

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045208.D
 Acq On : 07 Oct 2021 13:42
 Operator : SY/MD
 Sample : M4025-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP5

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: VU045208.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	33	43	55	rBV	51187	134834	10.45%	1.359%
2	1.600	75	81	102	rVB	195395	212841	16.50%	2.146%
3	1.893	165	172	184	rVB	137294	183510	14.22%	1.850%
4	2.562	367	380	400	rBV	268431	446027	34.57%	4.497%
5	2.687	415	419	421	rBV	217	171	0.01%	0.002%
6	2.761	436	442	443	rBV2	180	167	0.01%	0.002%
7	2.787	443	450	451	rBV2	1548	1538	0.12%	0.016%
8	3.192	564	576	588	rBV	2978	6675	0.52%	0.067%
9	3.346	621	624	628	rBV	271	275	0.02%	0.003%
10	3.481	663	666	673	rVB2	257	257	0.02%	0.003%
11	3.581	692	697	701	rBV3	354	335	0.03%	0.003%
12	3.719	736	740	746	rBB3	226	261	0.02%	0.003%
13	3.835	769	776	780	rVB2	217	251	0.02%	0.003%
14	3.861	780	784	787	rBV	263	203	0.02%	0.002%
15	3.941	804	809	812	rBV2	183	260	0.02%	0.003%
16	4.005	827	829	836	rVB	298	290	0.02%	0.003%
17	4.038	836	839	841	rBV2	200	152	0.01%	0.002%
18	4.073	846	850	852	rBV2	233	190	0.01%	0.002%
19	4.134	863	869	872	rVV2	197	232	0.02%	0.002%
20	4.211	889	893	896	rBV2	181	219	0.02%	0.002%
21	4.314	920	925	927	rBV2	152	158	0.01%	0.002%
22	4.520	983	989	992	rBV2	173	214	0.02%	0.002%
23	4.629	1007	1023	1054	rBV	140176	328981	25.50%	3.317%
24	4.832	1083	1086	1090	rVB3	263	193	0.01%	0.002%
25	5.067	1139	1159	1185	rBV	226329	496456	38.48%	5.005%
26	5.221	1203	1207	1211	rVB	292	214	0.02%	0.002%
27	5.292	1223	1229	1237	rVB3	634	1184	0.09%	0.012%
28	5.343	1242	1245	1251	rVB2	222	231	0.02%	0.002%
29	5.375	1251	1255	1257	rBV	221	161	0.01%	0.002%
30	5.494	1287	1292	1294	rBV2	207	223	0.02%	0.002%
31	5.552	1305	1310	1320	rVB	207	345	0.03%	0.003%
32	5.729	1341	1365	1387	rBV2	482333	1290323	100.00%	13.008%
33	6.021	1452	1456	1461	rVB3	418	466	0.04%	0.005%
34	6.047	1461	1464	1468	rBV2	371	368	0.03%	0.004%
35	6.202	1506	1512	1513	rBV	151	147	0.01%	0.001%
36	6.253	1513	1528	1545	rBV	380454	714122	55.34%	7.199%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045208.D
 Acq On : 07 Oct 2021 13:42
 Operator : SY/MD
 Sample : M4025-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP5

