Application Note 410000019-B

拉曼光法定受染白酒中甲醇的含量

保消者免受受染料的危害

一个令人担的全球凸了入非法造的酒精可能造成的重危害。用工溶(即木醇)制并作酒精料的家用蒸酒通常含有甲醇。成分会致失明,入后会致死亡。在多个大洲造成了致命的后果[1-3]。
捷克共和国的折点出在2012年9月。在20人因食用甲醇含量危的烈酒而死亡后,烈性酒的售被禁止[2]。在使用不同的工具行了尽的研究后,捷克共和国拉曼光法作定和定量受染烈酒中甲醇的方法。
本用告了拉曼光是用的理想的原因,并展示了甲醇朗姆酒拉曼分析的真例子。

INTRODUCTION

Raman spectroscopy is a fast and easy analytical tool for quantifying the amount of methanol contamination present in alcoholic beverages. It is an ideal method for the discrimination of very similar molecules like ethanol (CH_3CH_2OH) and methanol (CH_3OH), as shown in **Figure 1**.

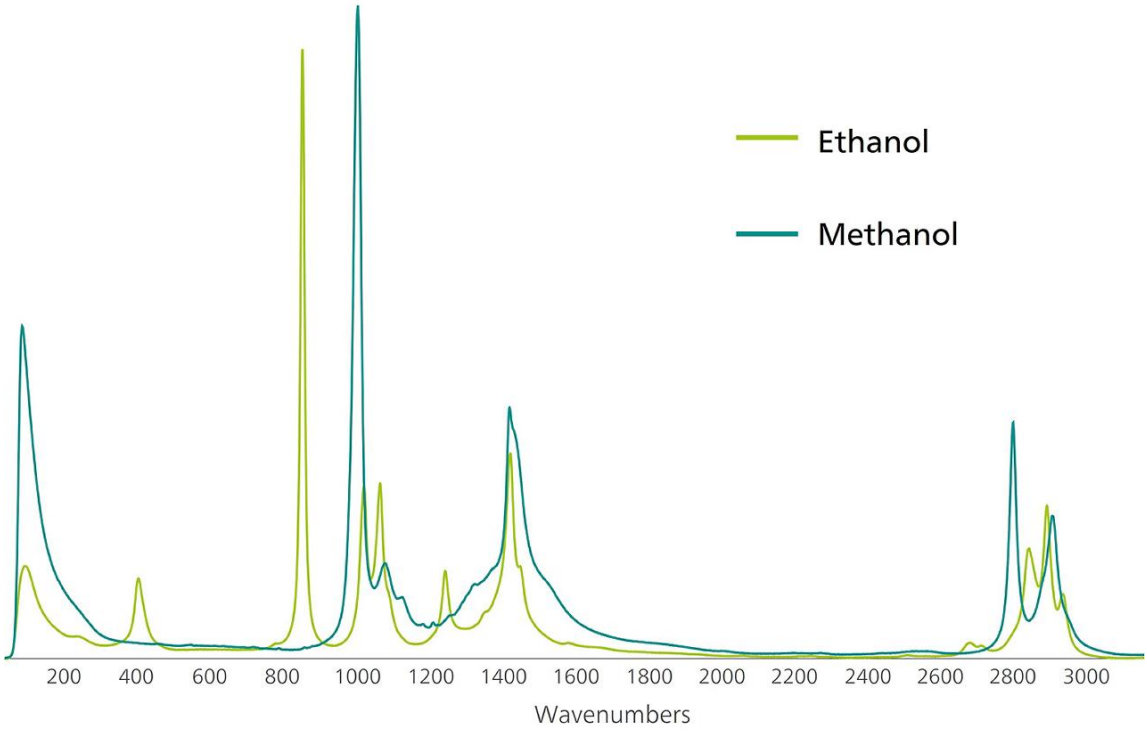
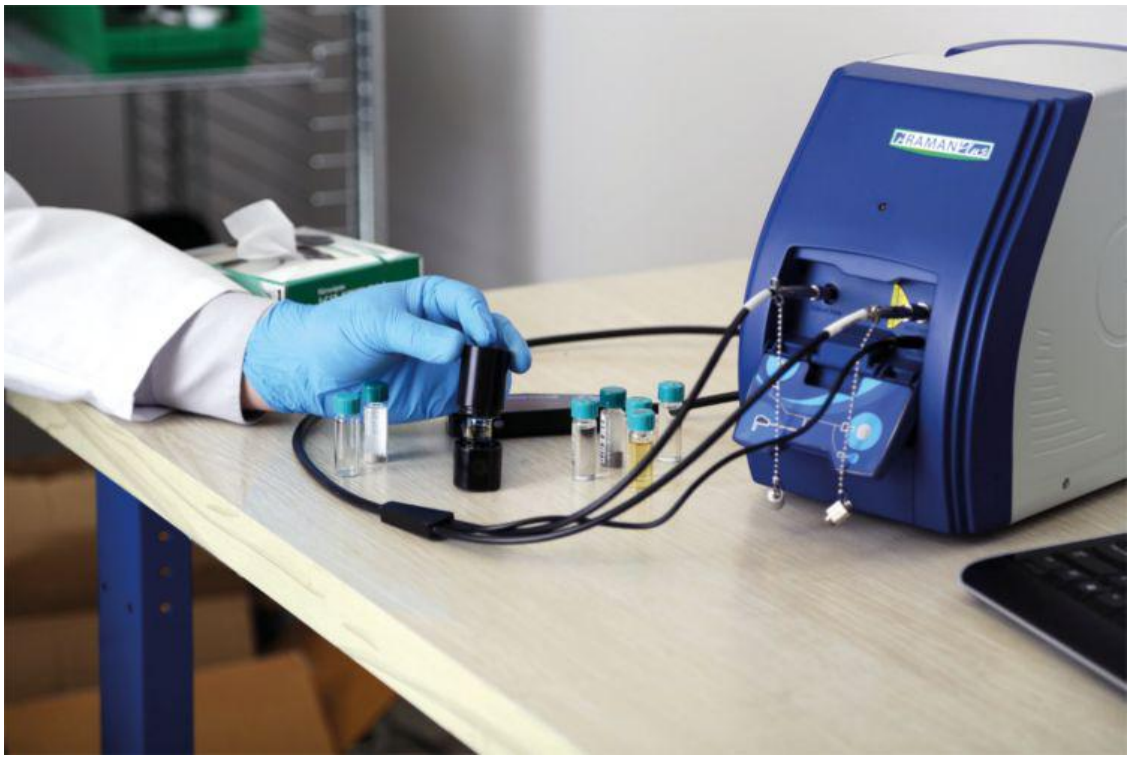


