

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053631.D
 Acq On : 11 Apr 2023 13:36
 Operator : JC/MD
 Sample : 02251-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD2

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	34	40	55	rBV	20984	34982	3.98%	0.511%
2	1.597	74	80	94	rBV	92238	105240	11.96%	1.536%
3	1.909	170	177	195	rVB	81639	114245	12.99%	1.668%
4	2.565	369	381	396	rBV	147954	243750	27.71%	3.559%
5	2.787	446	450	451	rBV	594	474	0.05%	0.007%
6	3.038	523	528	529	rBV2	501	417	0.05%	0.006%
7	3.311	610	613	616	rBV2	270	231	0.03%	0.003%
8	3.546	684	686	688	rBV	165	71	0.01%	0.001%
9	3.565	689	692	695	rVV	285	151	0.02%	0.002%
10	3.723	738	741	744	rBV	311	207	0.02%	0.003%
11	3.764	752	754	759	rVB	230	102	0.01%	0.001%
12	3.945	808	810	811	rBV	151	67	0.01%	0.001%
13	4.089	851	855	858	rBV	283	236	0.03%	0.003%
14	4.218	893	895	898	rBV	237	116	0.01%	0.002%
15	4.510	982	986	987	rBV	186	137	0.02%	0.002%
16	4.613	1006	1018	1046	rBV	62862	151772	17.25%	2.216%
17	4.896	1104	1106	1110	rBV2	323	235	0.03%	0.003%
18	4.919	1110	1113	1117	rVV2	273	277	0.03%	0.004%
19	4.990	1131	1135	1137	rBV	224	188	0.02%	0.003%
20	5.060	1140	1157	1177	rVV2	140426	311858	35.45%	4.553%
21	5.253	1215	1217	1218	rBV	170	44	0.01%	0.001%
22	5.305	1230	1233	1236	rVB2	291	212	0.02%	0.003%
23	5.321	1236	1238	1242	rBV	253	187	0.02%	0.003%
24	5.456	1277	1280	1283	rVB	321	160	0.02%	0.002%
25	5.485	1283	1289	1297	rBB2	270	433	0.05%	0.006%
26	5.578	1316	1318	1320	rVB	136	35	0.00%	0.001%
27	5.594	1320	1323	1327	rVB	202	114	0.01%	0.002%
28	5.616	1328	1330	1332	rBV	175	81	0.01%	0.001%
29	5.719	1341	1362	1397	rBV2	274352	789176	89.72%	11.522%
30	6.047	1461	1464	1469	rVB	223	146	0.02%	0.002%
31	6.073	1469	1472	1477	rBV2	188	147	0.02%	0.002%
32	6.134	1488	1491	1494	rVB	370	243	0.03%	0.004%
33	6.163	1495	1500	1501	rBV	176	177	0.02%	0.003%
34	6.243	1512	1525	1545	rBV	281864	529568	60.20%	7.731%
35	6.475	1593	1597	1601	rBV2	277	307	0.03%	0.004%
36	6.526	1609	1613	1616	rVB4	1113	824	0.09%	0.012%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053631.D
 Acq On : 11 Apr 2023 13:36
 Operator : JC/MD
 Sample : 02251-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD2

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\SFAMULM033123WMA.M
 Title : VOC Analysis

