

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044786.D
 Acq On : 31 Jan 2025 11:06
 Operator : JC/MD
 Sample : Q1162-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

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\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	21	25	36	rBV	21008	36094	3.78%	0.516%
2	1.367	42	46	61	rVB	114393	134565	14.08%	1.923%
3	1.648	88	92	101	rVB	72234	88753	9.29%	1.269%
4	2.300	193	199	210	rVB	205340	329346	34.46%	4.708%
5	2.635	252	254	255	rBV	477	347	0.04%	0.005%
6	2.709	265	266	271	rBV2	311	330	0.03%	0.005%
7	2.776	274	277	280	rBV2	852	1261	0.13%	0.018%
8	2.830	284	286	287	rBV2	359	231	0.02%	0.003%
9	2.940	298	304	311	rVB2	3196	7035	0.74%	0.101%
10	3.105	329	331	332	rBV	401	244	0.03%	0.003%
11	3.172	335	342	346	rBV2	379	979	0.10%	0.014%
12	3.227	349	351	354	rBV2	305	306	0.03%	0.004%
13	3.416	379	382	383	rBV2	563	500	0.05%	0.007%
14	3.434	383	385	387	rVB2	603	507	0.05%	0.007%
15	3.672	422	424	425	rBV2	428	244	0.03%	0.003%
16	3.769	436	440	444	rBV2	343	467	0.05%	0.007%
17	3.842	449	452	453	rBV	283	237	0.02%	0.003%
18	3.946	467	469	472	rBV	441	401	0.04%	0.006%
19	4.007	477	479	481	rBV2	382	307	0.03%	0.004%
20	4.080	490	491	494	rBV	284	259	0.03%	0.004%
21	4.251	518	519	523	rVB	337	318	0.03%	0.005%
22	4.288	523	525	528	rBV	277	313	0.03%	0.004%
23	4.379	538	540	542	rBV	377	230	0.02%	0.003%
24	4.452	545	552	569	rBV	57190	176262	18.44%	2.519%
25	4.940	628	632	633	rBV2	310	309	0.03%	0.004%
26	4.958	633	635	636	rBV	370	242	0.03%	0.003%
27	5.043	639	649	667	rVV	119932	369521	38.67%	5.282%
28	5.354	698	700	701	rBV	345	261	0.03%	0.004%
29	5.519	725	727	728	rBV2	419	255	0.03%	0.004%
30	5.665	748	751	752	rBV	371	337	0.04%	0.005%
31	5.696	754	756	758	rVB	276	267	0.03%	0.004%
32	5.732	758	762	766	rBV	523	764	0.08%	0.011%
33	5.763	766	767	770	rVB	441	368	0.04%	0.005%
34	5.958	786	799	826	rBV2	318118	955673	100.00%	13.660%
35	6.232	842	844	848	rBV	242	397	0.04%	0.006%
36	6.293	853	854	857	rVV2	473	346	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044786.D
 Acq On : 31 Jan 2025 11:06
 Operator : JC/MD
 Sample : Q1162-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

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\SFAMXML012825WMA.M
 Title : VOC Analysis

