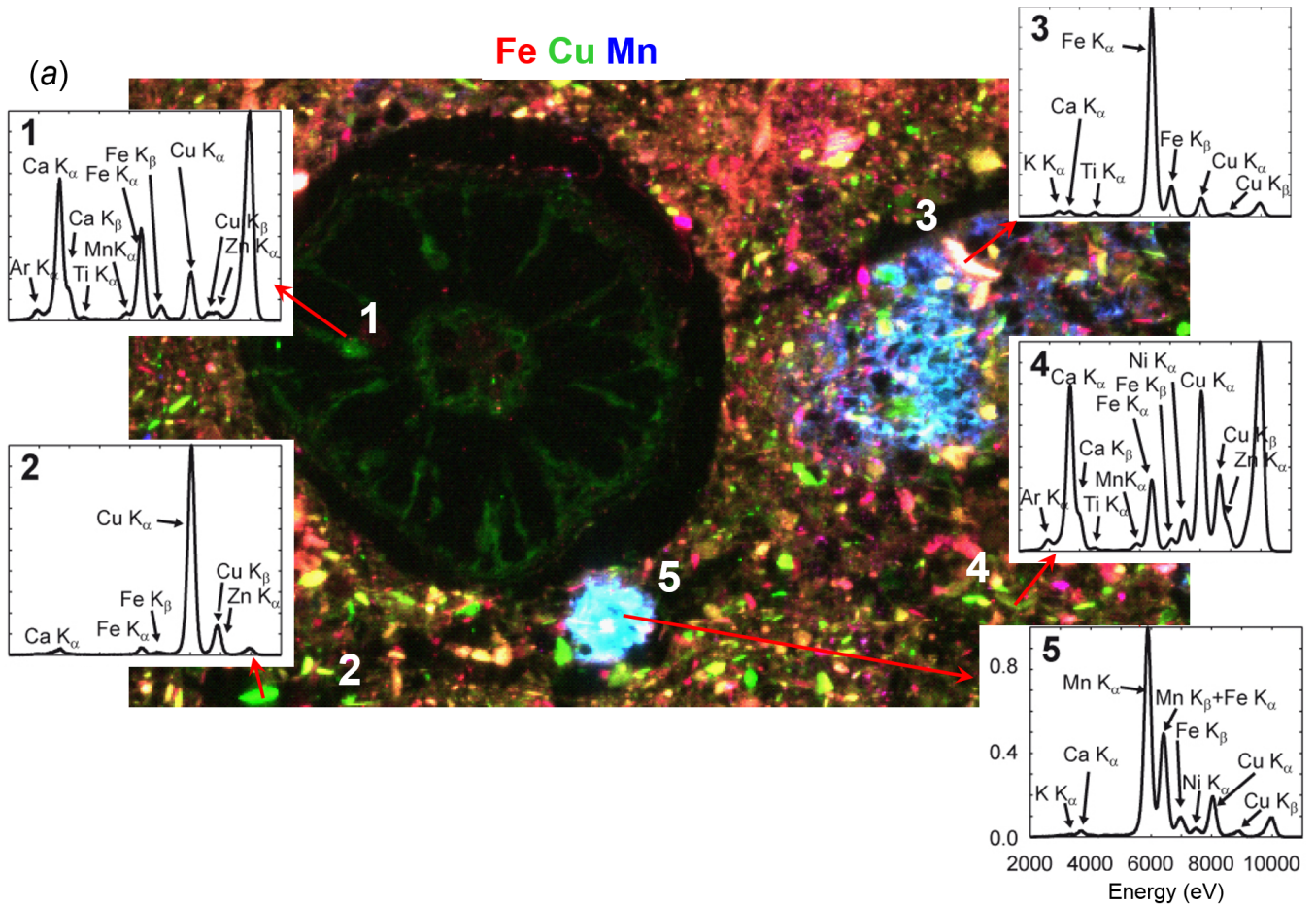