

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044696.D
 Acq On : 22 Jan 2025 15:09
 Operator : JC/MD
 Sample : Q1130-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

Signal : TIC: VX044696.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	22	25	32	rBV	21935	34054	3.54%	0.521%
2	1.367	43	46	62	rVB	103365	151707	15.77%	2.319%
3	1.648	89	92	97	rBV	26226	33043	3.43%	0.505%
4	2.294	192	198	208	rVB	170760	268010	27.86%	4.097%
5	2.410	216	217	218	rBV	669	416	0.04%	0.006%
6	2.458	224	225	229	rVB4	557	662	0.07%	0.010%
7	2.495	229	231	233	rBV3	1167	1365	0.14%	0.021%
8	2.940	299	304	313	rVB3	3710	9120	0.95%	0.139%
9	3.434	378	385	390	rBV2	5852	13788	1.43%	0.211%
10	3.605	410	413	414	rBV3	385	432	0.04%	0.007%
11	3.830	449	450	454	rBV3	476	582	0.06%	0.009%
12	3.964	470	472	475	rBV	379	311	0.03%	0.005%
13	4.019	479	481	483	rVV2	588	544	0.06%	0.008%
14	4.068	487	489	493	rVB	645	664	0.07%	0.010%
15	4.098	493	494	496	rBV	521	338	0.04%	0.005%
16	4.123	496	498	501	rBV2	460	448	0.05%	0.007%
17	4.251	517	519	520	rVB	931	493	0.05%	0.008%
18	4.275	520	523	526	rBV4	595	819	0.09%	0.013%
19	4.452	545	552	573	rBV2	58303	194583	20.22%	2.974%
20	4.757	600	602	605	rVB2	481	308	0.03%	0.005%
21	5.043	637	649	666	rBV2	119451	379770	39.47%	5.805%
22	5.293	688	690	692	rBV2	491	280	0.03%	0.004%
23	5.366	701	702	705	rBV3	839	1026	0.11%	0.016%
24	5.537	727	730	733	rBV4	701	1278	0.13%	0.020%
25	5.683	752	754	756	rBV2	500	465	0.05%	0.007%
26	5.775	767	769	770	rVB2	535	267	0.03%	0.004%
27	5.854	778	782	784	rBV4	530	708	0.07%	0.011%
28	5.879	784	786	787	rBV2	411	389	0.04%	0.006%
29	5.958	787	799	820	rVV2	321835	962108	100.00%	14.707%
30	6.232	842	844	846	rBV2	403	439	0.05%	0.007%
31	6.439	876	878	880	rVB2	745	488	0.05%	0.007%
32	6.580	899	901	903	rVB2	442	345	0.04%	0.005%
33	6.635	907	910	911	rBV2	392	477	0.05%	0.007%
34	6.750	920	929	954	rBV	209306	534501	55.56%	8.171%
35	7.080	982	983	984	rBV	603	360	0.04%	0.006%
36	7.299	1011	1019	1039	rBV	195662	442526	46.00%	6.765%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044696.D
 Acq On : 22 Jan 2025 15:09
 Operator : JC/MD
 Sample : Q1130-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

