

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081221\
 Data File : VX023669.D
 Acq On : 12 Aug 2021 13:04
 Operator : JC/MD
 Sample : M3364-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK95

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_X\Method\SFAMXML081121WMA.M
 Title : VOC Analysis

Signal : TIC: VX023669.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	27	32	42	rBV	30393	85926	8.71%	1.090%
2	1.368	43	46	53	rVB	102407	111735	11.32%	1.418%
3	1.666	91	95	102	rVB	81144	103239	10.46%	1.310%
4	2.307	194	200	209	rBV	193477	321318	32.56%	4.077%
5	2.386	209	213	222	rVB	8641	16025	1.62%	0.203%
6	2.453	222	224	226	rBV2	450	384	0.04%	0.005%
7	2.502	230	232	233	rBV	497	495	0.05%	0.006%
8	2.764	274	275	276	rBV	508	318	0.03%	0.004%
9	2.947	300	305	319	rVB2	4892	12023	1.22%	0.153%
10	3.117	331	333	336	rBV2	308	372	0.04%	0.005%
11	3.282	358	360	362	rBV2	304	268	0.03%	0.003%
12	3.465	388	390	394	rBV2	238	376	0.04%	0.005%
13	4.014	477	480	481	rBV	428	393	0.04%	0.005%
14	4.233	512	516	517	rBV2	572	709	0.07%	0.009%
15	4.373	537	539	540	rVB	451	234	0.02%	0.003%
16	4.465	545	554	567	rBV	92322	258415	26.19%	3.279%
17	5.068	641	653	667	rVV	128235	388732	39.39%	4.932%
18	5.391	703	706	708	rBV	496	484	0.05%	0.006%
19	5.458	715	717	718	rBV2	264	222	0.02%	0.003%
20	5.501	722	724	725	rBV	308	261	0.03%	0.003%
21	5.653	743	749	750	rBV3	246	249	0.03%	0.003%
22	5.800	771	773	776	rBV3	182	229	0.02%	0.003%
23	5.977	790	802	819	rBV2	333350	986770	100.00%	12.520%
24	6.202	837	839	842	rVB2	379	350	0.04%	0.004%
25	6.233	842	844	847	rBV	251	274	0.03%	0.003%
26	6.361	858	865	873	rBV5	1002	2653	0.27%	0.034%
27	6.470	879	883	887	rVB3	259	403	0.04%	0.005%
28	6.605	902	905	907	rBV3	458	613	0.06%	0.008%
29	6.769	920	932	943	rBV	294607	684131	69.33%	8.680%
30	6.976	965	966	969	rBV2	248	279	0.03%	0.004%
31	7.111	982	988	995	rBV4	2581	5844	0.59%	0.074%
32	7.190	999	1001	1003	rBV	308	290	0.03%	0.004%
33	7.318	1011	1022	1032	rBV	205500	454837	46.09%	5.771%
34	7.586	1064	1066	1068	rVV	425	445	0.05%	0.006%
35	7.696	1082	1084	1087	rBV2	298	397	0.04%	0.005%
36	7.720	1087	1088	1093	rVB2	338	401	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081221\
 Data File : VX023669.D
 Acq On : 12 Aug 2021 13:04
 Operator : JC/MD
 Sample : M3364-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK95

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_X\Method\SFAMXML081121WMA.M
 Title : VOC Analysis

