

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011222\
 Data File : VV024336.D
 Acq On : 12 Jan 2022 17:35
 Operator : SY/MD
 Sample : N1053-27ME
 Misc : 6.56g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLL4ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024336.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	76	83	97	rBV	133897	135546	14.71%	1.921%
2	1.568	157	164	177	rBV	107586	123010	13.35%	1.743%
3	2.108	322	332	356	rVB	239744	351570	38.16%	4.982%
4	2.343	401	405	407	rBV2	186	151	0.02%	0.002%
5	2.446	435	437	440	rVB	363	145	0.02%	0.002%
6	2.709	516	519	524	rVB2	193	149	0.02%	0.002%
7	2.947	589	593	596	rBB2	270	234	0.03%	0.003%
8	3.082	632	635	640	rBV2	256	310	0.03%	0.004%
9	3.169	659	662	665	rBV	266	219	0.02%	0.003%
10	3.227	678	680	683	rVB2	260	165	0.02%	0.002%
11	3.253	684	688	690	rBV	159	161	0.02%	0.002%
12	3.436	740	745	746	rBV	271	218	0.02%	0.003%
13	3.474	754	757	760	rVB2	265	192	0.02%	0.003%
14	3.503	763	766	768	rBV	194	152	0.02%	0.002%
15	3.603	793	797	799	rBV2	281	193	0.02%	0.003%
16	3.629	802	805	809	rVB2	204	187	0.02%	0.003%
17	3.844	867	872	876	rBV	156	234	0.03%	0.003%
18	3.886	876	885	922	rBV	54526	170284	18.49%	2.413%
19	4.262	999	1002	1006	rBV	277	327	0.04%	0.005%
20	4.349	1013	1029	1057	rBV	157740	388416	42.16%	5.504%
21	4.545	1087	1090	1093	rVB	520	344	0.04%	0.005%
22	4.568	1093	1097	1099	rBV2	416	349	0.04%	0.005%
23	4.777	1159	1162	1165	rBV	171	157	0.02%	0.002%
24	4.860	1184	1188	1191	rBB2	257	224	0.02%	0.003%
25	4.899	1194	1200	1202	rBV	297	369	0.04%	0.005%