37	7.701	1081	1085	1086	rBV2	422	596	0.06%	0.009%
38	7.714	1086	1087	1089	rVB2	591	280	0.03%	0.004%
39	7.762	1094	1095	1098	rBV2	286	293	0.03%	0.004%
40	7.860	1110	1111	1113	rVB2	619	354	0.04%	0.005%
41	7.915	1119	1120	1122	rBV2	480	408	0.04%	0.006%
42	7.951	1122	1126	1128	rBV4	688	1055	0.11%	0.016%
43	8.025	1136	1138	1142	rVB3	474	372	0.04%	0.006%
44	8.110	1150	1152	1154	rBV2	371	350	0.04%	0.005%
45	8.134	1154	1156	1160	rVB3	782	802	0.08%	0.012%
46	8.232	1170	1172	1173	rBV	425	344	0.04%	0.005%
47	8.317	1181	1186	1202	rBV	139998	241313	25.08%	3.689%
48	8.640	1233	1239	1263	rBV	427852	745154	77.45%	11.391%
49	8.945	1284	1289	1304	rBV	94787	150962	15.69%	2.308%
50	9.238	1335	1337	1338	rBV	428	305	0.03%	0.005%
51	9.384	1356	1361	1387	rBV	191836	357981	37.21%	5.472%
52	9.701	1410	1413	1418	rVB3	2490	3660	0.38%	0.056%
53	9.799	1427	1429	1430	rVB2	622	397	0.04%	0.006%
54	9.823	1430	1433	1436	rBV3	514	880	0.09%	0.013%
55	10.049	1465	1470	1486	rBV	394908	583261	60.62%	8.916%
56	10.250	1500	1503	1504	rBV3	534	524	0.05%	0.008%
57	10.457	1534	1537	1539	rBV2	340	324	0.03%	0.005%
58	10.573	1554	1556	1559	rBV2	286	360	0.04%	0.006%
59	10.987	1622	1624	1625	rBV	530	313	0.03%	0.005%
60	11.091	1638	1641	1642	rBV2	510	611	0.06%	0.009%
61	11.146	1649	1650	1652	rBV	455	388	0.04%	0.006%
62	11.189	1652	1657	1670	rVV	325669	433748	45.08%	6.630%
63	11.372	1685	1687	1690	rVB3	627	416	0.04%	0.006%
64	11.396	1690	1691	1694	rBV	248	300	0.03%	0.005%
65	11.487	1703	1706	1707	rBV2	457	406	0.04%	0.006%
66	11.573	1717	1720	1721	rBV2	460	411	0.04%	0.006%
67	11.652	1731	1733	1734	rVB2	567	312	0.03%	0.005%
68	11.768	1750	1752	1753	rBV	396	346	0.04%	0.005%
69	11.835	1762	1763	1765	rBV2	371	314	0.03%	0.005%
70	11.963	1782	1784	1785	rBV	390	271	0.03%	0.004%
71	12.018	1788	1793	1807	rVV	344902	449709	46.74%	6.874%
72	12.195	1819	1822	1823	rVB2	683	629	0.07%	0.010%
73	12.243	1828	1830	1831	rVB	477	304	0.03%	0.005%
74	12.316	1837	1842	1852	rBV	404622	511545	53.17%	7.820%
75	12.646	1894	1896	1898	rVB	599	385	0.04%	0.006%
76	12.701	1904	1905	1912	rVB3	456	733	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044696.D
 Acq On : 22 Jan 2025 15:09
 Operator : JC/MD
 Sample : Q1130-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

77	12.761	1912	1915	1917	rBV3	752	860	0.09%	0.013%
78	12.877	1931	1934	1935	rBV2	338	366	0.04%	0.006%
79	12.993	1952	1953	1954	rBV	489	270	0.03%	0.004%
80	13.042	1959	1961	1963	rVB2	797	538	0.06%	0.008%
81	13.066	1963	1965	1968	rBV2	667	879	0.09%	0.013%
82	13.188	1984	1985	1988	rBV2	377	398	0.04%	0.006%
83	13.225	1988	1991	1997	rVB3	538	860	0.09%	0.013%
84	13.274	1997	1999	2002	rBV2	373	524	0.05%	0.008%
85	13.365	2012	2014	2016	rBV3	517	553	0.06%	0.008%
86	13.487	2032	2034	2037	rBV3	351	345	0.04%	0.005%
87	13.633	2057	2058	2062	rBV2	463	489	0.05%	0.007%
88	13.926	2104	2106	2109	rBV2	368	316	0.03%	0.005%
89	14.078	2129	2131	2132	rBV	471	288	0.03%	0.004%
90	14.127	2136	2139	2142	rVB4	948	1439	0.15%	0.022%
91	14.158	2142	2144	2146	rBV2	350	301	0.03%	0.005%
92	14.322	2169	2171	2174	rBV3	445	544	0.06%	0.008%
93	14.383	2177	2181	2182	rVB3	480	358	0.04%	0.005%
94	14.840	2254	2256	2258	rBV2	490	492	0.05%	0.008%
95	15.145	2304	2306	2308	rVB3	952	750	0.08%	0.011%
96	15.170	2308	2310	2311	rBV2	697	669	0.07%	0.010%
97	15.529	2367	2369	2370	rBV2	836	599	0.06%	0.009%
98	15.901	2428	2430	2431	rBV	705	396	0.04%	0.006%
99	16.377	2505	2508	2510	rBV3	595	673	0.07%	0.010%
100	16.682	2556	2558	2561	rBV3	664	584	0.06%	0.009%