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	6.539	1608	1617	1627	rVB9	2474	4608	0.36%	0.046%
38	6.587	1627	1632	1635	rVB2	208	166	0.01%	0.002%
39	6.603	1635	1637	1641	rBV	141	153	0.01%	0.002%
40	6.697	1650	1666	1687	rBV	304791	588926	45.64%	5.937%
41	6.806	1695	1700	1709	rVB3	862	1252	0.10%	0.013%
42	6.960	1744	1748	1749	rBV	198	145	0.01%	0.001%
43	7.121	1795	1798	1804	rVV2	167	208	0.02%	0.002%
44	7.182	1810	1817	1827	rVB5	952	1641	0.13%	0.017%
45	7.250	1835	1838	1843	rVB2	186	189	0.01%	0.002%
46	7.475	1901	1908	1912	rBV2	185	226	0.02%	0.002%
47	7.568	1924	1937	1954	rBV	153431	266928	20.69%	2.691%
48	7.677	1968	1971	1973	rVV4	452	309	0.02%	0.003%
49	7.693	1973	1976	1981	rVB2	620	540	0.04%	0.005%
50	7.854	2021	2026	2027	rBV2	211	175	0.01%	0.002%
51	7.902	2027	2041	2056	rVV	594045	1016817	78.80%	10.251%
52	7.973	2056	2063	2073	rVB	8913	14062	1.09%	0.142%
53	8.182	2116	2128	2146	rVV	108572	178040	13.80%	1.795%
54	8.320	2167	2171	2180	rVB3	425	680	0.05%	0.007%
55	8.362	2180	2184	2186	rBV2	244	210	0.02%	0.002%
56	8.391	2189	2193	2198	rBV2	152	159	0.01%	0.002%
57	8.475	2211	2219	2230	rBV3	761	1515	0.12%	0.015%
58	8.533	2233	2237	2243	rBV	189	270	0.02%	0.003%
59	8.581	2247	2252	2253	rBV2	164	143	0.01%	0.001%
60	8.636	2257	2269	2303	rBV	420433	739015	57.27%	7.450%
61	8.832	2326	2330	2335	rBV2	230	207	0.02%	0.002%
62	8.893	2344	2349	2355	rBV	322	427	0.03%	0.004%
63	9.102	2410	2414	2417	rBV2	221	206	0.02%	0.002%
64	9.147	2421	2428	2431	rBV2	215	271	0.02%	0.003%
65	9.420	2499	2513	2550	rVB	552602	898720	69.65%	9.060%
66	9.545	2550	2552	2555	rBV	192	141	0.01%	0.001%
67	9.578	2557	2562	2565	rBV2	228	241	0.02%	0.002%
68	9.661	2582	2588	2590	rBV	211	248	0.02%	0.003%
69	9.693	2590	2598	2606	rVV4	1086	1635	0.13%	0.016%
70	9.764	2615	2620	2623	rVB2	283	248	0.02%	0.003%
71	9.816	2631	2636	2638	rBV	207	232	0.02%	0.002%
72	10.028	2699	2702	2705	rBV	183	159	0.01%	0.002%
73	10.047	2705	2708	2711	rVB	261	202	0.02%	0.002%
74	10.070	2711	2715	2717	rBV2	209	182	0.01%	0.002%
75	10.417	2819	2823	2826	rBV	247	229	0.02%	0.002%
76	10.504	2848	2850	2855	rBV2	170	182	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045208.D
 Acq On : 07 Oct 2021 13:42
 Operator : SY/MD
 Sample : M4025-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP5

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	10.677	2895	2904	2912	rVV3	1571	2242	0.17%	0.023%
78	10.761	2917	2930	2950	rVB	430867	693547	53.75%	6.992%
79	10.838	2950	2954	2958	rBV2	157	149	0.01%	0.002%
80	10.867	2960	2963	2968	rVB	322	295	0.02%	0.003%
81	10.896	2968	2972	2976	rBV2	403	410	0.03%	0.004%
82	11.092	3029	3033	3035	rBV	269	209	0.02%	0.002%
83	11.455	3141	3146	3147	rBV	821	569	0.04%	0.006%
84	11.581	3182	3185	3188	rBV	257	149	0.01%	0.002%
85	11.696	3212	3221	3227	rBV4	855	1064	0.08%	0.011%
86	11.815	3245	3258	3278	rVV	514587	800983	62.08%	8.075%
87	11.938	3293	3296	3297	rBV2	388	257	0.02%	0.003%
88	11.976	3301	3308	3314	rVB2	887	1310	0.10%	0.013%
89	12.195	3363	3376	3397	rBV	539933	873160	67.67%	8.803%
90	12.368	3426	3430	3433	rBV2	300	268	0.02%	0.003%
91	12.616	3502	3507	3509	rBV2	219	214	0.02%	0.002%
92	12.767	3551	3554	3557	rBV2	197	152	0.01%	0.002%
93	13.391	3743	3748	3750	rBV2	185	159	0.01%	0.002%
94	13.497	3775	3781	3783	rBV2	258	251	0.02%	0.003%
95	13.587	3806	3809	3815	rBV2	226	298	0.02%	0.003%
96	14.140	3973	3981	3984	rBV	242	357	0.03%	0.004%
97	14.426	4066	4070	4073	rBV2	365	352	0.03%	0.004%
98	14.520	4096	4099	4101	rBV2	261	188	0.01%	0.002%
99	14.774	4175	4178	4179	rBV	237	151	0.01%	0.002%
100	14.966	4235	4238	4241	rBV2	250	192	0.01%	0.002%