26	4.963	1218	1220	1223	rVB2	263	148	0.02%	0.002%
27	5.047	1226	1246	1278	rBV2	348982	921188	100.00%	13.053%
28	5.339	1329	1337	1340	rBV2	492	628	0.07%	0.009%
29	5.445	1366	1370	1374	rBV	412	385	0.04%	0.005%
30	5.471	1374	1378	1381	rVB2	265	240	0.03%	0.003%
31	5.497	1382	1386	1389	rBV2	355	262	0.03%	0.004%
32	5.616	1410	1423	1450	rBV	275181	552185	59.94%	7.824%
33	5.908	1503	1514	1533	rVB4	13962	29878	3.24%	0.423%
34	6.015	1541	1547	1549	rBV3	249	263	0.03%	0.004%
35	6.069	1549	1564	1583	rBV	198371	404984	43.96%	5.738%
36	6.275	1626	1628	1636	rVB2	259	256	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW011222\
 Data File : VW024336.D
 Acq On : 12 Jan 2022 17:35
 Operator : SY/MD
 Sample : N1053-27ME
 Misc : 6.56g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLL4ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	6.400	1664	1667	1668	rBV	270	197	0.02%	0.003%
38	6.458	1682	1685	1690	rBV2	314	318	0.03%	0.005%
39	6.497	1695	1697	1698	rBV2	388	157	0.02%	0.002%
40	6.613	1731	1733	1736	rVB	263	147	0.02%	0.002%
41	6.632	1736	1739	1744	rBV3	229	196	0.02%	0.003%
42	6.667	1747	1750	1753	rVV3	268	201	0.02%	0.003%
43	6.693	1755	1758	1762	rBV2	277	166	0.02%	0.002%
44	6.712	1762	1764	1768	rBV2	259	165	0.02%	0.002%
45	6.760	1777	1779	1786	rVB2	148	152	0.02%	0.002%
46	6.844	1803	1805	1808	rBV2	215	160	0.02%	0.002%
47	6.986	1838	1849	1878	rBV	111915	206206	22.38%	2.922%
48	7.159	1901	1903	1908	rVB3	392	297	0.03%	0.004%
49	7.185	1908	1911	1914	rBV	308	240	0.03%	0.003%
