

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049290.D
 Acq On : 18 Jun 2022 18:45
 Operator : SY/MD
 Sample : N3395-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0153

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\SFAMULM061022WMA.M

Title : VOC Analysis

Signal : TIC: VU049290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	34	43	58	rBV	18261	45820	4.44%	0.512%
2	1.597	74	80	96	rVB	128714	144761	14.04%	1.619%
3	1.912	170	178	195	rVB	99820	128017	12.41%	1.432%
4	2.568	369	382	395	rBV	200424	323778	31.40%	3.621%
5	2.758	431	441	446	rBV	1030	1865	0.18%	0.021%
6	2.781	446	448	450	rBV2	395	273	0.03%	0.003%
7	2.851	468	470	474	rBV3	310	270	0.03%	0.003%
8	2.893	480	483	489	rVB2	406	334	0.03%	0.004%
9	2.929	489	494	498	rBV2	223	232	0.02%	0.003%
10	3.038	522	528	529	rBV3	447	374	0.04%	0.004%
11	3.273	599	601	605	rVB	301	245	0.02%	0.003%
12	3.302	605	610	613	rBV2	471	421	0.04%	0.005%
13	3.356	621	627	632	rBV3	185	261	0.03%	0.003%
14	3.543	682	685	690	rVB	310	280	0.03%	0.003%
15	3.572	690	694	702	rBV3	360	473	0.05%	0.005%
16	3.996	823	826	831	rBV2	316	342	0.03%	0.004%
17	4.054	841	844	847	rVV	315	227	0.02%	0.003%
18	4.131	864	868	870	rBV2	299	238	0.02%	0.003%
19	4.199	886	889	893	rVB2	441	366	0.04%	0.004%
20	4.224	893	897	900	rBV	327	315	0.03%	0.004%
21	4.343	927	934	937	rBV3	215	311	0.03%	0.003%
22	4.398	946	951	954	rBV3	275	231	0.02%	0.003%
23	4.520	987	989	993	rVB2	367	229	0.02%	0.003%
24	4.620	1006	1020	1047	rBV	127224	310925	30.15%	3.477%
25	4.941	1116	1120	1123	rBV2	251	207	0.02%	0.002%
26	5.063	1141	1158	1179	rBV	189895	414861	40.23%	4.639%
27	5.372	1238	1254	1281	rBV	232998	481303	46.68%	5.382%
28	5.546	1304	1308	1312	rVB2	286	233	0.02%	0.003%
29	5.575	1312	1317	1320	rBV3	273	267	0.03%	0.003%
30	5.726	1338	1364	1391	rBV2	379736	1031161	100.00%	11.531%
31	5.970	1436	1440	1442	rBV3	320	209	0.02%	0.002%
32	6.015	1449	1454	1457	rVB3	317	218	0.02%	0.002%
33	6.038	1457	1461	1464	rBV3	388	289	0.03%	0.003%
34	6.063	1464	1469	1473	rVB3	305	259	0.03%	0.003%
35	6.195	1499	1510	1512	rBV3	410	536	0.05%	0.006%
36	6.250	1512	1527	1556	rVV	350725	677691	65.72%	7.578%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049290.D
 Acq On : 18 Jun 2022 18:45
 Operator : SY/MD
 Sample : N3395-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0153

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\SFAMULM061022WMA.M
 Title : VOC Analysis

