

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
 Data File : VU045166.D
 Acq On : 05 Oct 2021 23:56
 Operator : SY/MD
 Sample : M3996-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A42

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: VU045166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.501	37	50	74	rBV	268612	1225116	94.73%	10.560%
2	1.912	173	178	201	rVB	143030	208595	16.13%	1.798%
3	2.572	370	383	404	rBV	259513	430622	33.30%	3.712%
4	2.803	444	455	463	rBV	4641	8682	0.67%	0.075%
5	3.192	567	576	592	rVB	16287	37539	2.90%	0.324%
6	3.359	615	628	651	rVB	116570	228958	17.70%	1.973%
7	3.861	773	784	795	rVV4	1554	3367	0.26%	0.029%
8	4.067	843	848	853	rVB2	253	238	0.02%	0.002%
9	4.099	853	858	861	rBV	174	188	0.01%	0.002%
10	4.218	892	895	900	rBV2	175	203	0.02%	0.002%
11	4.346	932	935	939	rVB2	184	154	0.01%	0.001%
12	4.427	955	960	963	rVB2	156	186	0.01%	0.002%
13	4.568	995	1004	1010	rBV4	1497	2917	0.23%	0.025%
14	4.636	1010	1025	1059	rVV2	147562	538567	41.65%	4.642%
15	4.957	1121	1125	1129	rBV2	201	276	0.02%	0.002%
16	5.002	1135	1139	1142	rBV3	142	155	0.01%	0.001%
17	5.070	1143	1160	1185	rVV	229217	499917	38.66%	4.309%
18	5.195	1196	1199	1200	rBV2	377	220	0.02%	0.002%
19	5.288	1224	1228	1229	rBV2	390	201	0.02%	0.002%
20	5.459	1277	1281	1285	rBV2	164	218	0.02%	0.002%
21	5.533	1299	1304	1308	rBV2	223	251	0.02%	0.002%
22	5.732	1343	1366	1399	rBV2	477983	1293215	100.00%	11.147%
23	5.877	1407	1411	1416	rBV5	329	305	0.02%	0.003%
24	6.253	1512	1528	1544	rBV	379313	714646	55.26%	6.160%
25	6.546	1609	1619	1633	rVB3	12812	23085	1.79%	0.199%
26	6.697	1650	1666	1687	rBV	304047	590035	45.63%	5.086%
27	6.806	1695	1700	1704	rVB3	530	598	0.05%	0.005%
28	6.935	1737	1740	1744	rBV	210	201	0.02%	0.002%
29	7.038	1769	1772	1773	rVV2	418	267	0.02%	0.002%
30	7.060	1777	1779	1785	rVB2	390	326	0.03%	0.003%
31	7.185	1807	1818	1831	rVB4	2191	4126	0.32%	0.036%
32	7.243	1831	1836	1840	rBV2	190	248	0.02%	0.002%
33	7.337	1861	1865	1870	rVB2	179	215	0.02%	0.002%
34	7.385	1876	1880	1886	rBV2	221	334	0.03%	0.003%
35	7.571	1925	1938	1958	rVV	163393	285941	22.11%	2.465%
36	7.693	1968	1976	1983	rVB2	1347	2002	0.15%	0.017%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
 Data File : VU045166.D
 Acq On : 05 Oct 2021 23:56
 Operator : SY/MD
 Sample : M3996-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A42

