

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021934.D
 Acq On : 23 Aug 2021 16:35
 Operator : SY/MD
 Sample : M3486-05ME
 Misc : 4.39g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AB8ME

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\SFAMVLM081621WMA.M

Title : VOC Analysis

Signal : TIC: VV021934.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	112	rVB	123736	183693	13.42%	1.663%
2	2.072	311	321	334	rBV	273419	388655	28.40%	3.519%
3	2.494	445	452	464	rVB2	17852	29503	2.16%	0.267%
4	2.879	570	572	575	rBV	325	162	0.01%	0.001%
5	2.899	575	578	582	rBV3	326	231	0.02%	0.002%
6	2.995	606	608	609	rBV	521	213	0.02%	0.002%
7	3.066	626	630	633	rBV	261	272	0.02%	0.002%
8	3.233	679	682	686	rVB	374	216	0.02%	0.002%
9	3.256	686	689	692	rBV2	253	214	0.02%	0.002%
10	3.288	697	699	702	rVB2	442	230	0.02%	0.002%
11	3.407	733	736	739	rBV2	303	207	0.02%	0.002%
12	3.542	774	778	780	rBV3	271	176	0.01%	0.002%
13	3.571	780	787	790	rVV3	230	275	0.02%	0.002%
14	3.590	790	793	796	rVB2	295	188	0.01%	0.002%
15	3.670	815	818	822	rBV	390	295	0.02%	0.003%
16	3.738	838	839	850	rVB3	364	405	0.03%	0.004%
17	3.895	873	888	932	rBV3	74717	296321	21.65%	2.683%
18	4.346	1012	1028	1056	rBV	195144	522008	38.15%	4.726%
19	4.596	1104	1106	1108	rBV2	387	197	0.01%	0.002%
20	4.703	1137	1139	1142	rVV2	548	297	0.02%	0.003%
21	4.715	1142	1143	1147	rVV2	324	192	0.01%	0.002%
22	4.760	1154	1157	1160	rBV2	385	283	0.02%	0.003%
23	4.776	1160	1162	1167	rVB2	632	379	0.03%	0.003%