37	6.449	1586	1589	1594	rBV3	371	323	0.03%	0.004%
38	6.539	1606	1617	1630	rBV7	2593	5444	0.53%	0.061%
39	6.690	1649	1664	1687	rBV	254789	493396	47.85%	5.517%
40	6.800	1694	1698	1699	rBV2	433	227	0.02%	0.003%
41	6.957	1745	1747	1752	rVB2	320	228	0.02%	0.003%
42	7.128	1797	1800	1804	rBV2	294	253	0.02%	0.003%
43	7.189	1811	1819	1832	rVB3	1624	2916	0.28%	0.033%
44	7.362	1869	1873	1876	rBV2	387	312	0.03%	0.003%
45	7.452	1893	1901	1905	rVB2	426	607	0.06%	0.007%
46	7.475	1905	1908	1910	rBV	362	251	0.02%	0.003%
47	7.504	1914	1917	1921	rVB2	346	238	0.02%	0.003%
48	7.565	1921	1936	1954	rBV	137104	241123	23.38%	2.696%
49	7.694	1968	1976	1985	rVB7	1104	2101	0.20%	0.023%
50	7.735	1986	1989	1993	rBV3	285	237	0.02%	0.003%
51	7.793	2001	2007	2008	rBV2	420	422	0.04%	0.005%
52	7.896	2026	2039	2059	rBV	469421	820832	79.60%	9.179%
53	8.057	2086	2089	2096	rVB4	647	502	0.05%	0.006%
54	8.121	2106	2109	2112	rVB2	398	238	0.02%	0.003%
55	8.179	2115	2127	2150	rBV	91463	158577	15.38%	1.773%
56	8.279	2157	2158	2163	rVB2	368	233	0.02%	0.003%
57	8.305	2163	2166	2172	rBV4	568	478	0.05%	0.005%
58	8.475	2214	2219	2222	rVB3	514	380	0.04%	0.004%
59	8.562	2242	2246	2249	rBV3	384	230	0.02%	0.003%
60	8.632	2256	2268	2305	rBV	360586	692967	67.20%	7.749%
61	8.864	2338	2340	2347	rVB2	279	207	0.02%	0.002%
62	8.983	2373	2377	2381	rBV3	221	230	0.02%	0.003%
63	9.202	2442	2445	2449	rBV2	315	234	0.02%	0.003%
64	9.266	2461	2465	2468	rVB2	338	239	0.02%	0.003%
65	9.337	2482	2487	2490	rBV	376	339	0.03%	0.004%
66	9.417	2499	2512	2533	rBV	500195	822353	79.75%	9.196%
67	9.571	2554	2560	2565	rVB4	512	590	0.06%	0.007%
68	9.661	2583	2588	2591	rVV3	670	620	0.06%	0.007%
69	9.694	2594	2598	2605	rVB4	999	1362	0.13%	0.015%
70	9.800	2629	2631	2636	rVB2	268	248	0.02%	0.003%
71	9.870	2648	2653	2656	rBV2	263	324	0.03%	0.004%
72	10.025	2695	2701	2704	rBV2	209	287	0.03%	0.003%
73	10.095	2718	2723	2726	rVB4	549	520	0.05%	0.006%
74	10.121	2726	2731	2736	rVB2	282	356	0.03%	0.004%
75	10.153	2736	2741	2744	rBV3	285	336	0.03%	0.004%
76	10.179	2746	2749	2756	rVB2	456	544	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049290.D
 Acq On : 18 Jun 2022 18:45
 Operator : SY/MD
 Sample : N3395-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0153

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\SFAMULM061022WMA.M
 Title : VOC Analysis

77	10.269	2773	2777	2783	rVB2	426	407	0.04%	0.005%
78	10.314	2787	2791	2794	rVB3	279	216	0.02%	0.002%
79	10.369	2799	2808	2809	rBV	372	443	0.04%	0.005%
80	10.755	2915	2928	2951	rVV	350634	578598	56.11%	6.470%
81	10.890	2963	2970	2979	rBV3	921	1627	0.16%	0.018%
82	11.092	3031	3033	3038	rVB4	325	247	0.02%	0.003%
83	11.401	3125	3129	3131	rBV2	294	251	0.02%	0.003%
84	11.430	3135	3138	3142	rVV3	267	220	0.02%	0.002%
85	11.581	3181	3185	3188	rBV2	328	349	0.03%	0.004%
86	11.812	3244	3257	3277	rBV	485908	772612	74.93%	8.640%
87	12.192	3362	3375	3394	rBV	467586	763887	74.08%	8.542%
88	12.697	3526	3532	3536	rBV2	345	423	0.04%	0.005%
89	12.722	3537	3540	3543	rBV2	246	216	0.02%	0.002%
90	12.780	3554	3558	3562	rBV3	651	622	0.06%	0.007%
91	13.246	3700	3703	3709	rVB3	333	272	0.03%	0.003%
92	13.436	3757	3762	3767	rBV2	467	590	0.06%	0.007%
93	13.700	3839	3844	3847	rVB2	423	331	0.03%	0.004%
94	14.102	3966	3969	3974	rBV2	518	483	0.05%	0.005%
95	14.333	4038	4041	4042	rBV	410	199	0.02%	0.002%
96	14.520	4096	4099	4101	rBV	291	210	0.02%	0.002%
97	14.697	4151	4154	4158	rBV3	205	200	0.02%	0.002%
98	14.825	4191	4194	4199	rVB3	306	226	0.02%	0.003%
99	15.590	4430	4432	4434	rBV	416	247	0.02%	0.003%
100	16.494	4711	4713	4716	rBV3	833	544	0.05%	0.006%

