

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040221\
 Data File : VV020880.D
 Acq On : 02 Apr 2021 16:16
 Operator : SY/MD
 Sample : M1859-15ME
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG554ME

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_V\Method\SOMVLM032321WMA.M

Title : VOC Analysis

Signal : TIC: VV020880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	77	83	102	rVB	295893	355468	10.69%	1.532%
2	1.571	159	165	180	rVB	188773	291875	8.78%	1.258%
3	2.085	318	325	343	rVB	814855	1169296	35.18%	5.040%
4	2.670	504	507	509	rBV	510	329	0.01%	0.001%
5	2.715	518	521	524	rBV3	675	534	0.02%	0.002%
6	2.773	526	539	561	rVV3	39785	93842	2.82%	0.404%
7	2.895	575	577	579	rBV	593	315	0.01%	0.001%
8	2.979	600	603	608	rVB3	777	658	0.02%	0.003%
9	2.998	608	609	611	rBV	427	195	0.01%	0.001%
10	3.011	611	613	614	rBV	814	409	0.01%	0.002%
11	3.059	624	628	634	rBV4	907	985	0.03%	0.004%
12	3.088	634	637	638	rBV4	276	152	0.00%	0.001%
13	3.149	653	656	659	rBV2	546	273	0.01%	0.001%
14	3.185	664	667	672	rBV	609	438	0.01%	0.002%
15	3.214	672	676	677	rBV3	567	334	0.01%	0.001%
16	3.272	691	694	695	rBV	301	155	0.00%	0.001%
17	3.416	737	739	741	rBV	276	154	0.00%	0.001%
18	3.471	752	756	760	rVB3	674	463	0.01%	0.002%
19	3.490	760	762	766	rVB2	532	366	0.01%	0.002%
20	3.519	766	771	773	rBV	860	519	0.02%	0.002%
21	3.532	773	775	778	rVB2	607	308	0.01%	0.001%
22	3.571	783	787	788	rBV3	663	405	0.01%	0.002%
23	3.719	830	833	837	rBV2	719	570	0.02%	0.002%
24	3.767	843	848	852	rVB3	643	610	0.02%	0.003%
25	3.793	852	856	859	rVB3	476	384	0.01%	0.002%
26	3.812	859	862	866	rBV2	399	260	0.01%	0.001%
27	3.834	866	869	872	rVB2	255	179	0.01%	0.001%
28	3.850	872	874	876	rBV2	478	275	0.01%	0.001%
29	3.873	877	881	883	rVB2	614	405	0.01%	0.002%
30	3.921	883	896	924	rBV2	108248	471362	14.18%	2.032%
31	4.349	1015	1029	1065	rVB	532069	1372686	41.29%	5.917%
32	4.764	1154	1158	1160	rBV3	584	453	0.01%	0.002%
33	4.834	1177	1180	1182	rBV2	769	601	0.02%	0.003%
34	4.963	1219	1220	1222	rBV	472	157	0.00%	0.001%
35	5.043	1227	1245	1284	rBV2	1329458	3324202	100.00%	14.328%
36	5.317	1328	1330	1331	rBV	602	237	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040221\
 Data File : VV020880.D
 Acq On : 02 Apr 2021 16:16
 Operator : SY/MD
 Sample : M1859-15ME
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG554ME

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_V\Method\SOMVLM032321WMA.M
 Title : VOC Analysis

