

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021276.D
 Acq On : 04 May 2021 17:37
 Operator : SY/MD
 Sample : M2209-19ME 400X
 Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7F5ME

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\SFAMVLM050321WMA.M

Title : VOC Analysis

Signal : TIC: VV021276.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	100	rVB	180447	191265	9.11%	1.068%
2	1.568	158	164	173	rVB	175775	191954	9.14%	1.072%
3	2.108	323	332	344	rBV	422416	603009	28.72%	3.368%
4	2.278	383	385	387	rBV3	1680	1031	0.05%	0.006%
5	2.320	395	398	405	rVB6	1835	1530	0.07%	0.009%
6	2.404	421	424	427	rBV4	1568	1280	0.06%	0.007%
7	2.741	524	529	530	rBV3	1156	878	0.04%	0.005%
8	2.815	550	552	555	rVB2	1508	774	0.04%	0.004%
9	2.838	555	559	562	rBV2	1619	1121	0.05%	0.006%
10	2.860	564	566	571	rBV3	1191	992	0.05%	0.006%
11	3.050	620	625	630	rVB7	1785	1709	0.08%	0.010%
12	3.101	638	641	644	rBV4	1418	1182	0.06%	0.007%
13	3.175	661	664	667	rBV5	1854	1252	0.06%	0.007%
14	3.282	693	697	700	rBV4	1837	1273	0.06%	0.007%
15	3.368	720	724	728	rBV7	1159	1059	0.05%	0.006%
16	3.568	783	786	789	rBV3	1086	765	0.04%	0.004%
17	3.635	804	807	811	rVV5	1339	1021	0.05%	0.006%
18	3.725	831	835	838	rBV4	1191	975	0.05%	0.005%
19	3.844	868	872	875	rBV3	1373	905	0.04%	0.005%
20	3.902	879	890	917	rBV	128866	423321	20.16%	2.365%
21	4.272	1000	1005	1007	rBV5	2118	1483	0.07%	0.008%
22	4.352	1016	1030	1055	rBV	379961	917962	43.72%	5.128%
23	4.587	1100	1103	1108	rBV5	2667	2337	0.11%	0.013%
24	4.777	1159	1162	1167	rBV5	1560	1168	0.06%	0.007%
25	4.806	1167	1171	1174	rBV4	1122	882	0.04%	0.005%
26	4.918	1199	1206	1207	rBV5	1123	1288	0.06%	0.007%
27	4.960	1217	1219	1222	rBV3	1395	965	0.05%	0.005%
28	5.050	1230	1247	1274	rBV3	802955	2099637	100.00%	11.728%
29	5.404	1353	1357	1358	rBV2	1250	806	0.04%	0.005%
30	5.436	1364	1367	1370	rVB3	1868	1185	0.06%	0.007%
31	5.535	1395	1398	1404	rBV6	1615	1547	0.07%	0.009%
32	5.622	1412	1425	1450	rBV	815829	1642196	78.21%	9.173%
33	5.912	1505	1515	1534	rVB4	43459	94579	4.50%	0.528%
34	5.982	1534	1537	1542	rBV7	3619	3007	0.14%	0.017%
35	6.008	1542	1545	1549	rVB5	1986	1586	0.08%	0.009%
36	6.076	1553	1566	1592	rBV2	454740	939253	44.73%	5.247%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021276.D
 Acq On : 04 May 2021 17:37
 Operator : SY/MD
 Sample : M2209-19ME 400X
 Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7F5ME

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\SFAMVLM050321WMA.M
 Title : VOC Analysis

