

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033838.D
 Acq On : 23 Jan 2024 18:45
 Operator : SY/MD
 Sample : P1191-16 50X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMT0

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: VV033838.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	51	rBV	37012	42045	4.38%	0.639%
2	1.281	68	75	90	rBV2	113255	129733	13.51%	1.971%
3	1.529	145	152	170	rVB	77431	94562	9.84%	1.436%
4	2.059	308	317	335	rVB	158544	235276	24.49%	3.574%
5	2.185	353	356	361	rVB4	672	596	0.06%	0.009%
6	2.243	369	374	377	rBV2	442	478	0.05%	0.007%
7	2.449	432	438	444	rVB3	1024	1205	0.13%	0.018%
8	2.561	462	473	483	rBV2	1400	2668	0.28%	0.041%
9	2.699	507	516	530	rVV3	8482	15384	1.60%	0.234%
10	3.156	653	658	662	rBV2	94	102	0.01%	0.002%
11	3.352	715	719	720	rBV	130	119	0.01%	0.002%
12	3.429	738	743	744	rBV2	189	195	0.02%	0.003%
13	3.465	750	754	757	rBV2	214	213	0.02%	0.003%
14	3.487	757	761	766	rVV2	224	280	0.03%	0.004%
15	3.526	771	773	778	rBV	161	161	0.02%	0.002%
16	3.664	813	816	825	rVB2	148	136	0.01%	0.002%
17	3.812	843	862	905	rBV2	353570	960541	100.00%	14.590%
18	4.146	963	966	969	rVB2	303	205	0.02%	0.003%
19	4.162	969	971	976	rBV3	186	118	0.01%	0.002%
20	4.249	983	998	1029	rBV	109016	277285	28.87%	4.212%
21	4.407	1044	1047	1053	rVB3	720	808	0.08%	0.012%
22	4.432	1053	1055	1060	rVV3	231	141	0.01%	0.002%
23	4.461	1060	1064	1066	rVB2	224	127	0.01%	0.002%
24	4.477	1066	1069	1075	rVB4	430	366	0.04%	0.006%
25	4.529	1082	1085	1087	rBV	258	157	0.02%	0.002%
26	4.561	1090	1095	1097	rBV2	214	124	0.01%	0.002%
27	4.619	1110	1113	1117	rBV2	203	216	0.02%	0.003%
28	4.957	1202	1218	1253	rBV2	261036	699538	72.83%	10.625%
29	5.201	1292	1294	1298	rVB3	175	129	0.01%	0.002%
30	5.391	1347	1353	1354	rBV	263	240	0.02%	0.004%
31	5.468	1374	1377	1378	rBV	238	138	0.01%	0.002%
32	5.532	1386	1397	1428	rBV	254055	524956	54.65%	7.974%
33	5.841	1480	1493	1516	rVB5	13105	29363	3.06%	0.446%
34	5.921	1516	1518	1522	rVB2	232	167	0.02%	0.003%
35	5.989	1526	1539	1567	rBV	152951	317233	33.03%	4.819%
36	6.153	1589	1590	1593	rVB	402	132	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033838.D
 Acq On : 23 Jan 2024 18:45
 Operator : SY/MD
 Sample : P1191-16 50X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMT0