50	7.201	1914	1916	1917	rBV	371	176	0.02%	0.002%
51	7.265	1933	1936	1940	rBB	170	159	0.02%	0.002%
52	7.317	1940	1952	1971	rBV	432290	748419	81.24%	10.605%
53	7.622	2037	2047	2070	rVV2	79488	141383	15.35%	2.003%
54	7.802	2100	2103	2105	rBV	277	210	0.02%	0.003%
55	7.876	2123	2126	2128	rVV3	296	195	0.02%	0.003%
56	8.088	2182	2192	2235	rBV	204952	403406	43.79%	5.716%
57	8.358	2273	2276	2279	rBV2	291	300	0.03%	0.004%
58	8.423	2289	2296	2302	rBV4	960	1557	0.17%	0.022%
59	8.612	2352	2355	2357	rBV2	234	146	0.02%	0.002%
60	8.629	2357	2360	2363	rVV	307	232	0.03%	0.003%
61	8.725	2388	2390	2395	rBV2	235	215	0.02%	0.003%
62	8.751	2395	2398	2401	rVV	225	180	0.02%	0.003%
63	8.767	2401	2403	2406	rVB	336	214	0.02%	0.003%
64	8.850	2418	2429	2454	rBV	414015	665505	72.24%	9.430%
65	9.101	2504	2507	2510	rBV	229	199	0.02%	0.003%
66	9.146	2516	2521	2523	rBV3	1206	1192	0.13%	0.017%
67	9.317	2570	2574	2577	rBV	253	224	0.02%	0.003%
68	9.397	2596	2599	2603	rVB	342	231	0.03%	0.003%
69	9.423	2604	2607	2611	rBV	229	215	0.02%	0.003%
70	9.883	2746	2750	2753	rBV	273	236	0.03%	0.003%
71	9.995	2782	2785	2787	rBV	287	232	0.03%	0.003%
72	10.127	2819	2826	2834	rBV5	1694	2853	0.31%	0.040%
73	10.214	2842	2853	2872	rBV	267075	415050	45.06%	5.881%
74	10.548	2955	2957	2960	rVB3	391	177	0.02%	0.003%
75	10.574	2960	2965	2966	rBV3	717	590	0.06%	0.008%
76	10.744	3014	3018	3019	rBV	314	181	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW011222\
 Data File : VW024336.D
 Acq On : 12 Jan 2022 17:35
 Operator : SY/MD
