

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
 Data File : VV021944.D
 Acq On : 25 Aug 2021 12:58
 Operator : SY/MD
 Sample : M3518-08ME
 Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AZ4ME

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: VV021944.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	112	rVB	119937	170180	12.92%	1.594%
2	2.079	314	323	335	rBV	253498	364048	27.63%	3.410%
3	2.494	447	452	465	rVB3	9950	16531	1.25%	0.155%
4	2.664	502	505	510	rBV2	433	404	0.03%	0.004%
5	2.879	569	572	574	rBV	253	155	0.01%	0.001%
6	2.979	600	603	607	rBV2	475	412	0.03%	0.004%
7	3.069	628	631	634	rBV2	563	435	0.03%	0.004%
8	3.117	641	646	647	rBV2	349	219	0.02%	0.002%
9	3.130	647	650	651	rVV2	376	191	0.01%	0.002%
10	3.211	671	675	678	rBV2	283	161	0.01%	0.002%
11	3.307	703	705	708	rVB2	301	152	0.01%	0.001%
12	3.323	708	710	714	rVB	482	249	0.02%	0.002%
13	3.449	747	749	754	rVB2	351	249	0.02%	0.002%
14	3.474	754	757	762	rVB2	266	175	0.01%	0.002%
15	3.503	764	766	769	rBV	240	161	0.01%	0.002%
16	3.616	799	801	806	rBV3	382	303	0.02%	0.003%
17	3.645	808	810	813	rVB	427	194	0.01%	0.002%
18	3.664	813	816	819	rBV3	257	184	0.01%	0.002%
19	3.738	836	839	841	rBV2	610	322	0.02%	0.003%
20	3.751	841	843	846	rVV	316	146	0.01%	0.001%
21	3.809	857	861	866	rBV3	439	416	0.03%	0.004%
22	3.892	877	887	921	rBV	65519	265625	20.16%	2.488%
23	4.346	1013	1028	1062	rBV	183828	503578	38.22%	4.717%
24	4.638	1117	1119	1123	rBV3	407	262	0.02%	0.002%
25	4.664	1125	1127	1128	rBV3	542	242	0.02%	0.002%
26	4.702	1137	1139	1142	rBV2	315	191	0.01%	0.002%
27	4.799	1165	1169	1170	rBV2	265	164	0.01%	0.002%
28	4.857	1181	1187	1191	rBV	606	488	0.04%	0.005%
29	4.895	1196	1199	1200	rBV	369	222	0.02%	0.002%
30	4.934	1209	1211	1216	rBV2	394	330	0.03%	0.003%
31	5.040	1228	1244	1281	rBV2	516983	1317414	100.00%	12.339%
32	5.342	1327	1338	1349	rBV7	3904	10290	0.78%	0.096%
33	5.516	1390	1392	1393	rBV2	335	146	0.01%	0.001%
34	5.571	1407	1409	1410	rBV	270	146	0.01%	0.001%
35	5.616	1410	1423	1456	rVV	421362	897451	68.12%	8.406%
36	5.834	1489	1491	1492	rBV	394	187	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
 Data File : VV021944.D
 Acq On : 25 Aug 2021 12:58
 Operator : SY/MD
 Sample : M3518-08ME
 Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AZ4ME

