

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045207.D
 Acq On : 07 Oct 2021 13:18
 Operator : SY/MD
 Sample : M4025-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP4

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\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU045207.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	54	rBV	16115	35991	2.80%	0.363%
2	1.600	74	81	91	rVB	190513	202092	15.74%	2.036%
3	1.896	165	173	183	rVB	136109	180510	14.06%	1.819%
4	2.562	367	380	398	rBV	265580	450418	35.08%	4.538%
5	2.764	439	443	444	rBV	409	306	0.02%	0.003%
6	2.793	444	452	456	rVV5	1046	1850	0.14%	0.019%
7	3.102	545	548	551	rBV2	229	196	0.02%	0.002%
8	3.153	560	564	565	rBV	238	202	0.02%	0.002%
9	3.192	565	576	590	rVB2	3015	6711	0.52%	0.068%
10	3.327	616	618	623	rVB3	288	155	0.01%	0.002%
11	3.414	640	645	648	rBV2	300	294	0.02%	0.003%
12	3.485	663	667	669	rBV2	239	184	0.01%	0.002%
13	3.501	669	672	676	rVB2	212	149	0.01%	0.002%
14	3.604	700	704	706	rBV	244	180	0.01%	0.002%
15	3.819	765	771	774	rVB2	240	267	0.02%	0.003%
16	3.842	774	778	785	rVB	261	261	0.02%	0.003%
17	3.874	785	788	791	rBV	348	313	0.02%	0.003%
18	3.989	821	824	827	rVB	284	208	0.02%	0.002%
19	4.009	827	830	834	rBV2	203	202	0.02%	0.002%
20	4.073	843	850	852	rVV2	148	161	0.01%	0.002%
21	4.198	883	889	893	rBV	192	298	0.02%	0.003%
22	4.314	918	925	928	rBV	236	316	0.02%	0.003%
23	4.433	959	962	965	rVB	224	168	0.01%	0.002%
24	4.539	992	995	1002	rBV2	233	292	0.02%	0.003%
25	4.629	1006	1023	1048	rBV	139665	339479	26.44%	3.420%
26	4.809	1077	1079	1084	rBV2	227	163	0.01%	0.002%
27	5.067	1140	1159	1184	rBV	228346	497295	38.73%	5.010%
28	5.282	1224	1226	1227	rBV	448	211	0.02%	0.002%
29	5.314	1227	1236	1250	rVB5	2433	4898	0.38%	0.049%
30	5.530	1298	1303	1306	rBV2	185	158	0.01%	0.002%
31	5.555	1306	1311	1314	rVV2	122	157	0.01%	0.002%
32	5.729	1342	1365	1391	rBV2	477345	1284156	100.00%	12.937%
33	6.012	1451	1453	1458	rBV3	165	182	0.01%	0.002%
34	6.095	1475	1479	1480	rBV	281	205	0.02%	0.002%
35	6.140	1490	1493	1495	rBV2	213	143	0.01%	0.001%
36	6.253	1513	1528	1551	rBV	381003	709396	55.24%	7.147%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045207.D
 Acq On : 07 Oct 2021 13:18
 Operator : SY/MD
 Sample : M4025-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP4

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\SFAMULM092321WMA.M
 Title : VOC Analysis