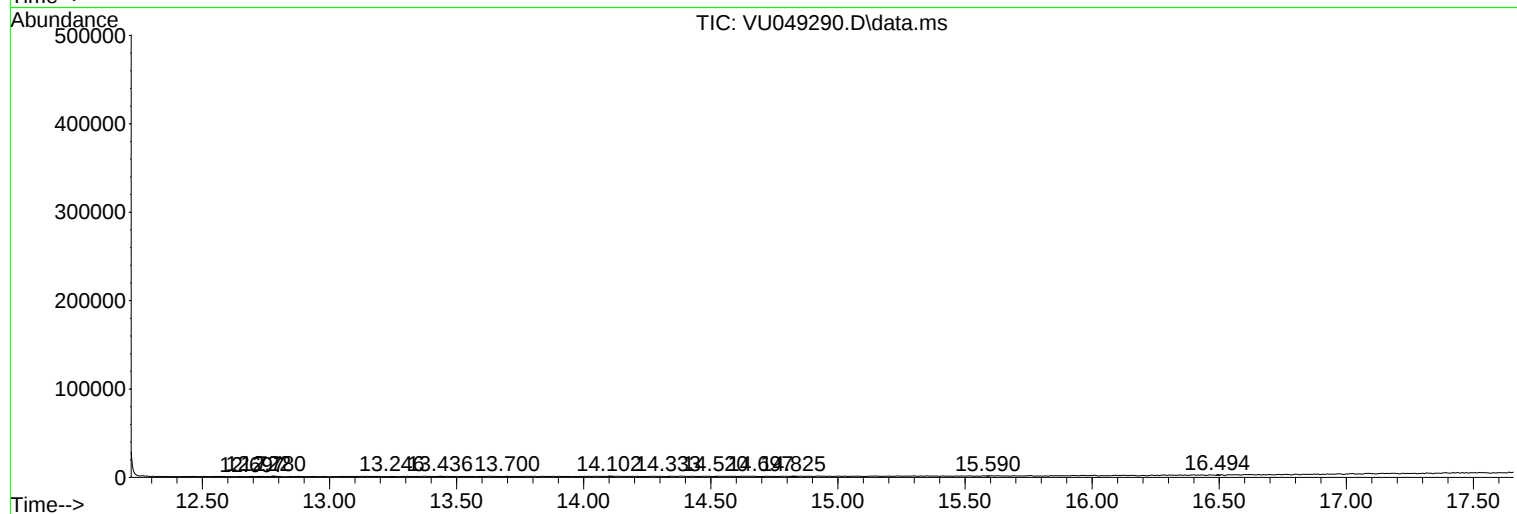
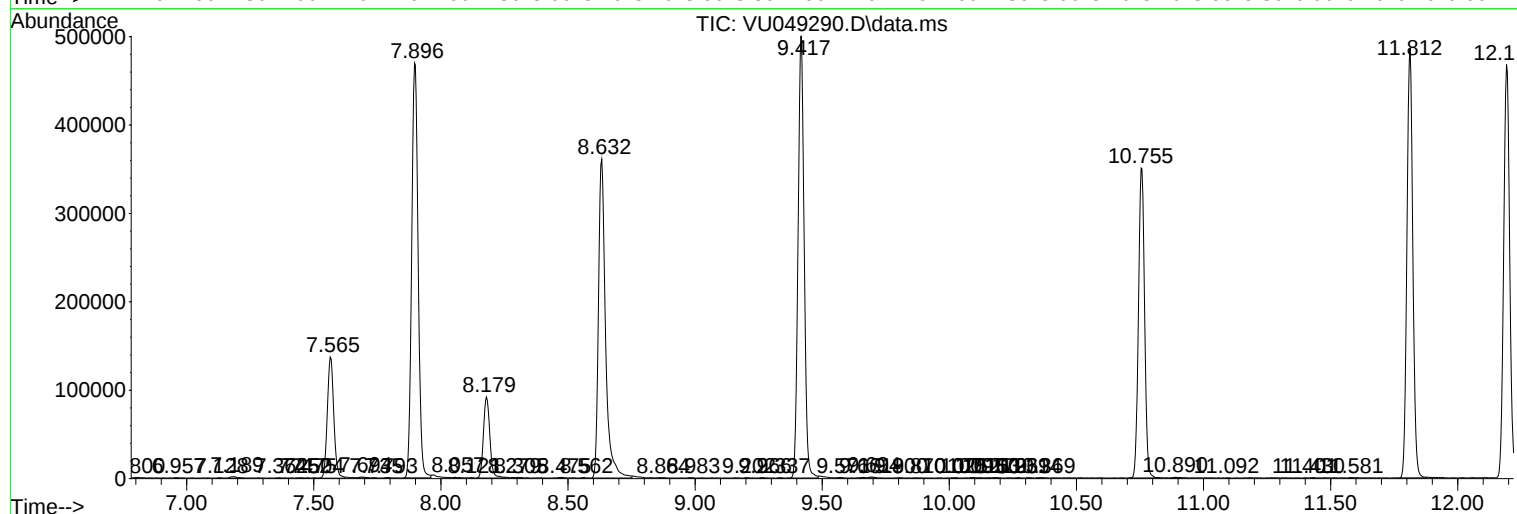
