SUPPORTING INFORMATION

Workflow for the Supervised Learning of Chemical Data—Efficient Data Reduction-Multivariate Curve Resolution (EDR-MCR)

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Contents

Supporting Text.

Practical notes on the application of EDR-MCR

Note 1:

EDR is presented as one of several possible solution methods that can be used to accomplish dimension reduction and dataset splitting, and therefore other methods can be applied subsequent to the application of MCR. Therefore, the steps for data splitting (step 1-1 displayed in Scheme 1) and variable selection (combination of steps 1-1 and 1-2 displayed in Scheme 1) that were performed by the EDR method shown in Scheme 1 can be replaced with other potential methods such as KS and random sampling[10-14] for the selection of representative data samples, and with approaches[5] such as minimum redundancy, maximum relevance (mRmR) and *Relief-F* for variable selection.

Note 2:

Depending on the properties of the data, the number of MCR components can be lower than, equal to or higher than the number of classes. In the instance where the number of components is higher than the number of classes, those that fulfil the constraint will have the class information embedded within them, because the equality constraint applies for the number of profiles that corresponds to the number of classes. When the number of components is lower than the number of classes, the equality constraint for the class profiles can still be applied. However, some of the class profiles will have information for more than one class.

Note 3:

Bilinearity is the basic principal that underlies MCR methods. Thus, MCR is useful for supervised learning for datasets which fulfill the bilinearity requirement similar to other bilinear decomposition methods (such as PLS), and it exhibits limitations when deviations from linearity are not small.[33-35] In this work, the focus was to introduce MCR methods for discriminant analysis and classification, and thus bilinear datasets were examined. Future work will focus on in-depth investigations of the utility of the approach for analysis of a range of data types that exhibit varying levels of non-linearity.

Nighshade species

This data DART-HRMS of the seeds of 24 plant species, all of which contain the psychoactive principles atropine (*m/z* 290.17) and scopolamine (*m/z* 304.14). These plants are taxonomically related and are members of five genera in the Solanaceae (nightshade) family: *Atropa* (3 species): *A. baetica*, *A. belladonna and*, *A. komarovii*; *Brugmansia* (5 species): *B. arborea*, *B. aurea*, *B. sanguinea*, *B. suaveolens* and *B. versicolor*; *Datura* (9 species): *D. ceratocaula*, *D. discolor*, *D. ferox*, *D. inoxia*, *D. leichhardtii*, *D. metel*, *D. quercifolia*, *D. stramonium* and *D. wrightii*; *Hyoscyamus* (5 species): *H. albus*, *H. aureus*, *H. muticus*, *H. niger* and *H. pusillus*; *Mandragora* (2 species): *M. autumnalis* and *M.officinarum*.

Mass spectral data were collected in positive-ion mode using a DART-SVP ion source (Ion Sense, Saugus, MA, USA) coupled to a JEOL AccuTOF mass spectrometer (JEOL USA, Peabody, MA, USA). After data binning (with a bin width 15 mmu) and using a relative abundance cutoff of 0.2%, the generated data matrix had 219 rows and 2976 columns.

Strategy on comparison of different methods

First, the datasets were explored for any possible outlier samples using PCA along with Hotelling's T-square and Qres measures to avoid their selection as training samples. The PCs that explained 99.9% of the data variance were used for the application of Hotelling's T-square and Qres methods. Then the datasets were divided into training and test sets using, independently, iterative random sampling (IRS; 100 iterations), Kennard-Stone (KS) and EDR-step 1-1 methods to reveal the impact of data splitting variability on model validation performance. The training versus test sample split ratios used for KS and IRS for each class were 70:30 for iris, wine and CRC datasets, and 80:20 for the nightshade data set. Independent of the data splitting strategy used, the resulting training and test sets were reduced in variable dimension using variables identified in step 1-2 of the EDR strategy. The number of important PCs that were used for building the convex spaces in EDR strategy were selected based on the measure of the data variance that was explained by the PCs.

The reduced datasets were analyzed by the described MCR method and various other machine learning techniques for comparison. Specifically, partial least square-discriminant analysis (PLS-DA) and error-correcting output code (ECOC) multiclass models using linear discriminant analysis (LDA), K-nearest neighbors (KNN), classification and regression trees (CART), and support vector machines (SVM) were investigated for comparison with MCR. ECOCs, which combine multiple binary classifiers to solve multi-class classification problems, are an ensemble-learning framework shown to reduce the bias and variance errors of the underlying classifiers.[47] The hyper-parameters of the ECOC models are: linear coefficient threshold and regularization parameters for LDA; the number of neighbors and the distance function for KNN; the maximum number of leaves for CART; and the box constraint and kernel scale of the linear kernel function for SVM. The Bayesian optimization method was used to compute optimal hyper-parameters of the ECOC models by minimizing the loss of test set prediction ability. The predicted class label for a sample corresponds to the minimum expected classification cost among all classes. The parameter that should be optimized for PLS-DA is the number of latent variables. For MCR, a critical element of the under- or overfitting of the data is the number of MCR components. The importance of MCR components can be assessed using eigenvalues or the contributions derived from PCA analysis. The optimal number of MCR components has been estimated based on MCR lack of fit- and test set prediction errors. It has been studied that it can be determined using a number of different strategies.[43] Class labels of the training set were imposed in the form of a hard equality constraint into the MCR process. The non-negativity constraint was applied in iterations of MCR-ALS on both $\mathbf{C}$ and $\mathbf{W}^T$ profiles. The proficiencies of the methods in training an accurate classification model were compared using the following classification performance characteristics: accuracy (correct classification rate), error rate (1 – accuracy), weighted-F1-score (i.e. the weighted average of precision and sensitivity), sensitivity (i.e. 1 – false negative rate (*type II error*)), specificity (1 – false positive rate (*type I error*)), and precision.

Supporting Figures.

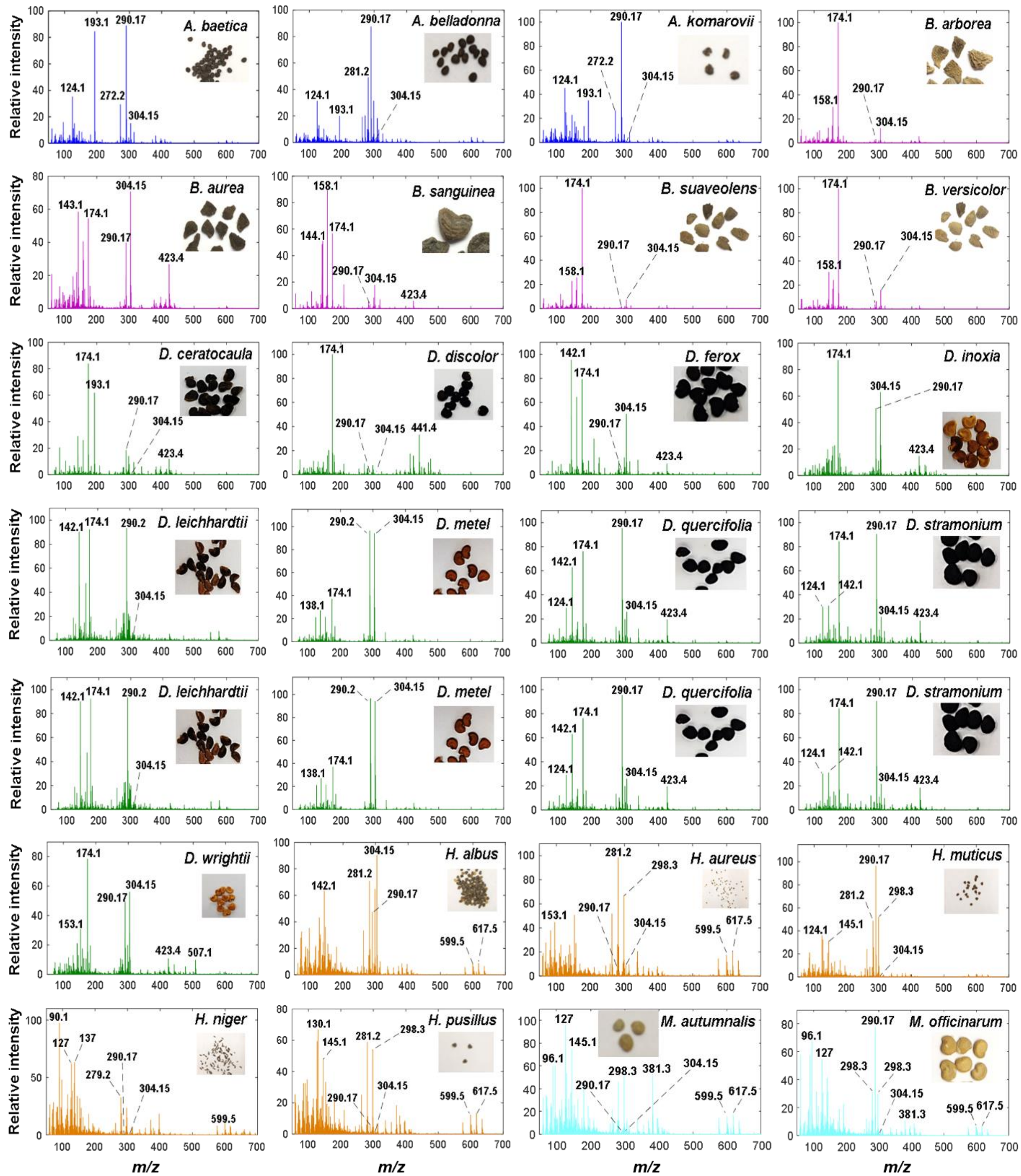

Figure S1. Representative DART high-resolution mass spectra of the seed species represented in this study. The figure is reprinted with permission from Beyramysoltan, S.; Abdul-Rahman, N. -H.; Musah, R. A., Call it a "nightshade"—A hierarchical classification approach to identification of hallucinogenic Solanaceae spp. using DART-HRMS-derived chemical signatures. *Talanta* 2019, *204*, 739-746, Supplementary Material. Copyright © 2019 Elsevier B.V.

A B

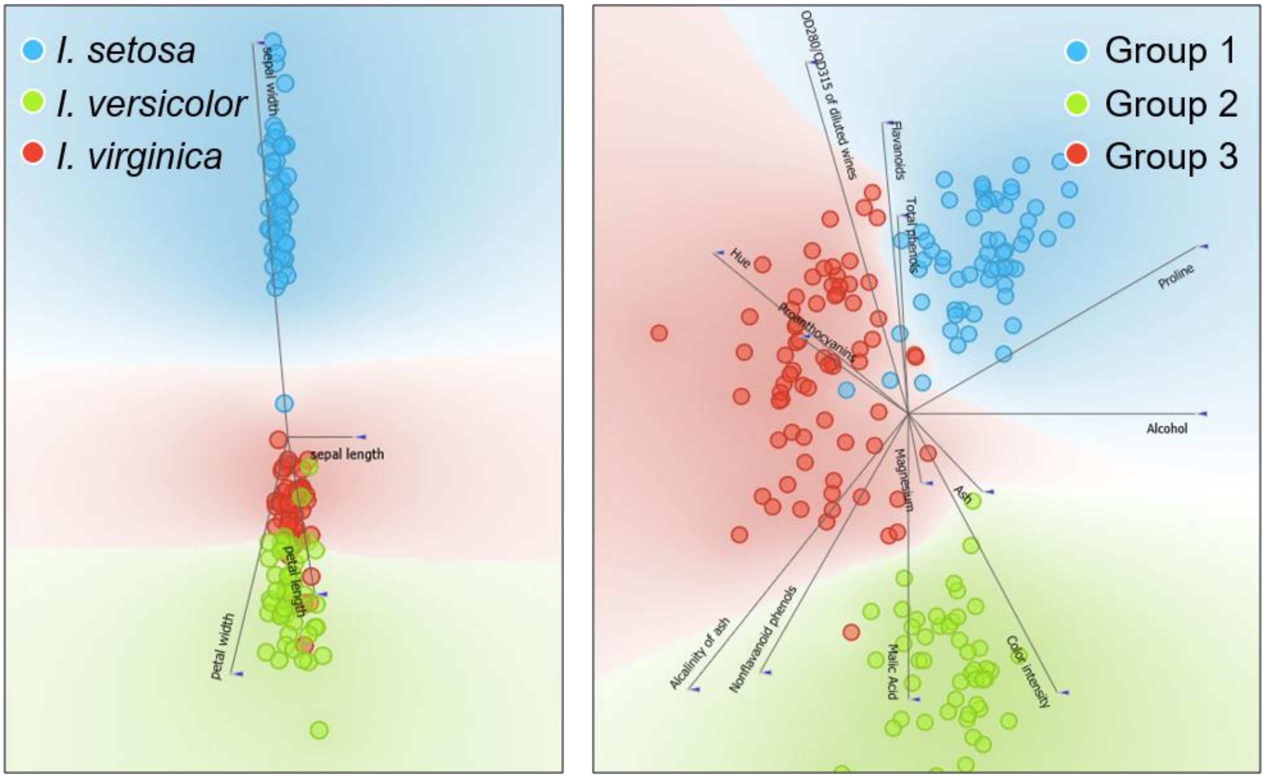

Figure S2. Visual representations of the variables for iris flower (A) and wine (B) datasets, rendered in FreeViz. Freevis (an application in Orange toolbox, which was implemented in Python) enables supervised multivariate visualization of the data by optimizing a linear projection and displaying the projected data in a 2D plot. The lines arising from the origin in each plot and the circles represent projections of the features of the base vectors and data samples, respectively. For ease of visualization the data are colored-coded by class, and the visualization space is colored based on the class-computed probability. For the iris dataset, blue, red and green correspond to *I. setosa*, *I. versicolor* and *I. virginica* classes respectively. For the wine dataset, blue, red and green correspond to the Group 1, Group 2 and Group 3 classes respectively. In panel A, *I. virginica* and *I. versicolor* (green and red respectively) are contained within a single cluster. In panel B, for the wine data set, clear discrimination between the classes is observed.