 Sample : N1053-27ME
 Misc : 6.56g/5.0mL/100ul/5.0ml/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLL4ME

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

77	10.879	3057	3060	3063	rBV	404	280	0.03%	0.004%
78	10.921	3066	3073	3082	rVB5	1889	2909	0.32%	0.041%
79	11.037	3105	3109	3112	rBV2	323	324	0.04%	0.005%
80	11.088	3118	3125	3129	rBV2	316	501	0.05%	0.007%
81	11.146	3138	3143	3151	rVB4	1087	1273	0.14%	0.018%
82	11.185	3152	3155	3157	rBV	248	184	0.02%	0.003%
83	11.249	3163	3175	3195	rBV	417399	646002	70.13%	9.154%
84	11.368	3208	3212	3213	rBV2	784	491	0.05%	0.007%
85	11.497	3248	3252	3259	rVB2	263	321	0.03%	0.005%
86	11.574	3273	3276	3278	rBV	432	276	0.03%	0.004%
87	11.622	3280	3291	3315	rVV	461412	719378	78.09%	10.193%
88	11.738	3325	3327	3330	rBV	470	320	0.03%	0.005%
89	11.789	3337	3343	3353	rVB3	2837	3848	0.42%	0.055%
90	11.847	3359	3361	3362	rBV3	464	203	0.02%	0.003%
91	12.005	3408	3410	3412	rBV	334	212	0.02%	0.003%
92	12.056	3422	3426	3429	rBV2	220	210	0.02%	0.003%
93	12.091	3434	3437	3439	rBV2	415	251	0.03%	0.004%
94	12.593	3591	3593	3597	rVB2	566	304	0.03%	0.004%
95	13.024	3725	3727	3731	rVB	353	202	0.02%	0.003%
96	13.387	3838	3840	3841	rBV	365	165	0.02%	0.002%
97	13.513	3873	3879	3891	rVB3	1681	2660	0.29%	0.038%
98	14.014	4030	4035	4039	rBV3	420	479	0.05%	0.007%
99	14.034	4039	4041	4044	rBV	418	220	0.02%	0.003%
100	14.104	4057	4063	4065	rBV2	353	361	0.04%	0.005%

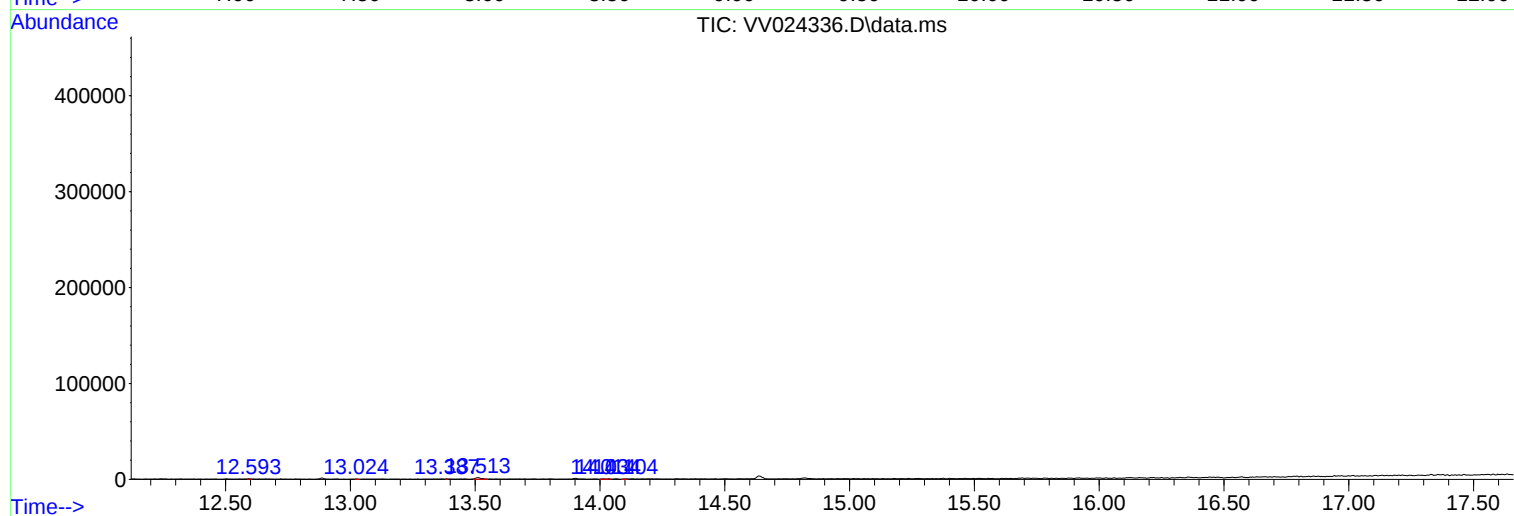
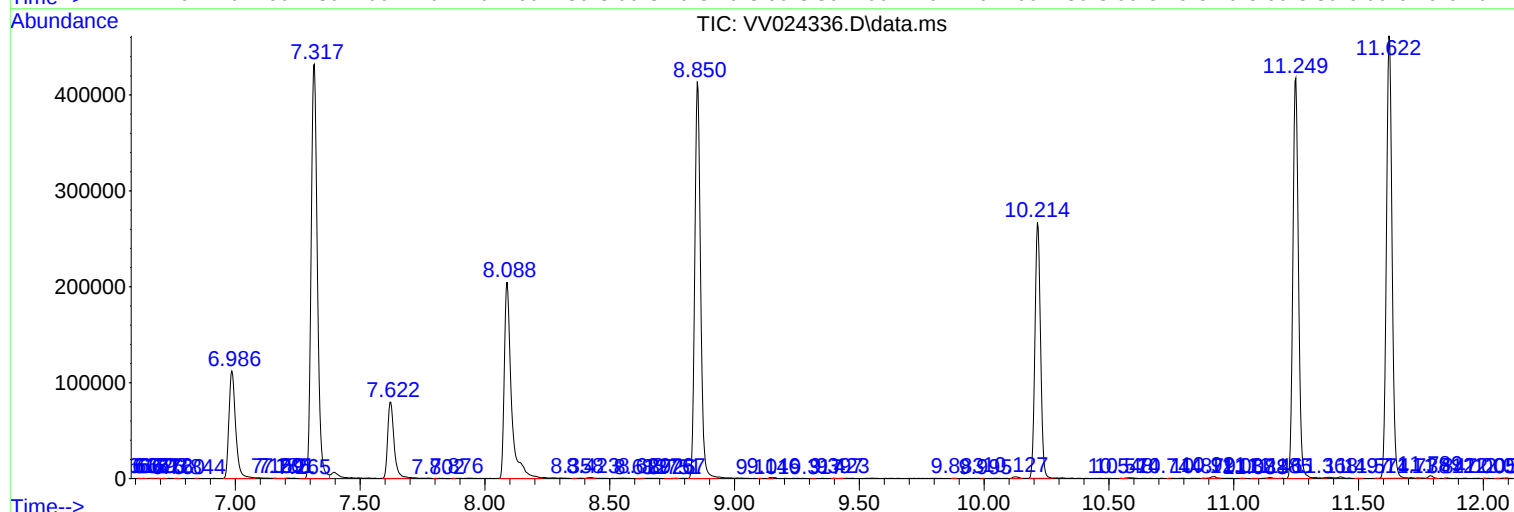
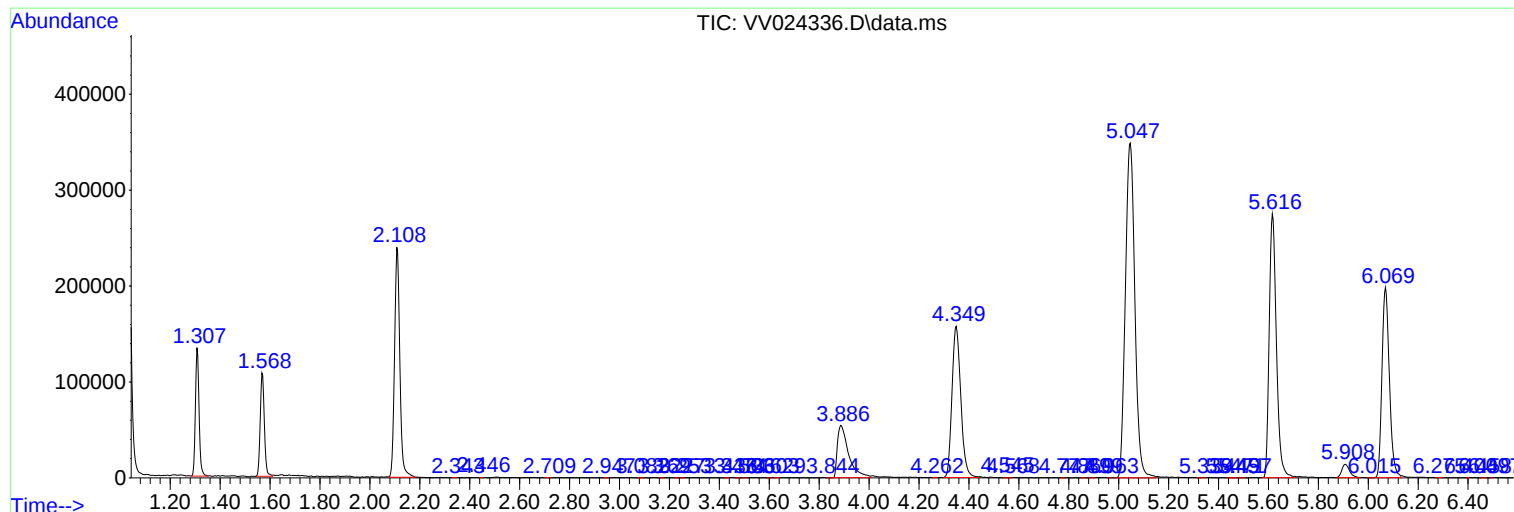