24	4.821	1168	1176	1180	rBV3	399	422	0.03%	0.004%
25	4.844	1180	1183	1186	rVB	476	214	0.02%	0.002%
26	4.879	1191	1194	1197	rBV	391	293	0.02%	0.003%
27	4.895	1197	1199	1202	rBV2	293	168	0.01%	0.002%
28	4.947	1214	1215	1217	rBV	336	171	0.01%	0.002%
29	5.040	1227	1244	1288	rBV2	551537	1368434	100.00%	12.389%
30	5.333	1328	1335	1350	rBV7	5013	12183	0.89%	0.110%
31	5.455	1371	1373	1378	rVB3	852	650	0.05%	0.006%
32	5.477	1378	1380	1382	rBV3	597	276	0.02%	0.002%
33	5.539	1397	1399	1402	rBV	251	172	0.01%	0.002%
34	5.612	1409	1422	1454	rBV	434435	917877	67.07%	8.310%
35	5.857	1495	1498	1501	rBV	401	327	0.02%	0.003%
36	5.902	1501	1512	1533	rVV3	26853	60640	4.43%	0.549%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021934.D
 Acq On : 23 Aug 2021 16:35
 Operator : SY/MD
 Sample : M3486-05ME
 Misc : 4.39g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AB8ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	6.069	1551	1564	1590	rVB	286098	600241	43.86%	5.434%
38	6.349	1647	1651	1652	rBV	487	332	0.02%	0.003%
39	6.391	1660	1664	1665	rBV2	322	191	0.01%	0.002%
40	6.532	1703	1708	1712	rBV3	385	411	0.03%	0.004%
41	6.625	1734	1737	1738	rBV3	389	169	0.01%	0.002%
42	6.712	1763	1764	1769	rVB3	547	308	0.02%	0.003%
43	6.741	1769	1773	1777	rBV4	411	357	0.03%	0.003%
44	6.828	1798	1800	1805	rVV3	284	204	0.01%	0.002%
45	6.902	1820	1823	1825	rBV	289	159	0.01%	0.001%
46	6.934	1829	1833	1836	rVB3	394	361	0.03%	0.003%
47	6.989	1836	1850	1875	rBV	157977	314663	22.99%	2.849%
48	7.252	1930	1932	1934	rBV3	410	198	0.01%	0.002%