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	6.178	1594	1598	1604	rVB2	500	602	0.06%	0.009%
38	6.207	1604	1607	1612	rBV2	299	271	0.03%	0.004%
39	6.252	1618	1621	1626	rVB2	169	153	0.02%	0.002%
40	6.275	1626	1628	1632	rBV2	168	119	0.01%	0.002%
41	6.304	1635	1637	1641	rVB	161	126	0.01%	0.002%
42	6.329	1641	1645	1648	rBV2	173	206	0.02%	0.003%
43	6.471	1685	1689	1695	rBV	219	337	0.04%	0.005%
44	6.606	1727	1731	1733	rBV3	292	304	0.03%	0.005%
45	6.628	1736	1738	1740	rVV	202	106	0.01%	0.002%
46	6.641	1740	1742	1745	rVB	239	119	0.01%	0.002%
47	6.780	1781	1785	1792	rBV2	238	354	0.04%	0.005%
48	6.915	1817	1827	1859	rBV	86524	165044	17.18%	2.507%
49	7.095	1881	1883	1889	rVB2	205	174	0.02%	0.003%
50	7.120	1889	1891	1895	rBV2	170	140	0.01%	0.002%
51	7.169	1904	1906	1911	rBV3	172	123	0.01%	0.002%
52	7.243	1918	1929	1952	rBV	311342	548264	57.08%	8.328%
53	7.554	2016	2026	2057	rBV	59271	107047	11.14%	1.626%
54	7.702	2069	2072	2080	rVB2	451	511	0.05%	0.008%
55	7.744	2080	2085	2088	rBV2	267	220	0.02%	0.003%
56	7.763	2089	2091	2093	rVV2	206	99	0.01%	0.002%
57	7.776	2093	2095	2101	rVB2	218	176	0.02%	0.003%
58	7.802	2101	2103	2107	rBV	184	144	0.01%	0.002%
59	7.908	2127	2136	2150	rBV4	9665	17186	1.79%	0.261%
60	8.024	2163	2172	2214	rBV	160156	314630	32.76%	4.779%
61	8.214	2229	2231	2232	rBV2	356	156	0.02%	0.002%
62	8.316	2260	2263	2266	rBV3	155	123	0.01%	0.002%
63	8.333	2266	2268	2273	rVB2	251	193	0.02%	0.003%
64	8.362	2273	2277	2278	rBV2	292	187	0.02%	0.003%
65	8.394	2284	2287	2290	rBV	210	179	0.02%	0.003%
66	8.429	2295	2298	2301	rBV2	164	116	0.01%	0.002%
67	8.506	2319	2322	2324	rVB	198	115	0.01%	0.002%
68	8.525	2324	2328	2331	rBV2	158	118	0.01%	0.002%
69	8.783	2397	2408	2440	rBV	384068	629373	65.52%	9.560%
70	9.017	2479	2481	2488	rVB3	187	181	0.02%	0.003%
71	9.532	2637	2641	2643	rBV2	134	108	0.01%	0.002%
72	9.628	2667	2671	2676	rBV2	115	145	0.02%	0.002%
73	9.709	2692	2696	2698	rBV	204	188	0.02%	0.003%
74	10.005	2786	2788	2790	rBV	180	125	0.01%	0.002%
75	10.152	2822	2834	2855	rBV	202851	319796	33.29%	4.857%
76	10.570	2960	2964	2968	rBV2	144	135	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033838.D
 Acq On : 23 Jan 2024 18:45
 Operator : SY/MD
 Sample : P1191-16 50X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMT0

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	10.847	3048	3050	3056	rVB2	135	119	0.01%	0.002%
78	11.185	3145	3155	3181	rBV	402307	620905	64.64%	9.431%
79	11.500	3249	3253	3256	rBV	154	116	0.01%	0.002%
80	11.561	3260	3272	3289	rBV	325312	515331	53.65%	7.827%
81	11.709	3314	3318	3319	rBV2	256	180	0.02%	0.003%
82	12.426	3537	3541	3549	rVB2	197	208	0.02%	0.003%
83	12.471	3550	3555	3559	rBV2	131	145	0.02%	0.002%
84	12.574	3584	3587	3592	rVB2	124	103	0.01%	0.002%
85	12.599	3592	3595	3597	rBV	126	97	0.01%	0.001%
86	13.467	3857	3865	3872	rVB	326	608	0.06%	0.009%
87	13.773	3957	3960	3962	rBV	244	105	0.01%	0.002%
88	13.863	3986	3988	3993	rVB	234	142	0.01%	0.002%
89	13.924	4002	4007	4008	rBV2	239	221	0.02%	0.003%
90	13.982	4020	4025	4026	rBV	445	388	0.04%	0.006%
91	14.043	4040	4044	4047	rBV2	215	155	0.02%	0.002%
92	14.127	4068	4070	4073	rBV2	194	101	0.01%	0.002%
93	14.188	4085	4089	4092	rBV2	192	144	0.01%	0.002%
94	14.258	4107	4111	4112	rBV	226	174	0.02%	0.003%
95	14.602	4216	4218	4220	rBV	184	112	0.01%	0.002%
96	14.943	4320	4324	4326	rBV3	421	222	0.02%	0.003%
97	14.995	4337	4340	4345	rBV3	263	236	0.02%	0.004%
98	15.162	4390	4392	4396	rBV4	307	228	0.02%	0.003%
99	15.361	4451	4454	4458	rVB4	386	297	0.03%	0.005%
100	15.866	4607	4611	4614	rBV4	502	433	0.05%	0.007%