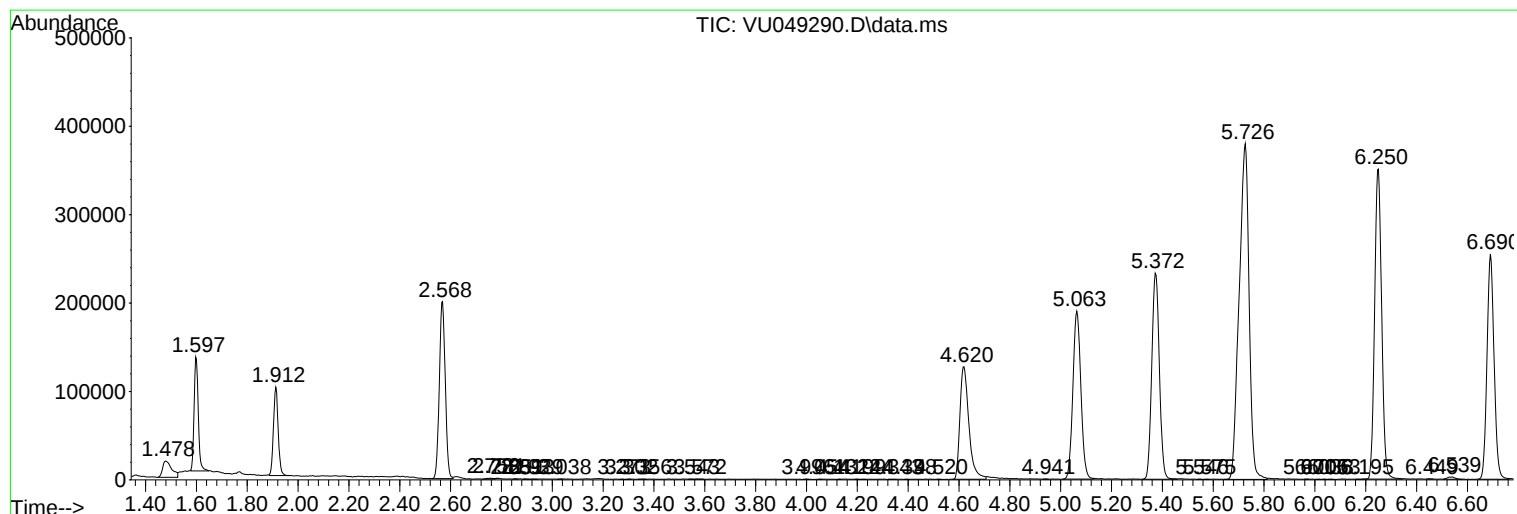
Sum of corrected areas: 8942546

