

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
 Data File : VV033893.D
 Acq On : 26 Jan 2024 17:57
 Operator : SY/MD
 Sample : P1252-05
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMS6

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: VV033893.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	53	rBV	76337	85815	11.09%	1.238%
2	1.282	67	75	111	rBV3	278538	420478	54.36%	6.064%
3	1.529	145	152	168	rVB	83266	106181	13.73%	1.531%
4	2.060	307	317	345	rVB	175385	276434	35.74%	3.987%
5	2.233	363	371	385	rVB5	2223	4597	0.59%	0.066%
6	2.288	385	388	391	rBV3	266	164	0.02%	0.002%
7	2.320	396	398	405	rVB3	235	176	0.02%	0.003%
8	2.439	433	435	437	rBV	290	205	0.03%	0.003%
9	2.513	454	458	463	rVV2	252	262	0.03%	0.004%
10	2.564	466	474	476	rBV3	528	693	0.09%	0.010%
11	2.699	508	516	528	rBV2	5923	10334	1.34%	0.149%
12	2.931	584	588	591	rBV2	185	185	0.02%	0.003%
13	3.079	631	634	636	rBV2	177	132	0.02%	0.002%
14	3.198	667	671	675	rBV	185	154	0.02%	0.002%
15	3.310	703	706	710	rBV2	270	176	0.02%	0.003%
16	3.355	716	720	723	rBV	275	216	0.03%	0.003%
17	3.433	740	744	747	rBV2	155	141	0.02%	0.002%
18	3.510	766	768	776	rVB2	332	395	0.05%	0.006%
19	3.558	776	783	787	rVB	307	395	0.05%	0.006%
20	3.587	787	792	797	rBV2	252	389	0.05%	0.006%
21	3.625	801	804	809	rVB2	273	251	0.03%	0.004%
22	3.658	809	814	820	rBV	179	282	0.04%	0.004%
23	3.690	821	824	828	rVB2	252	186	0.02%	0.003%
24	3.812	845	862	893	rBV2	280385	773458	100.00%	11.155%
25	4.159	967	970	974	rBV2	482	357	0.05%	0.005%
26	4.179	974	976	980	rVV3	318	252	0.03%	0.004%
27	4.249	982	998	1031	rVV	109165	277673	35.90%	4.005%
28	4.494	1071	1074	1081	rVB3	477	455	0.06%	0.007%
29	4.561	1093	1095	1099	rVB3	268	159	0.02%	0.002%
30	4.638	1116	1119	1123	rBV3	287	246	0.03%	0.004%
31	4.687	1130	1134	1138	rVB	253	167	0.02%	0.002%
32	4.899	1196	1200	1202	rBV2	185	152	0.02%	0.002%
33	4.957	1202	1218	1248	rBV2	262898	693685	89.69%	10.005%
34	5.375	1346	1348	1352	rVB2	187	151	0.02%	0.002%
35	5.532	1386	1397	1426	rBV	275741	560399	72.45%	8.082%
36	5.719	1452	1455	1461	rBV2	313	254	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
 Data File : VV033893.D
 Acq On : 26 Jan 2024 17:57
 Operator : SY/MD
 Sample : P1252-05
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMS6

