

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045229.D
 Acq On : 07 Oct 2021 23:52
 Operator : SY/MD
 Sample : M4138-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F5

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: VU045229.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	31	39	54	rBV	188396	302390	23.19%	2.944%
2	1.597	75	80	105	rVB	182564	219937	16.87%	2.141%
3	1.893	164	172	191	rVB	135402	184890	14.18%	1.800%
4	2.562	368	380	397	rBV	242318	406372	31.16%	3.957%
5	2.713	424	427	431	rBV	239	168	0.01%	0.002%
6	2.781	439	448	464	rVB3	3585	7593	0.58%	0.074%
7	2.951	493	501	504	rBV2	392	467	0.04%	0.005%
8	3.022	519	523	526	rBV	169	148	0.01%	0.001%
9	3.044	527	530	531	rBV	269	187	0.01%	0.002%
10	3.186	564	574	587	rBV2	1695	3998	0.31%	0.039%
11	3.282	602	604	608	rVB2	195	139	0.01%	0.001%
12	3.314	608	614	615	rBV	241	162	0.01%	0.002%
13	3.363	627	629	635	rVB	197	165	0.01%	0.002%
14	3.453	652	657	659	rVV2	177	171	0.01%	0.002%
15	3.597	697	702	706	rBV	198	270	0.02%	0.003%
16	3.691	724	731	735	rBV2	172	194	0.01%	0.002%
17	3.745	743	748	750	rVV2	173	176	0.01%	0.002%
18	3.758	750	752	759	rVB2	237	204	0.02%	0.002%
19	3.803	763	766	772	rVB2	241	212	0.02%	0.002%
20	3.845	775	779	782	rBV2	164	143	0.01%	0.001%
21	3.996	821	826	829	rBV2	144	152	0.01%	0.001%
22	4.099	853	858	863	rBV2	249	313	0.02%	0.003%
23	4.157	869	876	884	rVB2	167	300	0.02%	0.003%
24	4.192	884	887	891	rBV	211	214	0.02%	0.002%
25	4.244	899	903	905	rBV	171	151	0.01%	0.001%
26	4.359	935	939	941	rBV	201	159	0.01%	0.002%
27	4.414	950	956	960	rBV2	205	286	0.02%	0.003%
28	4.478	973	976	980	rBV	249	183	0.01%	0.002%
29	4.514	983	987	990	rBV	219	237	0.02%	0.002%
30	4.629	1008	1023	1051	rBV	146872	345434	26.49%	3.363%
31	4.858	1090	1094	1098	rBV2	175	180	0.01%	0.002%
32	4.893	1103	1105	1110	rVB3	192	194	0.01%	0.002%
33	4.999	1135	1138	1142	rVV	252	257	0.02%	0.003%
34	5.067	1142	1159	1185	rVV	229850	500471	38.38%	4.873%
35	5.173	1188	1192	1198	rVB2	392	422	0.03%	0.004%
36	5.289	1222	1228	1230	rBV2	437	538	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045229.D
 Acq On : 07 Oct 2021 23:52
 Operator : SY/MD
 Sample : M4138-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F5

