USE OF HPLC IN COMBINATION WITH DIFFERENT CHEMOMETRIC METHODS FOR THE DETERMINATION OF HOP VARIETIES

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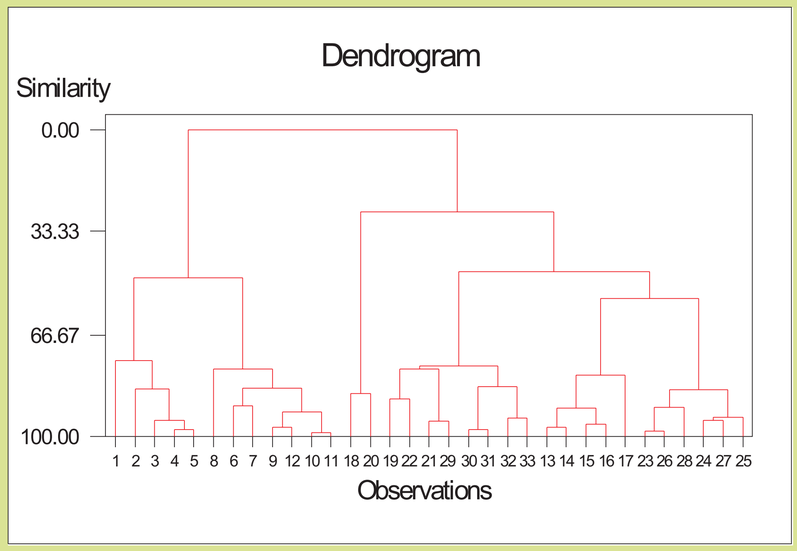
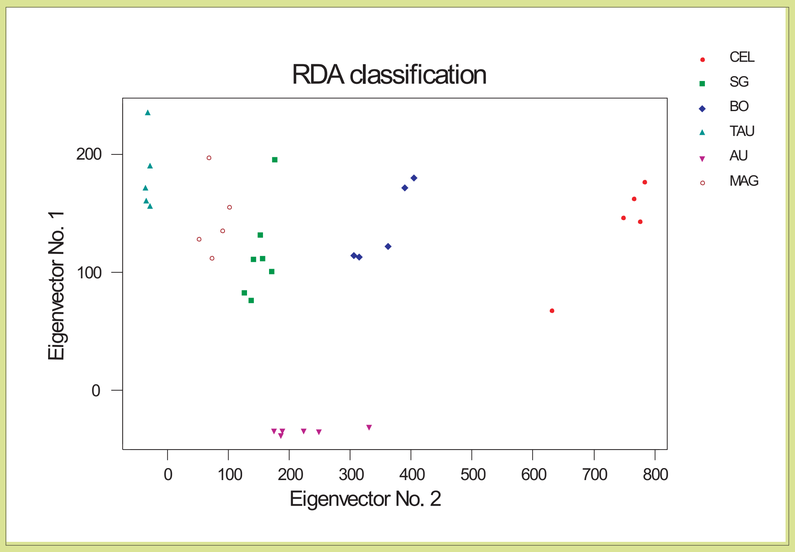
INTRODUCTION

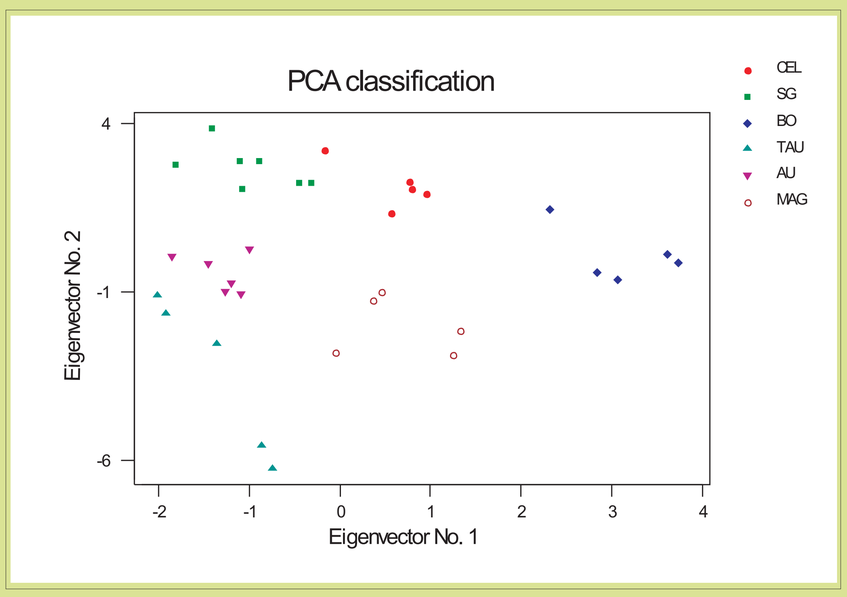
In agro-food chemistry, the application of chemometric methods for the characterisation or classification of products according to origin, quality or variety is very atractive and has already been widely used.
In the present work we explore the use of HPLC method in combination with Principal Component Analysis (PCA), Hierarchical clustering (HC), Linear Discriminant Analysis (LDA), and Regulised Discriminant Analysis (RDA) for the possibility of the classification of hop samples according to the six different varieties Celeia (CEL), Savinjski Golding (SG), Bobek (BO), Taurus (TAU), Aurora (AU), and Magnum (MAG). The amounts of particular and total alfa- and beta-acids, ratios between total amounts of alfa- and beta-acids, ratios of cohumulone and colupulone in alfa-and beta-acids and the Lead conductance value of hops determined according to the instructions in Methods 7.7 and 7.4 in Analytica EBC (1) were used as the input parameters to different chemometric methods.
We compare chemometric methods to find the optimal one for the discrimination between different groups of hops regarding the variety due to the simplicity, efficiency and time needed for analysis.



