

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
 Data File : VU045272.D
 Acq On : 09 Oct 2021 19:00
 Operator : SY/MD
 Sample : M4138-08DL 100X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F8DL

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045272.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	22482	45034	2.69%	0.358%
2	1.601	74	81	95	rVB	197903	213681	12.78%	1.699%
3	1.896	164	173	184	rBV	137267	186666	11.16%	1.484%
4	2.562	368	380	399	rBV	261551	446420	26.69%	3.550%
5	2.800	445	454	466	rVB3	988	2281	0.14%	0.018%
6	2.858	470	472	478	rVB2	360	307	0.02%	0.002%
7	2.941	494	498	499	rBV	248	183	0.01%	0.001%
8	2.957	499	503	505	rVV3	283	278	0.02%	0.002%
9	3.047	523	531	540	rBV3	3093	5618	0.34%	0.045%
10	3.128	552	556	559	rBV2	218	230	0.01%	0.002%
11	3.189	566	575	588	rBV3	1505	3262	0.20%	0.026%
12	3.266	595	599	601	rBV2	189	175	0.01%	0.001%
13	3.420	643	647	650	rBV	180	203	0.01%	0.002%
14	3.568	689	693	698	rVB2	223	205	0.01%	0.002%
15	3.703	732	735	740	rVB2	265	214	0.01%	0.002%
16	3.752	745	750	753	rBV2	189	170	0.01%	0.001%
17	3.790	759	762	765	rBV	202	173	0.01%	0.001%
18	3.871	778	787	796	rBV2	799	1442	0.09%	0.011%
19	4.105	858	860	866	rBV	140	172	0.01%	0.001%
20	4.202	887	890	893	rVB2	222	175	0.01%	0.001%
21	4.279	910	914	920	rVB2	264	303	0.02%	0.002%
22	4.408	950	954	958	rBV	178	206	0.01%	0.002%
23	4.626	1007	1022	1052	rBV	146957	347362	20.77%	2.762%
24	4.896	1102	1106	1108	rBV2	199	190	0.01%	0.002%
25	4.996	1132	1137	1142	rVV4	1052	1634	0.10%	0.013%
26	5.067	1143	1159	1187	rVB	225204	491890	29.41%	3.911%
27	5.295	1223	1230	1238	rVB3	676	1158	0.07%	0.009%
28	5.385	1251	1258	1262	rVV3	383	422	0.03%	0.003%
29	5.588	1316	1321	1324	rBV2	251	286	0.02%	0.002%
30	5.633	1331	1335	1339	rVB2	263	262	0.02%	0.002%
31	5.729	1343	1365	1389	rBV2	483027	1292210	77.26%	10.275%
32	6.121	1480	1487	1490	rBV2	306	428	0.03%	0.003%
33	6.253	1513	1528	1546	rBV	352934	661971	39.58%	5.264%
34	6.462	1585	1593	1595	rBV3	179	276	0.02%	0.002%
35	6.526	1607	1613	1623	rVB4	1737	2982	0.18%	0.024%
36	6.571	1623	1627	1630	rBV	276	223	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
 Data File : VU045272.D
 Acq On : 09 Oct 2021 19:00
 Operator : SY/MD
 Sample : M4138-08DL 100X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F8DL

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\SFAMULM092321WMA.M
 Title : VOC Analysis

