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

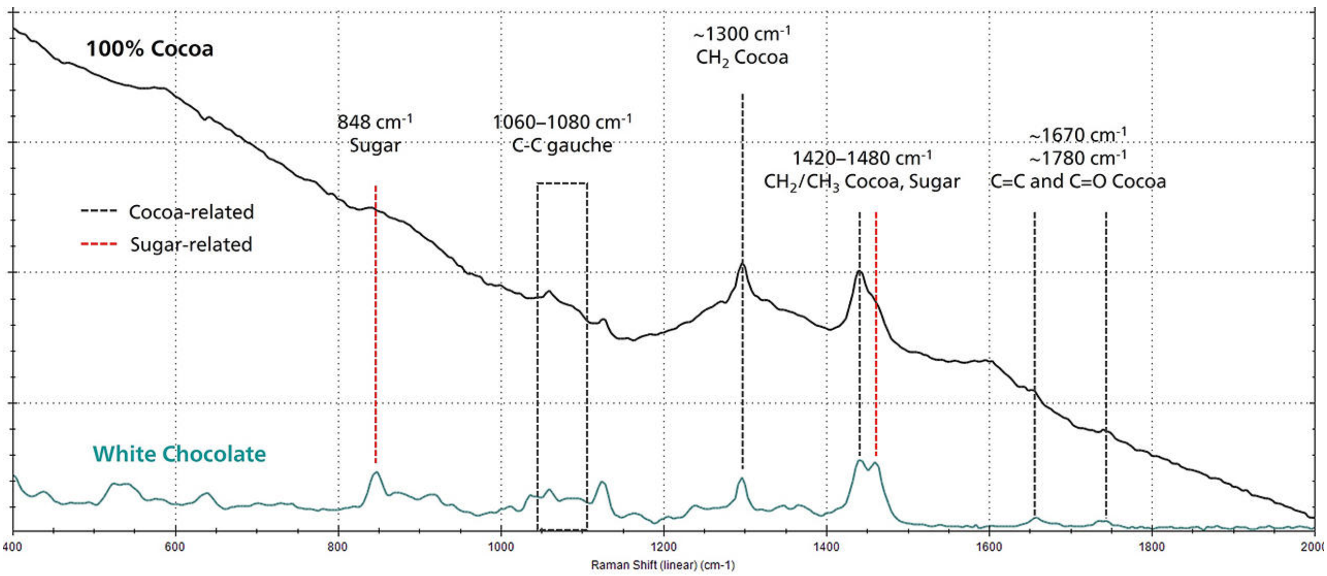

Figure 1. Representative Raman spectra of 100% cocoa and white chocolate (no math treatment).

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.

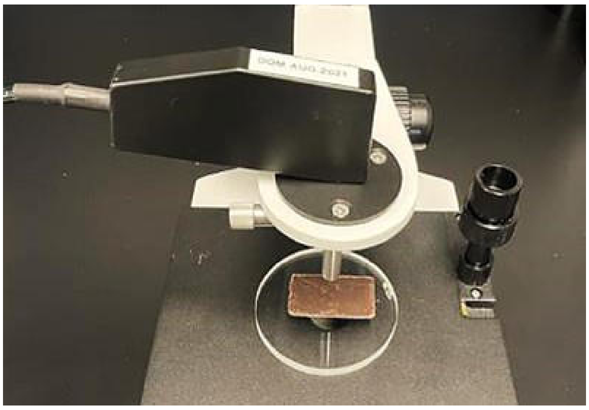

Figure 3. A chocolate sample on the probe holder.

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%.

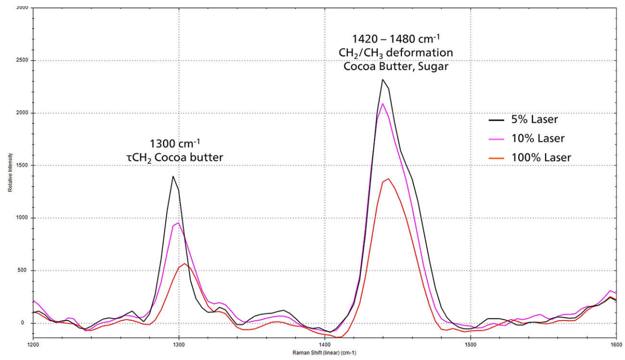

Figure 4a. Close-up view of Raman peaks from 100% chocolate measured with 1064 nm laser at 5%, 10%, and 15% laser power.

However, melting is not the sole indicator of heat-induced structural changes. Even white chocolate exhibited subtle crystallinity shifts in the 1060–1100 cm1 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.