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	5.844	1485	1494	1508	rBV6	7149	14914	1.93%	0.215%
38	5.989	1527	1539	1566	rVV	152235	315256	40.76%	4.547%
39	6.108	1574	1576	1579	rVB2	420	197	0.03%	0.003%
40	6.159	1589	1592	1598	rVB5	562	574	0.07%	0.008%
41	6.227	1610	1613	1616	rBV2	230	136	0.02%	0.002%
42	6.445	1678	1681	1685	rVB2	312	258	0.03%	0.004%
43	6.468	1685	1688	1693	rBV2	241	263	0.03%	0.004%
44	6.606	1724	1731	1733	rBV2	171	212	0.03%	0.003%
45	6.722	1762	1767	1773	rVB2	162	179	0.02%	0.003%
46	6.915	1816	1827	1856	rBV	89607	164138	21.22%	2.367%
47	7.124	1890	1892	1895	rBV	253	146	0.02%	0.002%
48	7.169	1902	1906	1908	rBV2	268	167	0.02%	0.002%
49	7.243	1918	1929	1954	rBV	309721	547332	70.76%	7.894%
50	7.555	2016	2026	2052	rBV	59432	105348	13.62%	1.519%
51	7.866	2120	2123	2125	rBV	226	185	0.02%	0.003%
52	7.915	2135	2138	2142	rBV2	270	187	0.02%	0.003%
53	7.989	2157	2161	2163	rBV	186	177	0.02%	0.003%
54	8.024	2163	2172	2211	rBV	192505	353249	45.67%	5.095%
55	8.294	2253	2256	2260	rBV3	283	269	0.03%	0.004%
56	8.423	2293	2296	2301	rVB2	243	211	0.03%	0.003%
57	8.448	2301	2304	2306	rBV2	252	176	0.02%	0.003%
58	8.542	2330	2333	2340	rBV	234	161	0.02%	0.002%
59	8.786	2397	2409	2456	rBV	409614	685261	88.60%	9.883%
60	9.027	2481	2484	2489	rBV2	208	211	0.03%	0.003%
61	9.146	2515	2521	2525	rBV2	198	260	0.03%	0.004%
62	9.297	2565	2568	2570	rBV2	198	129	0.02%	0.002%
63	9.342	2576	2582	2583	rBV	174	147	0.02%	0.002%
64	9.825	2728	2732	2735	rBV2	192	153	0.02%	0.002%
65	9.892	2749	2753	2759	rBV2	167	202	0.03%	0.003%
66	9.979	2776	2780	2786	rBV2	186	253	0.03%	0.004%
67	10.153	2823	2834	2861	rBV	213324	336160	43.46%	4.848%
68	10.304	2878	2881	2882	rBV	274	159	0.02%	0.002%
69	10.323	2883	2887	2896	rVB3	610	753	0.10%	0.011%
70	10.365	2896	2900	2904	rBV2	169	185	0.02%	0.003%
71	10.487	2934	2938	2942	rBV3	310	219	0.03%	0.003%
72	10.683	2995	2999	3003	rBV3	276	262	0.03%	0.004%
73	10.834	3042	3046	3050	rBV	179	153	0.02%	0.002%
74	10.915	3069	3071	3078	rVB2	188	142	0.02%	0.002%
75	11.005	3096	3099	3102	rBV2	207	163	0.02%	0.002%
76	11.185	3145	3155	3180	rBV	427062	671544	86.82%	9.685%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
 Data File : VV033893.D
 Acq On : 26 Jan 2024 17:57
 Operator : SY/MD
 Sample : P1252-05
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMS6

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	11.374	3209	3214	3220	rVB3	290	387	0.05%	0.006%
78	11.407	3220	3224	3228	rBV2	164	149	0.02%	0.002%
79	11.561	3260	3272	3293	rBV	325470	512244	66.23%	7.388%
80	11.728	3322	3324	3327	rVB2	289	143	0.02%	0.002%
81	11.902	3375	3378	3383	rBV2	160	133	0.02%	0.002%
82	12.046	3420	3423	3427	rBB2	212	164	0.02%	0.002%
83	12.506	3563	3566	3574	rBV2	254	329	0.04%	0.005%
84	12.937	3697	3700	3703	rVB	269	177	0.02%	0.003%
85	12.963	3703	3708	3713	rBV2	294	352	0.05%	0.005%
86	13.361	3829	3832	3837	rBV2	196	177	0.02%	0.003%
87	13.503	3872	3876	3878	rBV	174	140	0.02%	0.002%
88	13.693	3933	3935	3938	rVB	322	179	0.02%	0.003%
89	13.988	4024	4027	4028	rBV2	395	165	0.02%	0.002%
90	14.017	4033	4036	4045	rVB	452	449	0.06%	0.006%
91	14.059	4045	4049	4050	rBV	200	144	0.02%	0.002%
92	14.172	4081	4084	4086	rBV2	238	160	0.02%	0.002%
93	14.323	4128	4131	4134	rVB2	435	320	0.04%	0.005%
94	14.342	4134	4137	4142	rBV2	302	330	0.04%	0.005%
95	14.365	4142	4144	4147	rBV2	288	187	0.02%	0.003%
96	14.503	4183	4187	4190	rBV3	225	202	0.03%	0.003%
97	15.107	4371	4375	4380	rBV3	512	391	0.05%	0.006%
98	15.188	4398	4400	4402	rBV2	367	182	0.02%	0.003%
99	15.525	4503	4505	4509	rVB2	270	132	0.02%	0.002%
100	15.824	4595	4598	4602	rBV3	692	653	0.08%	0.009%