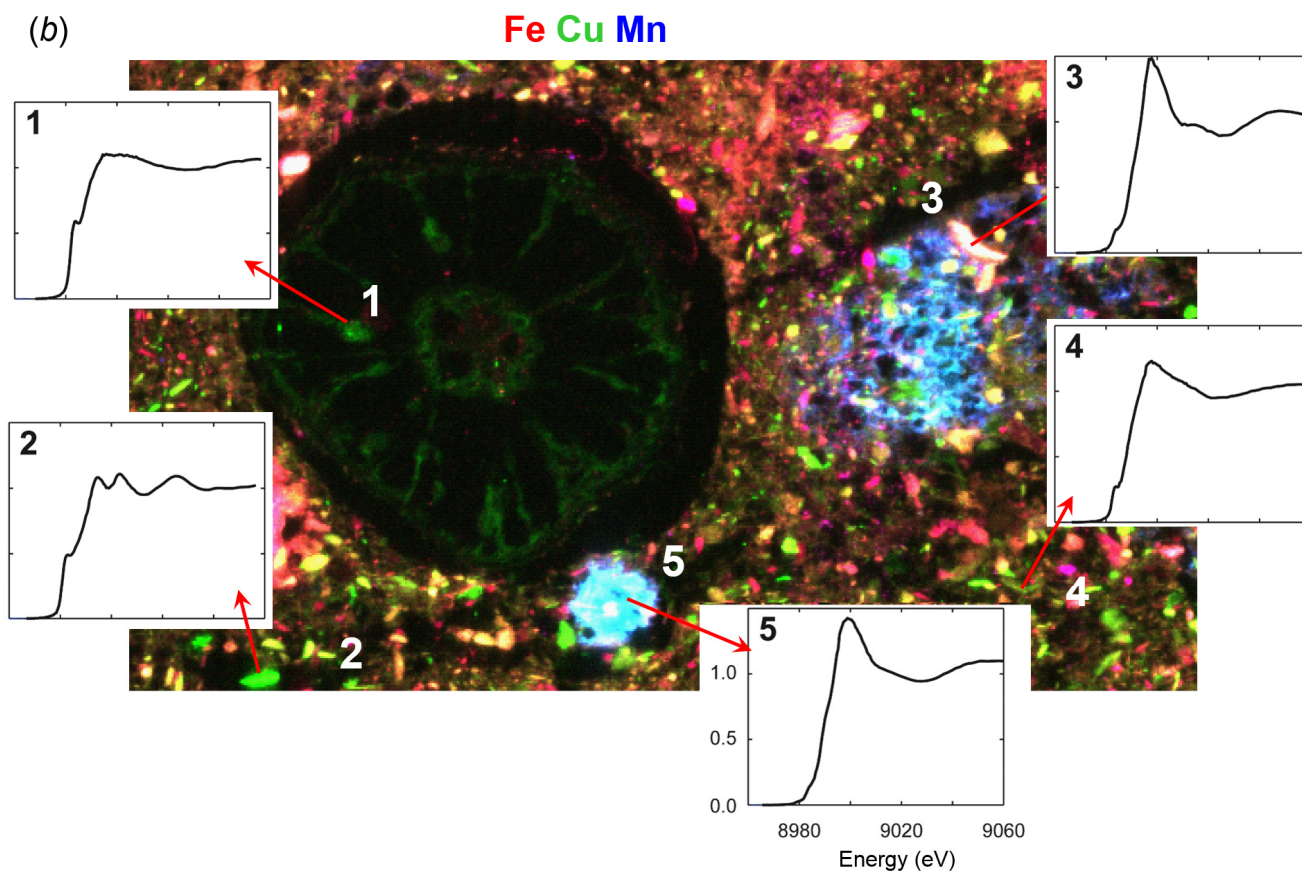# Supplementary material for

