

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
 Data File : VX025942.D
 Acq On : 21 Dec 2021 02:13
 Operator : JC/MD
 Sample : M5126-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0J11

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\SFAMXML122021WMA.M
 Title : VOC Analysis

Signal : TIC: VX025942.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	43	rBV	46348	146603	21.41%	2.737%
2	1.367	43	46	56	rVB	83581	98440	14.38%	1.838%
3	1.672	92	96	104	rVB	70753	94858	13.86%	1.771%
4	2.312	195	201	210	rBV	131827	221034	32.29%	4.126%
5	2.514	230	234	237	rBV2	790	1489	0.22%	0.028%
6	3.166	336	341	342	rBV2	185	210	0.03%	0.004%
7	3.263	355	357	359	rVB2	263	195	0.03%	0.004%
8	3.312	363	365	366	rBV	282	241	0.04%	0.004%
9	3.349	369	371	375	rBV2	203	244	0.04%	0.005%
10	3.526	398	400	402	rVB2	179	185	0.03%	0.003%
11	3.599	410	412	413	rBV2	359	289	0.04%	0.005%
12	3.715	427	431	432	rBV	260	303	0.04%	0.006%
13	3.751	435	437	440	rBV2	247	279	0.04%	0.005%
14	3.837	448	451	455	rBV2	223	243	0.04%	0.005%
15	3.946	467	469	471	rBV2	159	175	0.03%	0.003%
16	3.977	473	474	477	rVV	182	189	0.03%	0.004%
17	4.032	481	483	487	rBV2	160	260	0.04%	0.005%
18	4.263	519	521	524	rVB2	153	173	0.03%	0.003%
19	4.330	530	532	536	rBV3	144	204	0.03%	0.004%
20	4.458	544	553	567	rBV	50389	150961	22.05%	2.818%
21	4.647	583	584	588	rBV2	294	362	0.05%	0.007%
22	5.062	636	652	672	rVB2	88690	289400	42.27%	5.402%
23	5.617	740	743	744	rVB2	222	228	0.03%	0.004%
24	5.635	744	746	748	rBV	301	343	0.05%	0.006%
25	5.793	771	772	775	rVB	337	236	0.03%	0.004%
26	5.976	787	802	815	rBV2	229723	684629	100.00%	12.780%
27	6.208	839	840	844	rVB	223	226	0.03%	0.004%
28	6.549	894	896	899	rBV2	223	272	0.04%	0.005%
29	6.635	909	910	915	rVB2	220	247	0.04%	0.005%
30	6.763	922	931	944	rBV	143838	345162	50.42%	6.443%
31	7.062	977	980	982	rBV2	188	270	0.04%	0.005%
32	7.129	984	991	1001	rVV2	34303	75230	10.99%	1.404%
33	7.311	1011	1021	1033	rBV2	141521	312818	45.69%	5.839%
34	7.433	1033	1041	1054	rVB2	104782	212725	31.07%	3.971%
35	7.732	1088	1090	1092	rVB2	178	170	0.02%	0.003%
36	7.811	1100	1103	1107	rVB3	367	567	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
 Data File : VX025942.D
 Acq On : 21 Dec 2021 02:13
 Operator : JC/MD
 Sample : M5126-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0J11

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\SFAMXML122021WMA.M
 Title : VOC Analysis

