SPECTRAL_MVA help

Menu: **Open**

- Mat files containing spectra and variable (if no variable is present it is automatically generated in reverse scale – from Max to Min)

- open XPS VMS files – converted in Vision2 software

- open Casa VMS – vms files saved using "Simple VMS format" option in CasaXPS software

Menu: **Process**

- Smooth spectra using savitski golay smoothing – select an odd value for window (value >=3)-the larger the window, the more significant smoothing

- Shift spectra to the same position of Maximum – (with original accuracy of the data)

- Shift spectra to the same position of Maximum – (with 10x better accuracy than original data -if variable have a step in x-axis of 0.1, the spectra are interpolated to having step of 0.01, then the spectra are shifted and then converted back to original number of points. This prepares data for multivariate analysis which is sensitive to shift in data.)

- shift spectra to different values of Maximum –with original accuracy

- normalize spectra – click on the plot to chose the variable at which to normalize

- derivatize – 1st and 2nd derivative – choose smoothing value – odd value >3

- undo processing

Menu: **Save**:

- spectra that have been processed
- Results of PCA, MCR and Simplisma

To run the analysis

1. **PCA** – enter # of components to run the model with

   - add preprocessing or hit cancel

   - display scores and loadings or save PCA model

2. **Simplisma**- enter # of components and offset (>3 – the larger the value the less sensitive the method to noise). Mark start with 2nd derivative as a starting point for severally overlapped peaks. Hit Enter multiple times until final figures appear.

3. **MCR** – Hit MCR and choose initialization – random, or results from PCA or Simplisma. Choose # of components if random initialization. Choose nonnegatvity constraints for both spectra and concentration.