

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045264.D
 Acq On : 08 Oct 2021 20:13
 Operator : SY/MD
 Sample : M4025-21
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK001

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: VU045264.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	22981	43756	3.33%	0.455%
2	1.601	74	81	92	rVB	204466	212953	16.21%	2.216%
3	1.890	163	171	183	rVB	138853	188677	14.36%	1.963%
4	2.562	367	380	399	rBV	264823	448006	34.11%	4.662%
5	2.781	446	448	454	rVB2	290	312	0.02%	0.003%
6	2.954	497	502	508	rBV3	320	448	0.03%	0.005%
7	3.047	520	531	543	rVB2	5317	9835	0.75%	0.102%
8	3.118	550	553	556	rVB2	180	121	0.01%	0.001%
9	3.144	556	561	565	rBV	194	220	0.02%	0.002%
10	3.195	569	577	583	rBV3	538	918	0.07%	0.010%
11	3.234	586	589	596	rBV2	187	296	0.02%	0.003%
12	3.369	627	631	638	rBV	157	191	0.01%	0.002%
13	3.462	653	660	661	rBV2	190	203	0.02%	0.002%
14	3.533	678	682	685	rVB	210	181	0.01%	0.002%
15	3.649	714	718	720	rBV	156	144	0.01%	0.001%
16	3.703	730	735	738	rBV2	232	247	0.02%	0.003%
17	3.752	747	750	752	rBV	200	119	0.01%	0.001%
18	3.871	784	787	792	rBV	147	160	0.01%	0.002%
19	3.954	810	813	815	rVV2	165	116	0.01%	0.001%
20	3.986	819	823	829	rVB2	206	282	0.02%	0.003%
21	4.086	850	854	859	rBV	144	147	0.01%	0.002%
22	4.292	914	918	922	rBV2	184	160	0.01%	0.002%
23	4.321	922	927	932	rBV2	200	278	0.02%	0.003%
24	4.517	984	988	993	rBV2	222	281	0.02%	0.003%
25	4.629	1008	1023	1060	rBV	150570	352810	26.86%	3.671%
26	4.874	1094	1099	1101	rBV2	203	215	0.02%	0.002%
27	5.067	1140	1159	1179	rBV	227780	496833	37.82%	5.170%
28	5.211	1203	1204	1207	rVB	225	124	0.01%	0.001%
29	5.285	1223	1227	1228	rBV	469	358	0.03%	0.004%
30	5.372	1250	1254	1256	rBV2	269	167	0.01%	0.002%
31	5.385	1256	1258	1262	rVB2	251	134	0.01%	0.001%
32	5.639	1332	1337	1339	rBV	143	176	0.01%	0.002%
33	5.729	1343	1365	1383	rBV2	493190	1313603	100.00%	13.669%
34	6.115	1481	1485	1491	rBV3	361	373	0.03%	0.004%
35	6.170	1499	1502	1505	rBV	125	121	0.01%	0.001%
36	6.253	1512	1528	1549	rBV	329115	616189	46.91%	6.412%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045264.D
 Acq On : 08 Oct 2021 20:13
 Operator : SY/MD
 Sample : M4025-21
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK001