37	8.330	1180	1188	1200	rBV	82742	138353	20.21%	2.583%
38	8.470	1208	1211	1213	rBV2	360	382	0.06%	0.007%
39	8.512	1217	1218	1222	rVB	363	269	0.04%	0.005%
40	8.653	1234	1241	1248	rBV	343235	542374	79.22%	10.124%
41	8.951	1284	1290	1300	rVV	54426	79618	11.63%	1.486%
42	9.110	1311	1316	1317	rBV2	228	344	0.05%	0.006%
43	9.275	1339	1343	1348	rVB4	2032	2974	0.43%	0.056%
44	9.384	1356	1361	1373	rBV	211524	312866	45.70%	5.840%
45	9.585	1392	1394	1396	rVB	266	192	0.03%	0.004%
46	9.604	1396	1397	1399	rBV2	303	238	0.03%	0.004%
47	10.055	1465	1471	1482	rVV	322254	440905	64.40%	8.230%
48	10.152	1486	1487	1490	rVV	305	195	0.03%	0.004%
49	10.244	1498	1502	1505	rBV3	528	747	0.11%	0.014%
50	10.305	1507	1512	1516	rBV3	717	1239	0.18%	0.023%
51	10.348	1517	1519	1522	rVB2	223	213	0.03%	0.004%
52	10.512	1542	1546	1548	rVB2	230	345	0.05%	0.006%
53	10.537	1548	1550	1553	rBV2	241	308	0.04%	0.006%
54	10.646	1565	1568	1571	rVB3	384	416	0.06%	0.008%
55	10.744	1582	1584	1587	rBV2	230	246	0.04%	0.005%
56	10.780	1587	1590	1592	rVB2	306	325	0.05%	0.006%
57	10.939	1613	1616	1619	rVB2	184	247	0.04%	0.005%
58	10.969	1619	1621	1624	rBV2	266	304	0.04%	0.006%
59	11.122	1643	1646	1652	rVV2	1280	1707	0.25%	0.032%
60	11.195	1652	1658	1667	rVV	254781	329508	48.13%	6.151%
61	11.286	1671	1673	1674	rBV	355	269	0.04%	0.005%
62	11.323	1676	1679	1681	rVV2	637	598	0.09%	0.011%
63	11.427	1694	1696	1698	rBV2	171	189	0.03%	0.004%
64	11.475	1702	1704	1709	rVB2	538	763	0.11%	0.014%
65	11.750	1744	1749	1753	rBV4	1318	1785	0.26%	0.033%
66	11.823	1758	1761	1762	rBV2	218	224	0.03%	0.004%
67	11.933	1776	1779	1784	rVB3	957	1131	0.17%	0.021%
68	12.024	1788	1794	1803	rBV	309430	395639	57.79%	7.385%
69	12.091	1803	1805	1807	rVB2	264	196	0.03%	0.004%
70	12.122	1807	1810	1812	rBV2	686	802	0.12%	0.015%
71	12.219	1822	1826	1831	rBV	4022	5597	0.82%	0.104%
72	12.323	1836	1843	1857	rVB	351394	448869	65.56%	8.379%
73	12.433	1857	1861	1863	rBV2	383	466	0.07%	0.009%
74	12.493	1870	1871	1875	rVB	335	322	0.05%	0.006%
75	12.561	1879	1882	1885	rBV2	200	326	0.05%	0.006%
76	12.597	1887	1888	1892	rVB3	250	202	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
 Data File : VX025942.D
 Acq On : 21 Dec 2021 02:13
 Operator : JC/MD
 Sample : M5126-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0J11

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\SFAMXML122021WMA.M
 Title : VOC Analysis

77	12.762	1914	1915	1917	rVV2	340	222	0.03%	0.004%
78	13.115	1971	1973	1977	rVB	209	176	0.03%	0.003%
79	13.774	2080	2081	2085	rBV2	235	276	0.04%	0.005%
80	13.804	2085	2086	2089	rVV	214	244	0.04%	0.005%
81	13.877	2096	2098	2101	rVB2	170	191	0.03%	0.004%
82	13.963	2110	2112	2116	rVB2	193	191	0.03%	0.004%
83	14.341	2172	2174	2175	rVV	355	188	0.03%	0.004%
84	14.377	2176	2180	2183	rVV	217	276	0.04%	0.005%
85	14.621	2218	2220	2223	rBV2	231	297	0.04%	0.006%
86	14.658	2223	2226	2227	rVB	234	180	0.03%	0.003%
87	14.682	2227	2230	2231	rBV	291	223	0.03%	0.004%
88	14.944	2271	2273	2274	rBV	353	253	0.04%	0.005%
89	15.011	2281	2284	2287	rBV2	200	257	0.04%	0.005%
90	15.127	2299	2303	2304	rBV3	240	283	0.04%	0.005%
91	15.194	2312	2314	2318	rBV2	218	260	0.04%	0.005%
92	15.237	2318	2321	2322	rBV2	255	275	0.04%	0.005%
93	15.548	2369	2372	2375	rVB3	271	308	0.04%	0.006%
94	15.590	2375	2379	2382	rBV2	206	265	0.04%	0.005%
95	15.737	2402	2403	2405	rBV2	379	217	0.03%	0.004%
96	15.810	2413	2415	2417	rBV	262	231	0.03%	0.004%
97	16.133	2466	2468	2470	rBV2	320	364	0.05%	0.007%
98	16.377	2507	2508	2511	rVB	440	264	0.04%	0.005%
99	16.401	2511	2512	2515	rBV2	343	304	0.04%	0.006%
100	16.602	2544	2545	2548	rVB2	290	251	0.04%	0.005%

