

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053272.D
 Acq On : 17 Mar 2023 17:13
 Operator : JC/MD
 Sample : 01930-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFC1

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: VU053272.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	53	rBV	19081	32288	5.21%	0.713%
2	1.597	74	80	99	rVB	84409	96162	15.50%	2.123%
3	1.909	170	177	193	rVB	65637	89500	14.43%	1.976%
4	2.565	369	381	394	rBV	126434	203145	32.75%	4.484%
5	3.173	567	570	575	rBV3	332	327	0.05%	0.007%
6	3.218	581	584	587	rBV	239	121	0.02%	0.003%
7	3.588	696	699	702	rBV	224	132	0.02%	0.003%
8	3.832	773	775	777	rVB	144	37	0.01%	0.001%
9	3.899	793	796	801	rBV	190	107	0.02%	0.002%
10	4.125	863	866	872	rVB2	186	208	0.03%	0.005%
11	4.237	899	901	904	rBV	163	81	0.01%	0.002%
12	4.256	906	907	909	rVB	124	28	0.00%	0.001%
13	4.478	972	976	980	rBV2	197	193	0.03%	0.004%
14	4.555	998	1000	1005	rVB	203	124	0.02%	0.003%
15	4.613	1006	1018	1045	rBV	46162	110100	17.75%	2.430%
16	5.057	1140	1156	1181	rBV	113420	246139	39.68%	5.434%
17	5.182	1194	1195	1197	rVB	114	23	0.00%	0.001%
18	5.195	1197	1199	1202	rBV2	157	83	0.01%	0.002%
19	5.218	1205	1206	1207	rBV2	117	26	0.00%	0.001%
20	5.285	1224	1227	1230	rVB	262	176	0.03%	0.004%
21	5.530	1301	1303	1308	rBV	145	56	0.01%	0.001%
22	5.719	1341	1362	1386	rBV2	228013	620292	100.00%	13.693%
23	5.887	1412	1414	1418	rVB	163	77	0.01%	0.002%
24	5.951	1431	1434	1436	rBV	160	141	0.02%	0.003%
25	5.993	1445	1447	1451	rVB	185	94	0.02%	0.002%
26	6.015	1451	1454	1455	rBV	152	64	0.01%	0.001%
27	6.092	1473	1478	1481	rBV2	200	209	0.03%	0.005%
28	6.157	1495	1498	1500	rBV	246	156	0.03%	0.003%
29	6.243	1512	1525	1546	rBV	183843	344311	55.51%	7.601%
30	6.395	1569	1572	1576	rBV2	170	113	0.02%	0.002%
31	6.427	1581	1582	1583	rBV2	118	27	0.00%	0.001%
32	6.478	1595	1598	1603	rBV	213	140	0.02%	0.003%
33	6.523	1608	1612	1615	rBV2	189	111	0.02%	0.002%
34	6.536	1615	1616	1617	rVB2	113	22	0.00%	0.000%
35	6.684	1649	1662	1684	rVB	144511	280601	45.24%	6.194%
36	6.806	1697	1700	1701	rBV	405	224	0.04%	0.005%

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

37	7.153	1800	1808	1810	rBV	238	344	0.06%	0.008%
38	7.182	1813	1817	1818	rBV2	647	527	0.08%	0.012%
39	7.214	1825	1827	1830	rBV2	169	107	0.02%	0.002%
40	7.308	1854	1856	1857	rBV	108	61	0.01%	0.001%
41	7.330	1859	1863	1865	rBV	283	207	0.03%	0.005%
42	7.427	1891	1893	1894	rBV	146	80	0.01%	0.002%
43	7.452	1898	1901	1904	rVV	320	205	0.03%	0.005%
44	7.485	1908	1911	1913	rBV	185	93	0.01%	0.002%
45	7.562	1922	1935	1953	rBV2	80103	142120	22.91%	3.137%
46	7.690	1971	1975	1979	rBV3	657	647	0.10%	0.014%
47	7.774	1999	2001	2003	rBV	137	94	0.02%	0.002%
48	7.893	2025	2038	2065	rBV	284099	486524	78.43%	10.740%
49	8.073	2091	2094	2097	rVB	221	115	0.02%	0.003%
50	8.086	2097	2098	2099	rBV	119	31	0.00%	0.001%
51	8.176	2115	2126	2143	rBV	56577	92996	14.99%	2.053%
52	8.256	2149	2151	2157	rVB	174	92	0.01%	0.002%
53	8.279	2157	2158	2159	rBV	102	22	0.00%	0.000%
54	8.321	2168	2171	2173	rBV	128	113	0.02%	0.002%
55	8.375	2185	2188	2191	rBV2	218	161	0.03%	0.004%
56	8.546	2239	2241	2242	rBV2	135	39	0.01%	0.001%
57	8.626	2255	2266	2295	rBV2	138103	259977	41.91%	5.739%
58	8.851	2333	2336	2338	rBV	197	166	0.03%	0.004%
59	8.912	2354	2355	2356	rBV	228	73	0.01%	0.002%
60	8.925	2357	2359	2362	rVB2	217	144	0.02%	0.003%
61	9.025	2387	2390	2397	rVB	228	168	0.03%	0.004%
62	9.243	2456	2458	2459	rBV	115	29	0.00%	0.001%
63	9.414	2498	2511	2532	rBV	252520	415837	67.04%	9.180%
64	9.539	2547	2550	2552	rBV2	146	93	0.01%	0.002%
65	9.549	2552	2553	2554	rVV2	97	22	0.00%	0.000%
66	9.584	2562	2564	2565	rBV2	142	62	0.01%	0.001%
67	9.616	2571	2574	2576	rBV	174	148	0.02%	0.003%
68	9.758	2616	2618	2621	rBV	145	62	0.01%	0.001%
69	10.291	2781	2784	2788	rBV	194	127	0.02%	0.003%
70	10.391	2813	2815	2818	rVB	161	68	0.01%	0.002%
71	10.661	2897	2899	2901	rVB	199	80	0.01%	0.002%
72	10.751	2915	2927	2947	rBV	185754	296154	47.74%	6.538%
73	10.896	2969	2972	2975	rBV	185	106	0.02%	0.002%
74	11.111	3037	3039	3043	rVB	224	107	0.02%	0.002%
75	11.185	3060	3062	3063	rBV	123	47	0.01%	0.001%
76	11.336	3107	3109	3112	rBV	144	47	0.01%	0.001%