Sum of corrected areas: 7057376

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011222\
Data File : VV024336.D
Acq On : 12 Jan 2022 17:35
Operator : SY/MD
Sample : N1053-27ME
Misc : 6.56g/5.0mL/100ul/5.0ml/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLL4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011222\
Data File : VV024336.D
Acq On : 12 Jan 2022 17:35
Operator : SY/MD
Sample : N1053-27ME
Misc : 6.56g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLL4ME

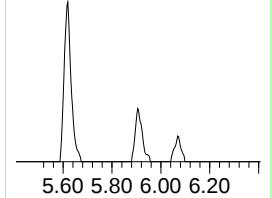
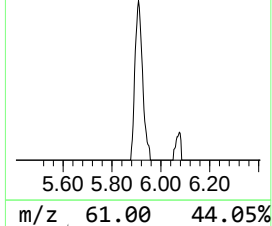
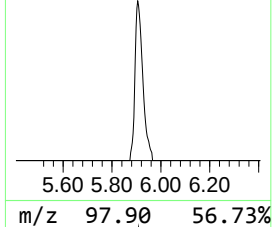
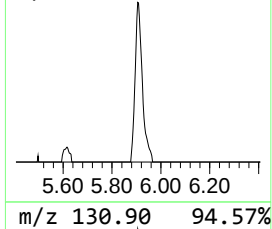
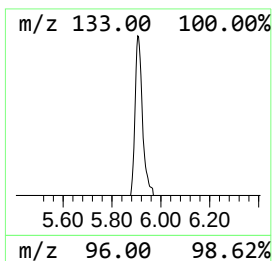
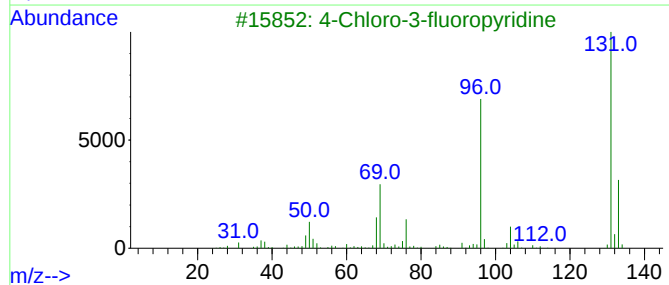
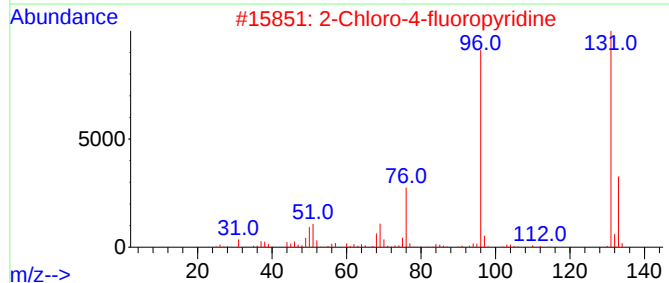
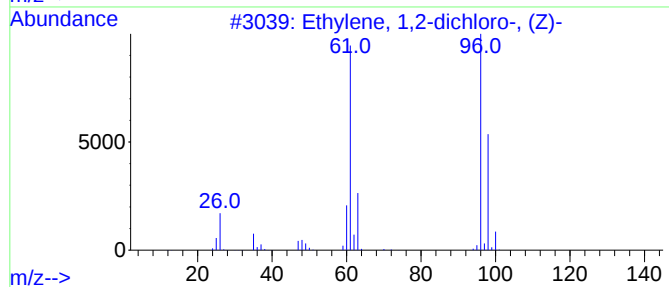
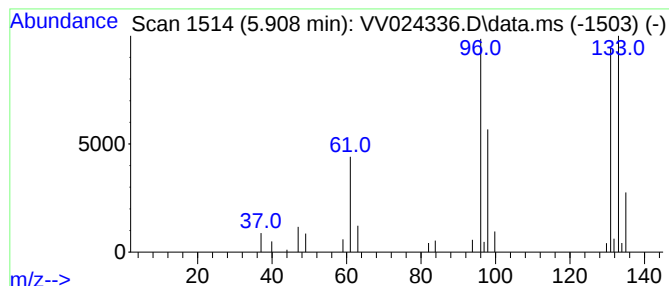
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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.
5.908	2.71 ug/L	29878	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	35
2			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	32
3			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011222\
Data File : VV024336.D
Acq On : 12 Jan 2022 17:35
Operator : SY/MD
Sample : N1053-27ME
Misc : 6.56g/5.0mL/100ul/5.0ml/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLL4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.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	5.908	2.7	ug/L	29878	1	5.616	552185	50.0