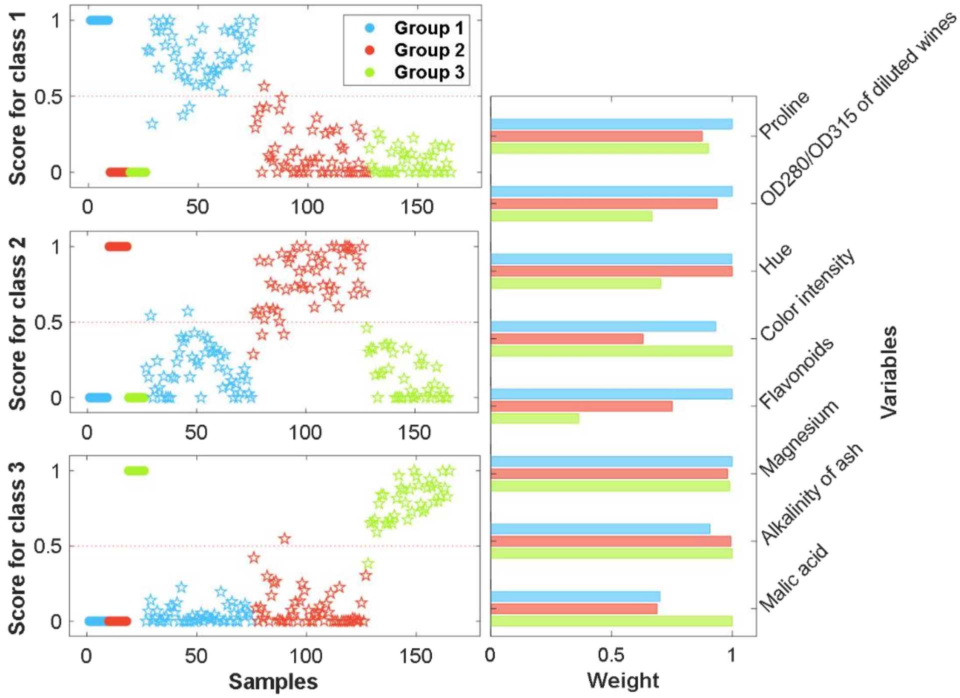

Figure S3. Class and weight profiles for the three classes of the wine dataset, resulting from the application of the EDR-MCR method. The samples belonging to the training and test sets are indicated with color-coded circles and stars respectively.

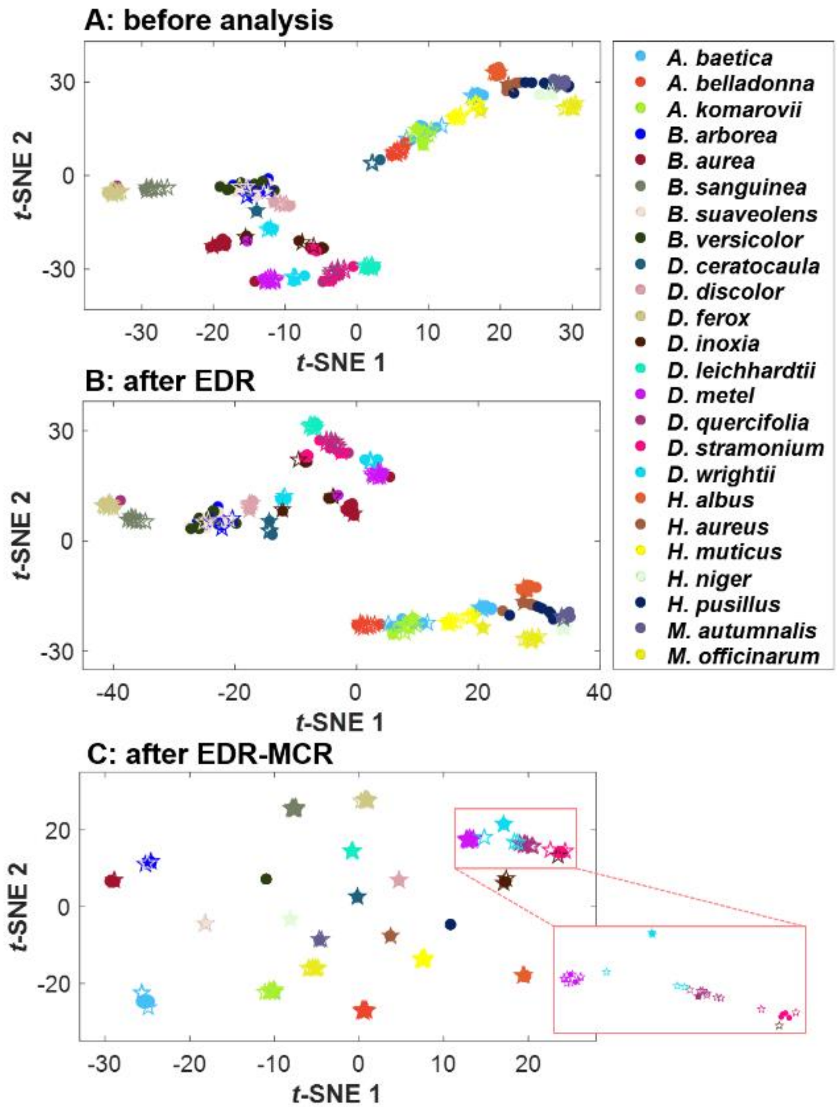

Figure S4. Comparative analysis of the clustering results obtained from the application of various approaches on nightshade species DART-HRMS data (i.e. matrix 219×2976). The samples belonging to training and test sets are illustrated with color-coded circles and stars respectively. A: Results obtained by projection of raw data in *t*-stochastic neighbor embedding space (*t*-SNE) space; B: Results obtained by projection in *t*-SNE space after applying EDR; C: Results obtained by projection in *t*-SNE space after applying EDR-MCR.

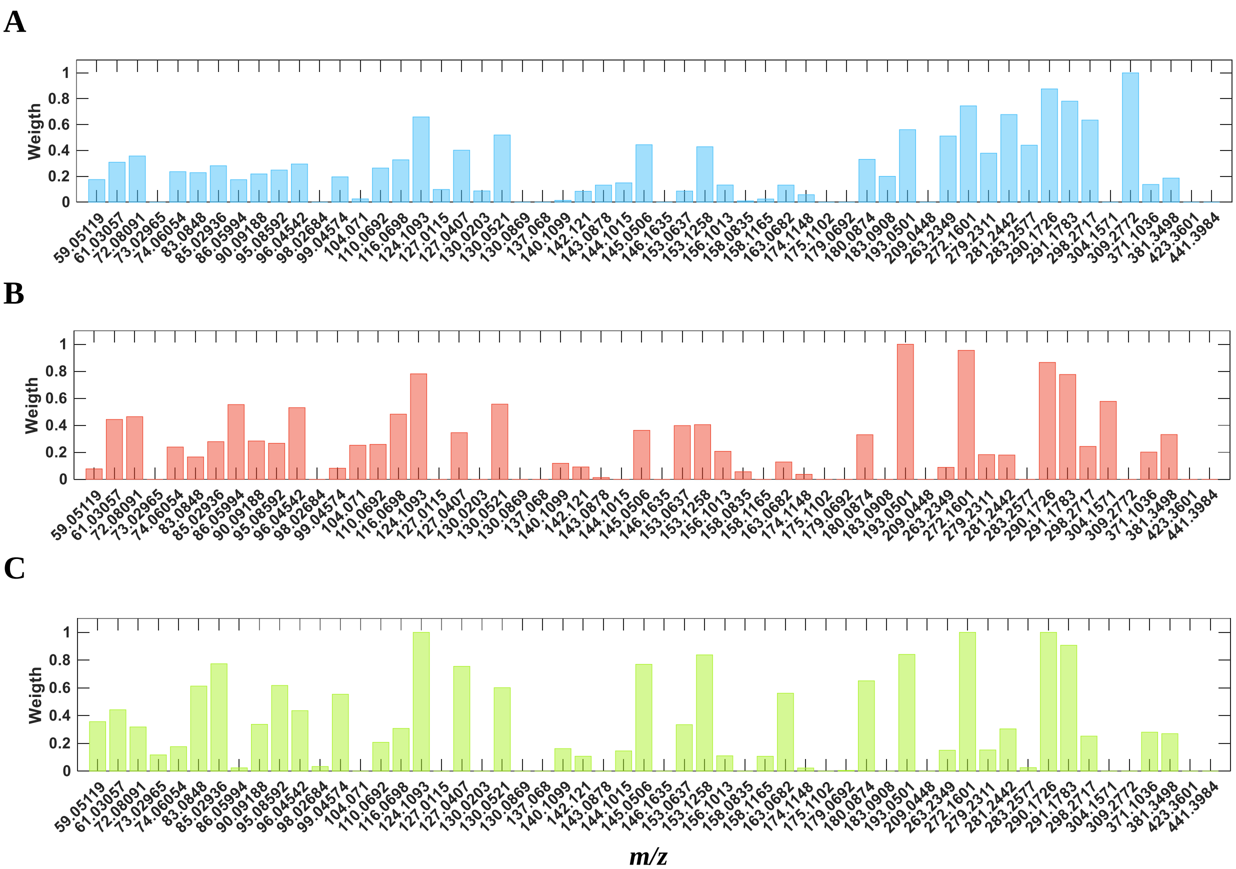

Figure S5. Scaled weight profiles of *Atropa* genus data, resolved by the EDR-MCR method. Panel A: *A. beatica*; Panel B: *A. belladonna*; Panel C *A. komarovii*.

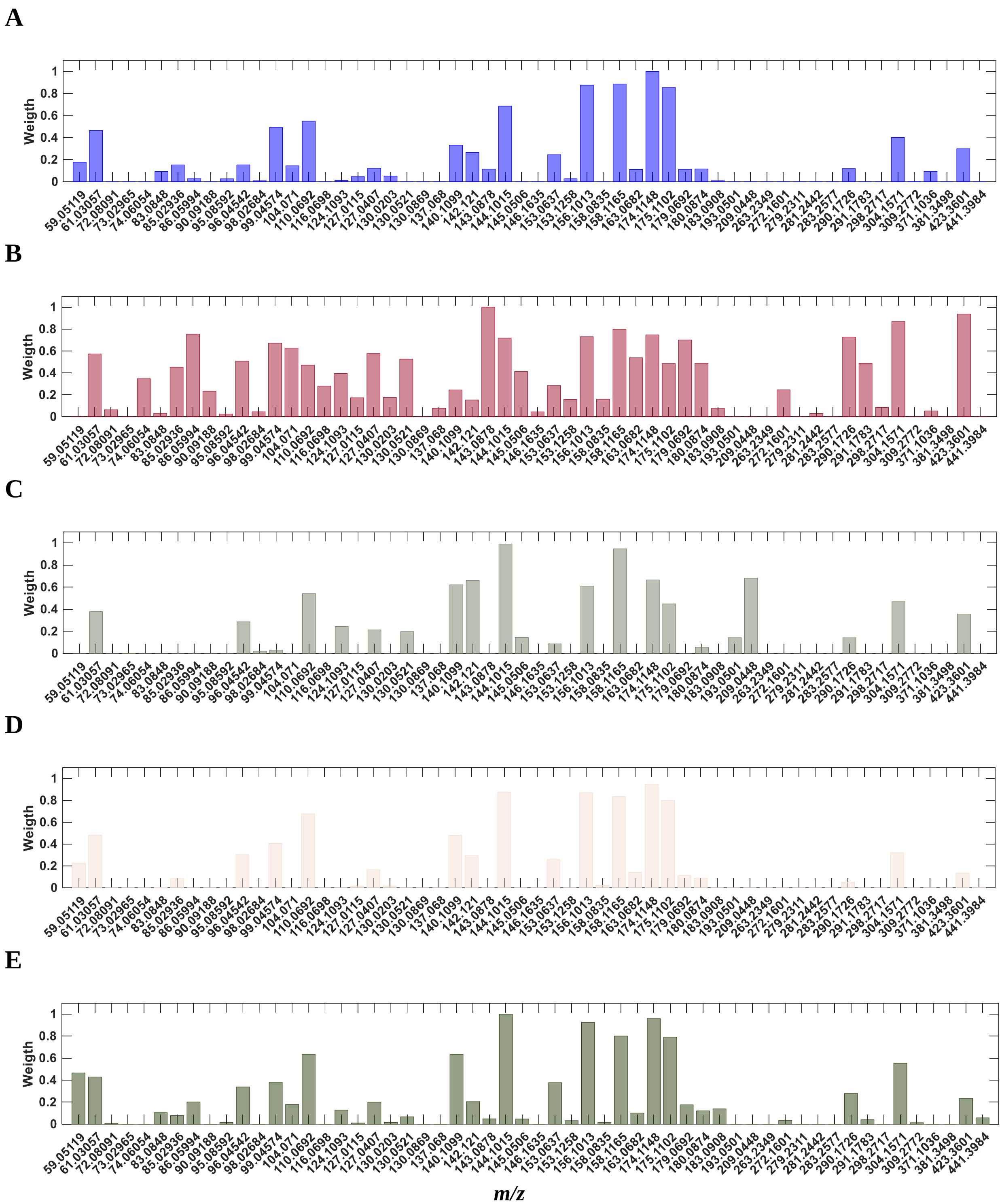

Figure S6. Scaled weight profiles of *Brugmansia* genus data, resolved by the EDR-MCR method. Panel A: *B. arborea*; Panel B: *B. aurea*; Panel C: *B. sanguinea*; Panel D: *B. suaveolens*; Panel E: *B. versicolor*.