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	5.905	1501	1513	1532	rBV	34233	75378	5.72%	0.706%
38	6.069	1552	1564	1594	rVB	271819	580409	44.06%	5.436%
39	6.349	1648	1651	1654	rBV2	374	181	0.01%	0.002%
40	6.368	1654	1657	1658	rVB2	355	203	0.02%	0.002%
41	6.387	1658	1663	1666	rBV2	354	321	0.02%	0.003%
42	6.439	1676	1679	1681	rBV2	354	167	0.01%	0.002%
43	6.458	1681	1685	1690	rVB2	388	408	0.03%	0.004%
44	6.484	1690	1693	1695	rBV2	259	179	0.01%	0.002%
45	6.519	1700	1704	1705	rBV	277	180	0.01%	0.002%
46	6.616	1731	1734	1735	rBV	385	217	0.02%	0.002%
47	6.641	1738	1742	1743	rBV2	624	451	0.03%	0.004%
48	6.796	1788	1790	1793	rVB2	294	141	0.01%	0.001%
49	6.815	1793	1796	1798	rVB2	564	242	0.02%	0.002%
50	6.825	1798	1799	1804	rVB2	378	234	0.02%	0.002%
51	6.860	1804	1810	1811	rBV2	269	179	0.01%	0.002%
52	6.892	1816	1820	1825	rBV3	304	301	0.02%	0.003%
53	6.937	1829	1834	1835	rBV3	493	322	0.02%	0.003%
54	6.989	1839	1850	1883	rBV	151306	302506	22.96%	2.833%
55	7.178	1906	1909	1912	rVB3	347	222	0.02%	0.002%
56	7.262	1933	1935	1939	rVB	523	296	0.02%	0.003%
57	7.317	1939	1952	1970	rBV	617890	1115101	84.64%	10.444%
58	7.625	2038	2048	2074	rBV	100367	204990	15.56%	1.920%
59	8.040	2174	2177	2179	rBV2	394	311	0.02%	0.003%
60	8.104	2185	2197	2228	rBV2	307212	668797	50.77%	6.264%
61	8.474	2310	2312	2314	rBV2	336	195	0.01%	0.002%
62	8.567	2339	2341	2342	rBV	462	207	0.02%	0.002%
63	8.661	2367	2370	2373	rBV2	274	262	0.02%	0.002%
64	8.763	2399	2402	2404	rBV	322	183	0.01%	0.002%
65	8.857	2418	2431	2463	rBV	655593	1133088	86.01%	10.613%
66	9.210	2537	2541	2544	rBV2	326	265	0.02%	0.002%
67	9.448	2612	2615	2620	rVB	317	182	0.01%	0.002%
68	9.689	2684	2690	2691	rBV2	381	303	0.02%	0.003%
69	9.751	2707	2709	2715	rVB3	289	257	0.02%	0.002%
70	9.783	2715	2719	2722	rBV3	235	223	0.02%	0.002%
71	9.869	2743	2746	2751	rVB2	289	218	0.02%	0.002%
72	9.995	2783	2785	2788	rVV2	454	246	0.02%	0.002%
73	10.014	2788	2791	2795	rVB2	487	358	0.03%	0.003%
74	10.072	2807	2809	2814	rVB	356	190	0.01%	0.002%
75	10.130	2818	2827	2841	rBV2	4868	8046	0.61%	0.075%
76	10.181	2841	2843	2844	rBV	395	206	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
 Data File : VV021944.D
 Acq On : 25 Aug 2021 12:58
 Operator : SY/MD
 Sample : M3518-08ME
 Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AZ4ME

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	10.223	2844	2856	2882	rBV	397529	631797	47.96%	5.917%
78	10.541	2952	2955	2958	rBV5	567	512	0.04%	0.005%
79	10.667	2988	2994	2998	rVB3	813	938	0.07%	0.009%
80	10.779	3026	3029	3031	rBV	253	152	0.01%	0.001%
81	10.879	3058	3060	3061	rBV	644	243	0.02%	0.002%
82	10.927	3067	3075	3084	rVB8	4293	7507	0.57%	0.070%
83	10.976	3089	3090	3093	rBV	280	168	0.01%	0.002%
84	11.021	3100	3104	3105	rBV2	420	274	0.02%	0.003%
85	11.033	3105	3108	3118	rVV4	1414	1864	0.14%	0.017%
86	11.075	3118	3121	3125	rVB3	312	233	0.02%	0.002%
87	11.149	3136	3144	3151	rBV3	3010	4240	0.32%	0.040%
88	11.210	3160	3163	3166	rBV	9549	6002	0.46%	0.056%
89	11.252	3166	3176	3197	rVV	794034	1224178	92.92%	11.466%
90	11.541	3263	3266	3269	rBV	552	353	0.03%	0.003%
91	11.628	3281	3293	3313	rBV	723038	1143798	86.82%	10.713%
92	11.850	3356	3362	3364	rBV4	1277	1167	0.09%	0.011%
93	12.178	3461	3464	3466	rBV	359	195	0.01%	0.002%
94	12.294	3497	3500	3504	rBV4	647	613	0.05%	0.006%
95	12.509	3565	3567	3572	rBV	324	275	0.02%	0.003%
96	12.590	3591	3592	3595	rBV2	634	328	0.02%	0.003%
97	12.654	3610	3612	3617	rVB2	531	366	0.03%	0.003%
98	12.680	3617	3620	3623	rBV2	565	333	0.03%	0.003%
99	12.792	3653	3655	3659	rBV2	420	295	0.02%	0.003%
100	13.075	3735	3743	3748	rBV7	2258	2838	0.22%	0.027%

