

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033776.D
 Acq On : 20 Jan 2024 00:46
 Operator : SY/MD
 Sample : P1189-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMR3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	32	39	59	rBV	142044	170374	22.71%	2.633%
2	1.278	65	74	100	rBV3	205469	356622	47.53%	5.511%
3	1.532	147	153	167	rVB	84988	104492	13.93%	1.615%
4	2.060	308	317	331	rVB	173936	256463	34.18%	3.963%
5	2.333	400	402	406	rBV	269	179	0.02%	0.003%
6	2.545	465	468	469	rBV2	300	175	0.02%	0.003%
7	2.706	516	518	521	rBV2	258	158	0.02%	0.002%
8	2.928	584	587	589	rBV	197	120	0.02%	0.002%
9	2.941	589	591	593	rVV2	232	162	0.02%	0.003%
10	2.966	597	599	602	rVV3	186	134	0.02%	0.002%
11	3.005	609	611	616	rVB2	156	147	0.02%	0.002%
12	3.066	628	630	633	rVB	271	132	0.02%	0.002%
13	3.089	634	637	639	rBV2	259	181	0.02%	0.003%
14	3.140	648	653	661	rBV3	138	158	0.02%	0.002%
15	3.484	756	760	763	rVV2	137	121	0.02%	0.002%
16	3.619	797	802	808	rBV	141	192	0.03%	0.003%
17	3.783	845	853	891	rBV	46369	130080	17.34%	2.010%
18	4.249	981	998	1029	rBV	116535	298983	39.85%	4.620%
19	4.449	1057	1060	1062	rBV2	278	190	0.03%	0.003%
20	4.564	1093	1096	1099	rBV2	161	144	0.02%	0.002%
21	4.635	1111	1118	1122	rVB3	163	206	0.03%	0.003%
22	4.667	1123	1128	1132	rBV3	248	251	0.03%	0.004%
23	4.690	1132	1135	1140	rVB3	246	202	0.03%	0.003%
24	4.809	1169	1172	1174	rBV	142	121	0.02%	0.002%