37	6.252	1618	1621	1631	rVB6	2381	2472	0.12%	0.014%
38	6.423	1672	1674	1677	rVB5	1569	832	0.04%	0.005%
39	6.455	1679	1684	1687	rBV6	1766	1357	0.06%	0.008%
40	6.484	1687	1693	1697	rBV9	1786	1613	0.08%	0.009%
41	6.506	1697	1700	1703	rBV3	1485	1058	0.05%	0.006%
42	6.632	1735	1739	1741	rBV4	1534	1184	0.06%	0.007%
43	6.667	1748	1750	1753	rBV4	1244	1039	0.05%	0.006%
44	6.889	1816	1819	1822	rBV3	892	743	0.04%	0.004%
45	6.992	1839	1851	1879	rBV2	284633	534814	25.47%	2.987%
46	7.195	1910	1914	1915	rBV3	1636	1134	0.05%	0.006%
47	7.268	1934	1937	1940	rBV5	1534	776	0.04%	0.004%
48	7.320	1942	1953	1972	rBV	991625	1716036	81.73%	9.586%
49	7.510	2008	2012	2014	rBV3	1917	1403	0.07%	0.008%
50	7.625	2038	2048	2070	rBV2	206451	368467	17.55%	2.058%
51	7.905	2132	2135	2139	rBV6	1664	1497	0.07%	0.008%
52	7.982	2148	2159	2171	rBV3	91138	161798	7.71%	0.904%
53	8.095	2183	2194	2225	rBV2	507108	985258	46.93%	5.504%
54	8.561	2336	2339	2344	rBV7	1472	1452	0.07%	0.008%
55	8.616	2352	2356	2359	rBV3	1705	1307	0.06%	0.007%
56	8.635	2359	2362	2366	rVV4	1268	858	0.04%	0.005%
57	8.696	2377	2381	2383	rBV4	1456	980	0.05%	0.005%
58	8.799	2410	2413	2415	rBV3	1519	1024	0.05%	0.006%
59	8.857	2418	2431	2452	rBV	1269962	2013236	95.88%	11.246%
60	9.018	2479	2481	2485	rBV4	1556	1324	0.06%	0.007%
61	9.085	2499	2502	2505	rVV4	1788	1332	0.06%	0.007%
62	9.130	2513	2516	2518	rBV4	1604	1028	0.05%	0.006%
63	9.233	2546	2548	2553	rBV3	1881	1715	0.08%	0.010%
64	9.516	2630	2636	2642	rBV6	1363	1526	0.07%	0.009%
65	9.571	2651	2653	2657	rBV3	912	771	0.04%	0.004%
66	9.593	2657	2660	2662	rBV3	1040	738	0.04%	0.004%
67	9.657	2677	2680	2684	rBV5	1952	1339	0.06%	0.007%
68	9.802	2723	2725	2728	rVB3	1364	775	0.04%	0.004%
69	9.828	2728	2733	2739	rBV6	2330	2667	0.13%	0.015%
70	9.924	2760	2763	2767	rBV5	1603	1185	0.06%	0.007%
71	9.982	2775	2781	2783	rBV5	1356	1551	0.07%	0.009%
72	10.034	2792	2797	2800	rBV6	1951	1711	0.08%	0.010%
73	10.053	2800	2803	2806	rVB2	1789	1065	0.05%	0.006%
74	10.223	2842	2856	2877	rBV	680671	1076469	51.27%	6.013%
75	10.317	2882	2885	2886	rBV3	1742	826	0.04%	0.005%
76	10.651	2986	2989	2992	rBV4	998	757	0.04%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021276.D
 Acq On : 04 May 2021 17:37
 Operator : SY/MD
 Sample : M2209-19ME 400X
 Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7F5ME

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\SFAMVLM050321WMA.M
 Title : VOC Analysis

77	10.709	3003	3007	3008	rBV2	1333	893	0.04%	0.005%
78	10.764	3021	3024	3026	rBV4	1512	739	0.04%	0.004%
79	10.924	3068	3074	3086	rBV4	4667	8664	0.41%	0.048%
80	11.034	3105	3108	3111	rVB3	1513	799	0.04%	0.004%
81	11.104	3127	3130	3133	rBV3	1557	1245	0.06%	0.007%
82	11.255	3166	3177	3203	rBV	1279806	1978126	94.21%	11.050%
83	11.545	3262	3267	3269	rBV5	1416	1187	0.06%	0.007%
84	11.632	3282	3294	3319	rBV	1194354	1854261	88.31%	10.358%
85	11.834	3351	3357	3362	rBV9	2035	2518	0.12%	0.014%
86	12.001	3405	3409	3410	rBV3	1663	1021	0.05%	0.006%
87	12.075	3429	3432	3437	rBV6	1093	958	0.05%	0.005%
88	12.931	3693	3698	3702	rBV5	960	1089	0.05%	0.006%
89	13.188	3772	3778	3781	rBV5	1663	1445	0.07%	0.008%
90	13.220	3786	3788	3791	rBV2	1553	793	0.04%	0.004%
91	13.304	3811	3814	3819	rVB5	1573	895	0.04%	0.005%
92	13.362	3830	3832	3836	rBV5	1226	933	0.04%	0.005%
93	13.519	3874	3881	3882	rBV5	1826	1813	0.09%	0.010%
94	13.870	3985	3990	3993	rBV6	2391	2467	0.12%	0.014%
95	13.995	4025	4029	4031	rBV4	1990	1332	0.06%	0.007%
96	14.037	4040	4042	4043	rBV2	1940	845	0.04%	0.005%
97	14.107	4062	4064	4067	rBV4	1220	802	0.04%	0.004%
98	14.214	4095	4097	4099	rBV3	1525	876	0.04%	0.005%
99	15.236	4409	4415	4418	rVB6	2473	2913	0.14%	0.016%
100	15.567	4516	4518	4520	rBV2	2331	1116	0.05%	0.006%