37	6.336	859	861	864	rVB	534	551	0.06%	0.008%
38	6.360	864	865	868	rBV2	461	421	0.04%	0.006%
39	6.427	875	876	879	rBV	407	376	0.04%	0.005%
40	6.586	899	902	906	rBV2	227	352	0.04%	0.005%
41	6.757	919	930	954	rBV	254481	640925	67.07%	9.161%
42	7.177	998	999	1004	rBV2	533	708	0.07%	0.010%
43	7.299	1011	1019	1037	rBV	191439	430569	45.05%	6.155%
44	7.476	1046	1048	1052	rVB2	785	872	0.09%	0.012%
45	7.513	1052	1054	1055	rBV2	398	244	0.03%	0.003%
46	7.567	1062	1063	1065	rBV	294	233	0.02%	0.003%
47	7.604	1065	1069	1070	rVB2	394	331	0.03%	0.005%
48	7.634	1070	1074	1075	rVB2	280	311	0.03%	0.004%
49	7.671	1075	1080	1081	rVB2	339	374	0.04%	0.005%
50	7.683	1081	1082	1085	rBV2	294	336	0.04%	0.005%
51	7.762	1091	1095	1097	rBV	438	466	0.05%	0.007%
52	7.781	1097	1098	1101	rVV	437	352	0.04%	0.005%
53	8.177	1162	1163	1165	rBV	525	399	0.04%	0.006%
54	8.214	1167	1169	1172	rBV	389	468	0.05%	0.007%
55	8.238	1172	1173	1176	rVB2	432	292	0.03%	0.004%
56	8.323	1180	1187	1204	rBV	129678	231709	24.25%	3.312%
57	8.525	1219	1220	1222	rBV	440	326	0.03%	0.005%
58	8.646	1233	1240	1263	rBV	433855	742298	77.67%	10.610%
59	8.945	1284	1289	1303	rBV	89060	142489	14.91%	2.037%
60	9.207	1330	1332	1336	rVB2	320	362	0.04%	0.005%
61	9.256	1338	1340	1343	rBV2	392	448	0.05%	0.006%
62	9.384	1356	1361	1383	rBV	211526	340000	35.58%	4.860%
63	9.652	1403	1405	1408	rBV	427	439	0.05%	0.006%
64	9.774	1424	1425	1428	rBV	312	312	0.03%	0.004%
65	10.049	1465	1470	1492	rBV	524569	734032	76.81%	10.492%
66	10.384	1521	1525	1526	rBV2	251	371	0.04%	0.005%
67	10.402	1526	1528	1530	rVV	374	281	0.03%	0.004%
68	10.421	1530	1531	1534	rVV	407	293	0.03%	0.004%
69	10.475	1539	1540	1542	rBV	508	372	0.04%	0.005%
70	10.567	1551	1555	1556	rBV	330	341	0.04%	0.005%
71	10.738	1581	1583	1585	rVB2	342	298	0.03%	0.004%
72	10.957	1618	1619	1624	rBV2	372	466	0.05%	0.007%
73	11.018	1627	1629	1632	rVB	359	243	0.03%	0.003%
74	11.055	1632	1635	1638	rBV2	355	508	0.05%	0.007%
75	11.103	1640	1643	1649	rBV2	482	975	0.10%	0.014%
76	11.189	1651	1657	1667	rBV	335713	423600	44.32%	6.055%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044786.D
 Acq On : 31 Jan 2025 11:06
 Operator : JC/MD
 Sample : Q1162-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

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\SFAMXML012825WMA.M
 Title : VOC Analysis

77	11.451	1696	1700	1701	rBV2	201	274	0.03%	0.004%
78	11.597	1721	1724	1727	rBV2	301	379	0.04%	0.005%
79	11.701	1739	1741	1743	rBV2	305	240	0.03%	0.003%
80	11.762	1748	1751	1755	rBV	482	499	0.05%	0.007%
81	11.798	1755	1757	1759	rVB2	324	259	0.03%	0.004%
82	12.018	1788	1793	1804	rVV	499387	615034	64.36%	8.791%
83	12.237	1827	1829	1831	rBV	360	293	0.03%	0.004%
84	12.317	1837	1842	1854	rBV	446079	560632	58.66%	8.014%
85	12.695	1902	1904	1907	rVB2	351	325	0.03%	0.005%
86	12.762	1911	1915	1920	rVB2	1839	2153	0.23%	0.031%
87	12.993	1951	1953	1955	rBV2	404	390	0.04%	0.006%
88	13.127	1972	1975	1977	rBV2	320	418	0.04%	0.006%
89	13.188	1984	1985	1989	rBV	349	245	0.03%	0.004%
90	13.353	2009	2012	2013	rBV	385	337	0.04%	0.005%
91	13.463	2027	2030	2031	rBV	237	248	0.03%	0.004%
92	13.481	2031	2033	2036	rVB	325	242	0.03%	0.003%
93	13.511	2036	2038	2041	rBV2	297	330	0.03%	0.005%
94	13.792	2080	2084	2086	rBV2	392	513	0.05%	0.007%
95	13.902	2101	2102	2105	rBV2	602	714	0.07%	0.010%
96	14.127	2134	2139	2144	rBV	2687	3717	0.39%	0.053%
97	14.243	2155	2158	2159	rBV	299	387	0.04%	0.006%
98	14.298	2165	2167	2171	rVB2	291	352	0.04%	0.005%
99	14.584	2211	2214	2217	rBV3	448	572	0.06%	0.008%
100	15.029	2283	2287	2289	rBV2	439	420	0.04%	0.006%