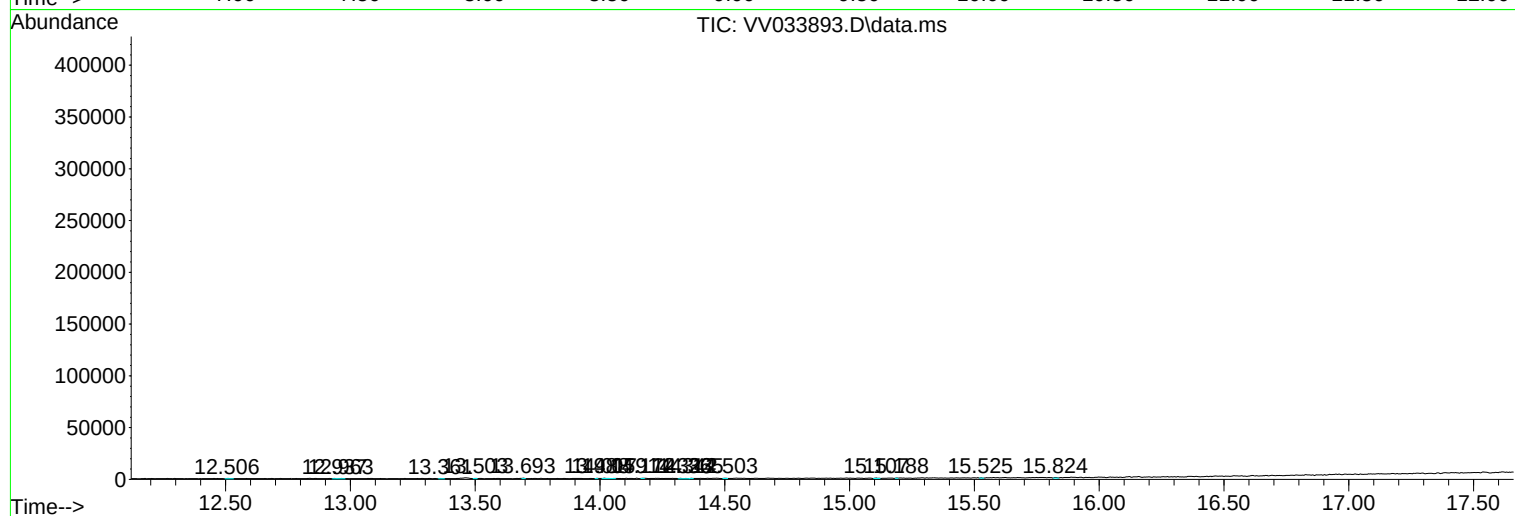
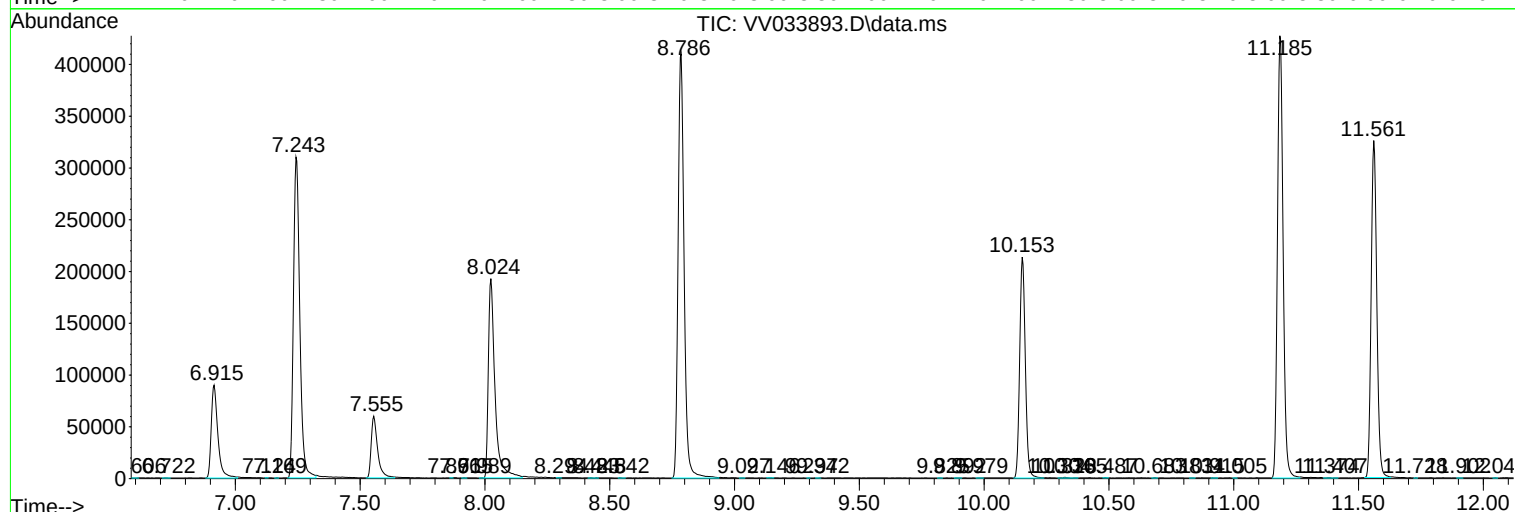