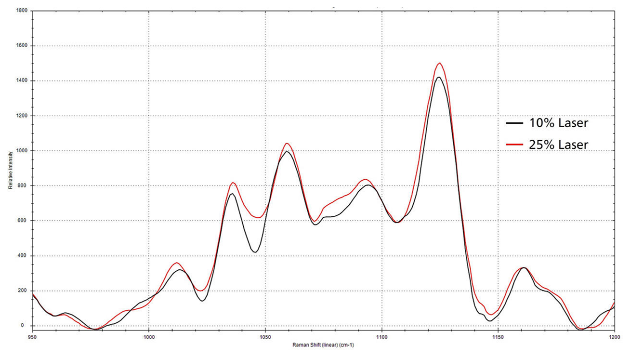

Figure 4b. White chocolate's gauche chain extension region measured with 10% and 25% laser power, demonstrating the difference between laser powers.

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 cm1. This suggests that Raman effectively determines sugar content for QC measurements. Cocoa-related ingredients exhibit characteristic Raman bands around 1300 cm1 and 1420–1480 cm1. Confining a Partial Least Squares (PLS) model to these spectral regions resulted in the most accurate predictive model for cocoa content analysis.

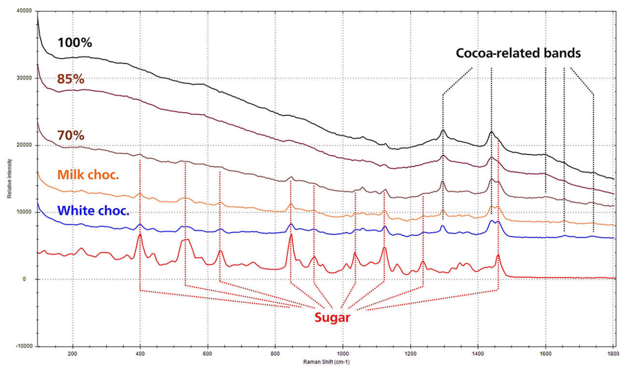

Figure 5. Raman spectra of 100% cocoa, 85% cocoa, 70% cocoa, milk chocolate, white chocolate, and sugar. Data collection method: laser power 5%, integration time 120 s, average 3.

PLS model performance and predictive accuracy

PLS models built from key peaks between 1200–1600 cm1 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.

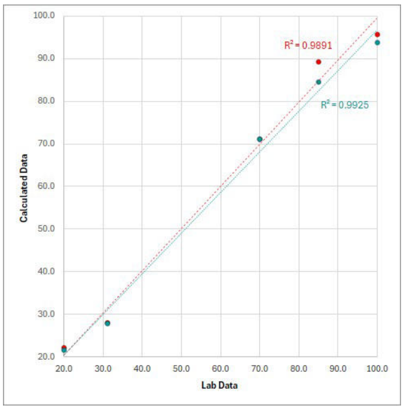

Figure 6a. PLS calibration model and model statistics of cacao solids and cocoa butter.

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.

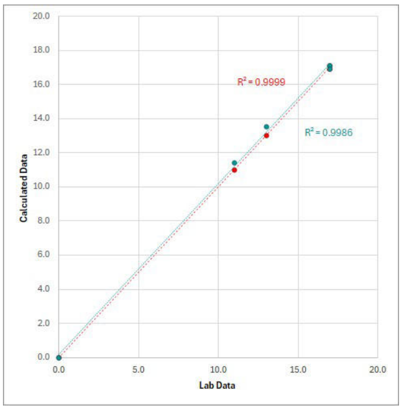

Figure 6b. PLS calibration model and model statistics of sugar content in different samples.

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).

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CONFIGURATION

i-Raman NxG 1064

i-Raman NxG 1064 是一款高性能 Raman 光谱仪,专为应对最具挑战性和最复杂的样品类型而设计。它采用 1064 nm 激光器,拥有 100-2500 cm1 的宽光谱范围,其卓越之处在于能显著减弱荧光干扰,因此非常适合分析高荧光、色泽鲜艳的样品或天然产物,这些样品通常会给常规 Raman 系统带来困扰。

这一先进技术能够实现快速、精确的测量,即使对于制药、保健品和石油行业中常见的复杂样品也不例外。其多功能配置(包括能够透过不透明容器进行透射测量)可在那些必须抑制荧光的严格质量控制流程中提供卓越的结果。

i-Raman NxG 1064 是需对复杂质控样品进行可靠、无荧光 Raman 分析的用户的最佳选择。

了解这款近红外激光器何以助您应对最具挑战性的质控测量:

- 高灵敏度光谱仪可在数秒内输出结果,并能检测到最微弱的 Raman 信号。
- 近红外激光器可轻松测量深色与高着色度样品。
- 可与包括小管支架、比色皿支架、浸入式探头和透射适配器在内的多种附件兼容的柔性光纤探头。
- 功能强大的 SpecSuite 软件,不仅便于轻松采集 Raman 数据,还可用于建立量化模型、进行谱库识别以及执行常规分析。
- 结构紧凑,可堆叠设计,有效节省宝贵的实验台空间。

与 Metrohm 实验室级拉曼探头(包括实验室级探头杆、工业级浸入式探头杆和透视探头杆)配合使用的探头支架。提供手动 XYZ 轴粗调和细调功能。