49	7.317	1940	1952	1970	rBV	646864	1157548	84.59%	10.480%
50	7.625	2037	2048	2071	rBV	103757	208684	15.25%	1.889%
51	7.844	2115	2116	2119	rBV	322	159	0.01%	0.001%
52	7.950	2144	2149	2153	rVB3	491	379	0.03%	0.003%
53	7.982	2153	2159	2162	rBV4	1804	1769	0.13%	0.016%
54	8.053	2175	2181	2183	rBV	573	515	0.04%	0.005%
55	8.108	2185	2198	2233	rBV2	302945	699781	51.14%	6.336%
56	8.439	2298	2301	2305	rBV3	319	196	0.01%	0.002%
57	8.497	2317	2319	2323	rVB3	641	353	0.03%	0.003%
58	8.567	2336	2341	2343	rBV3	307	244	0.02%	0.002%
59	8.725	2387	2390	2394	rVB2	258	159	0.01%	0.001%
60	8.857	2416	2431	2455	rBV	648399	1135237	82.96%	10.278%
61	9.114	2507	2511	2516	rBV3	703	758	0.06%	0.007%
62	9.288	2559	2565	2567	rBV2	409	307	0.02%	0.003%
63	9.394	2597	2598	2603	rVB2	293	152	0.01%	0.001%
64	9.416	2603	2605	2608	rBV2	291	217	0.02%	0.002%
65	9.439	2608	2612	2614	rVV2	342	229	0.02%	0.002%
66	9.455	2615	2617	2623	rVB2	468	248	0.02%	0.002%
67	9.651	2676	2678	2682	rBV2	301	201	0.01%	0.002%
68	9.709	2694	2696	2699	rBV2	382	212	0.02%	0.002%
69	9.760	2707	2712	2715	rVB2	283	233	0.02%	0.002%
70	9.825	2727	2732	2735	rBV	406	364	0.03%	0.003%
71	9.870	2743	2746	2748	rBV	360	211	0.02%	0.002%
72	9.963	2773	2775	2779	rBV2	352	260	0.02%	0.002%
73	10.014	2788	2791	2793	rBV2	330	212	0.02%	0.002%
74	10.130	2820	2827	2842	rVB4	4905	8099	0.59%	0.073%
75	10.223	2844	2856	2876	rBV	411614	677501	49.51%	6.134%
76	10.455	2925	2928	2933	rBV2	565	545	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