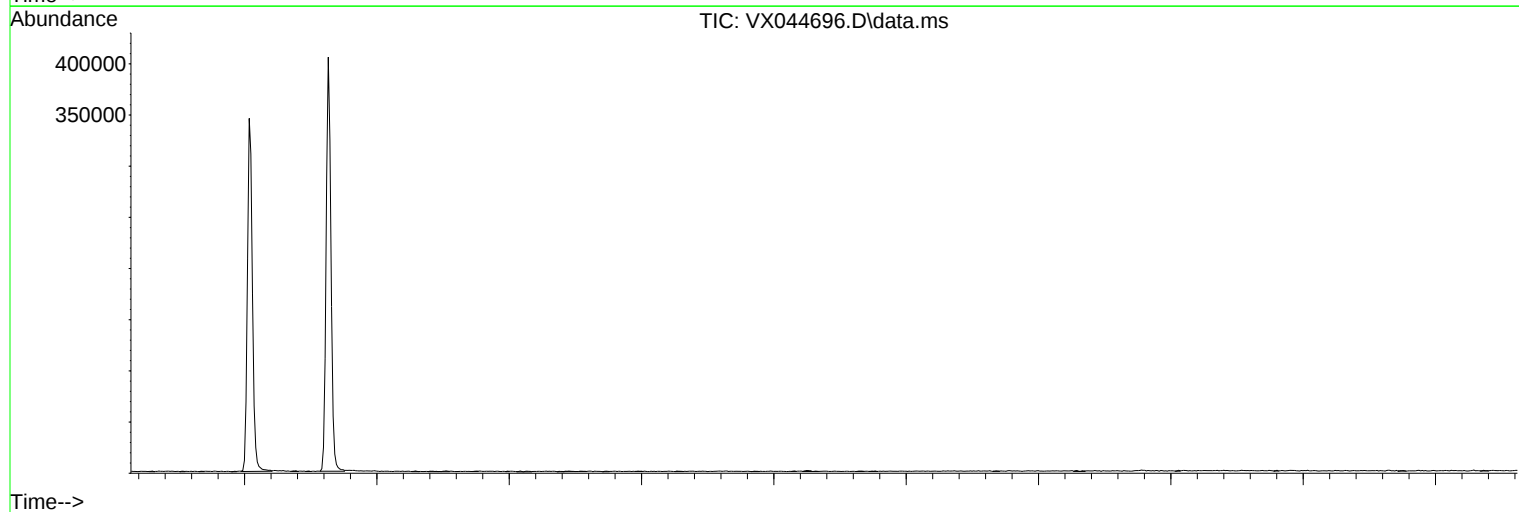
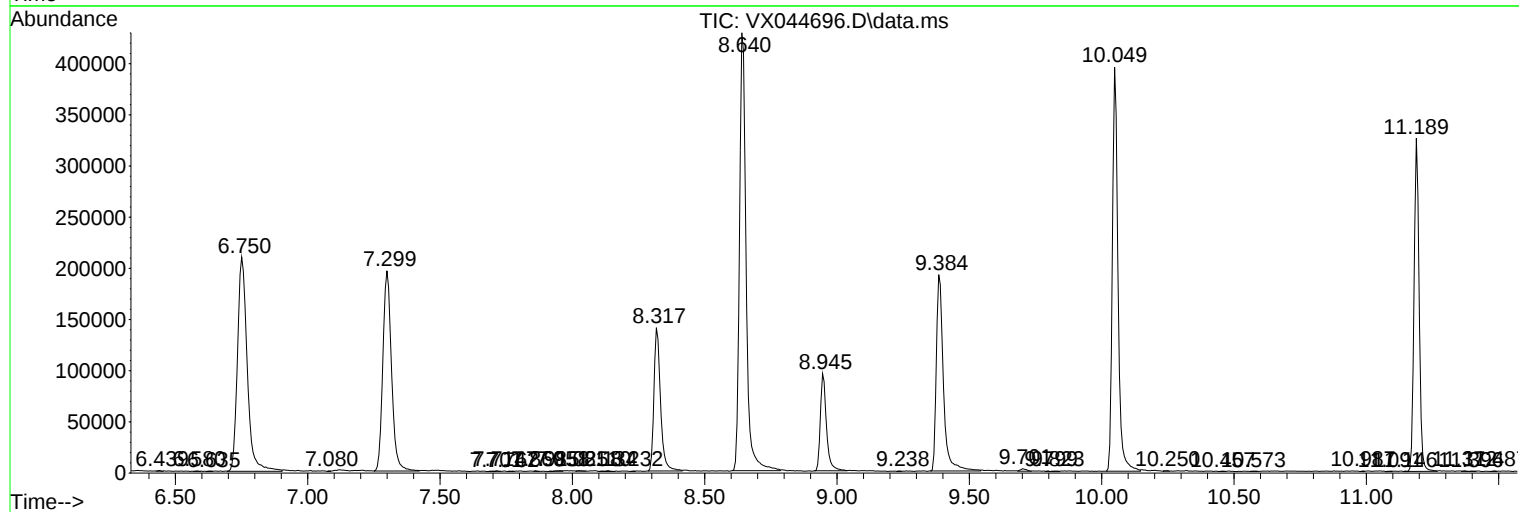