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	5.729	1341	1365	1387	rBV2	484824	1304068	100.00%	12.697%
38	6.038	1457	1461	1463	rBV2	283	222	0.02%	0.002%
39	6.115	1482	1485	1486	rBV2	236	155	0.01%	0.002%
40	6.157	1493	1498	1504	rBV3	361	431	0.03%	0.004%
41	6.253	1511	1528	1547	rBV	374611	696974	53.45%	6.786%
42	6.533	1609	1615	1621	rVB6	1446	2155	0.17%	0.021%
43	6.694	1651	1665	1689	rBV	304767	597996	45.86%	5.822%
44	6.813	1697	1702	1710	rVB4	904	1043	0.08%	0.010%
45	7.051	1769	1776	1783	rVB	652	775	0.06%	0.008%
46	7.099	1788	1791	1794	rBV2	173	150	0.01%	0.001%
47	7.124	1794	1799	1804	rBV2	131	144	0.01%	0.001%
48	7.182	1811	1817	1830	rVB4	1475	2151	0.16%	0.021%
49	7.462	1898	1904	1905	rBV2	227	203	0.02%	0.002%
50	7.568	1924	1937	1956	rBV	166325	285113	21.86%	2.776%
51	7.690	1968	1975	1978	rBV4	1009	1379	0.11%	0.013%
52	7.719	1980	1984	1991	rVB6	1565	2095	0.16%	0.020%
53	7.803	2004	2010	2013	rVV2	299	389	0.03%	0.004%
54	7.903	2026	2041	2054	rBV	599617	1004621	77.04%	9.781%
55	7.973	2054	2063	2078	rVB	35224	60589	4.65%	0.590%
56	8.182	2116	2128	2145	rVV	116493	193039	14.80%	1.879%
57	8.243	2145	2147	2154	rVB3	335	321	0.02%	0.003%
58	8.440	2206	2208	2212	rVB	237	164	0.01%	0.002%
59	8.472	2212	2218	2219	rBV	775	727	0.06%	0.007%
60	8.636	2257	2269	2299	rBV	431130	760940	58.35%	7.409%
61	8.931	2357	2361	2364	rBV2	168	169	0.01%	0.002%
62	9.099	2410	2413	2418	rVB	177	154	0.01%	0.001%
63	9.420	2499	2513	2546	rBV	538274	871984	66.87%	8.490%
64	9.571	2551	2560	2576	rBV	19141	30051	2.30%	0.293%
65	9.693	2587	2598	2612	rBV	62650	102707	7.88%	1.000%
66	9.912	2663	2666	2670	rBV	184	200	0.02%	0.002%
67	10.105	2715	2726	2739	rBV2	15524	24187	1.85%	0.235%
68	10.501	2841	2849	2850	rBV	269	364	0.03%	0.004%
69	10.536	2857	2860	2864	rBV2	187	229	0.02%	0.002%
70	10.594	2873	2878	2881	rBV2	206	229	0.02%	0.002%
71	10.674	2894	2903	2911	rBV3	2360	3416	0.26%	0.033%
72	10.761	2917	2930	2949	rVB	436451	699236	53.62%	6.808%
73	10.886	2967	2969	2970	rBV	384	184	0.01%	0.002%
74	10.896	2970	2972	2976	rVB4	620	366	0.03%	0.004%
75	10.960	2989	2992	2998	rVV2	193	240	0.02%	0.002%
76	11.002	2998	3005	3010	rVV3	638	998	0.08%	0.010%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045229.D
 Acq On : 07 Oct 2021 23:52
 Operator : SY/MD
 Sample : M4138-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F5

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	11.028	3010	3013	3022	rVB	352	422	0.03%	0.004%
78	11.092	3030	3033	3039	rVB2	495	421	0.03%	0.004%
79	11.118	3039	3041	3046	rBV2	382	245	0.02%	0.002%
80	11.295	3093	3096	3099	rBV	229	222	0.02%	0.002%
81	11.382	3119	3123	3126	rBV2	214	158	0.01%	0.002%
82	11.468	3138	3150	3161	rVB5	2805	4888	0.37%	0.048%
83	11.623	3195	3198	3205	rVB3	830	956	0.07%	0.009%
84	11.700	3216	3222	3227	rVB4	1131	1358	0.10%	0.013%
85	11.816	3245	3258	3279	rBV	492432	762063	58.44%	7.420%
86	11.941	3293	3297	3302	rBV4	759	872	0.07%	0.008%
87	11.973	3302	3307	3315	rVB2	1679	2262	0.17%	0.022%
88	12.028	3321	3324	3328	rBV2	188	150	0.01%	0.001%
89	12.066	3328	3336	3344	rBV4	2238	3776	0.29%	0.037%
90	12.195	3360	3376	3393	rBV	524043	857193	65.73%	8.346%
91	12.336	3417	3420	3426	rVB3	554	433	0.03%	0.004%
92	12.517	3462	3476	3483	rVB6	1836	3567	0.27%	0.035%
93	12.552	3483	3487	3489	rBV	175	161	0.01%	0.002%
94	12.623	3505	3509	3510	rBV	216	164	0.01%	0.002%
95	12.832	3568	3574	3580	rVB3	878	1342	0.10%	0.013%
96	13.041	3637	3639	3644	rBV	162	145	0.01%	0.001%
97	13.266	3705	3709	3712	rVB	248	196	0.02%	0.002%
98	13.462	3766	3770	3774	rBV	242	318	0.02%	0.003%
99	14.066	3955	3958	3959	rBV	275	157	0.01%	0.002%
100	14.092	3962	3966	3974	rVB2	1204	1428	0.11%	0.014%

