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SPECTRA OF THE MONTH

COMPARISON OF CHOCOLATE TYPES UTILIZING ABSORBANCE SPECTROSCOPY

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INTRO

BACKGROUND OF APPLICATION

Valentine's Day is one of the most popular holidays both nationally and globally. The holiday of romance as we know it began around the 14th century as a celebration of love and a time to give affectionate greetings and gifts, the most popular of which being beautiful-smelling flowers or sweet-tasting chocolates. While the term 'chocolate' includes a very broad category of sweets, the specifications of what defines certain chocolates can be very strict. Any chocolate defined as 'milk chocolate' must contain at least 12% milk and 10% chocolate liquor, which includes cocoa butter and cocoa solids. While this is the minimum, higher quality milk chocolates may contain as much as 30-40% cocoa. The remaining contents may be a combination of sugar, vanilla, emulsifiers, and other flavorings. White chocolate must contain at least 14% milk and 20% cocoa butter but contains no cocoa solids, which removes the fruity and bitter tastes associated with other chocolate types. Dark chocolate must contain at least 35% chocolate liquor, with this percentage often being closer to 60-70% and as high as the mid-90 percentages, and no milk, though trace amounts are usually present. While these chocolate variants an often be distinguished by their visible hue and their brittleness, the required content percentages mean they can also be identified by their molecular composition. This type of characterization can be done using many methods, including NIR spectroscopy.

FIGURE 1: Five chocolate samples and reference tile used for the experiment (from left to right: milk chocolate, cheap milk chocolate, white chocolate, dark chocolate with 78% cacao, dark chocolate with 92% cacao, and white reference tile

This experiment aims to measure differences between five different types of chocolate, including milk chocolate, cheap milk chocolate, white chocolate, dark chocolate with 78% cacao, and dark chocolate with 92% cacao (Figure 1). A white reference tile will be used as a reference material. Measurements will be taken in the near-infrared (NIR) spectral range to avoid trivial measurement differences such as color.

DESCRIPTION OF SPECTROSCOPY SETUP

The setup for this experiment (Figure 2) was based around the AvaSpec-NIR256-1.7-EVO. Specifically for measurements in the NIR range up to 1.7 µm, this model pairs our high-sensitivity optical bench with next generation electronics for exceptional performance, including 0.53 ms/scan sample speed and integration times as fast as 10 µs. The AvaSpec-NIR256-1.7-EVO is equipped with our trusted InGaAs (Indium-Gallium-Arsenide) array detector and our ultra low-noise electronics board with both USB3.0 and Giga-Ethernet connection ports onboard. Additional features include multiple grating and replaceable slit options, as well as digital and analog I/O ports, which can be used to control the shutter or pulse of connected light sources and the gain setting of the spectrometer, with either High Sensitivity or Low Noise.