 Data File : VV021934.D
 Acq On : 23 Aug 2021 16:35
 Operator : SY/MD
 Sample : M3486-05ME
 Misc : 4.39g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AB8ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

77	10.744	3013	3018	3020	rBV2	404	342	0.02%	0.003%
78	10.837	3044	3047	3050	rBV3	548	382	0.03%	0.003%
79	11.037	3100	3109	3116	rBV5	1396	2247	0.16%	0.020%
80	11.152	3136	3145	3152	rBV4	2566	4286	0.31%	0.039%
81	11.252	3164	3176	3195	rBV	800579	1240847	90.68%	11.234%
82	11.628	3281	3293	3313	rBV	748699	1165753	85.19%	10.554%
83	11.792	3336	3344	3352	rBV5	7860	11476	0.84%	0.104%
84	11.892	3373	3375	3377	rBV	346	161	0.01%	0.001%
85	11.914	3378	3382	3384	rVB2	683	549	0.04%	0.005%
86	12.197	3467	3470	3472	rBV3	418	273	0.02%	0.002%
87	12.310	3503	3505	3508	rBV3	543	280	0.02%	0.003%
88	12.387	3525	3529	3530	rBV2	788	562	0.04%	0.005%
89	12.461	3549	3552	3554	rVV3	747	493	0.04%	0.004%
90	12.596	3588	3594	3595	rBV3	1282	1222	0.09%	0.011%
91	12.889	3679	3685	3697	rVB4	5095	6990	0.51%	0.063%
92	12.976	3708	3712	3713	rBV2	346	300	0.02%	0.003%
93	13.040	3727	3732	3735	rBV5	1164	1223	0.09%	0.011%
94	13.091	3746	3748	3751	rVB	526	213	0.02%	0.002%
95	13.336	3820	3824	3825	rBV2	323	228	0.02%	0.002%
96	13.487	3868	3871	3873	rBV2	616	390	0.03%	0.004%
97	13.519	3874	3881	3891	rVB5	3018	5195	0.38%	0.047%
98	13.754	3949	3954	3961	rVB5	1793	2212	0.16%	0.020%
99	13.792	3962	3966	3971	rBV4	500	513	0.04%	0.005%
100	14.284	4117	4119	4121	rBV	475	199	0.01%	0.002%

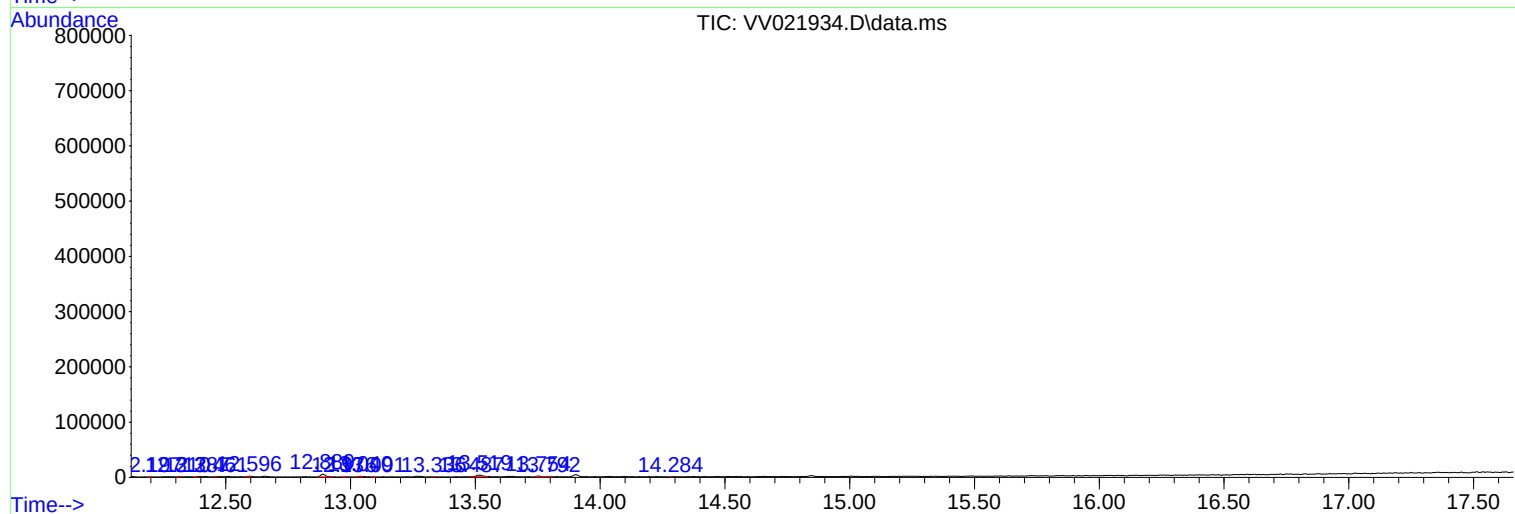