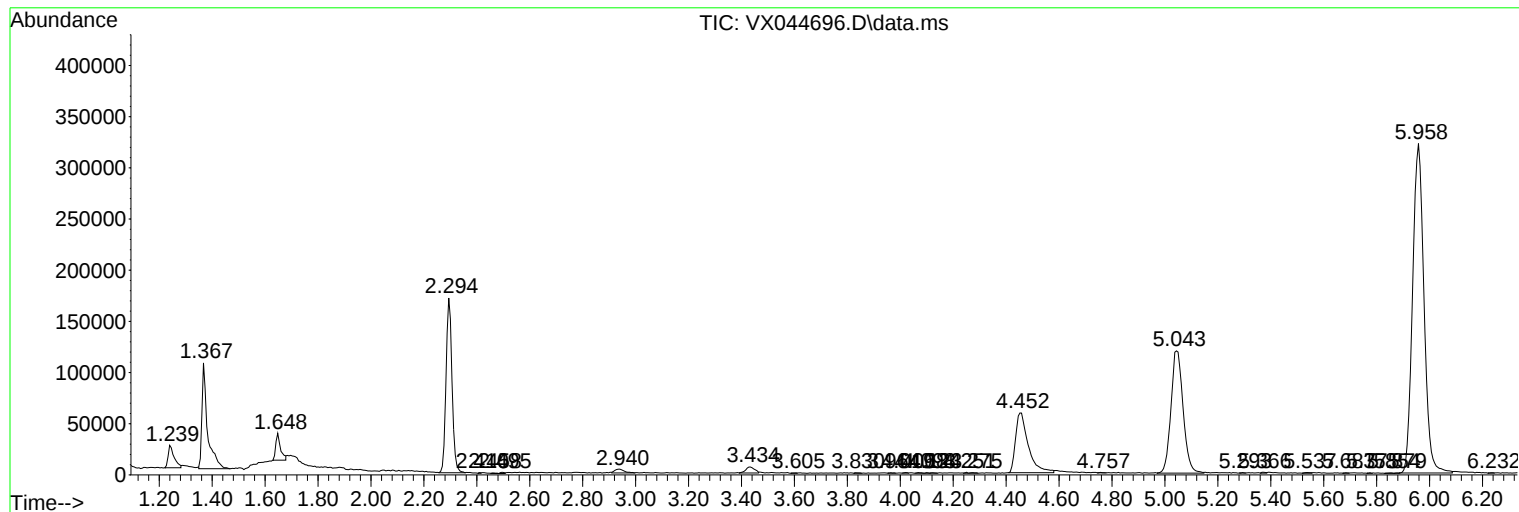
Sum of corrected areas: 6541721