Sum of corrected areas: 6583600

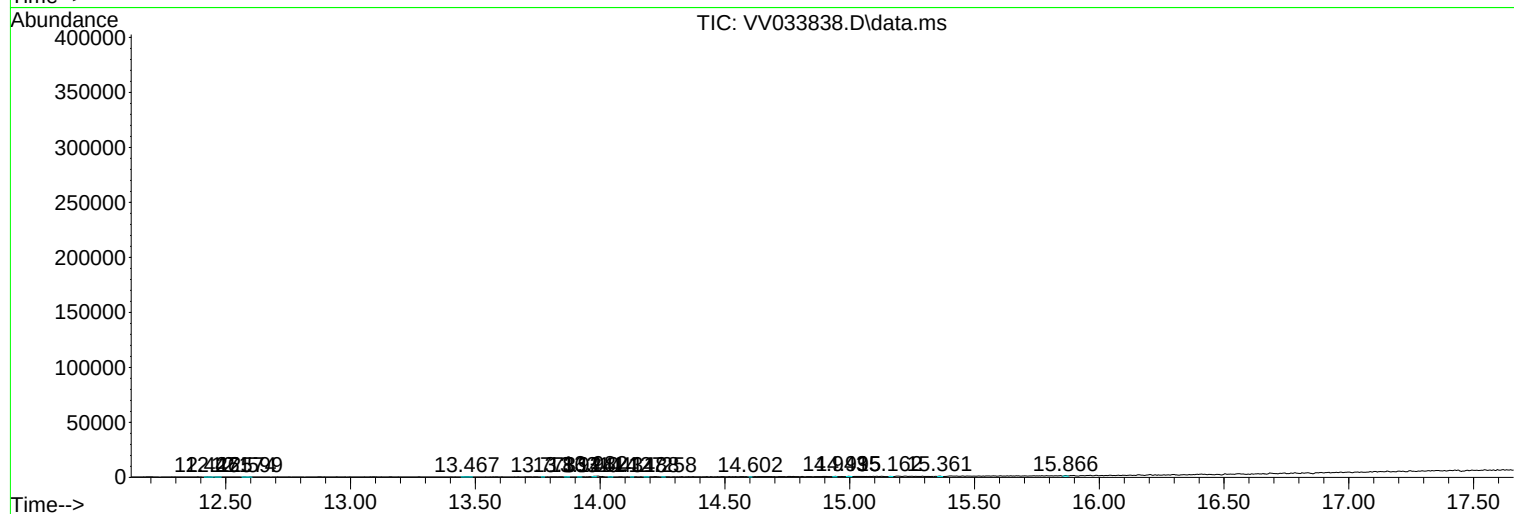
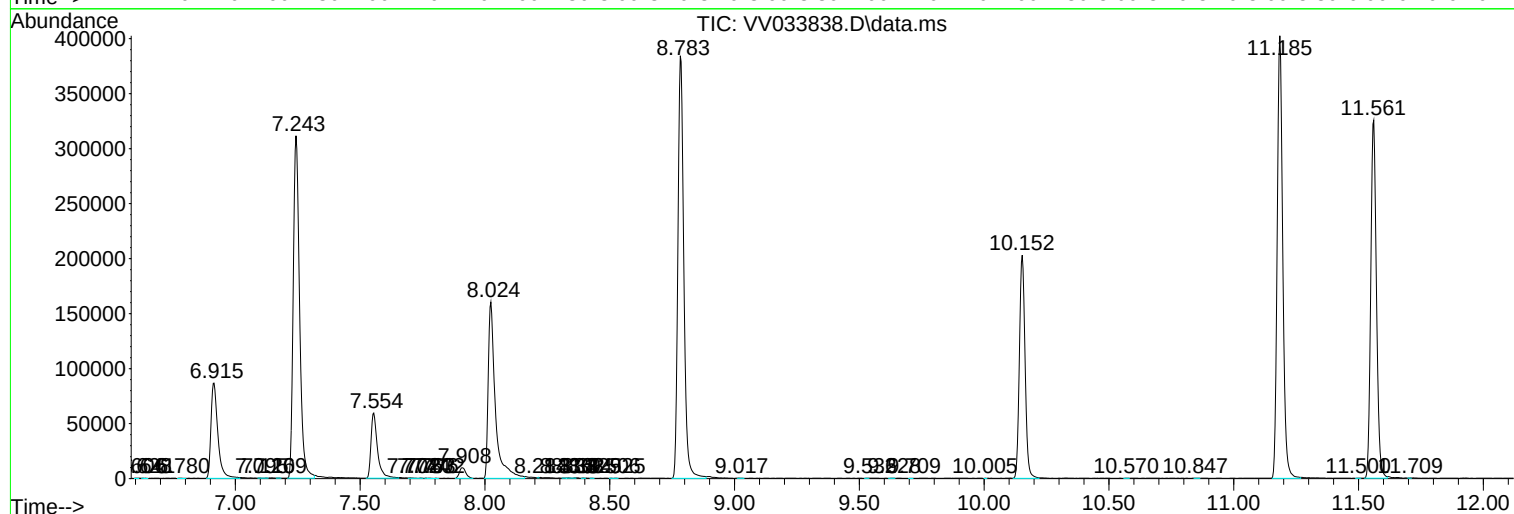
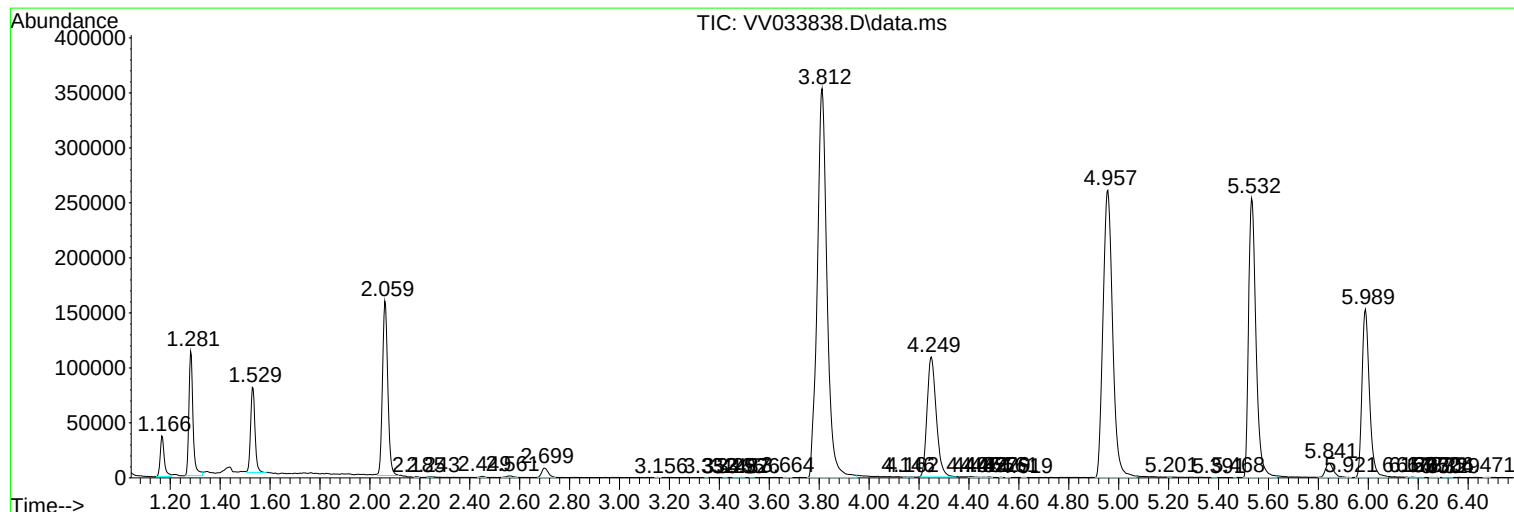
Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
Data File : VV033838.D
Acq On : 23 Jan 2024 18:45
Operator : SY/MD
Sample : P1191-16 50X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMT0

