

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045188.D
 Acq On : 06 Oct 2021 16:14
 Operator : SY/MD
 Sample : M4024-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COANO

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: VU0451188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	32	39	57	rBV	125756	216768	17.04%	2.220%
2	1.600	75	81	102	rVB	167134	199156	15.66%	2.039%
3	1.899	167	174	195	rVB	126045	180219	14.17%	1.845%
4	2.565	368	381	396	rBV	241024	406567	31.96%	4.163%
5	2.771	435	445	465	rVB	11253	22190	1.74%	0.227%
6	2.845	465	468	472	rBV	368	290	0.02%	0.003%
7	2.948	492	500	511	rBV3	978	2070	0.16%	0.021%
8	2.996	512	515	520	rVV3	229	186	0.01%	0.002%
9	3.051	525	532	540	rVB2	839	1195	0.09%	0.012%
10	3.128	553	556	560	rBV	196	222	0.02%	0.002%
11	3.192	561	576	591	rVB	14141	31217	2.45%	0.320%
12	3.395	635	639	646	rBV2	260	402	0.03%	0.004%
13	3.440	650	653	657	rVB2	224	206	0.02%	0.002%
14	3.494	667	670	675	rBV2	203	232	0.02%	0.002%
15	3.591	697	700	706	rVB3	534	621	0.05%	0.006%
16	3.629	707	712	717	rBV	232	278	0.02%	0.003%
17	3.793	761	763	769	rVB2	231	204	0.02%	0.002%
18	3.922	799	803	806	rBV2	211	223	0.02%	0.002%
19	3.973	814	819	822	rBV	197	199	0.02%	0.002%
20	4.018	829	833	836	rBV2	234	214	0.02%	0.002%
21	4.063	843	847	851	rVB2	194	192	0.02%	0.002%
22	4.089	851	855	858	rBV2	271	235	0.02%	0.002%
23	4.115	858	863	871	rVB2	200	303	0.02%	0.003%
24	4.510	978	986	993	rBV	264	467	0.04%	0.005%
25	4.629	1004	1023	1047	rBV	145070	349395	27.47%	3.578%
26	4.761	1062	1064	1072	rVB3	570	408	0.03%	0.004%
27	4.977	1123	1131	1133	rBV2	388	378	0.03%	0.004%
28	5.067	1143	1159	1182	rVV	223464	486348	38.23%	4.980%
29	5.195	1196	1199	1201	rBV2	424	313	0.02%	0.003%
30	5.285	1223	1227	1228	rBV2	558	345	0.03%	0.004%
31	5.372	1251	1254	1255	rBV	342	180	0.01%	0.002%
32	5.571	1314	1316	1324	rVB2	365	362	0.03%	0.004%
33	5.616	1324	1330	1335	rBV2	243	363	0.03%	0.004%
34	5.729	1343	1365	1389	rBV2	471364	1272011	100.00%	13.026%
35	6.083	1472	1475	1479	rBV	240	238	0.02%	0.002%
36	6.253	1513	1528	1544	rBV	366498	686753	53.99%	7.032%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045188.D
 Acq On : 06 Oct 2021 16:14
 Operator : SY/MD
 Sample : M4024-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COANO