25	4.957	1199	1218	1251	rBV3	281589	750346	100.00%	11.596%
26	5.191	1289	1291	1292	rBV	298	149	0.02%	0.002%
27	5.346	1335	1339	1343	rBV3	201	197	0.03%	0.003%
28	5.410	1352	1359	1361	rBV3	283	236	0.03%	0.004%
29	5.474	1374	1379	1383	rBV3	192	180	0.02%	0.003%
30	5.532	1386	1397	1429	rBV	277691	565957	75.43%	8.746%
31	5.838	1486	1492	1493	rBV4	996	893	0.12%	0.014%
32	5.905	1508	1513	1514	rBV	168	154	0.02%	0.002%
33	5.989	1526	1539	1568	rBV	164815	342683	45.67%	5.296%
34	6.150	1585	1589	1592	rBV3	581	453	0.06%	0.007%
35	6.185	1596	1600	1604	rVB2	288	218	0.03%	0.003%
36	6.326	1640	1644	1647	rBV2	137	123	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033776.D
 Acq On : 20 Jan 2024 00:46
 Operator : SY/MD
 Sample : P1189-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMR3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

37	6.375	1657	1659	1666	rVB2	205	120	0.02%	0.002%
38	6.516	1696	1703	1705	rBV2	162	182	0.02%	0.003%
39	6.596	1724	1728	1729	rBV2	292	173	0.02%	0.003%
40	6.667	1747	1750	1753	rVB2	211	150	0.02%	0.002%
41	6.915	1816	1827	1853	rBV	85138	160662	21.41%	2.483%
42	7.149	1893	1900	1906	rVB5	519	812	0.11%	0.013%
43	7.194	1912	1914	1918	rVB	226	145	0.02%	0.002%
44	7.243	1918	1929	1957	rBV	340622	602070	80.24%	9.304%
45	7.555	2017	2026	2056	rBV2	56917	103194	13.75%	1.595%
46	7.741	2081	2084	2087	rVB3	300	167	0.02%	0.003%
47	7.760	2087	2090	2095	rVB2	215	159	0.02%	0.002%
48	7.789	2095	2099	2102	rVB2	238	152	0.02%	0.002%
