

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031523\
 Data File : VU053205.D
 Acq On : 15 Mar 2023 17:03
 Operator : JC/MD
 Sample : 01929-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFE2

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: VU053205.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	34	42	72	rBV	60640	151422	27.53%	3.722%
2	1.600	75	81	94	rVB	81808	95725	17.41%	2.353%
3	1.915	172	179	192	rVB	64610	84163	15.30%	2.068%
4	2.568	369	382	395	rBV	121577	197808	35.97%	4.862%
5	3.041	526	529	530	rBV2	347	193	0.04%	0.005%
6	3.285	602	605	607	rBV	207	125	0.02%	0.003%
7	3.504	670	673	675	rBV	176	108	0.02%	0.003%
8	3.591	697	700	702	rBV2	257	162	0.03%	0.004%
9	3.764	751	754	755	rBV	146	67	0.01%	0.002%
10	3.780	756	759	763	rVB	227	149	0.03%	0.004%
11	3.996	824	826	828	rBV2	124	68	0.01%	0.002%
12	4.166	876	879	881	rBV	320	221	0.04%	0.005%
13	4.256	904	907	909	rBV	146	91	0.02%	0.002%
14	4.366	939	941	942	rBV	146	44	0.01%	0.001%
15	4.433	956	962	965	rBV2	243	315	0.06%	0.008%
16	4.488	977	979	980	rBV2	133	56	0.01%	0.001%
17	4.581	1005	1008	1010	rBV	227	148	0.03%	0.004%
18	4.623	1010	1021	1052	rBV	34971	94011	17.09%	2.311%
19	4.877	1097	1100	1101	rBV2	252	153	0.03%	0.004%
20	4.906	1106	1109	1112	rBV	175	129	0.02%	0.003%
21	4.951	1120	1123	1125	rBV	147	88	0.02%	0.002%
22	5.057	1140	1156	1181	rBV	101985	220158	40.03%	5.411%
23	5.301	1230	1232	1234	rVB	283	69	0.01%	0.002%
24	5.349	1245	1247	1249	rVB	183	79	0.01%	0.002%
25	5.414	1264	1267	1271	rBV2	158	101	0.02%	0.002%
26	5.439	1271	1275	1277	rBV2	194	165	0.03%	0.004%
27	5.501	1292	1294	1297	rVB	160	65	0.01%	0.002%
28	5.610	1324	1328	1329	rBV2	286	227	0.04%	0.006%
29	5.652	1338	1341	1342	rBV	229	148	0.03%	0.004%
30	5.719	1342	1362	1383	rVV2	203365	549936	100.00%	13.516%
31	5.909	1418	1421	1422	rBV	224	127	0.02%	0.003%
32	6.066	1468	1470	1474	rBV2	133	86	0.02%	0.002%
33	6.108	1480	1483	1485	rBV	348	232	0.04%	0.006%
34	6.156	1494	1498	1499	rBV	260	119	0.02%	0.003%
35	6.185	1504	1507	1510	rBV	221	138	0.03%	0.003%
36	6.243	1513	1525	1541	rBV	130211	244243	44.41%	6.003%