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	6.391	1568	1571	1576	rVB2	405	319	0.03%	0.003%
38	6.417	1576	1579	1582	rBV2	240	240	0.02%	0.002%
39	6.546	1608	1619	1629	rVB5	8384	15711	1.24%	0.161%
40	6.620	1636	1642	1643	rBV2	293	254	0.02%	0.003%
41	6.697	1650	1666	1685	rBV	299912	584520	45.95%	5.986%
42	6.796	1692	1697	1699	rBV4	457	451	0.04%	0.005%
43	7.021	1761	1767	1769	rBV2	170	200	0.02%	0.002%
44	7.044	1769	1774	1775	rBV3	401	347	0.03%	0.004%
45	7.099	1786	1791	1793	rBV2	227	230	0.02%	0.002%
46	7.182	1804	1817	1828	rBV4	2028	3648	0.29%	0.037%
47	7.520	1918	1922	1924	rBV2	254	184	0.01%	0.002%
48	7.568	1924	1937	1957	rVV	152890	261906	20.59%	2.682%
49	7.690	1969	1975	1982	rVB3	1139	1868	0.15%	0.019%
50	7.902	2027	2041	2056	rBV	574465	976396	76.76%	9.998%
51	7.973	2056	2063	2073	rVB2	9508	16367	1.29%	0.168%
52	8.182	2117	2128	2143	rBV	107098	174262	13.70%	1.784%
53	8.423	2200	2203	2208	rBV2	240	218	0.02%	0.002%
54	8.462	2208	2215	2217	rBV2	293	278	0.02%	0.003%
55	8.529	2231	2236	2239	rVB2	197	224	0.02%	0.002%
56	8.555	2240	2244	2247	rBV3	497	374	0.03%	0.004%
57	8.636	2256	2269	2302	rBV	416217	727376	57.18%	7.448%
58	8.938	2358	2363	2366	rBV	253	181	0.01%	0.002%
59	9.182	2435	2439	2442	rBV	184	213	0.02%	0.002%
60	9.420	2498	2513	2531	rBV	530347	851907	66.97%	8.724%
61	9.562	2553	2557	2558	rBV	354	240	0.02%	0.002%
62	9.574	2558	2561	2566	rVB3	568	582	0.05%	0.006%
63	9.693	2591	2598	2611	rVB3	3038	4446	0.35%	0.046%
64	9.748	2611	2615	2618	rBV	281	223	0.02%	0.002%
65	9.771	2618	2622	2625	rBV2	239	217	0.02%	0.002%
66	9.793	2625	2629	2633	rBV2	224	243	0.02%	0.002%
67	9.928	2668	2671	2676	rVB2	258	236	0.02%	0.002%
68	9.963	2676	2682	2684	rBV2	248	274	0.02%	0.003%
69	10.105	2719	2726	2734	rVB3	884	1351	0.11%	0.014%
70	10.221	2758	2762	2764	rBV2	211	208	0.02%	0.002%
71	10.336	2795	2798	2803	rBV	253	231	0.02%	0.002%
72	10.423	2820	2825	2828	rBV2	232	244	0.02%	0.002%
73	10.571	2868	2871	2877	rVB2	249	280	0.02%	0.003%
74	10.674	2898	2903	2912	rVB3	1581	2168	0.17%	0.022%
75	10.761	2916	2930	2953	rBV	423525	675138	53.08%	6.913%
76	10.841	2953	2955	2960	rVB	205	180	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045188.D
 Acq On : 06 Oct 2021 16:14
 Operator : SY/MD
 Sample : M4024-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN0

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	10.954	2984	2990	2992	rBV	205	235	0.02%	0.002%
78	11.124	3041	3043	3048	rVB2	470	338	0.03%	0.003%
79	11.250	3078	3082	3086	rBV	201	232	0.02%	0.002%
80	11.468	3141	3150	3161	rBV7	1717	3111	0.24%	0.032%
81	11.635	3194	3202	3209	rVB3	1020	1240	0.10%	0.013%
82	11.700	3213	3222	3227	rBV4	1045	1354	0.11%	0.014%
83	11.815	3245	3258	3281	rVB	480618	748552	58.85%	7.665%
84	11.906	3281	3286	3290	rVV2	479	406	0.03%	0.004%
85	11.944	3296	3298	3299	rVV	598	336	0.03%	0.003%
86	11.976	3303	3308	3315	rVB4	1394	1675	0.13%	0.017%
87	12.063	3331	3335	3336	rBV2	643	444	0.03%	0.005%
88	12.195	3361	3376	3392	rBV	519267	836107	65.73%	8.562%
89	12.336	3417	3420	3423	rBV3	293	195	0.02%	0.002%
90	12.407	3437	3442	3445	rBV	301	260	0.02%	0.003%
91	12.648	3512	3517	3524	rVB2	325	380	0.03%	0.004%
92	12.787	3557	3560	3565	rBV2	253	222	0.02%	0.002%
93	13.092	3653	3655	3658	rBV	227	178	0.01%	0.002%
94	13.298	3714	3719	3721	rBV2	229	213	0.02%	0.002%
95	13.571	3801	3804	3807	rBV	250	230	0.02%	0.002%
96	13.735	3851	3855	3858	rBV2	293	249	0.02%	0.003%
97	13.770	3861	3866	3868	rBV	289	282	0.02%	0.003%
98	13.870	3892	3897	3900	rBV2	336	392	0.03%	0.004%
99	13.918	3909	3912	3916	rBV	479	418	0.03%	0.004%
100	14.092	3958	3966	3978	rVB	2573	3590	0.28%	0.037%