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	6.324	1549	1550	1553	rBV2	230	116	0.01%	0.001%
38	6.530	1605	1614	1627	rBV3	4631	8398	0.64%	0.087%
39	6.694	1651	1665	1685	rBV	312250	603776	45.96%	6.283%
40	6.809	1696	1701	1703	rBV3	634	561	0.04%	0.006%
41	6.964	1743	1749	1752	rBV2	254	242	0.02%	0.003%
42	7.047	1768	1775	1785	rVB3	702	1199	0.09%	0.012%
43	7.179	1808	1816	1828	rBV4	1308	2301	0.18%	0.024%
44	7.266	1837	1843	1847	rVB2	186	271	0.02%	0.003%
45	7.346	1864	1868	1876	rBV2	136	238	0.02%	0.002%
46	7.462	1901	1904	1910	rVB2	213	228	0.02%	0.002%
47	7.507	1915	1918	1920	rBV2	218	171	0.01%	0.002%
48	7.568	1925	1937	1955	rBV	166869	286519	21.81%	2.981%
49	7.690	1970	1975	1984	rVB2	980	1220	0.09%	0.013%
50	7.816	2008	2014	2016	rBV	245	298	0.02%	0.003%
51	7.903	2026	2041	2056	rBV	594649	1005672	76.56%	10.465%
52	7.970	2057	2062	2075	rVB2	7975	12604	0.96%	0.131%
53	8.079	2094	2096	2098	rBV	229	132	0.01%	0.001%
54	8.118	2105	2108	2114	rBV2	178	210	0.02%	0.002%
55	8.182	2115	2128	2142	rBV	117935	193046	14.70%	2.009%
56	8.420	2199	2202	2204	rBV	199	159	0.01%	0.002%
57	8.520	2228	2233	2236	rVB2	172	189	0.01%	0.002%
58	8.536	2236	2238	2241	rBV2	151	117	0.01%	0.001%
59	8.639	2256	2270	2313	rBV	433747	771850	58.76%	8.031%
60	8.864	2337	2340	2341	rBV	171	120	0.01%	0.001%
61	8.919	2352	2357	2359	rBV	244	200	0.02%	0.002%
62	9.240	2454	2457	2461	rBV	269	235	0.02%	0.002%
63	9.343	2484	2489	2491	rBV2	181	186	0.01%	0.002%
64	9.420	2500	2513	2533	rBV	478737	775061	59.00%	8.065%
65	9.575	2556	2561	2564	rBV2	448	508	0.04%	0.005%
66	9.629	2574	2578	2581	rBV2	174	183	0.01%	0.002%
67	9.697	2590	2599	2606	rBV3	1521	2421	0.18%	0.025%
68	9.896	2659	2661	2663	rBV	181	128	0.01%	0.001%
69	9.989	2688	2690	2692	rBV2	218	143	0.01%	0.001%
70	10.079	2716	2718	2721	rBV	156	145	0.01%	0.002%
71	10.237	2764	2767	2771	rBV2	158	127	0.01%	0.001%
72	10.452	2830	2834	2837	rBV2	154	159	0.01%	0.002%
73	10.645	2885	2894	2895	rBV	265	362	0.03%	0.004%
74	10.674	2895	2903	2912	rVB2	2954	4357	0.33%	0.045%
75	10.761	2917	2930	2949	rVV	437531	701118	53.37%	7.295%
76	10.870	2957	2964	2967	rBV3	533	636	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045264.D
 Acq On : 08 Oct 2021 20:13
 Operator : SY/MD
 Sample : M4025-21
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK001

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	10.960	2989	2992	2997	rVB2	154	150	0.01%	0.002%
78	11.002	3003	3005	3009	rBV2	209	141	0.01%	0.001%
79	11.050	3016	3020	3022	rBV2	157	137	0.01%	0.001%
80	11.118	3035	3041	3045	rVB5	544	579	0.04%	0.006%
81	11.150	3045	3051	3056	rVB4	472	513	0.04%	0.005%
82	11.201	3065	3067	3070	rVB2	264	164	0.01%	0.002%
83	11.462	3139	3148	3157	rBV6	2304	3414	0.26%	0.036%
84	11.549	3172	3175	3178	rBV2	144	134	0.01%	0.001%
85	11.697	3215	3221	3228	rVB4	1053	1572	0.12%	0.016%
86	11.745	3231	3236	3240	rBV2	197	234	0.02%	0.002%
87	11.816	3245	3258	3274	rBV	430441	678888	51.68%	7.064%
88	11.944	3289	3298	3302	rBV5	1223	1743	0.13%	0.018%
89	11.976	3302	3308	3315	rVB3	2199	3063	0.23%	0.032%
90	12.195	3360	3376	3395	rBV	525373	851577	64.83%	8.861%
91	12.336	3414	3420	3425	rVB5	692	754	0.06%	0.008%
92	12.468	3458	3461	3467	rVB2	309	332	0.03%	0.003%
93	12.504	3468	3472	3474	rBV2	189	141	0.01%	0.001%
94	12.639	3509	3514	3523	rBV2	482	636	0.05%	0.007%
95	12.790	3557	3561	3564	rBV	234	238	0.02%	0.002%
96	12.944	3606	3609	3615	rBV2	210	287	0.02%	0.003%
97	14.098	3965	3968	3970	rBV	299	144	0.01%	0.001%
98	14.333	4038	4041	4047	rBV	314	301	0.02%	0.003%
99	14.578	4114	4117	4121	rBV3	339	285	0.02%	0.003%
100	14.623	4129	4131	4133	rBV	218	129	0.01%	0.001%

