



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

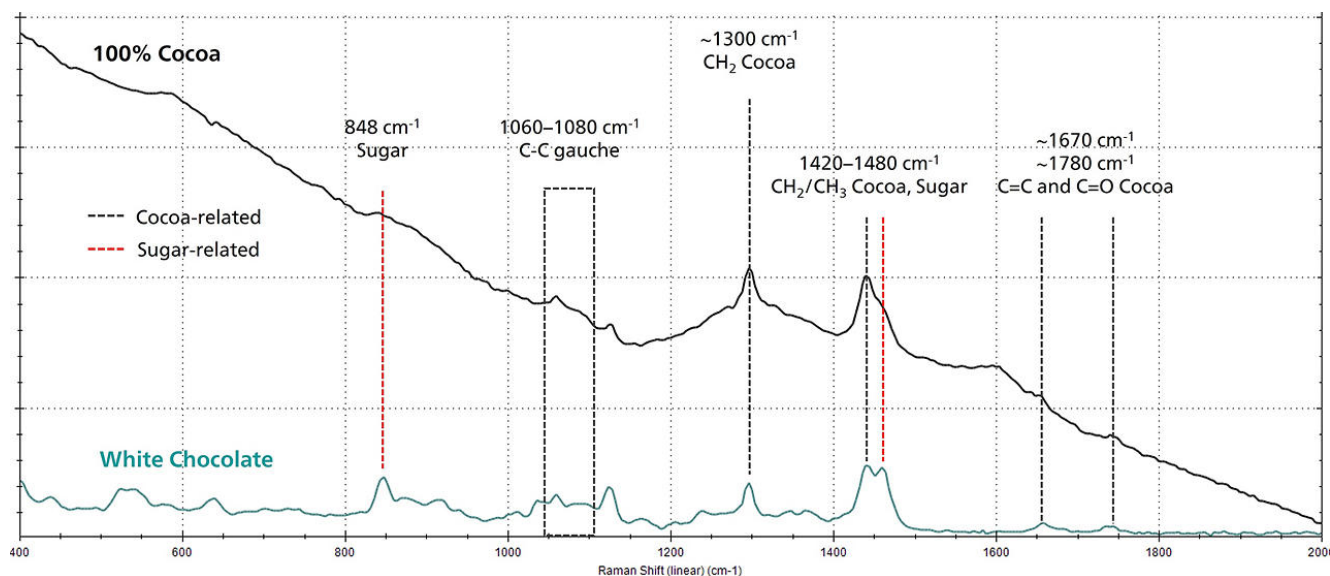


Figure 1. Representative Raman spectra of 100% cocoa and white chocolate (no math treatment).

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%.

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.

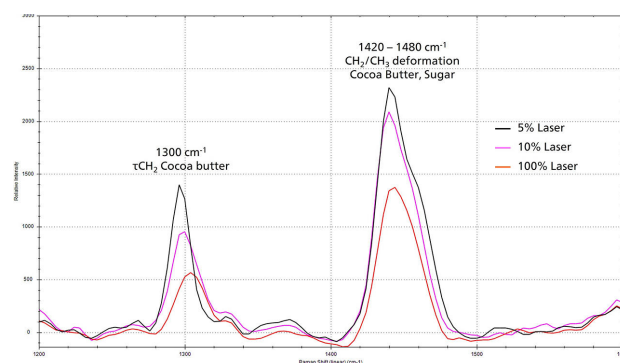


Figure 4a. Close-up view of Raman peaks from 100% chocolate measured with 1064 nm laser at 5%, 10%, and 15% laser power.

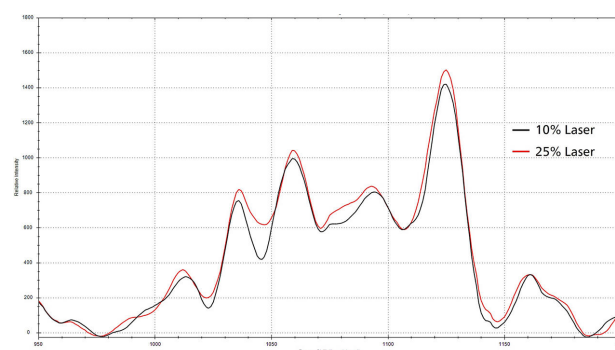


Figure 4b. White chocolate's gauche chain extension region measured with 10% and 25% laser power, demonstrating the difference between laser powers.