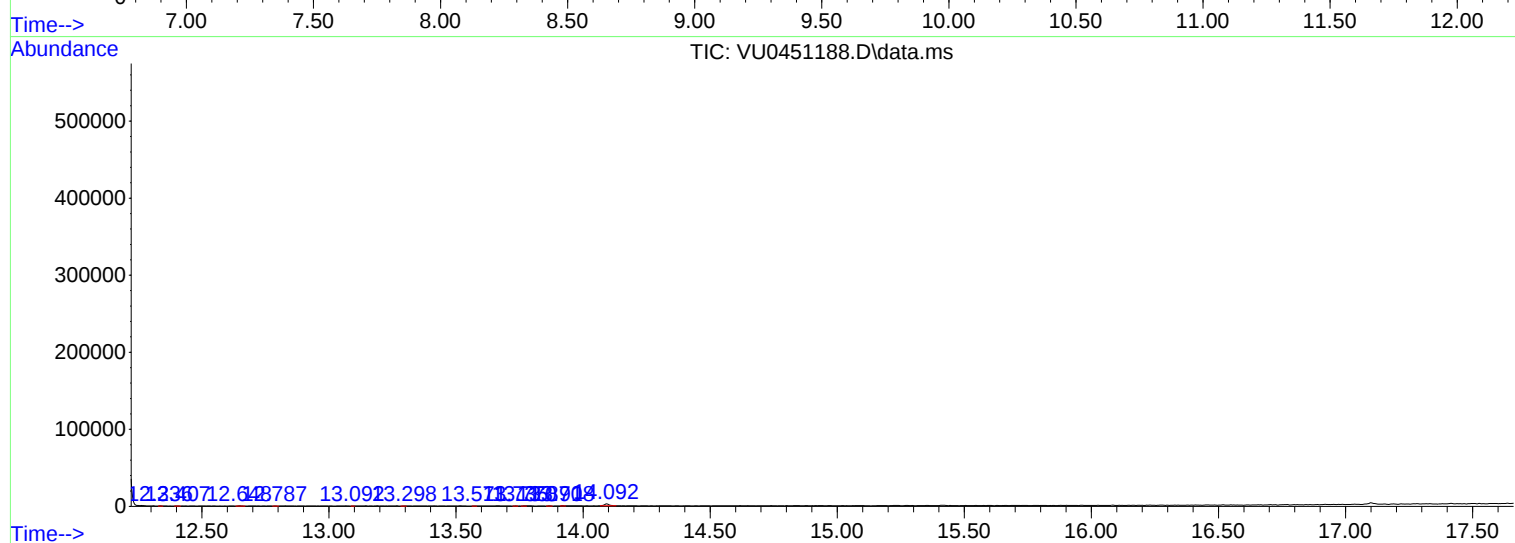
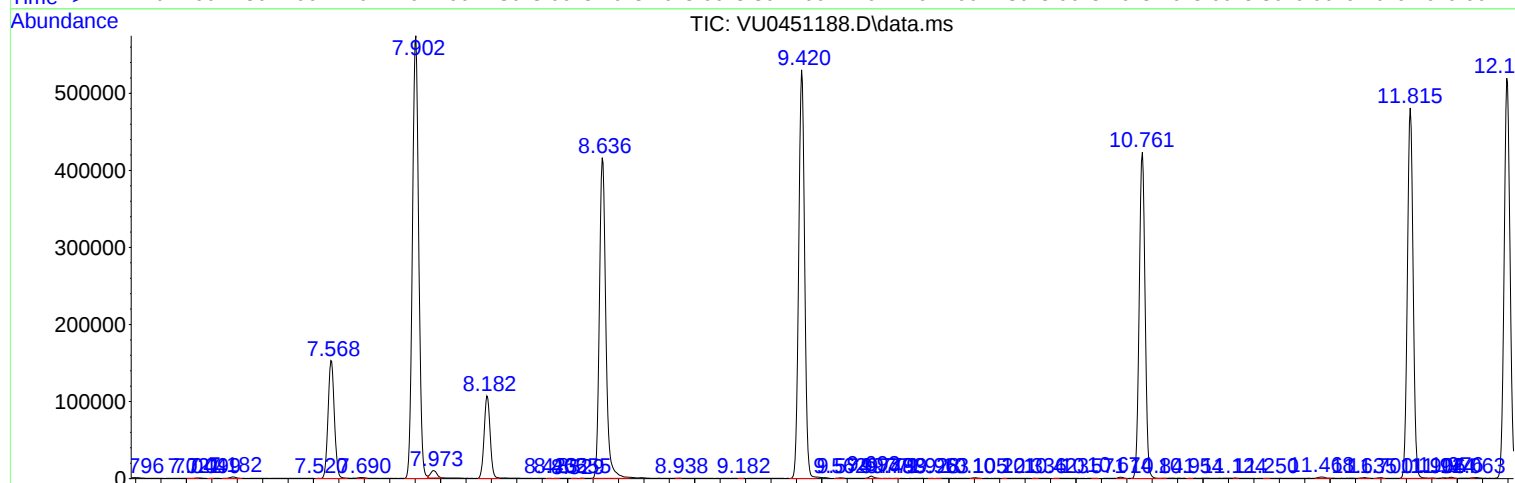