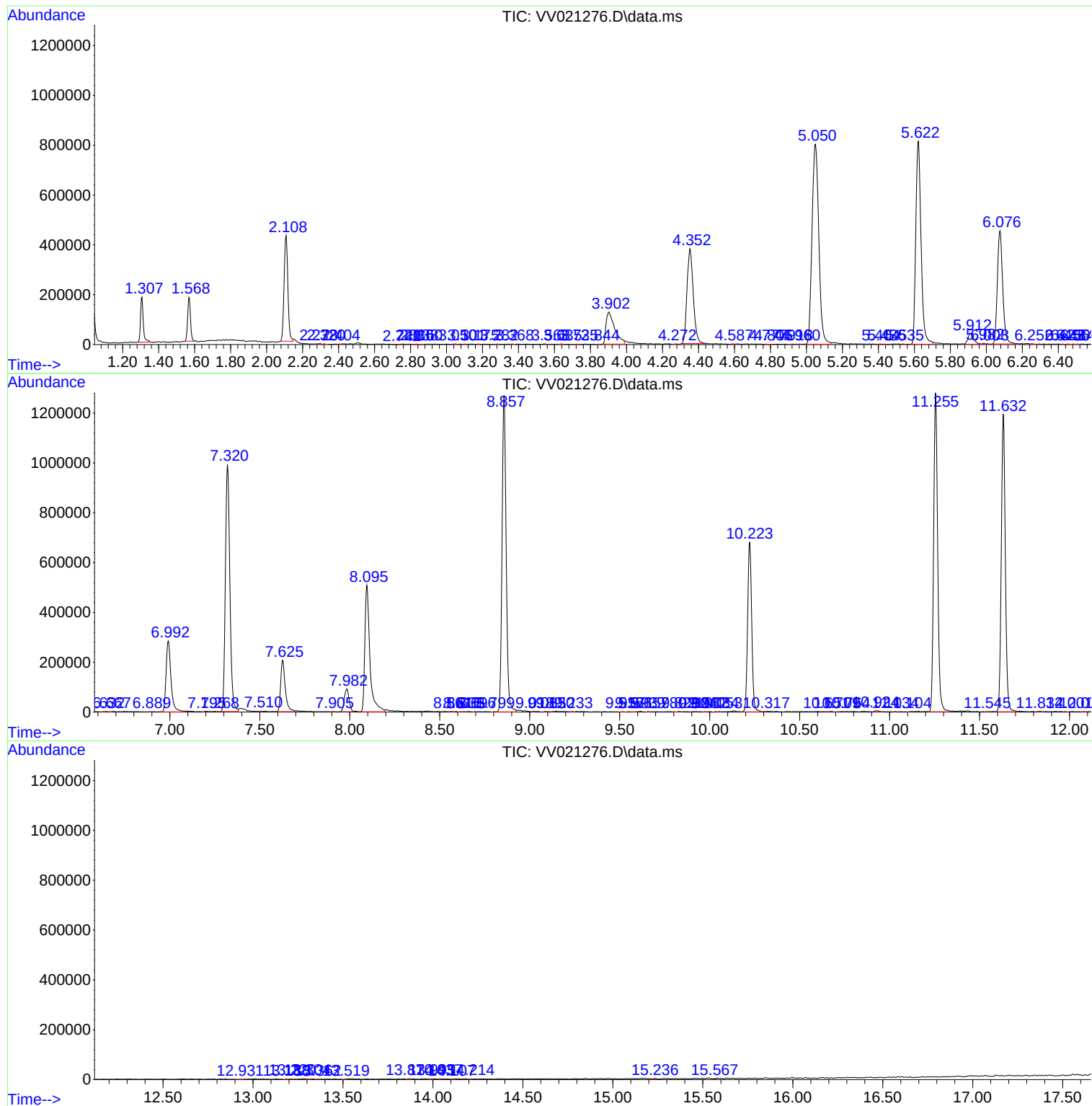
Sum of corrected areas: 17902024

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
Data File : VV021276.D
Acq On : 04 May 2021 17:37
Operator : SY/MD
Sample : M2209-19ME 400X
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7F5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
Data File : VV021276.D
Acq On : 04 May 2021 17:37
Operator : SY/MD
Sample : M2209-19ME 400X
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7F5ME