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\VV012324\
Data File : VV033838.D
Acq On : 23 Jan 2024 18:45
Operator : SY/MD
Sample : P1191-16 50X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMT0

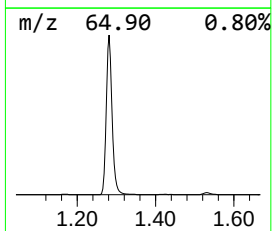
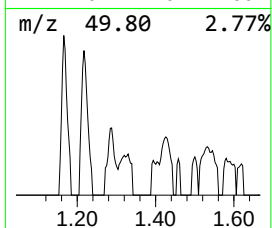
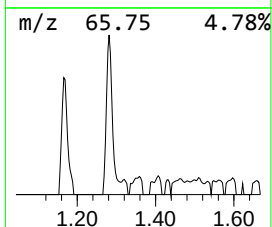
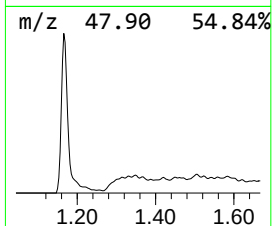
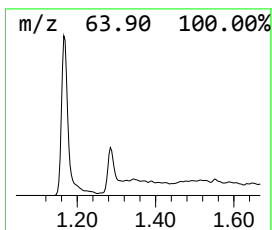
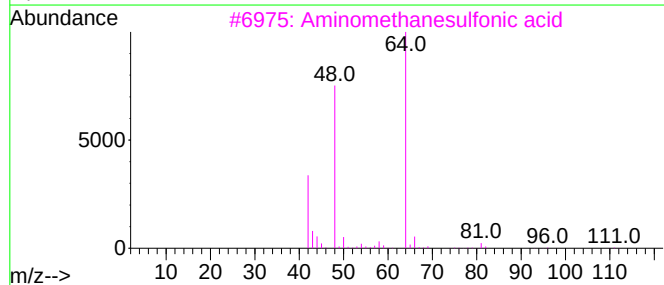
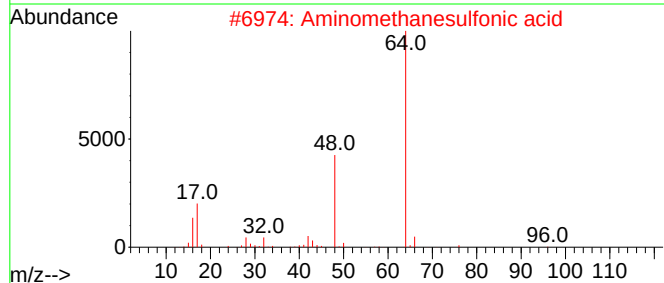
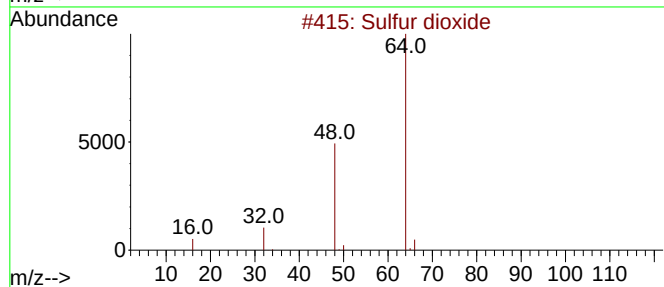
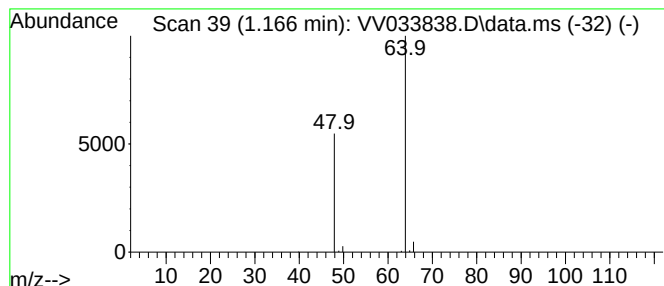
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	4.00 ug/L	42045	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	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
Data File : VV033838.D
Acq On : 23 Jan 2024 18:45
Operator : SY/MD
Sample : P1191-16 50X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMT0

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	4.0	ug/L	42045	1	5.532	524956	50.0