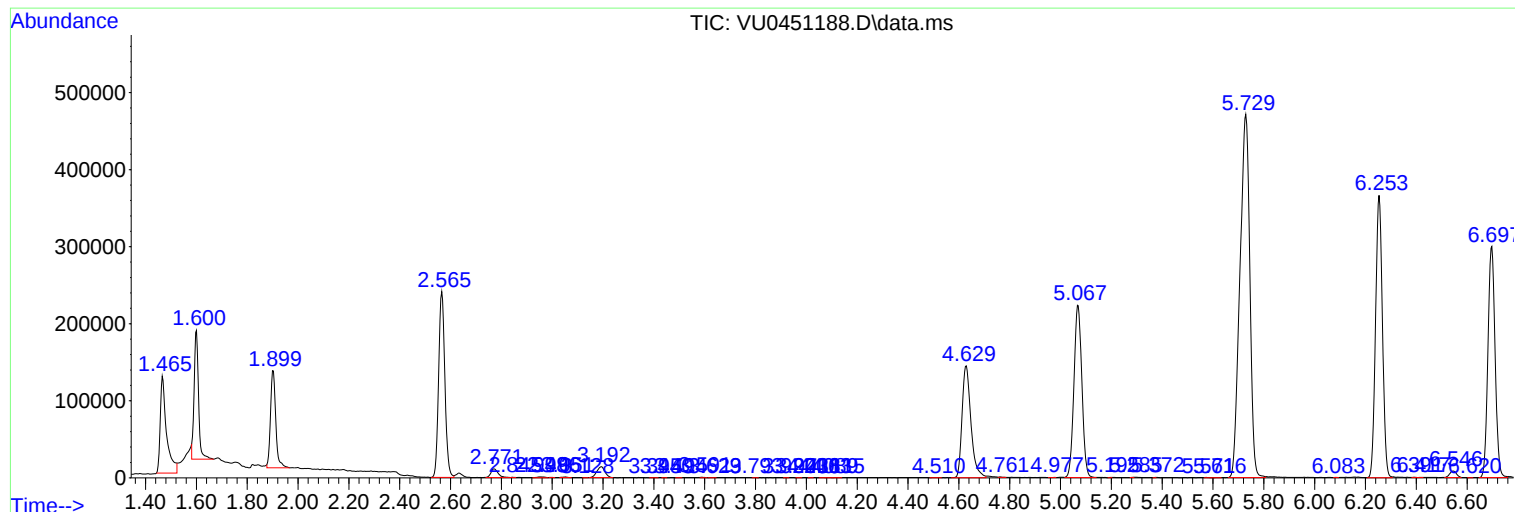
Sum of corrected areas: 9765524