49	7.915	2132	2138	2147	rVB4	1669	2187	0.29%	0.034%
50	7.957	2147	2151	2155	rVB2	181	139	0.02%	0.002%
51	8.024	2163	2172	2205	rBV	172417	328861	43.83%	5.082%
52	8.239	2237	2239	2252	rVB4	526	552	0.07%	0.009%
53	8.304	2257	2259	2261	rBV2	255	151	0.02%	0.002%
54	8.439	2297	2301	2302	rBV2	246	154	0.02%	0.002%
55	8.471	2308	2311	2315	rBV	204	139	0.02%	0.002%
56	8.545	2331	2334	2339	rBV	133	128	0.02%	0.002%
57	8.593	2347	2349	2358	rVB2	252	221	0.03%	0.003%
58	8.635	2358	2362	2364	rBV	171	137	0.02%	0.002%
59	8.674	2370	2374	2378	rBV2	157	143	0.02%	0.002%
60	8.783	2398	2408	2441	rBV	419927	688541	91.76%	10.640%
61	9.037	2481	2487	2490	rBV2	139	146	0.02%	0.002%
62	9.857	2737	2742	2746	rVB	242	218	0.03%	0.003%
63	10.153	2822	2834	2859	rBV	218864	340774	45.42%	5.266%
64	10.239	2859	2861	2864	rVB2	276	137	0.02%	0.002%
65	10.268	2868	2870	2875	rVB3	194	129	0.02%	0.002%
66	10.313	2877	2884	2885	rBV3	258	279	0.04%	0.004%
67	10.429	2917	2920	2926	rBV2	176	217	0.03%	0.003%
68	11.185	3144	3155	3184	rBV	441030	680067	90.63%	10.509%
69	11.561	3260	3272	3297	rBV	353987	561252	74.80%	8.673%
70	11.712	3315	3319	3322	rVB3	343	263	0.04%	0.004%
71	11.731	3322	3325	3329	rVB3	185	133	0.02%	0.002%
72	11.908	3374	3380	3382	rBV	126	138	0.02%	0.002%
73	11.963	3395	3397	3399	rBV2	230	158	0.02%	0.002%
74	12.291	3495	3499	3503	rBV2	151	152	0.02%	0.002%
75	12.429	3536	3542	3544	rBV2	117	134	0.02%	0.002%