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 Title : VOC Analysis

37	6.449	1587	1589	1591	rBV	172	84	0.02%	0.002%
38	6.510	1606	1608	1609	rBV	157	43	0.01%	0.001%
39	6.607	1635	1638	1640	rBV	233	139	0.03%	0.003%
40	6.639	1646	1648	1649	rBV	148	58	0.01%	0.001%
41	6.684	1649	1662	1682	rVV2	125432	246979	44.91%	6.070%
42	6.790	1694	1695	1698	rBV2	364	232	0.04%	0.006%
43	6.845	1710	1712	1717	rBV2	198	145	0.03%	0.004%
44	6.886	1723	1725	1726	rBV2	248	108	0.02%	0.003%
45	6.951	1742	1745	1748	rVB2	179	121	0.02%	0.003%
46	7.012	1759	1764	1767	rBV2	227	217	0.04%	0.005%
47	7.185	1811	1818	1825	rBV3	679	1018	0.19%	0.025%
48	7.446	1897	1899	1903	rBV2	145	93	0.02%	0.002%
49	7.562	1923	1935	1954	rBV	73757	131185	23.85%	3.224%
50	7.893	2025	2038	2059	rBV	256533	444537	80.83%	10.925%
51	8.176	2115	2126	2145	rBV	51239	87539	15.92%	2.151%
52	8.307	2164	2167	2169	rBV	158	107	0.02%	0.003%
53	8.385	2188	2191	2195	rVB2	326	279	0.05%	0.007%
54	8.414	2195	2200	2207	rBV	242	449	0.08%	0.011%
55	8.552	2241	2243	2247	rBV	262	226	0.04%	0.006%
56	8.629	2256	2267	2294	rBV2	113485	219867	39.98%	5.404%
57	8.809	2321	2323	2328	rVB2	190	142	0.03%	0.003%
58	8.867	2338	2341	2342	rBV2	166	72	0.01%	0.002%
59	9.012	2383	2386	2390	rVB	158	94	0.02%	0.002%
60	9.217	2448	2450	2454	rVB	200	118	0.02%	0.003%
61	9.243	2455	2458	2463	rVB	195	125	0.02%	0.003%
62	9.266	2463	2465	2470	rBV	170	132	0.02%	0.003%
63	9.327	2481	2484	2487	rBV	101	73	0.01%	0.002%
64	9.349	2488	2491	2494	rBV2	191	130	0.02%	0.003%
65	9.414	2496	2511	2530	rBV	185916	307585	55.93%	7.560%
66	9.545	2550	2552	2556	rVV	273	124	0.02%	0.003%
67	9.568	2556	2559	2563	rVB2	174	123	0.02%	0.003%
68	9.674	2590	2592	2594	rBV	183	78	0.01%	0.002%
69	9.873	2652	2654	2658	rBV2	252	157	0.03%	0.004%
70	10.002	2692	2694	2697	rBB	166	68	0.01%	0.002%
71	10.063	2710	2713	2716	rBV2	219	146	0.03%	0.004%
72	10.108	2724	2727	2728	rBV2	164	78	0.01%	0.002%
73	10.214	2757	2760	2762	rBV	179	106	0.02%	0.003%
74	10.484	2839	2844	2846	rBV2	432	298	0.05%	0.007%
75	10.751	2915	2927	2941	rBV	163055	260453	47.36%	6.401%
76	10.889	2967	2970	2974	rBV	316	161	0.03%	0.004%

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Peak Location: TOP

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

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77	10.970	2993	2995	3003	rVB2	221	281	0.05%	0.007%
78	11.015	3007	3009	3011	rBV	170	58	0.01%	0.001%
79	11.095	3031	3034	3036	rBV2	229	136	0.02%	0.003%
80	11.131	3042	3045	3047	rBV	229	141	0.03%	0.003%
81	11.179	3057	3060	3065	rBV2	210	192	0.03%	0.005%
82	11.388	3121	3125	3131	rBV2	278	344	0.06%	0.008%
83	11.458	3145	3147	3149	rBV	181	101	0.02%	0.002%
84	11.491	3155	3157	3165	rBV	235	242	0.04%	0.006%
85	11.806	3244	3255	3279	rBV	204157	331619	60.30%	8.150%
86	12.111	3347	3350	3352	rBV	211	101	0.02%	0.002%
87	12.188	3362	3374	3391	rBV	238684	388727	70.69%	9.554%
88	12.629	3509	3511	3514	rBV	168	58	0.01%	0.001%
89	12.693	3528	3531	3535	rBV	221	185	0.03%	0.005%
90	12.857	3579	3582	3583	rBV	197	102	0.02%	0.003%
91	12.960	3611	3614	3619	rBV	271	277	0.05%	0.007%
92	13.159	3673	3676	3677	rBV	202	120	0.02%	0.003%
93	13.240	3697	3701	3704	rBV2	257	203	0.04%	0.005%
94	13.291	3715	3717	3720	rBV	172	74	0.01%	0.002%
95	13.487	3775	3778	3782	rBV	252	187	0.03%	0.005%
96	13.616	3815	3818	3821	rVB2	277	188	0.03%	0.005%
97	13.886	3900	3902	3903	rBV2	220	78	0.01%	0.002%
98	14.786	4179	4182	4185	rBV2	206	150	0.03%	0.004%
99	14.873	4207	4209	4211	rBV	314	177	0.03%	0.004%
100	14.995	4243	4247	4248	rBV2	314	237	0.04%	0.006%

