

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045228.D
 Acq On : 07 Oct 2021 23:28
 Operator : SY/MD
 Sample : M4138-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F6

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: VU045228.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	30	39	54	rBV	302964	488101	37.59%	4.463%
2	1.597	76	80	123	rVB	218068	341306	26.29%	3.121%
3	1.896	166	173	185	rVB	133768	179363	13.81%	1.640%
4	2.562	367	380	397	rBV	253677	427241	32.91%	3.906%
5	2.703	421	424	429	rBV3	251	227	0.02%	0.002%
6	2.781	439	448	459	rVV4	2722	5727	0.44%	0.052%
7	2.855	467	471	476	rBV2	213	266	0.02%	0.002%
8	2.951	496	501	503	rBV2	356	369	0.03%	0.003%
9	3.044	527	530	535	rVB3	682	621	0.05%	0.006%
10	3.144	556	561	565	rBV2	281	336	0.03%	0.003%
11	3.189	568	575	585	rVB3	1398	2619	0.20%	0.024%
12	3.498	666	671	675	rBV2	244	241	0.02%	0.002%
13	3.736	741	745	750	rBV2	231	312	0.02%	0.003%
14	3.842	771	778	781	rBV2	178	230	0.02%	0.002%
15	3.912	797	800	804	rBV2	148	171	0.01%	0.002%
16	3.954	811	813	818	rVB2	199	164	0.01%	0.001%
17	4.060	840	846	852	rBV	189	166	0.01%	0.002%
18	4.108	857	861	865	rVB	262	210	0.02%	0.002%
19	4.629	1008	1023	1050	rBV	145236	341357	26.29%	3.121%
20	4.954	1122	1124	1131	rVB3	310	327	0.03%	0.003%
21	4.986	1131	1134	1137	rBV	338	240	0.02%	0.002%
22	5.067	1143	1159	1178	rVV	227199	492310	37.92%	4.501%
23	5.234	1208	1211	1217	rBV3	210	226	0.02%	0.002%
24	5.285	1223	1227	1228	rBV2	436	277	0.02%	0.003%
25	5.334	1238	1242	1245	rVB2	222	210	0.02%	0.002%
26	5.350	1245	1247	1251	rBV	210	194	0.01%	0.002%
27	5.375	1252	1255	1261	rVB3	316	335	0.03%	0.003%
28	5.417	1265	1268	1273	rVB2	229	216	0.02%	0.002%
29	5.452	1273	1279	1281	rBV	253	223	0.02%	0.002%
30	5.497	1285	1293	1297	rBV	179	226	0.02%	0.002%
31	5.729	1342	1365	1399	rBV2	482157	1298362	100.00%	11.871%
32	6.044	1460	1463	1467	rBV3	302	221	0.02%	0.002%
33	6.115	1481	1485	1490	rBV3	400	374	0.03%	0.003%
34	6.166	1497	1501	1505	rVB3	176	178	0.01%	0.002%
35	6.253	1512	1528	1552	rBV	376533	706656	54.43%	6.461%
36	6.359	1555	1561	1564	rBV3	324	372	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045228.D
 Acq On : 07 Oct 2021 23:28
 Operator : SY/MD
 Sample : M4138-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F6