76	12.522	3568	3571	3575	rBV2	301	198	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033776.D
 Acq On : 20 Jan 2024 00:46
 Operator : SY/MD
 Sample : P1189-16
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMR3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

77	12.673	3615	3618	3621	rVV2	203	131	0.02%	0.002%
78	13.387	3838	3840	3842	rBV	298	194	0.03%	0.003%
79	13.641	3917	3919	3928	rVB2	160	166	0.02%	0.003%
80	13.680	3928	3931	3933	rBV2	222	154	0.02%	0.002%
81	13.760	3953	3956	3959	rVB	237	134	0.02%	0.002%
82	13.783	3959	3963	3966	rBV	172	162	0.02%	0.003%
83	13.844	3979	3982	3986	rVB2	246	166	0.02%	0.003%
84	13.866	3986	3989	3990	rBV	198	120	0.02%	0.002%
85	14.046	4041	4045	4047	rBV3	226	163	0.02%	0.003%
86	14.085	4048	4057	4061	rBV5	3551	6124	0.82%	0.095%
87	14.185	4086	4088	4091	rBV3	441	234	0.03%	0.004%
88	14.252	4106	4109	4113	rVB2	534	365	0.05%	0.006%
89	14.287	4117	4120	4123	rBV3	403	288	0.04%	0.004%
90	14.345	4136	4138	4142	rVB2	343	187	0.02%	0.003%
91	14.374	4142	4147	4148	rBV2	161	143	0.02%	0.002%
92	14.448	4168	4170	4175	rVV3	264	191	0.03%	0.003%
93	14.471	4175	4177	4182	rVB3	444	261	0.03%	0.004%
94	14.606	4216	4219	4222	rBV2	289	260	0.03%	0.004%
95	14.857	4294	4297	4299	rBV	249	184	0.02%	0.003%
96	14.914	4312	4315	4318	rBV2	272	135	0.02%	0.002%
97	15.130	4379	4382	4385	rBV2	328	320	0.04%	0.005%
98	15.275	4425	4427	4428	rBV2	354	136	0.02%	0.002%
99	15.574	4515	4520	4522	rBV4	498	522	0.07%	0.008%