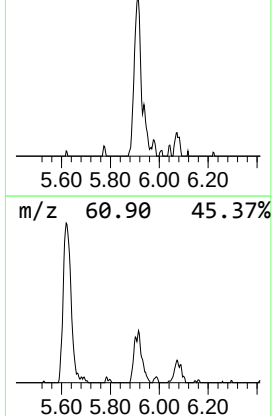
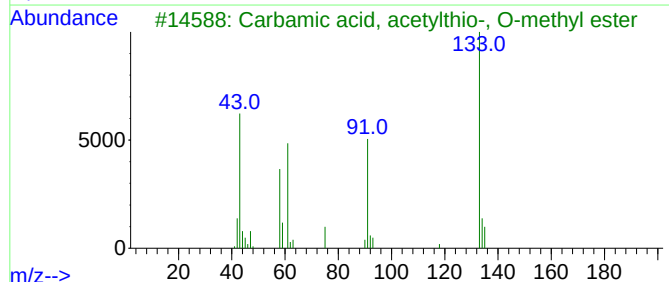
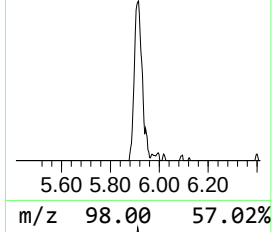
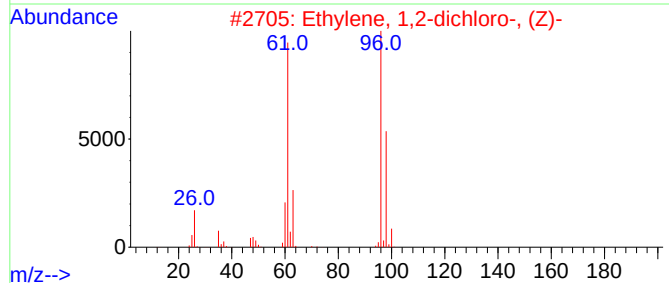
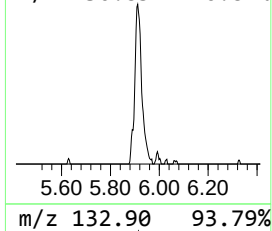
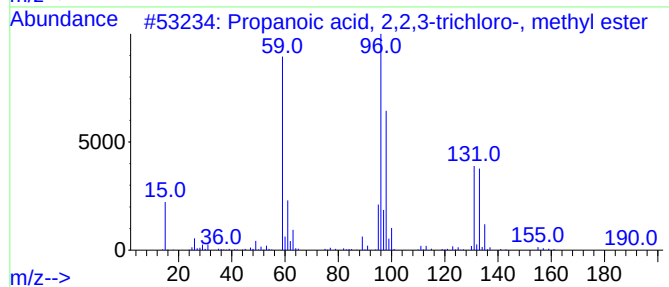
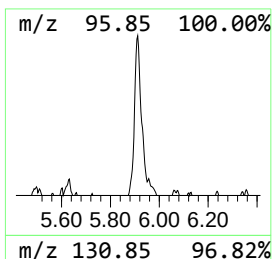
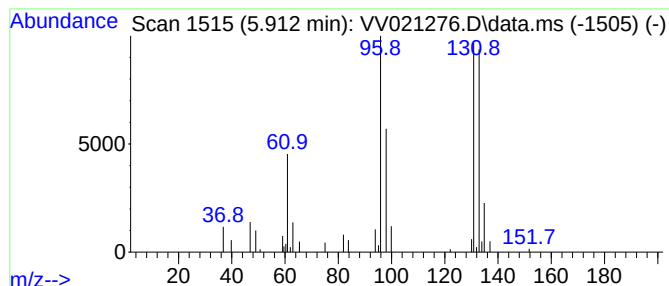
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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.
5.912	2.88 ug/L	94579	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	28
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	27
3			Carbamic acid, acetylthio-, O-me...	133	C4H7NO2S	016696-87-0	12
4			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	9
5			Acetylthiosemicarbazide	133	C3H7N3OS	002302-88-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
Data File : VV021276.D
Acq On : 04 May 2021 17:37
Operator : SY/MD
Sample : M2209-19ME 400X
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7F5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.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	5.912	2.9	ug/L	94579	1	5.622	1642200	50.0