37	6.546	1606	1619	1635	rVB	77039	144209	11.23%	1.453%
38	6.610	1635	1639	1641	rBV2	276	155	0.01%	0.002%
39	6.694	1651	1665	1688	rBV	302625	586448	45.67%	5.908%
40	6.806	1696	1700	1701	rBV2	395	322	0.03%	0.003%
41	7.044	1768	1774	1776	rBV2	345	374	0.03%	0.004%
42	7.089	1783	1788	1791	rBV2	144	149	0.01%	0.002%
43	7.185	1810	1818	1824	rVV4	1203	1738	0.14%	0.018%
44	7.301	1851	1854	1858	rBV	172	168	0.01%	0.002%
45	7.356	1867	1871	1873	rBV2	279	235	0.02%	0.002%
46	7.420	1889	1891	1895	rVB2	212	148	0.01%	0.001%
47	7.462	1901	1904	1909	rBV2	203	184	0.01%	0.002%
48	7.491	1909	1913	1918	rBV2	177	175	0.01%	0.002%
49	7.568	1925	1937	1962	rVB	156269	268200	20.89%	2.702%
50	7.693	1969	1976	1980	rVV3	697	924	0.07%	0.009%
51	7.732	1984	1988	1990	rBV2	169	148	0.01%	0.001%
52	7.902	2026	2041	2055	rBV	598220	1018675	79.33%	10.263%
53	7.973	2057	2063	2077	rVB	8480	14068	1.10%	0.142%
54	8.182	2115	2128	2144	rVV	110652	180283	14.04%	1.816%
55	8.478	2212	2220	2223	rVV2	395	524	0.04%	0.005%
56	8.636	2257	2269	2296	rBV	420621	734252	57.18%	7.397%
57	9.028	2387	2391	2397	rBV	272	394	0.03%	0.004%
58	9.137	2420	2425	2428	rVB	164	166	0.01%	0.002%
59	9.156	2428	2431	2436	rBV	292	288	0.02%	0.003%
60	9.420	2500	2513	2533	rBV	543416	884105	68.85%	8.907%
61	9.574	2556	2561	2566	rVB2	268	341	0.03%	0.003%
62	9.697	2591	2599	2607	rVB3	920	1473	0.11%	0.015%
63	9.777	2620	2624	2630	rBV2	162	196	0.02%	0.002%
64	9.845	2641	2645	2647	rBV2	266	247	0.02%	0.002%
65	9.973	2682	2685	2690	rBV2	215	233	0.02%	0.002%
66	10.230	2759	2765	2768	rBV	254	310	0.02%	0.003%
67	10.263	2772	2775	2780	rVB2	183	207	0.02%	0.002%
68	10.301	2782	2787	2790	rBV	150	167	0.01%	0.002%
69	10.671	2895	2902	2913	rVB3	1588	2516	0.20%	0.025%
70	10.761	2916	2930	2949	rBV	429465	688833	53.64%	6.940%
71	10.867	2959	2963	2965	rBV	390	262	0.02%	0.003%
72	10.883	2965	2968	2970	rVV2	298	232	0.02%	0.002%
73	10.896	2970	2972	2977	rVB3	496	349	0.03%	0.004%
74	10.922	2977	2980	2987	rBV2	251	280	0.02%	0.003%
75	11.089	3028	3032	3037	rBV3	243	259	0.02%	0.003%
76	11.172	3055	3058	3061	rBV2	179	163	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045207.D
 Acq On : 07 Oct 2021 13:18
 Operator : SY/MD
 Sample : M4025-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP4

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\SFAMULM092321WMA.M

Title : VOC Analysis

77	11.214	3067	3071	3075	rVB2	246	194	0.02%	0.002%
78	11.237	3075	3078	3081	rVB	245	152	0.01%	0.002%
79	11.253	3081	3083	3087	rVB2	239	180	0.01%	0.002%
80	11.285	3087	3093	3094	rBV	243	240	0.02%	0.002%
81	11.324	3101	3105	3108	rBV	271	267	0.02%	0.003%
82	11.465	3140	3149	3158	rBV4	1129	2078	0.16%	0.021%
83	11.565	3178	3180	3184	rBV2	162	144	0.01%	0.001%
84	11.693	3217	3220	3225	rBV2	567	573	0.04%	0.006%
85	11.751	3232	3238	3240	rBV2	227	274	0.02%	0.003%
86	11.815	3245	3258	3278	rVV	502211	793860	61.82%	7.998%
87	11.973	3303	3307	3308	rBV2	634	426	0.03%	0.004%
88	12.195	3363	3376	3393	rBV	537600	874028	68.06%	8.805%
89	12.478	3461	3464	3466	rVV	239	174	0.01%	0.002%
90	12.764	3549	3553	3554	rBV2	245	167	0.01%	0.002%
91	12.896	3589	3594	3598	rBV2	205	227	0.02%	0.002%
92	12.973	3615	3618	3619	rBV	326	206	0.02%	0.002%
93	13.031	3631	3636	3639	rBV2	362	363	0.03%	0.004%
94	13.082	3646	3652	3655	rBV2	299	326	0.03%	0.003%
95	13.172	3676	3680	3684	rBV2	242	229	0.02%	0.002%
96	13.375	3739	3743	3747	rBV2	306	348	0.03%	0.004%
97	13.449	3764	3766	3769	rBV	228	142	0.01%	0.001%
98	14.282	4023	4025	4028	rBV	212	140	0.01%	0.001%
99	14.336	4040	4042	4046	rBV	336	168	0.01%	0.002%
100	14.719	4155	4161	4165	rBV2	406	516	0.04%	0.005%

