



Adulterant Screen for Spectrum Software

Introduction

Detecting the presence of adulterants in your products has never been easier than it is with PerkinElmer FT-IR and NIR spectrometers using

Adulterant Screen in the Spectrum® 10 software. Adulterant Screen offers simple method development with a powerful algorithm to ensure detection, identification, and quantitation of materials that have been fraudulently or accidentally introduced into your product.

Your analysis is future-proofed, since new adulterants can be simply added by scanning a spectrum of the pure adulterant and adding it to your existing list of adulterants. No lengthy recalibration will be required. Adulterant Screen can be used on demand as a data processing command within Spectrum 10 software. It can also be easily incorporated into Spectrum 10 macros and Spectrum Touch methods to provide simple turnkey analyzer operation with PerkinElmer IR and NIR systems. These methods can incorporate additional Spectrum Quant methods to quantify materials in the product if it passes the Adulterant Screen.

Smart, Simple Detection of Adulterants

Adulterant Screen is ideal for laboratories that need to test products to prove that they are the correct product, and have not been contaminated or adulterated, without the need for extensive software training or methods development. The Spectrum 10 software is used to collect your IR or NIR data representing “good samples” spectra for your product. This consists of multiple spectra representing many sources of variation of your product, such as different batches, sources, grades of material, etc. These spectra define the boundaries of the acceptable product. You then collect the spectra of all known adulterants as pure materials. These spectra define your Adulterant Spectra.

Adulterant Screen requires virtually no additional training to get up and running (Figure 1). Method development can be fast-tracked thanks to the routines being embedded within the Spectrum 10 software, not as a separate software package.

For example, once the Material Spectra and Adulterant Spectra have been collected using Spectrum 10, incorporation into the method is achieved by simply using a File Selector to select the required spectra. The method is automatically generated by the software.

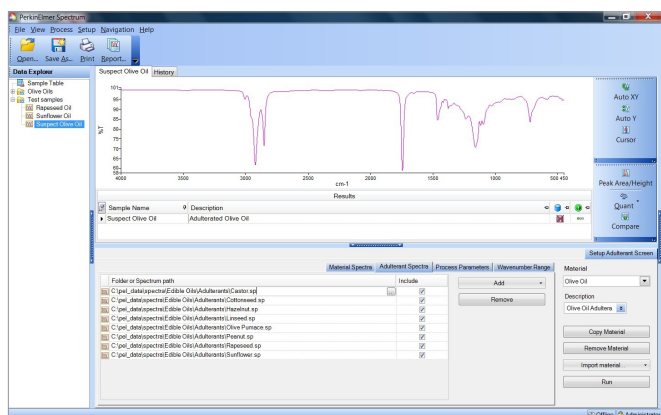


Figure 1. Adulterant Screen in the Spectrum 10 software

Accelerated Method Optimization

Adulterant Screen methods can be rapidly developed to detect and quantify the level of adulterants. Quantitative predictions are based on the pure spectra of adulterants and, do not require the preparation of calibration standards and methods. A suite of preprocessing algorithms are included to assist with common sampling variability issues and improve method robustness, accounting for spectral baseline effects and spectral regions of poor signal to noise. Blank regions can be incorporated to exclude spectral regions that do not contribute useful information to the method.

In addition, Pass/Fail limits can be set up based on the calculated concentration level of the adulterant.

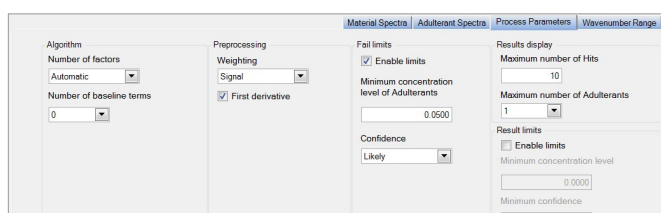


Figure 2. Adulterant Screen setup

The Adulterant Screen Algorithm

When a sample spectrum is scanned, the algorithm first compares it to a PCA model generated from the reference materials. This model is then augmented with each of the adulterant spectra. If including a given adulterant in the model greatly increases the fit of the sample spectrum, it is likely that the adulterant is actually present in the sample. The algorithm also accounts for contamination with multiple adulterants, searching for every

combination of up to three potential adulterants. The output of the algorithm is an estimated concentration, detection limit, and confidence indicator for each adulterant in the library.

