

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031523\
 Data File : VU053212.D
 Acq On : 15 Mar 2023 19:47
 Operator : JC/MD
 Sample : 01929-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFF1

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: VU053212.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	37	45	71	rBV	21627	64395	10.11%	1.159%
2	1.601	74	81	96	rVB2	167692	210011	32.96%	3.779%
3	1.913	171	178	197	rVB	74508	101188	15.88%	1.821%
4	2.568	369	382	395	rBV	140752	233648	36.67%	4.204%
5	2.787	445	450	452	rBV2	507	505	0.08%	0.009%
6	3.006	516	518	520	rBV	260	126	0.02%	0.002%
7	3.263	594	598	601	rVB2	225	151	0.02%	0.003%
8	3.282	601	604	610	rBV2	254	243	0.04%	0.004%
9	3.411	640	644	647	rBV2	176	146	0.02%	0.003%
10	3.546	684	686	689	rVB	187	79	0.01%	0.001%
11	3.565	689	692	694	rBV	271	136	0.02%	0.002%
12	3.581	694	697	700	rBV3	322	269	0.04%	0.005%
13	3.848	777	780	786	rVB2	164	173	0.03%	0.003%
14	3.941	807	809	812	rBV	139	97	0.02%	0.002%
15	3.986	819	823	829	rVB2	265	231	0.04%	0.004%
16	4.118	858	864	869	rBV2	352	420	0.07%	0.008%
17	4.186	883	885	887	rBV	185	83	0.01%	0.001%
18	4.202	887	890	893	rBV	126	73	0.01%	0.001%
19	4.279	912	914	916	rBV	131	81	0.01%	0.001%
20	4.327	926	929	932	rBV	269	234	0.04%	0.004%
21	4.379	943	945	948	rBV2	166	93	0.01%	0.002%
22	4.446	963	966	970	rBV	194	118	0.02%	0.002%
23	4.662	1009	1033	1057	rBV2	99221	331351	52.00%	5.962%
24	4.829	1082	1085	1089	rVB2	384	306	0.05%	0.006%
25	4.922	1112	1114	1118	rVB	374	232	0.04%	0.004%
26	4.951	1118	1123	1124	rBV2	347	304	0.05%	0.005%
27	5.057	1141	1156	1181	rVB	119979	257447	40.41%	4.632%
28	5.192	1194	1198	1202	rBV3	341	416	0.07%	0.007%
29	5.289	1224	1228	1231	rBV	485	399	0.06%	0.007%
30	5.623	1330	1332	1334	rBV	156	76	0.01%	0.001%
31	5.719	1341	1362	1388	rBV2	237474	637163	100.00%	11.465%
32	5.977	1439	1442	1444	rBV	195	125	0.02%	0.002%
33	5.996	1446	1448	1450	rBV2	136	74	0.01%	0.001%
34	6.041	1458	1462	1465	rBV3	308	213	0.03%	0.004%
35	6.096	1473	1479	1481	rBV2	189	168	0.03%	0.003%
36	6.131	1488	1490	1493	rVB2	231	109	0.02%	0.002%