37	5.455	1372	1373	1376	rVB2	1350	560	0.02%	0.002%
38	5.506	1386	1389	1390	rBV	453	226	0.01%	0.001%
39	5.574	1407	1410	1411	rBV2	467	296	0.01%	0.001%
40	5.619	1411	1424	1450	rBV	622664	1348304	40.56%	5.812%
41	5.854	1495	1497	1500	rBV2	623	355	0.01%	0.002%
42	5.908	1502	1514	1537	rVV3	38040	89020	2.68%	0.384%
43	6.072	1551	1565	1601	rBV	664754	1449071	43.59%	6.246%
44	6.384	1660	1662	1663	rBV	738	337	0.01%	0.001%
45	6.506	1697	1700	1701	rVV	575	268	0.01%	0.001%
46	6.519	1701	1704	1707	rVV2	734	486	0.01%	0.002%
47	6.564	1715	1718	1721	rBV5	917	682	0.02%	0.003%
48	6.754	1773	1777	1778	rBV3	1158	682	0.02%	0.003%
49	6.808	1791	1794	1799	rVB5	963	804	0.02%	0.003%
50	6.924	1827	1830	1833	rBV2	971	742	0.02%	0.003%
51	6.989	1839	1850	1883	rBV	371061	781687	23.52%	3.369%
52	7.316	1940	1952	1971	rBV	1519017	2770018	83.33%	11.940%
53	7.625	2038	2048	2077	rBV	244620	537271	16.16%	2.316%
54	7.844	2113	2116	2119	rBV3	1027	911	0.03%	0.004%
55	7.934	2141	2144	2145	rBV3	800	479	0.01%	0.002%
56	7.943	2145	2147	2149	rVV3	892	339	0.01%	0.001%
57	8.130	2187	2205	2246	rBV2	392790	1413585	42.52%	6.093%
58	8.693	2378	2380	2384	rBV2	924	460	0.01%	0.002%
59	8.860	2420	2432	2457	rBV	861385	1701676	51.19%	7.335%
60	9.043	2486	2489	2492	rVB4	1315	949	0.03%	0.004%
61	9.156	2521	2524	2529	rBV4	1734	1478	0.04%	0.006%
62	9.230	2544	2547	2549	rBV2	529	338	0.01%	0.001%
63	9.291	2563	2566	2569	rBV	831	646	0.02%	0.003%
64	9.349	2581	2584	2586	rBV3	710	377	0.01%	0.002%
65	9.484	2623	2626	2627	rBV2	422	260	0.01%	0.001%
66	9.558	2646	2649	2651	rBV	425	215	0.01%	0.001%
67	9.683	2686	2688	2691	rBV3	944	652	0.02%	0.003%
68	9.718	2695	2699	2702	rBV2	614	568	0.02%	0.002%
69	9.869	2743	2746	2752	rBV3	590	577	0.02%	0.002%
70	9.898	2753	2755	2756	rBV3	563	207	0.01%	0.001%
71	9.908	2756	2758	2763	rVV5	765	604	0.02%	0.003%
72	10.130	2820	2827	2840	rVB5	7746	12350	0.37%	0.053%
73	10.233	2843	2859	2879	rBV	940817	1633951	49.15%	7.043%
74	10.558	2956	2960	2961	rBV2	1371	719	0.02%	0.003%
75	10.644	2985	2987	2989	rBV	520	192	0.01%	0.001%
76	10.725	3010	3012	3014	rBV	441	185	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040221\
 Data File : VV020880.D
 Acq On : 02 Apr 2021 16:16
 Operator : SY/MD
 Sample : M1859-15ME
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG554ME

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_V\Method\SOMVLM032321WMA.M

Title : VOC Analysis

77	10.812	3035	3039	3044	rBV4	980	1124	0.03%	0.005%
78	10.927	3066	3075	3083	rVB4	7906	13176	0.40%	0.057%
79	11.001	3094	3098	3099	rBV	322	189	0.01%	0.001%
80	11.037	3105	3109	3110	rBV2	1373	913	0.03%	0.004%
81	11.114	3131	3133	3134	rBV	408	223	0.01%	0.001%
82	11.258	3167	3178	3197	rBV	1044120	1655577	49.80%	7.136%
83	11.535	3262	3264	3265	rBV	508	193	0.01%	0.001%
84	11.635	3283	3295	3315	rBV	1695134	2677453	80.54%	11.541%
85	11.950	3391	3393	3398	rBV4	815	539	0.02%	0.002%
86	11.972	3398	3400	3401	rBV	985	432	0.01%	0.002%
87	12.130	3447	3449	3450	rBV2	757	310	0.01%	0.001%
88	12.255	3483	3488	3490	rBV3	1431	1297	0.04%	0.006%
89	12.278	3493	3495	3496	rBV	765	313	0.01%	0.001%
90	12.487	3557	3560	3562	rBV3	1064	606	0.02%	0.003%
91	12.593	3589	3593	3596	rBV6	1264	1290	0.04%	0.006%
92	12.847	3667	3672	3675	rBV3	739	871	0.03%	0.004%
93	12.956	3704	3706	3709	rVB2	645	323	0.01%	0.001%
94	13.056	3735	3737	3739	rBV3	551	245	0.01%	0.001%
95	13.107	3750	3753	3755	rBV2	715	460	0.01%	0.002%
96	13.580	3898	3900	3903	rBV2	788	438	0.01%	0.002%
97	13.660	3923	3925	3927	rBV2	466	206	0.01%	0.001%
98	13.705	3937	3939	3944	rBV2	713	537	0.02%	0.002%
99	13.834	3976	3979	3981	rBV3	908	571	0.02%	0.002%
100	13.921	4003	4006	4007	rBV2	738	326	0.01%	0.001%