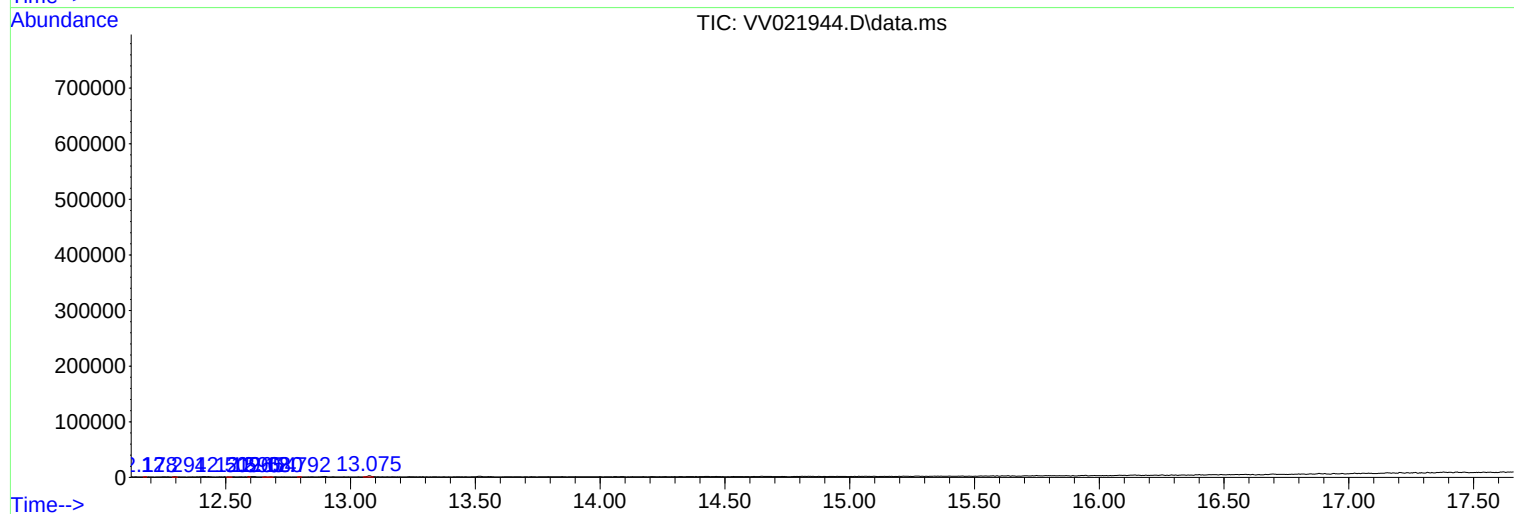
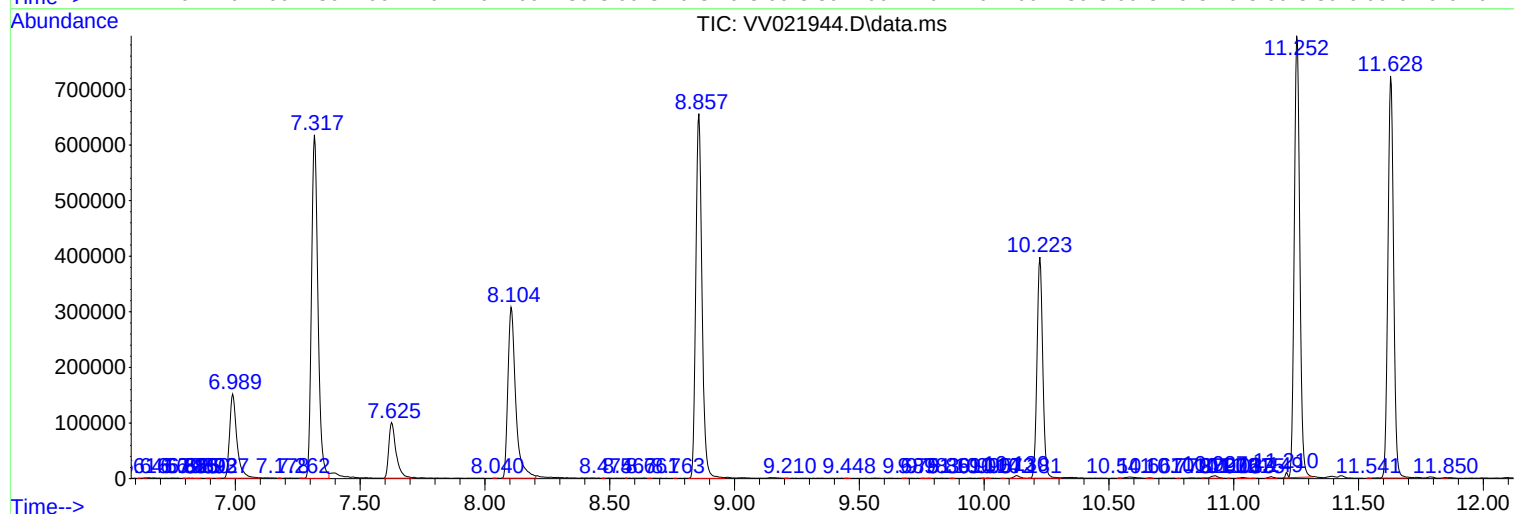
