

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081019\
 Data File : VU033737.D
 Acq On : 10 Aug 2019 23:59
 Operator : JC/SP
 Sample : VIBLK40
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK40

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\SOMULM080919WMA.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	1.389	86	93	110	rVB	182196	188528	17.53%	2.096%
2	1.547	135	142	153	rVB2	28733	38482	3.58%	0.428%
3	1.669	172	180	195	rBV	145475	177553	16.51%	1.974%
4	2.257	352	363	377	rVB	277833	420247	39.07%	4.672%
5	2.566	456	459	460	rBV	402	151	0.01%	0.002%
6	2.682	488	495	496	rBV2	997	986	0.09%	0.011%
7	2.711	501	504	506	rBV2	216	134	0.01%	0.001%
8	2.817	525	537	551	rBV	8452	17254	1.60%	0.192%
9	2.891	558	560	562	rVB	343	146	0.01%	0.002%
10	2.916	562	568	570	rBV2	308	384	0.04%	0.004%
11	3.087	620	621	626	rVB	235	136	0.01%	0.002%
12	3.112	626	629	633	rVB2	188	141	0.01%	0.002%
13	3.151	639	641	646	rVB2	235	127	0.01%	0.001%
14	3.199	653	656	659	rBV2	179	131	0.01%	0.001%
15	3.270	675	678	683	rVB2	195	147	0.01%	0.002%
16	3.318	688	693	699	rBV2	239	306	0.03%	0.003%
17	3.675	801	804	809	rVB2	150	151	0.01%	0.002%
18	3.701	809	812	817	rVB	164	127	0.01%	0.001%
19	3.797	836	842	847	rBV2	269	409	0.04%	0.005%
20	3.939	884	886	889	rBV	268	141	0.01%	0.002%
21	4.071	921	927	930	rBV2	267	313	0.03%	0.003%
22	4.148	938	951	987	rBV2	114969	327171	30.42%	3.637%
23	4.556	1075	1078	1080	rBV3	274	176	0.02%	0.002%
24	4.620	1080	1098	1122	rVV	183588	431572	40.12%	4.798%
25	4.801	1151	1154	1157	rBV3	341	216	0.02%	0.002%
26	4.865	1167	1174	1176	rBV2	761	758	0.07%	0.008%
27	4.942	1196	1198	1203	rVB	336	229	0.02%	0.003%
28	4.968	1203	1206	1207	rBV2	362	231	0.02%	0.003%
29	5.022	1221	1223	1227	rBV3	211	179	0.02%	0.002%
30	5.071	1234	1238	1240	rBV2	230	155	0.01%	0.002%
31	5.100	1244	1247	1253	rVB2	262	186	0.02%	0.002%
32	5.128	1253	1256	1259	rBV2	280	162	0.02%	0.002%
33	5.157	1262	1265	1270	rBV2	207	185	0.02%	0.002%
34	5.212	1279	1282	1286	rBV2	215	151	0.01%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081019\
 Data File : VU033737.D
 Acq On : 10 Aug 2019 23:59
 Operator : JC/SP
 Sample : VIBLK40
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK40

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\SOMULM080919WMA.M
 Title : VOC Analysis