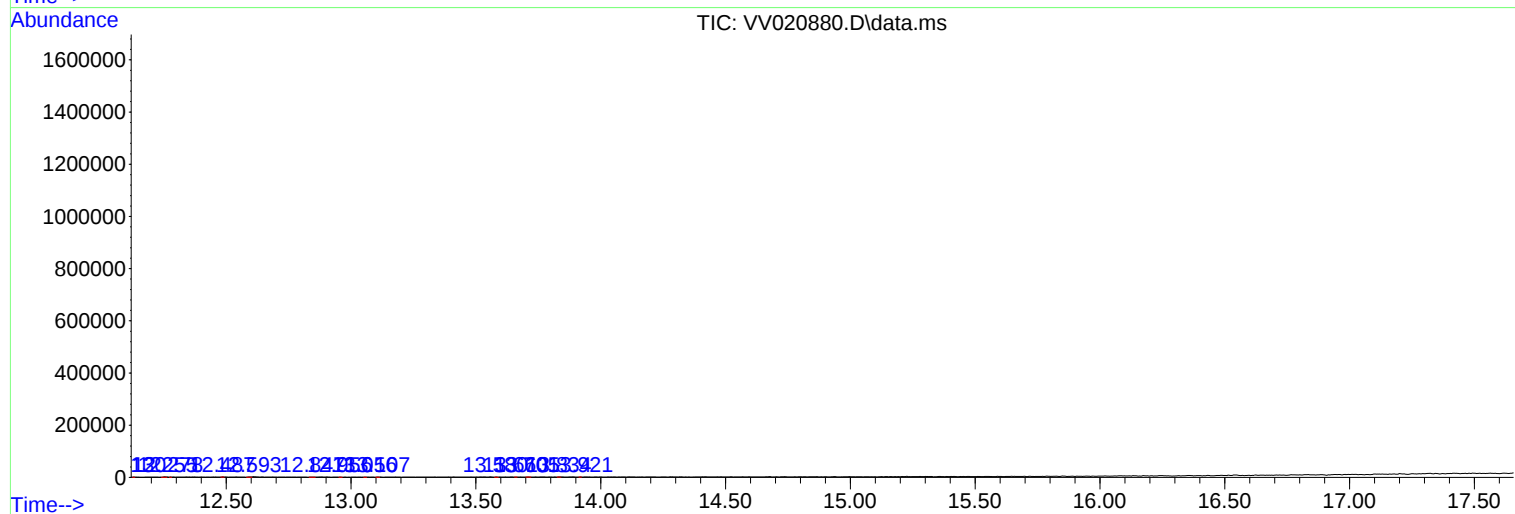
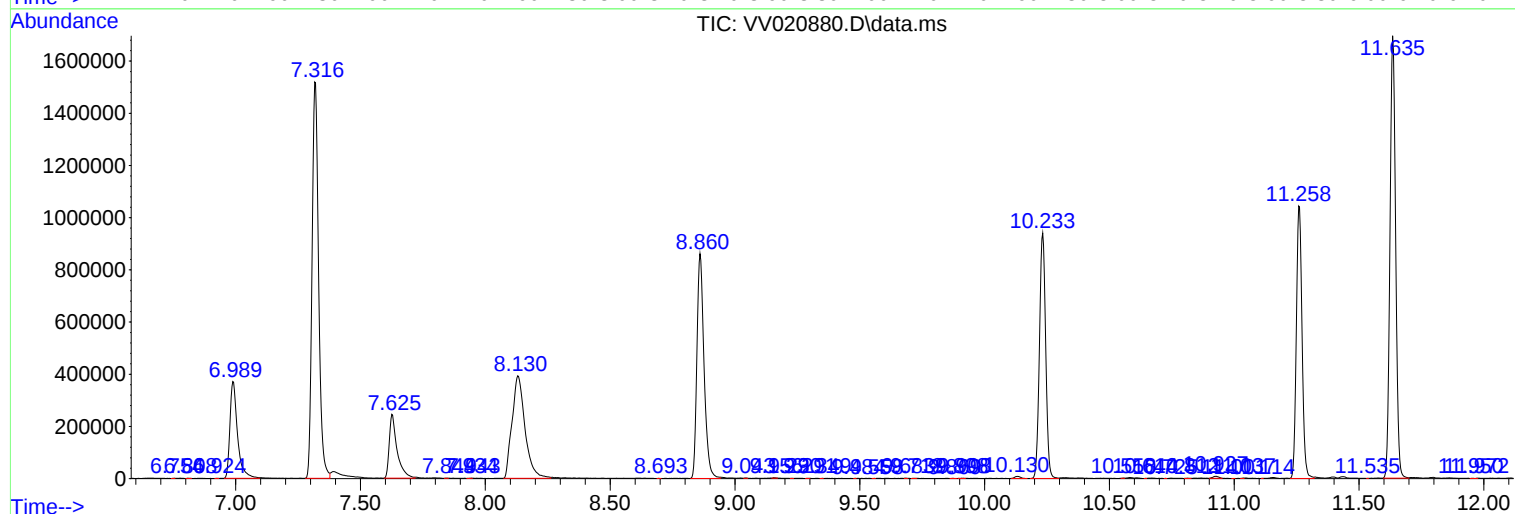