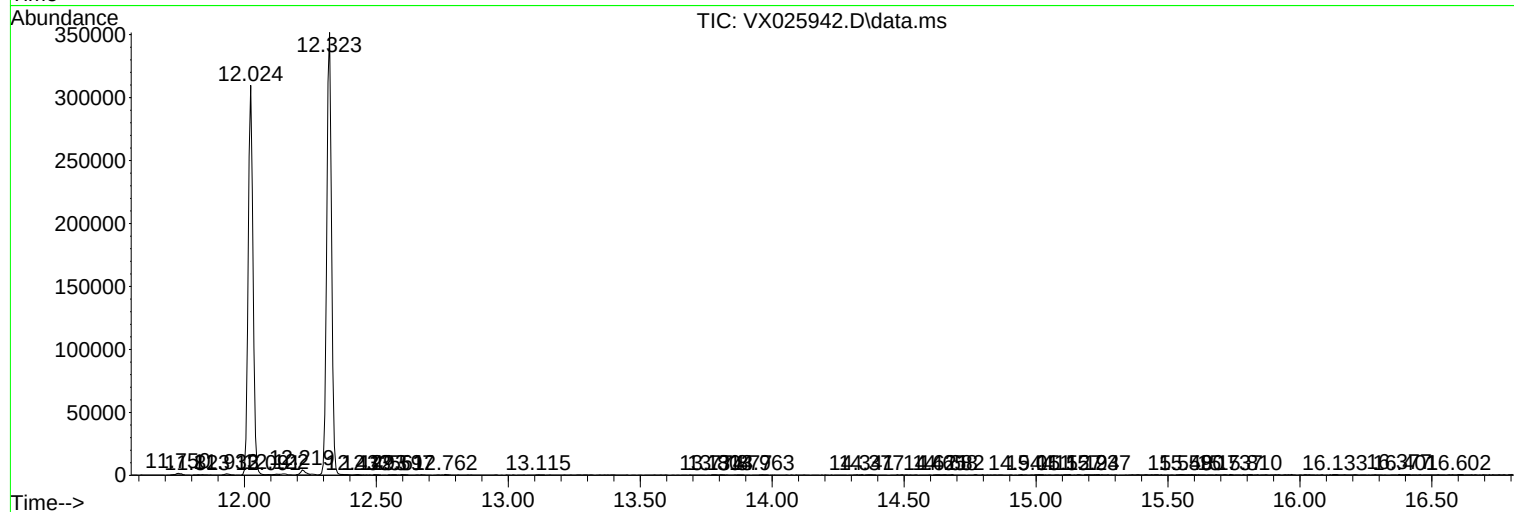
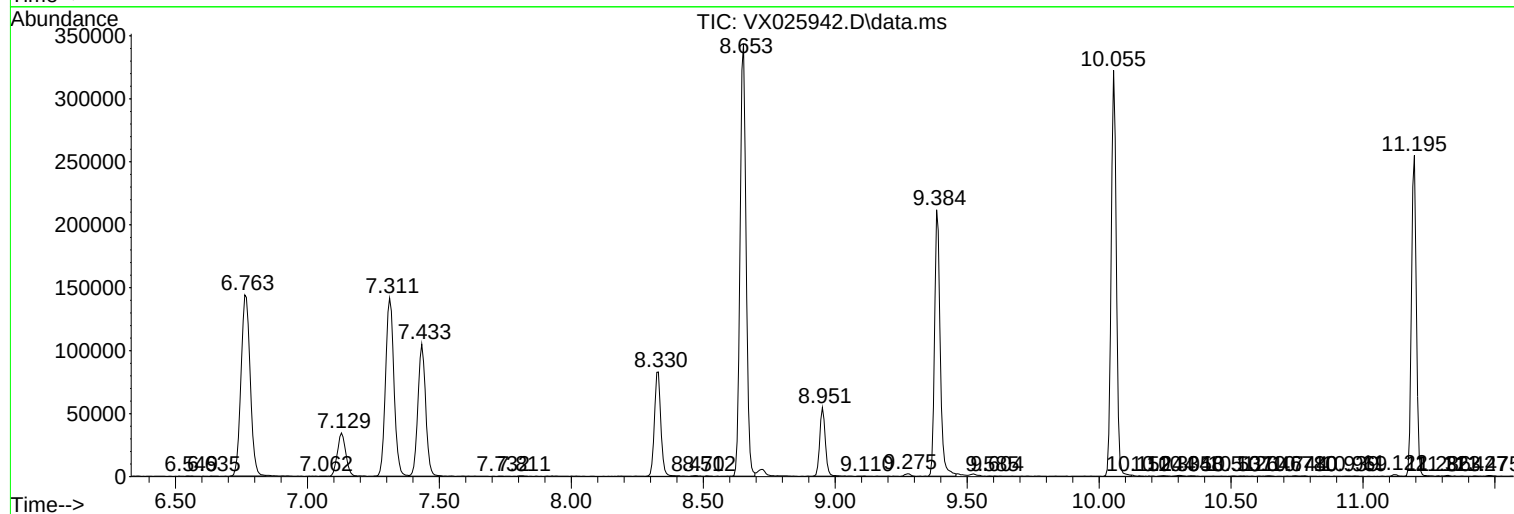
