Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044784.D
Acq On : 31 Jan 2025 10:08
Operator : JC/MD
Sample : VX0131MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK757

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\SFAMXLM012825WMA.M
Title : VOC Analysis

Signal : TIC: VX044784.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	39	rBV	21291	38249	4.09%	0.535%
2	1.368	42	46	60	rVB	114073	139918	14.98%	1.956%
3	1.648	88	92	102	rVB	72334	96282	10.30%	1.346%
4	2.300	192	199	209	rBV	199988	331085	35.44%	4.628%
5	2.502	227	232	238	rBV2	3678	5836	0.62%	0.082%
6	2.703	259	265	268	rBV4	1013	1824	0.20%	0.025%
7	2.788	273	279	284	rBV4	2712	4775	0.51%	0.067%
8	2.861	289	291	292	rBV	411	301	0.03%	0.004%
9	2.928	300	302	303	rBV	996	769	0.08%	0.011%
10	3.032	316	319	320	rBV2	270	293	0.03%	0.004%
11	3.105	323	331	339	rVV4	3361	10517	1.13%	0.147%
12	3.172	341	342	345	rBV2	376	417	0.04%	0.006%
13	3.428	381	384	385	rBV2	789	877	0.09%	0.012%
14	3.599	409	412	422	rVB3	1332	2944	0.32%	0.041%
15	3.678	422	425	426	rVV	619	477	0.05%	0.007%
16	3.739	433	435	440	rVB2	500	609	0.07%	0.009%
17	3.818	445	448	449	rBV	305	292	0.03%	0.004%
18	3.879	457	458	461	rBV2	318	354	0.04%	0.005%
19	4.038	482	484	487	rBV2	501	663	0.07%	0.009%
20	4.227	512	515	517	rBV	473	355	0.04%	0.005%
21	4.264	517	521	522	rBV	390	384	0.04%	0.005%
22	4.373	537	539	544	rBV2	333	501	0.05%	0.007%
23	4.453	544	552	569	rBV	55611	175695	18.80%	2.456%
24	4.891	618	624	630	rBV4	1126	2781	0.30%	0.039%
25	5.044	638	649	669	rVV	114907	364849	39.05%	5.100%
26	5.269	684	686	689	rVB	522	595	0.06%	0.008%
27	5.306	689	692	695	rBV3	420	538	0.06%	0.008%
28	5.379	695	704	710	rBV6	2045	6320	0.68%	0.088%
29	5.556	731	733	737	rVB2	681	577	0.06%	0.008%
30	5.647	746	748	750	rBV2	738	843	0.09%	0.012%
31	5.794	769	772	774	rBV	295	426	0.05%	0.006%
32	5.958	788	799	817	rBV2	310467	934324	100.00%	13.060%
33	6.312	855	857	860	rBV2	449	421	0.05%	0.006%
34	6.446	877	879	880	rBV	388	302	0.03%	0.004%
35	6.477	883	884	886	rVV	537	407	0.04%	0.006%
36	6.501	886	888	889	rVV	504	339	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044784.D
Acq On : 31 Jan 2025 10:08
Operator : JC/MD
Sample : VX0131MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK757

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\SFAMXLM012825WMA.M
Title : VOC Analysis