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	6.530	1609	1614	1626	rVB7	1610	2472	0.19%	0.023%
38	6.694	1651	1665	1688	rBV	304872	595436	45.86%	5.444%
39	6.806	1695	1700	1703	rBV4	373	419	0.03%	0.004%
40	6.877	1717	1722	1724	rBV2	243	160	0.01%	0.001%
41	7.044	1769	1774	1777	rBV2	330	381	0.03%	0.003%
42	7.115	1793	1796	1801	rBV2	142	159	0.01%	0.001%
43	7.182	1809	1817	1828	rVB5	1390	2071	0.16%	0.019%
44	7.391	1879	1882	1885	rVB2	228	189	0.01%	0.002%
45	7.430	1889	1894	1897	rVV2	177	184	0.01%	0.002%
46	7.568	1923	1937	1955	rVV	164494	284230	21.89%	2.599%
47	7.674	1964	1970	1971	rBV2	590	403	0.03%	0.004%
48	7.800	2003	2009	2016	rVB3	388	577	0.04%	0.005%
49	7.903	2027	2041	2054	rBV	585197	992588	76.45%	9.075%
50	7.973	2055	2063	2075	rVB	24748	41953	3.23%	0.384%
51	8.182	2116	2128	2148	rBV	116345	190587	14.68%	1.743%
52	8.378	2186	2189	2194	rVB2	285	214	0.02%	0.002%
53	8.475	2209	2219	2228	rBV3	988	1942	0.15%	0.018%
54	8.565	2244	2247	2250	rVB	206	163	0.01%	0.001%
55	8.636	2256	2269	2300	rBV	434448	756083	58.23%	6.913%
56	8.951	2364	2367	2375	rVB	140	178	0.01%	0.002%
57	9.420	2499	2513	2533	rBV	532948	860885	66.31%	7.871%
58	9.575	2548	2561	2580	rBV	72542	117163	9.02%	1.071%
59	9.697	2587	2599	2625	rVB	222551	367901	28.34%	3.364%
60	9.854	2646	2648	2653	rVB	247	176	0.01%	0.002%
61	9.886	2654	2658	2662	rVB2	208	181	0.01%	0.002%
62	10.105	2714	2726	2747	rBV	60115	97664	7.52%	0.893%
63	10.250	2767	2771	2776	rBV	216	249	0.02%	0.002%
64	10.343	2797	2800	2803	rBV	183	167	0.01%	0.002%
65	10.491	2837	2846	2854	rBV3	1717	2484	0.19%	0.023%
66	10.674	2895	2903	2910	rVB4	2106	2704	0.21%	0.025%
67	10.761	2917	2930	2950	rBV	435513	692446	53.33%	6.331%
68	10.854	2954	2959	2960	rBV2	199	162	0.01%	0.001%
69	10.909	2968	2976	2980	rBV4	1281	1509	0.12%	0.014%
70	11.005	2996	3006	3011	rBV3	2893	4485	0.35%	0.041%
71	11.092	3025	3033	3039	rBV3	1134	1635	0.13%	0.015%
72	11.211	3066	3070	3073	rVB2	192	162	0.01%	0.001%
73	11.234	3073	3077	3080	rBV3	619	489	0.04%	0.004%
74	11.295	3089	3096	3097	rBV3	1350	1206	0.09%	0.011%
75	11.468	3139	3150	3165	rVB3	7220	11830	0.91%	0.108%
76	11.574	3179	3183	3185	rBV	336	250	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045228.D
 Acq On : 07 Oct 2021 23:28
 Operator : SY/MD
 Sample : M4138-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F6

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	11.619	3193	3197	3206	rBV3	425	622	0.05%	0.006%
78	11.700	3215	3222	3228	rVB4	1036	1315	0.10%	0.012%
79	11.751	3236	3238	3242	rBV2	205	178	0.01%	0.002%
80	11.816	3245	3258	3276	rVV	462037	732287	56.40%	6.695%
81	11.899	3279	3284	3292	rVV4	2758	3187	0.25%	0.029%
82	11.941	3294	3297	3302	rVV3	992	1062	0.08%	0.010%
83	11.976	3302	3308	3318	rVB4	1659	2357	0.18%	0.022%
84	12.018	3318	3321	3324	rBV2	218	205	0.02%	0.002%
85	12.066	3329	3336	3343	rBV3	3257	4895	0.38%	0.045%
86	12.147	3357	3361	3362	rBV2	396	225	0.02%	0.002%
87	12.195	3363	3376	3395	rVB	502316	811600	62.51%	7.420%
88	12.356	3423	3426	3427	rBV	244	170	0.01%	0.002%
89	12.365	3427	3429	3432	rVB2	446	258	0.02%	0.002%
90	12.513	3456	3475	3493	rBV5	12371	28554	2.20%	0.261%
91	12.635	3507	3513	3514	rBV2	413	405	0.03%	0.004%
92	12.822	3557	3571	3584	rVB5	5340	11212	0.86%	0.103%
93	12.954	3606	3612	3616	rBV3	438	565	0.04%	0.005%
94	13.015	3625	3631	3642	rVB5	1216	2585	0.20%	0.024%
95	13.076	3646	3650	3653	rBV2	332	317	0.02%	0.003%
96	13.115	3658	3662	3665	rBV	169	183	0.01%	0.002%
97	14.092	3956	3966	3979	rBV2	6260	10162	0.78%	0.093%
98	14.629	4130	4133	4137	rBV2	395	382	0.03%	0.003%
99	14.777	4177	4179	4182	rBV	231	182	0.01%	0.002%
100	14.947	4229	4232	4235	rBV2	373	306	0.02%	0.003%

