

Supplementary File 1

Biplots show the particles in the projection plane of the two first principal components of the original coordinates. The colors of the circles represent the subclasses the corresponding particles belong to and are coded the same way as in fig. 4 and 5. The projected original coordinate axes are plotted in grey. By construction, the particles have the largest spread in this projection among all possible 2D projections. The biplot on the left is based on the particles in ILR transformed coordinates and demonstrates the separation of the particles best. The biplot on right is constructed from the original elementary coordinates, so that an interpretation in terms of elemental composition is possible.

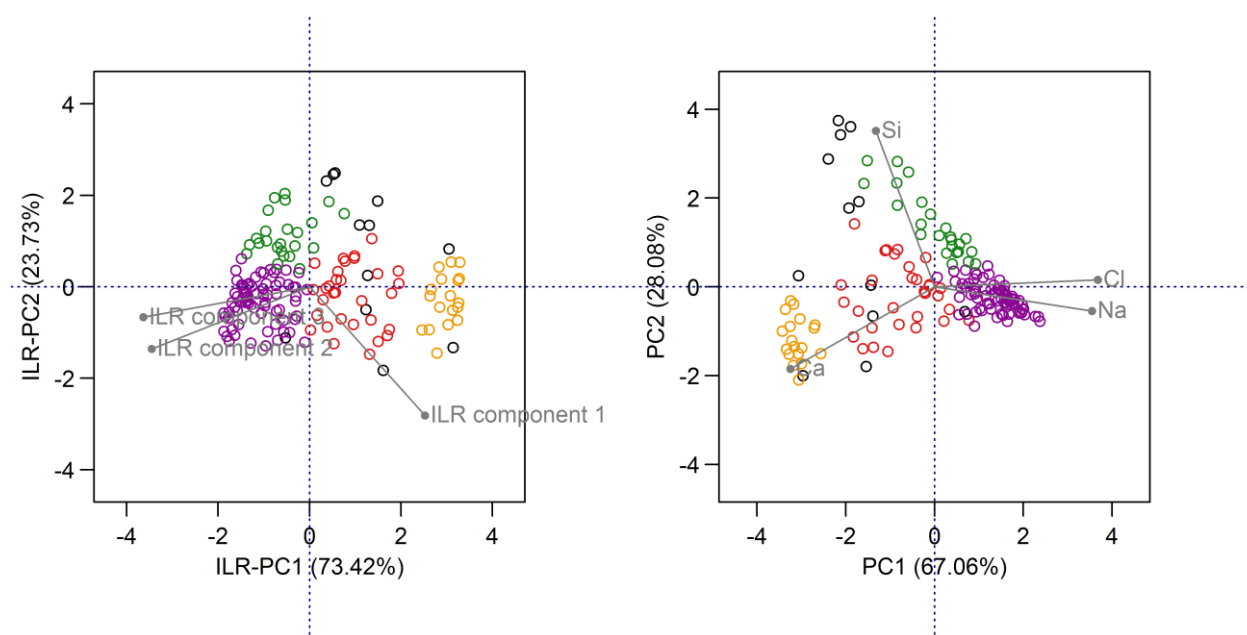


Figure 8. Biplots of the particles of the Si-Ca-Na-Cl main class in ILR transformed (left) and elemental coordinates (right). The subclasses the particles belong to are color-coded as described in fig. 4 of the publication.