37	6.571	1625	1627	1629	rBV	172	80	0.01%	0.001%
38	6.684	1649	1662	1686	rBV	174210	341995	38.88%	4.993%
39	6.957	1744	1747	1751	rBV2	194	113	0.01%	0.002%
40	6.977	1751	1753	1756	rBV	177	125	0.01%	0.002%
41	7.079	1781	1785	1790	rVV2	281	275	0.03%	0.004%
42	7.102	1790	1792	1794	rVB	129	70	0.01%	0.001%
43	7.147	1803	1806	1810	rBV	242	160	0.02%	0.002%
44	7.189	1810	1819	1823	rBV4	1041	1321	0.15%	0.019%
45	7.234	1830	1833	1835	rBV	198	119	0.01%	0.002%
46	7.269	1842	1844	1846	rBV	173	68	0.01%	0.001%
47	7.317	1857	1859	1864	rVB	170	81	0.01%	0.001%
48	7.433	1891	1895	1898	rVB	406	314	0.04%	0.005%
49	7.514	1917	1920	1921	rBV	300	177	0.02%	0.003%
50	7.562	1923	1935	1955	rVV	97442	171524	19.50%	2.504%
51	7.893	2025	2038	2070	rBV	354296	611663	69.54%	8.930%
52	8.057	2087	2089	2090	rBV	271	80	0.01%	0.001%
53	8.079	2094	2096	2099	rBV	197	92	0.01%	0.001%
54	8.128	2109	2111	2112	rBV	280	109	0.01%	0.002%
55	8.176	2115	2126	2148	rVV	65670	112064	12.74%	1.636%
56	8.263	2150	2153	2154	rVV	218	120	0.01%	0.002%
57	8.279	2155	2158	2162	rVB	325	212	0.02%	0.003%
58	8.366	2182	2185	2189	rVB2	237	177	0.02%	0.003%
59	8.401	2193	2196	2198	rBV	195	102	0.01%	0.001%
60	8.430	2203	2205	2206	rBV	187	54	0.01%	0.001%
61	8.446	2207	2210	2211	rVV	386	238	0.03%	0.003%
62	8.468	2213	2217	2227	rVB3	1604	1945	0.22%	0.028%
63	8.552	2240	2243	2247	rVB	318	199	0.02%	0.003%
64	8.626	2252	2266	2306	rBV	189144	348992	39.67%	5.095%
65	8.893	2346	2349	2351	rBV	197	139	0.02%	0.002%
66	8.989	2376	2379	2382	rBV	347	212	0.02%	0.003%
67	9.063	2399	2402	2409	rBV2	393	488	0.06%	0.007%
68	9.208	2444	2447	2448	rBV2	190	114	0.01%	0.002%
69	9.304	2475	2477	2482	rVB2	454	350	0.04%	0.005%
70	9.330	2482	2485	2486	rBV	318	212	0.02%	0.003%
71	9.414	2498	2511	2539	rBV2	388106	790798	89.90%	11.545%
72	9.600	2566	2569	2574	rVB2	232	218	0.02%	0.003%
73	9.787	2624	2627	2630	rBV	258	161	0.02%	0.002%
74	9.935	2670	2673	2677	rVB	388	256	0.03%	0.004%
75	10.044	2705	2707	2711	rBV	220	162	0.02%	0.002%
76	10.166	2743	2745	2749	rVB	403	179	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053631.D
 Acq On : 11 Apr 2023 13:36
 Operator : JC/MD
 Sample : 02251-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD2

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\SFAMULM033123WMA.M
 Title : VOC Analysis

77	10.189	2750	2752	2753	rBV	162	54	0.01%	0.001%
78	10.234	2764	2766	2770	rBV	251	183	0.02%	0.003%
79	10.478	2840	2842	2846	rBV	414	304	0.03%	0.004%
80	10.674	2901	2903	2904	rBV	152	52	0.01%	0.001%
81	10.751	2915	2927	2944	rBV	263941	417888	47.51%	6.101%
82	10.886	2965	2969	2978	rVB3	1423	2017	0.23%	0.029%
83	10.996	3001	3003	3004	rBV3	131	39	0.00%	0.001%
84	11.246	3079	3081	3083	rBV	218	73	0.01%	0.001%
85	11.275	3088	3090	3093	rBV2	173	125	0.01%	0.002%
86	11.337	3106	3109	3112	rVB	292	174	0.02%	0.003%
87	11.356	3113	3115	3117	rBV	199	122	0.01%	0.002%
88	11.742	3226	3235	3244	rBV	25392	38902	4.42%	0.568%
89	11.809	3244	3256	3285	rVB2	427279	879636	100.00%	12.842%
90	12.092	3340	3344	3347	rBV3	1055	889	0.10%	0.013%
91	12.189	3362	3374	3398	rBV2	391792	801649	91.13%	11.704%
92	12.340	3420	3421	3423	rVB	313	75	0.01%	0.001%
93	12.877	3585	3588	3590	rBV	255	185	0.02%	0.003%
94	12.931	3603	3605	3609	rVB	490	295	0.03%	0.004%
95	13.070	3645	3648	3650	rBV	310	196	0.02%	0.003%
96	13.391	3746	3748	3750	rBV	218	116	0.01%	0.002%
97	13.841	3879	3888	3904	rVB4	14489	23997	2.73%	0.350%
98	14.333	4032	4041	4053	rVB5	5593	9884	1.12%	0.144%
99	14.381	4053	4056	4060	rBV	397	351	0.04%	0.005%