37	6.694	1650	1665	1684	rBV	303174	586419	35.06%	4.663%
38	7.044	1769	1774	1775	rBV	368	293	0.02%	0.002%
39	7.176	1810	1815	1817	rBV3	930	791	0.05%	0.006%
40	7.282	1842	1848	1852	rVB2	208	286	0.02%	0.002%
41	7.308	1852	1856	1860	rBV2	177	222	0.01%	0.002%
42	7.333	1860	1864	1869	rVB2	193	202	0.01%	0.002%
43	7.356	1869	1871	1876	rBV2	195	181	0.01%	0.001%
44	7.388	1876	1881	1888	rVV2	183	276	0.02%	0.002%
45	7.568	1924	1937	1956	rBV	148431	255148	15.26%	2.029%
46	7.687	1970	1974	1984	rVB3	803	1200	0.07%	0.010%
47	7.735	1984	1989	1995	rBV2	199	250	0.01%	0.002%
48	7.796	2001	2008	2015	rBV4	1299	1514	0.09%	0.012%
49	7.903	2027	2041	2053	rBV	588609	992467	59.34%	7.892%
50	7.973	2053	2063	2083	rVB	127276	213551	12.77%	1.698%
51	8.182	2115	2128	2143	rBV	106202	173126	10.35%	1.377%
52	8.636	2256	2269	2313	rBV	428674	757887	45.31%	6.026%
53	8.922	2352	2358	2359	rBV	235	240	0.01%	0.002%
54	9.137	2418	2425	2430	rBV2	197	317	0.02%	0.003%
55	9.420	2499	2513	2534	rBV	509458	833451	49.83%	6.627%
56	9.574	2548	2561	2576	rBV	345415	544240	32.54%	4.328%
57	9.693	2585	2598	2629	rVB	1021522	1672515	100.00%	13.299%
58	10.105	2713	2726	2739	rBV	298584	476945	28.52%	3.792%
59	10.414	2816	2822	2824	rBV2	177	220	0.01%	0.002%
60	10.488	2836	2845	2855	rBV2	6690	9566	0.57%	0.076%
61	10.603	2877	2881	2887	rVB2	205	219	0.01%	0.002%
62	10.642	2887	2893	2894	rBV	298	222	0.01%	0.002%
63	10.674	2896	2903	2910	rVV3	1638	2177	0.13%	0.017%
64	10.761	2916	2930	2951	rVB	426964	684223	40.91%	5.441%
65	10.909	2968	2976	2985	rVB2	2287	3523	0.21%	0.028%
66	10.957	2985	2991	2994	rBV2	176	199	0.01%	0.002%
67	11.002	2997	3005	3011	rBV	7438	11411	0.68%	0.091%
68	11.089	3024	3032	3044	rVB3	3105	4890	0.29%	0.039%
69	11.179	3057	3060	3065	rVB2	309	293	0.02%	0.002%
70	11.234	3074	3077	3080	rVB2	308	188	0.01%	0.001%
71	11.295	3088	3096	3105	rVB2	3614	4787	0.29%	0.038%
72	11.468	3141	3150	3163	rVB2	14451	21575	1.29%	0.172%
73	11.539	3169	3172	3178	rVB2	204	194	0.01%	0.002%
74	11.581	3182	3185	3188	rVB	357	252	0.02%	0.002%
75	11.645	3199	3205	3206	rBV2	181	201	0.01%	0.002%
76	11.700	3219	3222	3225	rVB	457	282	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
 Data File : VU045272.D
 Acq On : 09 Oct 2021 19:00
 Operator : SY/MD
 Sample : M4138-08DL 100X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F8DL

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\SFAMULM092321WMA.M
 Title : VOC Analysis

77	11.748	3234	3237	3239	rBV	381	232	0.01%	0.002%
78	11.816	3245	3258	3274	rBV	474607	744594	44.52%	5.921%
79	11.896	3276	3283	3292	rVV	4965	7117	0.43%	0.057%
80	11.951	3296	3300	3301	rVV2	391	319	0.02%	0.003%
81	11.973	3303	3307	3316	rVB4	1409	1835	0.11%	0.015%
82	12.095	3339	3345	3354	rVB2	1774	2678	0.16%	0.021%
83	12.195	3363	3376	3394	rBV	519141	845007	50.52%	6.719%
84	12.603	3500	3503	3506	rBV	343	291	0.02%	0.002%
85	13.008	3625	3629	3631	rBV2	294	254	0.02%	0.002%
86	13.224	3692	3696	3699	rBV2	379	326	0.02%	0.003%
87	13.349	3732	3735	3738	rBV2	211	201	0.01%	0.002%
88	13.407	3748	3753	3756	rBV2	281	262	0.02%	0.002%
89	13.504	3779	3783	3787	rBV2	228	246	0.01%	0.002%
90	13.687	3837	3840	3842	rBV	254	186	0.01%	0.001%
91	13.915	3907	3911	3914	rBV	308	310	0.02%	0.002%
92	14.095	3956	3967	3977	rBV	2885	4332	0.26%	0.034%
93	14.301	4027	4031	4032	rBV	337	223	0.01%	0.002%
94	14.333	4037	4041	4048	rVB4	503	849	0.05%	0.007%
95	14.552	4103	4109	4112	rBV2	335	445	0.03%	0.004%
96	14.584	4116	4119	4126	rVB2	454	474	0.03%	0.004%
97	14.725	4160	4163	4166	rBV	257	211	0.01%	0.002%
98	14.899	4211	4217	4221	rBV3	328	432	0.03%	0.003%
99	14.983	4240	4243	4249	rVB3	429	475	0.03%	0.004%
100	15.237	4319	4322	4326	rBV2	304	279	0.02%	0.002%