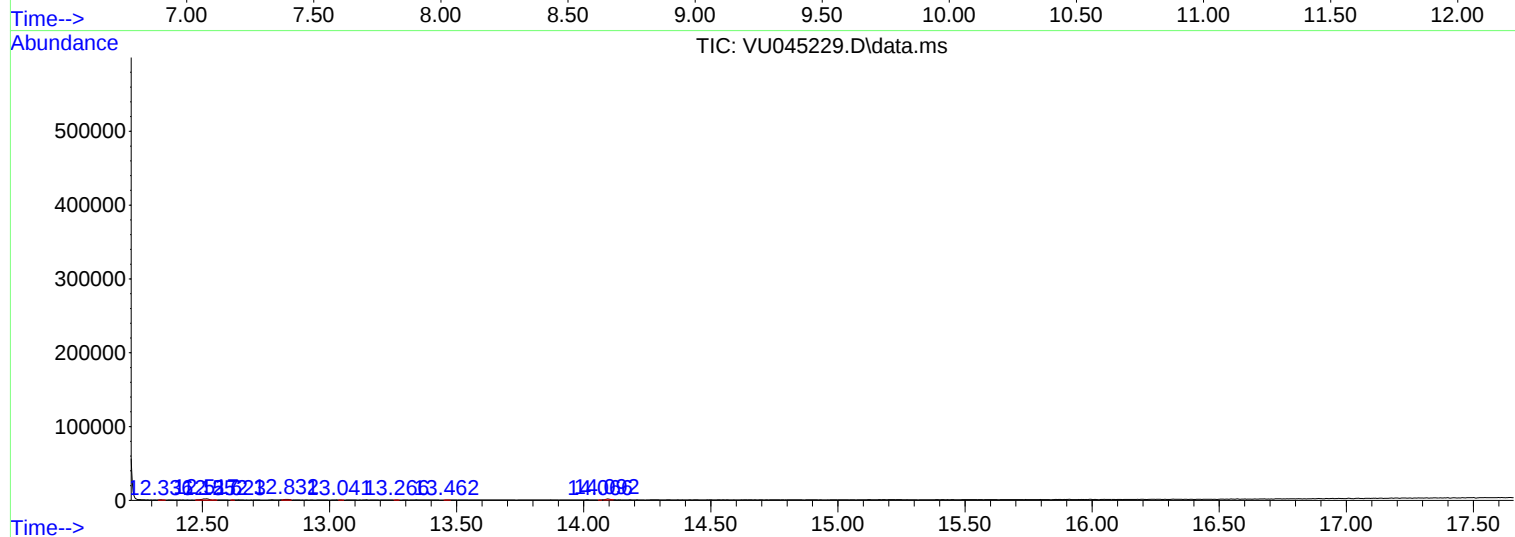
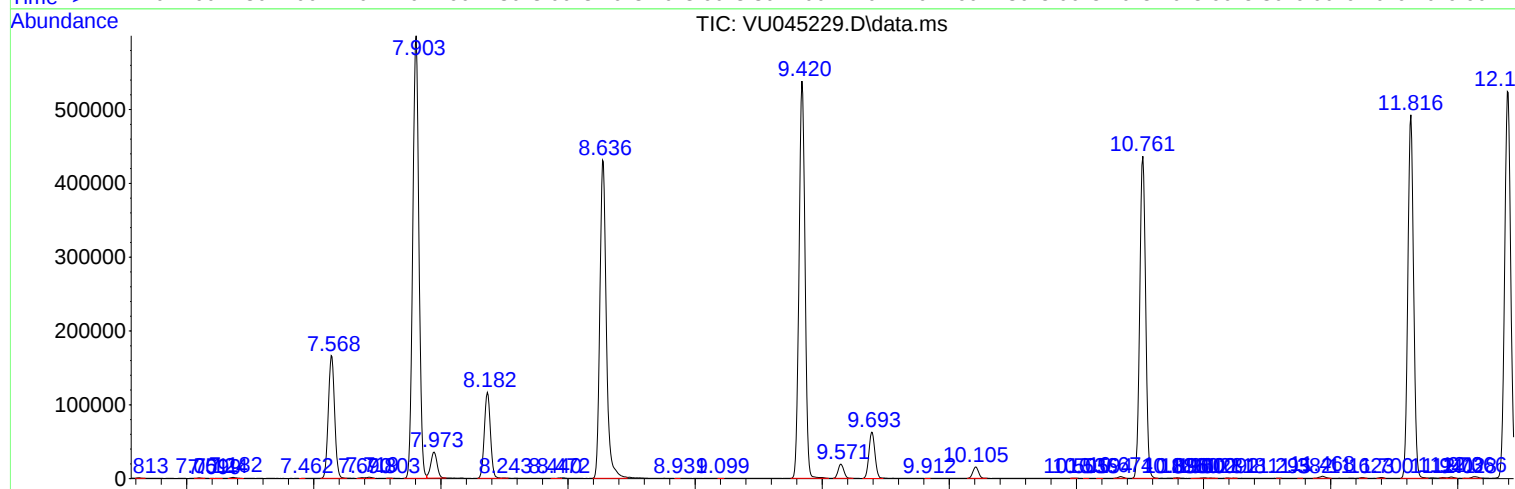