35	5.315	1292	1314	1336	rBV2	369405	1075684	100.00%	11.959%
36	5.469	1359	1362	1364	rVB	512	282	0.03%	0.003%
37	5.489	1364	1368	1372	rBV3	302	237	0.02%	0.003%
38	5.588	1395	1399	1403	rBV2	238	204	0.02%	0.002%
39	5.723	1438	1441	1444	rBV	301	290	0.03%	0.003%
40	5.772	1451	1456	1459	rBV3	297	357	0.03%	0.004%
41	5.794	1459	1463	1467	rVB2	293	328	0.03%	0.004%
42	5.865	1470	1485	1513	rBV	373877	737724	68.58%	8.202%
43	5.997	1524	1526	1530	rVB2	432	295	0.03%	0.003%
44	6.161	1566	1577	1586	rVB9	3163	6311	0.59%	0.070%
45	6.206	1586	1591	1593	rVB2	163	132	0.01%	0.001%
46	6.225	1594	1597	1599	rBV2	309	199	0.02%	0.002%
47	6.254	1602	1606	1610	rBV2	269	301	0.03%	0.003%
48	6.309	1610	1623	1648	rBV	237364	481192	44.73%	5.350%
49	6.643	1725	1727	1731	rVB2	290	151	0.01%	0.002%
50	6.665	1731	1734	1737	rBV2	290	279	0.03%	0.003%
51	6.717	1745	1750	1752	rBV	180	129	0.01%	0.001%
52	6.765	1762	1765	1770	rBV2	240	262	0.02%	0.003%
53	6.833	1782	1786	1789	rBV2	182	142	0.01%	0.002%
54	6.881	1793	1801	1804	rVB2	197	243	0.02%	0.003%
55	6.929	1810	1816	1819	rBV2	196	244	0.02%	0.003%
56	7.006	1837	1840	1845	rVB2	266	200	0.02%	0.002%
57	7.077	1857	1862	1863	rBV	238	184	0.02%	0.002%
58	7.132	1875	1879	1881	rVB	274	161	0.01%	0.002%
59	7.151	1881	1885	1888	rBV	292	239	0.02%	0.003%
60	7.209	1888	1903	1933	rBV	127424	232911	21.65%	2.589%
61	7.418	1964	1968	1969	rBV	318	189	0.02%	0.002%
62	7.472	1982	1985	1989	rBV3	250	164	0.02%	0.002%
63	7.546	1995	2008	2036	rBV	492242	862424	80.17%	9.588%
64	7.833	2086	2097	2127	rBV	90853	159916	14.87%	1.778%
65	8.164	2190	2200	2203	rBV2	520	788	0.07%	0.009%
66	8.209	2210	2214	2215	rBV2	318	179	0.02%	0.002%
67	8.238	2221	2223	2226	rBV2	215	126	0.01%	0.001%
68	8.292	2229	2240	2277	rBV	339659	595375	55.35%	6.619%
69	8.537	2314	2316	2320	rVB2	281	155	0.01%	0.002%
70	8.601	2327	2336	2337	rBV4	2240	2214	0.21%	0.025%
71	8.804	2396	2399	2400	rBV	249	150	0.01%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081019\
Data File : VU033737.D
Acq On : 10 Aug 2019 23:59
Operator : JC/SP
Sample : VIBLK40
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK40

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\SOMULM080919WMA.M
Title : VOC Analysis

72	9.070	2469	2482	2521	rBV	569205	954276	88.71%	10.610%
73	9.296	2548	2552	2557	rBV3	249	291	0.03%	0.003%
74	9.321	2557	2560	2565	rVB3	334	250	0.02%	0.003%
75	9.421	2589	2591	2596	rBV2	133	135	0.01%	0.002%
76	9.472	2603	2607	2610	rBV2	211	178	0.02%	0.002%
77	9.636	2655	2658	2662	rBV2	338	336	0.03%	0.004%
78	9.675	2667	2670	2673	rVV2	290	270	0.03%	0.003%
79	9.691	2673	2675	2679	rVV2	436	297	0.03%	0.003%
80	9.710	2679	2681	2684	rVV2	230	130	0.01%	0.001%
81	9.736	2687	2689	2695	rBV2	212	206	0.02%	0.002%
82	9.794	2704	2707	2711	rBV3	194	159	0.01%	0.002%
83	9.935	2747	2751	2752	rBV2	216	163	0.02%	0.002%
84	10.189	2828	2830	2836	rBV2	327	313	0.03%	0.003%
85	10.283	2857	2859	2865	rVB2	247	243	0.02%	0.003%
86	10.414	2888	2900	2921	rBV	356240	576356	53.58%	6.408%
87	10.543	2936	2940	2944	rBV3	238	215	0.02%	0.002%
88	10.575	2947	2950	2952	rVB2	246	131	0.01%	0.001%
89	10.623	2963	2965	2971	rVB2	295	225	0.02%	0.003%
90	10.996	3075	3081	3082	rBV2	308	272	0.03%	0.003%
91	11.141	3123	3126	3128	rBV2	479	380	0.04%	0.004%
92	11.186	3136	3140	3141	rBV2	336	192	0.02%	0.002%
93	11.312	3175	3179	3185	rBV3	348	411	0.04%	0.005%
94	11.350	3188	3191	3193	rBV2	279	203	0.02%	0.002%
95	11.382	3198	3201	3204	rBV3	266	213	0.02%	0.002%
96	11.466	3215	3227	3249	rBV	578512	902712	83.92%	10.036%
97	11.842	3331	3344	3363	rBV	492012	786599	73.13%	8.745%
98	12.067	3411	3414	3423	rVB4	785	803	0.07%	0.009%
99	12.189	3448	3452	3454	rBV2	582	425	0.04%	0.005%
100	12.337	3496	3498	3504	rVB3	497	352	0.03%	0.004%

