

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033827.D
 Acq On : 23 Jan 2024 14:00
 Operator : SY/MD
 Sample : P1191-11
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ1

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: VV033827.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	52	rBV	45978	53732	7.04%	0.879%
2	1.282	68	75	91	rBV	99100	113237	14.83%	1.852%
3	1.532	146	153	167	rVB	87804	106050	13.89%	1.735%
4	2.060	307	317	333	rVB	181004	263606	34.53%	4.312%
5	2.179	352	354	356	rBV2	365	222	0.03%	0.004%
6	2.243	369	374	377	rBV2	730	760	0.10%	0.012%
7	2.503	452	455	457	rBV2	161	117	0.02%	0.002%
8	2.568	472	475	476	rBV	350	157	0.02%	0.003%
9	2.703	513	517	522	rBV3	623	639	0.08%	0.010%
10	2.892	569	576	577	rBV2	155	177	0.02%	0.003%
11	2.947	587	593	596	rBV2	177	169	0.02%	0.003%
12	3.146	652	655	659	rVB2	222	169	0.02%	0.003%
13	3.169	659	662	667	rBV2	164	210	0.03%	0.003%
14	3.240	681	684	686	rBV	168	121	0.02%	0.002%
15	3.381	722	728	732	rBV2	252	351	0.05%	0.006%
16	3.516	766	770	775	rBV2	300	322	0.04%	0.005%
17	3.584	786	791	794	rBV2	205	275	0.04%	0.004%
18	3.616	798	801	808	rBV2	246	312	0.04%	0.005%
19	3.658	808	814	819	rVB	198	267	0.03%	0.004%
20	3.683	819	822	825	rBB2	182	112	0.01%	0.002%
21	3.703	825	828	830	rBV	170	129	0.02%	0.002%
22	3.786	845	854	896	rBV3	48341	172651	22.62%	2.824%
23	3.995	917	919	923	rVB2	306	179	0.02%	0.003%
24	4.088	945	948	953	rVB2	290	213	0.03%	0.003%
25	4.249	982	998	1035	rBV	119227	304482	39.89%	4.981%
26	4.413	1047	1049	1055	rVB3	364	237	0.03%	0.004%
27	4.551	1090	1092	1096	rBV	297	186	0.02%	0.003%
28	4.957	1202	1218	1252	rBV2	283677	763392	100.00%	12.488%
29	5.301	1322	1325	1328	rBV2	243	199	0.03%	0.003%
30	5.352	1338	1341	1345	rBV	207	208	0.03%	0.003%
31	5.477	1376	1380	1383	rVB2	348	333	0.04%	0.005%
32	5.532	1386	1397	1432	rBV	255985	524348	68.69%	8.578%
33	5.744	1460	1463	1472	rBV3	267	356	0.05%	0.006%
34	5.780	1472	1474	1477	rVB2	209	121	0.02%	0.002%
35	5.844	1483	1494	1504	rBV7	5562	11669	1.53%	0.191%
36	5.899	1510	1511	1515	rBV3	164	114	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033827.D
 Acq On : 23 Jan 2024 14:00
 Operator : SY/MD
 Sample : P1191-11
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ1