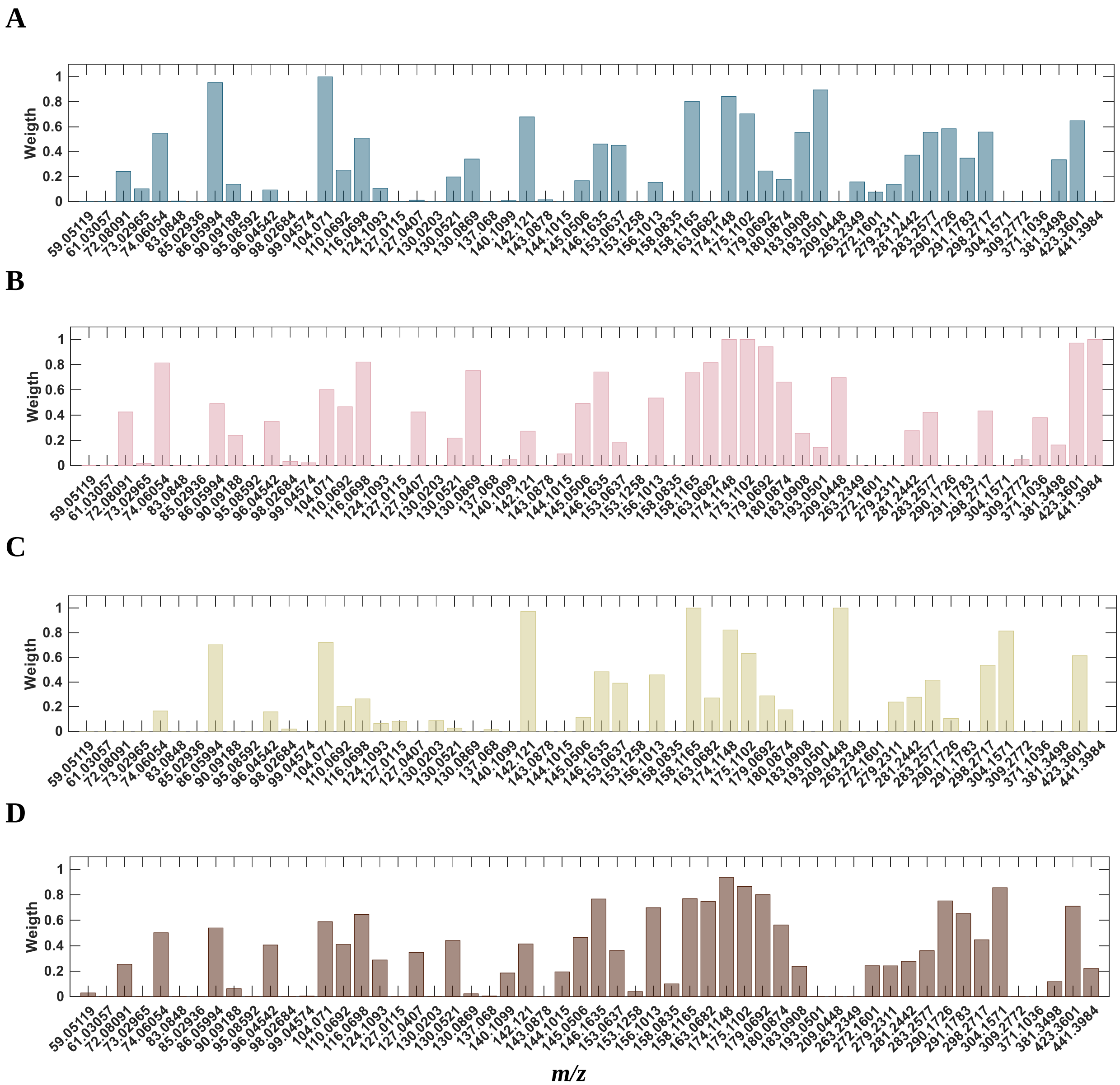

Figure S7. Scaled weight profiles of *Datura* genus data, resolved by the EDR-MCR method. Panel A: *D. ceratocaula*; Panel B: *D. discolor*; Panel C: *D. ferox*; Panel D: *D. inoxia*.

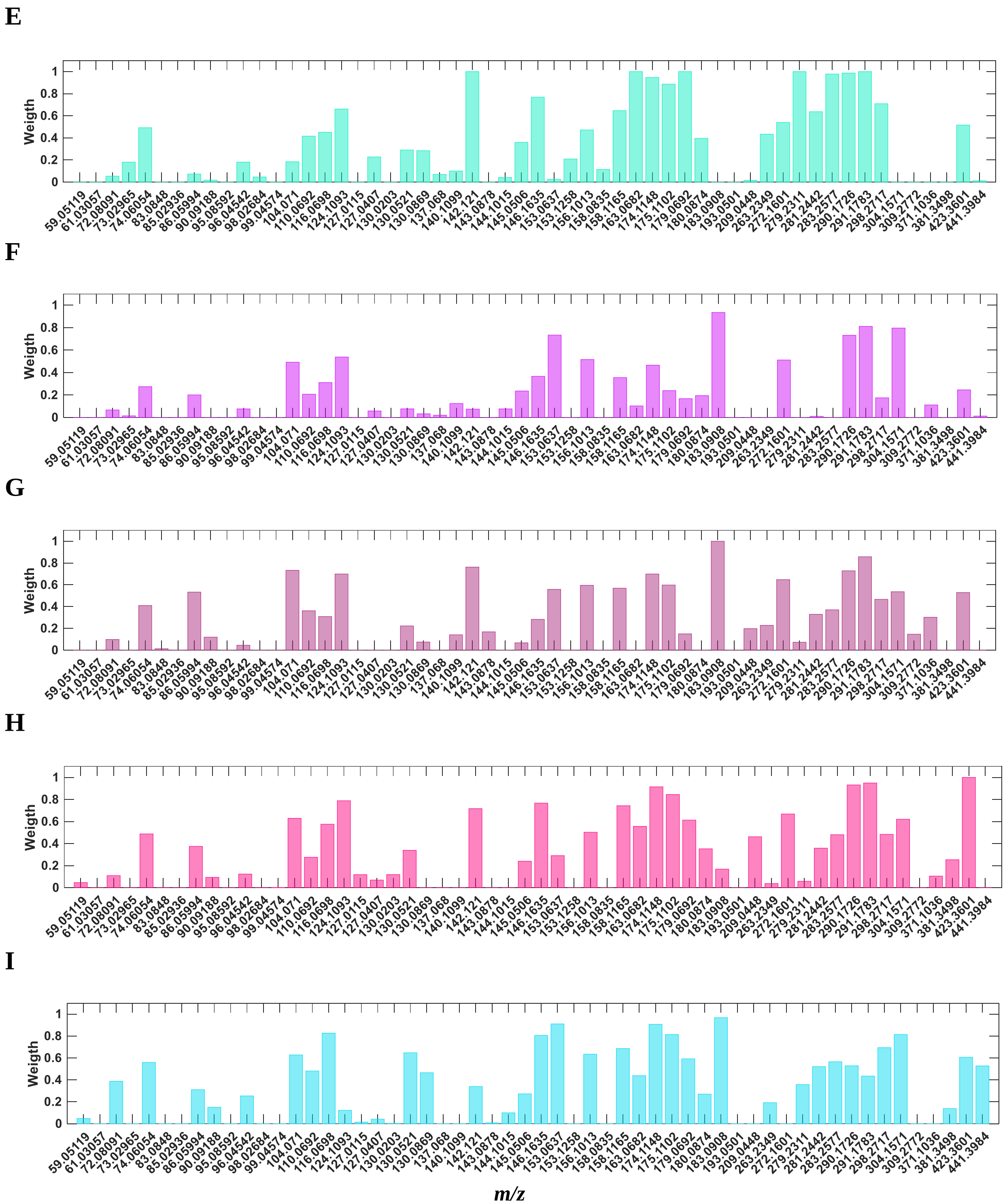

Figure S7 (continued). Scaled weight profiles of *Datura* genus data, resolved by the EDR-MCR method. Panel E: *D. leichhardtii*; Panel F: *D. metel*; Panel G: *D. quercifolia*; Panel H: *D. stramonium*; Panel I: *D. wrightii*.

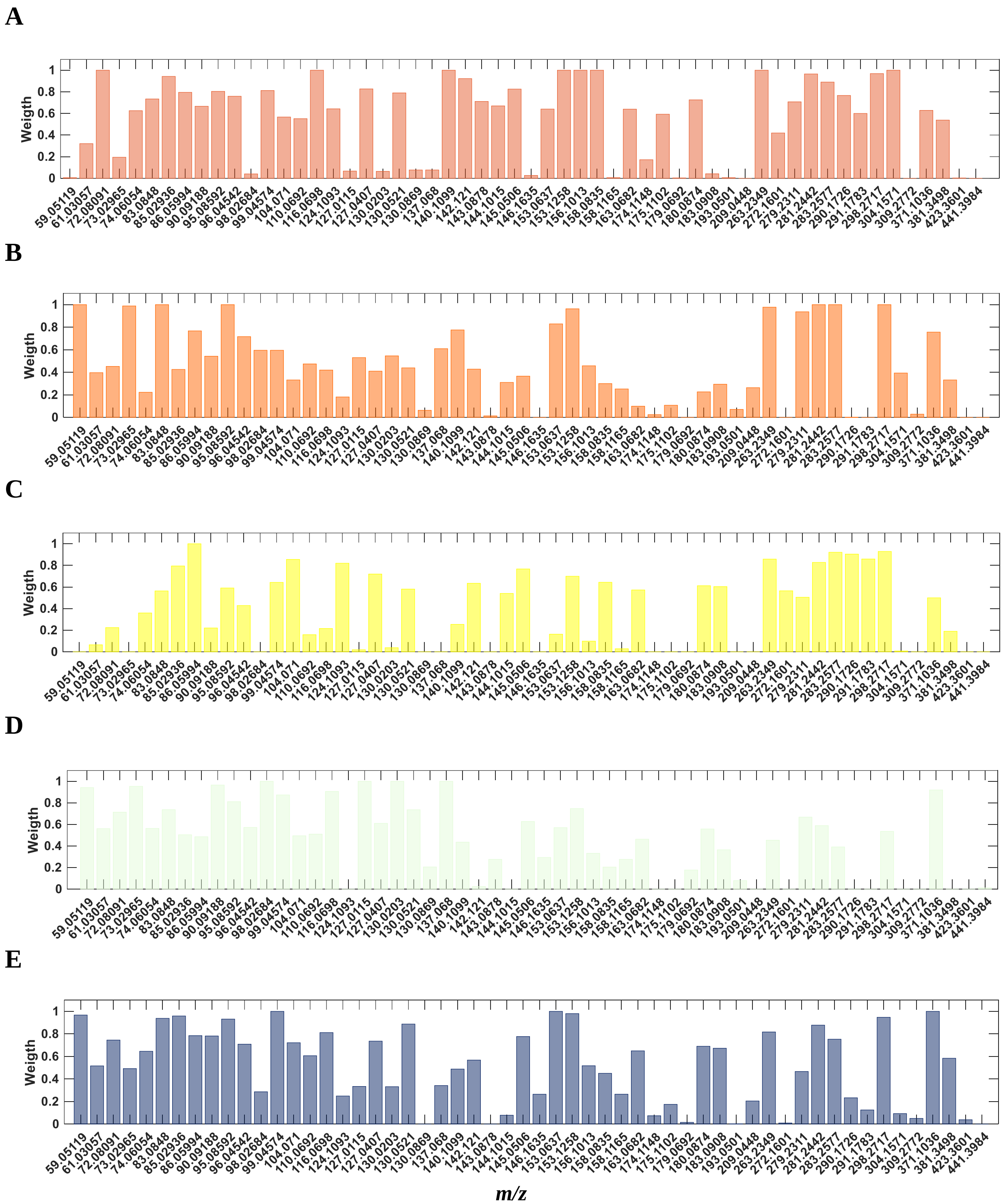

Figure S8. Weight profiles of *Hyoscyamus* genus data, resolved by the EDR-MCR method. Panel A: *H. albus*; Panel B: *H. aureus*; Panel C: *H. muticus*; Panel D: *H. niger*; Panel E: *H. pusillus*.

A

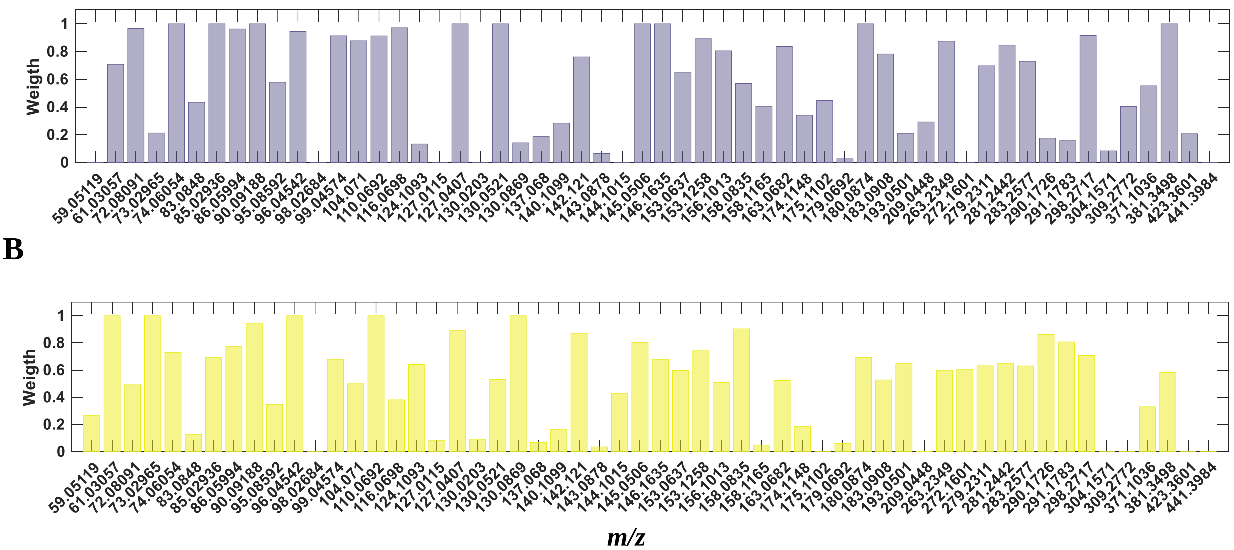

Figure S9. Weight profiles of *Mandragora* genus data, resolved by the EDR-MCR method. Panel A: *M. autumnalis*; Panel B: *M. officinarum*.

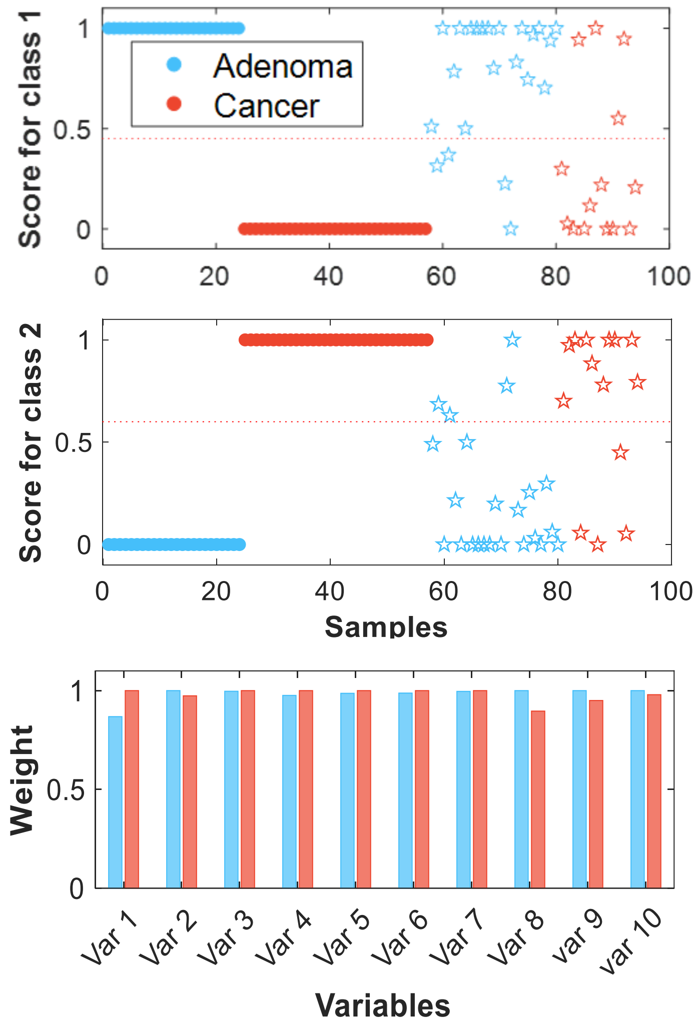

Figure S10. Class and weight profiles for the three classes of the colorectal cancer dataset resulting from the application of the EDR-MCR method. The samples belonging to the training and test sets are indicated with color-coded circles and stars respectively.

