Whiskey Analysis with Gas Chromatography

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1 Purpose

In this lab, we utilized a GC/FID to identify the presence and quantity of specific additives in two different brands of whiskey. Aside from alcohol proof, the presence of trace compounds (technically impurities) in the otherwise pure ethanol-water matrix is the only thing that differentiates alcoholic beverages from each other. Identifying these trace elements in a quantitative manner allows us to isolate the qualities that make each drink unique. In this lab, we tested Jim Beam and Jameson brand whiskey for the presence of 2-methyl-1-butanol, ethyl acetate, and 1-propanol.

2 Theory

Gas chromatography (also known as gas-liquid partition chromatography or vapor-phase chromatography) is a form of chromatography that utilizes differences in retention time of gases to separate a sample. To this end, a "mobile-phase" is chosen that will not interact with the sample, usually a relatively inert gas such as helium, argon, or nitrogen. This mobile-phase gas is then laced with sample and flowed through a tube lined with a "stationary-phase" substance, often consisting of a waxy nonpolar liquid or polymer (though differing stationary phases can be used depending on the situation); depending on the amount of intermolecular attraction between the stationary phase and each component of the sample, differing constituents will elute through the column at different times[1]. The more a specific component of the sample is attracted to the stationary phase, the longer it will take to elute through the entire column (thus, for a nonpolar stationary phase, more polar compounds will exit the column first. The detector used in this experiment is a Flame-Ionization Detector, which uses a flame placed at the end of the column to pyrolyse compounds exiting the GC; organic compounds pyrolysed in such a manner form charged products that are detectable by electron flow[2]. The combination of these two methods, also known as GC/FID, allows for the detection of many compounds with good separation and at outstanding sensitivities (as low as a few picograms per second retention[2]). However, this method is not able to detect all compounds universally;
many compounds that do not pyrolyse or do not form charged pyrolysis products are undetectable by this method, limiting its use largely to hydrocarbons and other organic molecules\(^1\). However, this precision comes at a price: because the FID’s signal is proportional to the number of carbon atoms pyrolysed (at least roughly speaking, with regards to hydrocarbons), it measures mass, not concentration; a single large hydrocarbon with many carbon atoms will send the same signal as many small hydrocarbons with the same total number of carbons. We can calculate the relative response factors by comparing the signal strengths (in peak area) of different concentrations of the same analyte, but to turn these into absolute data points instead of ratios we need to use an internal standard as a reference point. By measuring the signal strength of a specific compound in our unknown, and comparing it to the peak area of an internal standard of known concentration, we can determine the amount of unknown substance in our compound absolutely.

3 Experimental

In this lab, we prepared two whiskey samples with an internal 1-butanol standard, to act as the primary subjects of our analysis. For calibration purposes, we used serial dilutions to create 6 standard solutions of each of the unknowns we were looking for (2-methyl-1-butanol, ethyl acetate, and 1-propanol), along with our internal standard (1-butanol), ranging from 25 ppm to 1000 ppm (in increasing order: 25 ppm, 50 ppm, 100 ppm, 250 ppm, 500 ppm, and 1000 ppm). It is relevant to note that because all of the standards were of known concentration, an internal standard was unnecessary because no reference point was necessary. By plotting peak area against standard concentration, we were able to draw a calibration curve, to which we could fit a linear function that would allow us to find reference values of unknown concentrations in our samples (by applying the inverse of our regressed function to the peak area of our sample). To aid in calculation, we experimentally determined the density of the 40% ethanol solution we used to create the standards, simply by finding the mass of a fixed volume of ethanol (by taring out the container) and dividing it by the volume to get density.
4 Results and Discussion

This section contains only tabulated results from the Appendix. Derivations can be found in Appendix A on page 8. Raw data can be found in Appendix B on page 12.