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	7.902	2027	2041	2056	rBV	574516	991985	76.71%	8.550%
38	8.128	2106	2111	2115	rBV	244	195	0.02%	0.002%
39	8.182	2115	2128	2146	rBV	110564	190342	14.72%	1.641%
40	8.308	2165	2167	2170	rVB	340	168	0.01%	0.001%
41	8.449	2206	2211	2213	rBV	215	193	0.01%	0.002%
42	8.555	2233	2244	2258	rBV	128880	216584	16.75%	1.867%
43	8.639	2258	2270	2302	rBV	453304	800425	61.89%	6.899%
44	8.928	2355	2360	2366	rBV2	182	230	0.02%	0.002%
45	8.989	2376	2379	2384	rVB2	189	174	0.01%	0.001%
46	9.028	2384	2391	2394	rBV2	183	182	0.01%	0.002%
47	9.073	2399	2405	2406	rBV	142	172	0.01%	0.001%
48	9.105	2411	2415	2420	rVB2	218	184	0.01%	0.002%
49	9.134	2420	2424	2429	rBV2	196	214	0.02%	0.002%
50	9.205	2443	2446	2449	rBV	173	154	0.01%	0.001%
51	9.327	2480	2484	2488	rBV2	202	200	0.02%	0.002%
52	9.353	2488	2492	2497	rVB	285	295	0.02%	0.003%
53	9.420	2497	2513	2549	rBV	540194	886300	68.53%	7.639%
54	9.574	2559	2561	2564	rVV	367	245	0.02%	0.002%
55	9.693	2592	2598	2607	rBV5	892	1348	0.10%	0.012%
56	9.780	2615	2625	2635	rVB3	6122	9243	0.71%	0.080%
57	9.999	2687	2693	2696	rBV2	197	250	0.02%	0.002%
58	10.050	2705	2709	2716	rVB2	157	241	0.02%	0.002%
59	10.105	2721	2726	2729	rBV2	347	306	0.02%	0.003%
60	10.131	2729	2734	2737	rVB2	222	184	0.01%	0.002%
61	10.394	2813	2816	2819	rBV	208	192	0.01%	0.002%
62	10.478	2839	2842	2846	rBV	199	217	0.02%	0.002%
63	10.526	2848	2857	2873	rVV2	6854	12077	0.93%	0.104%
64	10.674	2889	2903	2915	rBV2	2736	4634	0.36%	0.040%
65	10.761	2915	2930	2948	rBV	420173	681376	52.69%	5.873%
66	10.867	2959	2963	2967	rBV	335	336	0.03%	0.003%
67	10.925	2978	2981	2986	rVB	370	273	0.02%	0.002%
68	10.957	2986	2991	2997	rBV	231	349	0.03%	0.003%
69	11.086	3030	3031	3035	rVB2	297	168	0.01%	0.001%
70	11.118	3037	3041	3043	rVV2	523	395	0.03%	0.003%
71	11.131	3043	3045	3046	rVV	384	194	0.02%	0.002%
72	11.156	3050	3053	3062	rVB	376	381	0.03%	0.003%
73	11.288	3087	3094	3096	rBV2	262	308	0.02%	0.003%
74	11.307	3097	3100	3104	rVB2	169	162	0.01%	0.001%
75	11.362	3113	3117	3120	rBV	252	209	0.02%	0.002%
76	11.462	3139	3148	3159	rBV6	1592	3019	0.23%	0.026%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
 Data File : VU045166.D
 Acq On : 05 Oct 2021 23:56
 Operator : SY/MD
 Sample : M3996-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A42

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	11.516	3162	3165	3171	rVB	264	314	0.02%	0.003%
78	11.610	3191	3194	3199	rVB2	181	184	0.01%	0.002%
79	11.668	3209	3212	3215	rBV	200	179	0.01%	0.002%
80	11.693	3215	3220	3228	rVB5	988	1352	0.10%	0.012%
81	11.764	3238	3242	3245	rBV2	241	169	0.01%	0.001%
82	11.816	3245	3258	3275	rBV	510552	810279	62.66%	6.984%
83	11.922	3288	3291	3293	rBV3	326	212	0.02%	0.002%
84	11.976	3303	3308	3313	rVB5	926	1276	0.10%	0.011%
85	12.066	3333	3336	3341	rBV3	307	299	0.02%	0.003%
86	12.195	3358	3376	3396	rBV	545532	877504	67.85%	7.563%
87	12.336	3415	3420	3423	rBV2	390	297	0.02%	0.003%
88	12.684	3525	3528	3532	rVB2	304	239	0.02%	0.002%
89	12.761	3547	3552	3556	rBV	550	619	0.05%	0.005%
90	12.864	3581	3584	3593	rVB2	218	283	0.02%	0.002%
91	13.224	3692	3696	3700	rBV2	234	219	0.02%	0.002%
92	13.250	3700	3704	3706	rBV	218	175	0.01%	0.002%
93	13.439	3759	3763	3769	rBV2	287	268	0.02%	0.002%
94	13.841	3885	3888	3890	rBV	187	156	0.01%	0.001%
95	13.986	3930	3933	3937	rBV2	278	240	0.02%	0.002%
96	14.092	3962	3966	3968	rBV3	445	390	0.03%	0.003%
97	14.304	4029	4032	4038	rBV2	198	193	0.01%	0.002%
98	14.735	4164	4166	4171	rBV2	292	239	0.02%	0.002%
99	14.918	4221	4223	4226	rBV	322	234	0.02%	0.002%
100	15.005	4246	4250	4254	rBV2	349	347	0.03%	0.003%