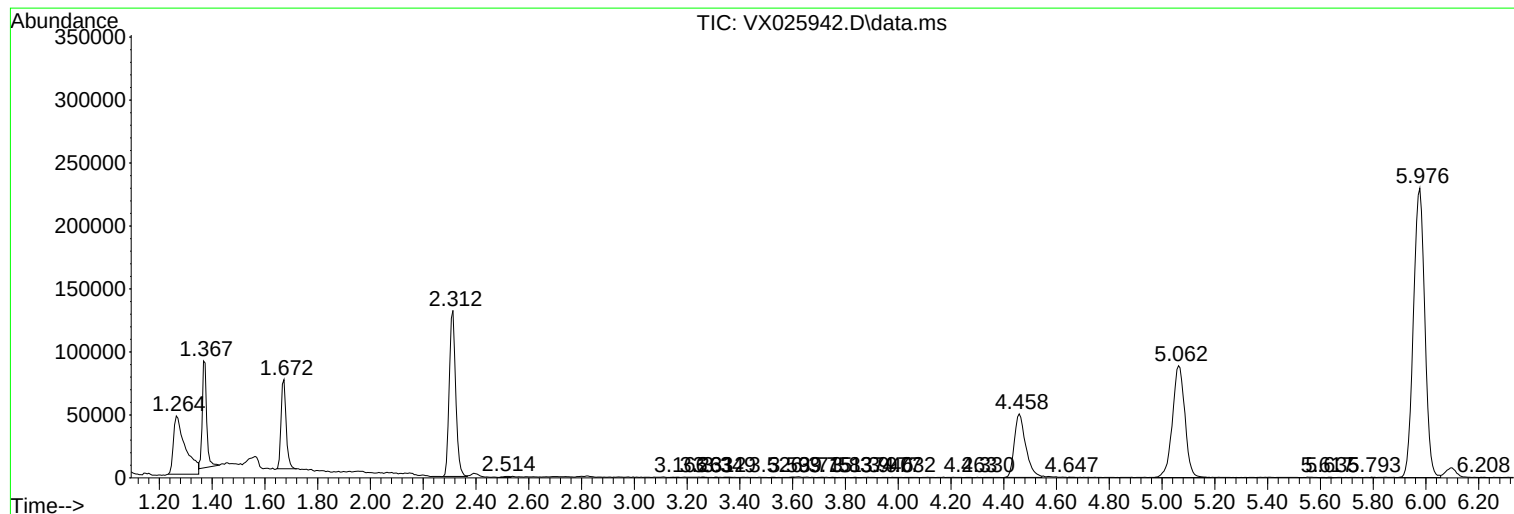
Sum of corrected areas: 5357149