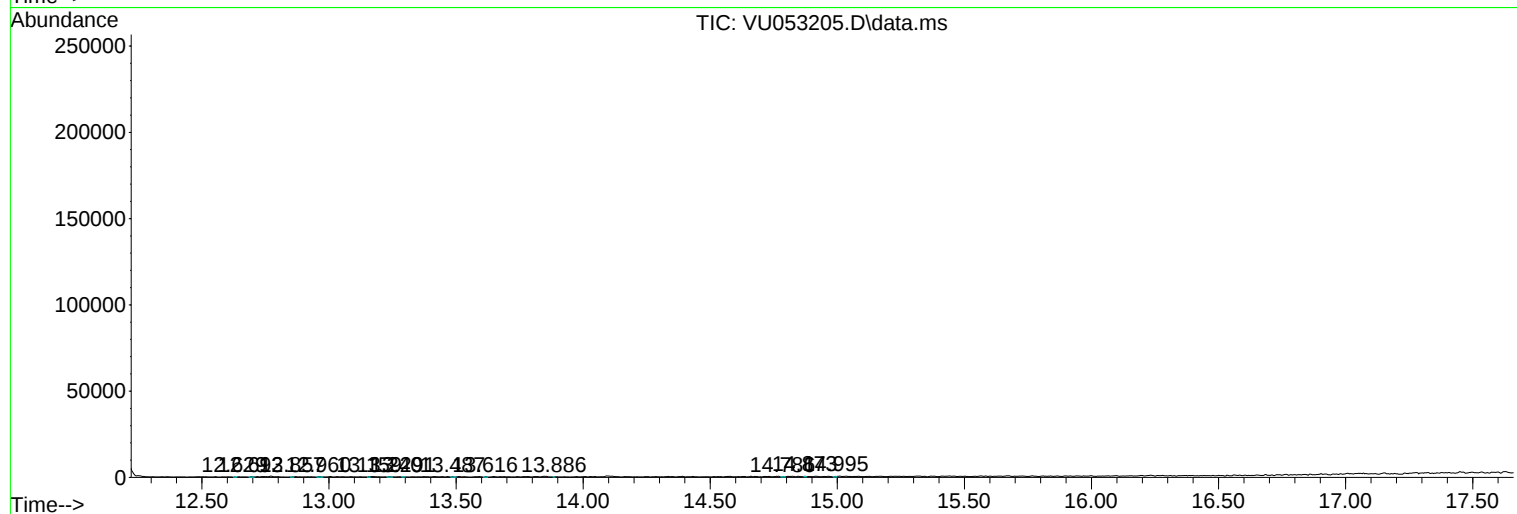
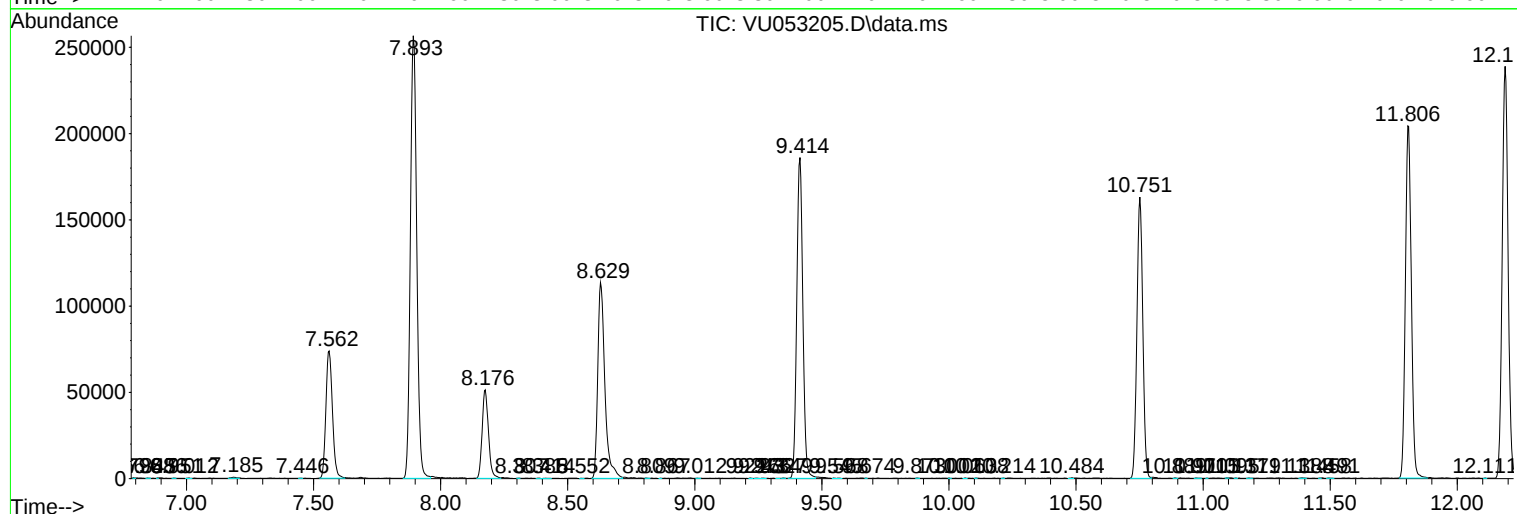
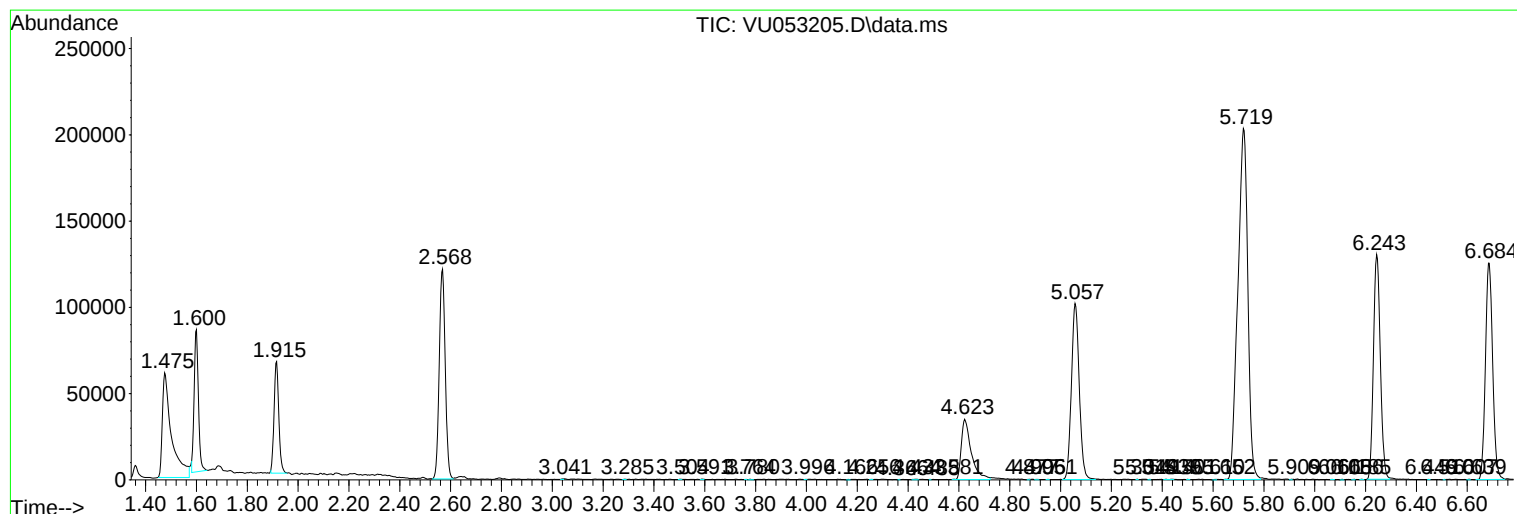
Sum of corrected areas: 4068806