100	16.252	4725	4731	4740	rVB4	3786	4932	0.66%	0.076%

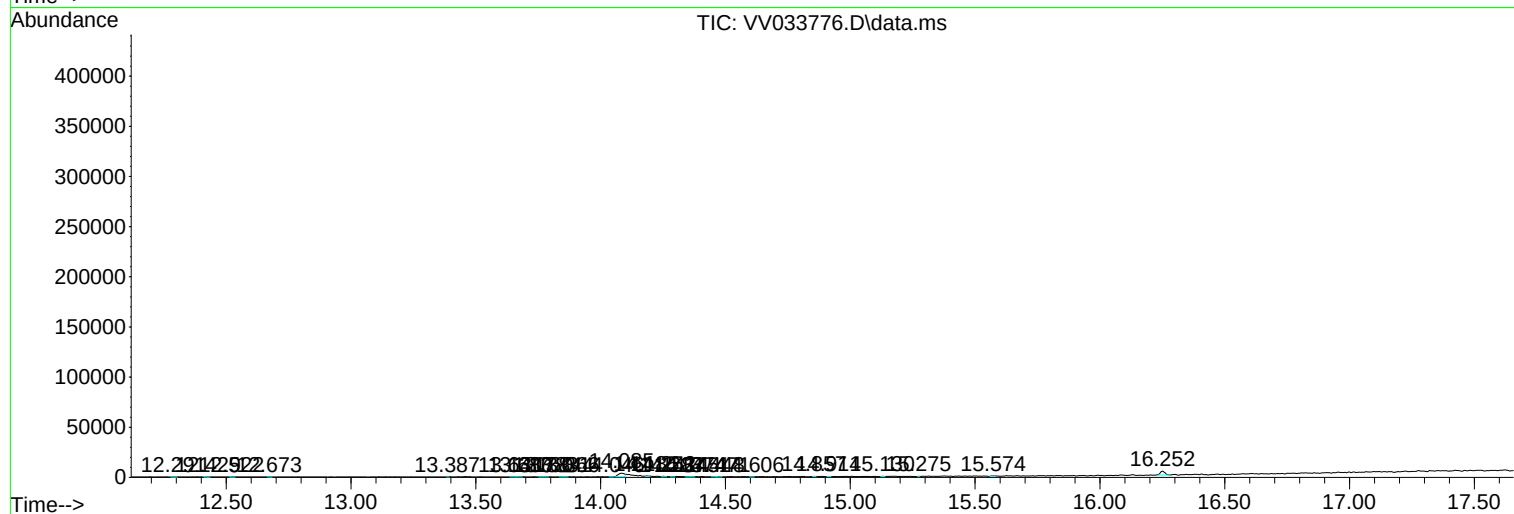
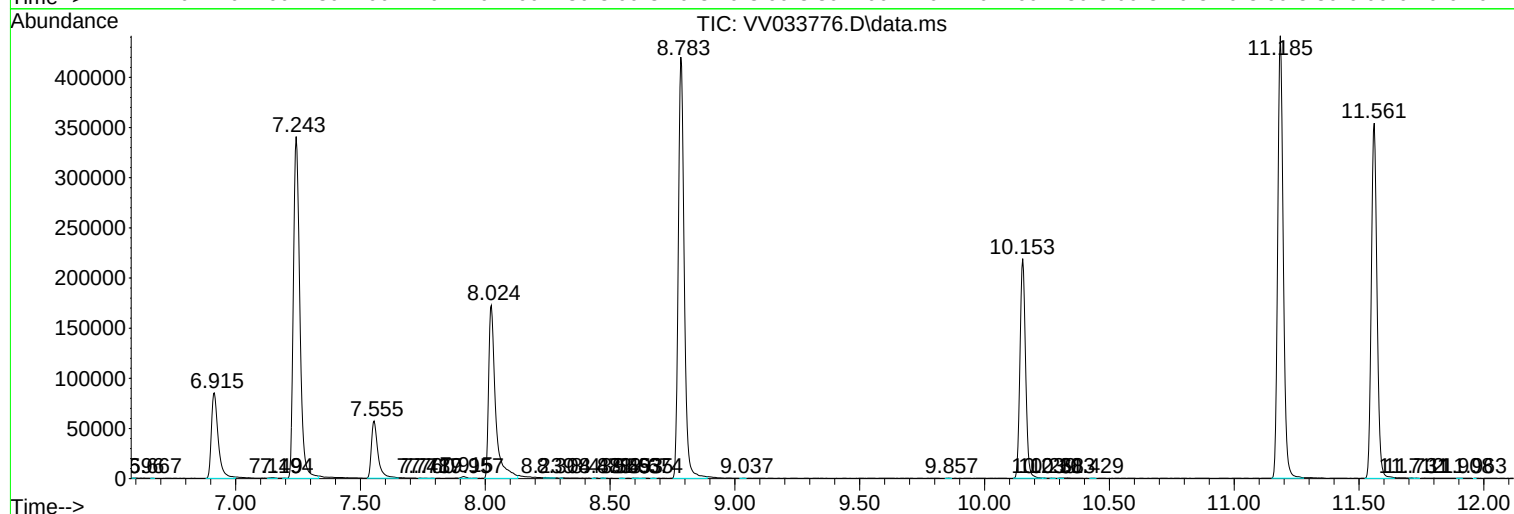
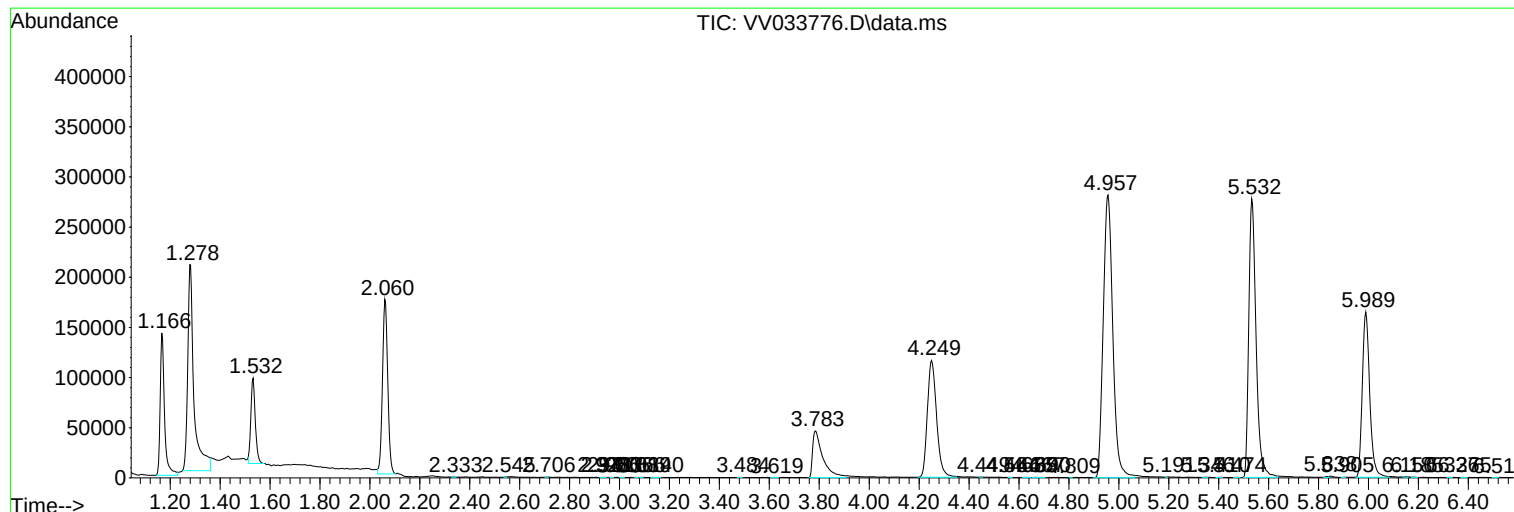
Sum of corrected areas: 6470982

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
Data File : VV033776.D
Acq On : 20 Jan 2024 00:46
Operator : SY/MD
Sample : P1189-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMR3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
Data File : VV033776.D
Acq On : 20 Jan 2024 00:46
Operator : SY/MD
Sample : P1189-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMR3

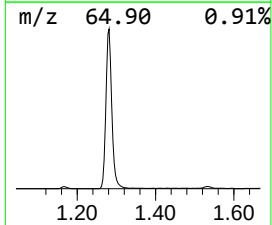
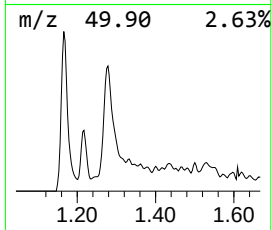
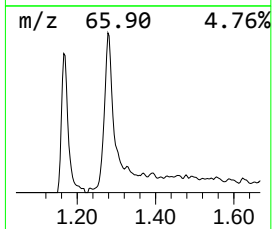
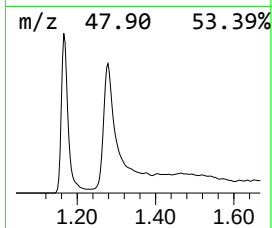
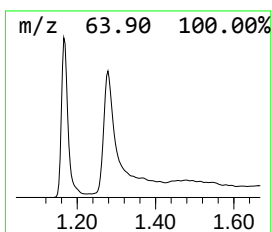
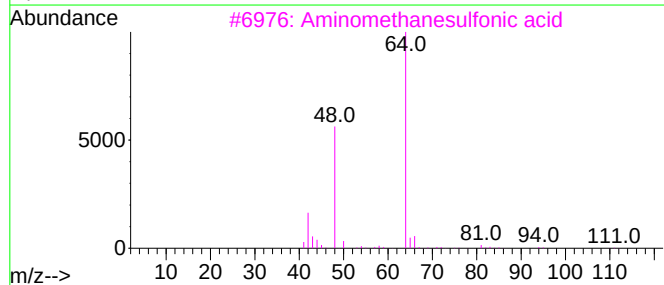
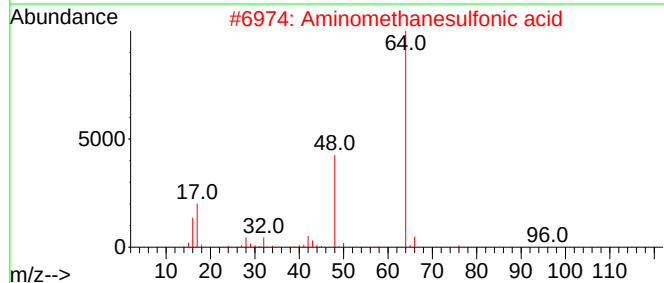
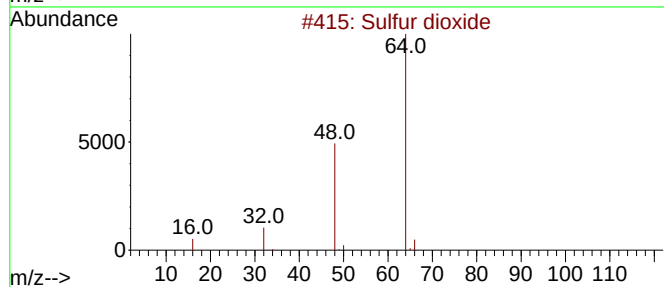
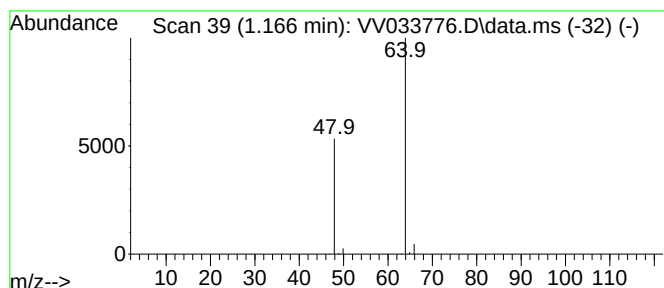
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
1.166	15.05 ug/L	170374	1,4-Difluorobenzene	5.532

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
Data File : VV033776.D
Acq On : 20 Jan 2024 00:46
Operator : SY/MD
Sample : P1189-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMR3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.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	1.166	15.1	ug/L	170374	1	5.532	565957	50.0