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	5.989	1525	1539	1566	rBV	166163	343096	44.94%	5.613%
38	6.162	1590	1593	1597	rVB3	437	347	0.05%	0.006%
39	6.564	1714	1718	1722	rVB2	140	115	0.02%	0.002%
40	6.754	1769	1777	1781	rBV2	216	393	0.05%	0.006%
41	6.860	1807	1810	1814	rBV	206	155	0.02%	0.003%
42	6.915	1814	1827	1853	rBV	96992	180997	23.71%	2.961%
43	7.111	1885	1888	1891	rVB2	352	223	0.03%	0.004%
44	7.143	1891	1898	1899	rBV2	455	414	0.05%	0.007%
45	7.156	1899	1902	1904	rBV2	235	145	0.02%	0.002%
46	7.185	1908	1911	1915	rVB2	336	220	0.03%	0.004%
47	7.243	1917	1929	1956	rBV	356134	621260	81.38%	10.163%
48	7.506	2009	2011	2017	rVB2	279	166	0.02%	0.003%
49	7.555	2017	2026	2047	rBV	64960	116517	15.26%	1.906%
50	7.725	2076	2079	2082	rBV3	381	266	0.03%	0.004%
51	7.754	2082	2088	2094	rBV3	295	408	0.05%	0.007%
52	7.847	2114	2117	2119	rBV	159	107	0.01%	0.002%
53	7.876	2119	2126	2129	rBV2	551	709	0.09%	0.012%
54	7.911	2129	2137	2151	rVB3	7820	13681	1.79%	0.224%
55	7.966	2151	2154	2163	rVB2	204	283	0.04%	0.005%
56	8.024	2163	2172	2217	rBV	165844	328542	43.04%	5.375%
57	8.365	2276	2278	2283	rVB3	381	279	0.04%	0.005%
58	8.397	2283	2288	2295	rBV	280	366	0.05%	0.006%
59	8.783	2397	2408	2442	rBV	383449	634114	83.07%	10.373%
60	8.973	2465	2467	2470	rVV2	260	156	0.02%	0.003%
61	9.063	2491	2495	2499	rVB	192	145	0.02%	0.002%
62	9.133	2513	2517	2523	rBV2	228	310	0.04%	0.005%
63	9.239	2545	2550	2553	rBV	185	181	0.02%	0.003%
64	9.355	2582	2586	2587	rBV2	212	155	0.02%	0.003%
65	9.641	2671	2675	2678	rBV2	203	151	0.02%	0.002%
66	10.153	2823	2834	2858	rBV	217571	337850	44.26%	5.527%
67	10.320	2880	2886	2887	rBV2	672	556	0.07%	0.009%
68	10.413	2912	2915	2917	rBV	196	119	0.02%	0.002%
69	10.738	3013	3016	3019	rBV	150	104	0.01%	0.002%
70	10.866	3053	3056	3062	rVB2	255	270	0.04%	0.004%
71	11.104	3127	3130	3134	rBV	146	138	0.02%	0.002%
72	11.185	3144	3155	3179	rBV	406322	629255	82.43%	10.294%
73	11.288	3186	3187	3192	rVB3	350	203	0.03%	0.003%
74	11.561	3260	3272	3300	rBV	358870	575220	75.35%	9.410%
75	11.709	3316	3318	3322	rVB2	347	230	0.03%	0.004%
76	11.728	3322	3324	3327	rBV2	201	116	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033827.D
 Acq On : 23 Jan 2024 14:00
 Operator : SY/MD
 Sample : P1191-11
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ1

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	11.802	3344	3347	3353	rBV	163	147	0.02%	0.002%
78	11.847	3358	3361	3367	rVB2	176	158	0.02%	0.003%
79	12.271	3490	3493	3496	rBV2	155	117	0.02%	0.002%
80	12.522	3568	3571	3575	rBV2	151	109	0.01%	0.002%
81	12.808	3656	3660	3665	rBV	164	170	0.02%	0.003%
82	12.853	3669	3674	3679	rBV2	221	296	0.04%	0.005%
83	13.172	3770	3773	3778	rBV2	164	155	0.02%	0.003%
84	13.265	3796	3802	3807	rBV2	231	331	0.04%	0.005%
85	13.455	3855	3861	3862	rBV2	278	296	0.04%	0.005%
86	13.506	3874	3877	3882	rBV2	144	157	0.02%	0.003%
87	13.908	3997	4002	4004	rBV2	199	213	0.03%	0.003%
88	14.046	4042	4045	4047	rBV2	226	142	0.02%	0.002%
89	14.066	4047	4051	4054	rBV2	192	190	0.02%	0.003%
90	14.162	4078	4081	4084	rBV	173	122	0.02%	0.002%
91	14.287	4118	4120	4121	rBV	353	123	0.02%	0.002%
92	14.361	4139	4143	4147	rBV3	268	322	0.04%	0.005%
93	14.471	4175	4177	4182	rVB	332	172	0.02%	0.003%
94	14.500	4182	4186	4188	rBV2	425	321	0.04%	0.005%
95	14.558	4201	4204	4206	rBV	291	161	0.02%	0.003%
96	14.818	4283	4285	4288	rVB	349	169	0.02%	0.003%
97	14.882	4302	4305	4308	rBV3	254	215	0.03%	0.004%
98	14.963	4327	4330	4333	rBV3	425	275	0.04%	0.004%
99	15.069	4361	4363	4366	rBV2	285	195	0.03%	0.003%
100	15.139	4381	4385	4389	rBV3	454	524	0.07%	0.009%