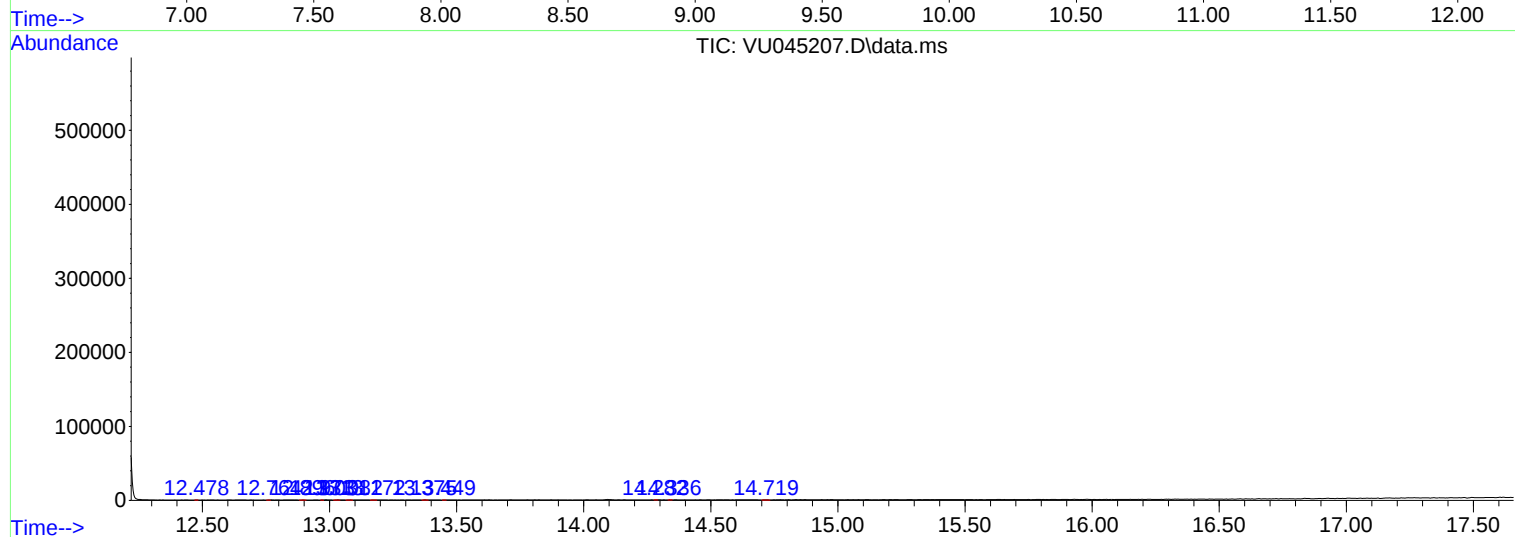
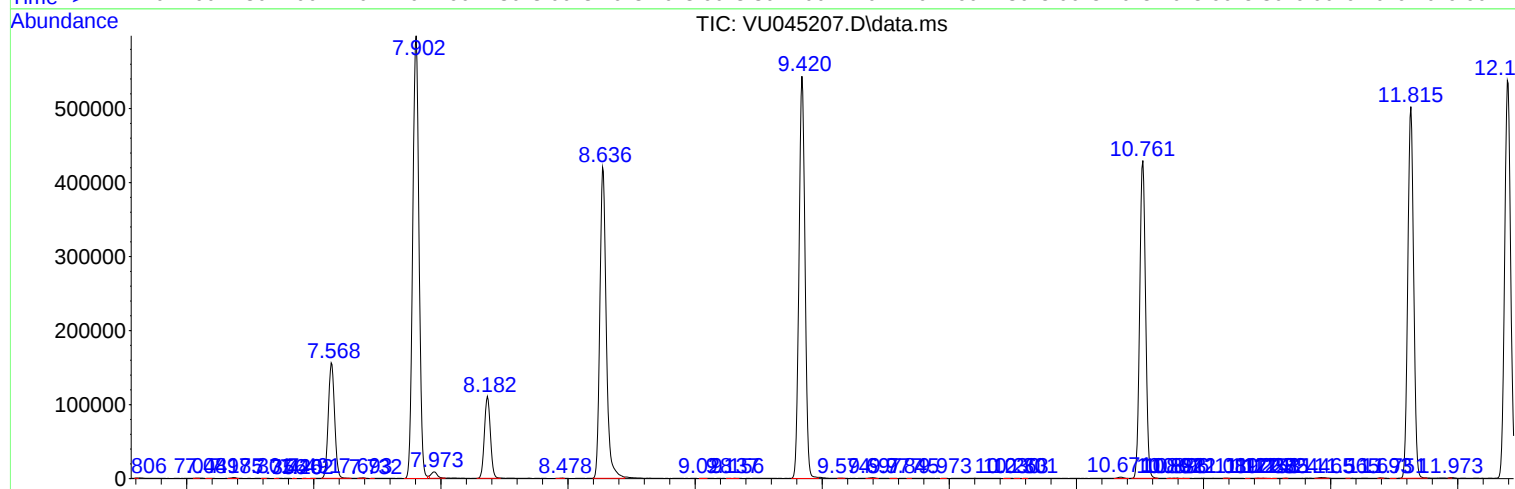