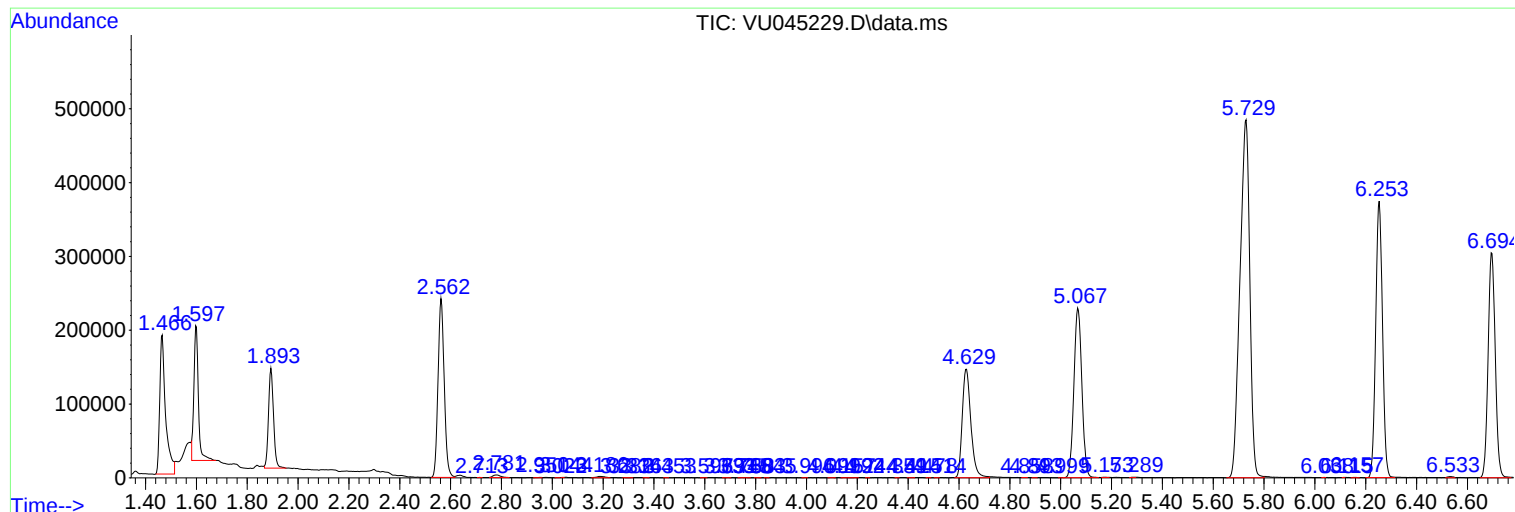
Sum of corrected areas: 10270932