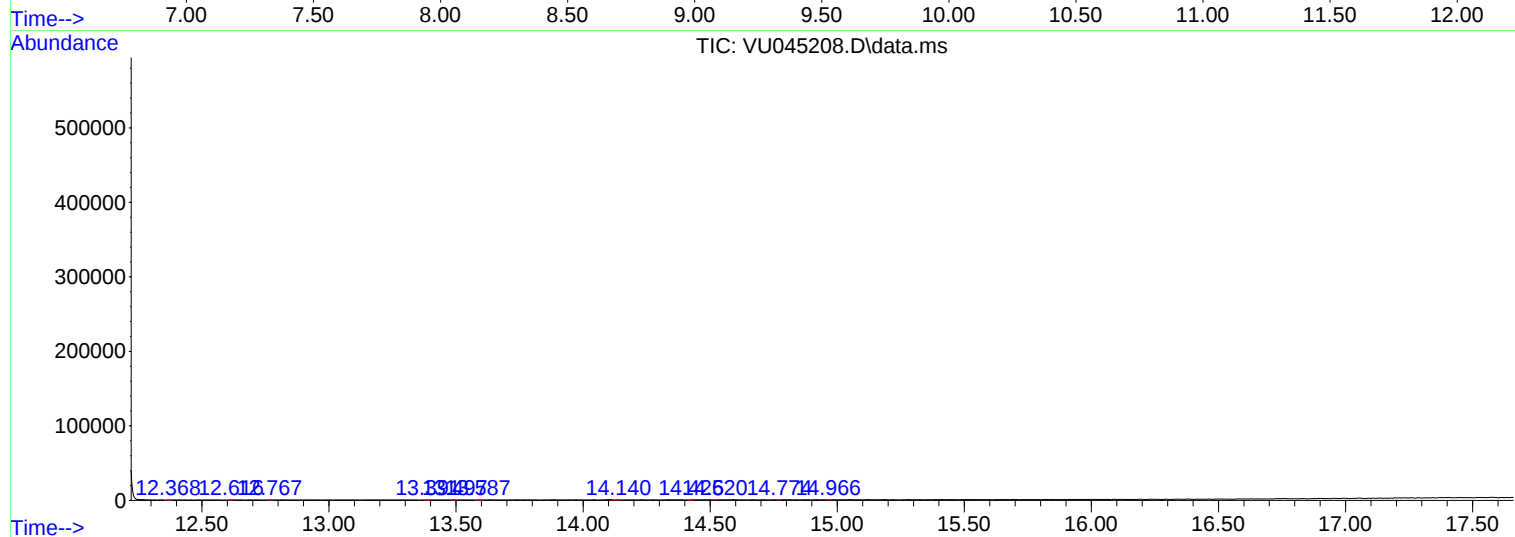
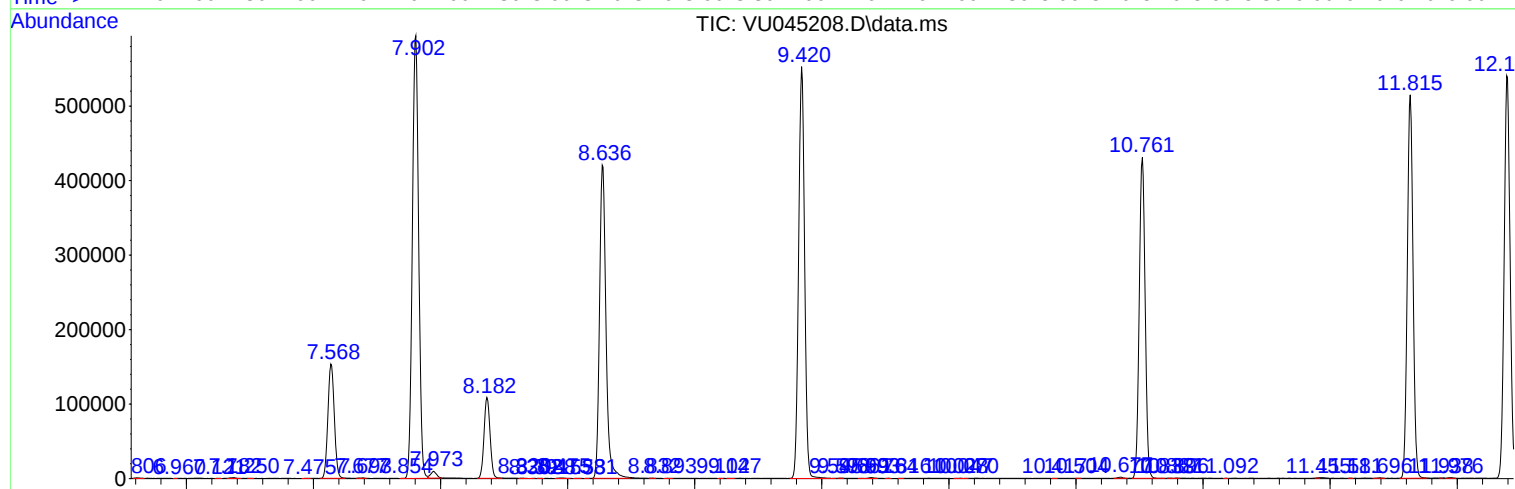