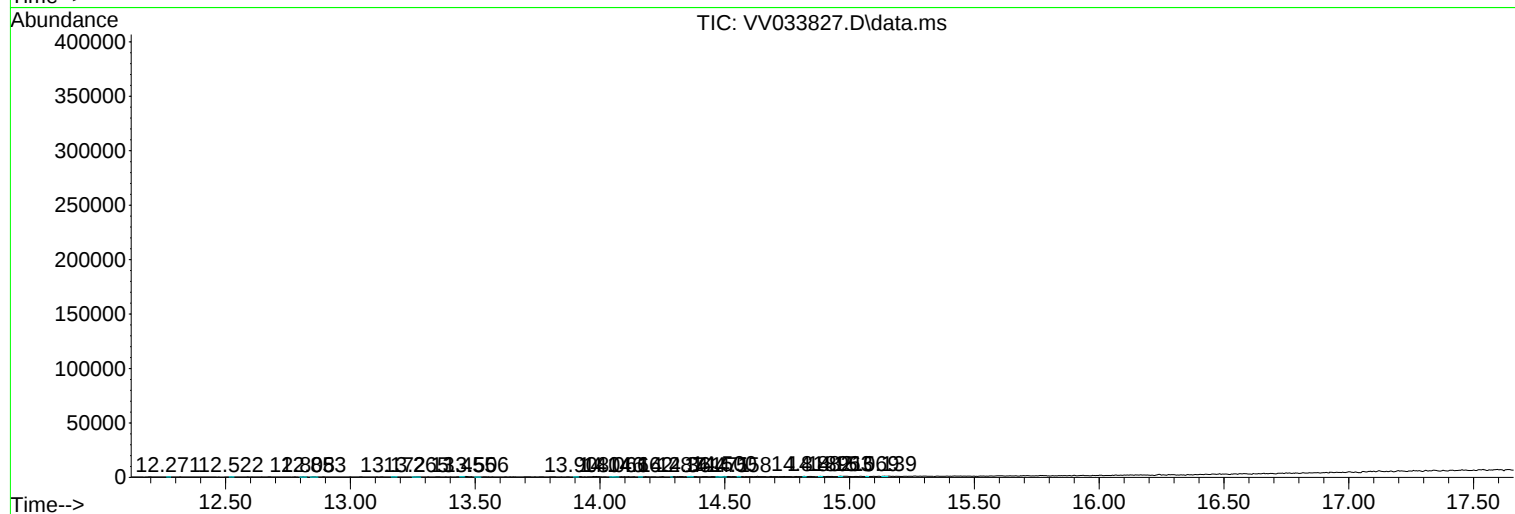
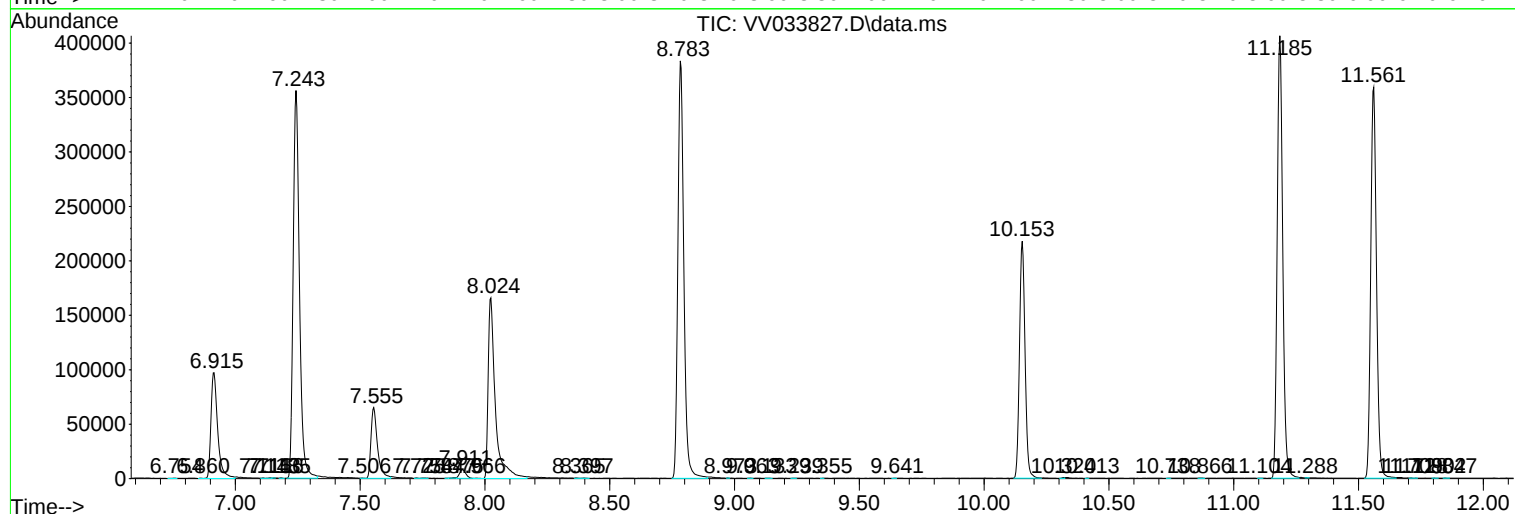