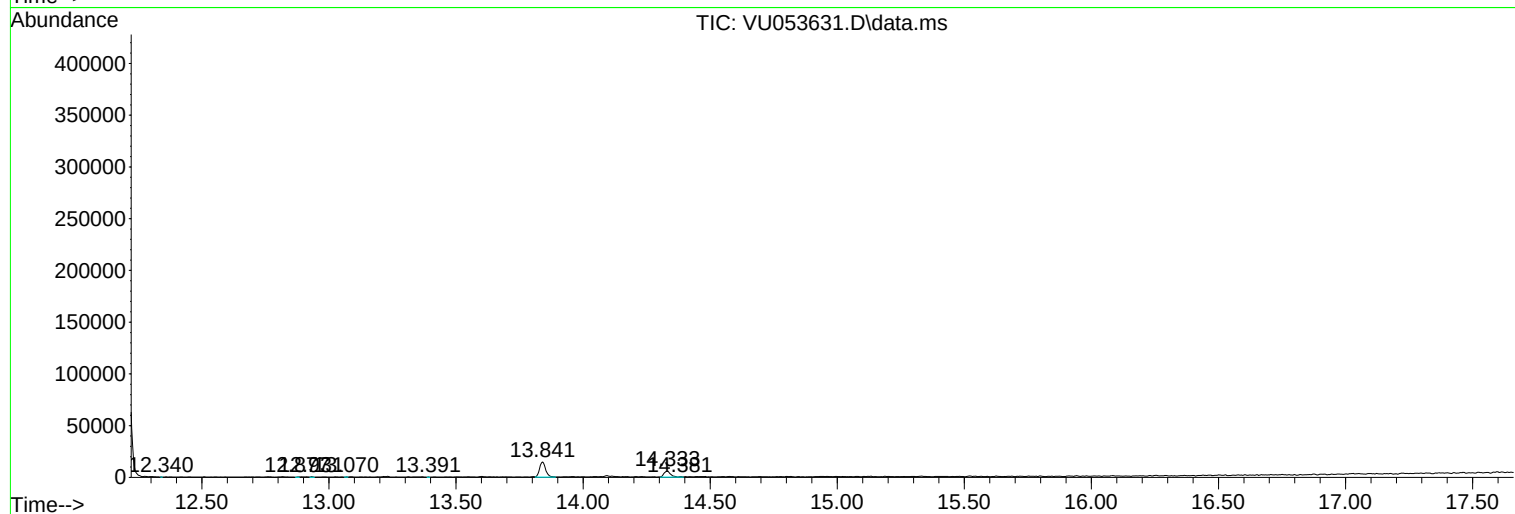
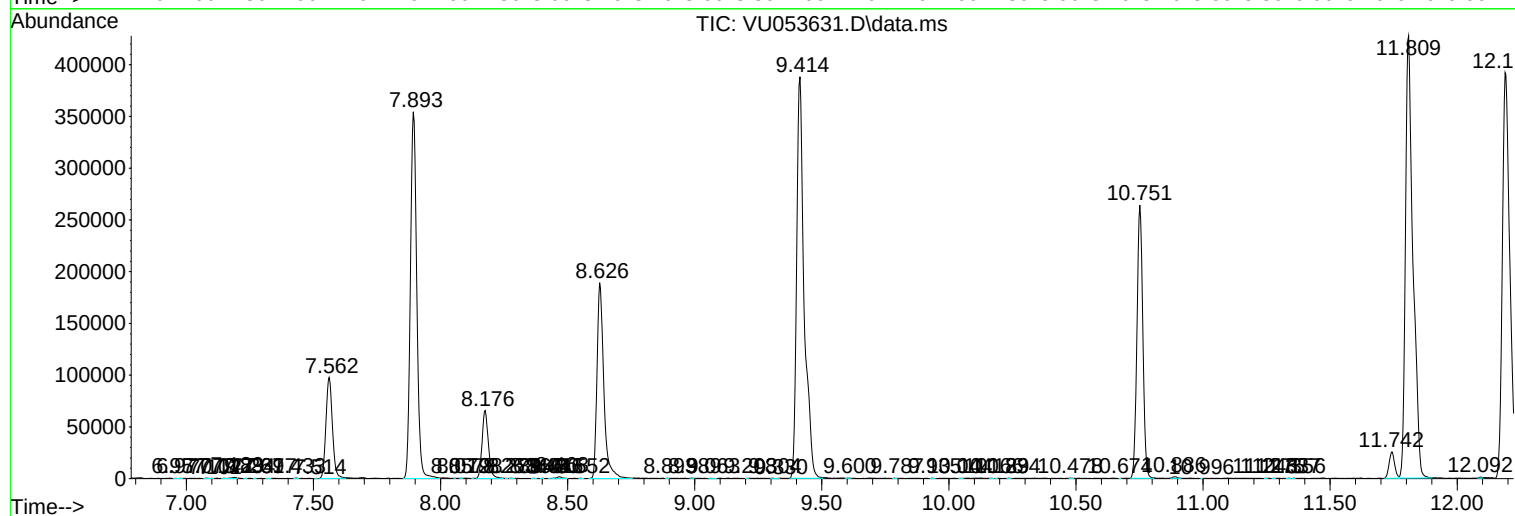
