

# Determining the composition of mineral-organic mixes by UV-vis-NIR diffuse reflectance spectroscopy (DRS)

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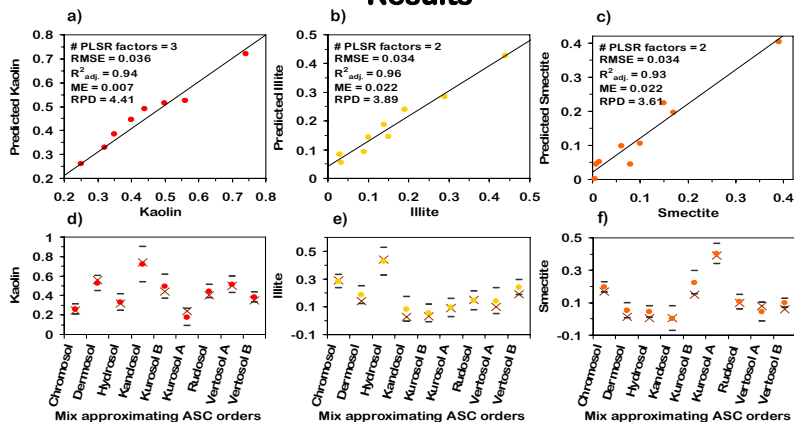
## Background & Aims

Quantifying the mineral composition of a soil is important, as is the development of a simple technique to do it. Conventional methods, e.g. X-ray diffraction (XRD) are primarily qualitative. Quantitative modifications such as X-ray powder diffraction (XRPD) are usually involved, time-consuming and expensive (e.g. Hillier et al., 2003). The aims of this paper are: (i) model mineral-organic mixes as a function of their ultraviolet (UV), visible (vis) and near infrared (NIR) diffuse reflectance spectra, (ii) predict mineral-organic composition of nine artificial mixes that approximate mineral-organic composition of Australian soils, and (iii) compare their spectra with those of corresponding Australian soils

## Methodology

We used a three-factor simplex lattice design with three levels - kaolinite (K), illite (I) and smectite (S) plus two levels of goethite (G) and a 50/50 mix of humic and fulvic acids (H-F). Quartz (Q) was also added. Other minerals were used as 'end member' in our models: attapulgite, bentonite, brucite, carbonate, chlorite, dickite, K-feldspar, gibbsite, halloysite, hectorite, limonite, metabentonite, mica, oligoclase, and vermiculite. Reflectance (R) spectra was measured using a UV-VIS-NIR (250 – 2500 nm) spectrometer (Cary 500, Varian Inc., CA, USA). Modelling by PLSR with LOO X-validation. Predictions of mineral-organic composition of nine artificial mineral-organic mixes that represent common Australian soils made by bagging-PLSR. PCA used to compare multivariate space of the nine mineral-organic mix spectra to the spectra of B2 horizons of Australian soils that correspond to similar orders. Data analysis using ParLeS v2.1 (Viscarra Rossel, 2005)

## Results



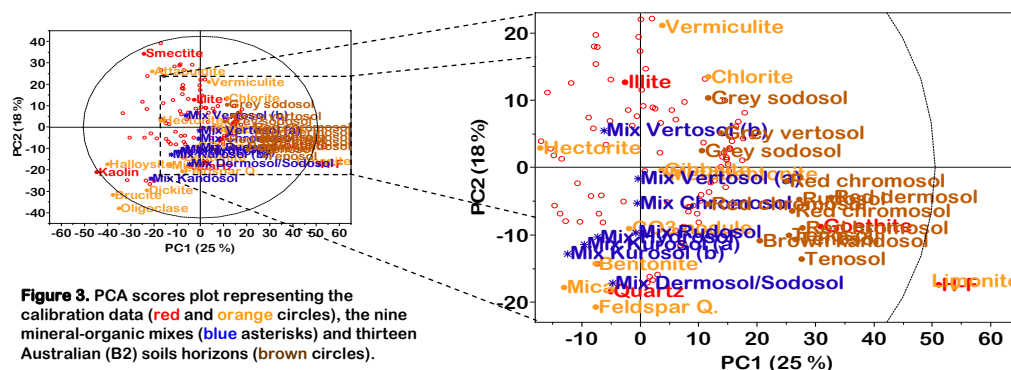
**Figure 2.** Bagging-PLSR predictions of K, I and S. (a), (b) and (c) show plots of actual vs. predicted, and (d), (e) and (f) the predictions (circles), their 95% confidence intervals (lines) and the actual values (crosses)

Bagging-PLSR accurately predicted the K, I, S composition of the nine artificial mixes (Fig. 2). Predictions of G, H-F and Q were poor (Table 1). This may be improved with a better experimental design.

**Table 1.** Assessment statistics for predictions of G, H-F mix and Q

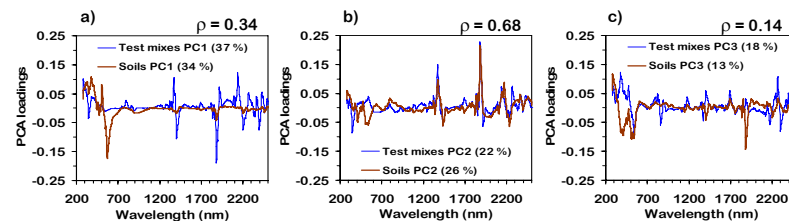
	#Factors	RMSE	ME	R <sup>2</sup> <sub>adj</sub>	RPD
G	2	0.036	0.032	0.55	0.36
H-F mix	5	0.028	0.023	0.60	0.38
Q	1	0.142	-0.134	0.16	0.18

Fig. 3 shows the PCA scores plot of the calibration data together with the nine artificial mineral-organic mixes and the Australian soils.



**Figure 3.** PCA scores plot representing the calibration data (red and orange circles), the nine mineral-organic mixes (blue asterisks) and thirteen Australian (B2) soils horizons (brown circles).

Fig. 4 compares the first three PCA loadings of the mixes and the Australian soils. The first 3 components explain ~ 75 % of the variation in the spectra



**Figure 4.** Comparison of the first 3 PCA loadings for the test mineral-organic mixes (Test mixes) and the thirteen Australian (B2) soil horizons (Soils). The correlation between the loadings is represented by the correlation coefficient ( $\rho$ )

## Conclusions

Accurate predictions of K, I and S. Biased predictions of G and the H-F (organic) mix. Multivariate space of Australian soil (B2) horizons and artificial mixes were similar, showing the potential of this methodology for rapid quantitative measurements of a soil's mineral-organic composition.