Supporting Tables

➢ Iris dataset results

Table S1. Analysis results for the iris dataset. A) number of selected variables; B) samples for the training/test sets for each class resulting from EDR; performance results for prediction of test samples with: C) MCR, D) LDA, E) KNN, F) CART, G) SVM and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S1.

A: Number of selected variables						
All 4 variables are important						
B: Number of selected samples for the training/test set						
Training set			19 (2 *I. setosa*, 9 *I. versicolor*, 8 *I. virginica*)			
Test set			125 (45 *I. setosa*, 38 *I. versicolor*, 42 *I. virginica*)			
C: Performance results for prediction of the test set with "MCR" Number of components: 3; constraints: hard equality and non-negativity.						
Training—Accuracy: 1.00; Not-assigned rate: 0.00			Test—Accuracy: 0.94; Not assigned rate: 0.06 (class assignment threshold 0.5)			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	0.87	1.00	0.93
Specificity	1.00	1.00	1.00	0.97	1.00	0.95
Precision	1.00	1.00	1.00	0.90	1.00	0.91
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 1e-6; regularization parameter: 0.002; coding design: ternary combinations.						
Training—Accuracy: 0.95; Not-assigned rate: 0.00			Test—Accuracy: 0.88; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	0.89	0.88	0.74
Specificity	1.00	1.00	0.90	0.87	1.00	0.95
Precision	1.00	1.00	0.90	0.76	1.00	0.89
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 3; distance function: "Euclidean"; coding design: ternary combinations.						
Training—Accuracy: 0.95; Not-assigned rate: 0.00			Test—Accuracy: 0.86; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.94	1.00	1.00	0.74
Specificity	1.00	1.00	1.00	0.87	0.96	1.00
Precision	1.00	1.00	1.00	0.72	0.87	1.00
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 3; coding design: ternary combinations.						
Training—Accuracy: 0.89; Not-assigned rate: 0.00			Test—Accuracy: 0.83; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	0.78	0.78	0.87	1.00	0.86
Specificity	0.94	0.94	1.00	0.83	0.91	0.99
Precision	0.67	0.88	1.00	0.69	0.89	0.97
G: Performance results for prediction of the test set with "SVM" Box constraint: 9.97e4; kernel scale of linear kernel function: 45.07; coding design: ternary combinations.						
Training—Accuracy: 1.00; Not-assigned rate: 0.00			Test—Accuracy: 0.92; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	1.00	1.00	0.76
Specificity	1.00	1.00	1.00	0.89	1.00	1.00
Precision	1.00	1.00	1.00	0.79	1.00	1.00

Table S1. Continued

H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 2.						
Training—Accuracy: 0.95; Not-assigned rate: 0.00			Test—Accuracy: 0.91; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.89	0.89	1.00	0.83
Specificity	1.00	1.00	1.00	0.92	0.91	0.95
Precision	1.00	1.00	1.00	0.83	0.89	090

Table S2. Analysis results for the iris dataset. A) number of selected variables; B) samples for the training/test sets for each class resulting from the Kennard-stone method; performance results for prediction of test samples with: C) MCR, D) LDA, E) KNN, F) CART, G) SVM and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S1-B.

A: Number of selected variables						
All 4 variables are important						
B: Number of selected samples for the training/test set						
Training set			99 (32 *I. setosa*, 32 *I. versicolor*, 35 *I. virginica*)			
Test set			45 (15 *I. setosa*, 15 *I. versicolor*, 15 *I. virginica*)			
C: Performance results for prediction of the test set with "MCR" Number of components: 3; constraints: hard equality and non-negativity.						
Training—Accuracy: 1.00; Not-assigned rate: 0.00			Test—Accuracy: 0.95; Not assigned rate: 0.04			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	0.85	1.00	1.00
Specificity	1.00	1.00	1.00	1.00	1.00	0.93
Precision	1.00	1.00	1.00	1.00	1.00	0.88
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 2.1e-5; regularization parameter: 0.41; coding design: ternary combinations.						
Training—Accuracy: 0.92; Not-assigned rate:0.00			Test—Accuracy: 1.00; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.84	1.00	0.91	1.00
Specificity	1.00	1.00	0.96	1.00	0.92	1.00
Precision	1.00	1.00	0.90	1.00	0.87	1.00
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 30; distance function: "Cosine"; coding design: ternary combinations.						
Training—Accuracy:0.96; Not-assigned rate: 0.00			Test—Accuracy: 1.00; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.91	1.00	0.97	1.00
Specificity	1.00	1.00	0.99	1.00	0.95	1.00
Precision	1.00	1.00	0.97	1.00	0.92	1.00
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 6.						
Training—Accuracy: 0.95; Not-assigned rate: 0.00			Test—Accuracy: 0.96; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.88	1.00	0.97	0.87
Specificity	1.00	1.00	0.99	0.93	0.94	1.00
Precision	1.00	1.00	0.97	0.88	0.89	1.00
G: Performance results for prediction of the test set with "SVM" Box constraint:59.2; kernel scale of linear kernel function: 0.09; coding design: ternary combinations.						
Training—Accuracy: 0.98; Not-assigned rate: 0.00			Test—Accuracy: 1.00; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.97	1.00	0.97	1.00
Specificity	1.00	1.00	0.99	1.00	0.98	1.00
Precision	1.00	1.00	0.97	1.00	0.97	1.00

Table S2. Continued

H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 2.						
Training—Accuracy: 0.96; Not-assigned rate: 0.00			Test—Accuracy: 0.98; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.91	1.00	0.97	0.93
Specificity	1.00	1.00	0.99	0.97	0.95	1.00
Precision	1.00	1.00	0.97	0.94	0.92	1.00

Table S3. Analysis results for the iris dataset. A) number of selected variables; B) samples for the training/test sets for each class resulting from random selection; performance results for prediction of test samples with: C) MCR, D) LDA, E) KNN, F) CART, G) SVM and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S1-C.

A: Number of selected variables	
All 4 variables are important	
B: Number of selected samples for the training/test set	
Training set	101 (33 *I. setosa*, 33 *I. versicolor*, 35 *I. virginica*)
Test set	43 (14 *I. setosa*, 14 *I. versicolor*, 15 *I. virginica*)

C: Performance results for prediction of the test set with "MCR"
Number of components: 3; constraints: hard equality and non-negativity.

Training—Accuracy: 1.00; Not-assigned rate: 0.00 | Test—Accuracy: 0.90; Not assigned rate: 0.00

	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	0.71	1.00	0.98
Specificity	1.00	1.00	1.00	0.99	1.00	0.86
Precision	1.00	1.00	1.00	0.97	1.00	0.79

D: Performance results for prediction of the test set with "LDA"
Linear coefficient threshold: 1.6e-6; regularization parameter: 0.09; coding design: ternary combinations.

Training—Accuracy: 0.98; Not-assigned rate: 0.00 | Test—Accuracy: 0.98; Not-assigned rate: 0.00

	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.96	0.96	0.98	0.98
Specificity	1.00	1.00	0.99	0.99	0.98	0.98
Precision	1.00	1.00	0.98	0.98	0.97	0.96

E: Performance results for prediction of the test set with "KNN"
Number of neighbors: 19; distance function: "cosine"; coding design: ternary combinations.

Training—Accuracy: 0.98; Not-assigned rate: 0.00 | Test—Accuracy: 0.98; Not-assigned rate: 0.00

	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.93	0.95	1.00	1.00
Specificity	1.00	1.00	1.00	1.00	0.97	0.97
Precision	1.00	1.00	1.00	1.00	0.94	0.95

F: Performance results for prediction of the test set with "CART"
Maximum number of leaves: 3.

Training—Accuracy: 0.97; Non-error rate: 0.00 | Test—Accuracy: 0.95; Non-error rate: 0.00

	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.94	0.93	0.98	0.92
Specificity	1.00	1.00	0.99	0.96	0.97	0.96
Precision	1.00	1.00	0.97	0.92	0.94	0.93

G: Performance results for prediction of the test set with "SVM"
Box constraint: 297; kernel scale of linear kernel function: 0.86; coding design: ternary combinations.

Training—Accuracy: 0.99; Not-assigned rate: 0.00 | Test—Accuracy: 0.96; Not-assigned rate: 0.00

	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.98	0.94	0.98	0.95
Specificity	1.00	1.00	0.99	0.97	0.99	0.97
Precision	1.00	1.00	0.98	0.94	0.98	0.95

Table S3. Continued

H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 2.						
Training—Accuracy: 0.97; Not-assigned rate: 0.00			Test—Accuracy: 0.96; Not-assigned rate: 0.00			
	I. setosa		*I. versicolor*		*I. virginica*	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.93	0.94	0.97	0.95
Specificity	1.00	1.00	0.98	0.97	0.96	0.97
Precision	1.00	1.00	0.97	0.94	0.93	0.95

➢ Wine dataset results

Table S4. Analysis results for the wine dataset. A) Number of selected variables; B) samples for the training/test set for each class resulting from EDR; performance results for prediction of test samples with C) MCR, D) LDA, E) KNN, F) CART, G) SVM, and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S2-A.

A: Number of selected variables

The 8 variables are importance: malic acid, alkalinity of ash, magnesium, flavonoids, color intensity, hue, OD280/OD315 of diluted wines, proline

B: Number of selected samples for the training/test set

Training set	59 (7 group 1, 32 group 2, 20 group 3)
Test set	106 (51 group 1, 29 group 2, 26 group 3)

C: Performance results for prediction of the test set with "MCR" (4 components is used)
Number of components: 4; constraints: hard equality and non-negativity.

Training—Accuracy: 1.00; Not-assigned rate: 0.00. | Test—Accuracy: 0.97; Not assigned rate: 0.01 (class assignment threshold 0.5)

	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	0.96	1.00	0.97	1.00	1.00
Specificity	1.00	0.98	1.00	0.97	1.00	1.00
Precision	1.00	0.98	1.00	0.93	1.00	1.00

D: Performance results for prediction of the test set with "LDA"
Linear coefficient threshold: 1.62e-6; regularization parameter: 0.09; coding design: ternary combinations.

Training—Accuracy: 0.97; Not-assigned rate: 0.00. | Test—Accuracy: 1.00; Not-assigned rate: 0.00.

	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.94	1.00	1.00	1.00
Specificity	1.00	1.00	1.00	1.00	0.95	1.00
Precision	1.00	1.00	1.00	1.00	0.91	1.00

E: Performance results for prediction of the test set with "KNN"
Number of neighbors: 3; distance function: "Euclidean"; coding design: ternary combinations.

Training—Accuracy: 0.95; Not-assigned rate: 0.00. | Test—Accuracy: 0.97; Not-assigned rate: 0.00.

	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	0.86	0.94	0.97	1.00	0.95	1.00
Specificity	1.00	1.00	0.93	0.96	0.97	1.00
Precision	1.00	1.00	0.94	0.91	0.95	1.00

F: Performance results for prediction of the test set with "CART"
Maximum number of leaves: 5; coding design: ternary combinations.

Training—Accuracy: 0.93; Not-assigned rate: 0.00. | Test—Accuracy: 0.90; Not-assigned rate: 0.00.

	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	0.71	0.78	0.97	1.00	0.95	1.00
Specificity	1.00	1.00	0.89	0.86	0.97	1.00
Precision	1.00	1.00	0.91	0.73	0.95	1.00

G: Performance results for prediction of the test set with "SVM"
Box constraint: 9.9e4; kernel scale of linear kernel function: 88.09; coding design: ternary combinations.

Training—Accuracy:0.98; Not-assigned rate: 0.00. | Test—Accuracy: 0.99; Not-assigned rate: 0.00.

	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	0.98	1.00	1.00	0.95	1.00
Specificity	1.00	1.00	0.96	0.99	1.00	1.00
Precision	1.00	1.00	0.97	0.97	1.00	1.00

Table S4. Continued

H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 4.						
Training—Accuracy:0.93; Not-assigned rate: 0.00.			Test—Accuracy: 0.98; Not-assigned rate: 0.00.			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	0.86	0.96	0.91	1.00	1.00	1.00
Specificity	0.98	1.00	0.96	0.97	0.95	1.00
Precision	0.86	1.00	0.97	0.93	0.91	1.00

Table S5. Analysis results for the wine dataset. A) Number of selected variables; B) samples for the training/test sets for each class resulting from the Kennard-Stone method; performance results for prediction of test samples with: C) MCR, D) LDA, E) KNN, F) CART, G) SVM and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S2-B.