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.

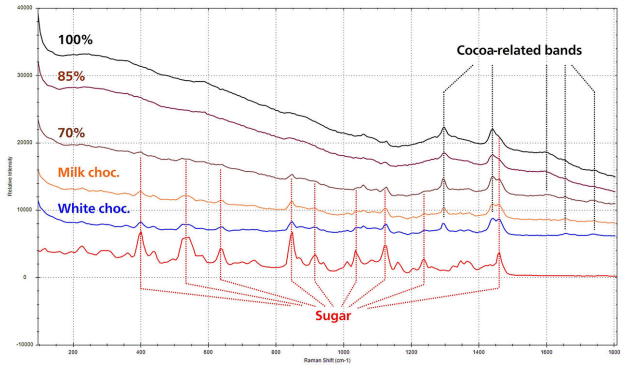


Figure 5. Raman spectra of 100% cocoa, 85% cocoa, 70% cocoa, milk chocolate, white chocolate, and sugar. Data collection method: laser power 5%, integration time 120 s, average 3.

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.

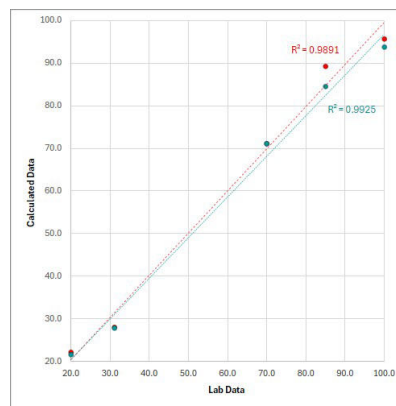


Figure 6a. PLS calibration model and model statistics of cacao solids and cocoa butter.

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.

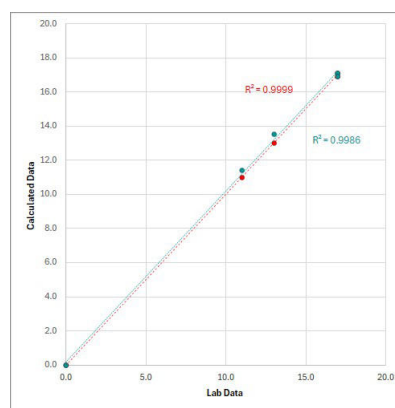


Figure 6b. PLS calibration model and model statistics of sugar content in different samples.

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

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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.
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3. *Chocolates, Truffles, and Delicious Gifts: Buy Online | Lindt Shop Intl.*
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i-Raman NxG 1064

i-Raman NxG 1064は、最も分析が困難で複雑なサンプルタイプ向けに特別に設計された高性能ラマン分光計です。1064 nmレーザーと100~2500 cm⁻¹の広いスペクトル範囲を備え、蛍光の妨害の影響を大幅に低減します。そのため、従来のラマンシステムでは分析が困難な、蛍光強度の高い、鮮やかな色をした、あるいは天然物の分析に最適です。

この高度な機能により、医薬品、栄養補助食品、石油分野でよく見られる難しいサンプルでも、迅速かつ正確な寸法が可能になります。不透明なキャニスターを通しての透過寸法も可能なその多用途なセットアップにより、蛍光の抑制が不可欠な厳格な品質コントロールプロセスで優れた結果が得られます。

i-Raman NxG 1064は、難しい品質コントロールサンプルに対して信頼性の高い蛍光フリーのラマン分析を必要とするユーザーにとって最適な選択肢です。

この近赤外線レーザーが、最も困難な品質コントロール寸法にどのように役立つかをご覧ください：

- 高感度分光計は数秒で結果を提供し、最も弱いラマン信号も検出できます。
- 近赤外線レーザーは色の濃いサンプルや暗いサンプルも簡単に測定します。
- バイアルホルダー、キュベットホルダー、浸漬プローブ、透過アダプターなど、さまざまな付属品と互換性のある柔軟なグラスファイバープローブです。
- 強力なSpecSuiteソフトウェアは、定量モデルの構築、スペクトルライブラリによる識別、日常的な分析に加えて、ラマンデータの収集を容易にします。
- コンパクトで積み重ね可能なので貴重なベンチスペースを節約できます。



ラボグレードのシャフト、産業用グレードの浸漬シャフト、透過シャフトを含む Metrohm のラボグレードラマンプローブとともに使用するためのプローブホルダーです。XYZの粗調整および微調整を手動で行うことができます。