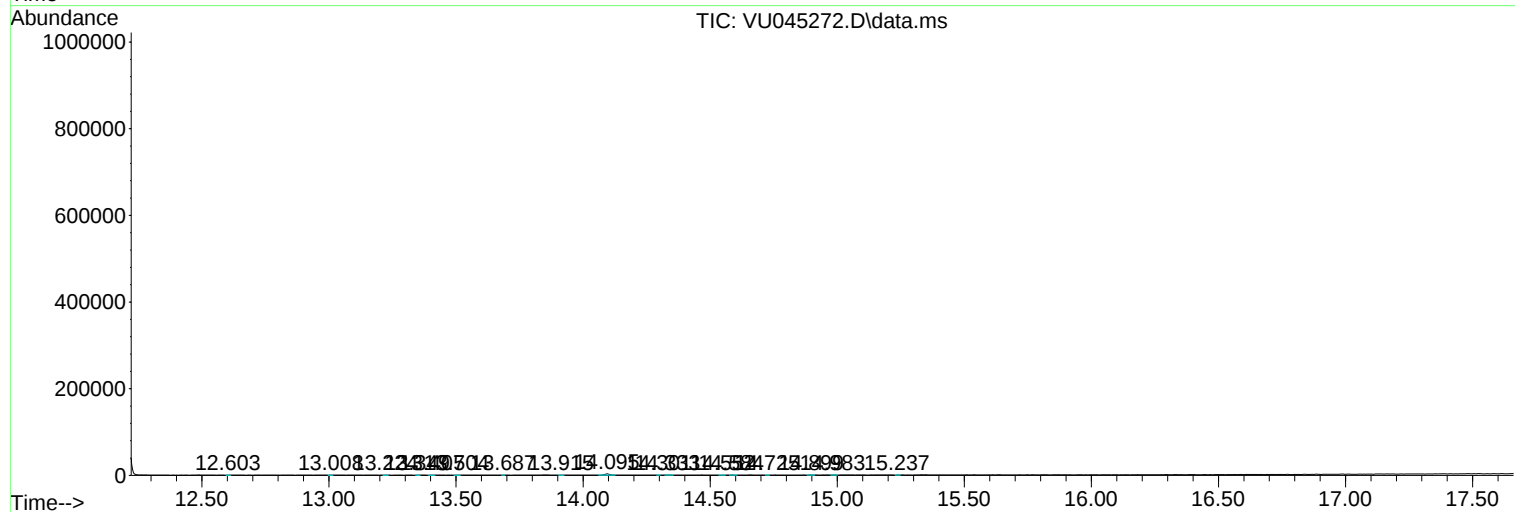
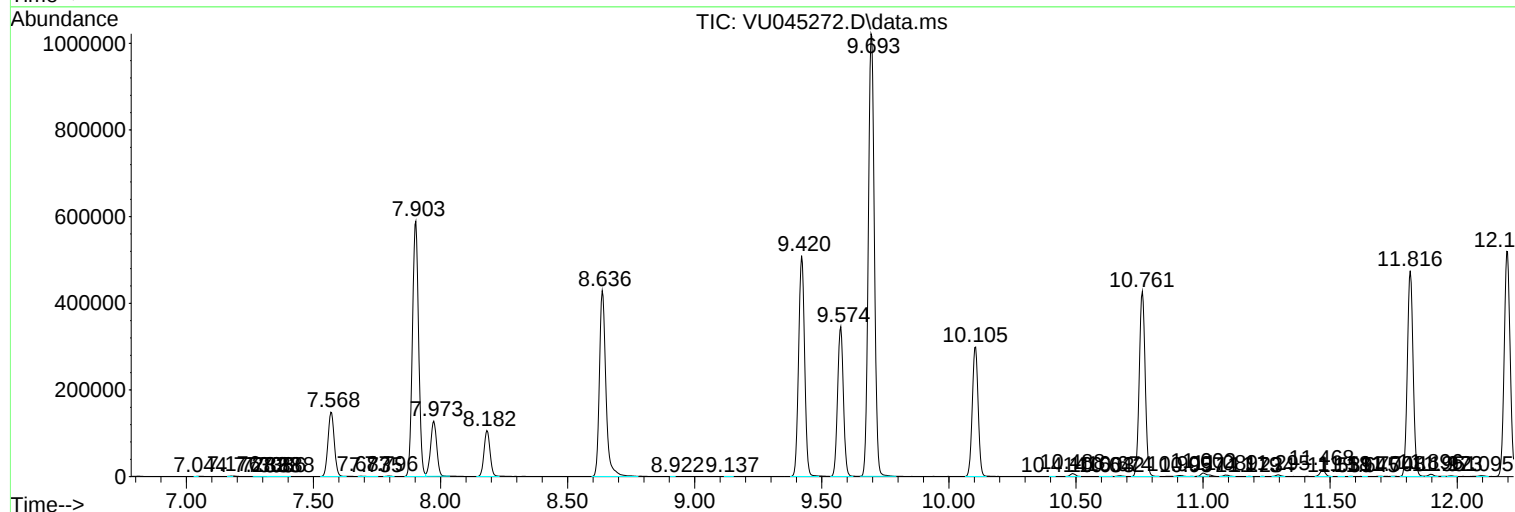