A: Number of selected variables						
All 4 variables are important						
B: Number of selected samples for the training/test set						
Training set			114 (40 group 1, 42 group 2, 30 group 3)			
Test set			51 (18 group 1, 19 group 2, 14 group 3)			
C: Performance results for prediction of the test set with "MCR" Number of components: 3; constraints: hard equality and non-negativity.						
Training—Accuracy: 1.00; Not-assigned rate: 0.00			Test—Accuracy: 0.98; Not assigned rate: 0.00 (class assignment threshold)			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	0.95	1.00	1.00
Specificity	1.00	0.97	1.00	1.00	1.00	1.00
Precision	1.00	0.95	1.00	1.00	1.00	1.00
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 2e-5; regularization parameter: 0.41; coding design: ternary combinations.						
Training—Accuracy: 0.97; Not-assigned rate: 0.00			Test—Accuracy: 1.00; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.93	1.00	1.00	1.00
Specificity	1.00	1.00	1.00	1.00	0.96	1.00
Precision	1.00	1.00	1.00	1.00	0.91	1.00
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 25; distance function: "cityblock"; coding design: ternary combinations.						
Training—Accuracy: 0.98; Not-assigned rate: 0.00			Test—Accuracy: 1.00; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.98	1.00	0.97	1.00
Specificity	1.00	1.00	0.99	1.00	0.99	1.00
Precision	1.00	1.00	0.98	1.00	0.97	1.00
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 3; coding design: ternary combinations.						
Training—Accuracy: 1.00; Non-error rate: 0.00			Test—Accuracy: 0.96; Non-error rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	0.95	1.00	0.93
Specificity	1.00	0.97	1.00	0.97	1.00	1.00
Precision	1.00	0.95	1.00	0.95	1.00	1.00
G: Performance results for prediction of the test set with "SVM" Box constraint: 12.05; kernel scale of linear kernel function:.5.07; coding design: ternary combinations.						
Training—Accuracy: 1.00; Not-assigned rate: 0.00			Test—Accuracy: 1.00; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	1.00	1.00	1.00	1.00
Specificity	1.00	1.00	1.00	1.00	0.99	1.00
Precision	1.00	1.00	1.00	1.00	0.97	1.00

Table S5. Continued

H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 4.						
Training—Accuracy: 0.95; Not-assigned rate: 0.00			Test—Accuracy: 0.98; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	0.95	1.00	0.90	0.95	1.00	1.00
Specificity	0.97	0.97	0.97	1.00	0.98	1.00
Precision	0.95	0.95	0.95	1.00	0.94	1.00

Table S6. Analysis results for the wine dataset. A) Number of selected variables; B) samples for the training/test sets for each class resulting from random selection; performance results for prediction of test samples with: C) MCR, D) LDA, E) KNN, F) CART, G) SVM and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S2-C.

A: Number of selected variables						
All 4 variables are important						
B: Number of selected samples for the training/test set						
Training set			116 (41 group 1, 42 group 2, 33 group 3)			
Test set			49 (17 group 1, 19 group 2, 13 group 3)			
C: Performance results for prediction of the test set with "MCR" Number of components: 3; constraints: hard equality and non-negativity.						
Training—Accuracy: 1.00; Not-assigned rate: 0.00			Test—Accuracy: 0.93; Not assigned rate: 0.00 (class assignment threshold)			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	0.95	1.00	0.88	1.00	0.98
Specificity	1.00	0.96	1.00	0.96	1.00	0.98
Precision	1.00	0.93	1.00	0.94	1.00	0.94
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 2.8e-6; regularization parameter: 0.45; coding design: ternary combinations.						
Training—Accuracy: 0.98; Not-assigned rate: 0.00			Test—Accuracy: 0.97; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.96	0.92	1.00	1.00
Specificity	0.99	0.98	1.00	1.00	0.98	0.97
Precision	0.99	0.97	1.00	1.00	0.96	0.93
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 3; distance function: "Euclidean"; coding design: ternary combinations.						
Training—Accuracy: 0.99; Not-assigned rate: 0.00			Test—Accuracy: 0.98; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.97	0.95	0.99	0.98
Specificity	0.99	0.99	1.00	0.99	0.99	0.99
Precision	0.99	0.98	0.99	0.99	0.98	0.97
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 2; coding design: ternary combinations.						
Training—Accuracy: 0.99; Non-error rate: 0.00			Test—Accuracy: 0.94; Non-error rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	0.99	0.96	0.99	0.92	0.99	0.93
Specificity	1.00	0.98	0.99	0.95	1.00	0.97
Precision	1.00	0.97	0.98	0.91	0.99	0.93
G: Performance results for prediction of the test set with "SVM" Box constraint: 1.03e-5; kernel scale of linear kernel function: 0.007; coding design: ternary combinations.						
Training—Accuracy: 0.99; Not-assigned rate: 0.00			Test—Accuracy: 0.98; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	1.00	1.00	0.97	0.96	0.99	0.98
Specificity	0.99	0.99	1.00	0.99	0.99	0.99
Precision	0.99	0.98	1.00	0.99	0.98	0.97

Table S6. Continued

H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 4.						
Training—Accuracy: 0.96; Not-assigned rate: 0.00			Test—Accuracy: 0.94; Not-assigned rate: 0.00			
	Group 1		Group 2		Group 3	
	Training	Test	Training	Test	Training	Test
Sensitivity	0.96	0.97	0.92	0.89	1.00	0.98
Specificity	0.97	0.96	0.98	0.97	0.98	0.98
Precision	0.95	0.93	0.96	0.95	0.96	0.94

➢ Nightshade plant family DART-HRMS dataset results (for 24 species)

Table S7. Vertices that were computed for the convex sets in PCA space resulting in: A) important variables; B) number of samples in each class that were partitioned into training and test sets using EDR.

A: Selected *m/z* values (56 in total)		
59.0512, 61.0306, 72.0809, 73.0296, 74.0605, 83.0848, 85.0294, 86.0599, 90.0919, 95.0859, 96.0454, 98.0268, 99.0457, 104.0710, 110.0692, 116.0698, 124.1093, 127.0115, 127.0407, 130.0203, 130.0521, 130.0869, 137.0680, 140.1099, 142.1210, 143.0878, 144.1015, 145.0506, 146.1635, 153.0637, 153.1258, 156.1013, 158.0835, 158.1165, 163.0682, 174.1148, 175.1102, 179.0692, 180.0874, 183.0908, 193.0501, 209.0448, 263.2349, 272.1601, 279.2311, 281.2442, 283.2577, 290.1726, 291.1783, 298.2717, 304.1571, 309.2772, 371.1036, 381.3498, 423.3601, 441.3984		
B: Number of selected samples for training/test sets		
	Training set (109)	Test set (110)
A. beatica	13	5
A. belladonna	2	8
A. komarovii	2	8
B .arborea	7	3
B. aurea	8	2
B. sanguinea	2	8
B. suaveolens	5	3
B. versicolor	8	0
D. ceratocaula	2	3
D. discolor	2	5
D. ferox	2	8
D. inoxia	7	3
D. leichhardtii	2	6
D. metel	2	9
D. quercifolia	2	8
D. stramonium	8	2
D. wrightii	5	5
H. albus	6	3
H. aureus	5	1
H. muticus	2	8
H. niger	2	2
H. pusillus	7	0
M. autumnalis	6	2
M. officinarum	2	8

Table S8. Performance result for A: KNN; and B: CART for prediction of the training set resulting from EDR for the nightshade family dataset.

Method	**A: KNN** Number of neighbors: 2; distance function: "correlation"; coding design: sparse ternary combinations. Not-assigned rate: 0.00.			**B: CART** Maximum number of leaves: 5. coding design: sparse ternary combinations. Not-assigned rate: 0.00.		
Accuracy	0.82			1.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	0.97	0.81	1.00	1.00	1.00
A. belladonna	0.50	1.00	1.00	1.00	1.00	1.00
A. komarovii	0.00	0.99	0.00	1.00	1.00	1.00
B .arborea	1.00	0.98	0.78	1.00	1.00	1.00
B. aurea	0.88	1.00	1.00	1.00	1.00	1.00
B. sanguinea	0.00	0.98	0.00	1.00	1.00	1.00
B. suaveolens	0.60	1.00	1.00	1.00	1.00	1.00
B. versicolor	0.75	0.98	0.75	1.00	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	0.50	1.00	1.00	1.00	1.00	1.00
D. inoxia	0.86	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	0.50	1.00	1.00	1.00	1.00	1.00
D. quercifolia	0.00	1.00	0.00	1.00	1.00	1.00
D. stramonium	1.00	0.98	0.80	1.00	1.00	1.00
D. wrightii	1.00	0.97	0.63	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	0.97	0.63	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	0.00	1.00	0.00	1.00	1.00	1.00
H. pusillus	0.86	0.98	0.75	1.00	1.00	1.00
M. autumnalis	0.83	1.00	1.00	1.00	1.00	1.00
M. officinarum	0.50	1.00	1.00	1.00	1.00	1.00

Table S9. Performance results for A: LDA and B: PLS-DA for prediction of the training set resulting from EDR for the nightshade family dataset.

Method	**A: LDA** Linear coefficient threshold: 1.57e-6; regularization parameter: 0.05; coding design: sparse ternary combinations. Not-assigned rate: 0.00.			**B: PLS-DA** Number of latent variables: 25. Not-assigned rate: 0.00.		
Accuracy	1.00			0.95		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	1.00	1.00	1.00	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	1.00	1.00	1.00	1.00	1.00	1.00
B .arborea	1.00	1.00	1.00	0.86	0.98	0.75
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	1.00	1.00	1.00	0.50	1.00	1.00
B. suaveolens	1.00	1.00	1.00	0.40	1.00	1.00
B. versicolor	1.00	1.00	1.00	1.00	0.97	0.73
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S10. Performance results for A: SVM; and B: MCR for prediction of the training set resulting from EDR for the nightshade family dataset.

Method	**A: SVM** Box constraint: 120.63; kernel scale of linear kernel function: 0.50; coding design: sparse ternary combinations. Not-assigned rate: 0.00.			**B: MCR** Component numbers: 24; constraints: hard equality and non-negativity. Not-assigned rate: 0.00.		
Accuracy	1.00			1.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	1.00	1.00	1.00	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	1.00	1.00	1.00	1.00	1.00	1.00
B .arborea	1.00	1.00	1.00	1.00	1.00	1.00
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	1.00	1.00	1.00	1.00	1.00	1.00
B. suaveolens	1.00	1.00	1.00	1.00	1.00	1.00
B. versicolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S11. Performance results for A: KNN; and B: CART for prediction of the test set resulting from EDR for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-A.

Method	**A: KNN**			**B: CART**		
	Accuracy: 0.62; Not-assigned rate: 0.00.			Accuracy: 0.61; Not-assigned rate: 0.00.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	0.89	0.29	1.00	0.90	0.33
A. belladonna	0.50	1.00	1.00	0.88	1.00	1.00
A. komarovii	0.00	0.98	0.00	0.13	0.99	0.50
B .arborea	0.33	0.99	0.50	0.67	0.97	0.40
B. aurea	1.00	0.99	0.67	1.00	0.98	0.50
B. sanguinea	0.63	0.99	0.83	0.00	0.99	0.00
B. suaveolens	0.67	0.98	0.50	0.67	0.99	0.67
B. versicolor	No test sample	0.99	No test sample	No test sample	0.95	No test sample
D. ceratocaula	0.67	1.00	1.00	0.67	1.00	1.00
D. discolor	1.00	1.00	1.00	0.60	1.00	1.00
D. ferox	0.88	1.00	1.00	0.88	1.00	1.00
D. inoxia	1.00	0.97	0.50	1.00	0.93	0.27
D. leichhardtii	1.00	1.00	1.00	1.00	0.99	0.86
D. metel	0.11	1.00	1.00	0.22	1.00	1.00
D. quercifolia	0.00	1.00	0.00	0.00	1.00	0.00
D. stramonium	1.00	0.89	0.14	1.00	0.94	0.22
D. wrightii	1.00	0.97	0.63	0.80	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	0.63	1.00	1.00
H. niger	0.00	1.00	0.00	1.00	1.00	1.00
H. pusillus	No test sample	0.97	No test sample	No test sample	0.99	No test sample
M. autumnalis	1.00	0.99	0.67	1.00	0.98	0.50
M. officinarum	0.5	1	1	0.75	1.00	1.00

Table S12. Performance results for A: LDA; and B: PLS-DA for prediction of the test set resulting from EDR for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-A.

Method	**A: LDA**			**B: PLS-DA**		
	Accuracy: 0.80; Not-assigned rate: 0.00.			Accuracy: 0.82; Not-assigned rate: 0.00.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	0.95	0.50	1.00	0.94	0.45
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	0.38	1.00	1.00	0.25	1.00	1.00
B .arborea	0.67	1.00	1.00	0.33	0.98	0.33
B. aurea	1.00	1.00	1.00	1.00	0.99	0.67
B. sanguinea	1.00	1.00	1.00	0.88	0.99	0.88
B. suaveolens	0.67	1.00	1.00	0.33	0.98	0.33
B. versicolor	No test sample	0.98	No test sample	No test sample	1.00	No test sample
D. ceratocaula	1.00	1.00	1.00	0.67	1.00	1.00
D. discolor	0.80	1.00	1.00	0.80	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	0.97	0.50	1.00	0.99	0.75
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	0.44	1.00	1.00	0.56	1.00	1.00
D. quercifolia	0.13	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	0.95	0.29	1.00	1.00	1.00
D. wrightii	1.00	0.94	0.45	1.00	0.96	0.56
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	0.99	0.89	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	No test sample	1.00	No test sample	No test sample	1.00	No test sample
M. autumnalis	1.00	1.00	1.00	1.00	0.98	0.50
M. officinarum	0.75	1.00	1.00	0.75	1.00	1.00

Table S13. Performance results for A: SVM; and B: MCR for prediction of the test set resulting from EDR for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-A.

Method	**A: SVM**			**B: MCR**		
	Accuracy: 0.80; Not-assigned rate: 0.00.			Accuracy: 0.96; Not-assigned rate: 0.05.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	0.95	0.50	0.80	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	0.38	1.00	1.00	1.00	0.99	0.89
B .arborea	0.33	0.98	0.33	0.67	0.99	0.67
B. aurea	1.00	0.99	0.67	1.00	1.00	1.00
B. sanguinea	1.00	1.00	1.00	1.00	1.00	1.00
B. suaveolens	0.33	0.99	0.50	0.67	0.99	0.67
B. versicolor	No test sample	1.00	No test sample	No test sample	1.00	No test sample
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	0.98	0.60	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	0.56	1.00	1.00	1.00	1.00	1.00
D. quercifolia	0.13	1.00	1.00	1.00	0.99	0.89
D. stramonium	1.00	0.94	0.25	1.00	1.00	1.00
D. wrightii	1.00	0.97	0.63	0.67	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	0.99	0.89	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	No test sample	1.00	No test sample	No test sample	1.00	0.00
M. autumnalis	1.00	0.99	0.67	1.00	1.00	1.00
M. officinarum	0.75	1.00	1.00	1.00	1.00	1.00

Table S14. Number of samples in each class for nightshade data that were partitioned into training and test sets using Kennard-Stone method.

Number of selected samples for training/test sets		
	Training set (170)	Test set (49)
A. beatica	14	4
A. belladonna	8	2
A. komarovii	8	2
B .arborea	8	2
B. aurea	8	2
B. sanguinea	8	2
B. suaveolens	6	2
B. versicolor	6	2
D. ceratocaula	4	1
D. discolor	5	2
D. ferox	8	2
D. inoxia	8	2
D. leichhardtii	6	2
D. metel	8	3
D. quercifolia	8	2
D. stramonium	8	2
D. wrightii	8	2
H. albus	7	2
H. aureus	4	2
H. muticus	8	2
H. niger	3	1
H. pusillus	5	2
M. autumnalis	6	2
M. officinarum	8	2

Table S15. Performance result for A: KNN; and B: CART for prediction of the training set resulting from the Kennard-Stone method for the nightshade family dataset.