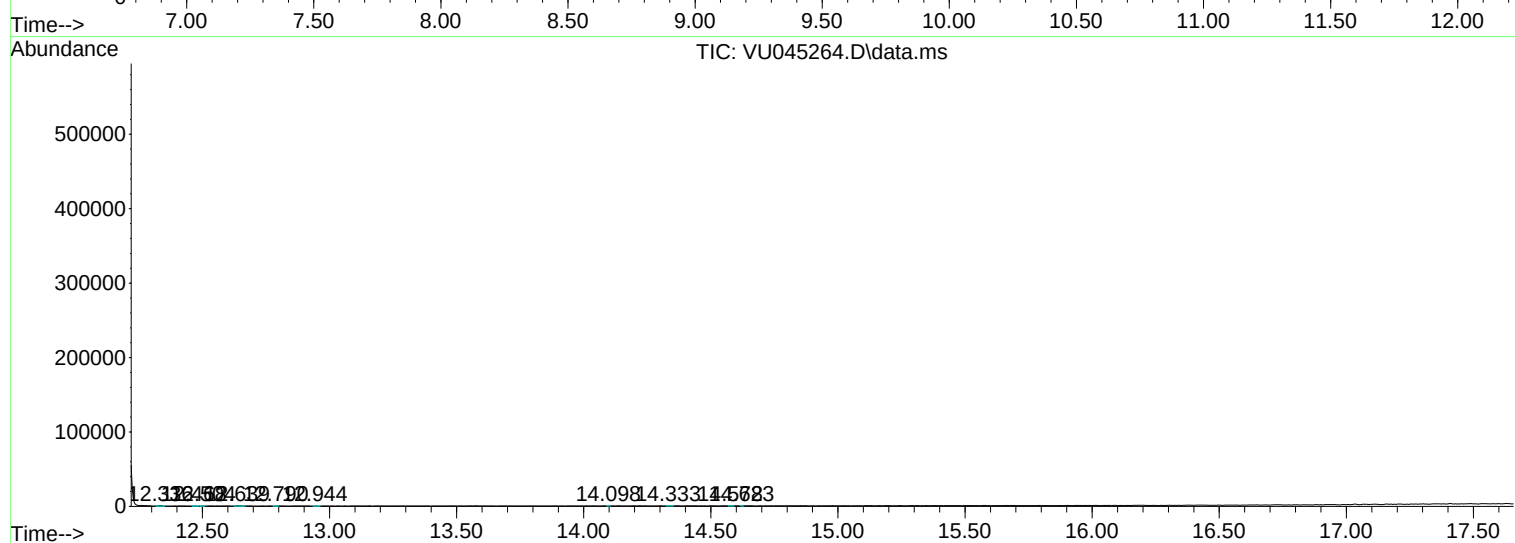
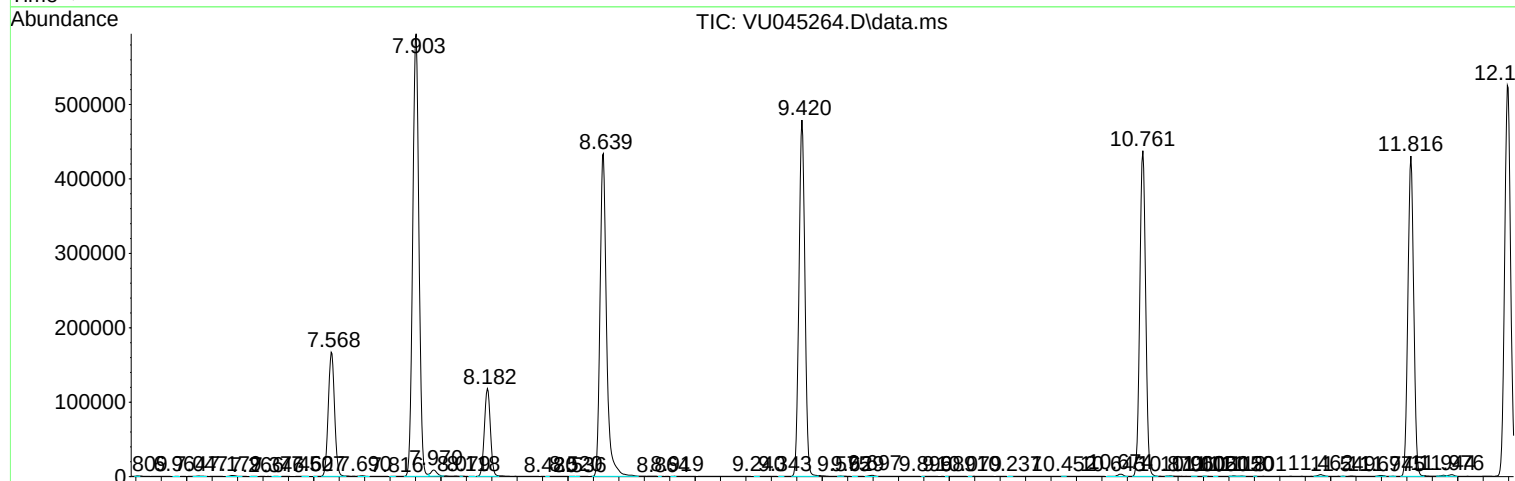