4.1 [Relative] Response Factor Analysis

4.1.1 Results

<table>
<thead>
<tr>
<th>Compound</th>
<th>Formula</th>
<th>$f_i$</th>
<th>$F_i$</th>
<th>Carbon/Oxygen ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>EtAc</td>
<td>C$_4$H$_8$O$_2$</td>
<td>0.0587</td>
<td>1.00</td>
<td>2</td>
</tr>
<tr>
<td>PrOH</td>
<td>C$_3$H$_6$O</td>
<td>0.0641</td>
<td>1.09</td>
<td>3</td>
</tr>
<tr>
<td>BuOH</td>
<td>C$<em>4$H$</em>{10}$O</td>
<td>0.0766</td>
<td>1.30</td>
<td>4</td>
</tr>
<tr>
<td>MeBuOH</td>
<td>C$<em>5$H$</em>{12}$O</td>
<td>0.0971</td>
<td>1.65</td>
<td>5</td>
</tr>
</tbody>
</table>

(*$f_i$ is absolute response factor, and $F_i$ is relative response factor*)

4.1.2 Discussion

The response factors$^1$ (summarized in the above table) tell us much about the sensitivity of the FID to the various analytes. The fact that simply sorting by increasing carbon to oxygen ratio places the compounds in order of increasing response factor is no coincidence; rather, it tells us that the FID more efficiently detects longer-chain hydrocarbons with less substitution than smaller, more substituted alkyls. In fact, if we multiply the standard response factor $f_i$ by a factor of 51.5 (an arbitrary number that conveniently scales up), we find that nearly all the hydrocarbons have integral response factors that approximate the number of carbons in their skeleton, with the highly substituted ethyl acetate having the lowest $f_i$ due to the greatest number of heteroatoms in its structure. Whereas retention time tells us how much each structure prefers to bond to the stationary phase in the column (longer retention time = larger affinity to stationary phase), response factor merely indicates to us the affinity of the sample to the FID, vis-à-vis the structure of the compound (FIDs are more responsive to long-chain hydrocarbons with fewer substituents).

$^1$Calculations in section A.3 on page 9.
4.2 Calculated Sample Analyte Concentrations

4.2.1 Results

<table>
<thead>
<tr>
<th>Analyte</th>
<th>Jameson</th>
<th>Jim Beam</th>
</tr>
</thead>
<tbody>
<tr>
<td>EtAc</td>
<td>52.48 ppm</td>
<td>$5.25 \times 10^{-5}$</td>
</tr>
<tr>
<td>PrOH</td>
<td>80.99 ppm</td>
<td>$8.11 \times 10^{-5}$</td>
</tr>
<tr>
<td>MeBuOH</td>
<td>176.69 ppm</td>
<td>$1.77 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

4.2.2 Discussion

Armed with this data\(^2\), we can identify the chemical "fingerprint" of the whiskeys we sampled, in terms of the relative concentrations of each of the three analytes we looked at. Perhaps the most significant difference we can identify between the two beverages is a nearly tenfold increase in concentration of 2-methyl-1-butanol from Jameson to Jim Beam, along with a corresponding increase in mixing ratio. We are also able to see that Jim Beam contains approximately thrice as much ethyl acetate per unit volume as Jameson. Finally, we can note that the two brands of whiskeys have nearly identical 1-propanol mixing ratios. There are several explanations for the significant differences in these trace compounds: they may be unintentional adulterants, and Jameson brand whiskey has a more thorough filtration process; alternatively, these compounds may be intentionally left in the drink to add aroma or flavor, and Jim Beam brand whiskey is subject to processes that bring out these qualities (or perhaps they are directly added to the drink). Whichever of these reasons is the cause for the differing chemical footprints of Jim Beam and Jameson, it is likely that the treatment of 1-propanol between the brands is similar if not identical, because the final mixing ratios of this analyte are very similar.