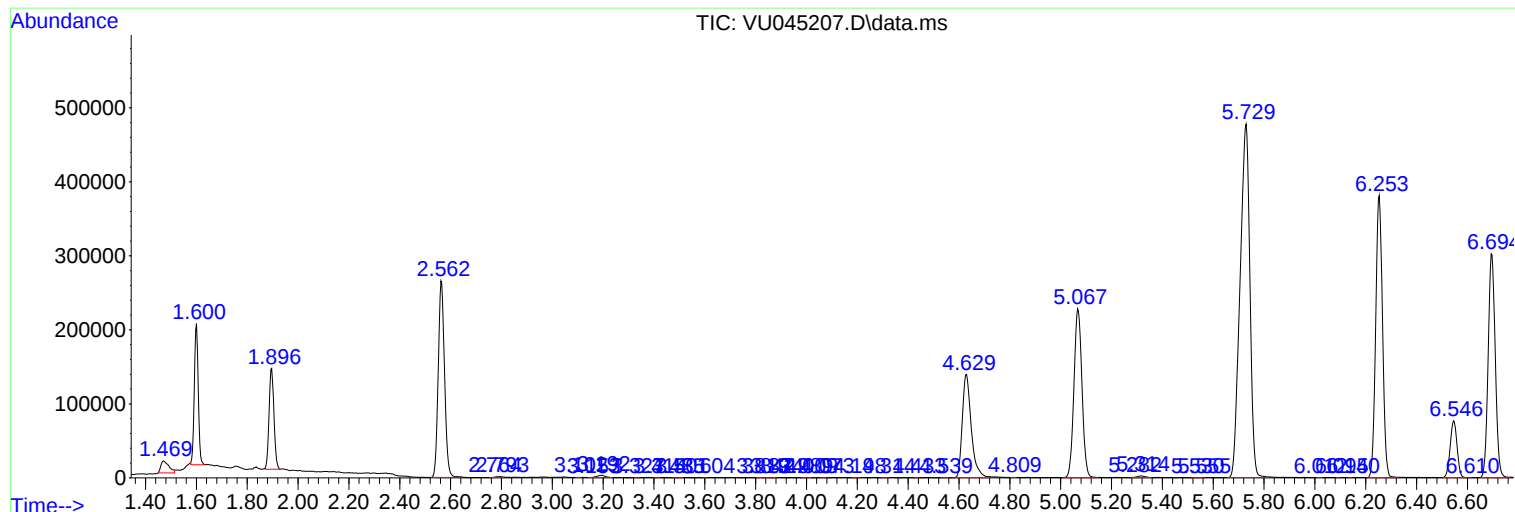
Sum of corrected areas: 9925989