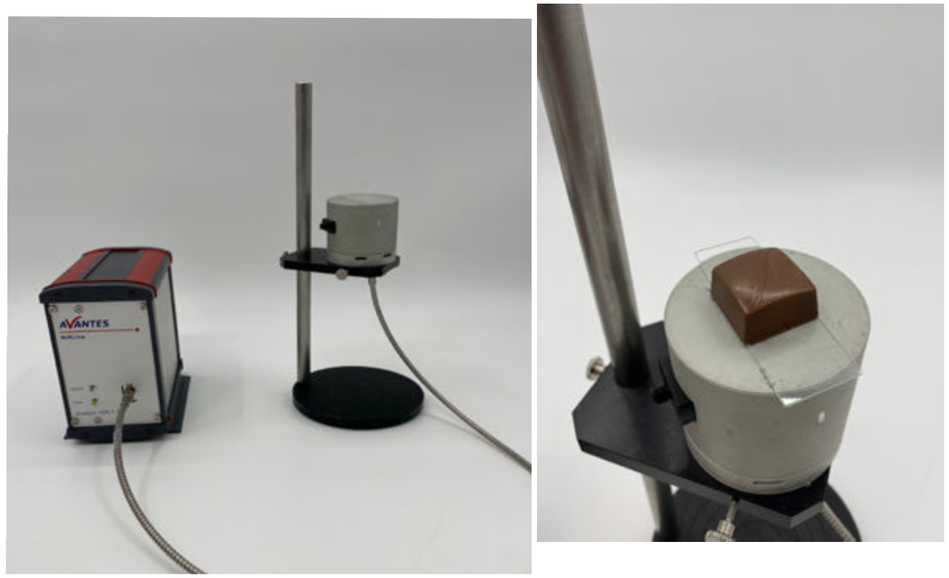

FIGURE 2 Spectroscopy setup (left). Close-up of the integrating sphere and chocolate sample (right).

The light source used for this experiment was a built-in halogen light in our AvaSphere-50-LS-HAL-12V integrating sphere. While specifically designed for reflection applications, this integrating sphere is also useful for low reflecting materials and NIR spectral measurements, where signal strength can be limited. The built-in halogen light source provides diffused halogen light on the sample without the losses associated with fiber-optic coupling, with up to 160 times more light on the sample compared to our standard reflectance integrating sphere. The AvaSphere-50-LS-HAL-12V has an internal diameter of 50 mm, a 10 mm sample port, an SMA-terminated reference port, and a direct collimated SMA-port for collection of the signal with any of our AvaSpec spectrometers.

Other accessories used for this experiment included a glass slide to separate the chocolate samples from the integrating sphere entrance, a white reference tile (WS-2) to compare each chocolate sample against, and a 600-micron core fiber optic cable (FC-UVIR600-1-BX) to connect the integrating sphere to the spectrometer.

DESCRIPTION OF METHODOLOGY

Each sample was a piece of chocolate broken from a larger chocolate bar except the cheap milk chocolate sample, which was its own piece of chocolate. Each sample was stored in a drawer in a room with a temperature around 70°F to ensure no melting or blooming occurred. When analyzed, each chocolate sample was individually placed on a glass slide that was then placed over the sample port of the integrating sphere (Figure 2). This glass slide prevented any small amount of chocolate from entering the integrating sphere and potentially contaminating the sphere. Additionally, this made measurement distance more consistent, which in turn resulted in more accurate comparisons between samples. The white reference tile was measured first to set our reference, and it was also placed on a glass slide to ensure consistency in measuring distance.

For data analysis, we used the absorbance mode in AvaSoft, our exclusive custom software package. This mode is specifically designed for absorbance applications, where the reference measurement will report 0 A.U. (absorbance units) and 5 A.U. when the light source is turned off. In this experiment, the white reference tile was used as the reference. We used an integration time of approximately 3 milliseconds, which can be adjusted to increase or decrease the amount of light being measured at one time and affects the overall magnitude of the reported spectrum. We set averaging to 100, meaning one hundred values were averaged together to provide more consistent spectra results. This high number of averages is more feasible when the integration time is lower.

TEST DATA AND RESULTS

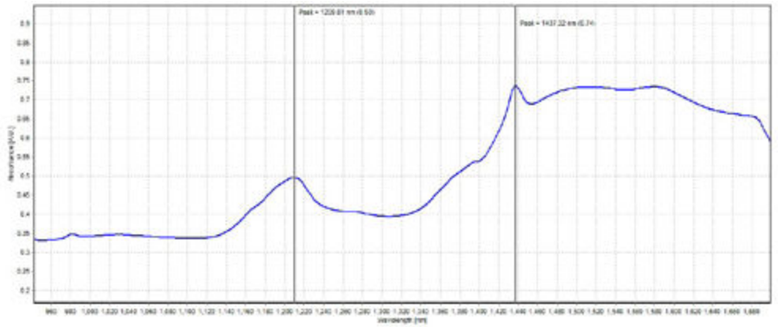

FIGURE 3: Absorbance spectrum of milk chocolate sample (peaks at 1209.81 nm and 1437.32 nm with magnitudes of 0.50 A.U. and 0.74 A.U., respectively).