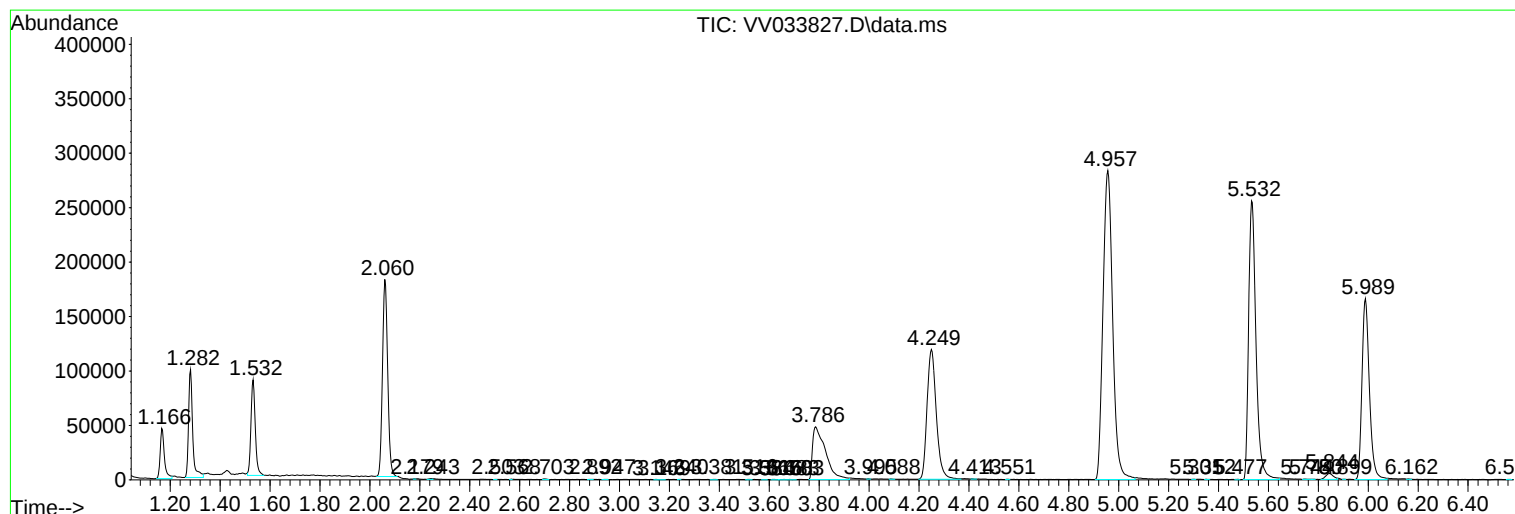
Sum of corrected areas: 6112864