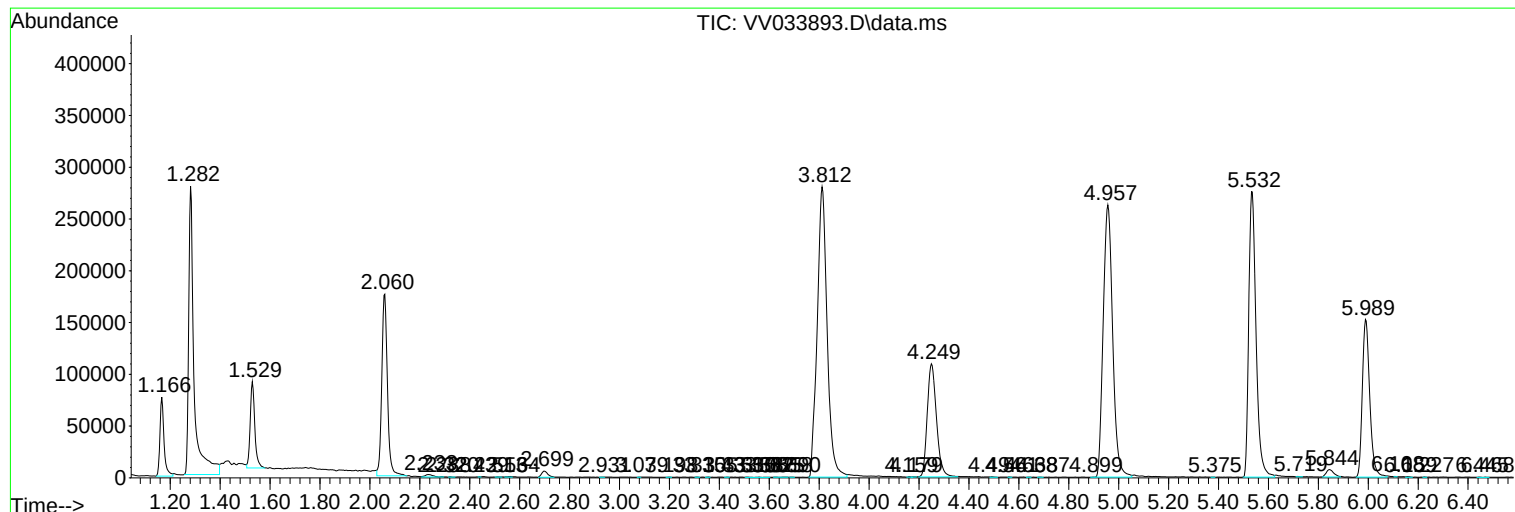
Sum of corrected areas: 6933629