37	7.818	1099	1104	1108	rVV2	475	1087	0.11%	0.014%
38	7.934	1115	1123	1128	rBV3	2279	4223	0.43%	0.054%
39	8.001	1131	1134	1136	rBV2	294	341	0.03%	0.004%
40	8.080	1143	1147	1148	rVB	232	267	0.03%	0.003%
41	8.330	1181	1188	1199	rBV	133826	216801	21.97%	2.751%
42	8.470	1206	1211	1216	rBV3	1511	2568	0.26%	0.033%
43	8.653	1234	1241	1249	rBV	521935	797191	80.79%	10.115%
44	8.726	1249	1253	1259	rVB	7603	11539	1.17%	0.146%
45	8.952	1284	1290	1303	rBV	96435	146036	14.80%	1.853%
46	9.153	1319	1323	1326	rBV4	216	368	0.04%	0.005%
47	9.202	1330	1331	1334	rBV	379	260	0.03%	0.003%
48	9.275	1339	1343	1348	rBV3	1144	1581	0.16%	0.020%
49	9.391	1356	1362	1378	rBV	407582	590291	59.82%	7.490%
50	9.756	1419	1422	1425	rBV	443	445	0.05%	0.006%
51	9.781	1425	1426	1430	rVB2	315	293	0.03%	0.004%
52	10.055	1465	1471	1483	rBV	595951	809722	82.06%	10.274%
53	10.244	1499	1502	1505	rBV4	460	687	0.07%	0.009%
54	10.305	1507	1512	1517	rVB4	1273	2056	0.21%	0.026%
55	10.354	1517	1520	1521	rVB2	348	227	0.02%	0.003%
56	10.378	1521	1524	1525	rBV	318	439	0.04%	0.006%
57	10.537	1548	1550	1553	rVV3	300	356	0.04%	0.005%
58	10.640	1564	1567	1570	rBV2	510	701	0.07%	0.009%
59	10.921	1609	1613	1615	rBV2	255	361	0.04%	0.005%
60	11.122	1642	1646	1652	rVV2	3715	4673	0.47%	0.059%
61	11.195	1652	1658	1666	rBV	379537	476625	48.30%	6.047%
62	11.451	1696	1700	1701	rBV2	664	654	0.07%	0.008%
63	11.543	1713	1715	1721	rBV4	388	602	0.06%	0.008%
64	11.634	1728	1730	1735	rVB3	569	592	0.06%	0.008%
65	11.707	1740	1742	1743	rBV	293	284	0.03%	0.004%
66	11.750	1745	1749	1757	rVB3	3144	4523	0.46%	0.057%
67	11.847	1760	1765	1771	rVB4	928	1856	0.19%	0.024%
68	11.933	1771	1779	1784	rBV5	1828	3325	0.34%	0.042%
69	12.024	1789	1794	1800	rBV	582059	697743	70.71%	8.853%
70	12.219	1823	1826	1830	rBV3	779	1233	0.12%	0.016%
71	12.323	1837	1843	1853	rVB	518686	647821	65.65%	8.220%
72	12.427	1857	1860	1864	rBV3	1068	1368	0.14%	0.017%
73	12.488	1866	1870	1872	rVB3	769	1027	0.10%	0.013%
74	12.579	1882	1885	1886	rBV3	266	279	0.03%	0.004%
75	12.817	1921	1924	1927	rVB2	450	511	0.05%	0.006%
76	12.853	1927	1930	1936	rVB2	329	609	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081221\
 Data File : VX023669.D
 Acq On : 12 Aug 2021 13:04
 Operator : JC/MD
 Sample : M3364-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK95

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_X\Method\SFAMXML081121WMA.M
 Title : VOC Analysis

77	12.914	1939	1940	1943	rVB	313	298	0.03%	0.004%
78	12.951	1943	1946	1950	rBV3	319	494	0.05%	0.006%
79	13.012	1954	1956	1959	rVB2	390	408	0.04%	0.005%
80	13.061	1959	1964	1969	rVB4	809	1141	0.12%	0.014%
81	13.116	1969	1973	1975	rBV2	446	549	0.06%	0.007%
82	13.402	2017	2020	2021	rBV2	340	412	0.04%	0.005%
83	13.652	2059	2061	2063	rVB	405	301	0.03%	0.004%
84	13.683	2063	2066	2067	rBV2	317	297	0.03%	0.004%
85	13.719	2070	2072	2074	rVV2	253	249	0.03%	0.003%
86	13.780	2078	2082	2085	rBV2	706	972	0.10%	0.012%
87	13.902	2100	2102	2106	rVB	416	419	0.04%	0.005%
88	14.036	2121	2124	2126	rVB2	295	318	0.03%	0.004%
89	14.061	2126	2128	2130	rBV2	292	247	0.03%	0.003%
90	14.182	2145	2148	2150	rBV2	212	333	0.03%	0.004%
91	14.249	2156	2159	2160	rBV2	273	260	0.03%	0.003%
92	14.359	2175	2177	2178	rBV2	331	268	0.03%	0.003%
93	14.451	2190	2192	2193	rVB2	327	230	0.02%	0.003%
94	14.597	2214	2216	2219	rBV3	232	269	0.03%	0.003%
95	14.877	2260	2262	2265	rVB2	503	375	0.04%	0.005%
96	15.377	2342	2344	2345	rBV2	596	362	0.04%	0.005%
97	15.963	2438	2440	2442	rVV3	523	233	0.02%	0.003%
98	15.987	2442	2444	2449	rVB3	510	554	0.06%	0.007%
99	16.188	2476	2477	2480	rBV2	334	264	0.03%	0.003%
100	16.749	2567	2569	2573	rBV3	445	548	0.06%	0.007%