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
Data File : VV033827.D
Acq On : 23 Jan 2024 14:00
Operator : SY/MD
Sample : P1191-11
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMQ1

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 : VV033827.D
Acq On : 23 Jan 2024 14:00
Operator : SY/MD
Sample : P1191-11
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMQ1

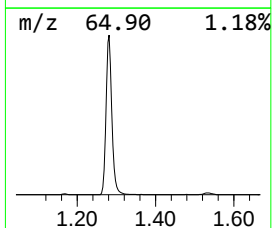
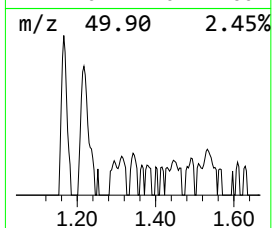
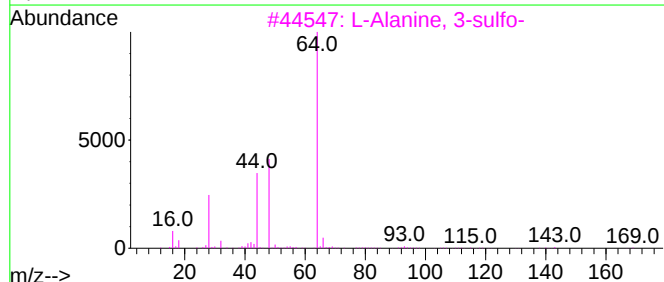
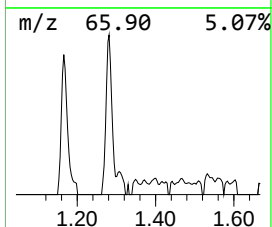
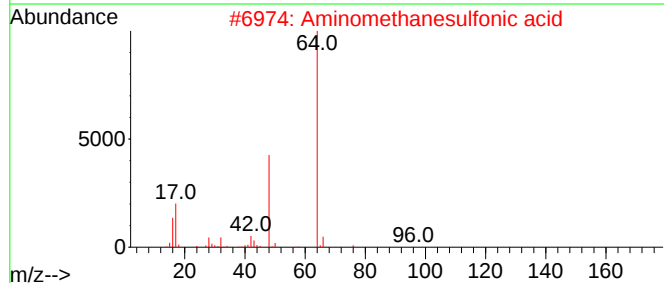
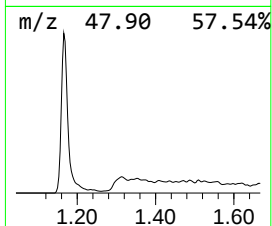
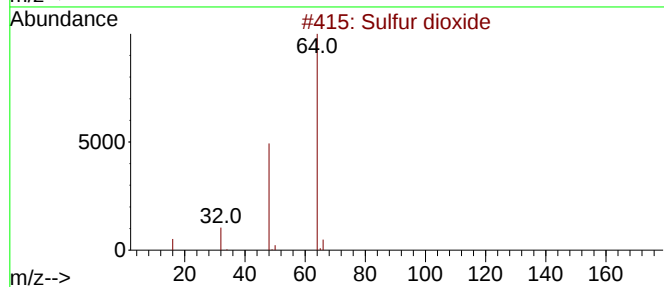
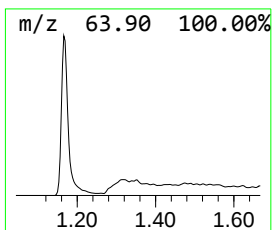
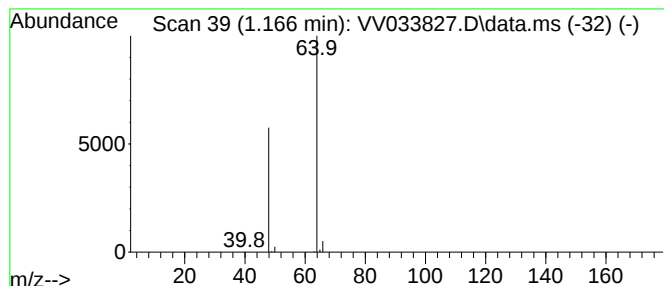
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	5.12 ug/L	53732	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
Data File : VV033827.D
Acq On : 23 Jan 2024 14:00
Operator : SY/MD
Sample : P1191-11
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMQ1

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	5.1	ug/L	53732	1	5.532	524348	50.0