

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
 Data File : VU033918.D
 Acq On : 22 Aug 2019 22:39
 Operator : JC/SP
 Sample : K4454-17
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK01

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_U\METHOD\SOMULM082219WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.174	22	26	35	rBV2	7483	7453	0.30%	0.040%
2	1.280	51	59	69	rBV	41711	81223	3.32%	0.441%
3	1.389	86	93	106	rVB	371008	380721	15.56%	2.066%
4	1.666	172	179	192	rVB	287118	356054	14.55%	1.932%
5	2.254	351	362	376	rVB	591734	890102	36.37%	4.830%
6	2.424	412	415	418	rBV4	699	412	0.02%	0.002%
7	2.505	437	440	443	rVB	598	337	0.01%	0.002%
8	2.601	467	470	473	rBV2	563	482	0.02%	0.003%
9	2.678	486	494	501	rBV6	2522	4144	0.17%	0.022%
10	2.820	536	538	542	rVB3	361	244	0.01%	0.001%
11	2.929	569	572	575	rVV3	502	331	0.01%	0.002%
12	2.958	575	581	583	rVV3	838	785	0.03%	0.004%
13	3.006	590	596	601	rVB3	570	565	0.02%	0.003%
14	3.035	601	605	606	rBV2	466	357	0.01%	0.002%
15	3.048	606	609	615	rBV3	314	378	0.02%	0.002%
16	3.083	615	620	625	rBV2	913	1100	0.04%	0.006%
17	3.199	653	656	659	rVB	524	292	0.01%	0.002%
18	3.309	685	690	691	rBV	445	276	0.01%	0.001%
19	3.408	716	721	724	rBV3	362	378	0.02%	0.002%
20	3.636	789	792	800	rVB2	323	365	0.01%	0.002%
21	3.765	826	832	838	rBV3	401	501	0.02%	0.003%
22	3.845	844	857	859	rBV3	261	539	0.02%	0.003%
23	3.871	859	865	868	rBV3	352	323	0.01%	0.002%
24	3.939	881	886	891	rBV	479	370	0.02%	0.002%
25	4.096	932	935	938	rBV2	312	270	0.01%	0.001%
26	4.148	939	951	994	rBV	205050	583957	23.86%	3.169%
27	4.466	1047	1050	1052	rBV2	572	497	0.02%	0.003%
28	4.550	1073	1076	1079	rBV3	615	434	0.02%	0.002%
29	4.620	1079	1098	1125	rVV	399766	957185	39.12%	5.194%
30	4.862	1169	1173	1185	rVB6	2245	3672	0.15%	0.020%
31	4.961	1198	1204	1205	rBV4	659	533	0.02%	0.003%
32	5.180	1268	1272	1274	rBV	463	346	0.01%	0.002%
33	5.315	1288	1314	1348	rBV2	825895	2447052	100.00%	13.279%
34	5.633	1410	1413	1415	rBV3	645	383	0.02%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
 Data File : VU033918.D
 Acq On : 22 Aug 2019 22:39
 Operator : JC/SP
 Sample : K4454-17
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK01

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_U\METHOD\SOMULM082219WMA.M
 Title : VOC Analysis