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
Data File : VX044696.D
Acq On : 22 Jan 2025 15:09
Operator : JC/MD
Sample : Q1130-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
Data File : VX044696.D
Acq On : 22 Jan 2025 15:09
Operator : JC/MD
Sample : Q1130-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

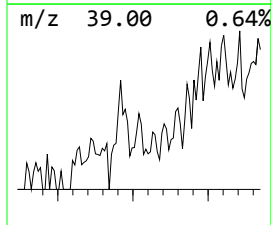
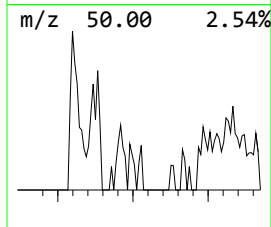
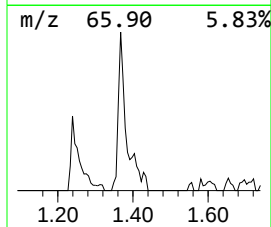
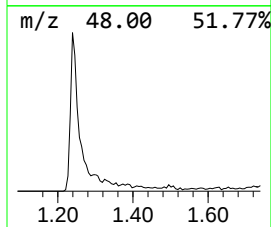
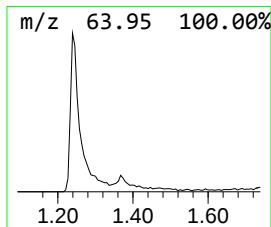
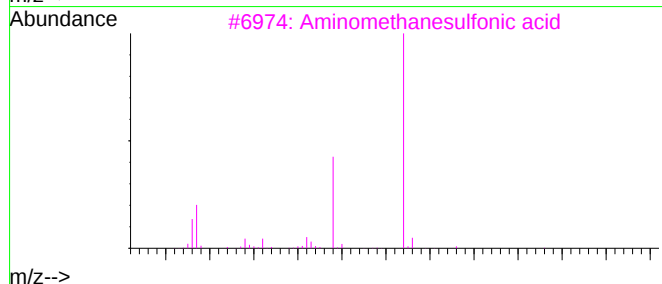
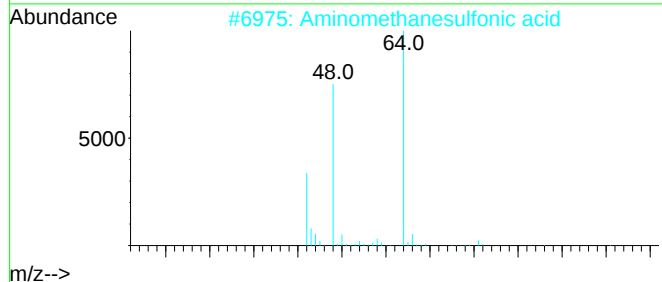
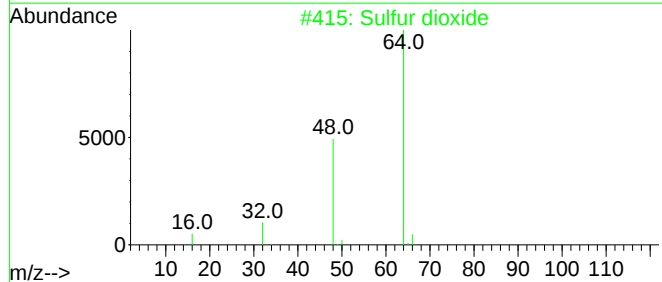
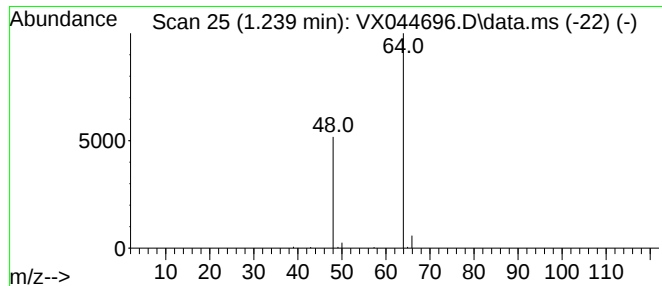
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012125WMA.M
Quant Title : VOC Analysis

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	3.19 ug/L	34054	1,4-Difluorobenzene	6.750

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\VX012225\
Data File : VX044696.D
Acq On : 22 Jan 2025 15:09
Operator : JC/MD
Sample : Q1130-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.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	3.2	ug/L	34054	1	6.750	534501	50.0