# Supplementary material

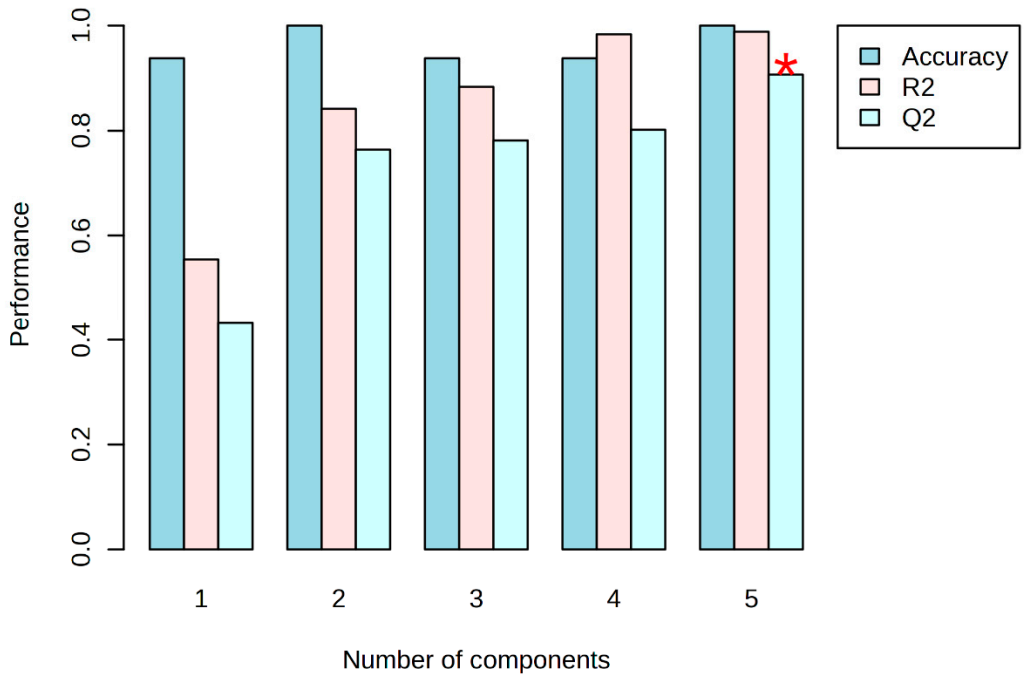


**Figure S1.** Performance indicators for the evaluation of the PLS-DA.

The outcomes of the leave one out cross-validation (LOOCV), using five components, expressed as accuracy =1.00, $Q^2$ = 0.91, and $R^2$ = 0.98, are summarized. The accuracy, with a maximum theoretical value of 1, is the capability of the model to correctly classify the samples. While the $R^2$ parameter indicates how well the PLS-DA model explains the current dataset, $Q^2$ provides a qualitative measure of consistency between the predicted and actual data.

* The red star (asterisk) indicates the best classifier optimized with 5 components and achieving the highest accuracy.