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
Data File : VV033893.D
Acq On : 26 Jan 2024 17:57
Operator : SY/MD
Sample : P1252-05
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS6

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\VV012624\
Data File : VV033893.D
Acq On : 26 Jan 2024 17:57
Operator : SY/MD
Sample : P1252-05
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS6

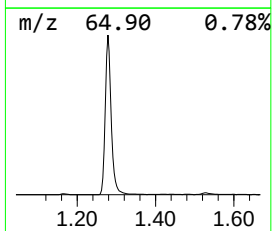
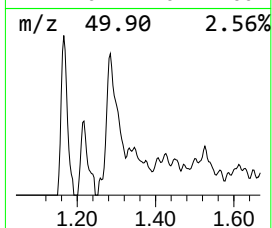
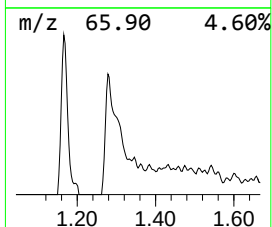
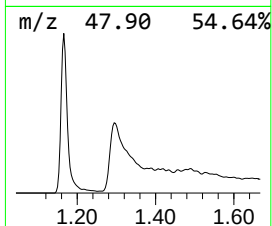
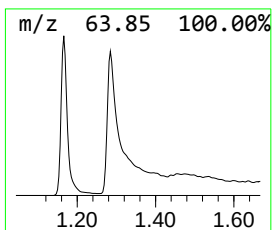
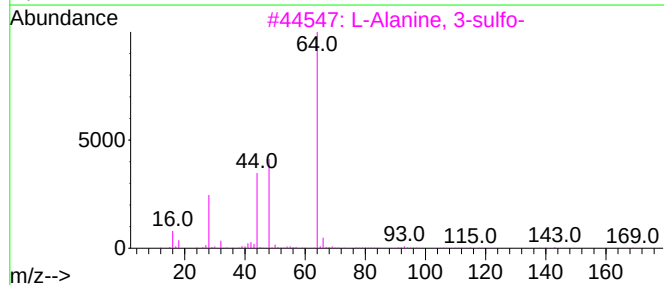
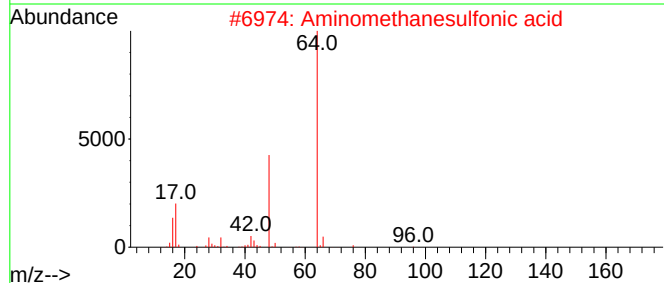
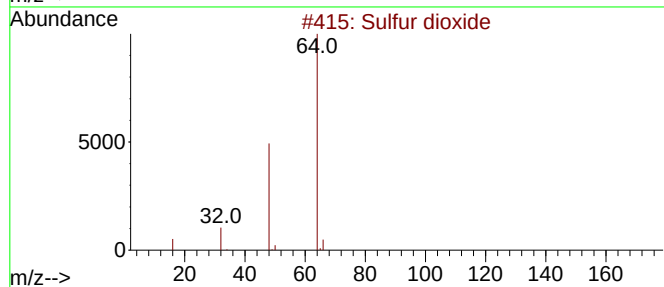
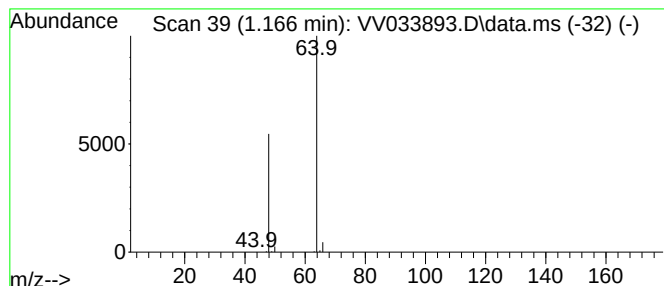
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	7.66 ug/L	85815	1,4-Difluorobenzene	5.535

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\VV012624\
Data File : VV033893.D
Acq On : 26 Jan 2024 17:57
Operator : SY/MD
Sample : P1252-05
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS6

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	7.7	ug/L	85815	1	5.535	560399	50.0