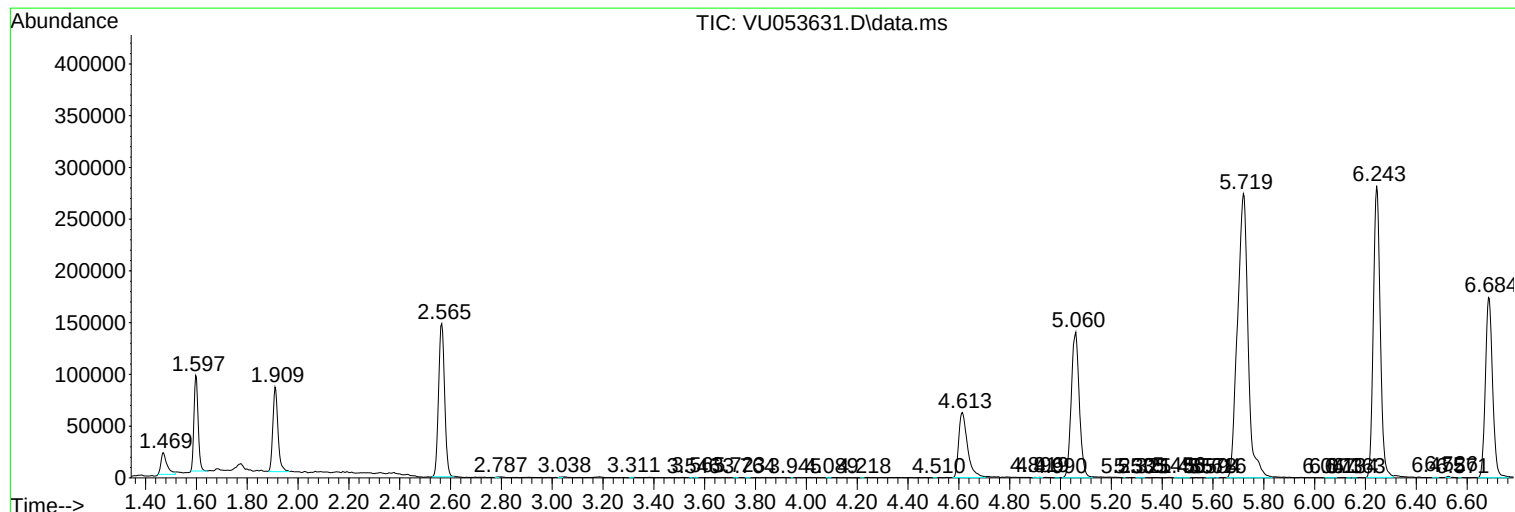
Sum of corrected areas: 6849574