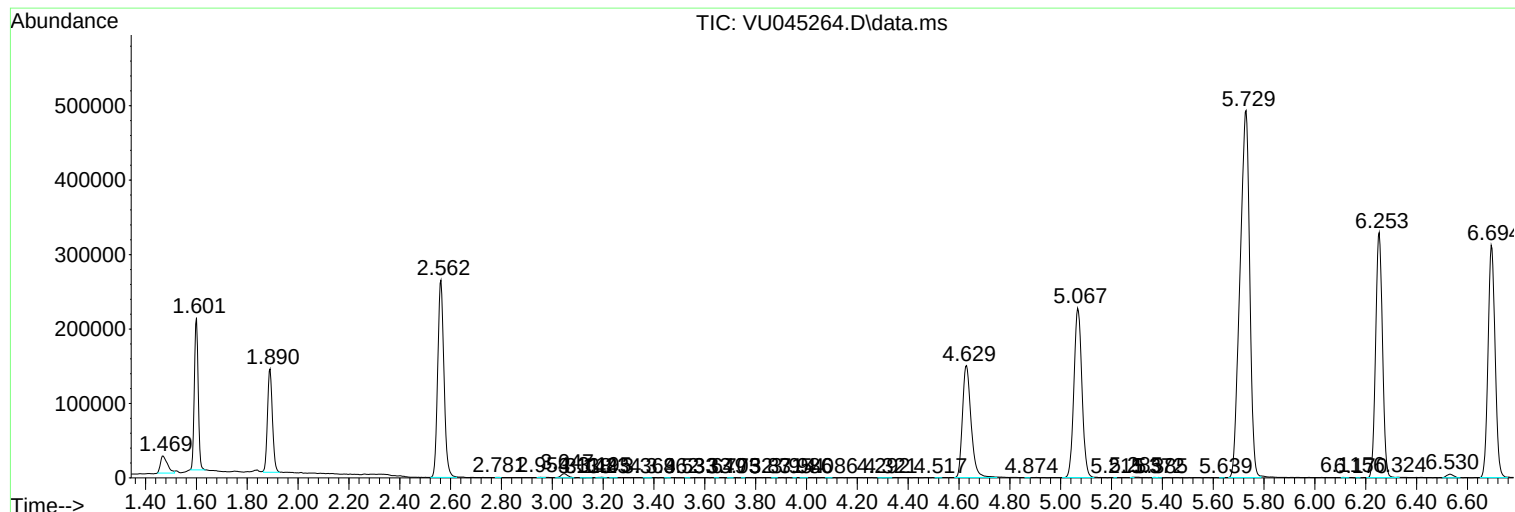
Sum of corrected areas: 9610316