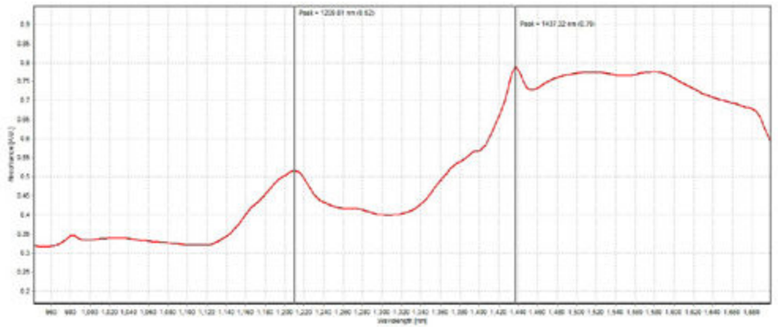

FIGURE 4: Absorbance spectrum of cheap milk chocolate sample peaks at 1209.81 nm and 1437.32 nm with magnitudes of 0.52 A.U. and 0.79 A.U., respectively).

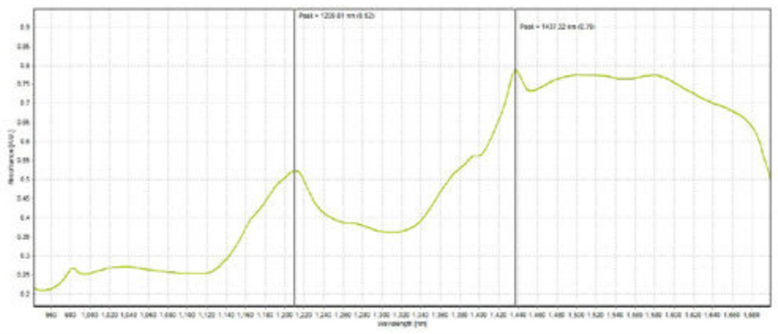

FIGURE 5: Absorbance spectrum of white chocolate sample (peaks at 1209.81 nm and 1437.32 nm with magnitudes of 0.52 A.U. and 0.79 A.U., respectively).

TEST DATA AND RESULTS

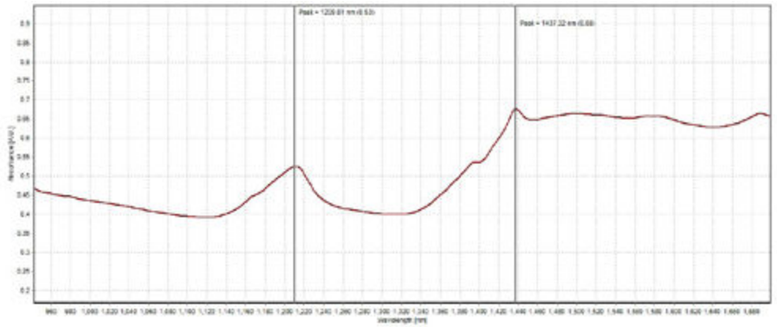

FIGURE 6: Absorbance spectrum of dark chocolate sample with 78% cacao (peaks at 1209.81 nm and 1437.32 nm with magnitudes of 0.53 A.U. and 0.68 A.U., respectively).

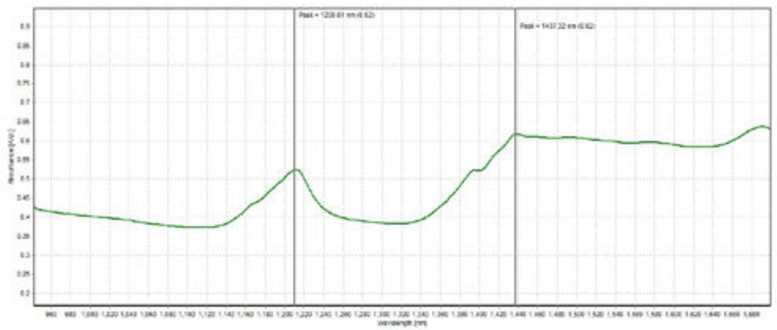

FIGURE 7: Spectrum of dark chocolate sample with 92% cacao (peaks at 1128.26 nm and 1322.60 nm with magnitudes of 34303.70 counts and 48289.00 counts, respectively).

