

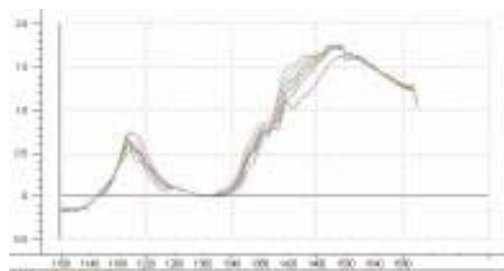


The Unscrambler® Accessory Pack for Spectroscopy

- Orthogonal Signal Correction can generate improved models particularly with large amounts of variance not related to the property of interest. Models will have fewer components for easy interpretation.
- Sample Selection for Calibration Transfer saves time by allowing calibration of instruments using fewer calibration samples. This function also facilitates the development of more robust models reducing the need to recalibrate.
- Deresolv Smoothing Function can be used to change the apparent resolution of an instrument. It can also be chosen as a smoothing alternative to Savitzky-Golay which is in The Unscrambler®.

Orthogonal Signal Correction (OSC)

This function calculates the orthogonal signal correction parameters for preprocessing a spectral data prior to developing a PLS model. In situations where the PLS model captures a very large amount of predictor block (X) variance in the first factor but gets very little of the predicted variable (y or Y), it can be very useful to remove extraneous variance from X that is unrelated to y. OSC does this by finding directions in X that describe large amounts of variance while being orthogonal to y. Models are built on OSC corrected data, then the OSC correction is applied before application of the PLS models to new data.



NIR spectra of different alcohols

Deresolv Smoothing Function

On occasion, one may wish to standardize a lower resolution instrument to a higher resolution instrument. In such an instance, it may be more effective to mathematically lower the resolution of the higher resolution instrument prior to forming the transfer model. The Deresolv Smoothing Function can be used to change the apparent resolution of an instrument and may also generate some beneficial noise reduction. This function works by FFTing the spectra, convolving it with an impulse of specified width, then back FFTing the result.

Sample Selection for Calibration Transfer

In calibration transfer, the relationship between the responses of two instruments is obtained using spectra from a set of standardization samples or using a subset of samples from the Instrument 1 calibration set. Tools are incorporated for applying previously defined standardizations and for selecting data for new ones. Selection of this subset can be performed with this function, which chooses samples based on their leverage, or uniqueness, within the group of spectra.

The Unscrambler® Accessory Pack for Spectroscopy is developed in collaboration with



CAMO continues its commitment to bring you today's most powerful modeling advancements and innovations. Our first The Unscrambler® Accessory Pack not only shows the flexibility and strength of the new features adopted into The Unscrambler® but also demonstrates CAMO's ability to understand, respond to, and satisfy customer needs more rapidly.

The Unscrambler® Accessory Pack for Spectroscopy requires The Unscrambler® 7.6.



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