37	6.629	907	909	915	rVB2	313	428	0.05%	0.006%
38	6.751	920	929	950	rBV	244446	609659	65.25%	8.522%
39	7.074	980	982	983	rVV2	283	284	0.03%	0.004%
40	7.123	985	990	998	rVB5	2532	6912	0.74%	0.097%
41	7.300	1010	1019	1036	rBV	189619	434272	46.48%	6.070%
42	7.550	1059	1060	1063	rBV2	326	288	0.03%	0.004%
43	7.824	1099	1105	1110	rBV3	1839	3329	0.36%	0.047%
44	8.318	1180	1186	1199	rBV	130845	235508	25.21%	3.292%
45	8.525	1218	1220	1222	rBV	372	425	0.05%	0.006%
46	8.574	1224	1228	1233	rBV2	3524	5598	0.60%	0.078%
47	8.641	1233	1239	1249	rBV	427419	723322	77.42%	10.111%
48	8.946	1283	1289	1305	rBV	94671	149883	16.04%	2.095%
49	9.159	1319	1324	1329	rVB5	2587	4960	0.53%	0.069%
50	9.275	1338	1343	1349	rVB2	3861	6133	0.66%	0.086%
51	9.324	1349	1351	1353	rBV	537	516	0.06%	0.007%
52	9.378	1356	1360	1379	rBV	209259	338101	36.19%	4.726%
53	9.610	1394	1398	1404	rVB3	1880	3045	0.33%	0.043%
54	9.659	1404	1406	1408	rBV2	346	342	0.04%	0.005%
55	9.695	1410	1412	1415	rBV2	469	578	0.06%	0.008%
56	9.787	1426	1427	1431	rBV2	449	299	0.03%	0.004%
57	9.952	1451	1454	1457	rBV2	215	365	0.04%	0.005%
58	10.049	1465	1470	1485	rBV	516590	723196	77.40%	10.109%
59	10.195	1490	1494	1500	rVB	5562	8210	0.88%	0.115%
60	10.305	1508	1512	1516	rBV2	4989	7744	0.83%	0.108%
61	10.640	1562	1567	1578	rBV3	6750	16530	1.77%	0.231%
62	10.799	1590	1593	1599	rVB3	1573	2399	0.26%	0.034%
63	10.854	1599	1602	1605	rBV2	335	405	0.04%	0.006%
64	10.964	1615	1620	1630	rBV	6476	9598	1.03%	0.134%
65	11.189	1651	1657	1664	rBV	344074	442232	47.33%	6.182%
66	11.451	1695	1700	1707	rBV2	6314	8805	0.94%	0.123%
67	11.634	1728	1730	1731	rBV	312	313	0.03%	0.004%
68	11.756	1745	1750	1755	rVB2	5796	8286	0.89%	0.116%
69	11.969	1781	1785	1788	rVV2	5084	6128	0.66%	0.086%
70	12.018	1788	1793	1805	rVV	509290	628339	67.25%	8.783%
71	12.317	1837	1842	1853	rBV	466865	593801	63.55%	8.300%
72	12.579	1883	1885	1891	rVB2	332	396	0.04%	0.006%
73	12.671	1897	1900	1901	rBV	345	321	0.03%	0.004%
74	12.762	1910	1915	1918	rBV4	1440	2224	0.24%	0.031%
75	12.945	1939	1945	1950	rBV4	945	2043	0.22%	0.029%
76	13.067	1963	1965	1968	rBV2	302	344	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044784.D
Acq On : 31 Jan 2025 10:08
Operator : JC/MD
Sample : VX0131MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK757

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\SFAMXLM012825WMA.M
Title : VOC Analysis

77	13.116	1968	1973	1980	rVV3	4085	5659	0.61%	0.079%
78	13.183	1983	1984	1987	rVB2	378	309	0.03%	0.004%
79	13.347	2009	2011	2016	rVB2	304	420	0.04%	0.006%
80	13.591	2047	2051	2059	rVB3	3854	5833	0.62%	0.082%
81	13.780	2077	2082	2090	rVV	7091	11294	1.21%	0.158%
82	13.859	2094	2095	2097	rVB	789	406	0.04%	0.006%
83	13.896	2097	2101	2102	rBV	622	674	0.07%	0.009%
84	13.963	2108	2112	2117	rVB3	4945	6160	0.66%	0.086%
85	14.091	2127	2133	2135	rBV2	420	518	0.06%	0.007%
86	14.128	2135	2139	2144	rVV2	2661	3573	0.38%	0.050%
87	14.243	2157	2158	2162	rBV2	319	397	0.04%	0.006%
88	14.298	2165	2167	2170	rVV2	345	303	0.03%	0.004%
89	14.445	2188	2191	2194	rBV2	393	497	0.05%	0.007%
90	14.896	2263	2265	2268	rVV2	359	336	0.04%	0.005%
91	14.926	2268	2270	2273	rVB	556	548	0.06%	0.008%
92	15.048	2288	2290	2291	rVB	582	317	0.03%	0.004%
93	15.066	2291	2293	2296	rBV2	542	672	0.07%	0.009%
94	15.335	2335	2337	2339	rBV2	382	416	0.04%	0.006%
95	15.383	2343	2345	2351	rVB5	994	1404	0.15%	0.020%
96	15.755	2404	2406	2408	rBB2	458	317	0.03%	0.004%
97	15.871	2423	2425	2427	rBV2	503	413	0.04%	0.006%
98	16.524	2528	2532	2533	rBV2	406	519	0.06%	0.007%
99	16.670	2554	2556	2561	rBV4	580	973	0.10%	0.014%
100	16.761	2570	2571	2574	rBV2	511	458	0.05%	0.006%