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045207.D
Acq On : 07 Oct 2021 13:18
Operator : SY/MD
Sample : M4025-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AP4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045207.D
Acq On : 07 Oct 2021 13:18
Operator : SY/MD
Sample : M4025-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AP4

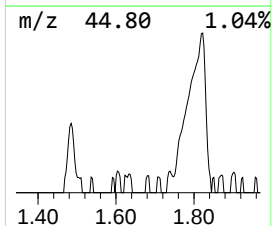
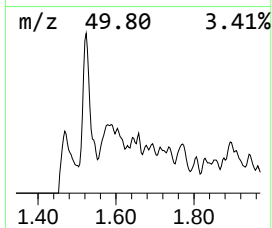
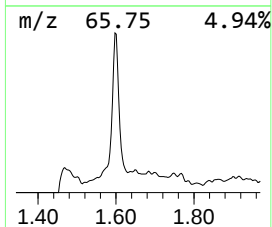
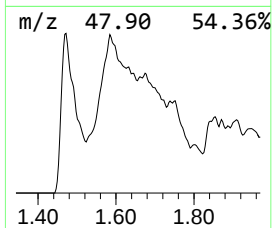
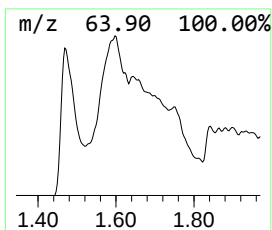
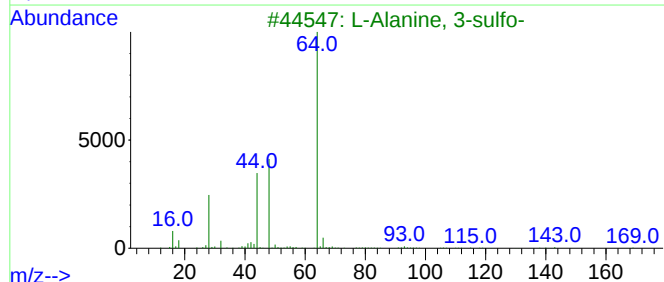
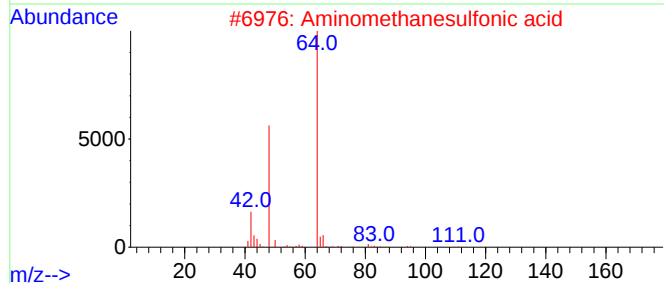
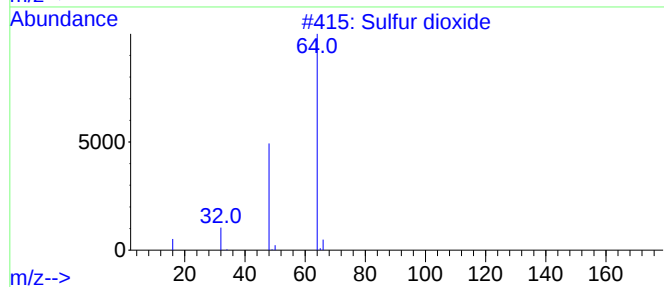
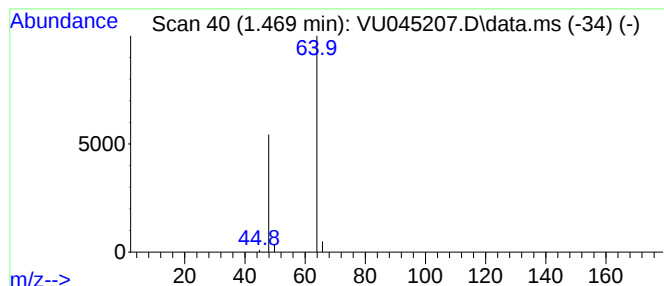
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	2.54 ug/L	35991	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045207.D
Acq On : 07 Oct 2021 13:18
Operator : SY/MD
Sample : M4025-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AP4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.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	2.5	ug/L	35991	1	6.253	709396	50.0