\(^2\)Calculations in section A.4 on page 9.
4.3 Predicted Sample Analyte Concentrations

<table>
<thead>
<tr>
<th>Sample→</th>
<th>Jameson</th>
<th>Jim Beam</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analyte↓</td>
<td>Concentration</td>
<td>Mixing Ratio</td>
</tr>
<tr>
<td>EtAc</td>
<td>52.31 ppm</td>
<td>$5.23 \times 10^{-5}$</td>
</tr>
<tr>
<td>PrOH</td>
<td>66.24 ppm</td>
<td>$6.62 \times 10^{-5}$</td>
</tr>
<tr>
<td>MeBuOH</td>
<td>214.20 ppm</td>
<td>$2.14 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

By plotting our calibration curves\(^3\) and fitting curves to them (again, see Appendix A on page 8 for graphs), we find ourselves with a linear correlation of astoundingly good fit (our lowest $R^2$ values is 0.997). The correlation function gives us a good way of relating peak area with concentration; by taking the peak areas of our samples and plugging them into the inverse of our regression, we can determine the corresponding concentration value on our trendline. These predicted values, based on interpolation (or extrapolation) of the 6 standard solutions we created, can be used to determine the accuracy of our calculated analyte concentrations; if our data is good, our calculated values should fall close to the trendline of our standards.

4.4 Accuracy and Error

<table>
<thead>
<tr>
<th>Sample→</th>
<th>Jameson</th>
<th>Jim Beam</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analyte↓</td>
<td>Calculated</td>
<td>Predicted</td>
</tr>
<tr>
<td>EtAc</td>
<td>52.48</td>
<td>52.31</td>
</tr>
<tr>
<td>PrOH</td>
<td>80.99</td>
<td>66.24</td>
</tr>
<tr>
<td>MeBuOH</td>
<td>176.69</td>
<td>214.195</td>
</tr>
</tbody>
</table>

Unfortunately, our deviation from the standard trendline is rather significant for all both 1-propanol and 2-methyl-1-butanol, though our ethyl acetate data aligns very well with the fit. The fact that our deviation from the expected values is similar for both whiskeys, even at different concentrations, hints at some sort of systematic error. A possible explanation for this could be inaccurate concentrations of our calibration standards;

\(^3\)Calculations in section A.5 on page 10.
because our samples were serially diluted from each other, if our original concentration was off, all of our following data points would be off by the same relative amount. This could cause our trendline to have an incorrect slope, while still fitting a linear curve very tightly. Properly executed, GC/FID should be an ideal tool for this sort of quantitative analysis, because the ethanol matrix of whiskey along with all the trace components are of a class that is easily detected by FID to high accuracy, due to the dominating presence of hydrocarbons in the sample. GC/FID works better than GC/MS for these sorts of samples because we are dealing with simple, ignitable compounds that pyrolyse easily, forming spectra that are far more identifiable than the electron-ionized alkyl ions created using GC/MS. While GC/MS is capable of analyzing a far greater variety of samples, it is at the cost of less precision on samples that FID can analyze. When the samples in question are mostly flammable, small-chain alkyl derivatives, GC/FID is the clear choice.

5 Conclusion

Though we have reason to doubt the accuracy of our standards, we nevertheless received answers that, while far from the theoretical limit on accuracy of a GC/FID, displayed relatively very reasonable fits and trends. We were able to accurately calculate the relative concentrations of various trace components of Jameson and Jim Beam brand whiskeys, and identified several characteristic features of each (notably, Jim Beam contains far greater concentrations of ethyl acetate and 2-methyl-1-butanol, but the two whiskeys contain almost identical quantities of 1-propanol). Unfortunately, though our relative values appeared accurate, there may be some systematic inaccuracy in our calibration curve, as both of our samples deviate from the expected linear fit by near-identical amounts. Despite this, we can still maintain relative confidence in our results, even if we don’t have perfect predicted values to back them up, simply because our relative data points fix extremely well. Though our data may not be good enough for an institute of standards (again, mostly due to the lack of accurate standards), we were still able to receive informative data regarding the importance of trace elements in alcohol differentiation, all
while honing our GC/FID and quantitative analysis skills for the future.