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
Data File : VU045188.D
Acq On : 06 Oct 2021 16:14
Operator : SY/MD
Sample : M4024-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COANO

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\VU100621\
Data File : VU045188.D
Acq On : 06 Oct 2021 16:14
Operator : SY/MD
Sample : M4024-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COANO

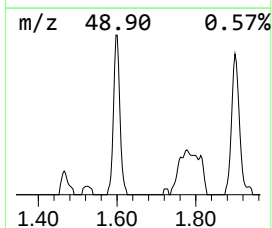
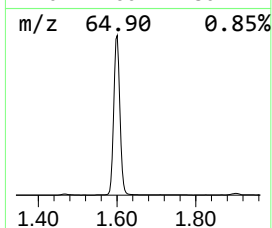
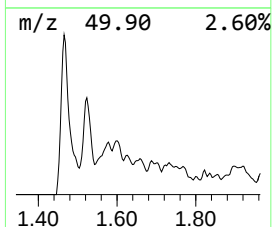
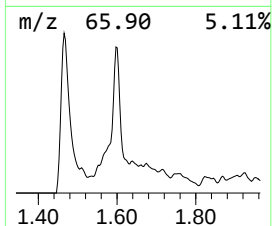
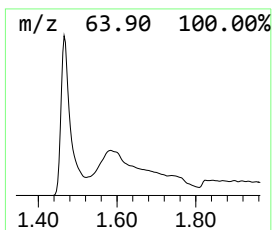
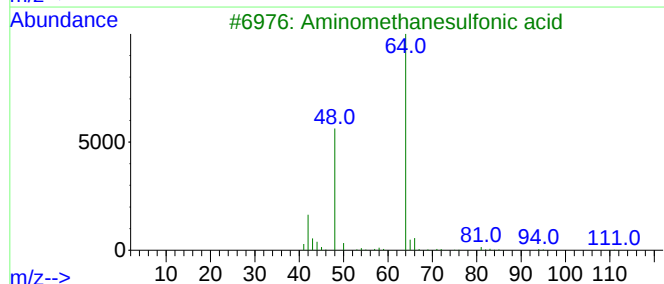
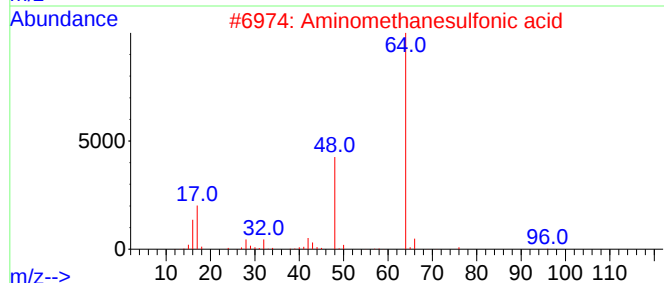
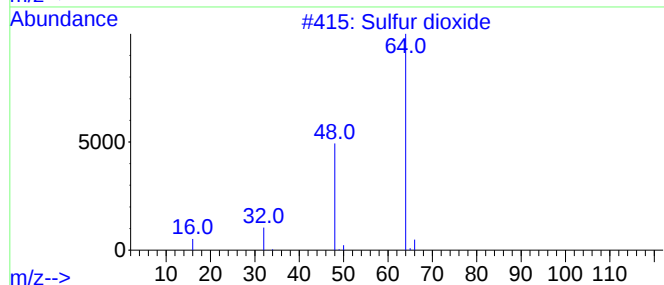
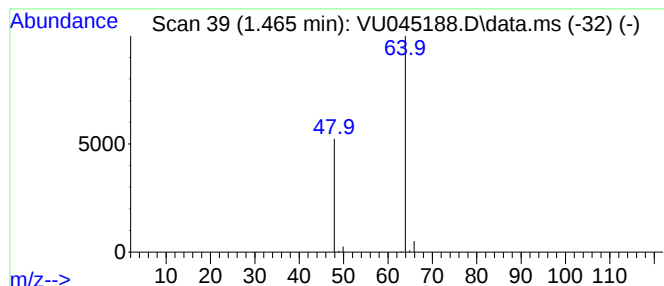
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.465	15.78 ug/L	216768	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
Data File : VU045188.D
Acq On : 06 Oct 2021 16:14
Operator : SY/MD
Sample : M4024-18
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COANO

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	1.465	15.8	ug/L	216768	1	6.253	686753	50.0