# Estimating the number of pure chemical components in a mixture by X-ray absorption spectroscopy

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Figure S1 : Tricolor (RGB) XRF maps of the distribution of Fe (red), Cu (green), and Mn (blue) in the rhizosphere of a paddy soil contaminated by Cu showing the diversity of the Cu forms. Five distinct Cu chemical associations and species were identified at selected points-of-interest by X-ray micro fluorescence (*a*) and Cu-XANES (*b*). These species (and probably others) are mixed in various proportions in the fine organo-clay matrix.
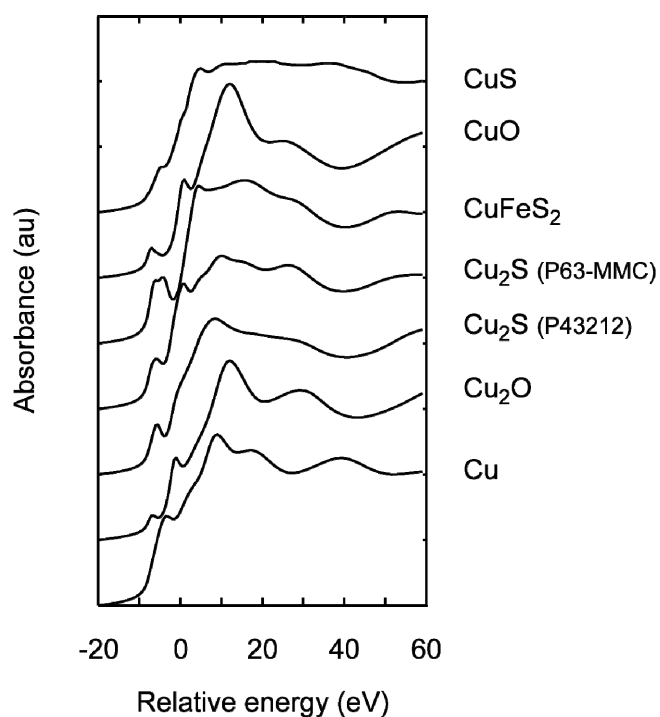
Figure S2 : Set of theoretical XANES spectra used to calculate the artificial mixtures.
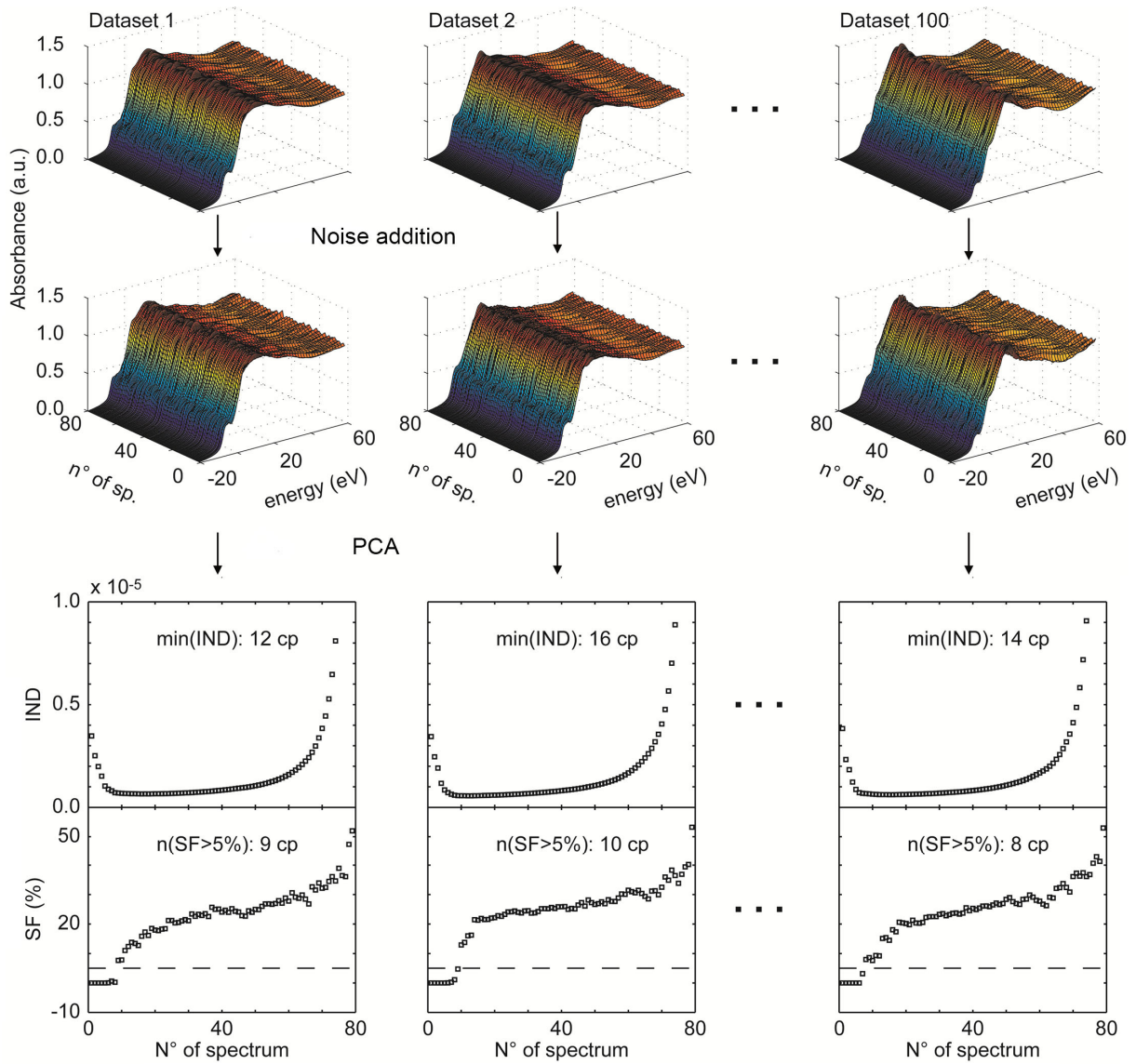
Figure S3 : Generation of the (*r*,*m*) synthetic mixtures and statistical analysis. Here *r* = 5 and *m* = 80.

Step 1: Random drawing of the *r* component spectra out of the seven theoretical spectra.

Step 2: Random drawing of each component weight with a normal law and rescaling to 1 the sum of weights.

Step 3: *m* replications of Step 2

Step 4: 100 replications of Steps 2+3

Step 5: Calculation of the mean and standard deviation of IND, F-test and the NSS-stat.