Sum of corrected areas: 10937325

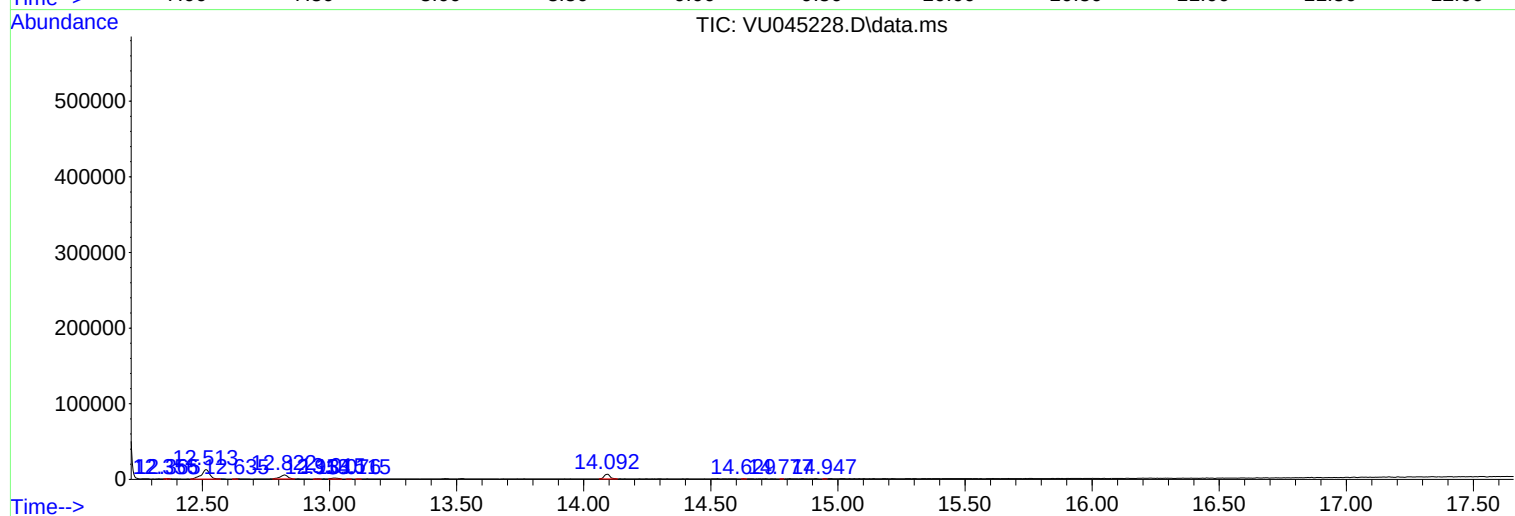
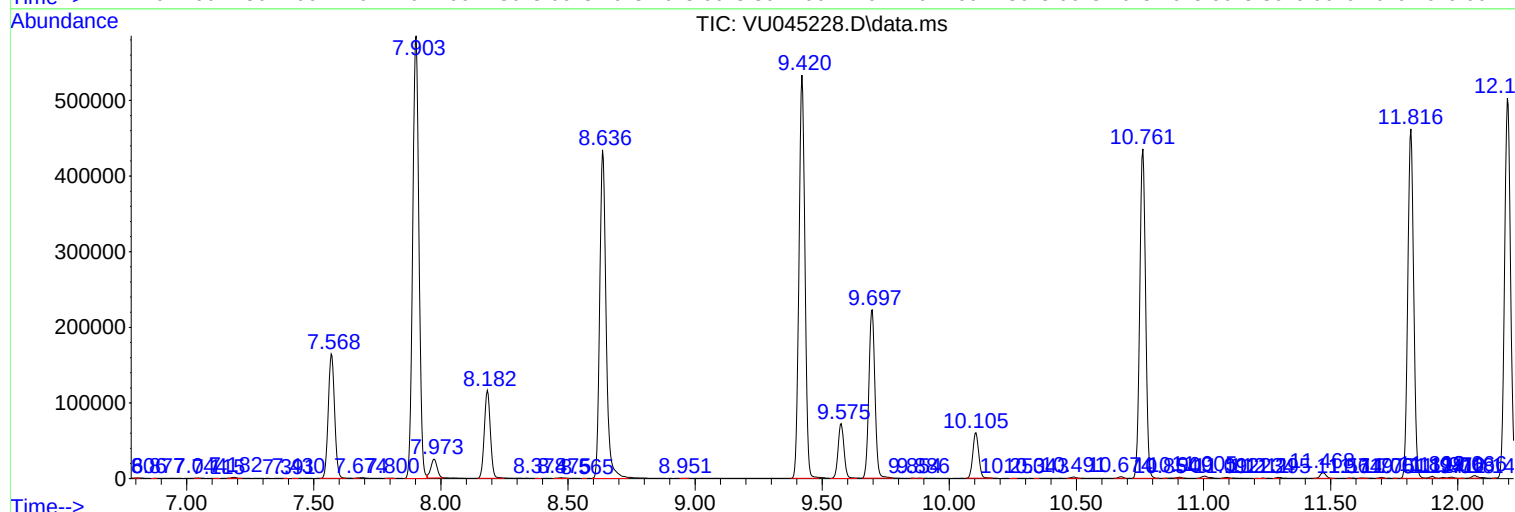
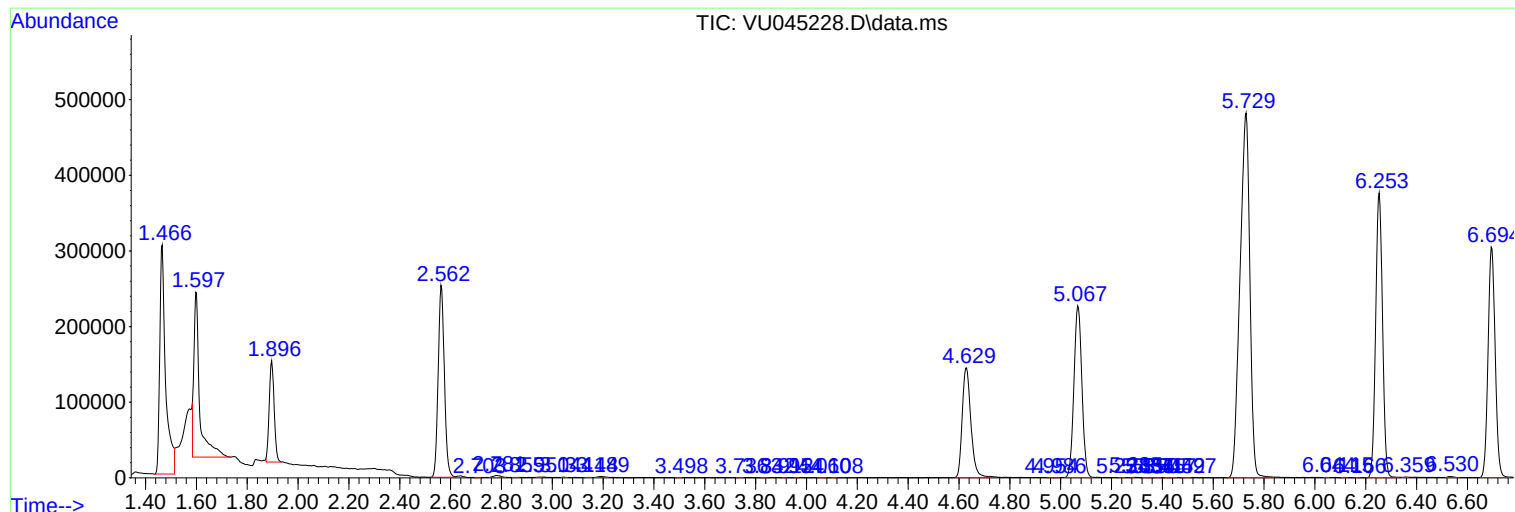
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045228.D
Acq On : 07 Oct 2021 23:28
Operator : SY/MD
Sample : M4138-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F6