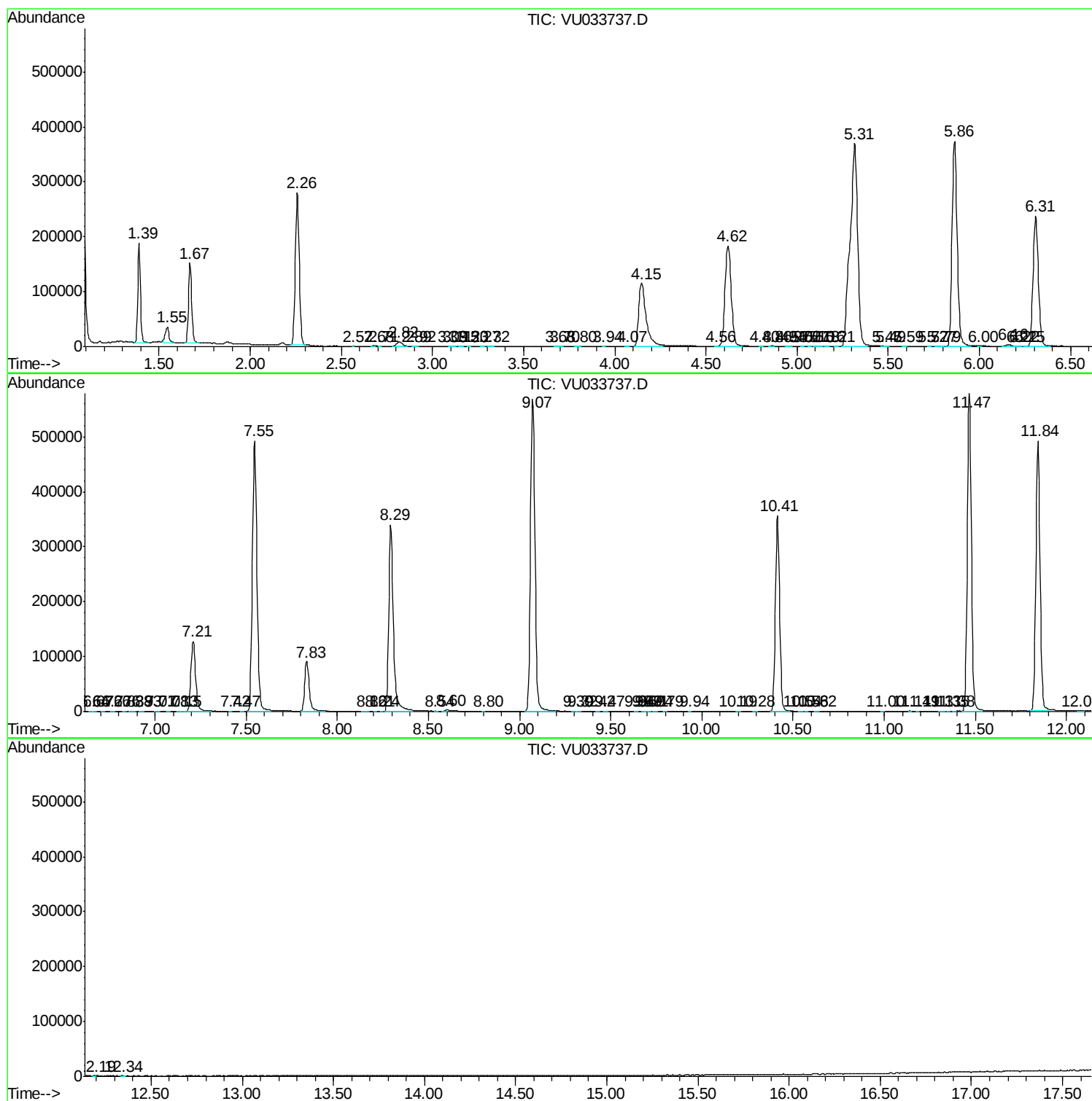
Sum of corrected areas: 8994462

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU081019\
Data File : VU033737.D
Acq On : 10 Aug 2019 23:59
Operator : JC/SP
Sample : VIBLK40
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK40

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080919WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU081019\
Data File : VU033737.D
Acq On : 10 Aug 2019 23:59
Operator : JC/SP
Sample : VIBLK40
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK40