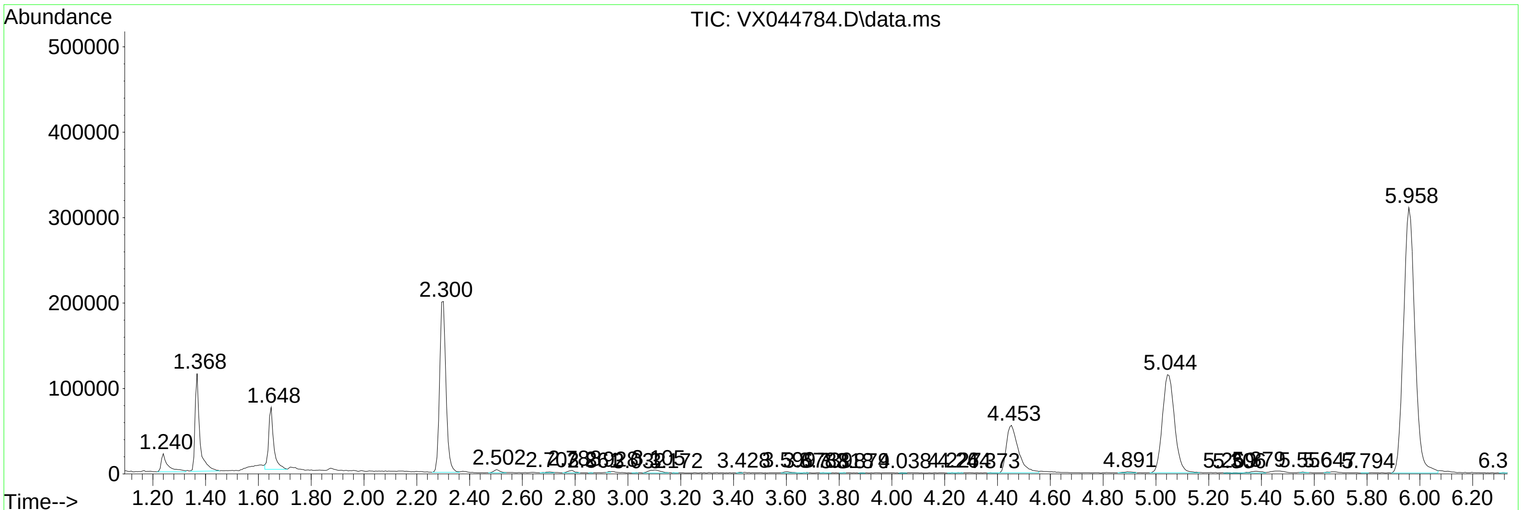
Sum of corrected areas: 7154116

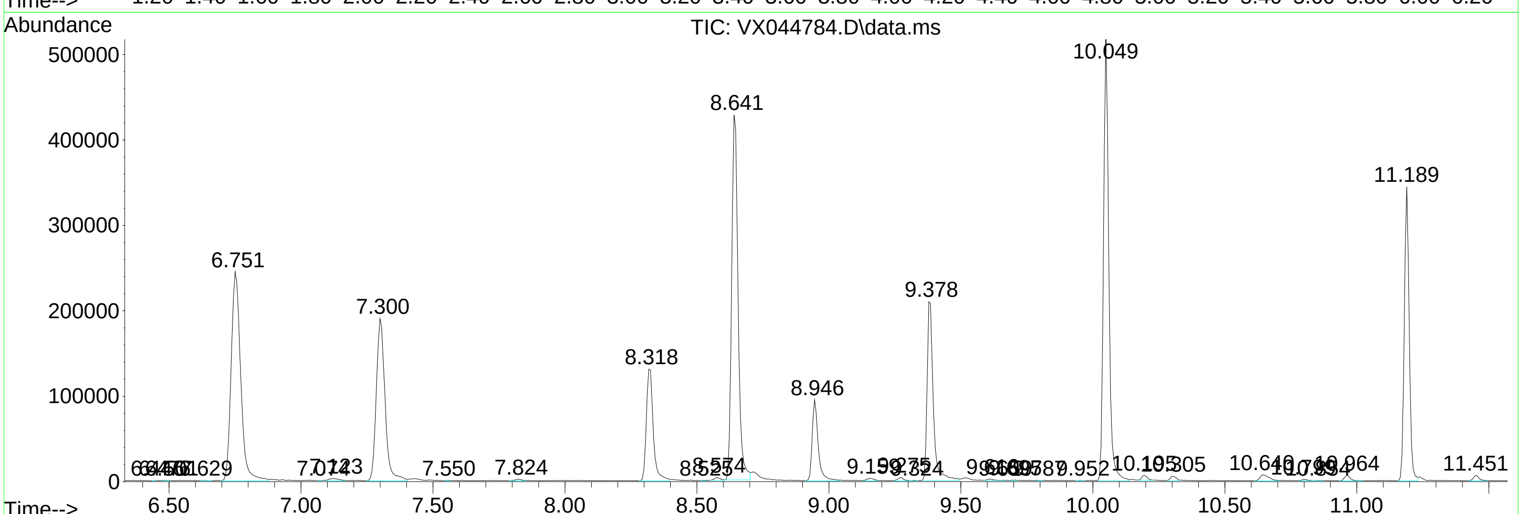
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044784.D