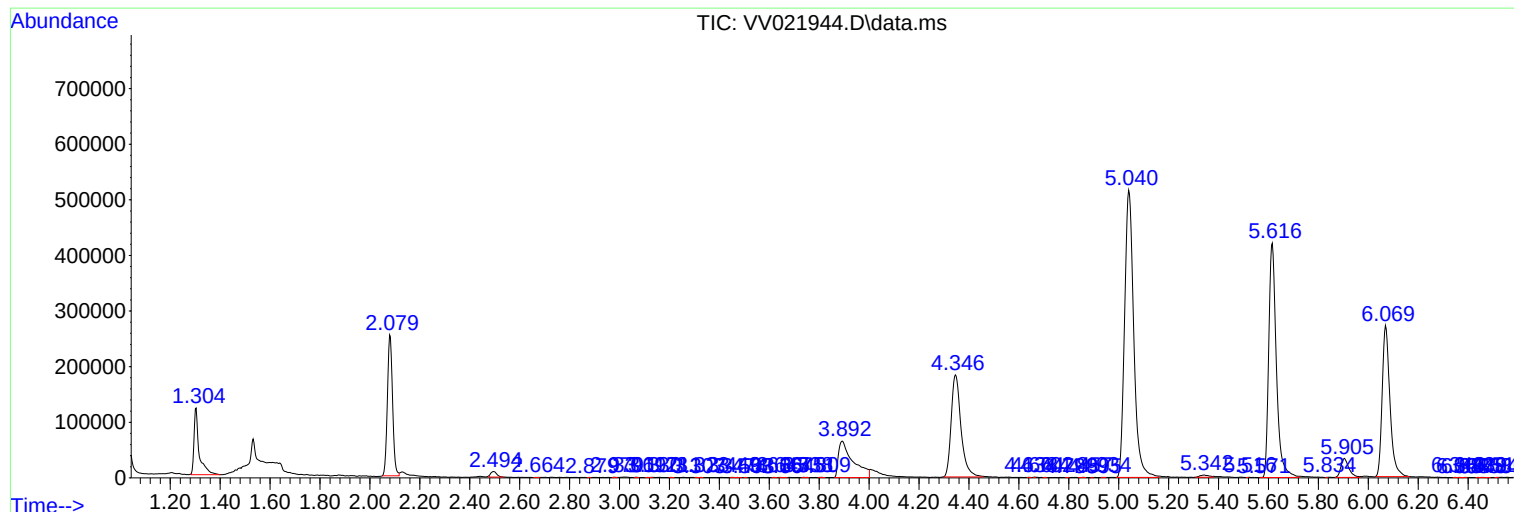
Sum of corrected areas: 10676857