Method	**A: KNN** Number of neighbors: 2; distance function: "cosine"; coding design: sparse ternary combinations. Not-assigned rate: 0.00			**B: CART** Maximum number of leaves: 6; coding design: sparse ternary combinations. Not-assigned rate: 0.00		
Accuracy	0.85			0.98		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	0.98	0.82	1.00	0.99	0.93
A. belladonna	0.88	1.00	1.00	1.00	1.00	1.00
A. komarovii	0.75	1.00	1.00	0.88	1.00	1.00
B .arborea	0.75	0.97	0.55	1.00	0.99	0.80
B. aurea	0.88	1.00	1.00	1.00	1.00	1.00
B. sanguinea	0.88	0.99	0.88	0.88	1.00	1.00
B. suaveolens	0.50	0.97	0.38	1.00	1.00	1.00
B. versicolor	0.00	0.99	0.00	0.83	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	0.99	0.89	1.00	1.00	1.00
D. inoxia	0.75	0.99	0.86	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	0.88	0.99	0.88	1.00	1.00	1.00
D. quercifolia	0.63	0.99	0.83	1.00	1.00	1.00
D. stramonium	1.00	0.98	0.67	1.00	1.00	1.00
D. wrightii	0.88	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	0.99	0.67	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	0.60	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S16. Performance results for A: LDA and B: PLS-DA for prediction of the training set resulting from the Kennard-Stone method for the nightshade family dataset.

Method	**A: LDA** Linear coefficient threshold: 1.86e-5; regularization parameter: 1.37e-4; coding design: sparse ternary combinations. Not-assigned rate: 0.00			**B: PLS-DA** Number of latent variables: 25 Not-assigned rate: 0.00		
Accuracy	0.99			0.96		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	1.00	1.00	0.86	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	1.00	1.00	1.00	1.00	0.99	0.80
B .arborea	1.00	0.99	0.89	0.88	0.98	0.70
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	0.88	1.00	1.00	0.88	1.00	1.00
B. suaveolens	1.00	1.00	1.00	0.67	0.99	0.80
B. versicolor	1.00	1.00	1.00	0.83	0.99	0.83
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S17. Performance results for A: SVM; and B: MCR for prediction of the training set resulting from Kennard-Stone method for the nightshade family dataset.

Method	**A: SVM** Box constraint: 12.92; kernel scale of linear kernel function: 0.97; coding design: sparse ternary combinations. Not-assigned rate:0.00			**B: MCR** Component numbers: 24; constraints: hard equality and non-negativity. Not-assigned rate: 0.00		
Accuracy	1.00			1.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	1.00	1.00	1.00	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	1.00	1.00	1.00	1.00	1.00	1.00
B .arborea	1.00	1.00	1.00	1.00	1.00	1.00
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	1.00	1.00	1.00	1.00	1.00	1.00
B. suaveolens	1.00	1.00	1.00	1.00	1.00	1.00
B. versicolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S18. Performance results for A: KNN; and B: CART for prediction of the test set resulting from the Kennard-Stone method for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-B.

Method	**A: KNN**			**B: CART**		
	Accuracy: 0.90; Not-assigned rate: 0.00.			Accuracy: 0.78; Not-assigned rate: 0.00.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	0.98	0.80	1.00	0.98	0.80
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	0.50	1.00	1.00	0.50	1.00	1.00
B .arborea	1.00	0.98	0.67	0.50	0.96	0.33
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	1.00	1.00	1.00	1.00	1.00	1.00
B. suaveolens	0.50	0.98	0.50	0.00	0.96	0.00
B. versicolor	0.50	1.00	1.00	0.50	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	0.98	0.50
D. discolor	1.00	1.00	1.00	0.00	1.00	0.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	0.00	1.00	0.00	0.50	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	0.98	0.75
D. quercifolia	1.00	1.00	1.00	1.00	0.98	0.67
D. stramonium	1.00	0.96	0.50	0.50	0.98	0.50
D. wrightii	1.00	1.00	1.00	1.00	0.98	0.67
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	0.98	0.67
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	0.50	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	0.50	1.00	1.00

Table S19. Performance results for A: LDA; and B: PLS-DA for prediction of the test set resulting from the Kennard-Stone method for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-B.

Method	**A: LDA**			**B: PLS-DA**		
	Accuracy: 0.92; Not-assigned rate: 0.00.			Accuracy: 0.94; Not-assigned rate: 0.00.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	1.00	1.00	1.00	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	1.00	1.00	1.00	1.00	1.00	1.00
B .arborea	1.00	0.96	0.50	1.00	0.98	0.67
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	1.00	1.00	1.00	1.00	1.00	1.00
B. suaveolens	0.50	0.98	0.50	0.50	0.98	0.50
B. versicolor	0.50	1.00	1.00	0.50	0.98	0.50
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	0.50	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	0.98	0.67	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	0.50	1.00	1.00	1.00	1.00	1.00
M. autumnalis	0.50	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S20. Performance results for A: SVM; and B: MCR for prediction of the test set resulting from the Kennard-Stone method for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-B.

Method	**A: SVM**			**B: MCR**		
	Accuracy: 0.92; Not-assigned rate: 0.00.			Accuracy: 0.90; Not-assigned rate: 0.00.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	1.00	1.00	1.00	0.50	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	1.00	1.00	1.00	1.00	0.96	0.50
B .arborea	0.00	0.96	0.00	0.50	0.98	0.50
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	1.00	0.98	0.67	1.00	1.00	1.00
B. suaveolens	0.50	0.98	0.50	0.50	0.96	0.33
B. versicolor	0.50	1.00	1.00	0.50	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S21. Number of samples in each class that were partitioned into training and test sets using random sampling.

Number of selected samples for training/test sets		
	Training set (176)	Test set (43)
A. beatica	15	3
A. belladonna	8	2
A. komarovii	8	2
B .arborea	7	3
B. aurea	8	2
B. sanguinea	8	2
B. suaveolens	7	1
B. versicolor	6	2
D. ceratocaula	4	1
D. discolor	6	1
D. ferox	8	2
D. inoxia	8	2
D. leichhardtii	7	1
D. metel	9	2
D. quercifolia	8	2
D. stramonium	8	2
D. wrightii	8	2
H. albus	8	1
H. aureus	5	1
H. muticus	7	3
H. niger	3	1
H. pusillus	6	1
M. autumnalis	7	1
M. officinarum	7	3

Table S22. Performance result for A: KNN; and B: CART for prediction of the training set resulting from 100 replicates of random selection for the nightshade family dataset.

Method	**A: KNN** Number of neighbors: 2; distance function: “correlation”; coding design: sparse ternary combinations. Not-assigned rate: 0.00			**B: CART** Maximum number of leaves: 2; coding design: sparse ternary combinations. Not-assigned rate: 0.00.		
Accuracy	0.90			1.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	0.99	0.99	0.90	1.00	1.00	1.00
A. belladonna	0.93	1.00	0.95	1.00	1.00	1.00
A. komarovii	0.87	1.00	0.99	0.99	1.00	1.00
B .arborea	0.67	0.98	0.61	0.99	1.00	0.94
B. aurea	0.91	1.00	1.00	1.00	1.00	1.00
B. sanguinea	0.90	1.00	0.97	0.94	1.00	1.00
B. suaveolens	0.70	0.97	0.52	1.00	1.00	1.00
B. versicolor	0.47	0.99	0.74	1.00	1.00	1.00
D. ceratocaula	0.90	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	0.99	1.00	1.00	1.00
D. ferox	1.00	1.00	0.91	1.00	1.00	1.00
D. inoxia	0.86	1.00	0.90	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	0.97	1.00	1.00	1.00
D. metel	0.91	1.00	0.92	1.00	1.00	1.00
D. quercifolia	0.86	0.99	0.83	1.00	1.00	1.00
D. stramonium	0.82	0.99	0.81	1.00	1.00	1.00
D. wrightii	0.98	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	0.99	0.99	0.76	1.00	1.00	1.00
H. muticus	1.00	1.00	0.98	1.00	1.00	1.00
H. niger	0.97	1.00	1.00	1.00	1.00	1.00
H. pusillus	0.74	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	0.99	1.00	1.00	1.00
M. officinarum	0.98	1.00	1.00	1.00	1.00	1.00

Table S23. Performance results for A: LDA and B: PLS-DA for prediction of the training set resulting from 100 replicates of random selection for the nightshade family dataset.

Method	**A: LDA** Linear coefficient threshold: 0.02; regularization parameter: 0.27; coding design: sparse ternary combinations. Not-assigned rate: 0.00.			**B: PLS-DA** Number of latent variables: 25. Not-assigned rate: 0.00.		
Accuracy	0.95			0.91		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	0.97	0.99	0.94	0.84	1.00	0.98
A. belladonna	0.95	1.00	0.95	0.96	1.00	0.90
A. komarovii	0.93	1.00	0.93	0.98	0.99	0.77
B .arborea	0.90	0.98	0.66	0.75	0.97	0.58
B. aurea	1.00	1.00	1.00	1.00	0.99	0.90
B. sanguinea	0.90	1.00	1.00	0.90	0.99	0.87
B. suaveolens	0.48	0.99	0.78	0.31	0.99	0.54
B. versicolor	0.96	0.99	0.88	0.55	0.99	0.60
D. ceratocaula	0.90	1.00	1.00	0.81	1.00	1.00
D. discolor	0.95	1.00	1.00	1.00	1.00	0.96
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	0.93	1.00	1.00	0.92	1.00	0.96
D. leichhardtii	1.00	1.00	0.96	1.00	1.00	1.00
D. metel	1.00	1.00	0.91	0.97	1.00	0.92
D. quercifolia	0.99	1.00	1.00	0.94	1.00	0.91
D. stramonium	1.00	1.00	0.99	0.94	1.00	0.94
D. wrightii	0.96	1.00	1.00	0.91	1.00	0.98
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S24. Performance results for A: SVM; and B: MCR for prediction of the training set resulting from 100 replicates of random selection for the nightshade family dataset.

Method	**A: SVM** Box constraint: 27.70; kernel scale of linear kernel function: 84.30; coding design: sparse ternary combinations. Not-assigned rate: 0.00.			**B: MCR** Component numbers: 25; constraints: hard equality and non-negativity. Not-assigned rate: 0.00.		
Accuracy	0.97			1.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	0.99	1.00	1.00	1.00	1.00	1.00
A. belladonna	1.00	1.00	1.00	1.00	1.00	1.00
A. komarovii	0.99	1.00	0.98	1.00	1.00	1.00
B .arborea	0.91	0.98	0.68	1.00	1.00	1.00
B. aurea	1.00	1.00	1.00	1.00	1.00	1.00
B. sanguinea	0.90	1.00	1.00	1.00	1.00	1.00
B. suaveolens	0.50	1.00	0.87	1.00	1.00	1.00
B. versicolor	1.00	0.99	0.87	1.00	1.00	1.00
D. ceratocaula	1.00	1.00	1.00	1.00	1.00	1.00
D. discolor	1.00	1.00	1.00	1.00	1.00	1.00
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	1.00	1.00	1.00	1.00	1.00	1.00
D. leichhardtii	1.00	1.00	1.00	1.00	1.00	1.00
D. metel	1.00	1.00	1.00	1.00	1.00	1.00
D. quercifolia	1.00	1.00	1.00	1.00	1.00	1.00
D. stramonium	1.00	1.00	1.00	1.00	1.00	1.00
D. wrightii	1.00	1.00	1.00	1.00	1.00	1.00
H. albus	1.00	1.00	1.00	1.00	1.00	1.00
H. aureus	1.00	1.00	1.00	1.00	1.00	1.00
H. muticus	1.00	1.00	1.00	1.00	1.00	1.00
H. niger	1.00	1.00	1.00	1.00	1.00	1.00
H. pusillus	1.00	1.00	1.00	1.00	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	1.00
M. officinarum	1.00	1.00	1.00	1.00	1.00	1.00

Table S25. Performance results for A: KNN; and B: CART for prediction of the test set resulting from 100 replicates of random selection for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-C.

Method	**A: KNN**			**B: CART**		
	Accuracy: 0.81; Not-assigned rate: 0.00.			Accuracy: 0.83; Not-assigned rate:.0.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	0.89	0.98	0.77	0.83	0.98	0.75
A. belladonna	0.93	0.99	0.81	0.95	1.00	1.00
A. komarovii	0.68	1.00	0.93	0.68	0.99	0.74
B .arborea	0.50	0.98	0.52	0.54	0.98	0.55
B. aurea	0.84	1.00	1.00	0.85	0.99	0.84
B. sanguinea	0.90	1.00	0.93	0.90	0.99	0.89
B. suaveolens	0.45	0.96	0.25	0.46	0.98	0.43
B. versicolor	0.14	0.99	0.33	0.37	0.99	0.40
D. ceratocaula	0.53	1.00	1.00	0.84	1.00	1.00
D. discolor	0.95	1.00	0.92	1.00	1.00	0.96
D. ferox	1.00	0.99	0.91	0.98	1.00	1.00
D. inoxia	0.70	0.99	0.88	0.52	0.99	0.79
D. leichhardtii	1.00	0.99	0.84	1.00	1.00	0.99
D. metel	0.93	0.99	0.87	1.00	0.99	0.83
D. quercifolia	0.75	0.98	0.69	0.98	0.99	0.80
D. stramonium	0.68	0.97	0.56	0.83	1.00	0.97
D. wrightii	0.88	1.00	0.99	0.84	0.99	0.86
H. albus	1.00	1.00	0.97	1.00	1.00	0.94
H. aureus	0.96	0.99	0.74	0.75	0.99	0.79
H. muticus	1.00	0.99	0.85	1.00	1.00	0.96
H. niger	0.89	1.00	1.00	0.74	1.00	0.82
H. pusillus	0.68	1.00	0.93	0.77	0.99	0.67
M. autumnalis	1.00	1.00	0.95	0.97	1.00	0.90
M. officinarum	0.85	1.00	1.00	0.97	1.00	0.99

Table S26. Performance results for A: LDA; and B: PLS-DA for prediction of the test set resulting from 100 replicates of random selection for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-C.