Figure 1. Raman spectra of pure ethanol (green) and pure methanol (blue).

Raman spectroscopy is superior to comparative technologies such as infrared spectroscopy (e.g., FTIR) because of its:

- ability to measure through optically transparent containers
- insensitivity to interference from water

These two key properties enable accurate detection of methanol down to approximately 1% by volume in the field with no need to open the bottles being tested.



EXPERIMENT

An in-house study measured commercially available coconut rum that was spiked with methanol in concentrations between 0.33% and 5.36%. The i-Raman® Plus, a sensitive high resolution laboratory system with a fiber-optic probe, was used to collect Raman spectra of the mixtures, shown in **Figure 2**. **Table 1** lists the relevant equipment and instrument settings used for this application study.

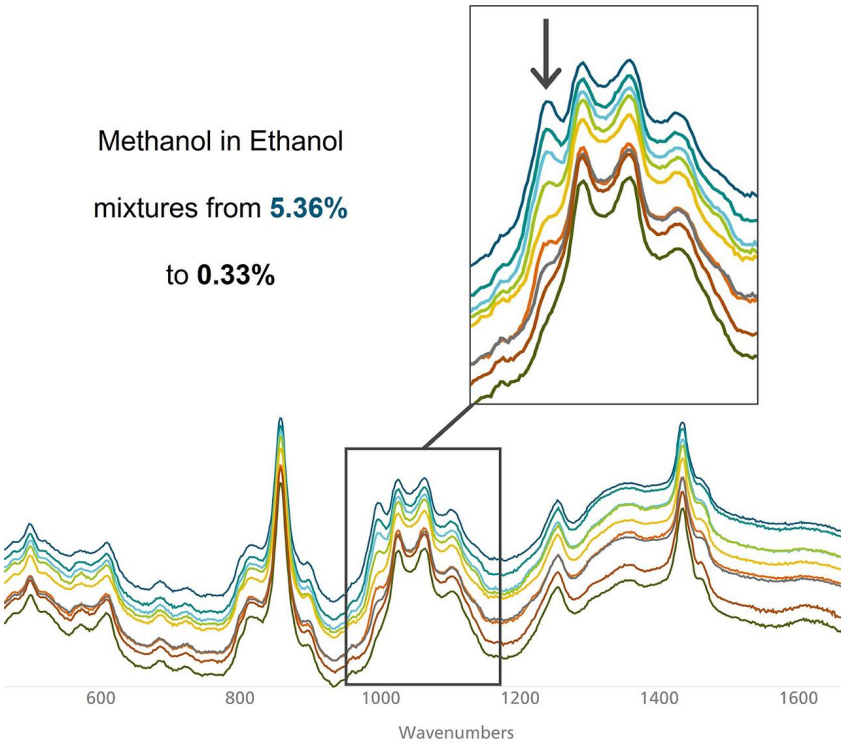


Figure 2. Raman spectra of methanol-laced rum with varying concentrations of methanol. Inlay: The peak noted with the arrow grows with increasing concentration of methanol.

The peak at around 1000 cm^{-1} visibly increases with increasing concentration of methanol, becoming significant at approximately 1%.

Table 1. Experimental parameters.

