Application Note AN-RS-052

Assessment of chocolate with Raman spectroscopy

Rapid quality control of different chocolate types

In 2024, the global chocolate market was valued at approximately $131 billion USD. It is projected to reach approximately $173 billion by 2030, implying a steady growth rate of roughly 4% [1]. This growth is driven by sustained consumer demand and is expected to continue rising.

Spectroscopy is increasingly utilized in chocolate manufacturing for quality control (QC), thanks to its ability to assess the composition of chocolate, providing a «fingerprint» spectrum that reveals its chemical details. Specifically, Raman can be used in QC to distinguish between types of chocolate, detect adulteration, measure crystallization and texture, and monitor the manufacturing process.

This Application Note outlines techniques for effectively collecting Raman spectra from various chocolates, providing a foundation for quality assessment and adulteration detection.

Raman spectra of chocolate bars with different cocoa content, including white chocolate (Lindt, Switzerland), were measured at a low (5%) laser power and long (120 s) integration time (Figure 1).

Specific chocolate sample types used in this study are summarized in Table 1. Laser power was adjusted based on the chocolate's cocoa content (ranging from white to 100%), not to exceed 15%, unless molten chocolate measurement was desired.

Table 1. Samples and important Raman peaks.

Sample	% Cocoa
Chocolate (various types)	100%
	85%
	70%
	Milk (~30%)
	White (20%)

EXPERIMENTAL OVERVIEW

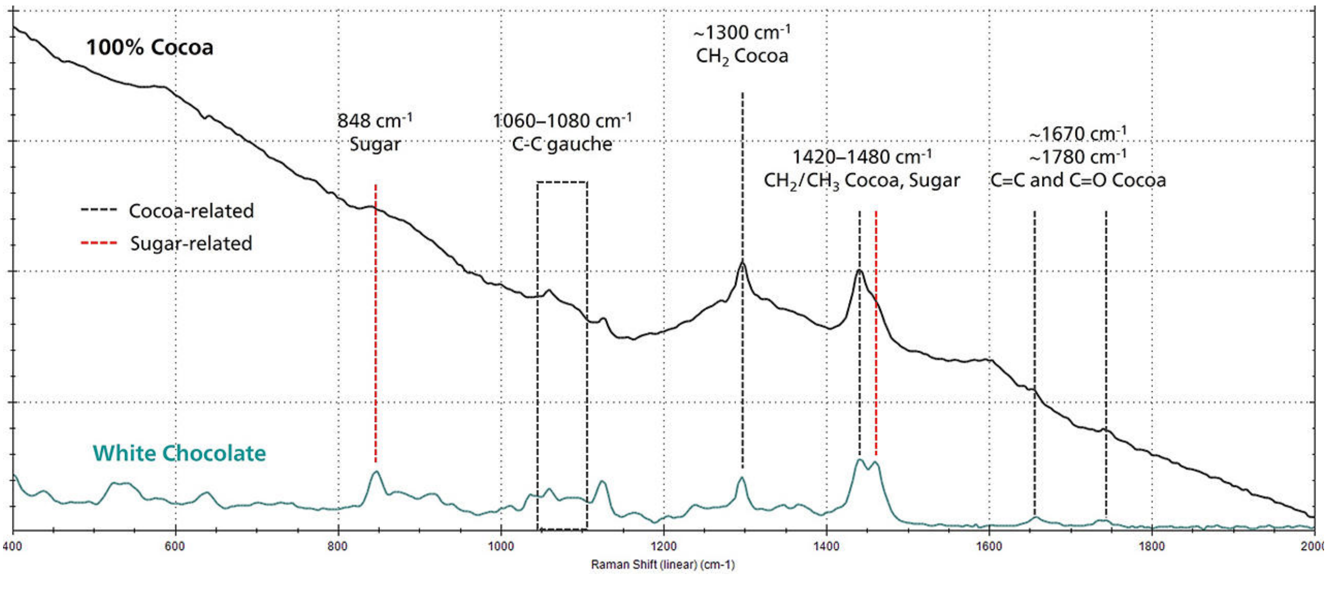

Figure 1. Representative Raman spectra of 100% cocoa and white chocolate (no math treatment).