Method	**A: LDA**			**B: PLS-DA**		
	Accuracy: 0.83; Not-assigned rate:.0.00			Accuracy: 0.79; Not-assigned rate:.0.00		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	0.89	0.98	0.77	0.78	0.99	0.81
A. belladonna	0.90	0.99	0.88	0.86	0.98	0.73
A. komarovii	0.73	0.99	0.82	0.80	0.98	0.72
B .arborea	0.69	0.97	0.54	0.58	0.97	0.53
B. aurea	0.85	1.00	0.98	0.87	1.00	0.92
B. sanguinea	0.90	1.00	0.99	0.90	0.99	0.89
B. suaveolens	0.13	0.98	0.18	0.11	0.98	0.12
B. versicolor	0.53	0.99	0.50	0.12	0.98	0.16
D. ceratocaula	0.75	1.00	0.99	0.39	1.00	0.98
D. discolor	0.77	1.00	1.00	0.87	0.99	0.66
D. ferox	1.00	1.00	1.00	1.00	1.00	0.98
D. inoxia	0.54	1.00	0.90	0.57	0.99	0.80
D. leichhardtii	1.00	0.99	0.82	1.00	1.00	0.93
D. metel	1.00	0.97	0.68	0.93	0.98	0.77
D. quercifolia	0.89	0.99	0.88	0.87	0.98	0.72
D. stramonium	0.94	0.99	0.86	0.68	0.99	0.87
D. wrightii	0.78	1.00	0.98	0.69	0.99	0.77
H. albus	1.00	1.00	0.96	1.00	1.00	0.85
H. aureus	0.94	0.99	0.78	0.85	0.99	0.80
H. muticus	1.00	0.99	0.89	1.00	1.00	0.96
H. niger	0.79	1.00	0.87	1.00	0.99	0.81
H. pusillus	0.83	0.99	0.81	0.68	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	0.98
M. officinarum	0.90	1.00	1.00	0.97	1.00	0.97

Table S27. Performance results for A: SVM; and B: MCR for prediction of the test set resulting from 100 replicates of random selection for the nightshade family dataset. The confusion matrices associated with the prediction of test samples are displayed in Appendix S3-C.

Method	**A: SVM**			**B: MCR**		
	Accuracy: 0.87; Not-assigned rate: 0.00.			Accuracy: 0.87; Not-assigned rate: 0.04.		
	Sensitivity	Specificity	Precision	Sensitivity	Specificity	Precision
A. beatica	0.90	0.99	0.84	0.61	1.00	1.00
A. belladonna	0.92	0.99	0.87	1.00	1.00	1.00
A. komarovii	0.85	0.99	0.85	1.00	0.97	0.64
B .arborea	0.71	0.97	0.60	0.47	0.98	0.53
B. aurea	0.87	0.99	0.89	1.00	1.00	0.96
B. sanguinea	0.82	1.00	0.97	0.90	1.00	1.00
B. suaveolens	0.09	0.99	0.16	0.53	0.97	0.34
B. versicolor	0.62	0.98	0.42	0.39	0.99	0.52
D. ceratocaula	0.76	1.00	1.00	1.00	1.00	1.00
D. discolor	0.96	1.00	0.99	1.00	0.99	0.85
D. ferox	1.00	1.00	1.00	1.00	1.00	1.00
D. inoxia	0.78	1.00	0.96	0.73	1.00	0.97
D. leichhardtii	1.00	1.00	0.99	1.00	1.00	1.00
D. metel	0.96	0.98	0.77	1.00	0.99	0.88
D. quercifolia	0.91	0.99	0.88	0.98	1.00	0.94
D. stramonium	0.98	1.00	1.00	0.99	1.00	0.97
D. wrightii	0.88	1.00	0.97	0.74	0.99	0.82
H. albus	0.98	1.00	0.97	1.00	1.00	1.00
H. aureus	0.81	1.00	0.86	0.87	0.99	0.78
H. muticus	1.00	1.00	0.95	1.00	1.00	1.00
H. niger	0.96	1.00	0.88	0.90	1.00	0.85
H. pusillus	0.83	1.00	0.88	0.77	1.00	1.00
M. autumnalis	1.00	1.00	1.00	1.00	1.00	0.93
M. officinarum	0.96	1.00	1.00	1.00	1.00	1.00

➢ NMR dataset

Table S28. Analysis results for the NMR dataset for colorectal cancer and adenoma samples. A) Number of selected variables; B) samples for the training/test sets resulting from EDR for each class; performance results for the prediction of test samples with C) MCR, D) LDA, E) KNN, F) CART, G) SVM, and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S4-A.

A: Number of selected variables				
10 variables are important				
B: Number of selected samples for the training/test set				
Training set	57 (24 adenoma, 33 cancer)			
Test set	37 (23 adenoma, 14 cancer)			
C: Performance results for prediction of the test set with "MCR" Number of components: 3; constraints: hard equality and non-negativity.				
Training—Accuracy: 1.00; Not-assigned rate: 0.03	Test—Accuracy: 0.78; Not-assigned rate: 0.00			
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	1.00	0.83	1.00	0.71
Specificity	1.00	0.71	1.00	0.83
Precision	1.00	0.83	1.00	0.71
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 0.06; regularization parameter: 0.15; coding design: one versus one.				
Training—Accuracy: 0.63; Not-assigned rate: 0.00	Test—Accuracy: 0.57; Not-assigned rate: 0.00			
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.50	0.39	0.73	0.86
Specificity	0.73	0.86	0.50	0.39
Precision	0.57	0.82	0.67	0.46
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 30; distance function: "minkowski"; coding design: one versus one.				
Training—Accuracy: 0.58; Not-assigned rate: 0.00	Test—Accuracy: 0.51; Not-assigned rate: 0.00			
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.33	0.26	0.76	0.93
Specificity	0.76	0.93	0.33	0.26
Precision	0.50	0.86	0.61	0.43
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 6; coding design: one versus one.				
Training—Accuracy: 0.85; Not-assigned rate: 0.00	Test—Accuracy: 0.68; Not-assigned rate: 0.00			
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.92	0.65	0.82	0.71
Specificity	0.82	0.71	0.92	0.65
Precision	0.79	0.79	0.93	0.56

Table S28. Continued

G: Performance results for prediction of the test set with "SVM" Box constraint: 864; kernel scale of linear kernel function: 0.05; coding design: one versus one.				
Training—Accuracy: 0.67; Not-assigned rate: 0.00		Test—Accuracy: 0.62; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.58	0.43	0.73	0.93
Specificity	0.73	0.93	0.58	0.43
Precision	0.61	0.91	0.71	0.50
H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 1.				
Training—Accuracy: 0.54; Not-assigned rate: 0.00		Test—Accuracy: 0.65; Non-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.71	0.83	0.42	0.36
Specificity	0.42	0.36	0.71	0.83
Precision	0.47	0.68	0.67	0.56

Table S29. Analysis results for the NMR dataset for colorectal cancer and adenoma samples. A) Number of selected variables; B) samples for the training/test sets resulting from the Kennard-stone method for each class; performance results for the prediction of test samples with C) MCR, D) LDA, E) KNN, F) CART, G) SVM, and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S4-B.

A: Number of selected variables				
10 variables are important				
B: Number of selected samples for the training/test set				
Training set		66 (31 adenoma, 35 cancer)		
Test set		28 (16 adenoma, 12 cancer)		
C: Performance results for prediction of the test set with "MCR" Number of components: 2; constraints: hard equality and non-negativity.				
Training—Accuracy: 1.00; Not-assigned rate: 0.00		Test—Accuracy: 0.61; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	1.00	0.50	1.00	0.69
Specificity	1.00	0.69	1.00	0.50
Precision	1.00	0.55	1.00	0.65
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 1.09e-6; regularization parameter: 0.01; coding design: one versus one.				
Training—Accuracy: 0.67; Not-assigned rate: 0.00		Test—Accuracy: 0.71; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.66	0.58	0.68	0.81
Specificity	0.68	0.81	0.66	0.58
Precision	0.70	0.70	0.64	0.72
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 14; distance function: "spearman"; coding design: one versus one.				
Training—Accuracy: 0.62; Not-assigned rate: 0.00		Test—Accuracy: 0.72; Not-assigned rate: 0.10		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.54	0.75	0.71	0.69
Specificity	0.71	0.69	0.54	0.75
Precision	0.68	0.69	0.58	0.75
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 6; coding design: one versus one.				
Training—Accuracy: 0.80; Not-assigned rate: 0.00		Test—Accuracy: 0.68; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.77	0.67	0.84	0.69
Specificity	0.84	0.69	0.77	0.67
Precision	0.84	0.62	0.76	0.73

Table S29. Continued

G: Performance results for prediction of the test set with "SVM" Box constraint: 220.97; kernel scale of linear kernel function: 0.001; coding design: one versus one.				
Training—Accuracy: 0.73; Not-assigned rate: 0.00		Test—Accuracy: 0.71; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.69	0.58	0.77	0.81
Specificity	0.77	0.81	0.69	0.58
Precision	0.77	0.70	0.69	0.72
H: Performance results for prediction of the test set with "PLS-DA" Number of latent variables: 1.				
Training—Accuracy: 0.62; Not-assigned rate: 0.000		Test—Accuracy: 0.50; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.46	0.17	0.81	0.75
Specificity	0.81	0.75	0.46	0.17
Precision	0.73	0.33	0.57	0.55

Table S30. Analysis results for the NMR dataset for colorectal cancer and adenoma samples. A) Number of selected variables; B) samples for the training/test sets resulting from random selection for each class; performance results for the prediction of test samples with C) MCR, D) LDA, E) KNN, F) CART, G) SVM, and H) PLS-DA. The confusion matrices associated with the prediction of test samples are displayed in Appendix S4-C.

A: Number of selected variables				
variables are important				
B: Number of selected samples for the training/test set				
Training set		66 (33 adenoma, 33 cancer)		
Test set		28 (14 adenoma, 14 cancer)		
C: Performance results for prediction of the test set with "MCR" Number of components: 2; constraints: hard equality and non-negativity.				
Training—Accuracy: 1.00; Not-assigned rate: 0.00		Test—Accuracy: 0.67; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	1.00	0.62	1.00	0.71
Specificity	1.00	0.71	1.00	0.62
Precision	1.00	0.68	1.00	0.65
D: Performance results for prediction of the test set with "LDA" Linear coefficient threshold: 0.21; regularization parameter: 0.49; coding design: one versus one.				
Training—Accuracy: 0.66; Not-assigned rate: 0.00		Test—Accuracy: 0.62; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.61	0.57	0.70	0.70
Specificity	0.70	0.70	0.61	0.57
Precision	0.67	0.63	0.64	0.61
E: Performance results for prediction of the test set with "KNN" Number of neighbors: 7; distance function: "cityblock"; coding design: one versus one.				
Training—Accuracy: 0.74; Not-assigned rate: 0.00		Test—Accuracy: 0.62; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.67	0.56	0.80	0.69
Specificity	0.80	0.69	0.67	0.56
Precision	0.77	0.64	0.71	0.61
F: Performance results for prediction of the test set with "CART" Maximum number of leaves: 4; coding design: one versus one.				
Training—Accuracy: 0.64; Not-assigned rate: 0.00		Test—Accuracy: 0.55; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.64	0.54	0.64	0.57
Specificity	0.64	0.57	0.64	0.54
Precision	0.64	0.56	0.64	0.56

Table S30. Continued

G: Performance results for prediction of the test set with “SVM” Box constraint: 10.95; kernel scale of linear kernel function: 0.02; coding design: one versus one.				
Training—Accuracy: 0.66; Not-assigned rate: 0.00		Test—Accuracy: 0.64; Not-assigned rate: 00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.56	0.55	0.77	0.73
Specificity	0.77	0.73	0.56	0.55
Precision	0.70	0.67	0.63	0.62
H: Performance results for prediction of the test set with “PLS-DA” Number of latent variables: 2.				
Training—Accuracy: 0.64; Not-assigned rate: 0.00		Test—Accuracy: 0.61; Not-assigned rate: 0.00		
	Adenoma		Cancer	
	Training	Test	Training	Test
Sensitivity	0.42	0.41	0.85	0.80
Specificity	0.85	0.80	0.42	0.41
Precision	0.74	0.68	0.60	0.58

Appendix.

Appendix S1-A. Confusion matrices associated with the prediction of test samples derived from EDR for the iris dataset.

LDA

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	45	0	0	0
	I. versicolor	0	34	4	0
	I. virginica	0	11	31	0

KNN

		Predicted			
Actual	*I. setosa*	*I. setosa*	*I. versicolor*	*I. virginica*	Not-assigned
	I. versicolor	45	0	0	0
	I. virginica	0	37	1	0
		0	16	26	0

CART

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	35	10	0	0
	I. versicolor	4	33	1	0
	I. virginica	1	5	36	0

SVM

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	45	0	0	0
	I. versicolor	0	38	0	0
	I. virginica	0	10	32	0

PLS-DA

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	45	0	0	0
	I. versicolor	0	34	4	0
	I. virginica	0	7	35	0

MCR

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	45	0	0	0
	I. versicolor	0	26	4	8
	I. virginica	0	3	39	0

Appendix S1-B. Confusion matrices associated with the prediction of test samples derived from Kennard-Stone for the iris dataset.

LDA

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	15	0	0	0
	I. versicolor	0	15	0	0
	I. virginica	0	0	15	0

KNN

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	15	0	0	0
	I. versicolor	0	15	0	0
	I. virginica	0	0	15	0

CART

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	15	0	0	0
	I. versicolor	0	15	0	0
	I. virginica	0	2	13	0

SVM

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	15	0	0	0
	I. versicolor	0	15	0	0
	I. virginica	0	0	15	0

PLS-DA

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	15	0	0	0
	I. versicolor	0	15	0	0
	I. virginica	0	1	14	0

MCR

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	15	0	0	0
	I. versicolor	0	11	2	2
	I. virginica	0	0	15	0

Appendix S1-C. Confusion matrices associated with the prediction of test samples derived from the random selection method for the iris dataset.

LDA

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	1400	0	0	0
	I. versicolor	0	1342	58	0
	I. virginica	0	30	1470	0

KNN

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	1400	0	0	0
	I. versicolor	0	1326	74	0
	I. virginica	0	2	1498	0

CART

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	1400	0	0	0
	I. versicolor	0	1296	104	0
	I. virginica	0	118	1382	0

SVM

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	1400	0	0	0
	I. versicolor	0	1318	82	0
	I. virginica	0	81	1419	0

PLS-DA

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	1400	0	0	0
	I. versicolor	0	1321	79	0
	I. virginica	0	78	1422	0

MCR

		Predicted			
		I. setosa	*I. versicolor*	*I. virginica*	Not-assigned
Actual	*I. setosa*	1400	0	0	0
	I. versicolor	0	921	382	97
	I. virginica	0	26	1474	0

Appendix S2-A. Confusion matrices associated with the prediction of test samples derived from EDR for the wine dataset.