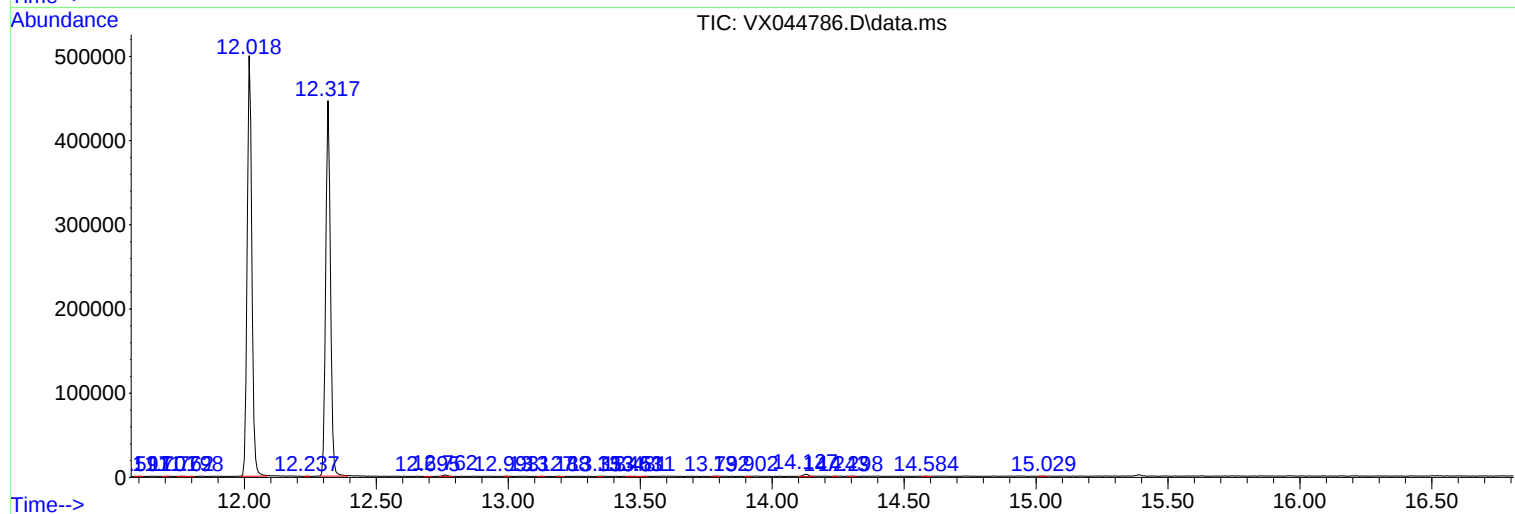
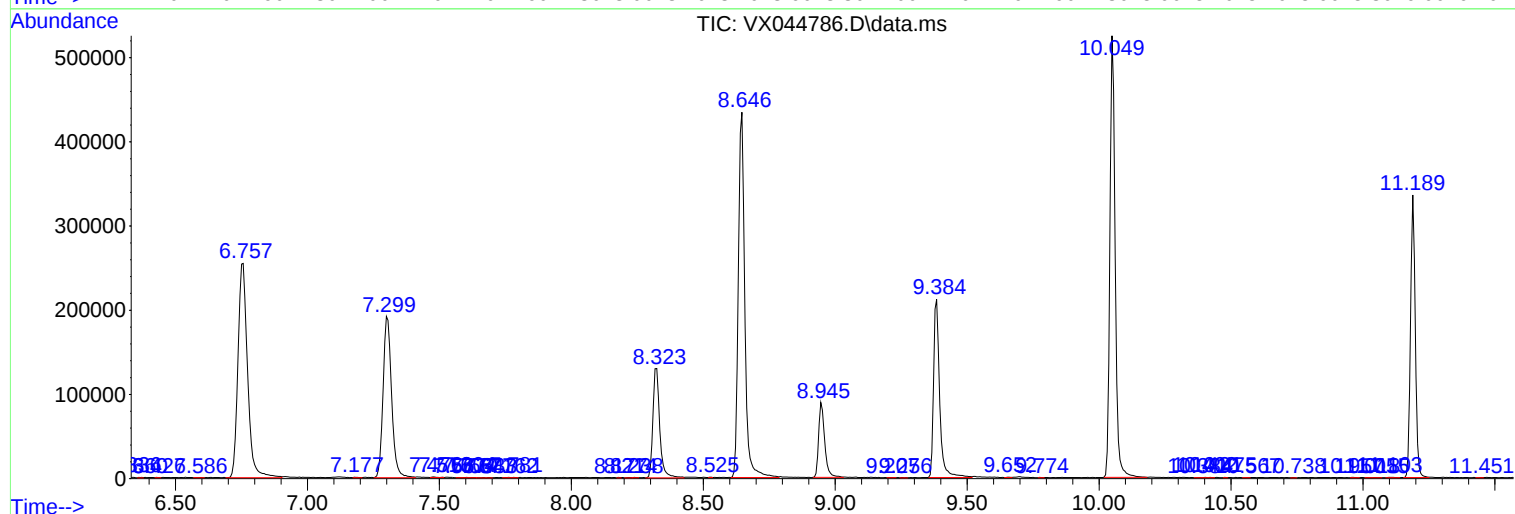