35	5.810	1465	1468	1470	rBV	434	251	0.01%	0.001%
36	5.861	1470	1484	1514	rBV	703653	1410217	57.63%	7.653%
37	6.157	1564	1576	1593	rVB5	14615	34182	1.40%	0.185%
38	6.308	1608	1623	1647	rBV	560599	1130590	46.20%	6.135%
39	6.501	1681	1683	1692	rVB6	885	1006	0.04%	0.005%
40	6.582	1705	1708	1712	rVB4	483	262	0.01%	0.001%
41	6.614	1715	1718	1725	rVB3	564	577	0.02%	0.003%
42	6.652	1728	1730	1734	rVB2	501	242	0.01%	0.001%
43	6.672	1734	1736	1740	rVB2	491	342	0.01%	0.002%
44	6.697	1740	1744	1746	rBV	330	233	0.01%	0.001%
45	6.726	1749	1753	1757	rVB2	442	415	0.02%	0.002%
46	6.752	1757	1761	1763	rBV4	740	488	0.02%	0.003%
47	6.807	1774	1778	1780	rBV3	382	278	0.01%	0.002%
48	6.832	1784	1786	1791	rBV2	471	362	0.01%	0.002%
49	6.865	1794	1796	1800	rVB2	518	358	0.01%	0.002%
50	6.984	1831	1833	1836	rVB2	483	288	0.01%	0.002%
51	7.042	1848	1851	1856	rBV3	551	513	0.02%	0.003%
52	7.096	1863	1868	1870	rBV3	391	332	0.01%	0.002%
53	7.209	1891	1903	1936	rBV	276130	514482	21.02%	2.792%
54	7.386	1955	1958	1959	rBV2	382	232	0.01%	0.001%
55	7.466	1979	1983	1984	rBV2	374	265	0.01%	0.001%
56	7.546	1993	2008	2042	rBV	1064405	1886015	77.07%	10.235%
57	7.832	2085	2097	2128	rBV	196779	350794	14.34%	1.904%
58	8.109	2180	2183	2184	rBV	415	238	0.01%	0.001%
59	8.122	2185	2187	2189	rVB2	695	328	0.01%	0.002%
60	8.148	2192	2195	2199	rBV3	540	423	0.02%	0.002%
61	8.180	2201	2205	2207	rBV2	465	361	0.01%	0.002%
62	8.205	2209	2213	2222	rVB6	2418	3862	0.16%	0.021%
63	8.295	2228	2241	2286	rBV2	628491	1239205	50.64%	6.725%
64	8.697	2360	2366	2367	rBV2	595	516	0.02%	0.003%
65	8.746	2379	2381	2387	rVB5	614	463	0.02%	0.003%
66	8.787	2392	2394	2397	rVB3	557	304	0.01%	0.002%
67	8.855	2410	2415	2417	rBV3	440	358	0.01%	0.002%
68	8.887	2420	2425	2427	rBV2	787	677	0.03%	0.004%
69	8.922	2432	2436	2438	rBV2	406	253	0.01%	0.001%
70	8.980	2449	2454	2455	rBV2	634	410	0.02%	0.002%
71	9.070	2466	2482	2526	rBV	1091474	1815053	74.17%	9.849%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082219\
 Data File : VU033918.D
 Acq On : 22 Aug 2019 22:39
 Operator : JC/SP
 Sample : K4454-17
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK01

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_U\METHOD\SOMULM082219WMA.M
 Title : VOC Analysis

72	9.363	2570	2573	2576	rBV4	532	368	0.02%	0.002%
73	9.427	2589	2593	2597	rBV4	327	299	0.01%	0.002%
74	9.469	2602	2606	2610	rBV2	486	485	0.02%	0.003%
75	9.617	2647	2652	2654	rBV2	492	418	0.02%	0.002%
76	9.707	2676	2680	2685	rBV3	480	430	0.02%	0.002%
77	9.800	2707	2709	2712	rBV3	658	336	0.01%	0.002%
78	9.816	2712	2714	2717	rBV2	484	283	0.01%	0.002%
79	9.910	2741	2743	2746	rVB2	570	298	0.01%	0.002%
80	10.012	2773	2775	2782	rVB4	377	344	0.01%	0.002%
81	10.061	2787	2790	2794	rBV3	666	474	0.02%	0.003%
82	10.131	2809	2812	2815	rBV2	341	272	0.01%	0.001%
83	10.215	2832	2838	2840	rBV2	432	479	0.02%	0.003%
84	10.302	2860	2865	2870	rVB4	583	611	0.02%	0.003%
85	10.331	2870	2874	2876	rBV4	377	357	0.01%	0.002%
86	10.414	2885	2900	2930	rBV	728987	1179248	48.19%	6.399%
87	10.553	2939	2943	2946	rBV4	625	544	0.02%	0.003%
88	10.723	2991	2996	2997	rBV2	482	386	0.02%	0.002%
89	10.839	3029	3032	3039	rVB3	454	561	0.02%	0.003%
90	10.990	3074	3079	3081	rBV3	575	549	0.02%	0.003%
91	11.067	3100	3103	3108	rVB3	842	552	0.02%	0.003%
92	11.270	3164	3166	3170	rBV2	395	320	0.01%	0.002%
93	11.379	3195	3200	3204	rBV6	942	986	0.04%	0.005%
94	11.466	3215	3227	3255	rBV	953821	1519784	62.11%	8.247%
95	11.842	3326	3344	3368	rBV	972989	1600369	65.40%	8.684%
96	12.508	3549	3551	3553	rBV2	399	246	0.01%	0.001%
97	12.778	3632	3635	3638	rBV2	677	601	0.02%	0.003%
98	12.877	3663	3666	3668	rBV3	763	445	0.02%	0.002%
99	13.134	3744	3746	3748	rBV2	484	263	0.01%	0.001%
100	13.350	3809	3813	3814	rBV2	683	441	0.02%	0.002%