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77	11.472	3150	3151	3152	rBV	100	23	0.00%	0.001%
78	11.703	3217	3223	3226	rBV2	214	249	0.04%	0.005%
79	11.809	3243	3256	3274	rBV	248555	394150	63.54%	8.701%
80	11.912	3286	3288	3290	rBV	198	108	0.02%	0.002%
81	12.082	3336	3341	3342	rBV	361	319	0.05%	0.007%
82	12.189	3362	3374	3394	rBV	253300	408948	65.93%	9.028%
83	12.359	3425	3427	3429	rBV	192	108	0.02%	0.002%
84	12.603	3499	3503	3505	rBV2	229	173	0.03%	0.004%
85	12.851	3577	3580	3582	rBV	217	128	0.02%	0.003%
86	13.008	3624	3629	3632	rBV2	215	175	0.03%	0.004%
87	13.693	3839	3842	3844	rBV	205	127	0.02%	0.003%
88	14.031	3944	3947	3949	rBV	216	108	0.02%	0.002%
89	14.394	4058	4060	4061	rBV	234	104	0.02%	0.002%
90	14.725	4159	4163	4168	rVB3	340	291	0.05%	0.006%
91	14.822	4189	4193	4195	rBV	342	249	0.04%	0.005%
92	15.108	4280	4282	4284	rBV	287	141	0.02%	0.003%
93	15.179	4302	4304	4306	rBV	244	115	0.02%	0.003%
94	15.192	4306	4308	4310	rBV	175	106	0.02%	0.002%
95	15.568	4423	4425	4427	rBV2	259	130	0.02%	0.003%
96	15.693	4458	4464	4470	rBV2	339	499	0.08%	0.011%