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045229.D
Acq On : 07 Oct 2021 23:52
Operator : SY/MD
Sample : M4138-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F5

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\VU100721\
Data File : VU045229.D
Acq On : 07 Oct 2021 23:52
Operator : SY/MD
Sample : M4138-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F5

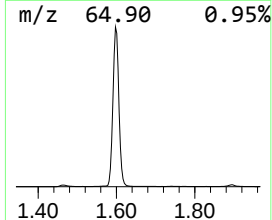
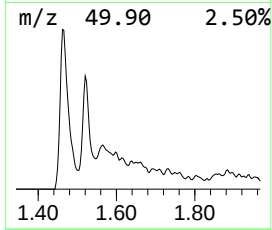
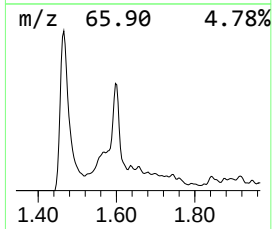
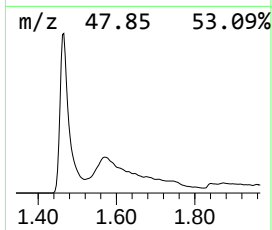
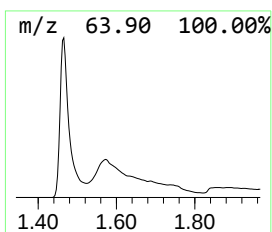
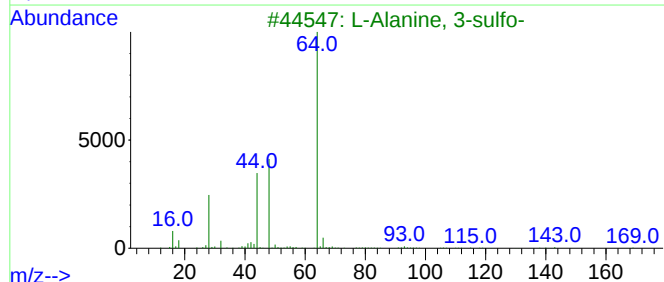
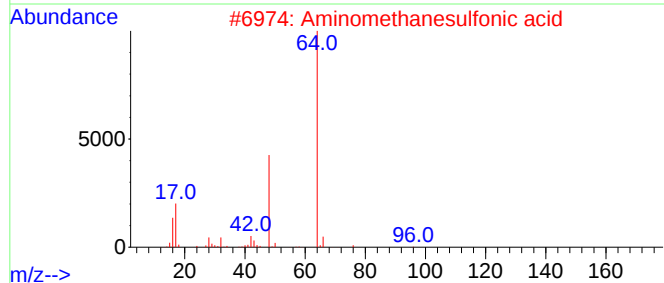
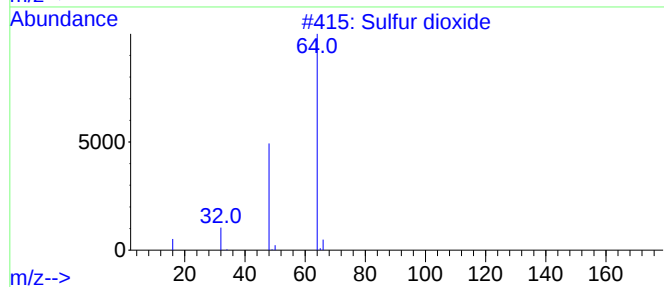
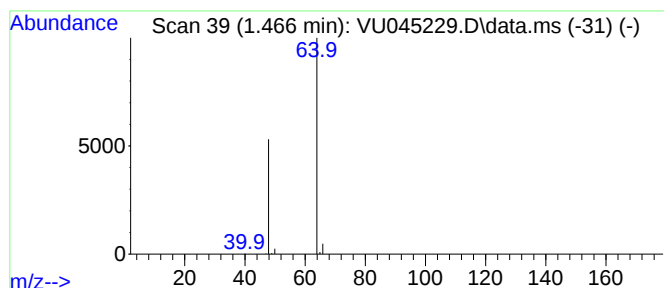
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	21.69 ug/L	302390	1,4-Difluorobenzene	6.253

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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045229.D
Acq On : 07 Oct 2021 23:52
Operator : SY/MD
Sample : M4138-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7F5

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	1.466	21.7	ug/L	302390	1	6.253	696974	50.0