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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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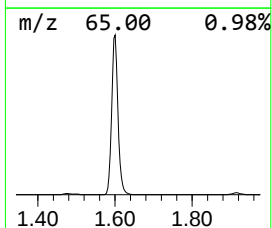
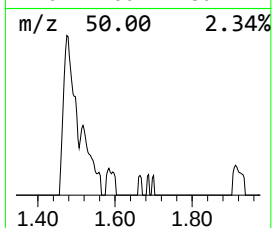
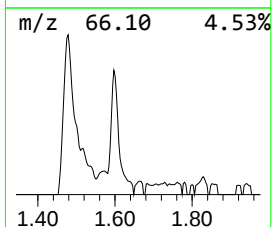
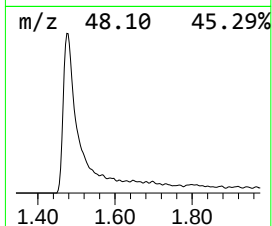
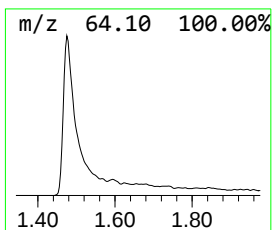
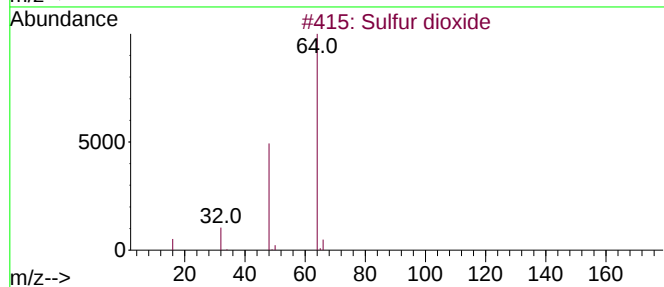
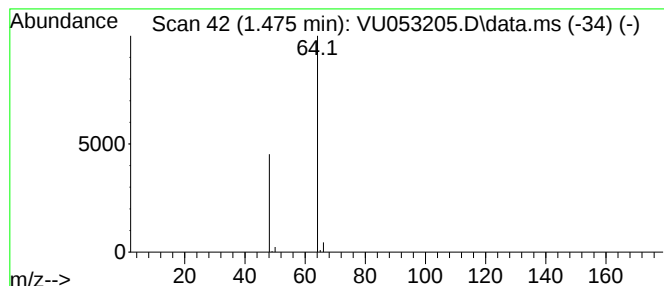
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	31.00 ug/L	151422	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			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	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.475	31.0	ug/L	151422	1	6.243	244243	50.0