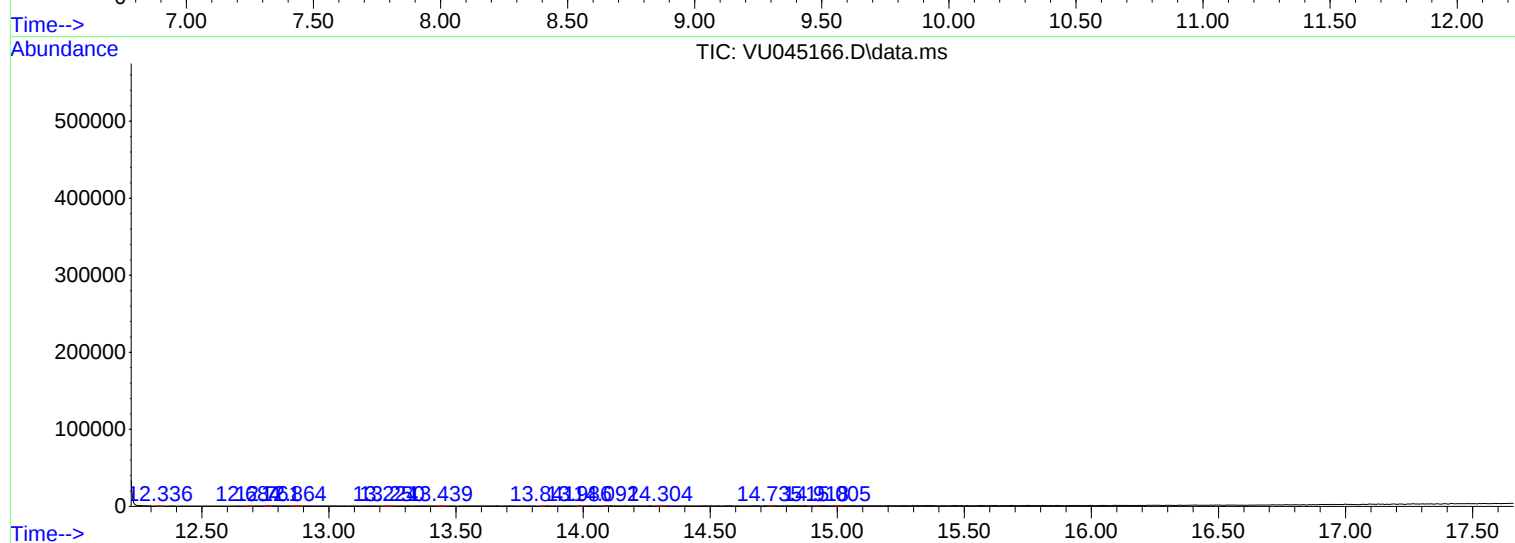
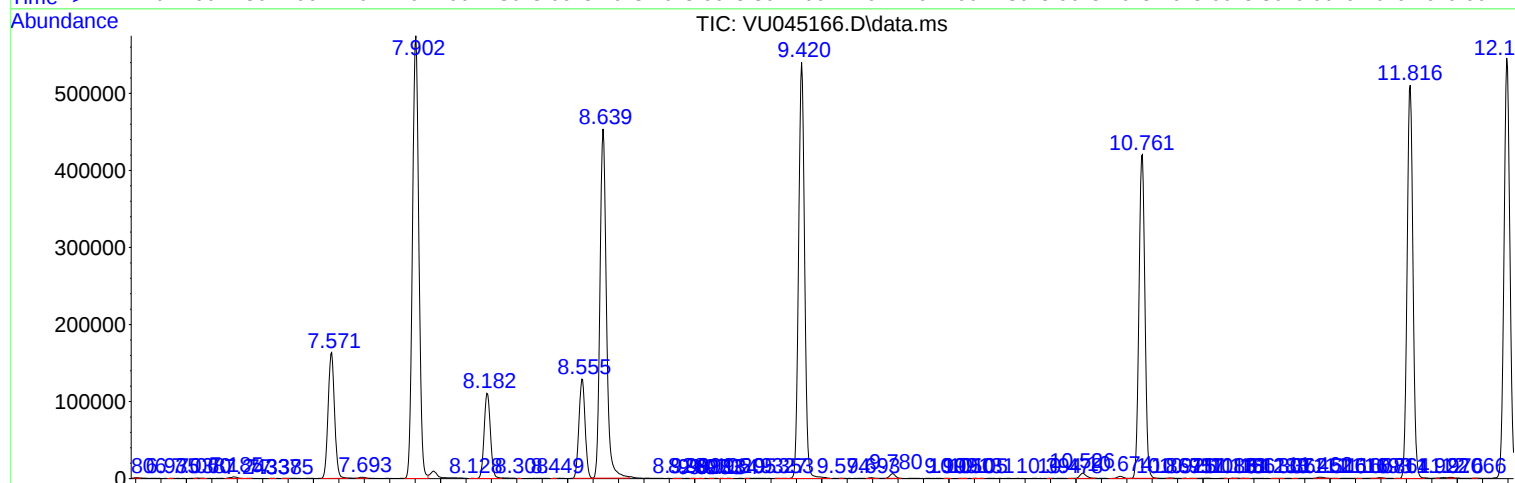