Acq On : 31 Jan 2025 10:08
Operator : JC/MD
Sample : VX0131MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

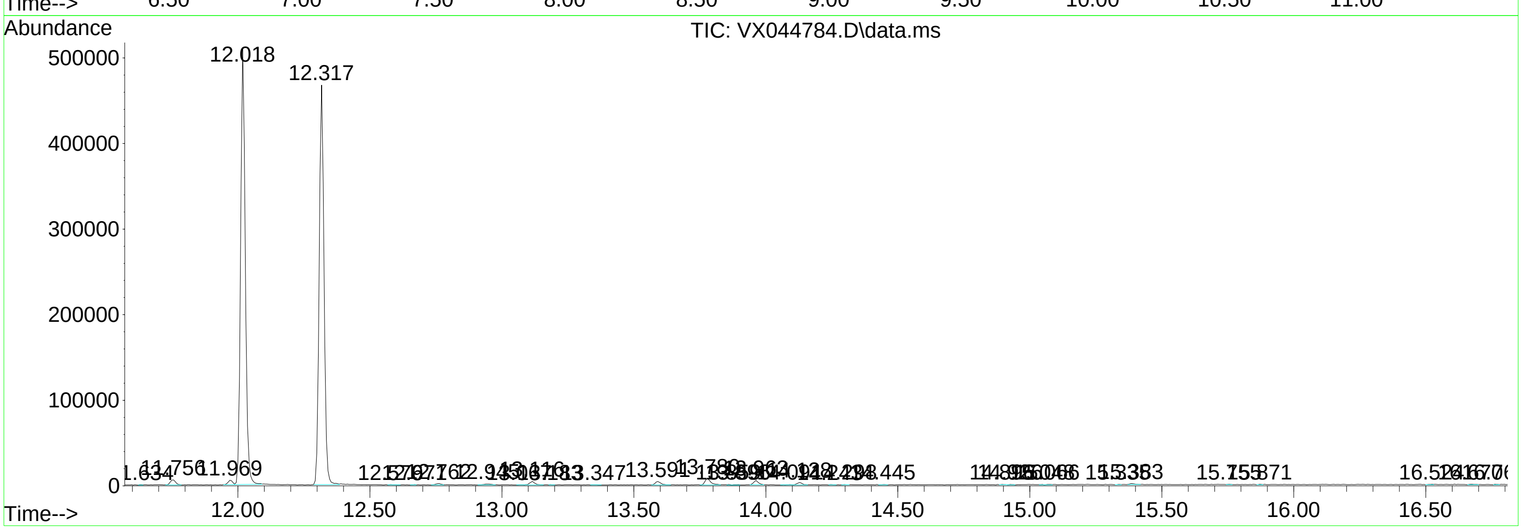
Instrument :
MSVOA_X
ClientSampleId :
VBLK757