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

37	6.176	1501	1504	1506	rVB	202	106	0.02%	0.002%
38	6.244	1512	1525	1546	rBV	195623	369699	58.02%	6.652%
39	6.449	1586	1589	1592	rVB	286	162	0.03%	0.003%
40	6.472	1593	1596	1599	rBV	254	221	0.03%	0.004%
41	6.536	1604	1616	1632	rBV	111937	210703	33.07%	3.791%
42	6.684	1649	1662	1684	rBV	149354	290712	45.63%	5.231%
43	6.793	1693	1696	1697	rBV2	309	197	0.03%	0.004%
44	6.848	1710	1713	1715	rBV	186	133	0.02%	0.002%
45	6.874	1717	1721	1726	rVV2	277	315	0.05%	0.006%
46	7.067	1778	1781	1784	rBV	130	76	0.01%	0.001%
47	7.224	1828	1830	1834	rBV2	175	133	0.02%	0.002%
48	7.369	1872	1875	1877	rVB	202	133	0.02%	0.002%
49	7.562	1923	1935	1955	rBV	88113	153989	24.17%	2.771%
50	7.636	1955	1958	1960	rVB2	245	160	0.03%	0.003%
51	7.793	2002	2007	2010	rBV3	244	257	0.04%	0.005%
52	7.893	2024	2038	2055	rBV	301981	516062	80.99%	9.286%
53	8.067	2090	2092	2097	rVB2	333	203	0.03%	0.004%
54	8.089	2097	2099	2102	rBV	146	69	0.01%	0.001%
55	8.112	2103	2106	2113	rVB	518	488	0.08%	0.009%
56	8.173	2113	2125	2144	rBV	59178	101265	15.89%	1.822%
57	8.285	2158	2160	2165	rBV	400	303	0.05%	0.005%
58	8.308	2165	2167	2169	rBV	156	71	0.01%	0.001%
59	8.404	2194	2197	2200	rBV	250	227	0.04%	0.004%
60	8.417	2200	2201	2204	rVB	293	131	0.02%	0.002%
61	8.436	2204	2207	2208	rBV	279	181	0.03%	0.003%
62	8.629	2256	2267	2294	rBV2	161687	300781	47.21%	5.412%
63	8.851	2333	2336	2340	rVB2	210	138	0.02%	0.002%
64	9.057	2396	2400	2404	rVB2	196	191	0.03%	0.003%
65	9.128	2416	2422	2423	rBV2	168	164	0.03%	0.003%
66	9.150	2427	2429	2430	rBV2	159	73	0.01%	0.001%
67	9.237	2454	2456	2461	rBV	184	110	0.02%	0.002%
68	9.356	2492	2493	2494	rBV	215	71	0.01%	0.001%
69	9.411	2498	2510	2532	rVV	278080	466727	73.25%	8.398%
70	9.575	2559	2561	2567	rVB	354	214	0.03%	0.004%
71	9.600	2567	2569	2572	rBV2	270	118	0.02%	0.002%
72	9.694	2595	2598	2602	rVB2	311	214	0.03%	0.004%
73	9.732	2607	2610	2612	rBV	183	132	0.02%	0.002%
74	10.044	2705	2707	2710	rBV	221	115	0.02%	0.002%
75	10.086	2718	2720	2721	rBV	213	91	0.01%	0.002%
76	10.124	2728	2732	2736	rVB	268	228	0.04%	0.004%

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Peak Location: TOP

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

77	10.314	2788	2791	2794	rVB2	290	191	0.03%	0.003%
78	10.337	2794	2798	2800	rBV	261	204	0.03%	0.004%
79	10.485	2841	2844	2845	rBV	163	93	0.01%	0.002%
80	10.616	2881	2885	2887	rBV2	236	203	0.03%	0.004%
81	10.751	2915	2927	2943	rBV	208988	329111	51.65%	5.922%
82	10.829	2949	2951	2954	rVB	172	80	0.01%	0.001%
83	10.973	2993	2996	2998	rBV	200	112	0.02%	0.002%
84	11.112	3037	3039	3042	rBV2	321	146	0.02%	0.003%
85	11.414	3131	3133	3137	rBV2	143	107	0.02%	0.002%
86	11.603	3188	3192	3194	rBV2	216	170	0.03%	0.003%
87	11.645	3201	3205	3209	rBV	244	180	0.03%	0.003%
88	11.806	3242	3255	3274	rBV	317241	503768	79.06%	9.065%
89	12.070	3328	3337	3347	rBV3	4491	9864	1.55%	0.177%
90	12.189	3362	3374	3393	rBV	281349	455098	71.43%	8.189%
91	12.311	3409	3412	3415	rBV2	202	141	0.02%	0.003%
92	12.449	3452	3455	3459	rBV2	262	256	0.04%	0.005%
93	12.603	3500	3503	3504	rBV2	225	137	0.02%	0.002%
94	12.655	3517	3519	3521	rBV2	230	134	0.02%	0.002%
95	13.150	3669	3673	3675	rBV	207	155	0.02%	0.003%
96	13.787	3868	3871	3873	rBV	179	90	0.01%	0.002%
97	13.877	3897	3899	3901	rBV	215	113	0.02%	0.002%
98	14.436	4071	4073	4078	rVB2	398	291	0.05%	0.005%
99	14.517	4094	4098	4101	rBV	313	321	0.05%	0.006%
100	14.764	4172	4175	4178	rBV2	372	258	0.04%	0.005%