The concentration estimate is based on the relative intensity of the library spectrum of the adulterant and the amount found in the sample spectrum without considering effective pathlength differences. As such, it is a semi-quantitative estimate. The detection limit estimate is expressed in the same terms. Finally, the reported confidence indicates the likelihood that the adulterant is actually present.

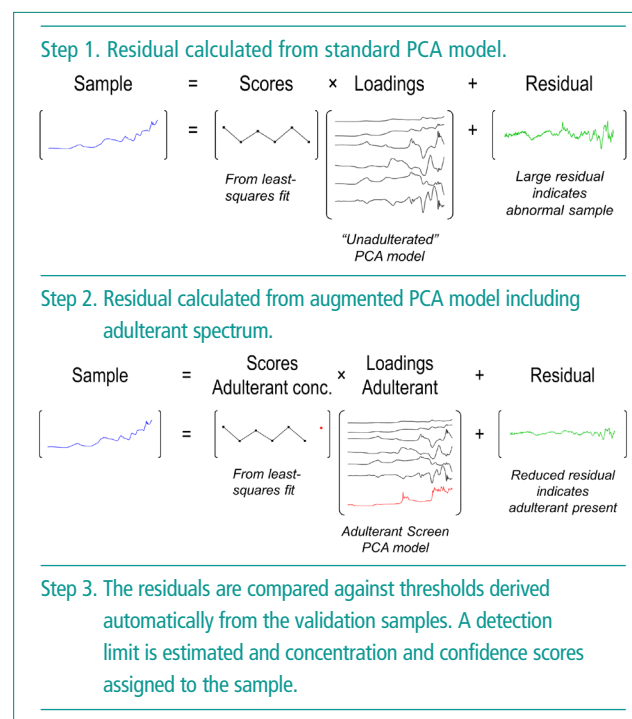


Figure 3. How Adulterant Screen works

Reporting of Adulterants

Adulterant Screen will attempt to detect the presence of known adulterants within your material and will report their presence if they are above the detection limit for that adulterant. A typical result screen for the adulteration of olive oil is shown in Figure 4.

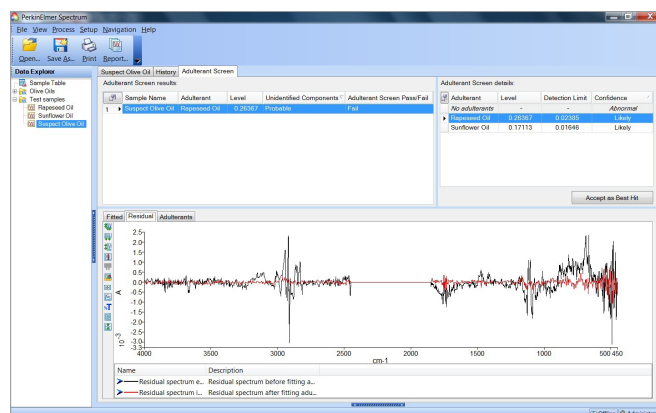


Figure 4. Result from Adulterant Screen for mid-IR spectra of olive oils

The residual spectra with and without the addition of the adulterants spectra will indicate the improvement obtained by adding in one or more adulterants.

The result will consist of a PASS/FAIL component, the identity of any adulterant(s), and the estimation of the concentration of the adulterant(s). This concentration estimation is based on the spectral contribution of the pure adulterant(s) within the total spectrum of the material being analysed. An additional confidence indicator makes the result even more definitive.