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
Data File : VU053631.D
Acq On : 11 Apr 2023 13:36
Operator : JC/MD
Sample : 02251-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COMD2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
Data File : VU053631.D
Acq On : 11 Apr 2023 13:36
Operator : JC/MD
Sample : 02251-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COMD2

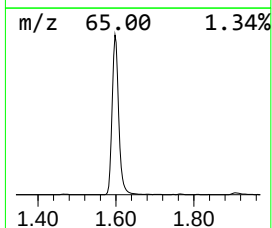
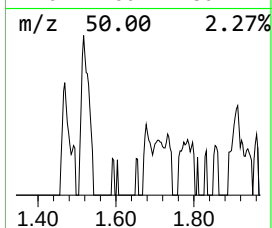
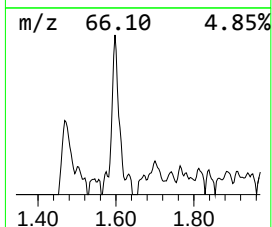
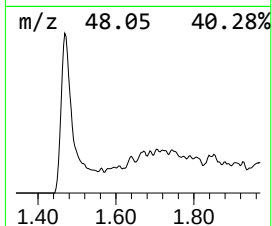
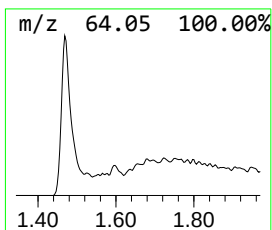
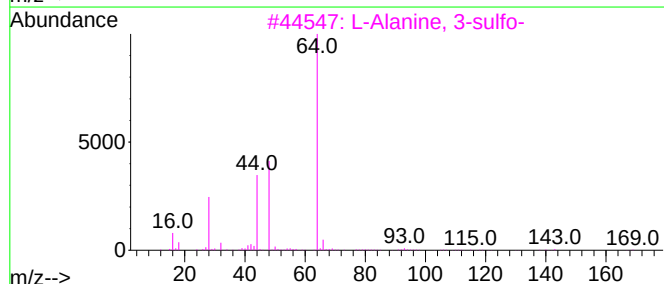
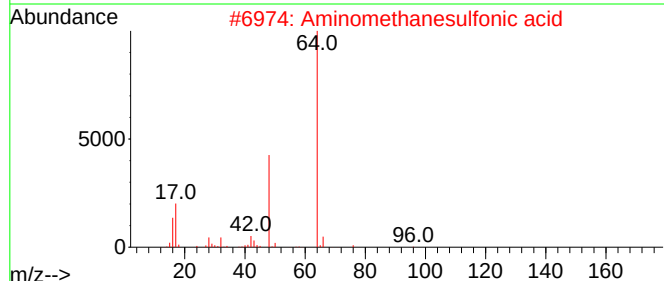
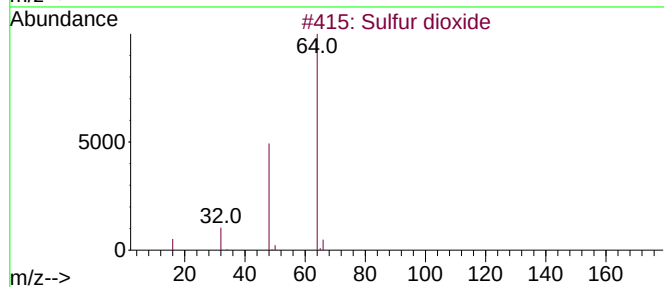
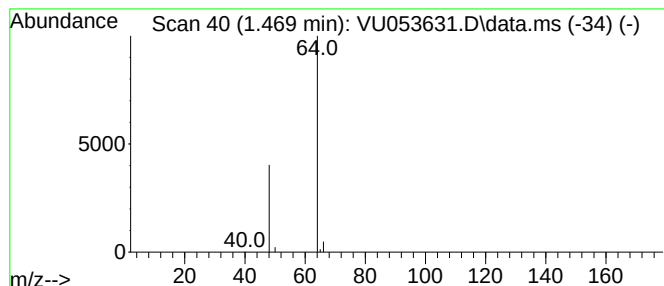
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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.
1.469	3.30 ug/L	34982	1,4-Difluorobenzene	6.243

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	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
Data File : VU053631.D
Acq On : 11 Apr 2023 13:36
Operator : JC/MD
Sample : 02251-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0MD2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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	1.469	3.3	ug/L	34982	1	6.243	529568	50.0