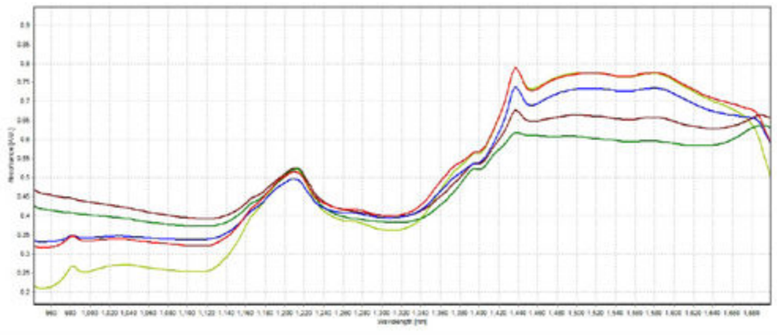

FIGURE 8: Absorbance spectra of milk chocolate sample (blue), cheap milk chocolate sample (red), white chocolate sample (light green), dark chocolate sample with 78% cacao (dark red), and dark chocolate sample with 92% cacao (dark green), shown together for comparison.

TEST DATA ANALYSIS

The absorbance spectra for all chocolate samples had measured peaks at 1209.81 nm and 1437.32 nm. The milk chocolate sample had absorbance values of 0.50 A.U. and 0.74 A.U. at each respective peak (Figure 3). The cheap milk chocolate sample had absorbance values of 0.52 A.U. and 0.79 A.U. at each respective peak (Figure 4). The white chocolate sample had absorbance values of 0.52 A.U. and 0.79 A.U. at each respective peak (Figure 5). The dark chocolate sample with 78% cacao had absorbance values of 0.53 A.U. and 0.68 A.U. at each respective peak (Figure 6). The dark chocolate sample with 92% cacao had absorbance values of 0.52 A.U. and 0.62 A.U. at each respective peak (Figure 7). A plot of all five spectra is also provided to illustrate the differences in peak intensity (Figure 8).

For the peak at 1209.81 nm, the dark chocolate sample with 78% cacao reported the highest absorbance value, followed by the dark chocolate sample with 92% cacao, the white chocolate sample, and the cheap milk chocolate sample. The milk chocolate sample had the absorbance value at this wavelength. It is not apparent what this peak is indicating without more complex analysis, though the second peak seen at 1437.32 nm may be more clear. At this peak, the white chocolate and cheap milk chocolate samples have the highest absorbance values, the milk chocolate sample has the next highest absorbance value, followed by the dark chocolate sample with 78% cacao, and ending with the dark chocolate sample with 92% cacao having the lowest absorbance value at this peak. Based on this relation, it could be hypothesized that this peak is an indicator of sugar content. Averaged for a 28g serving, the white chocolate has 15g of sugar, the cheap milk chocolate has 16g, the milk chocolate has 12g, the dark chocolate with 78% cacao has 5g, and the dark chocolate with 92% cacao has 2g of sugar. This is just one idea, as similar trends could be drawn from other ingredients such as milk solids and other added flavorings. As with the first observed peak, more complex analysis, such as chemometrics, could verify this hypothesis.

CONCLUSION

In conclusion, the present experiment highlights the differences that can be observed between different types of chocolate using NIR spectroscopy, though further analysis must be used to fully interpret and quantify these measured differences. The AvaSpec-NIR256-1.7-EVO is a highly versatile NIR spectrometer with plenty of available options to match the bandwidth and requirements fitting your application. The AvaSphere-50-LS-HAL-12V is specifically designed for reflectance measurements but is effective for any applications where limited signal strength may be an issue, such as NIR spectral measurements. Please contact Avantes for more information on the configuration that is best suited for your data collection.

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