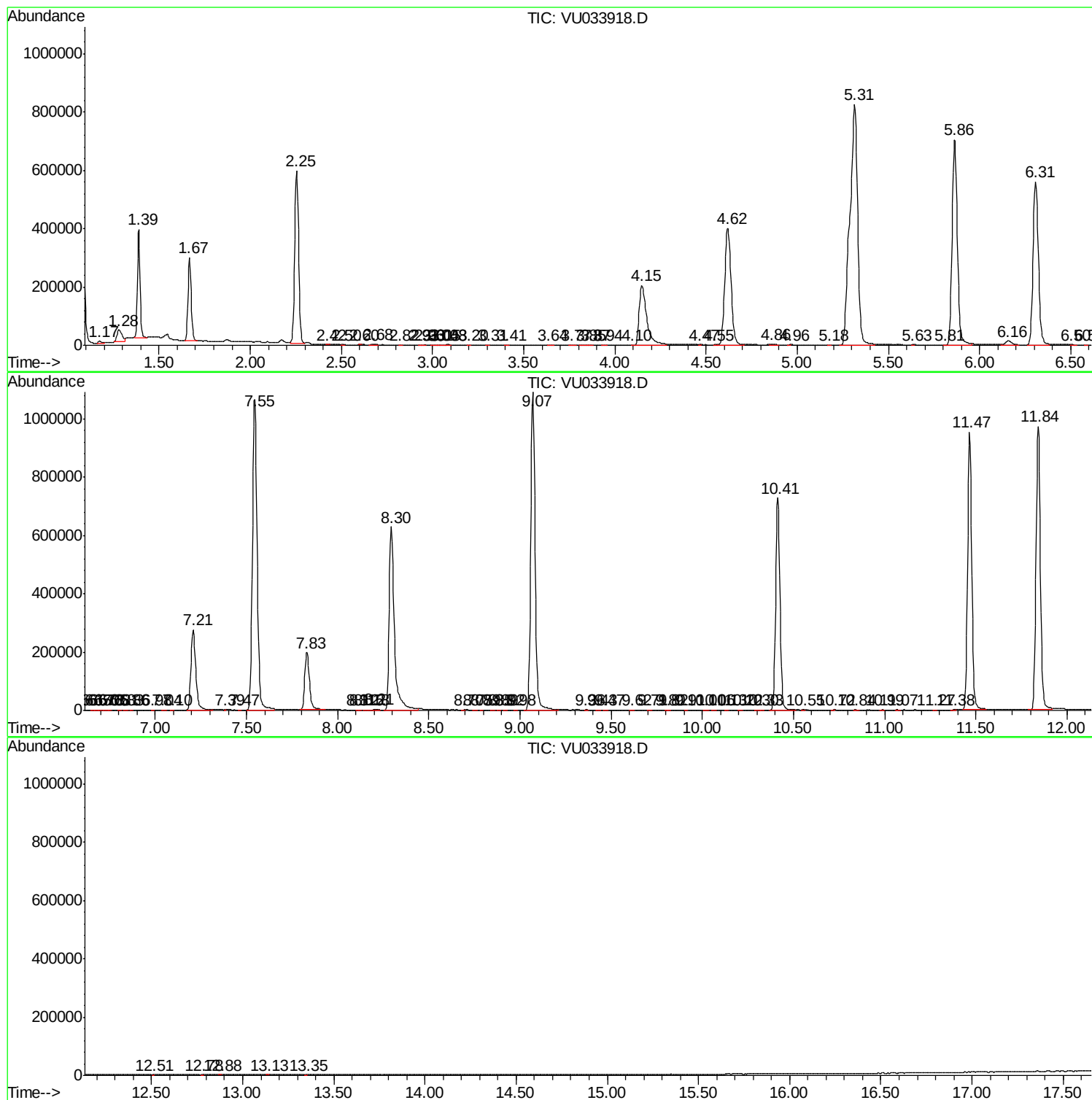
Sum of corrected areas: 18427985

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033918.D
Acq On : 22 Aug 2019 22:39
Operator : JC/SP
Sample : K4454-17
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VHBLK01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082219\
Data File : VU033918.D
Acq On : 22 Aug 2019 22:39
Operator : JC/SP
Sample : K4454-17
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 22 Sample Multiplier: 1