References


A Calculations

A.1 Integrated Peak Areas by Analyte

<table>
<thead>
<tr>
<th>Sample</th>
<th>2-Methyl-1-Butanol</th>
<th>Ethyl Acetate</th>
<th>1-Propanol</th>
<th>1-Butanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 ppm</td>
<td>2.02031</td>
<td>1.50115</td>
<td>1.89623</td>
<td>2.05119</td>
</tr>
<tr>
<td>50 ppm</td>
<td>3.34871</td>
<td>2.7806</td>
<td>3.37107</td>
<td>3.65682</td>
</tr>
<tr>
<td>100 ppm</td>
<td>8.42192</td>
<td>5.60155</td>
<td>6.33308</td>
<td>5.74012</td>
</tr>
<tr>
<td>250 ppm</td>
<td>19.41887</td>
<td>13.61902</td>
<td>16.1463</td>
<td>17.35356</td>
</tr>
<tr>
<td>500 ppm</td>
<td>41.13889</td>
<td>27.535</td>
<td>32.53373</td>
<td>35.27502</td>
</tr>
<tr>
<td>1000 ppm</td>
<td>80.19011</td>
<td>53.27674</td>
<td>71.27694</td>
<td>179.67223</td>
</tr>
<tr>
<td>100 ppm EtAc</td>
<td></td>
<td>16.52408</td>
<td></td>
<td>555.50897</td>
</tr>
<tr>
<td>100 ppm PrOH</td>
<td></td>
<td></td>
<td>12.68271</td>
<td>726.14496</td>
</tr>
<tr>
<td>Jameson</td>
<td>17.15689</td>
<td>3.08045</td>
<td>5.19168</td>
<td>719.90717</td>
</tr>
<tr>
<td>Jim Beam</td>
<td>138.06551</td>
<td>10.62693</td>
<td>5.0176</td>
<td>235.30447</td>
</tr>
</tbody>
</table>

8
A.2 Ethanol Density Calculation

<table>
<thead>
<tr>
<th>Trial</th>
<th>Density (g/mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.939</td>
</tr>
<tr>
<td>2</td>
<td>0.9417</td>
</tr>
<tr>
<td>3</td>
<td>0.940</td>
</tr>
</tbody>
</table>

\[ \bar{\mu} = \frac{x_1 + ... + x_n}{n} = 0.940 \text{ g/mL} \]

A.3 Response Factor Calibration

A.3.1 2-Methyl-1-Butanol

\[ 100 \text{ ppm(} \frac{v}{v} \text{)} = \frac{100 \mu L \text{ MeBuOH}}{1L \text{ solvent}} \times \frac{0.8152 \text{ mg \ MeBuOH}}{\mu L \text{ MeBuOH}} \times \frac{1L \text{ solvent}}{0.940 \text{ kg solvent}} = 86.72 \text{ mg solute} \text{ kg solvent} = 86.72 \text{ ppm(} \frac{m}{m} \text{)} \]

\[ f_{MeBuOH} = \frac{A_i}{A_{std}} f_{std} = \frac{5.60155}{86.72 \text{ ppm(} \frac{m}{m} \text{)}} \times 1 \text{ ppm} = 0.0971 \]

A.3.2 Ethyl Acetate

\[ 100 \text{ ppm(} \frac{v}{v} \text{)} = \frac{100 \mu L \text{ EtAc}}{1L \text{ solvent}} \times \frac{0.897 \text{ mg \ EtAc}}{\mu L \text{ EtAc}} \times \frac{1L \text{ solvent}}{0.940 \text{ kg solvent}} = 95.43 \text{ mg solute} \text{ kg solvent} = 95.43 \text{ ppm(} \frac{m}{m} \text{)} \]

\[ f_{EtAc} = \frac{A_i}{A_{std}} f_{std} = \frac{5.60155}{85.43 \text{ ppm(} \frac{m}{m} \text{)}} \times 1 \text{ ppm} = 0.0587 \]