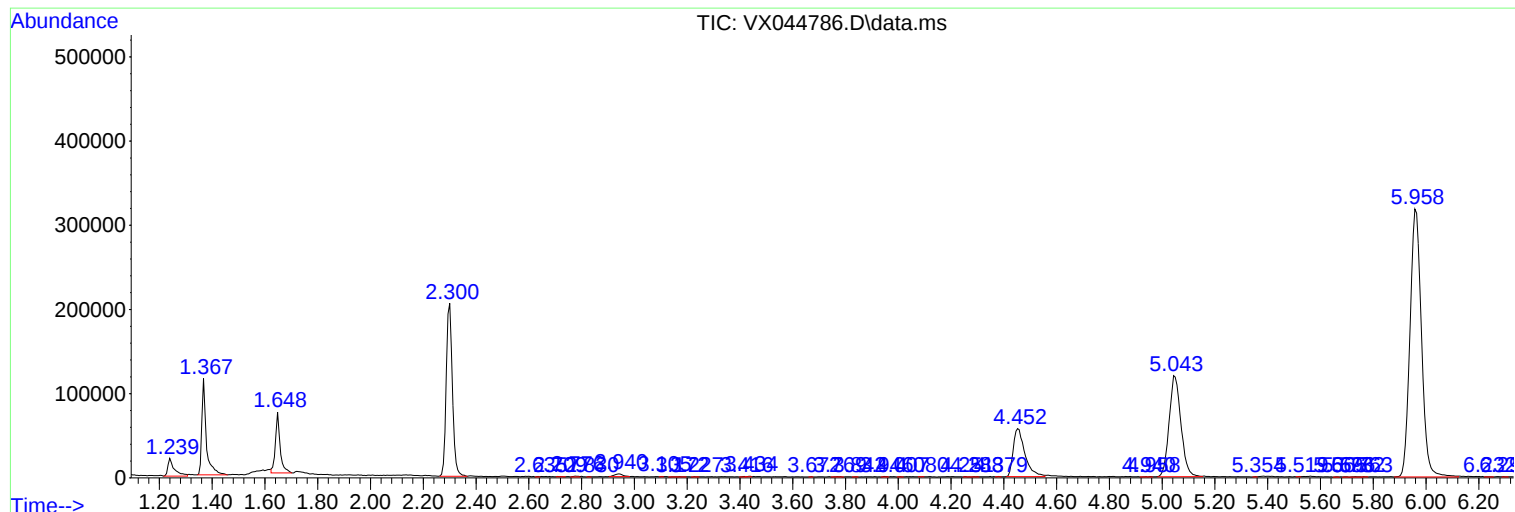
Sum of corrected areas: 6995992