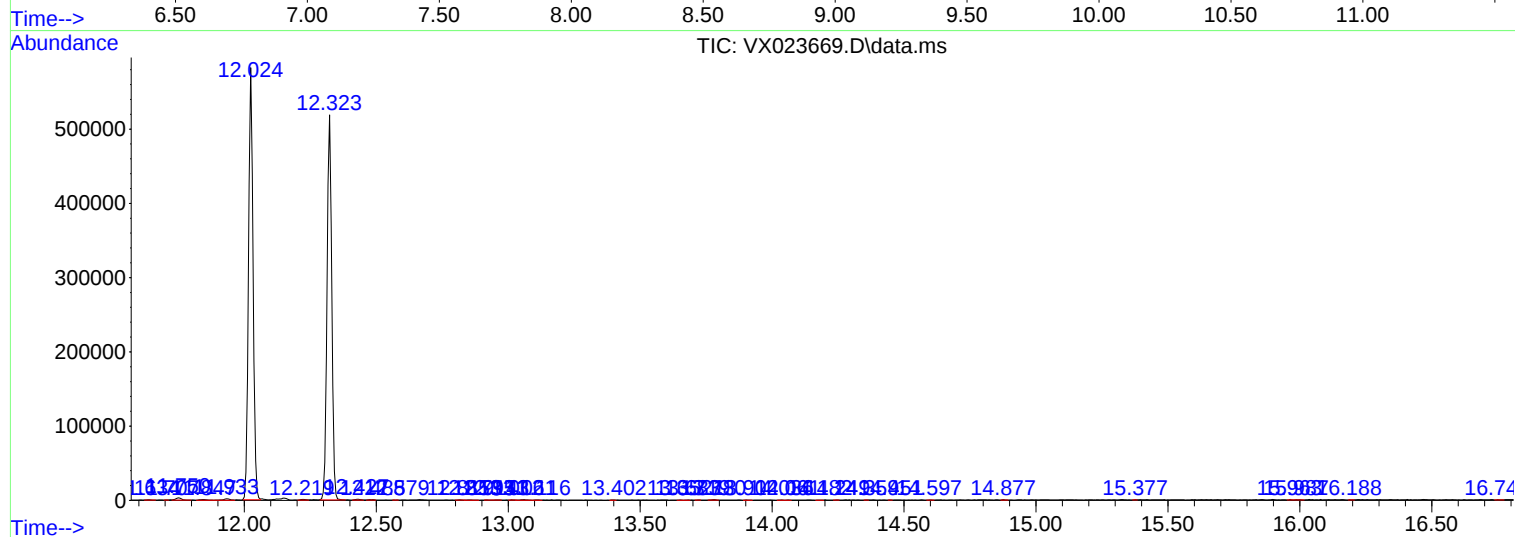
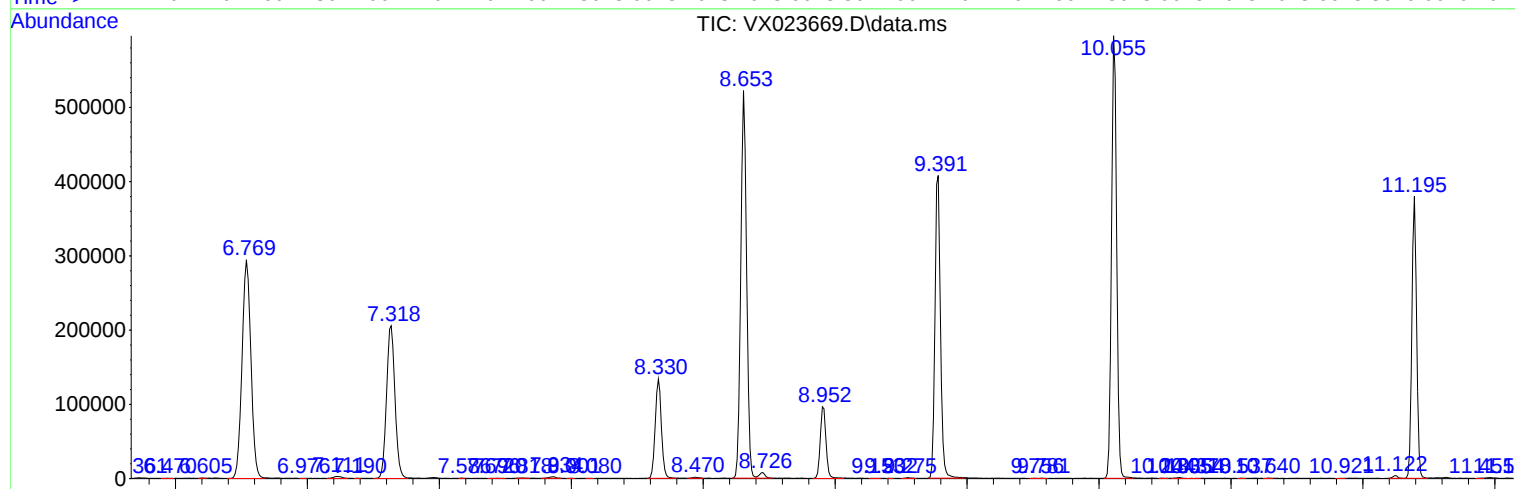