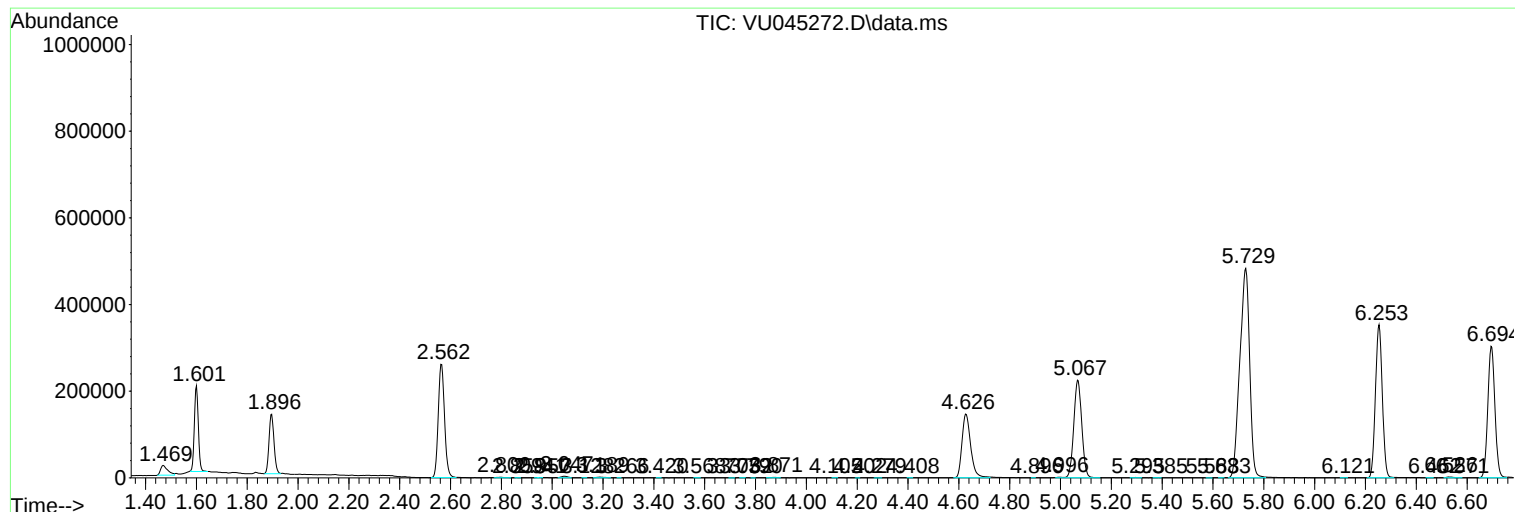
Sum of corrected areas: 12576213