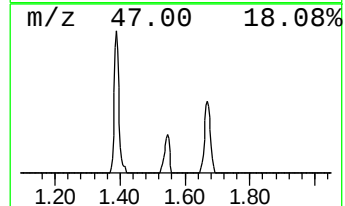
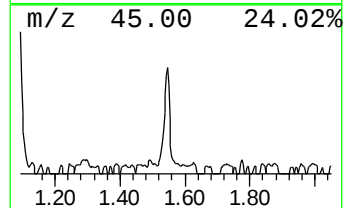
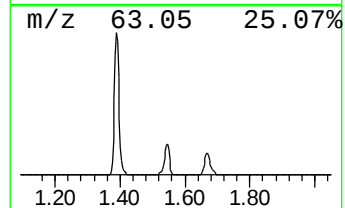
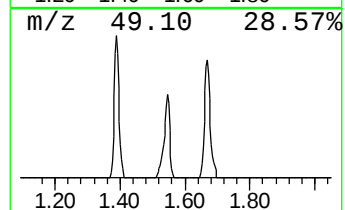
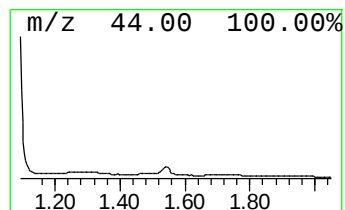
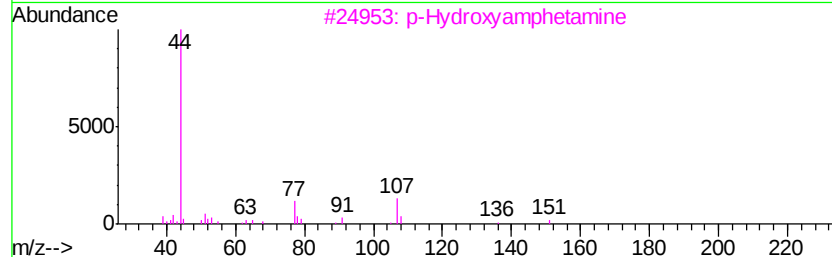
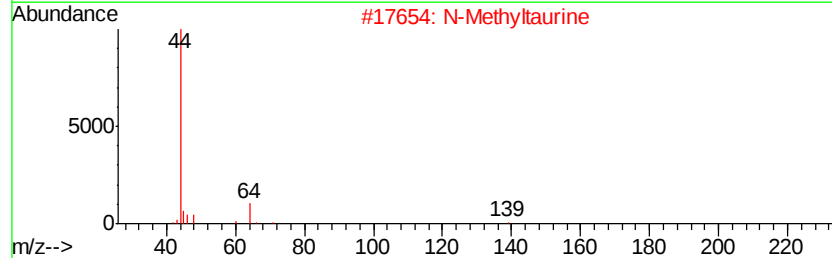
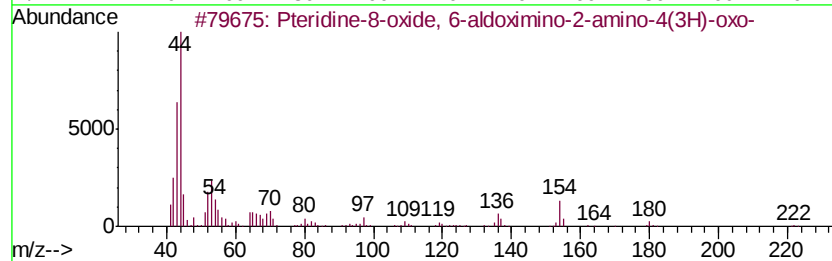
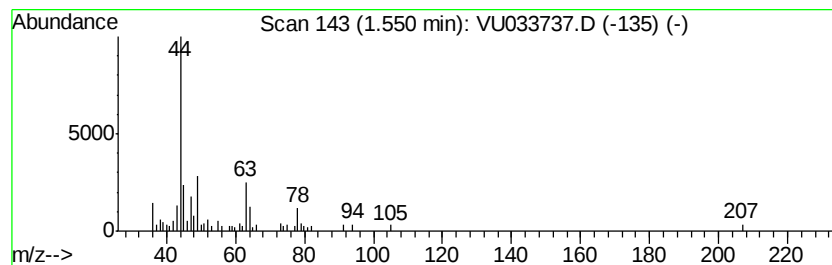
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	2.61 ug/L	38482	1,4-Difluorobenzene	5.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pteridine-8-oxide, 6-aldoximino-...	222	C7H6N6O3	023663-23-2	23
2		N-Methyltaurine	139	C3H9NO3S	000107-68-6	17
3		p-Hydroxyamphetamine	151	C9H13NO	000103-86-6	10
4		Boron trifluoride etherate	142	C4H10BF3O	000109-63-7	10
5		(R)-(-)-2-Amino-1-propanol	75	C3H9NO	035320-23-1	9



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081019\
Data File : VU033737.D
Acq On : 10 Aug 2019 23:59
Operator : JC/SP
Sample : VIBLK40
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK40

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080919WMA.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
unknown-01	1.55	2.6	ug/L	38482	1	5.86	737724	50.0