A.3.3 1-Propanol

\[ 100 \text{ ppm(} \frac{v}{v} \text{)} = \frac{100 \mu L \text{ PrOH}}{1L \text{ solvent}} \times \frac{0.803 \text{ mg \ PrOH}}{\mu L \text{ PrOH}} \times \frac{1L \text{ solvent}}{0.940 \text{ kg solvent}} = 85.43 \text{ mg solute} \text{ kg solvent} = 85.43 \text{ ppm(} \frac{m}{m} \text{)} \]

\[ f_{PrOH} = \frac{A_i}{A_{std}} f_{std} = \frac{6.33908}{85.43 \text{ ppm(} \frac{m}{m} \text{)}} \times 1 \text{ ppm} = 0.0641 \]

A.3.4 1-Butanol

\[ 100 \text{ ppm(} \frac{v}{v} \text{)} = \frac{100 \mu L \text{ BuOH}}{1L \text{ solvent}} \times \frac{0.81 \text{ mg \ BuOH}}{\mu L \text{ BuOH}} \times \frac{1L \text{ solvent}}{0.940 \text{ kg solvent}} = 86.17 \text{ mg solute} \text{ kg solvent} = 86.17 \text{ ppm(} \frac{m}{m} \text{)} \]

\[ f_{BuOH} = \frac{A_i}{A_{std}} f_{std} = \frac{5.74}{86.01217 \text{ ppm(} \frac{m}{m} \text{)}} \times 1 \text{ ppm} = 0.0766 \]

A.4 Calculated Analyte Concentrations and Mixing Ratios

A.4.1 Jameson

2-Methyl-1-Butanol  \[ r_i = \frac{n_i}{n_{tot} - n_i} \]

\[ \frac{17.15689}{0.0971} \times 1 \text{ ppm} = 176.69 \text{ ppm; } \frac{176.69 \text{ ppm}}{1 \times 10^6 \text{ ppm}} = 1.77 \times 10^{-4} \]
Ethyl Acetate \( r_i = \frac{n_i}{n_{\text{tot}} - n_i} \)

\[
\frac{3.08045}{0.0587} \times 1 \text{ ppm} = 52.48 \text{ ppm; } \frac{52.48 \text{ ppm}}{1 \times 10^6 \text{ ppm}} = 5.25 \times 10^{-5}
\]

1-Propanol \( r_i = \frac{n_i}{n_{\text{tot}} - n_i} \)

\[
\frac{5.19168}{0.0641} \times 1 \text{ ppm} = 80.99 \text{ ppm; } \frac{80.99 \text{ ppm}}{1 \times 10^6 \text{ ppm}} = 8.11 \times 10^{-5}
\]

A.4.2 Jim Beam

2-Methyl-1-Butanol \( r_i = \frac{n_i}{n_{\text{tot}} - n_i} \)

\[
\frac{138.06551}{0.0971} \times 1 \text{ ppm} = 1421.89 \text{ ppm; } \frac{1421.89 \text{ ppm}}{1 \times 10^6 \text{ ppm}} = 1.424 \times 10^{-3}
\]

Ethyl Acetate \( r_i = \frac{n_i}{n_{\text{tot}} - n_i} \)

\[
\frac{10.62693}{0.0587} \times 1 \text{ ppm} = 181.04 \text{ ppm; } \frac{181.04 \text{ ppm}}{1 \times 10^6 \text{ ppm}} = 1.81 \times 10^{-4}
\]

1-Propanol \( r_i = \frac{n_i}{n_{\text{tot}} - n_i} \)

\[
\frac{5.0176}{0.0641} \times 1 \text{ ppm} = 78.28 \text{ ppm; } \frac{78.28 \text{ ppm}}{1 \times 10^6 \text{ ppm}} = 7.82 \times 10^{-5}
\]