Equipment	Acquisition settings	
i-Raman Plus 785S	Laser Power	100
Vial holder (NR-LVH)	Int. time	20s
Vision Software	Average	1

This data was analyzed with Vision software, and a partial least squares (PLS) regression model was developed on normalized data. The two-factor model developed over the range from 920–1580 cm^{-1} gave the calibration curve shown in **Figure 3**, which has a root mean square error of cross-validation (RMSECV) of 0.1069 (**Table 2**). The R^2 value of 0.9977 shown in **Table 2** means that the Raman method used here can be used to confidently quantify the amount of methanol in a mixed alcohol sample.

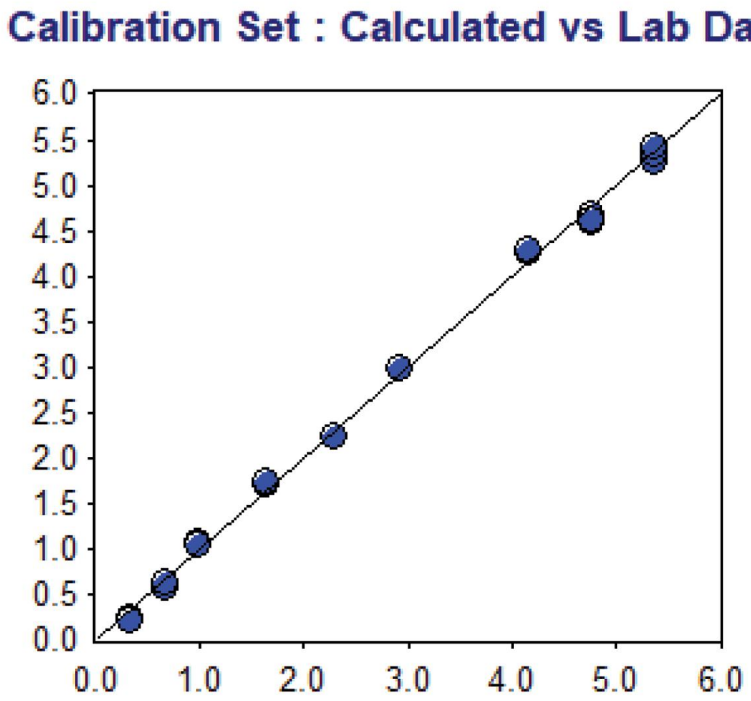


Figure 3. PLS regression model to predict the amount of methanol in rum.

Table 2. Regression parameters used for the development of the PLS model to determine methanol in rum with the i-Raman Plus 785S.

Parameter	Value
Spectral processing	Standard Normal Variate Savitzky-Golay derivative
R^2	0.9977
RMSEC	0.0976
RMSECV	0.1069

CONCLUSION

These results verify that Raman can be used for rapid, quantitative screening of dangerous adulterants in alcoholic beverages that pose a public safety risk. This technique can be expanded to investigate adulteration in other media such as food, petroleum, and pharmaceutical drugs [4].

REFERENCES

1. Lachenmeier, D. W.; Schoeberl, K.; Kanteres, F.; Is Contaminated Unrecorded Alcohol a Health Problem in the European Union? A Review of Existing and Methodological Outline for Future Studies. *Addiction* **2011**, *106* (s1), 20–30. https://doi.org/10.1111/j.1360-0443.2010.03322.x.
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4. Gryniewicz-Ruzicka, C. M.; Arzhantsev, S.; Pelster, L. N.; et al. Multivariate Calibration and Instrument Standardization for the Rapid Detection of Diethylene Glycol in Glycerin by Raman Spectroscopy. *Appl Spectrosc* **2011**, *65* (3), 334–341. https://doi.org/10.1366/10-05976.

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CONFIGURATION

i-Raman Plus 785S

i-Raman® Plus 785S 是我屡殊的 i-Raman 便携式拉曼光系列的一部分,其采用我新的智能光技。款便携式拉曼光使用了具有高量子效率、TE 冷却功能和高范的 CCD 列器,即使集成 30 分,也能提供出色的低噪声性能。因此,可以量弱的拉曼信号。

i-Raman Plus 785S 具有光范和高分辨率的独特合,其配置允在 65 cm^{-1} 至 3350 cm^{-1} 之行量。 系基面小,形式巧并且能耗低,故此可随随地行研究的拉曼分析。 i-Raman Plus 配有便于采的光探,并可以与一个比色皿支架、一个微、一个探支架的 XYZ 平移台、我公司内部的 BWIQ® 多量分析件和定件 BWID® 搭配使用。有了 i-Raman Plus,始可以使用高精度拉曼解决方案行定性和定量分析。

小管支架的配器，用于室量的拉曼探BAC100/BAC102,杆径 9.5 mm。与直径 15 mm 的小管兼容。一包有 6 个硼硅酸玻璃材的小管（15 mm)。

Vision 4.1

Vision 是一数据采集和方法件解决方案,用于 B&W Tek 便携式拉曼器、Metrohm XDS 室和程 NIRS 器的光分析和控制。用友好的形分析界面支持化学量学算法的用,以建、定和定量方法并行它。借助 Vision,可以存、管理、重新理和交数据。