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.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 : VX044784.D
Acq On : 31 Jan 2025 10:08
Operator : JC/MD
Sample : VX0131MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK757

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

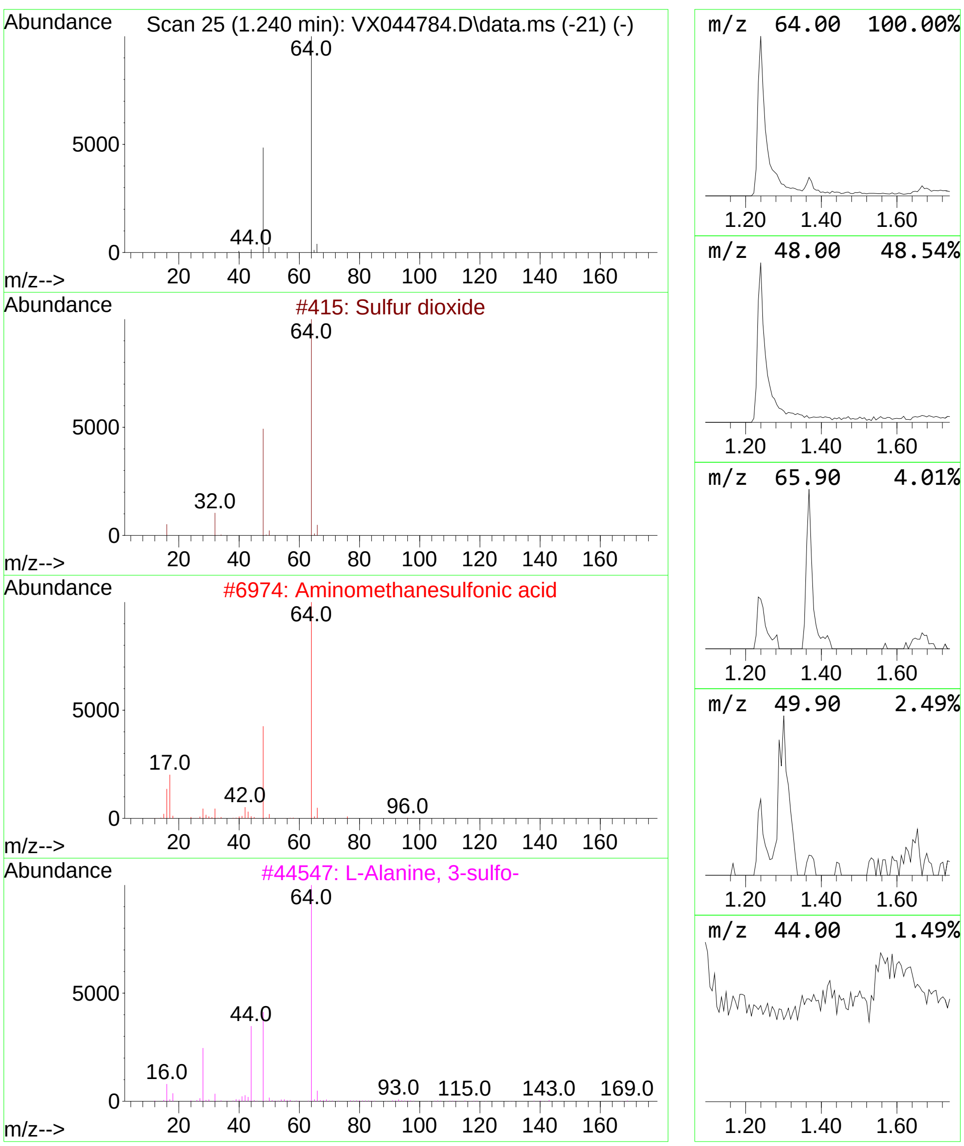
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.14 ug/L	38249	1,4-Difluorobenzene	6.751

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	4



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044784.D
Acq On : 31 Jan 2025 10:08
Operator : JC/MD
Sample : VX0131MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK757

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.240	3.1	ug/L	38249	1	6.751	609659	50.0