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\VU100721\
Data File : VU045228.D
Acq On : 07 Oct 2021 23:28
Operator : SY/MD
Sample : M4138-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F6

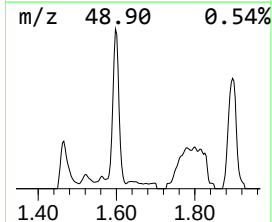
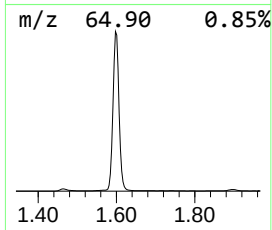
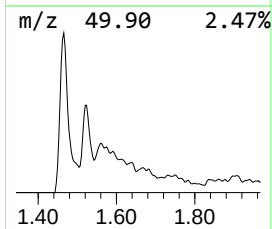
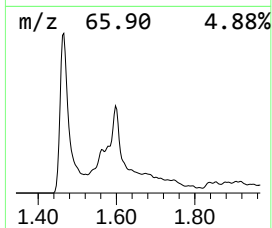
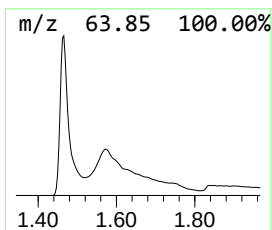
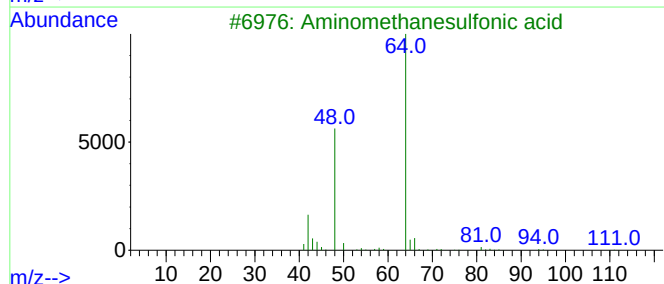
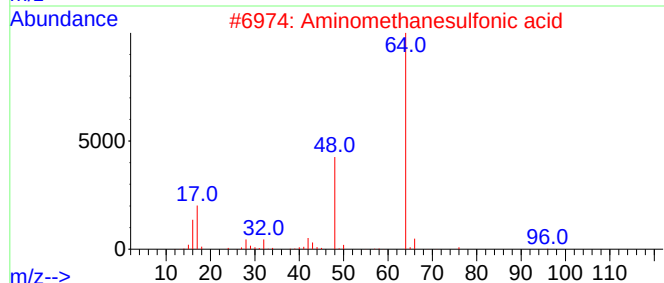
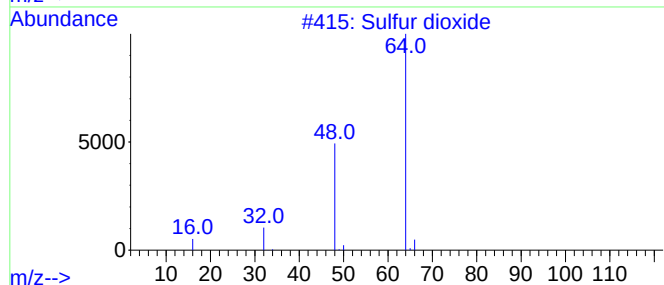
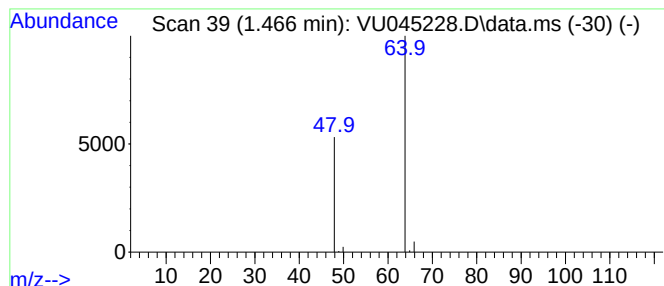
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	34.54 ug/L	488101	1,4-Difluorobenzene	6.253

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			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\VU100721\
Data File : VU045228.D
Acq On : 07 Oct 2021 23:28
Operator : SY/MD
Sample : M4138-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F6

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	1.466	34.5	ug/L	488101	1	6.253	706656	50.0