A.5 Predicted Analyte Concentrations and Mixing Ratios

A.5.1 2-Methyl-1-Butanol

![Calibration Curve of 2-Methyl-1-Butanol](image-url)

\[ f(x) = 0.0806380491x - 0.1154057467 \]

\[ R^2 = 0.999578592 \]
Jame son  \( f(x) = 0.08064x - 0.1154; 17.15689 = 0.08064x - 0.1154; x = 214.20 \text{ ppm}; \)
\[
\frac{214.20 \text{ ppm}}{1 \times 10^6 \text{ ppm} - 214.20 \text{ ppm}} = \frac{2.14 	imes 10^{-4}}{}
\]

Jim Beam  \( f(x) = 0.08064x - 0.1154; 138.06551 = 0.08064x - 0.1154; x = 1713.59 \text{ ppm}; \)
\[
\frac{1713.59 \text{ ppm}}{1 \times 10^6 \text{ ppm} - 1713.59 \text{ ppm}} = \frac{1.72 	imes 10^{-3}}{}
\]

A.5.2 Ethyl Acetate

![Calibration Curve of Ethyl Acetate](image)

Jame son  \( f(x) = 0.0532728x + 0.2939735; 3.08045 = 0.0532728x + 0.2939735; x = 52.31 \text{ ppm}; \)
\[
\frac{52.31 \text{ ppm}}{1 \times 10^6 \text{ ppm} - 52.31 \text{ ppm}} = 5.23 	imes 10^{-5}
\]

Jim Beam  \( f(x) = 0.0532728x + 0.2939735; 10.62693 = 0.0532728x + 0.2939735; x = 193.96 \text{ ppm}; \)
\[
\frac{193.96 \text{ ppm}}{1 \times 10^6 \text{ ppm} - 193.96 \text{ ppm}} = 1.94 	imes 10^{-4}
\]

A.5.3 1-Propanol

Jame son  \( f(x) = 0.0709324x - 0.8312747; 5.1916 = 0.0709324x - 0.8312747; x = 66.24 \text{ ppm}; \)
\[
\frac{66.24 \text{ ppm}}{1 \times 10^6 \text{ ppm} - 66.24 \text{ ppm}} = 6.62 	imes 10^{-5}
\]
Jim Beam \( f(x) = 0.0709324x - 0.8312747; \) 5.0176 = 0.0709324x - 0.8312747; \( x = 64.32 \) ppm; \( \frac{64.32 \text{ ppm}}{1 \times 10^6 \text{ ppm} - 64.32 \text{ ppm}} = 6.43 \times 10^{-5} \)

### A.6 Accuracy and Error

**Jameson** \( \frac{176.69 - 214.195}{214.195} \times 100\% = -17.5\% \text{ error} \)

**Jim Beam** \( \frac{1421.89 - 1713.594479}{1713.594479} \times 100\% = -17.1\% \text{ error} \)

**Jameson** \( \frac{52.48 - 52.30576021}{52.30576021} \times 100\% = 0.333\% \text{ error} \)

**Jim Beam** \( \frac{181.04 - 193.9629327}{193.9629327} \times 100\% = -6.66\% \text{ error} \)

**Jameson** \( \frac{80.99 - 66.23547047}{66.23547047} \times 100\% = 22.2\% \text{ error} \)

**Jim Beam** \( \frac{78.28 - 64.32108272}{64.32108272} \times 100\% = 21.7\% \text{ error} \)

### B Raw Data
Figure 1: GC/FID Report for 10 ppm standard
Figure 2: GC/FID Report for 25 ppm standard
Data File C:\HPCHEM\1\DATA\29JAN13\01881101.D  