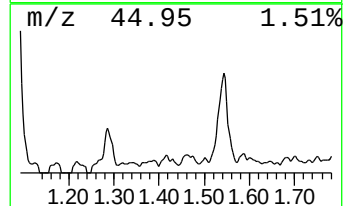
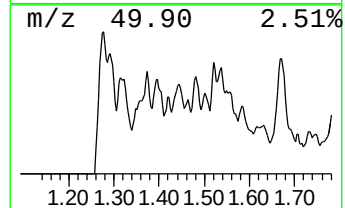
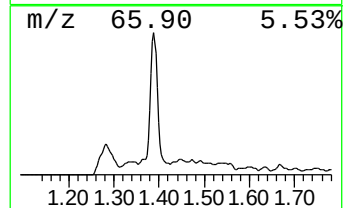
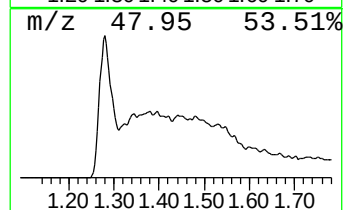
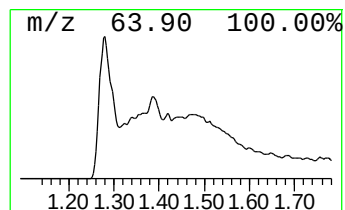
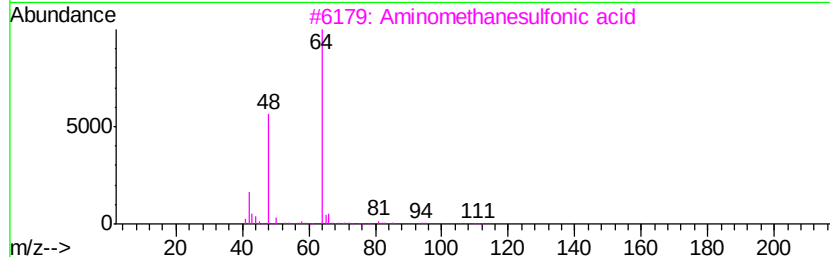
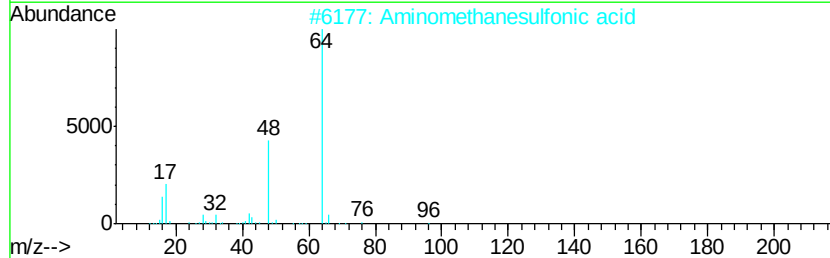
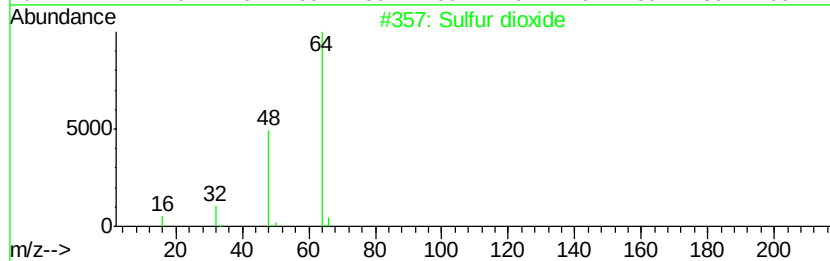
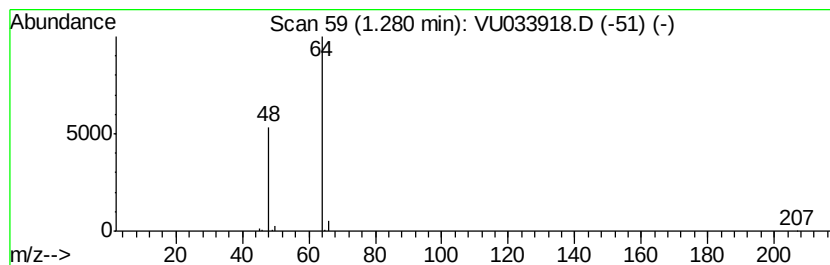
Instrument :
MSVOA_U
ClientSampleId :
VHBLK01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	2.88 ug/L	81223	1,4-Difluorobenzene	5.86
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 64
4		L-Alanine, 3-sulfo-	169 C3H7NO5S	000498-40-8 9
5		Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9 9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU082219\
Data File : VU033918.D
Acq On : 22 Aug 2019 22:39
Operator : JC/SP
Sample : K4454-17
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VHBLK01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082219WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Sulfur dioxide	1.28	2.9	ug/L	81223	1	5.86	1410220	50.0