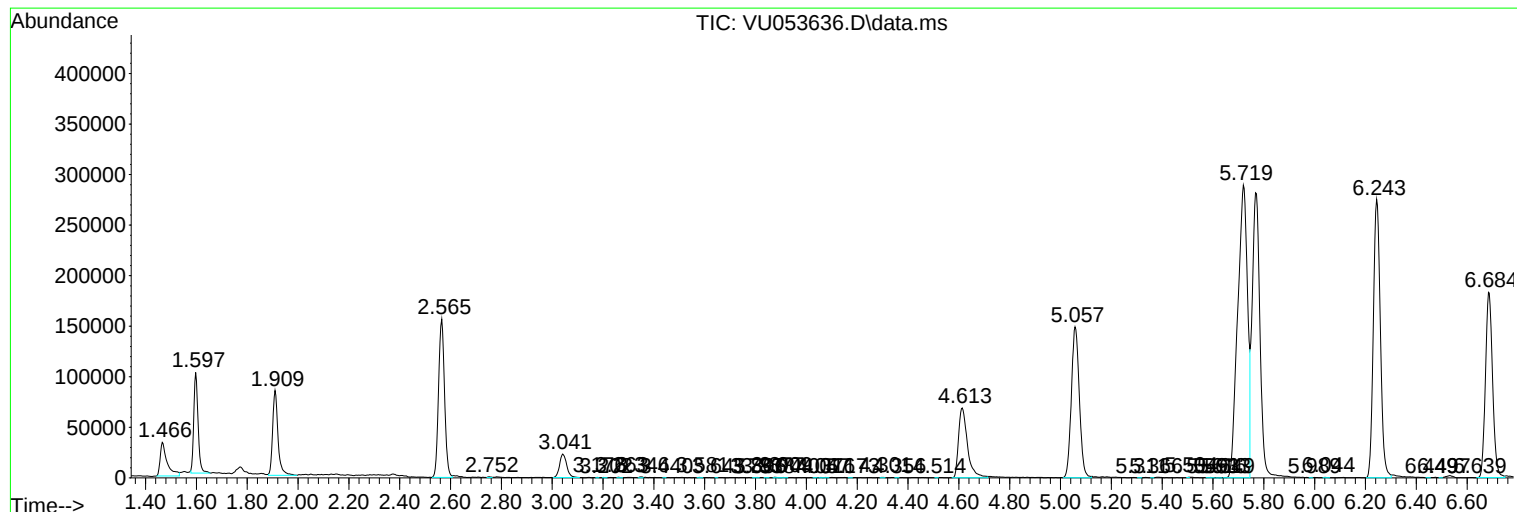
Sum of corrected areas: 6724389

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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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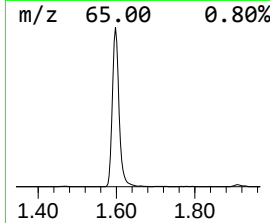
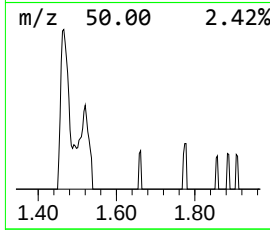
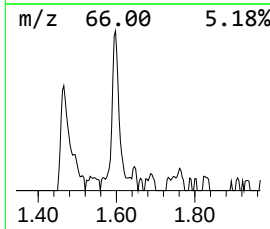
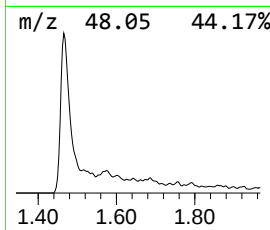
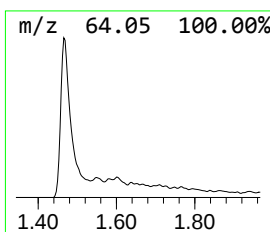
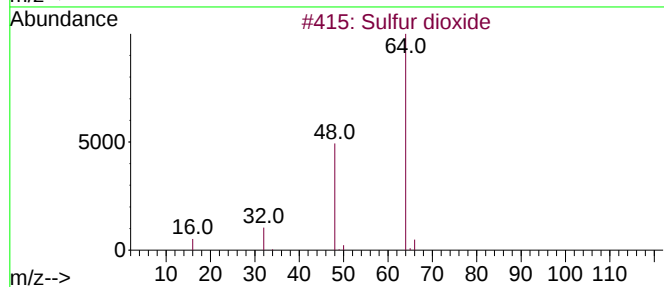
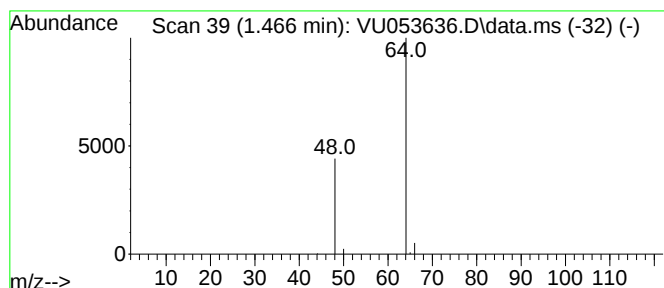
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	5.96 ug/L	62810	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			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	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	6.0	ug/L	62810	1	6.243	526843	50.0