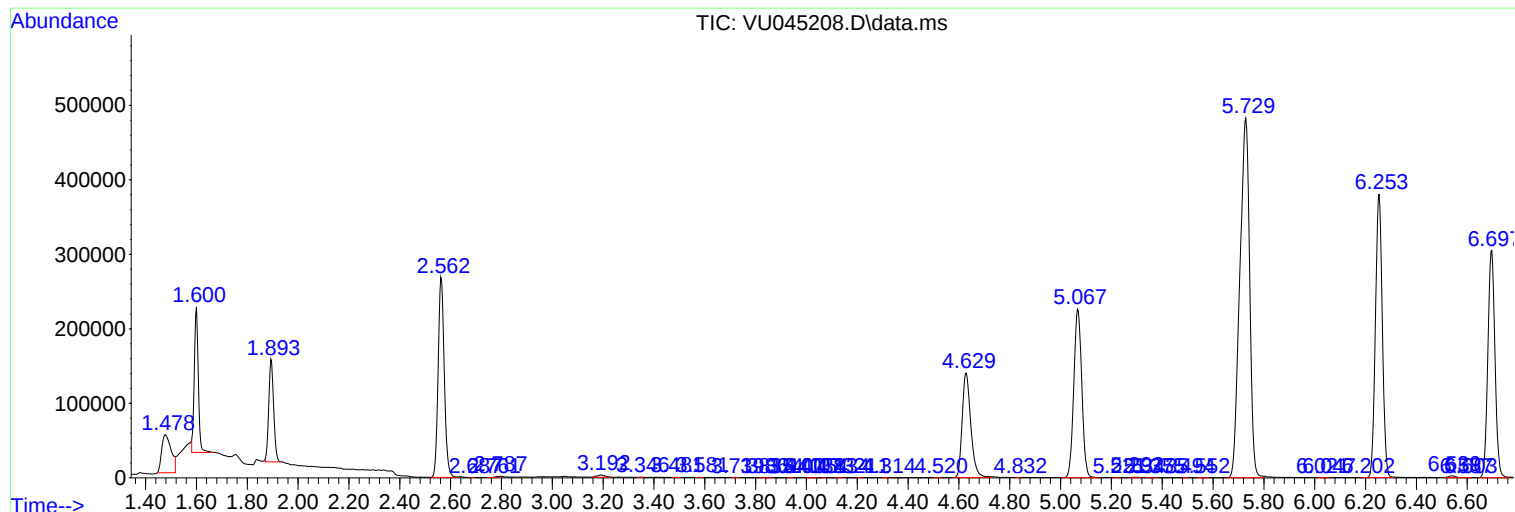
Sum of corrected areas: 9919307