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045264.D
Acq On : 08 Oct 2021 20:13
Operator : SY/MD
Sample : M4025-21
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VHBLK001

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\VU100821\
Data File : VU045264.D
Acq On : 08 Oct 2021 20:13
Operator : SY/MD
Sample : M4025-21
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VHBLK001

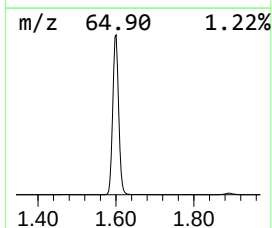
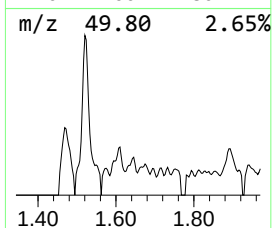
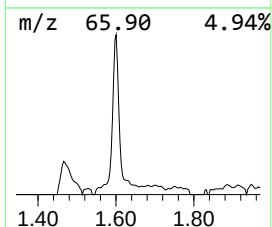
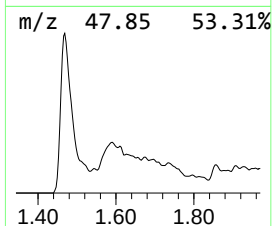
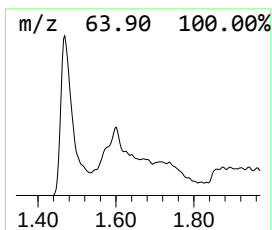
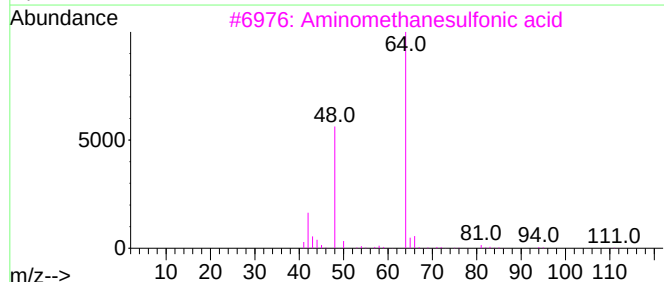
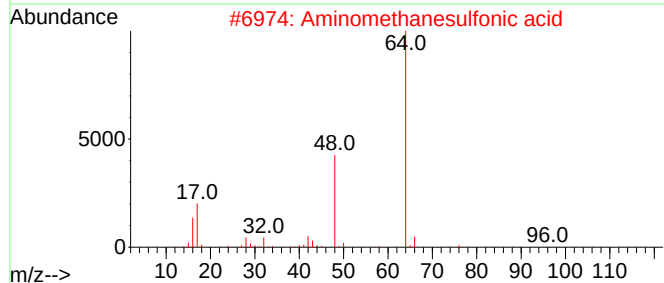
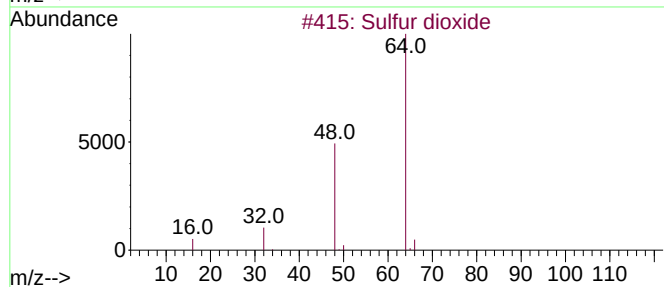
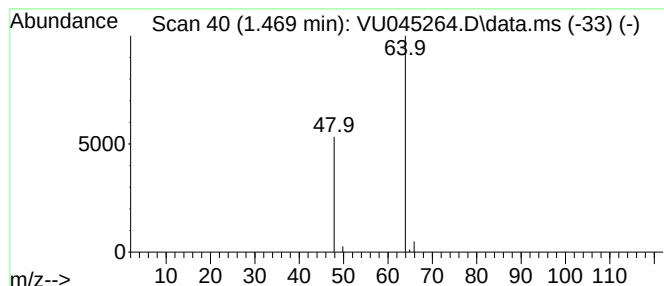
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.55 ug/L	43756	1,4-Difluorobenzene	6.253

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	64
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\VU100821\
Data File : VU045264.D
Acq On : 08 Oct 2021 20:13
Operator : SY/MD
Sample : M4025-21
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VHBLK001

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	3.5	ug/L	43756	1	6.253	616189	50.0