Put your Adulterant Screen Methods into Action

Adulterant Screen is just one of the many process options within the Spectrum 10 software and can be applied to any individual spectrum or multiple spectra, as required. Once the spectra to be analysed have been collected, simply click on Adulterant Screen.

It can also be used as a step within a Spectrum 10 Macro, allowing for complete method deployment from data collection through to a complete report, or output to a LIMS or Electronic Lab Notebook (ELN). The TIBCO Spotfire® data visualization and analysis software is the perfect environment for combining results from Adulterant Screen with data from other analytical techniques.

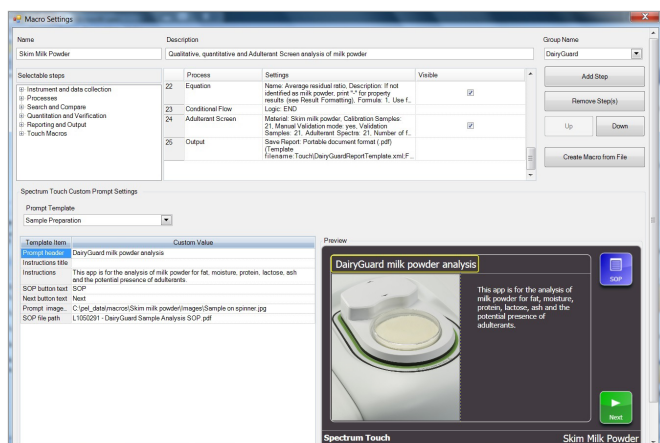


Figure 5. Setting up Adulterant Screen in a macro for milk powders on the PerkinElmer DairyGuard.

The Prompt screen allows the method developer to input free form text and to attach SOP instructions in local language to ensure the user follows standard procedures.

Using the unique Spectrum Touch interface allows simple touch/tap navigation through your analysis. Rather than the traditional point and click methods, to fully exploit modern touchscreen PC functionality (Figure 6). Performing Adulterant Screen, even on multiple spectra in Spectrum 10, can be a single-click operation.

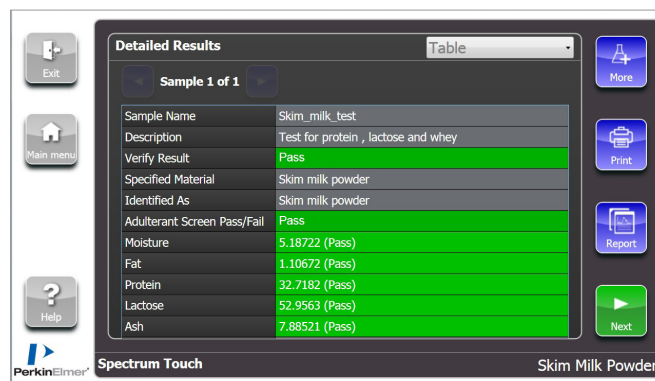


Figure 6. Spectrum Touch implementation of Adulterant Screen for milk powders

Adulterant Screen Ordering Information

Part Number	Description
L1101026	SPECTRUM ADULTERANT SCREEN – (1 User license) Spectrum Adulterant Screen is an add-on to Spectrum 10 that allows you to develop and execute screening methods for materials of concern.
L1101034	SPECTRUM ADULTERANT SCREEN (5 User license)
L1101035	SPECTRUM ADULTERANT SCREEN (10 User license)
L1101043	SPECTRUM ADULTERANT SCREEN ES (1 User license)
L1101044	SPECTRUM ADULTERANT SCREEN ES (5 User license)
L1101045	SPECTRUM ADULTERANT SCREEN ES (10 User license)
LX108875	SPECTRUM 10 Enhanced Security (ES) (1 User license)
L1101019	SPECTRUM 10 Enhanced Security (ES) (5 User license)
L1101020	SPECTRUM 10 Enhanced Security (ES) (10 User license)

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