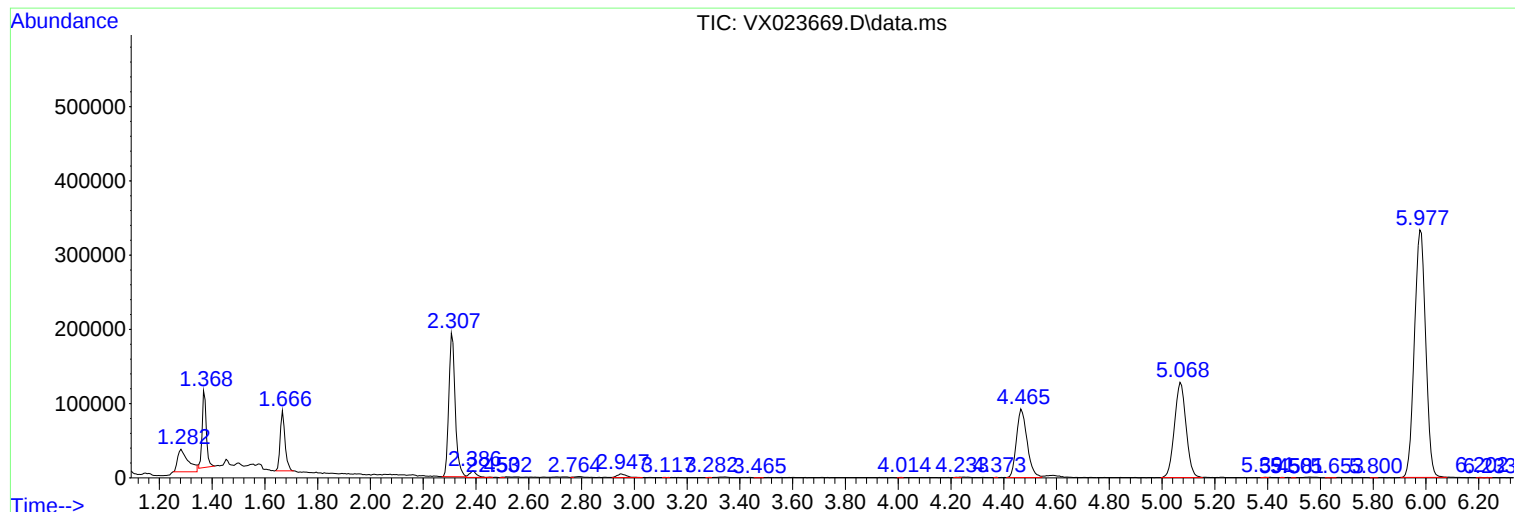
Sum of corrected areas: 7881460