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
Data File : VU049290.D
Acq On : 18 Jun 2022 18:45
Operator : SY/MD
Sample : N3395-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0153

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
Data File : VU049290.D
Acq On : 18 Jun 2022 18:45
Operator : SY/MD
Sample : N3395-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0153

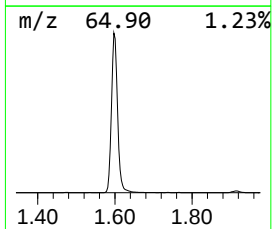
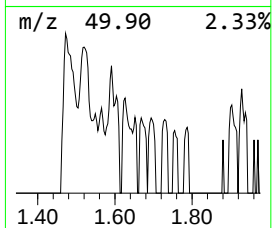
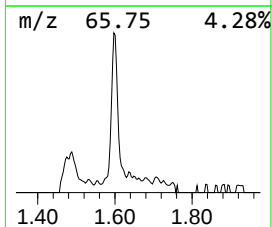
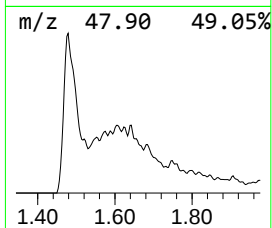
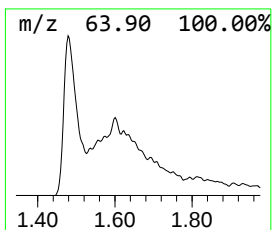
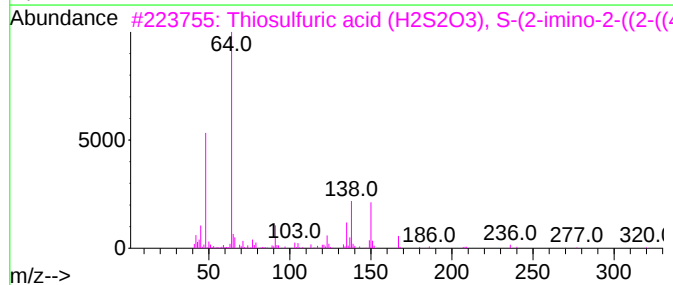
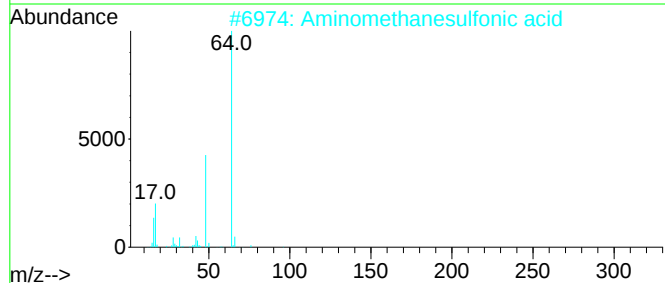
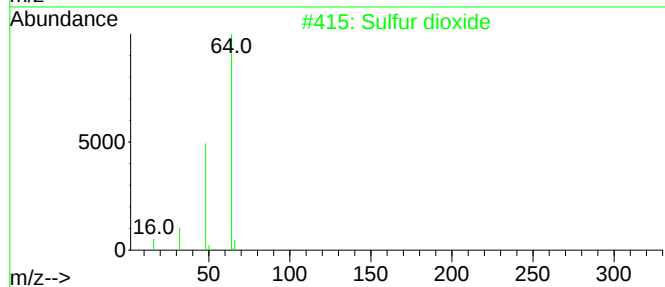
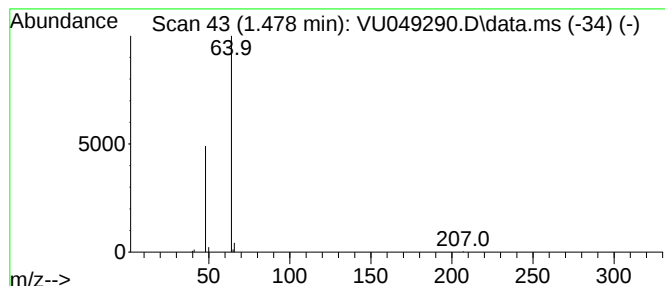
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	3.38 ug/L	45820	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9
4			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9
5			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
Data File : VU049290.D
Acq On : 18 Jun 2022 18:45
Operator : SY/MD
Sample : N3395-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0153

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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	1.478	3.4	ug/L	45820	1	6.250	677691	50.0