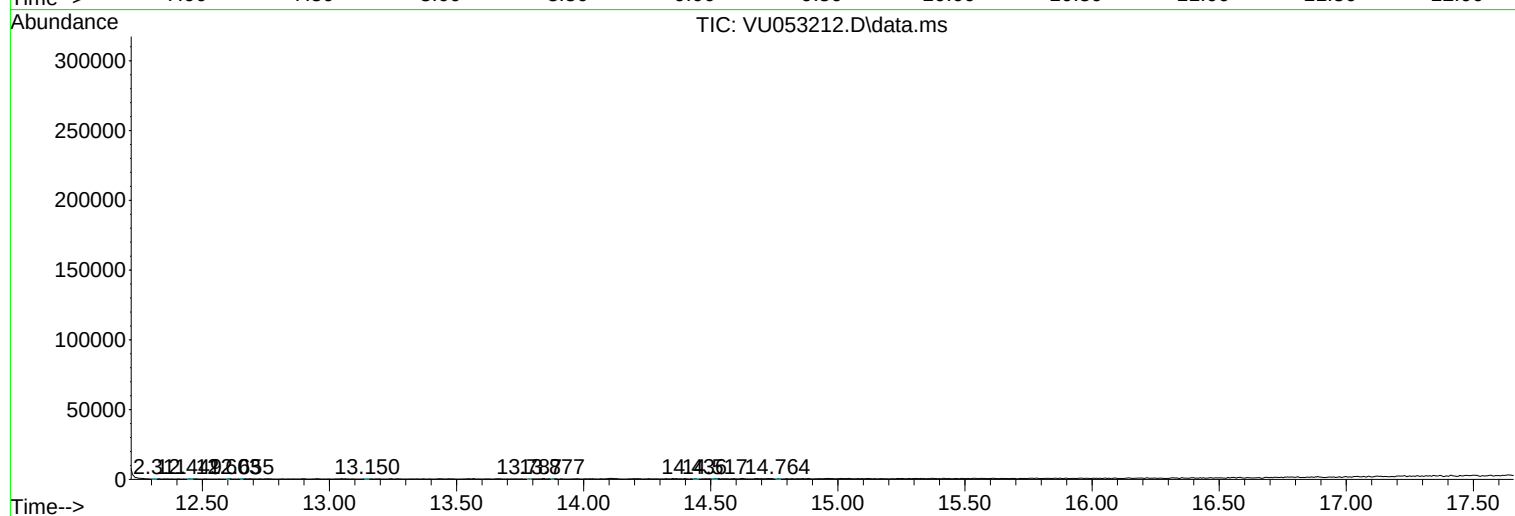
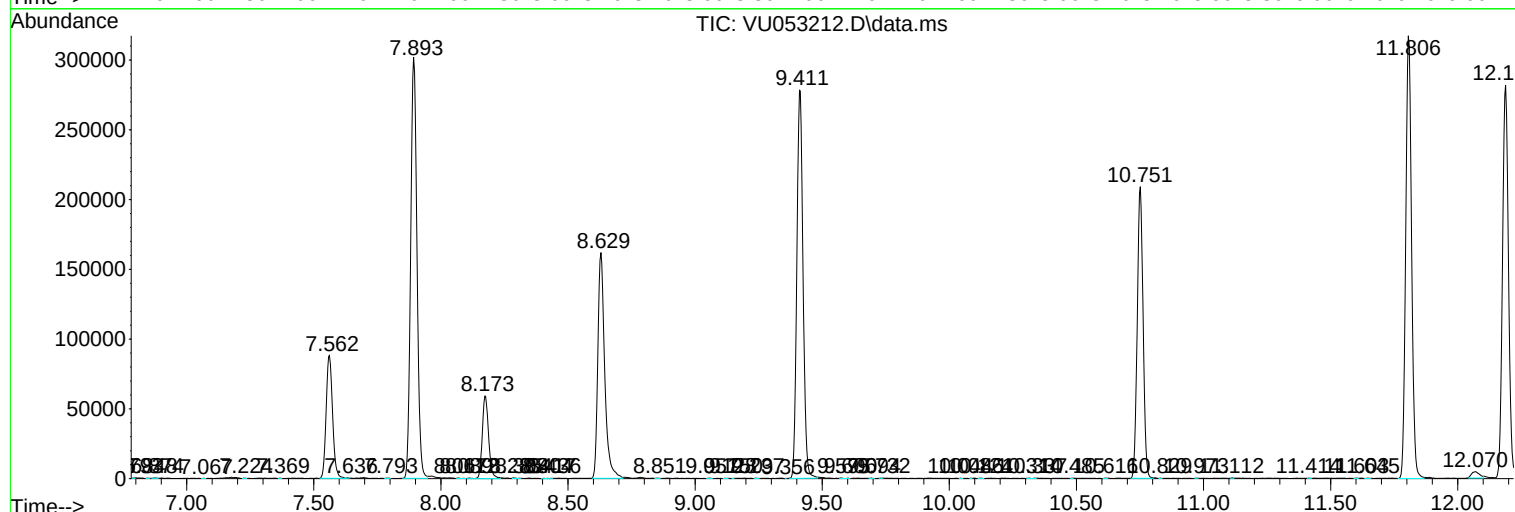