Injection Date : 1/29/2014 7:56:02 PM  Seq. Line :  11
Sample Name : JUJP50std  Location : Vial 10
Acq. Operator : Chem 105  Inj :  1
Acq. Instrument : DEG 6C  Inj Volume : 1 µL
Acq. Method : C:\HPCHEM\METHODS\C105 S13.M
Last Changed : 1/29/2014 2:05:32 PM by Chem 105
Analysis Method : C:\HPCHEM\METHODS\C105 S13.M
Last changed : 2/5/2014 2:00:12 PM by Chem 105
(modified after loading)
Chem 105 Whiskey Method

Arte Percent Report

Sorted By  :  Signal
Multiplier :  1.0000
Dilution  :  1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID2 E,

<table>
<thead>
<tr>
<th>#</th>
<th>[min]</th>
<th>[min]</th>
<th>[DA's]</th>
<th>[DA]</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.545</td>
<td>0.0509</td>
<td>2.2793E4</td>
<td>5726.41064</td>
<td>99.89955</td>
</tr>
<tr>
<td>2</td>
<td>4.148</td>
<td>0.0347</td>
<td>9.75901</td>
<td>5.1582</td>
<td>0.04277</td>
</tr>
<tr>
<td>3</td>
<td>5.265</td>
<td>0.0648</td>
<td>3.37107</td>
<td>5.14842e+1</td>
<td>0.01477</td>
</tr>
<tr>
<td>4</td>
<td>7.006</td>
<td>0.0573</td>
<td>2.78050</td>
<td>5.42413e+1</td>
<td>0.01216</td>
</tr>
<tr>
<td>5</td>
<td>9.470</td>
<td>0.1535</td>
<td>3.65682</td>
<td>3.97128e+1</td>
<td>0.01603</td>
</tr>
<tr>
<td>6</td>
<td>14.912</td>
<td>0.2143</td>
<td>3.34871</td>
<td>2.60439e+1</td>
<td>0.01468</td>
</tr>
</tbody>
</table>

Totals:  2.20167e+4  5731.94128

Results obtained with enhanced integrator!

Summed Peaks Report

Signal 1: FID2 E,

Final Summed Peaks Report

Signal 1: FID2 E,  

*** End of Report ***

Figure 3: GC/FID Report for 50 ppm standard
Data File C:\HPCHEM\1\DATA\23JOH13\019S1201.D
=================================================================
Injection Date : 1/29/2014 8:19:24 PM  Seq. Line : 12
Sample Name : JJ3P100std Location : Vial 19
Acc. Operator : Chem 105  Inj : 1
Acc. Instrument : DSA 6C  Inj Volume : 1 µl
Acc. Method : C:\HPCHEM\METHODS\c105 S13.M
Last Changed : 1/29/2014 2:05:32 PM by Chem 105
Analysis Method : C:\HPCHEM\METHODS\C105 S13.M
Last changed : 2/5/2014 1:38:14 PM by Chem 105
(modified after loading)
Chem 105 Whiskey Method
=================================================================

Artefact Report
=================================================================

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID2 E,

Peak Ret.Time Type Width Area Height Area
# [min] [min] [DA's] [DA] %
----|-----|-----|---------|-----|-----|-----|-----|
 1 3.547 PB  0.0499 2.27373e4  5750.386014 99.79786
 2 4.147 PP  0.0343 19.95820 7.34213 0.03760
 3 5.263 PB  0.0668 6.33308 1.13308 0.02760
 4 7.065 PP  0.0565 5.60155 1.31570 0.02459
 5 9.463 PB  0.1143 5.74012 6.49526e-1 0.02519
 6 14.921 MM  0.2546 8.42192 5.12225e-1 0.03967

Totals : 2.27833e4 5761.36261

Results obtained with enhanced integrator!
=================================================================

Summed Peaks Report
=================================================================

Signal 1: FID2 E,

Final Summed Peaks Report
=================================================================

Signal 1: FID2 E, *** End of Report ***

Figure 4: GC/FID Report for 100 ppm standard
Figure 5: GC/FID Report for 250 ppm standard
**Figure 6: GC/FID Report for 500 ppm standard**