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
Data File : VU045272.D
Acq On : 09 Oct 2021 19:00
Operator : SY/MD
Sample : M4138-08DL 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
Data File : VU045272.D
Acq On : 09 Oct 2021 19:00
Operator : SY/MD
Sample : M4138-08DL 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F8DL

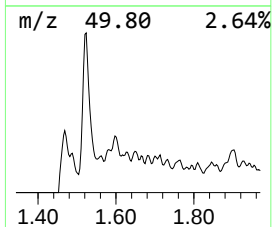
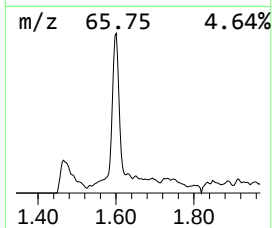
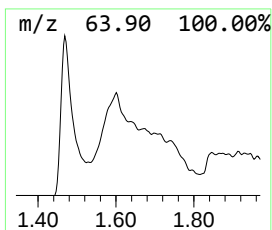
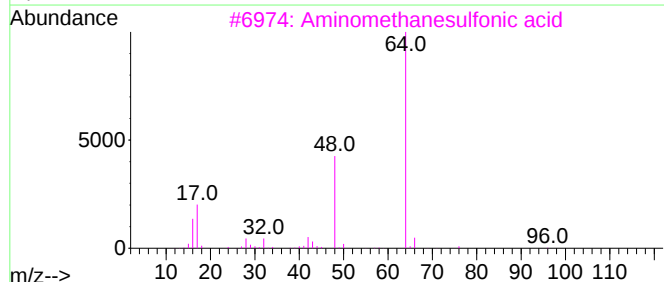
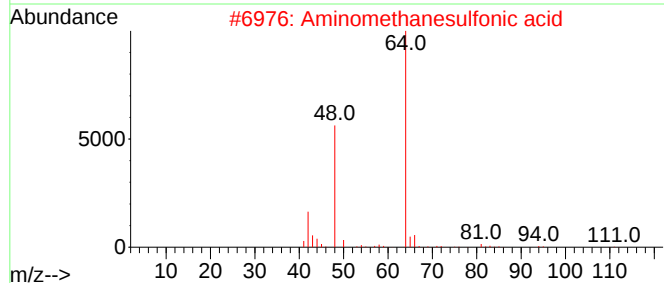
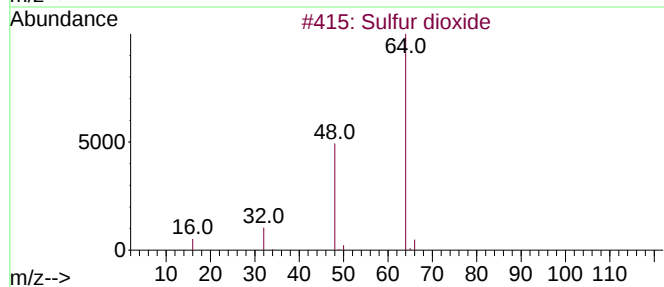
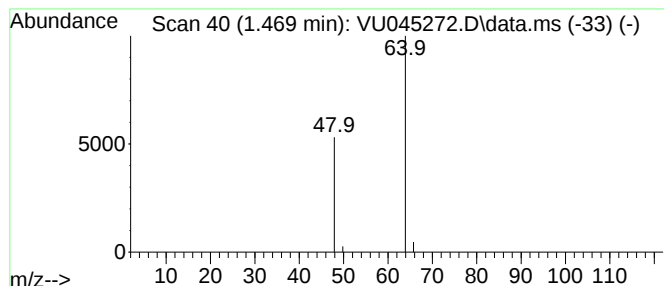
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.469	3.40 ug/L	45034	1,4-Difluorobenzene	6.253

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100921\
Data File : VU045272.D
Acq On : 09 Oct 2021 19:00
Operator : SY/MD
Sample : M4138-08DL 100X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	1.469	3.4	ug/L	45034	1	6.253	661971	50.0