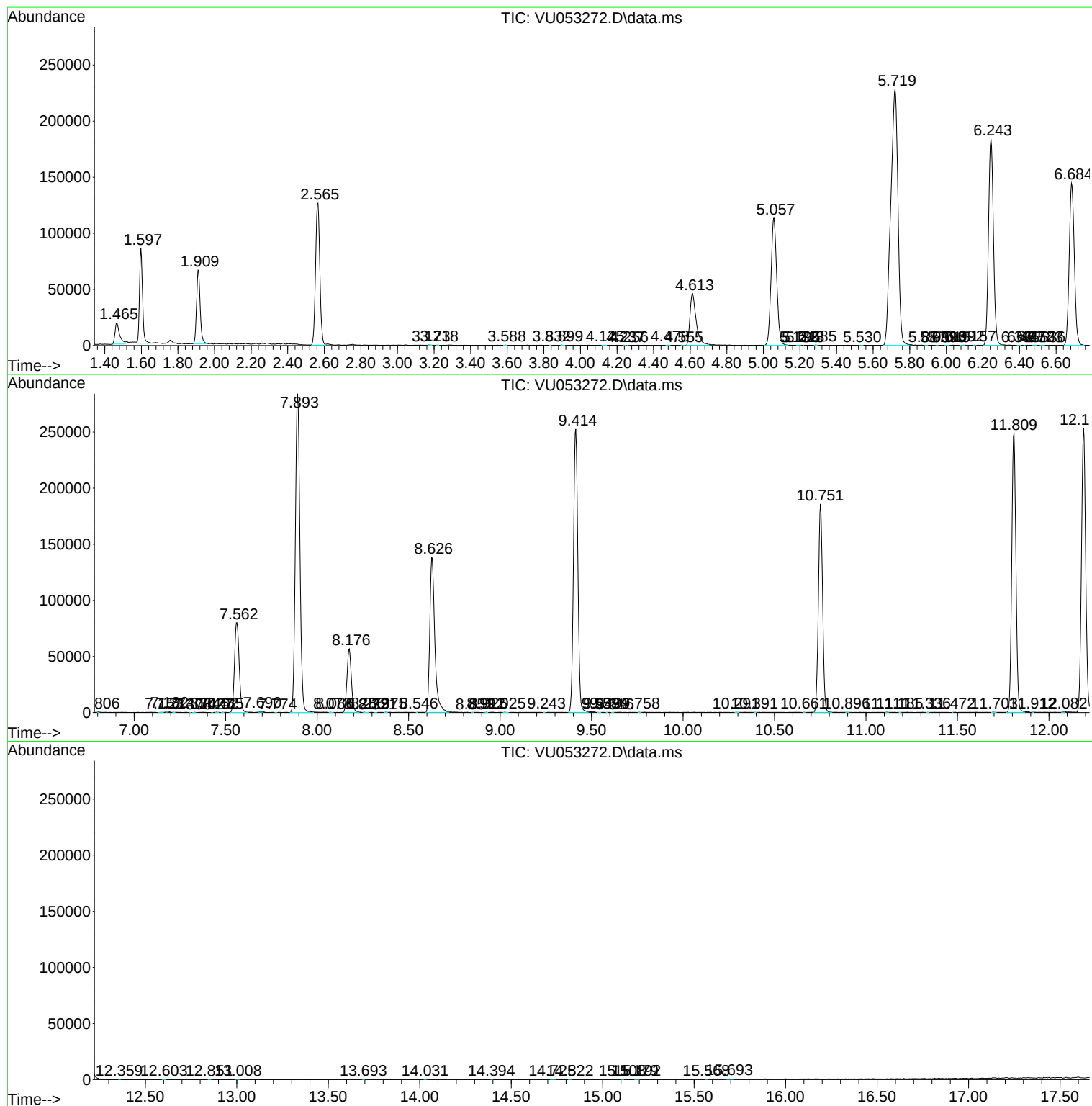
Sum of corrected areas: 4529984

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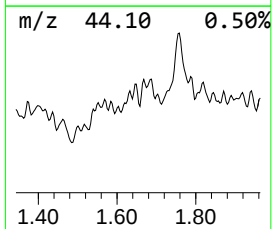
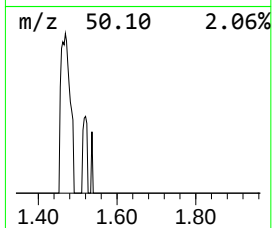
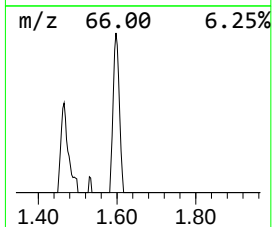
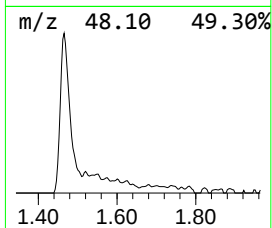
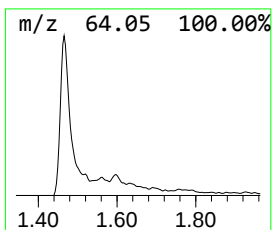
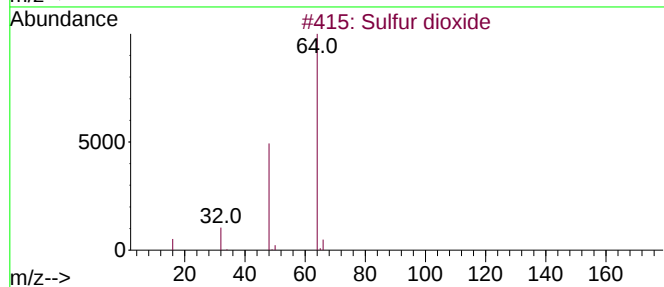
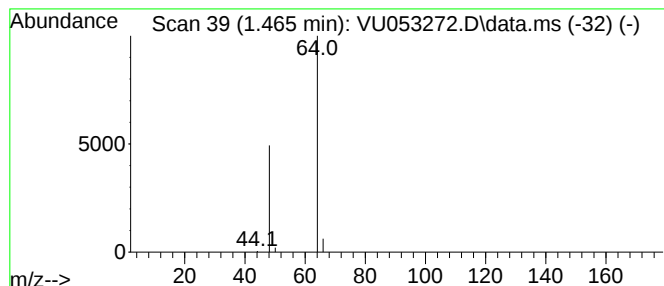
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	4.69 ug/L	32288	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
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	1.465	4.7	ug/L	32288	1	6.243	344311	50.0