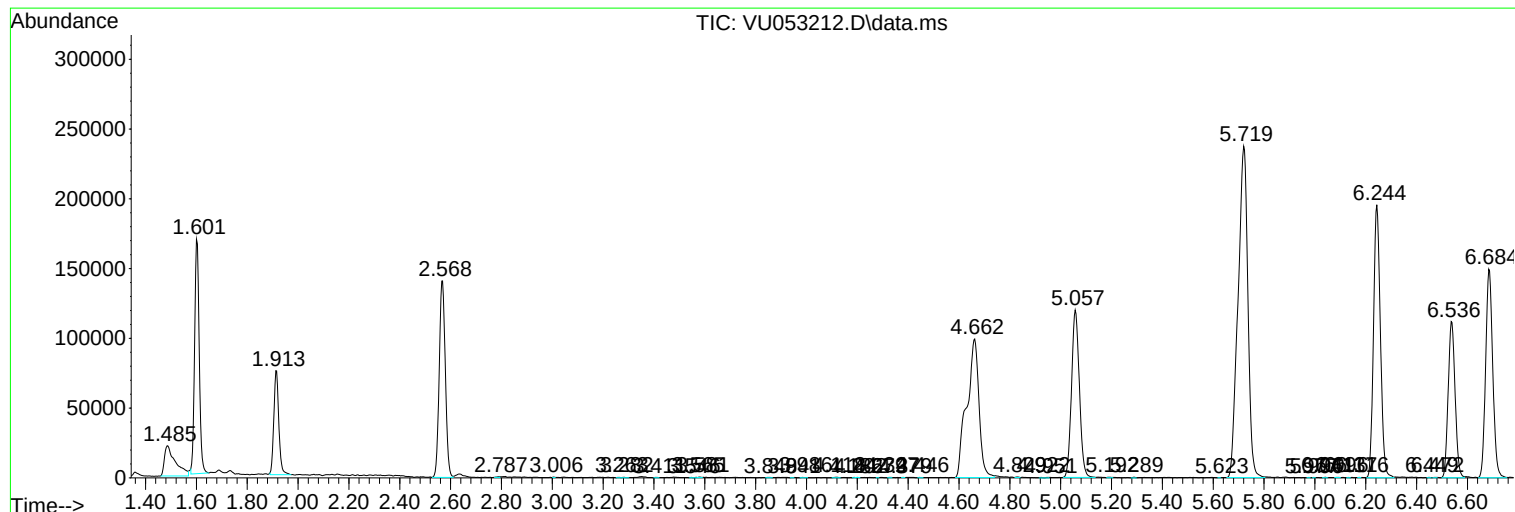
Sum of corrected areas: 5557469