Table 2. List of important peaks shown in Figure 1.*

Relation	Wavenumber (cm^{-1})
Cocoa-related	1060–1080
	~1300
	1420–1480
	~1670, ~1780
Sugar-related	<750, 848
	1460

METHOD

Raman data collection with an i-Raman NxG 1064 laboratory Raman system (Figure 2) was optimized by adjusting integration time and laser power (Table 3) to determine the best conditions to maximize signal strength and minimize risk of sample melting.

Figure 2. The i-Raman NxG 1064 and mounted fiber-optic probe from Metrohm were used in this study.

Table 3. System settings used for the analysis of different chocolate types by Raman spectroscopy.

Excitation wavelength	1064 nm
Laser power	5–15%
Integration time	>60 s
Accessories	Standard Sampling Probe Probe Holder with distance regulator
Software	SpecSuite

All chocolate samples were analyzed by placing a piece of chocolate on the stage with a Raman probe securely locked above the sample (Figure 3). The optimal working distance was determined by adjusting the probe's z-axis position while continuously monitoring the intensity of the Raman signal.
Once the optimal focal distance is found, a distance regulator helps the operator position the probe on the sample to ensure consistent and reliable measurement.

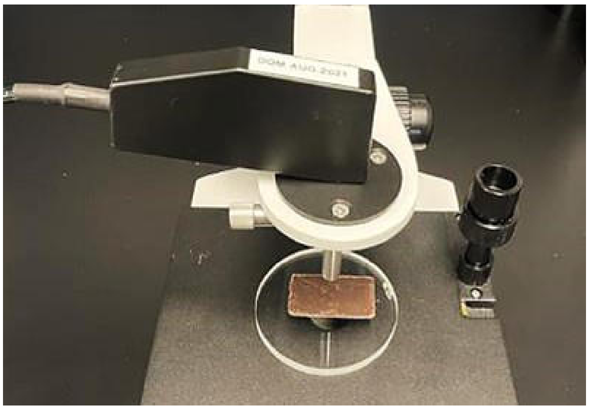

Figure 3. A chocolate sample on the probe holder.

RESULTS

Laser intensity and melting

Chocolate melts between 30–36 °C. 100% chocolate was used to establish the laser-induced melting threshold due to its darker color. The darker sample absorbs more laser light and, as a result, melts at lower powers and shorter exposure times.
Optimizing laser power is critical to prevent thermal damage or structural changes during measurement. Raman spectra collected at 5%, 10%, and 15% laser power revealed notable shifts in cocoa-related peaks (Figure 4a), with visible melting at 10%. Lighter-colored chocolates tolerated higher powers, generally up to 15%.

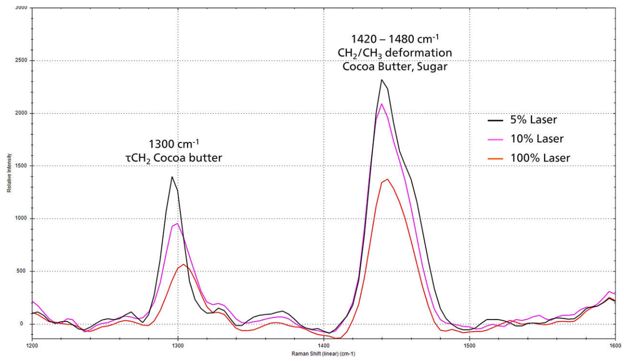

Figure 4a. Close-up view of Raman peaks from 100% chocolate measured with 1064 nm laser at 5%, 10%, and 15% laser power.

However, melting is not the sole indicator of heat-induced structural changes. Even white chocolate exhibited subtle crystallinity shifts in the 1060–1100 cm–1 range when laser power exceeded 10% (Figure 4b). These results highlight that chocolate can undergo thermal alteration at relatively low laser powers, emphasizing the need for careful power selection during quality assurance and quality control (QA/QC). Fluorescence rejection methods combined with lower-power 785 nm excitation offer potential solutions.