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081221\
Data File : VX023669.D
Acq On : 12 Aug 2021 13:04
Operator : JC/MD
Sample : M3364-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DBK95

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081221\
Data File : VX023669.D
Acq On : 12 Aug 2021 13:04
Operator : JC/MD
Sample : M3364-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DBK95

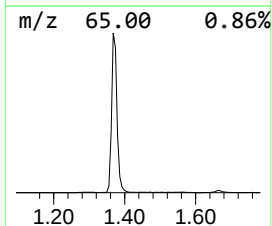
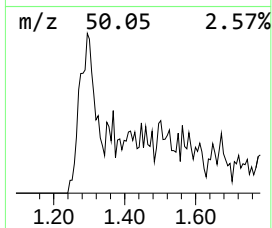
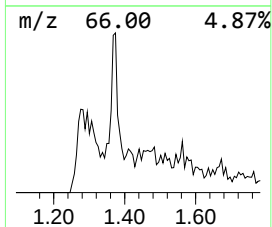
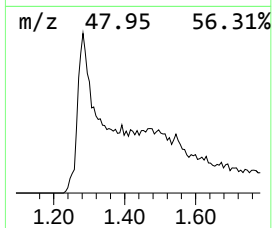
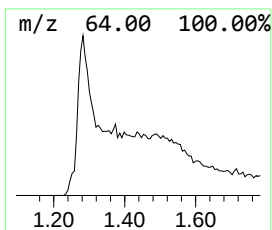
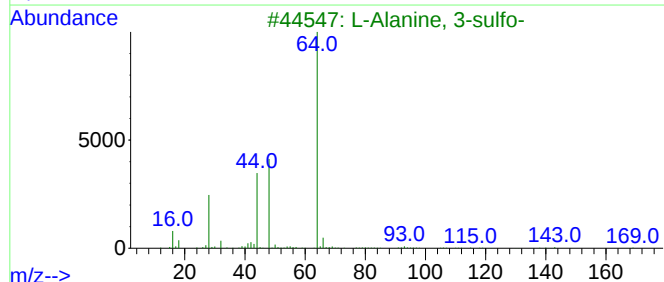
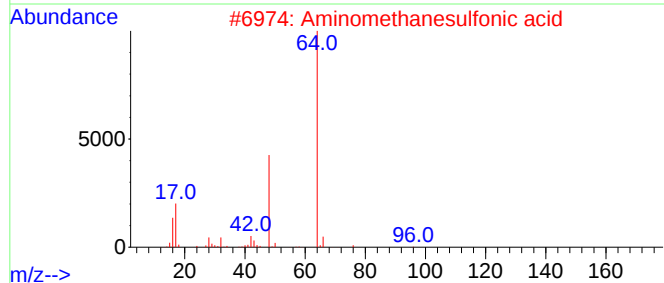
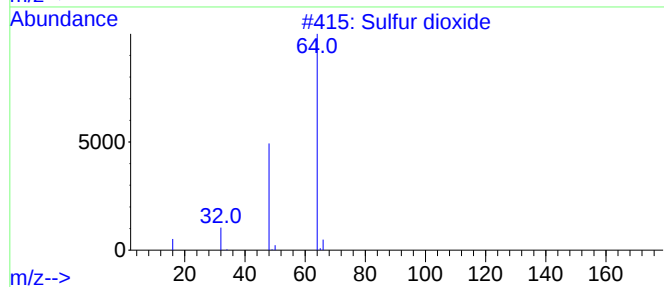
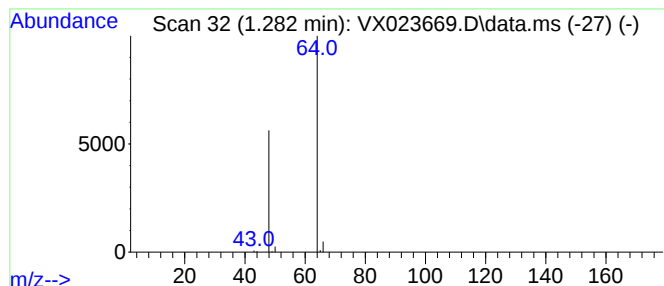
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.M
Quant Title : VOC Analysis

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.
1.282	6.28 ug/L	85926	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
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_X\Data\VX081221\
Data File : VX023669.D
Acq On : 12 Aug 2021 13:04
Operator : JC/MD
Sample : M3364-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DBK95

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.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	1.282	6.3	ug/L	85926	1	6.769	684131	50.0