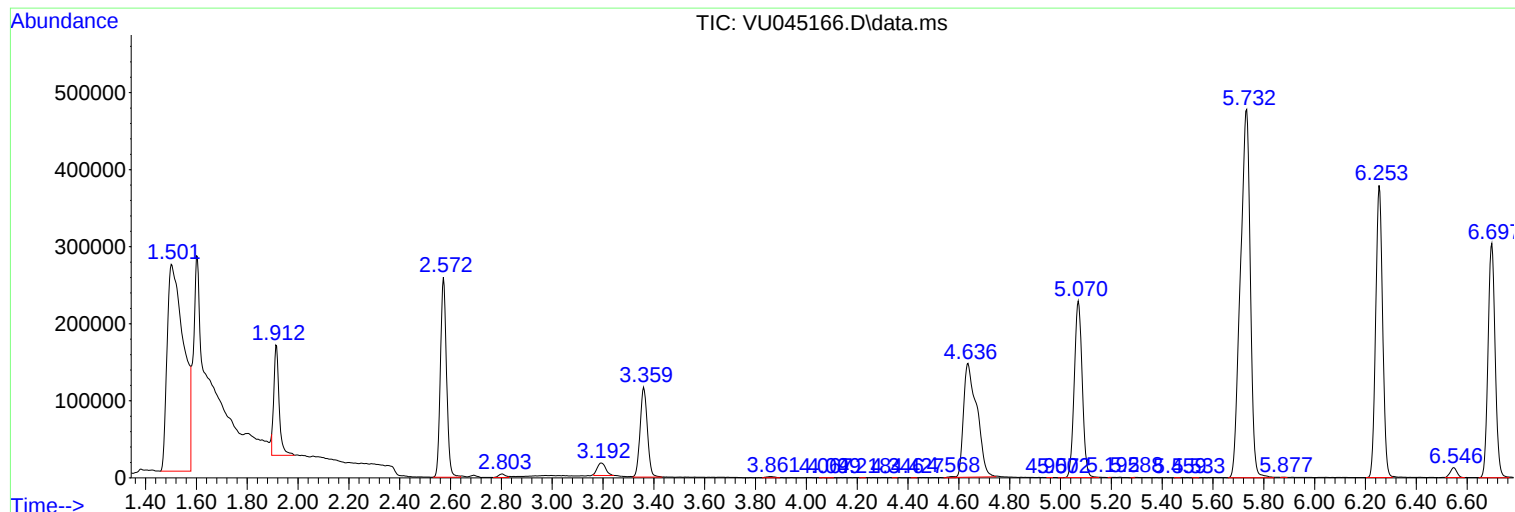
Sum of corrected areas: 11601885