LDA

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	51	0	0	0
	Group 2	0	29	0	0
	Group 3	0	0	26	0

KNN

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	48	3	0	0
	Group 2	0	29	0	0
	Group 3	0	0	26	0

CART

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	40	11	0	0
	Group 2	0	29	0	0
	Group 3	0	0	26	0

SVM

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	50	1	0	0
	Group 2	0	29	0	0
	Group 3	0	0	26	0

PLS-DA

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	49	2	0	0
	Group 2	0	29	0	0
	Group 3	0	0	26	0

MCR

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	48	2	0	1
	Group 2	1	28	0	0
	Group 3	0	0	26	0

Appendix S2-B. Confusion matrices associated with the prediction of test samples derived from Kennard-Stone for the wine dataset.

LDA

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	18	0	0	0
	Group 2	0	19	0	0
	Group 3	0	0	14	0

KNN

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	18	0	0	0
	Group 2	0	19	0	0
	Group 3	0	0	14	0

CART

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	18	0	0	0
	Group 2	1	18	0	0
	Group 3	0	1	13	0

SVM

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	18	0	0	0
	Group 2	0	19	0	0
	Group 3	0	0	14	0

PLS-DA

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	18	0	0	0
	Group 2	1	18	0	0
	Group 3	0	0	14	0

MCR

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	18	0	0	0
	Group 2	1	18	0	0
	Group 3	0	0	14	0

Appendix S2-C. Confusion matrices associated with the prediction of test samples derived from the random selection method for the wine dataset.

LDA

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	1731	0	0	0
	Group 2	48	1685	104	0
	Group 3	0	0	1332	0

KNN

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	1729	2	0	0
	Group 2	37	1753	47	0
	Group 3	0	22	1310	0

CART

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	1667	64	0	0
	Group 2	48	1692	97	0
	Group 3	1	96	1235	0

SVM

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	1731	0	0	0
	Group 2	32	1764	41	0
	Group 3	0	21	1311	0

PLS-DA

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	1672	59	0	0
	Group 2	117	1640	80	0
	Group 3	0	26	1306	0

MCR

		Predicted			
		Group 1	Group 2	Group3	Not-assigned
Actual	Group 1	1653	78	0	0
	Group 2	131	1617	89	0
	Group 3	0	32	1300	0

Appendix S3-A. Confusion matrices associated with the prediction of test samples derived from EDR for the nightshade dataset.

- **LDA**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**5**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**4**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**5**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**6**	**0**

➢ **KNN**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**4**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**1**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**5**	**2**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**7**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**1**	**0**	**3**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**4**	**0**

➢ **CART**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**7**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**7**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**2**	**0**	**0**	**1**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**0**	**0**	**1**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**7**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**7**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**1**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**6**	**0**

➢ **SVM**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**5**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**1**	**1**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**2**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**5**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**6**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**6**	**0**

➢ **PLS-DA**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**6**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**1**	**1**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**7**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**2**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**6**	**0**

- **MCR**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**4**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**2**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**7**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**9**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**8**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**7**	**1**

Appendix S3-B. Confusion matrices associated with the prediction of test samples derived from Kennard-Stone for the nightshade dataset.

- **LDA**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**

➢ KNN

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**1**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**

➢ CART

Actual	Predicted: *A. beatica*	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
A. beatica	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
A. belladonna	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
A. komarovii	**1**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B .arborea	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. sanguine	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. suaveolens	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**
H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**
H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**
M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**

- **SVM**

	Predicted																								
Actual	*A. beatica*	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
A. beatica	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
A. belladonna	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
A. komarovii	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B .arborea	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. sanguine	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. versicolor	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**
H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**
H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**
M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**

➢ PLS-DA

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**

➢ MCR

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**2**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**1**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**

Appendix S3-C. Confusion matrices associated with the prediction of test samples derived from the random selection method for the nightshade dataset.

➢ **LDA**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**280**	**0**	**35**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**21**	**193**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**59**	**1**	**159**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**149**	**0**	**0**	**52**	**15**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**5**	**182**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**0**	**24**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**23**	**0**	**199**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**70**	**0**	**0**	**15**	**33**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**31**	**3**	**2**	**18**	**60**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**25**	**0**	**0**	**0**	**0**	**0**	**0**	**85**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**96**	**0**	**0**	**22**	**0**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**214**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**13**	**0**	**0**	**0**	**114**	**2**	**53**	**11**	**17**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**115**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**223**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**23**	**195**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**14**	**205**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**13**	**0**	**27**	**0**	**9**	**169**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**107**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**109**	**4**	**3**	**0**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**219**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**21**	**0**	**90**	**3**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**9**	**0**	**11**	**98**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**114**	**0**	**0**
	M. officinarum	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**20**	**0**	**197**	**0**

- **KNN**

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	280	19	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0
	A. belladonna	15	200	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	A. komarovii	65	6	148	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	B .arborea	0	0	0	108	0	13	82	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	B. aurea	0	0	0	0	180	0	0	0	0	0	0	6	0	29	0	0	0	0	0	0	0	0	0	0	0
	B. sanguine	0	0	0	23	0	199	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	B. suaveolens	0	0	0	48	0	0	53	17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	B. versicolor	0	0	0	20	0	2	76	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	D. ceratocaula	0	21	0	1	0	0	0	0	60	10	0	0	0	0	0	22	0	0	0	0	0	0	0	0	0
	D. discolor	0	0	0	6	0	0	0	0	0	119	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	D. ferox	0	0	0	0	0	0	0	0	0	0	214	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	D. inoxia	0	0	0	0	0	0	1	2	0	0	0	149	0	0	0	58	2	0	0	0	0	0	0	0	0
	D. leichhardtii	0	0	0	0	0	0	0	0	0	0	0	0	115	0	0	0	0	0	0	0	0	0	0	0	0
	D. metel	0	0	0	0	0	0	0	0	0	0	0	15	0	208	0	0	0	0	0	0	0	0	0	0	0
	D. quercifolia	0	0	0	0	0	0	0	0	0	0	21	0	0	0	163	34	0	0	0	0	0	0	0	0	0
	D. stramonium	0	0	0	0	0	0	0	0	0	0	0	0	22	0	49	148	0	0	0	0	0	0	0	0	0
	D. wrightii	0	0	0	0	0	0	0	0	0	0	0	0	0	1	25	0	192	0	0	0	0	0	0	0	0
	H. albus	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	107	0	0	0	0	0	0	0
	H. aureus	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	111	0	0	0	0	0	0
	H. muticus	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	219	0	0	0	0	0
	H. niger	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	102	6	6	0	0
	H. pusillus	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	38	0	0	80	0	0	0
	M. autumnalis	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	114	0	0
	M. officinarum	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	34	0	0	0	186	0

➢ CART

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**263**	**0**	**49**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**
	A. belladonna	**10**	**205**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**70**	**0**	**149**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**117**	**19**	**17**	**32**	**31**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**5**	**1**	**0**	**1**	**183**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**0**	**1**	**0**	**0**	**2**	**6**	**11**	**1**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**21**	**0**	**199**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**39**	**0**	**3**	**54**	**22**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**31**	**0**	**4**	**37**	**42**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**2**	**0**	**1**	**0**	**0**	**0**	**96**	**0**	**0**	**3**	**0**	**0**	**9**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**125**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**210**	**0**	**0**	**0**	**0**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**9**	**0**	**0**	**7**	**0**	**0**	**0**	**110**	**1**	**36**	**12**	**2**	**27**	**0**	**0**	**2**	**0**	**6**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**115**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**223**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**214**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**0**	**2**	**0**	**2**	**29**	**182**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**24**	**0**	**5**	**5**	**0**	**183**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**107**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**1**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**87**	**2**	**9**	**16**	**0**	**0**	**0**
	H. muticus	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**218**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**1**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**13**	**1**	**84**	**9**	**1**	**3**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**9**	**1**	**2**	**91**	**10**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**1**	**0**	**1**	**0**	**111**	**0**	**0**
	M. officinarum	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**1**	**0**	**0**	**0**	**214**	**0**

➢ SVM

		Predicted																								
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**282**	**1**	**32**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. belladonna	**18**	**197**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**33**	**0**	**186**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**154**	**0**	**0**	**40**	**21**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**187**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**25**	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. sanguine	**0**	**0**	**0**	**23**	**0**	**183**	**0**	**16**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**67**	**0**	**0**	**11**	**40**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. versicolor	**0**	**0**	**0**	**11**	**10**	**5**	**17**	**71**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**23**	**0**	**0**	**0**	**0**	**0**	**0**	**87**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**3**	**0**	**0**	**0**	**0**	**0**	**120**	**0**	**1**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**214**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**20**	**0**	**0**	**0**	**165**	**0**	**3**	**23**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**115**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**0**	**213**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**20**	**198**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**215**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. wrightii	**0**	**0**	**0**	**0**	**12**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**14**	**0**	**0**	**191**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**105**	**0**	**0**	**0**	**2**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**94**	**6**	**9**	**7**	**0**	**0**	**0**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**219**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**110**	**4**	**0**	**0**	**0**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**15**	**0**	**5**	**98**	**0**	**0**	**0**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**114**	**0**	**0**
	M. officinarum	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**	**1**	**0**	**0**	**212**	**0**

➢ PLS-DA

Actual	Predicted: *A. beatica*	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
A. beatica	**247**	**0**	**68**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
A. belladonna	**29**	**184**	**1**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
A. komarovii	**20**	**24**	**175**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B .arborea	**0**	**0**	**0**	**126**	**2**	**0**	**52**	**32**	**0**	**0**	**0**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. aurea	**0**	**0**	**0**	**0**	**186**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**0**	**1**	**0**	**0**	**0**	**19**	**0**	**0**	**0**	**0**	**0**	**7**	**0**
B. sanguine	**0**	**0**	**0**	**18**	**0**	**199**	**5**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. suaveolens	**0**	**0**	**0**	**60**	**0**	**2**	**13**	**43**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
B. versicolor	**0**	**0**	**0**	**32**	**15**	**22**	**31**	**14**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. ceratocaula	**0**	**43**	**0**	**0**	**0**	**0**	**0**	**0**	**44**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**19**	**0**	**0**	**7**	**0**	**0**	**0**	**0**	**0**
D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**10**	**0**	**0**	**109**	**0**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**213**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**20**	**0**	**120**	**9**	**34**	**5**	**2**	**22**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**115**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**13**	**0**	**208**	**0**	**0**	**2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. quercifolia	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**190**	**21**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**	**4**	**0**	**0**	**61**	**150**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**35**	**0**	**1**	**0**	**25**	**6**	**0**	**151**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**107**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
H. aureus	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**3**	**0**	**99**	**1**	**9**	**0**	**0**	**0**	**0**
H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**219**	**0**	**0**	**0**	**0**	**0**
H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**114**	**0**	**0**	**0**	**0**
H. pusillus	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**24**	**0**	**11**	**80**	**2**	**0**	**0**
M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**114**	**0**	**0**
M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**6**	**0**	**0**	**213**	**0**

➢ MCR

		Predicted																							
		A. beatica	*A. belladonna*	*A. komarovii*	*B .arborea*	*B. aurea*	*B. sanguine*	*B. suaveolens*	*B. versicolor*	*D. ceratocaula*	*D. discolor*	*D. ferox*	*D. inoxia*	*D. leichhardtii*	*D. metel*	*D. quercifolia*	*D. stramonium*	*D. wrightii*	*H. albus*	*H. aureus*	*H. muticus*	*H. niger*	*H. pusillus*	*M. autumnalis*	*M. officinarum*	Not-assingned
Actual	*A. beatica*	**190**	**0**	**121**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**4**
	A. belladonna	**0**	**215**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	A. komarovii	**0**	**0**	**219**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B .arborea	**0**	**0**	**0**	**101**	**8**	**0**	**76**	**31**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. aurea	**0**	**0**	**0**	**0**	**187**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**28**
	B. sanguine	**0**	**0**	**0**	**22**	**0**	**199**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	B. suaveolens	**0**	**0**	**0**	**45**	**0**	**0**	**62**	**10**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**
	B. versicolor	**0**	**0**	**0**	**24**	**0**	**0**	**45**	**45**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ceratocaula	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**114**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. discolor	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**125**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. ferox	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**214**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. inoxia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**9**	**0**	**124**	**0**	**0**	**0**	**2**	**35**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**42**
	D. leichhardtii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**115**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	D. metel	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**208**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**15**
	D. quercifolia	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**189**	**4**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**25**
	D. stramonium	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**2**	**194**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**23**
	D. wrightii	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**13**	**0**	**4**	**0**	**28**	**11**	**0**	**156**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**6**
	H. albus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**107**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
	H. aureus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**98**	**0**	**15**	**0**	**0**	**0**	**3**
	H. muticus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**219**	**0**	**0**	**0**	**0**	**0**
	H. niger	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**10**	**0**	**94**	**0**	**0**	**0**	**10**
	H. pusillus	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**17**	**0**	**2**	**89**	**8**	**0**	**2**
	M. autumnalis	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**114**	**0**	**0**
	M. officinarum	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**220**	**0**

Appendix S4-A. Confusion matrices associated with the prediction of test samples derived from EDR for the CRC dataset.

LDA

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	9	14	0
	Cancer	2	12	0

KNN

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	6	17	0
	Cancer	1	13	0

CART

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	15	8	0
	Cancer	4	10	0

SVM

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	10	13	0
	Cancer	1	13	0

PLS-DA

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	19	4	0
	Cancer	9	5	0

MCR

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	19	4	0
	Cancer	4	10	0

Appendix S4-B. Confusion matrices associated with the prediction of test samples derived from Kennard-Stone for the CRC dataset.

LDA

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	13	3	0
	Cancer	5	7	0

KNN

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	9	4	3
	Cancer	3	9	0

CART

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	11	5	0
	Cancer	4	8	0

SVM

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	13	3	0
	Cancer	5	7	0

PLS-DA

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	12	4	0
	Cancer	10	2	0

MCR

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	11	5	0
	Cancer	6	6	0

Appendix S4-C. Confusion matrices associated with the prediction of test samples derived from the random selection method for the CRC dataset.

LDA

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	937	463	0
	Cancer	596	804	0

KNN

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	959	441	0
	Cancer	617	783	0

CART

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	797	603	0
	Cancer	647	753	0

SVM

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	1026	374	0
	Cancer	633	767	0

PLS-DA

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	1125	275	0
	Cancer	822	578	0

MCR

		Predicted		
		Adenoma	Cancer	Not-assigned
Actual	Adenoma	996	404	0
	Cancer	533	867	0