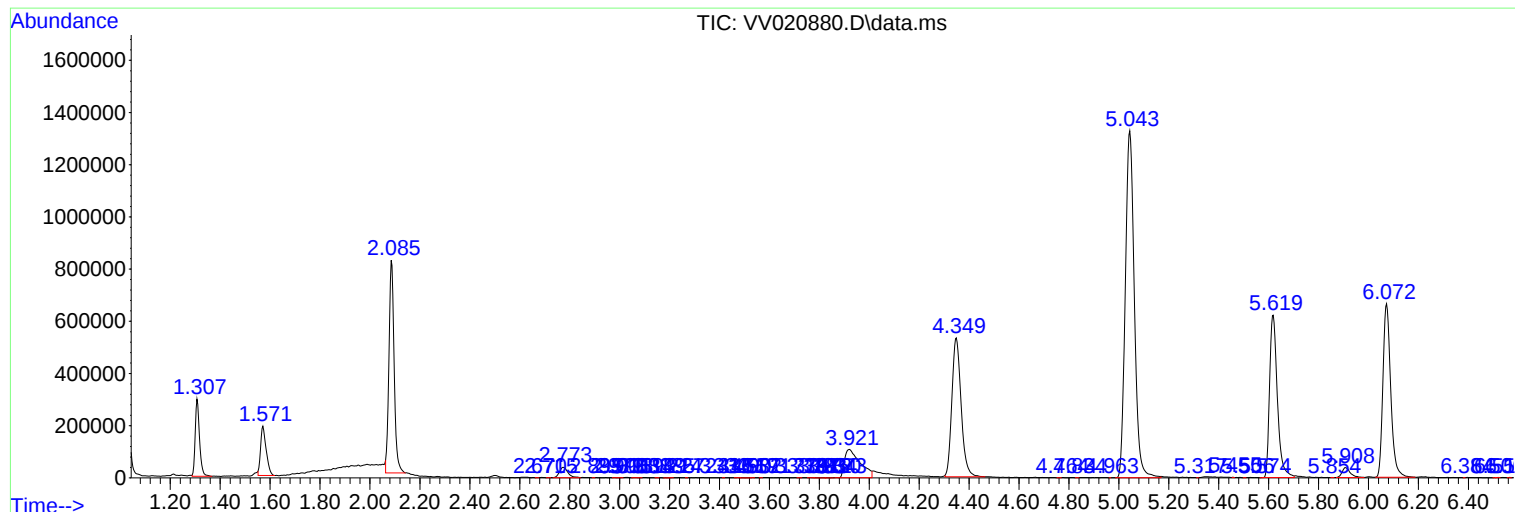
Sum of corrected areas: 23199993