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
Data File : VV021944.D
Acq On : 25 Aug 2021 12:58
Operator : SY/MD
Sample : M3518-08ME
Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
C0AZ4ME

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\VV082521\
Data File : VV021944.D
Acq On : 25 Aug 2021 12:58
Operator : SY/MD
Sample : M3518-08ME
Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AZ4ME

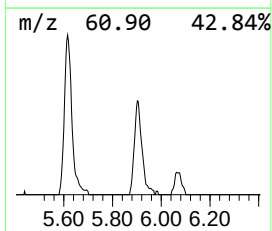
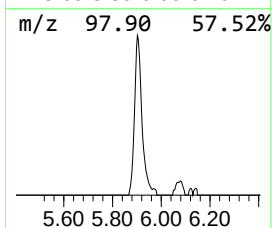
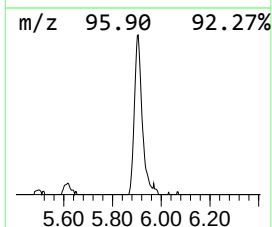
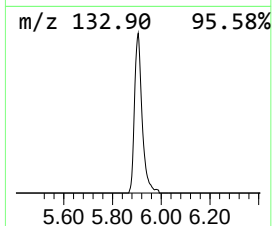
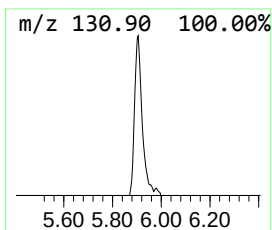
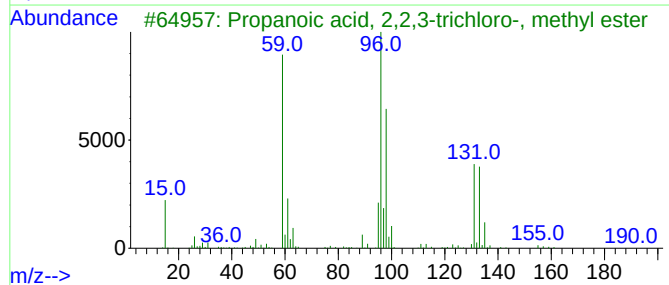
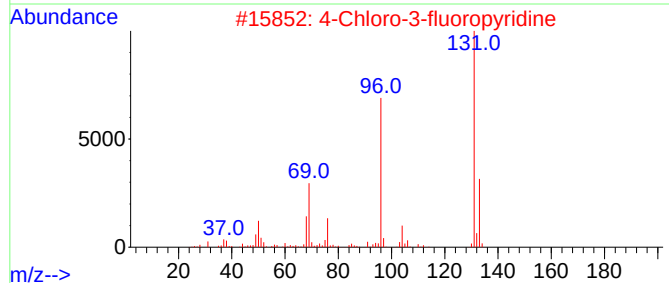
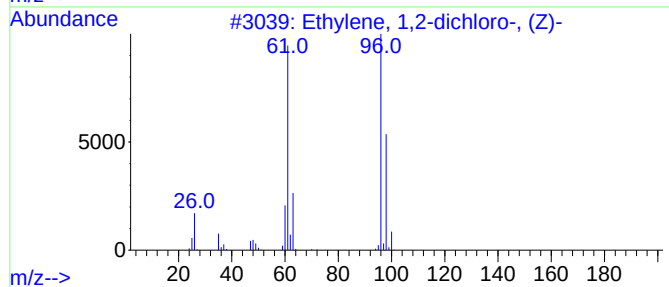
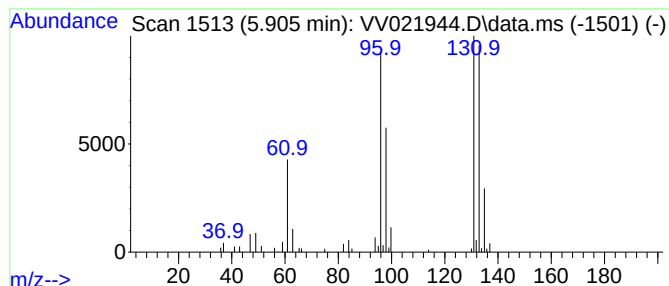
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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.
5.905	4.20 ug/L	75378	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	30
3			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	25
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
5			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082521\
Data File : VV021944.D
Acq On : 25 Aug 2021 12:58
Operator : SY/MD
Sample : M3518-08ME
Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AZ4ME

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	5.905	4.2	ug/L	75378	1	5.616	897451	50.0