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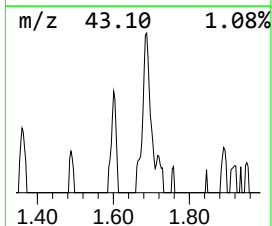
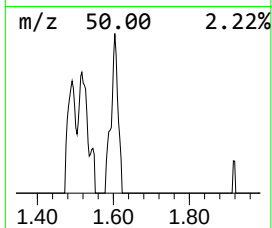
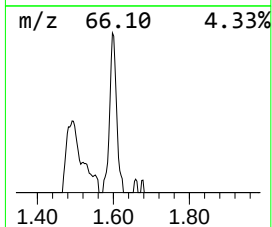
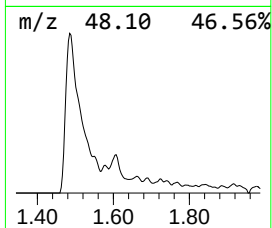
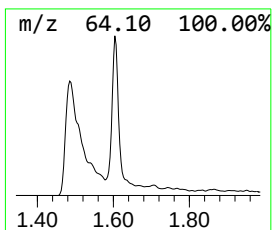
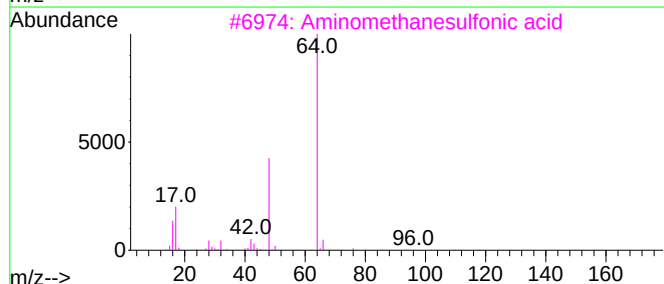
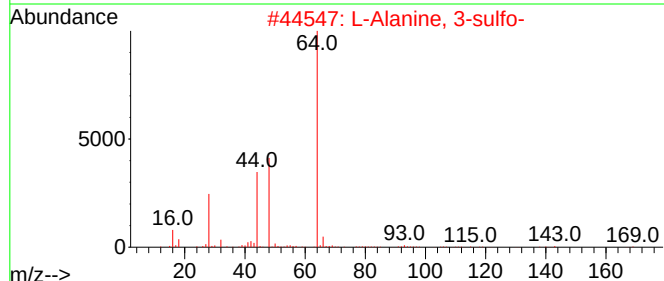
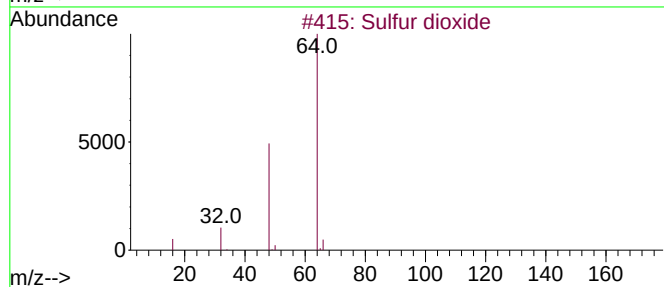
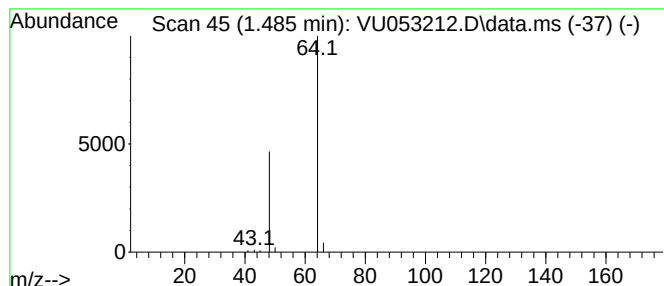
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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.
1.485	8.71 ug/L	64395	1,4-Difluorobenzene	6.244

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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	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	1.485	8.7	ug/L	64395	1	6.244	369699	50.0