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040221\
Data File : VV020880.D
Acq On : 02 Apr 2021 16:16
Operator : SY/MD
Sample : M1859-15ME
Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
BG554ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040221\
Data File : VV020880.D
Acq On : 02 Apr 2021 16:16
Operator : SY/MD
Sample : M1859-15ME
Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG554ME

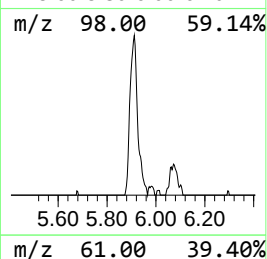
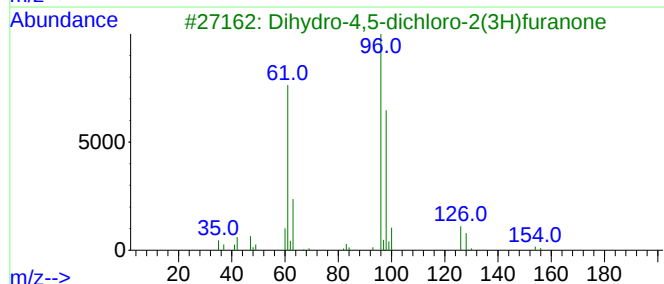
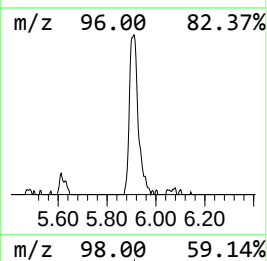
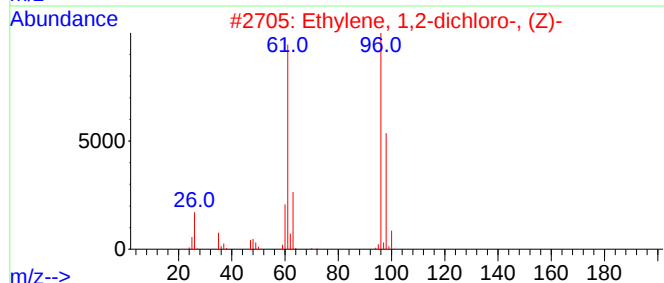
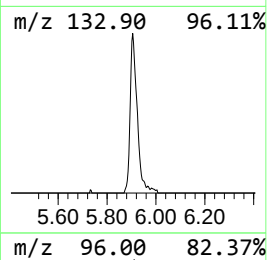
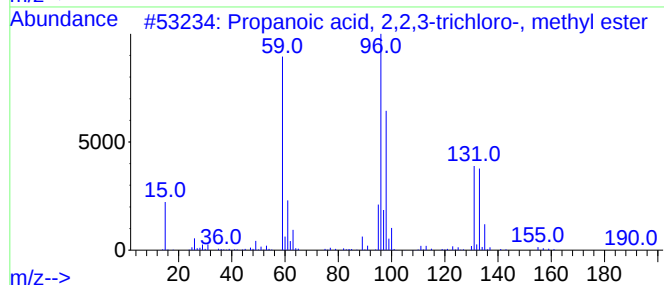
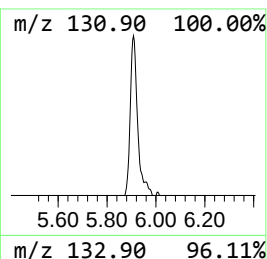
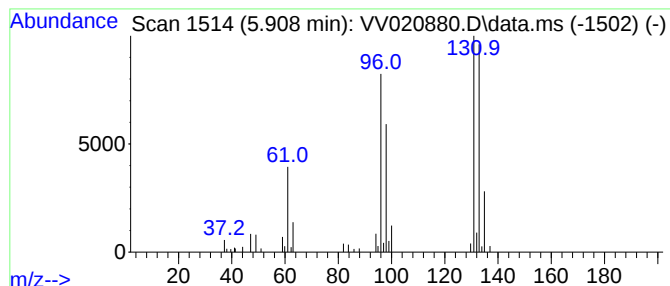
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

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.
5.908	3.30 ug/L	89020	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	45
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	27
3			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
4			1H-Imidazole, 1-ethyl-	96	C5H8N2	007098-07-9	9
5			N-Chlorosuccinimide	133	C4H4ClNO2	000128-09-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040221\
Data File : VV020880.D
Acq On : 02 Apr 2021 16:16
Operator : SY/MD
Sample : M1859-15ME
Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG554ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.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	5.908	3.3	ug/L	89020	1	5.619	1348300	50.0