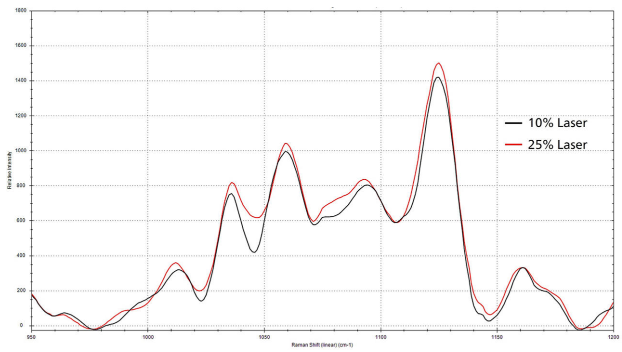

Figure 4b. White chocolate's gauche chain extension region measured with 10% and 25% laser power, demonstrating the difference between laser powers.

Chocolate generally consists of three primary components—cacao solids, cocoa butter, and sugar—in significantly different proportions, depending on the chocolate type. For instance, 100% chocolate contains no added sugar, whereas white chocolate lacks any cacao solids, but does contain cocoa butter. The other varieties fall between these extremes, with different cocoa and sugar content (Table 4).

Table 4. Cocoa and sugar content of different chocolates.

Chocolate Type	Cocoa (%)*	Sugar (g)**
White	20	16
Milk	31	17
70%	70	9
85%	85	4
100%	100	0

The major sugar peaks are clearly observed in white, milk, and 70% chocolates (Figure 5). However, in 85% chocolate, the only noticeable sugar-related spectral feature appears at 1460 cm–1. This suggests that Raman effectively determines sugar content for QC measurements. Cocoa-related ingredients exhibit characteristic Raman bands around 1300 cm–1 and 1420–1480 cm–1. Confining a Partial Least Squares (PLS) model to these spectral regions resulted in the most accurate predictive model for cocoa content analysis.

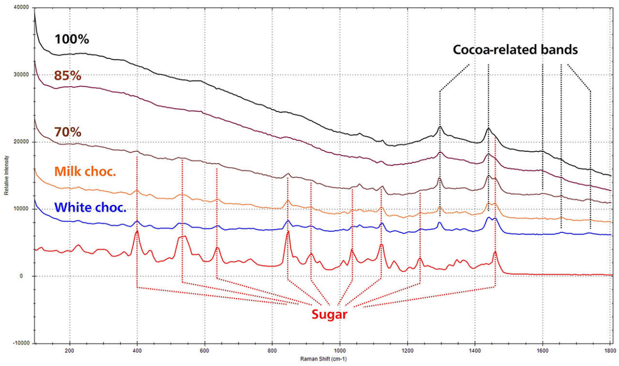

Figure 5. Raman spectra of 100% cocoa, 85% cocoa, 70% cocoa, milk chocolate, white chocolate, and sugar. Data collection method: laser power 5%, integration time 120 s, average 3.

PLS model performance and predictive accuracy

PLS models built from key peaks between 1200–1600 cm−1 in the Raman spectra of various chocolate types show strong agreement between predicted and measured cocoa content, with low standard error. This confirms Raman spectroscopy's effectiveness for routine cocoa content analysis (Figure 6a). Adding data points would enhance confidence in predictions at higher cocoa levels.

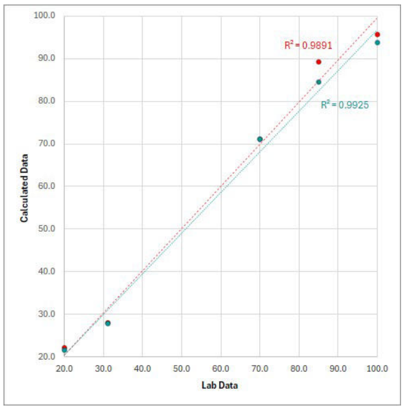

Figure 6a. PLS calibration model and model statistics of cacao solids and cocoa butter.