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045208.D
Acq On : 07 Oct 2021 13:42
Operator : SY/MD
Sample : M4025-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AP5

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 : VU045208.D
Acq On : 07 Oct 2021 13:42
Operator : SY/MD
Sample : M4025-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AP5

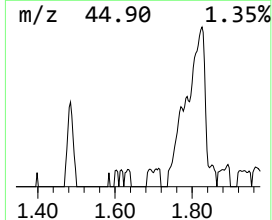
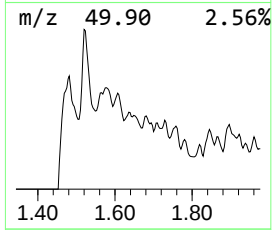
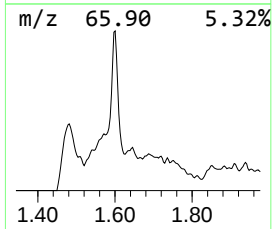
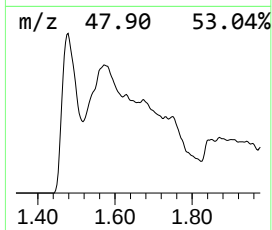
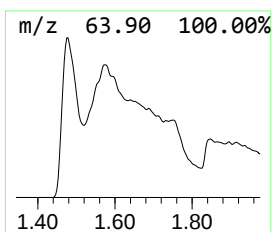
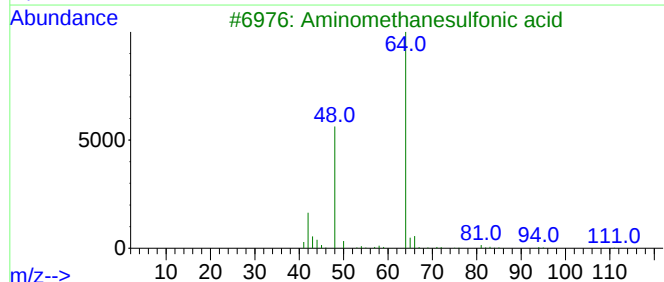
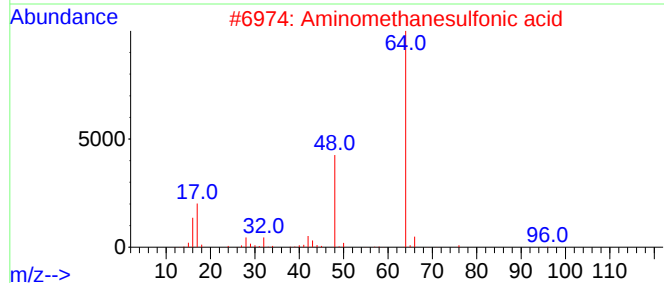
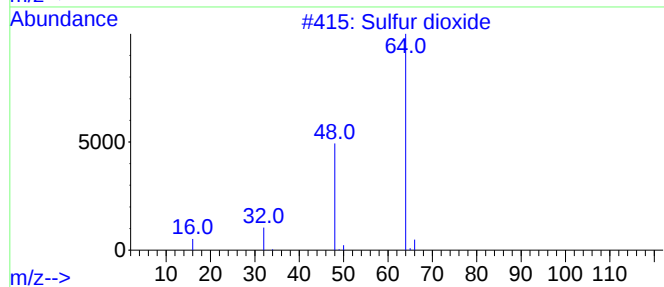
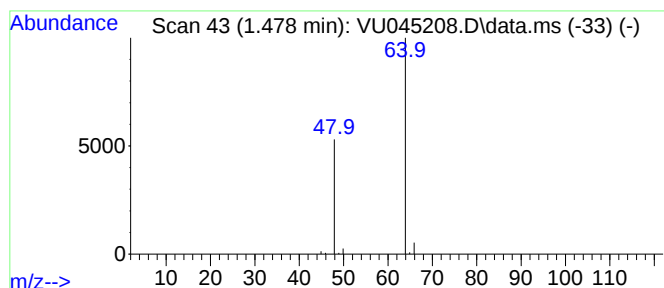
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.478	9.44 ug/L	134834	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	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045208.D
Acq On : 07 Oct 2021 13:42
Operator : SY/MD
Sample : M4025-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AP5

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	1.478	9.4	ug/L	134834	1	6.253	714122	50.0