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044786.D
Acq On : 31 Jan 2025 11:06
Operator : JC/MD
Sample : Q1162-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044786.D
Acq On : 31 Jan 2025 11:06
Operator : JC/MD
Sample : Q1162-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

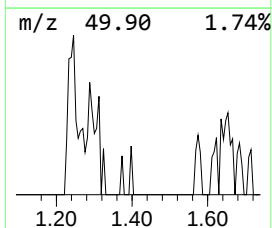
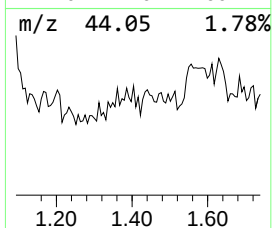
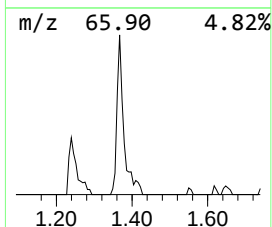
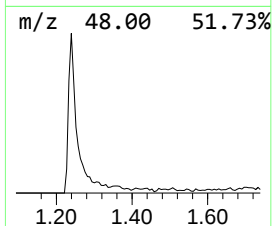
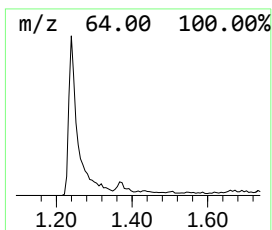
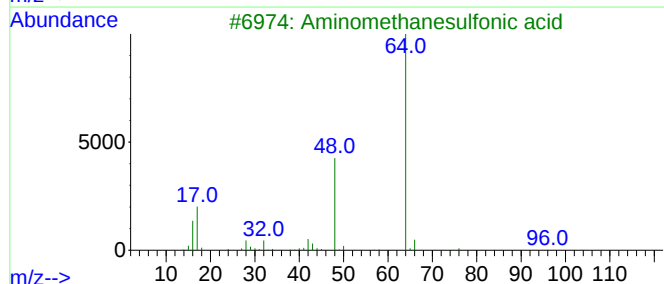
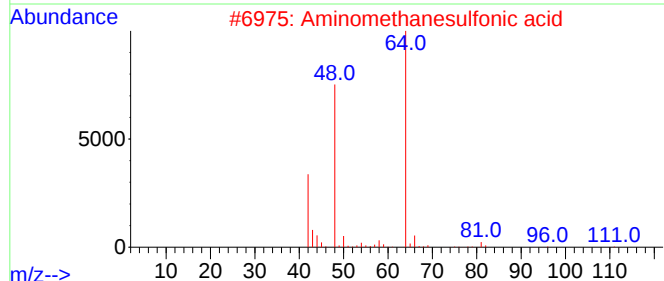
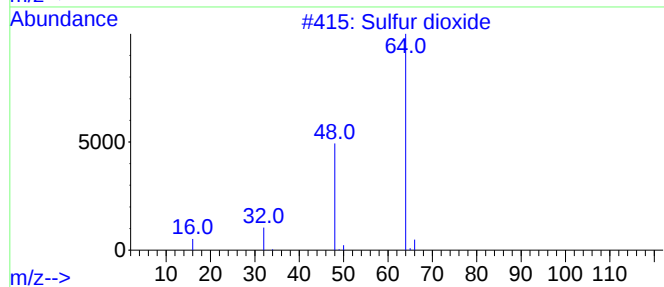
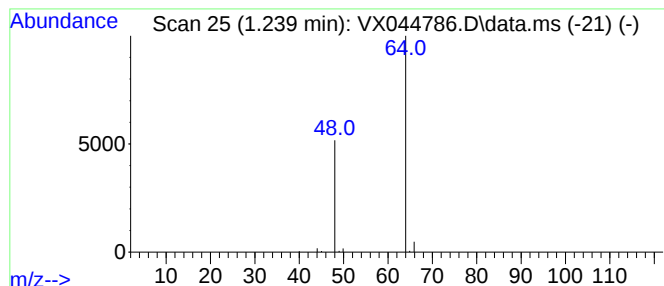
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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.
1.239	2.82 ug/L	36094	1,4-Difluorobenzene	6.757

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044786.D
Acq On : 31 Jan 2025 11:06
Operator : JC/MD
Sample : Q1162-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.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	1.239	2.8	ug/L	36094	1	6.757	640925	50.0