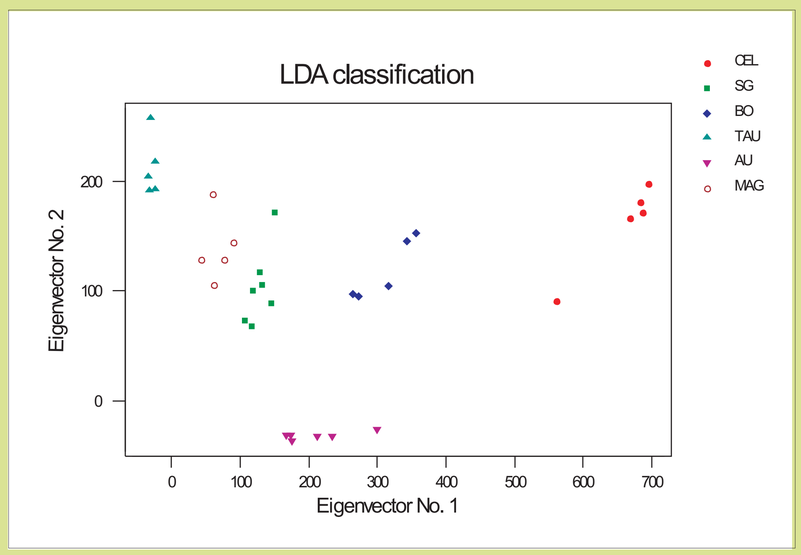
Dendrogram of the 33 objects represented by ten variables obtained by Ward's hierarchical clustering method with the use of Euclidean distances. Objects from 1-5 are CEL, 6-12, SG, 13-17 BO, 18-22 TAU, 23-28 AU, and 29-33 MAG hop samples.



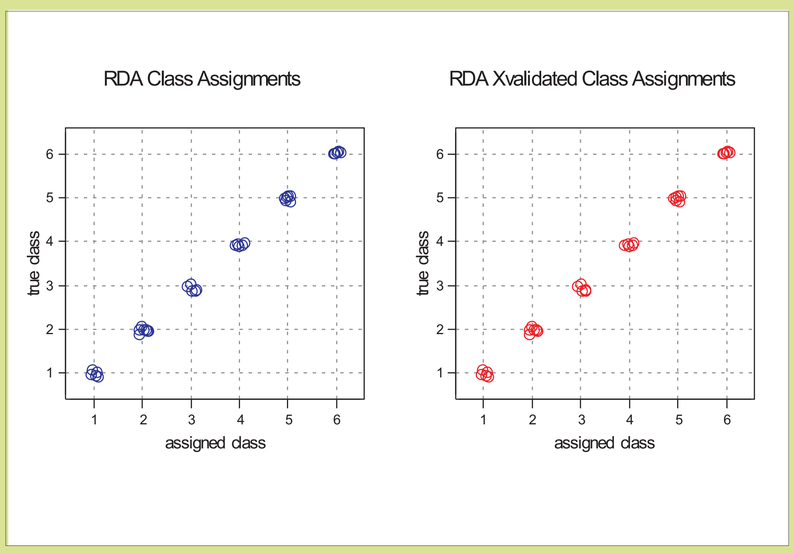
Projection of the 33 objects represented by ten variables onto the plot defined by the first two discriminant functions calculated with RDA.