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045166.D
Acq On : 05 Oct 2021 23:56
Operator : SY/MD
Sample : M3996-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4A42

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\VU100521\
Data File : VU045166.D
Acq On : 05 Oct 2021 23:56
Operator : SY/MD
Sample : M3996-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4A42

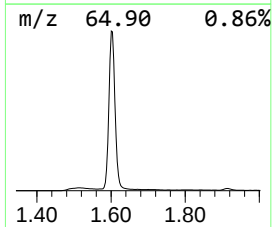
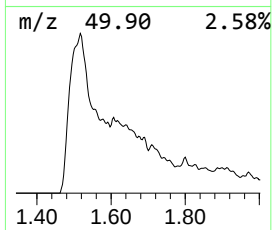
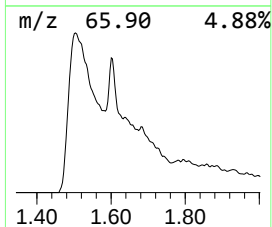
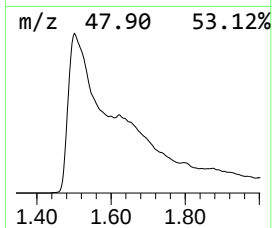
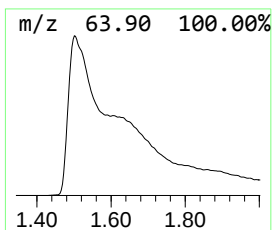
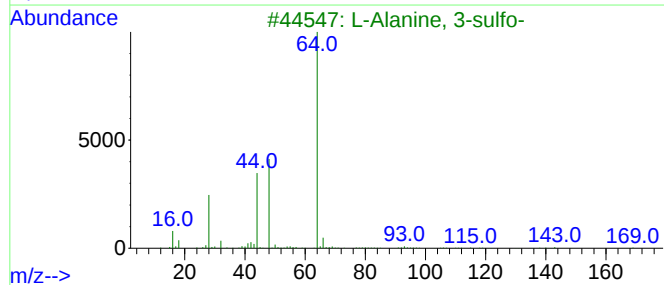
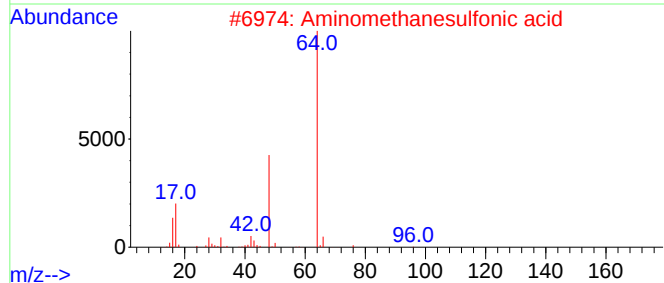
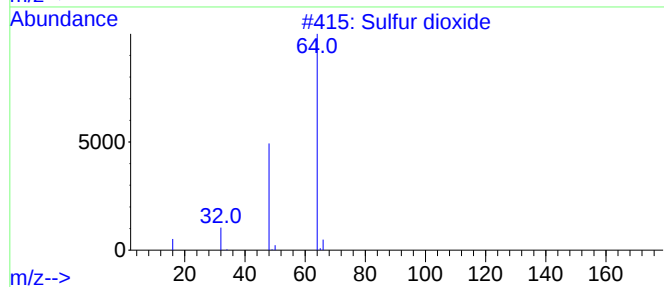
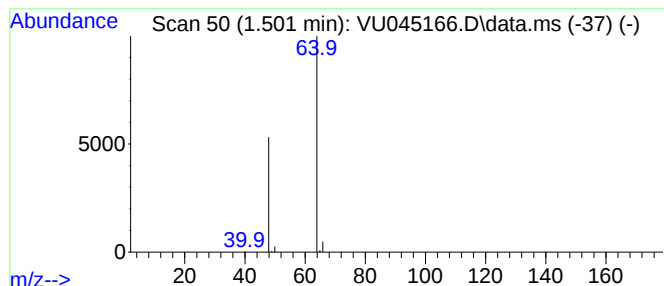
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.501	85.71 ug/L	1225120	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045166.D
Acq On : 05 Oct 2021 23:56
Operator : SY/MD
Sample : M3996-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4A42

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	1.501	85.7	ug/L	1225120	1	6.253	714646	50.0