The sugar content model demonstrates even greater predictive accuracy, attributed to distinct sugar peaks and the lack of temperature-related variation in sugar measurements. Sugar data may also refine predictions of cocoa-related content, as sugar's Raman intensity varies proportionally with cocoa content (Figure 6b). Both sugar and cocoa content are important QC parameters measurable via Raman spectroscopy.

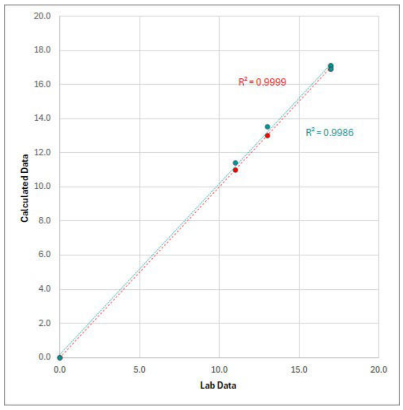

Figure 6b. PLS calibration model and model statistics of sugar content in different samples.

CONCLUSION

This study highlights the capability of Raman spectroscopy for rapid, nondestructive measurements of chocolate quality indicators. PLS models demonstrate high predictive accuracy for both cocoa-related materials and sugar content. Increasing the number of samples and testing a broader range of chocolates would further improve the robustness and accuracy of the model.

Overall, Raman spectroscopy, combined with chemometric modeling, offers a reliable QC method for routine and real-time chocolate analysis.

REFERENCES

1. marknteladvisors. *Chocolate Market Size, Share, Analysis and Industry Trend to 2030*.
2. Esmonde-White, K.; Lewis, M.; Lewis, I. R. Direct Measurement of Chocolate Components Using Dispersive Raman Spectroscopy at 1000 Nm Excitation. *Appl Spectrosc* **2023**, *77* (3), 320–326. https://doi.org/10.1177/00037028221147941.
3. *Chocolates, Truffles, and Delicious Gifts: Buy Online | Lindt Shop Intl.* https://www.chocolate.lindt.com/ (accessed 2025-08-17).

CONTACT

Metrohm UK & Ireland
Evenwood Close
WA71LZ Runcorn

info@metrohm.co.uk

CONFIGURATION

i-Raman NxG 1064

The i-Raman NxG 1064 is a high-performance Raman spectrometer purpose-built for the most challenging and complex sample types. Featuring a 1064 nm laser and a wide spectral range of 100–2500 cm−1, it excels at dramatically reducing fluorescence interference, making it ideal for analysis of highly fluorescent, brightly colored, or natural products that are problematic for conventional Raman systems.

This advanced capability enables rapid, accurate measurements, even with challenging samples often found in pharmaceuticals, nutraceuticals, and petroleum sectors. Its versatile setup—including the ability to perform see-through measurements through opaque containers - delivers excellent results in rigorous quality control processes where suppressing fluorescence is essential.

The i-Raman NxG 1064 is the preferred choice for users who need reliable, fluorescence-free Raman analysis of challenging quality control samples.

Discover how this near-infrared laser helps you make the most challenging quality control measurements:

- High-sensitivity spectrometers deliver results in seconds and can detect the weakest Raman signals.
- Near-IR laser measures highly colored and dark samples with ease.
- Flexible fiber optic probe compatible with a wide array of accessories including a vial holder, cuvette holder, immersion probe, and see-through adapter.
- Powerful SpecSuite software for easy Raman data collection in addition to quantitative model building, identification with spectral libraries, and routine analysis.
- Compact and stackable to save on valuable bench space.

Universal Raman Probe Holder

Probe holder for use with Metrohm's lab-grade Raman probes, including lab-grade shafts, industrial-grade immersion shafts, and see-through shafts. Provides manual coarse and fine XYZ adjustments.