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Data File C:\\HPChem\DATA\29JAN13\021B1401.D

Injection Date : 1/29/2014 9:06:14 PM  Seq. Line : 14
Sample Name : JJP500std  Location : Vial 21
Acq. Operator : Chem 105  Inj : 1
Acq. Instrument : DGA GC  Inj Volume : 1 μl
Sequence File : C:\HPChem\SEQUENCE\DEF GC.S
Method : C:\HPChem\METHODS\C105 S13.M
Last changed : 1/29/2014 2:05:32 PM by Chem 105
Chem 105 Whiskey Method

---

**Area Percent Report**

---

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

**Signal 1: FID2 E,**

<table>
<thead>
<tr>
<th>Peak RetTime</th>
<th>Type</th>
<th>Width</th>
<th>Area</th>
<th>Height</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PB</td>
<td>0.0493</td>
<td>2.2468664</td>
<td>5720.54229</td>
<td>96.94653</td>
</tr>
<tr>
<td>2</td>
<td>PP</td>
<td>0.0392</td>
<td>102.27948</td>
<td>37.94732</td>
<td>0.45042</td>
</tr>
<tr>
<td>3</td>
<td>PP</td>
<td>0.0706</td>
<td>33.53237</td>
<td>5.70139</td>
<td>0.14327</td>
</tr>
<tr>
<td>4</td>
<td>PP</td>
<td>0.0663</td>
<td>27.53500</td>
<td>6.57231</td>
<td>0.12126</td>
</tr>
<tr>
<td>5</td>
<td>PB</td>
<td>0.1485</td>
<td>35.27502</td>
<td>3.46438</td>
<td>0.15535</td>
</tr>
<tr>
<td>6</td>
<td>BB</td>
<td>0.2354</td>
<td>41.13869</td>
<td>2.55432</td>
<td>0.13117</td>
</tr>
</tbody>
</table>

Totals : 2.27074e4  5776.81201

Results obtained with enhanced integrator!

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**Summed Peaks Report**

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**Signal 1: FID2 E,**

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**Final Summed Peaks Report**

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**Signal 1: FID2 E,**

*** End of Report ***
Data File C: \HPChem\DATA\29JAN13\022B1501.D

Injection Date : 1/29/2014 9:29:33 PM  Seq. Line : 15
Sample Name : JWP1000std  Location : Vial 22
Acq. Operator : Chem 105  Inj. : 1
Acq. Instrument : DEA GC  Inj. Volume : 1 μl
Sequence File : C:\HPChem\\SEQUENCE\DEF GC.S
Method : C:\HPChem\\METHODS\C105 S13.M
Last changed : 1/29/2014 2:05:32 PM by Chem 105
Chrom 105 Whiskey Method

=================================================================

Area Percent Report
=================================================================

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID2 E,

<table>
<thead>
<tr>
<th>Peak RetTime Type Width</th>
<th>Area</th>
<th>Height</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 3.544 MB 0.0488 2.1860364 5635.385849 98.27188</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>2 5.256 PP 0.0659 71.27694 12.53314 0.32042</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 7.000 BP 0.0646 53.27674 12.86520 0.23950</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 9.435 PB 0.1328 179.67223 18.72349 0.80771</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 14.898 PB 0.2312 60.19011 5.15182 0.35049</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Totals : 2.22447e4 5685.15306

Results obtained with enhanced integrator!

=================================================================

Summed Peaks Report

=================================================================

Signal 1: FID2 E,

Final Summed Peaks Report

=================================================================

Signal 1: FID2 E,

*** End of Report ***

Figure 7: GC/FID Report for 1000 ppm standard
Figure 8: GC/FID Report for Ethyl Acetate standard
Figure 9: GC/FID Report for 2-Methyl-1-Butanol standard
Figure 10: GC/FID Report for 1-Propanol standard
Figure 11: GC/FID Report for Jameson sample
Figure 12: GC/FID Report for Jim Beam sample