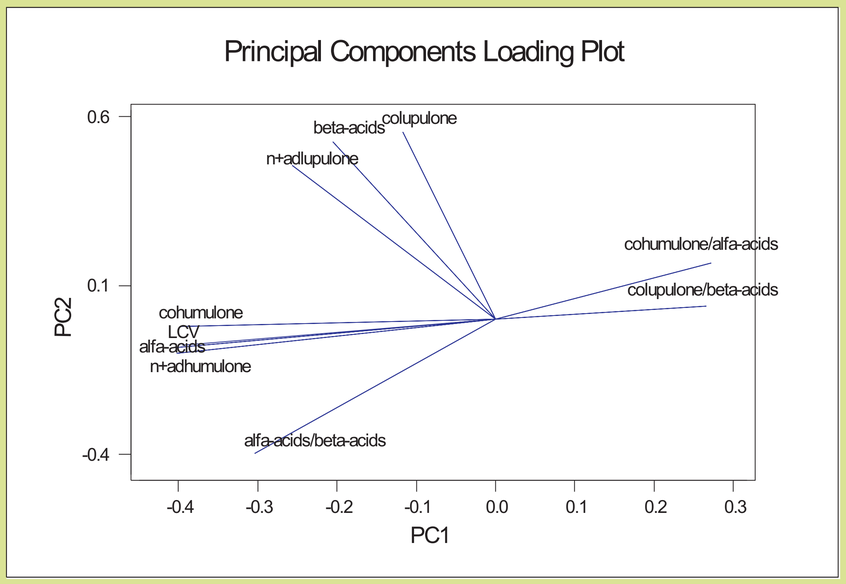
Projection of the 33 objects represented by ten variables onto the plot defined by the first two principal components PC1/PC2.



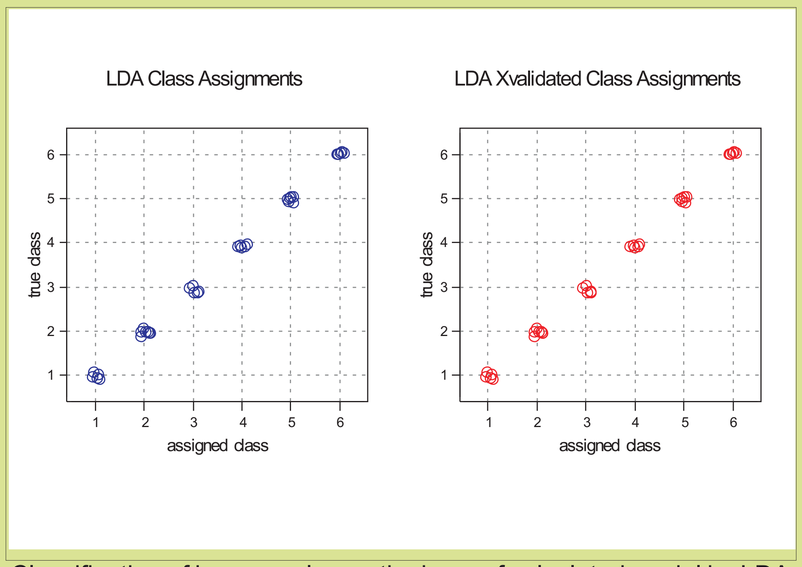
Projection of the 33 objects represented by ten variables onto the plot defined by the first two discriminant functions calculated with LDA.



Classification of hop samples on the base of calculated model by RDA and the result of cross validation of the calculated model.



Loading plot of the principal components.



Classification of hop samples on the base of calculated model by LDA and the result of cross validation of the calculated model.

CONCLUSIONS

PCA and HC were used as the examples of unsupervised methods to find out the importance of particular parameter to the grouping of samples. PCA and HC both gave comparable results for the separation of hop samples according to the varieties. In the case of PCA the best grouping was obtained by the use of Euclidean distances and Ward's linkage. Both PCA and HC methods gave the final results of 100 % correct grouping.
As the representative of supervised chemometric methods LDA and RDA were used. The models obtained from the application of both methods gave 100 % correct classification and also the prediction ability of the built models, determined with the test set and cross validation methods were very good.

REFERENCES

- Analytica - EBC, European Brewery Convention, Verlag Hans Carl Getranke-Fachverlag, Nurnberg, Germany, 1998.