

# Opadry verification using a handheld Raman analyzer

## Build custom PCA method for complex materials analysis

### Key Words

Qualitative analysis, Raman spectroscopy, PCA, pharmaceutical manufacturing, chemometrics, Opadry, tablet film coating

### Introduction

Pharmaceutical companies that manufacture tablets, capsules and other solid dosage forms use a film coating on their products to differentiate visual appearance, to improve the ability to swallow and to mask objectionable tastes or odors. Film coatings also reduce tablet breakage and chipping as well as provide protection from light, moisture and environmental gases.

Opadry®, manufactured by Colorcon®, is a customized, one-step film coating system that combines polymer, plasticizer and pigment, as required, in a dry concentrate. As the base polymer is clear, it is challenging to distinguish between colors. While the Thermo Scientific™ TruScan™ RM handheld Raman analyzer has a built-in multivariate residual analysis decision engine to identify most materials, more complex materials analysis requires users to build custom, advanced methods.

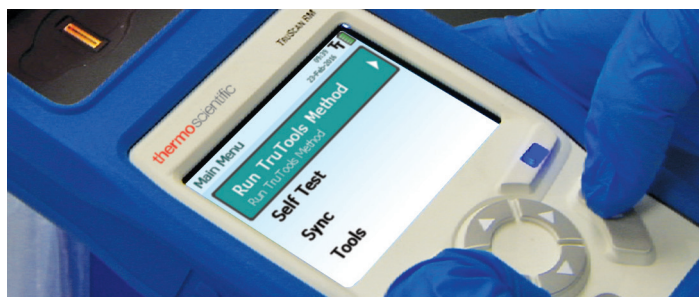
Thermo Scientific TruTools™ is an embedded chemometrics package for the TruScan RM analyzer. It enables users to create customized predictive applications, including classification, semi-quantitative and quantitative methods. TruTools leverages Solo, a chemometrics software package from Eigenvector Research Inc., which allows users to develop models that can be deployed onto the TruScan RM analyzer.

In this application, a Principal Component Analysis (PCA) method was found to be successful in identifying Opadry



orange from Opadry green. A TruTools PCA method produces a Pass or Fail result screen, based on the logic selected in the TruScan RM analyzer's WebAdmin functionality.

PCA method setting in WebAdmin allows users to make a decision based on either normalized hoteling ( $T^2$ ), normalized residual (Q), both or combined. Thus the user can control the PCA method's selectivity. For example, if normalized Q value will be used for the Pass/Fail criteria to identify raw materials, then any Q values higher than 1 will be considered as Fail. Usually, normalized Q value is more common than normalized  $T^2$  as the criteria for pass/fail indication, as Q value reflects the unusual variations outside the model.

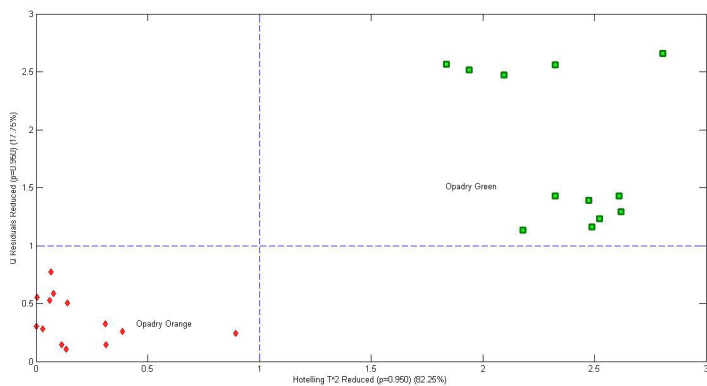


## Opadry Orange

- Acquisition Parameters:
  - Laser Power: 250 mW
  - Exposure Time: 200msec
  - Number of Coadds: 20
- Number of Scans: 13

### Eigenvector Solo Settings:

- Wavelength: 325.4-1867.2  $\text{cm}^{-1}$
- Pre-processing: Normalize (1-Norm, Area = 1), 1st Derivative (order: 2, window: 19 pt, incl only, tails: polyinterp), Mean Center
- Number of PCs: 1
- Cross validation: leave one out



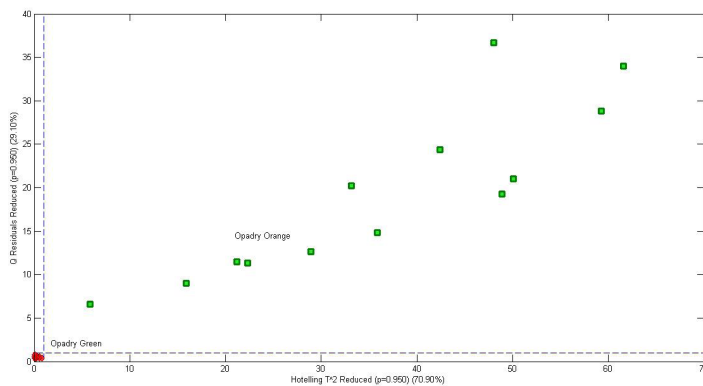
Cross Validated Opadry Orange PCA method against Opadry Green.

## Opadry Green

- Acquisition Parameters:
  - Laser Power: 250 mW
  - Exposure Time: 200msec
  - Number of Coadds: 20
- Number of Scans: 12

### Eigenvector Solo Settings:

- Wavelength: 289-1963.4  $\text{cm}^{-1}$
- Pre-processing: Normalize (1-Norm, Area = 1), 1st Derivative (order: 2, window: 19 pt, incl only, tails: polyinterp), Mean Center
- Number of PCs: 2
- Cross validation: venetian blinds w/ 5 splits and 1 sample per split



Cross Validated Opadry Green PCA method against Opadry Orange.

## Summary

Due to global supply chains and increased regulatory scrutiny, pharmaceutical manufacturers must ensure the quality of materials throughout the production process, as well as increase productivity and efficiency. The TruScan RM analyzer provides manufacturers with fast and accurate material verification, minimizing the need for time-consuming laboratory sampling tests. With the addition of the TruTools chemometrics package, the TruScan RM becomes a more powerful spectrometer, capable of identifying and quantifying more complex materials at the point of need.

**No. America**  
Boston, USA

**Central and So. America**  
Sao Paulo, Brazil

**Europe, Middle East, Africa**  
Munich, Germany

**Asia Pacific**  
Mumbai, India  
Shanghai, China  
Tokyo, Japan

Find out more at [thermofisher.com/truscanrm](http://thermofisher.com/truscanrm)

**ThermoFisher**  
SCIENTIFIC