Selection of calibration subset

# In OPUS

* Start Quant 2
* Click <Spectra> tab
  + Click <Add Spectra>
    - Navigate to folder containing spectra of potential calibrations samples (i.e. samples that have enough soil that they can be analysed by conventional laboratory methods if selected)
    - <Ctrl A> to select all spectra, followed by <Open>
  + Click <Set Sample Numbers>
    - In “Set Sample Numbers” dialog box:
      * Check “Set sample numbers according to file names”
      * Click <Set>
      * Click <Exit>
* Click <Parameters> tab
  + Under “Preprocessing in calibration regions” select “No spectral data preprocessing”
  + Check “Mean centering”
  + Under “Calibration regions” enter from 4000 to 600
  + Check “PCA”
  + Under “Factors” enter 10
  + Click <Factorize>
    - Wait for principal component analysis to run
  + Click <Show Scores>
    - Under “PCA Scores” dialog box
      * In “Automatic selection of subset” select all factors (1 to 10) under “Used Factors”
      * Decide on what percent of the samples are to be used for the calibration set. For example to select 100 samples out of 498 total samples (from seed sites) the percentage is about 20%
      * To select a calibration set of 20% of all the samples, enter 80% in “Subset in %:”
      * Click <Set Subset>
      * Under “Set subset samples on:” select “Test”
      * Click <Set Data Set> which will change 80% of the samples from ”Calibration” to “Test” on the “Spectra” tab
      * Click <Exit>
* Click <Spectra> tab
  + Some of the spectra are now labelled “Test” instead of “Calibration”
  + Highlight all spectra
  + Copy highlighted area <Ctrl C>
* Because you can only select a whole percentage in the calibration selection process, you may need to adjust the percentage entered (say from 80% to 79%). To do this, first reset all the spectra to “Calibration” and start the selection process again until you get the approximately number of calibration samples:
  + Click <Spectra> tab
    - Click “Set Data Set”
      * Click “Clear Test Spectra” which will change all the ‘Test’ spectra to ‘Calibration’.

## In Excel

* Start blank workbook
* Highlight cell A1
* Paste table from OPUS <Ctrl>V
* Highlight all pasted data
* Click <Data><Sort>
  + Select “Data Set” under “Sort by”
  + Click <Add level>
  + Select “File Name under “Sort by” on second line
    - The samples will be sorted so the calibration samples are at the top (in order of file name)
* Scroll down worksheet to line containing first sample with “Test” under “Data set”
* Highlight all rows below this with samples labelled “Test” using <Ctrl><Shift><↓>
* Click <Home><Delete><Rows> to delete rows with samples NOT in calibration set
* Move to cell A1
* For all columns except that with File Name:
  + Use <Home><Delete><Columns> to delete
* Finally use <Home><Delete>Rows> to delete row 1 (with the column headings)
  + There should now be only a list of the files names of the calibration spectra
* Save file as “Calibration list.CSV”