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
Data File : VX025942.D
Acq On : 21 Dec 2021 02:13
Operator : JC/MD
Sample : M5126-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0J11

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122021\
Data File : VX025942.D
Acq On : 21 Dec 2021 02:13
Operator : JC/MD
Sample : M5126-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0J11

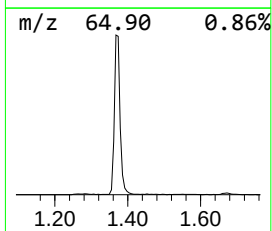
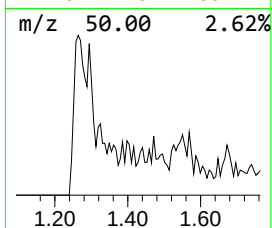
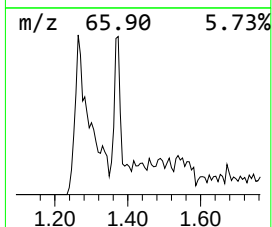
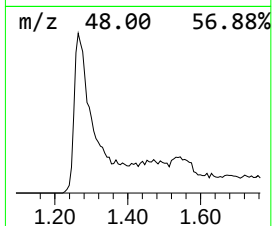
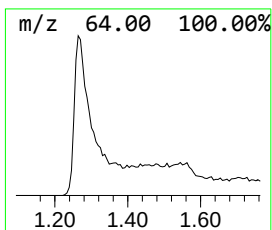
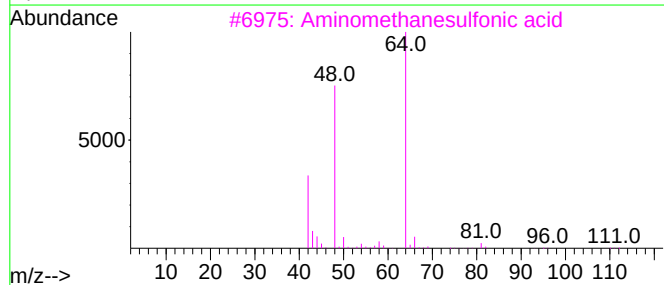
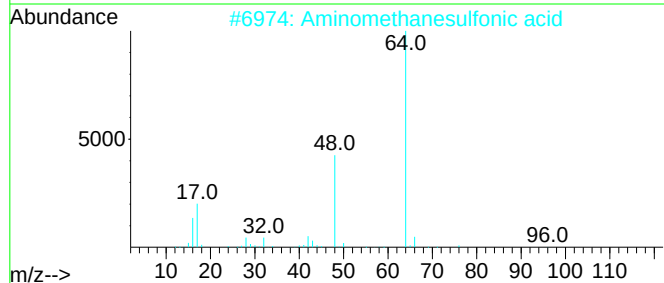
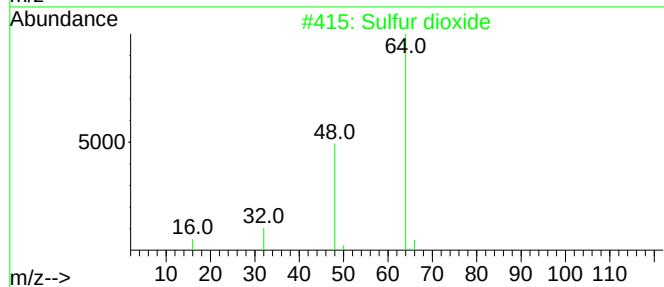
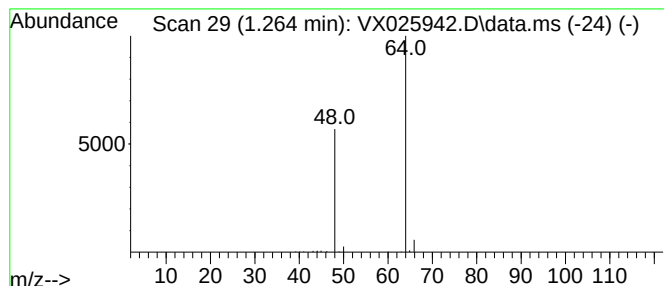
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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.
1.264	21.24 ug/L	146603	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			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\VX122021\
Data File : VX025942.D
Acq On : 21 Dec 2021 02:13
Operator : JC/MD
Sample : M5126-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0J11

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122021WMA.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	1.264	21.2	ug/L	146603	1	6.769	345162	50.0