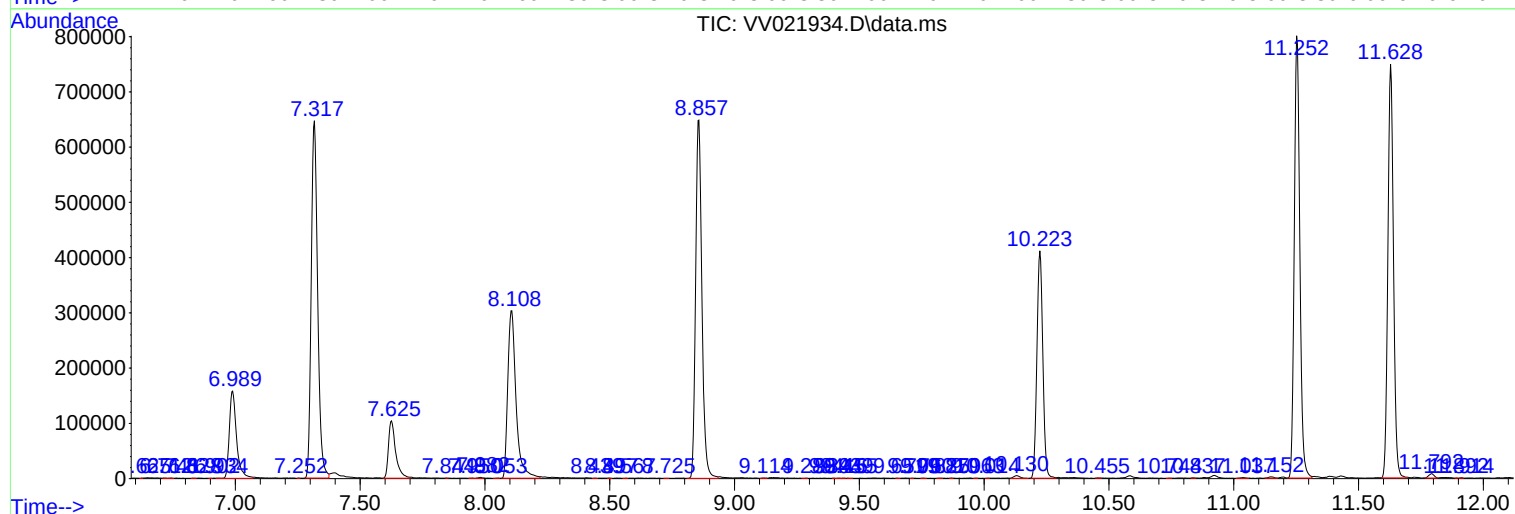
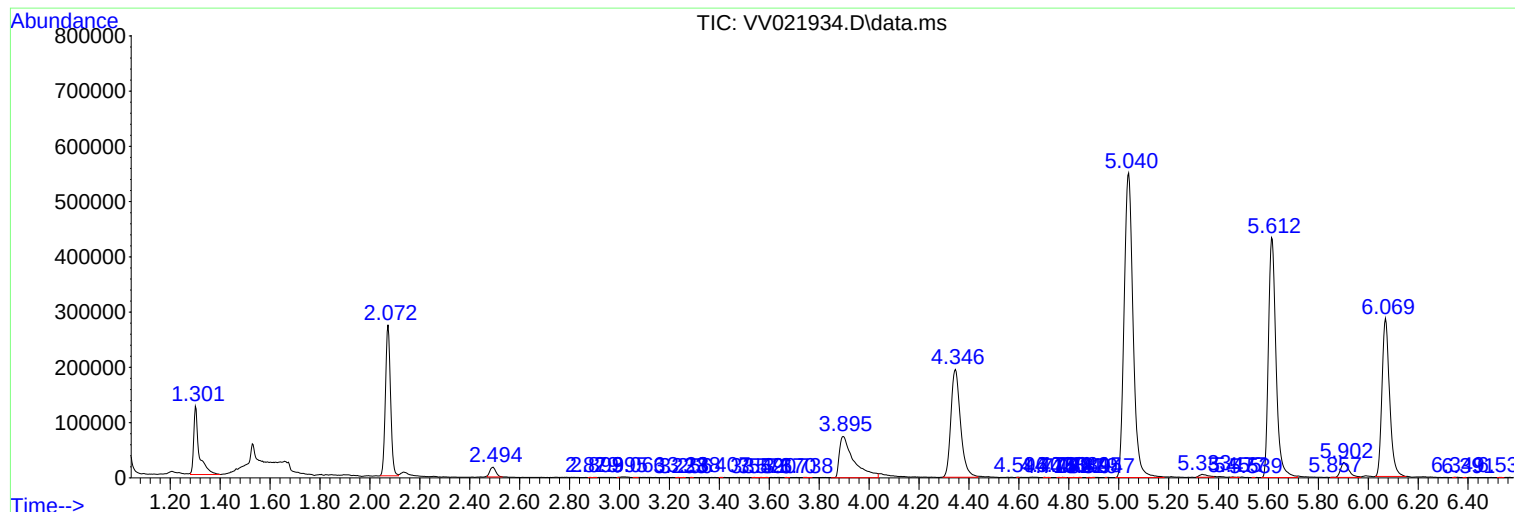
Sum of corrected areas: 11045142

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021934.D
Acq On : 23 Aug 2021 16:35
Operator : SY/MD
Sample : M3486-05ME
Misc : 4.39g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
C0AB8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021934.D
Acq On : 23 Aug 2021 16:35
Operator : SY/MD
Sample : M3486-05ME
Misc : 4.39g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB8ME

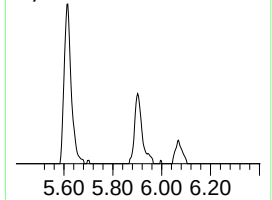
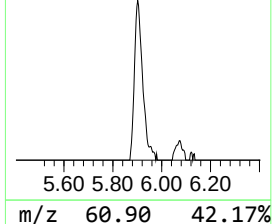
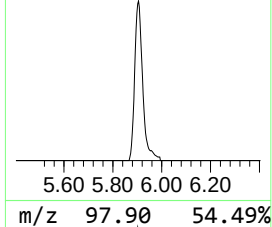
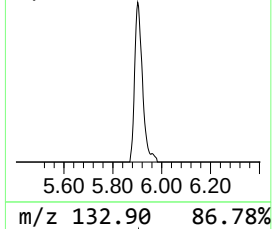
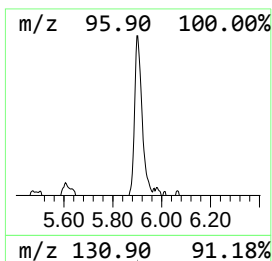
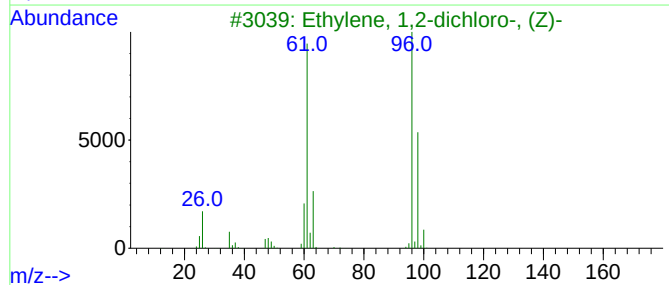
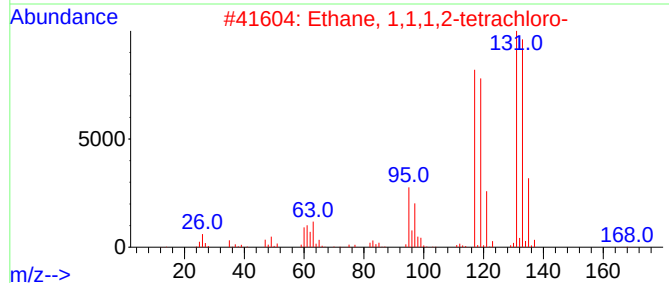
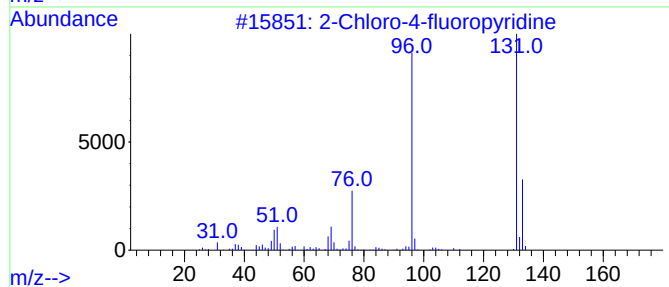
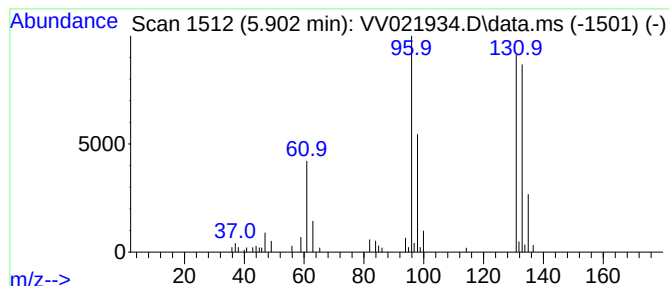
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.30 ug/L	60640	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	43
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5			Carbamic acid, acetylthio-, O-me...	133	C4H7NO2S	016696-87-0	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021934.D
Acq On : 23 Aug 2021 16:35
Operator : SY/MD
Sample : M3486-05ME
Misc : 4.39g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AB8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.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
unknown-01	5.902	3.3	ug/L	60640	1	5.616	917877	50.0