

The nitrate cellulose negatives: degradation study via chemometric methods

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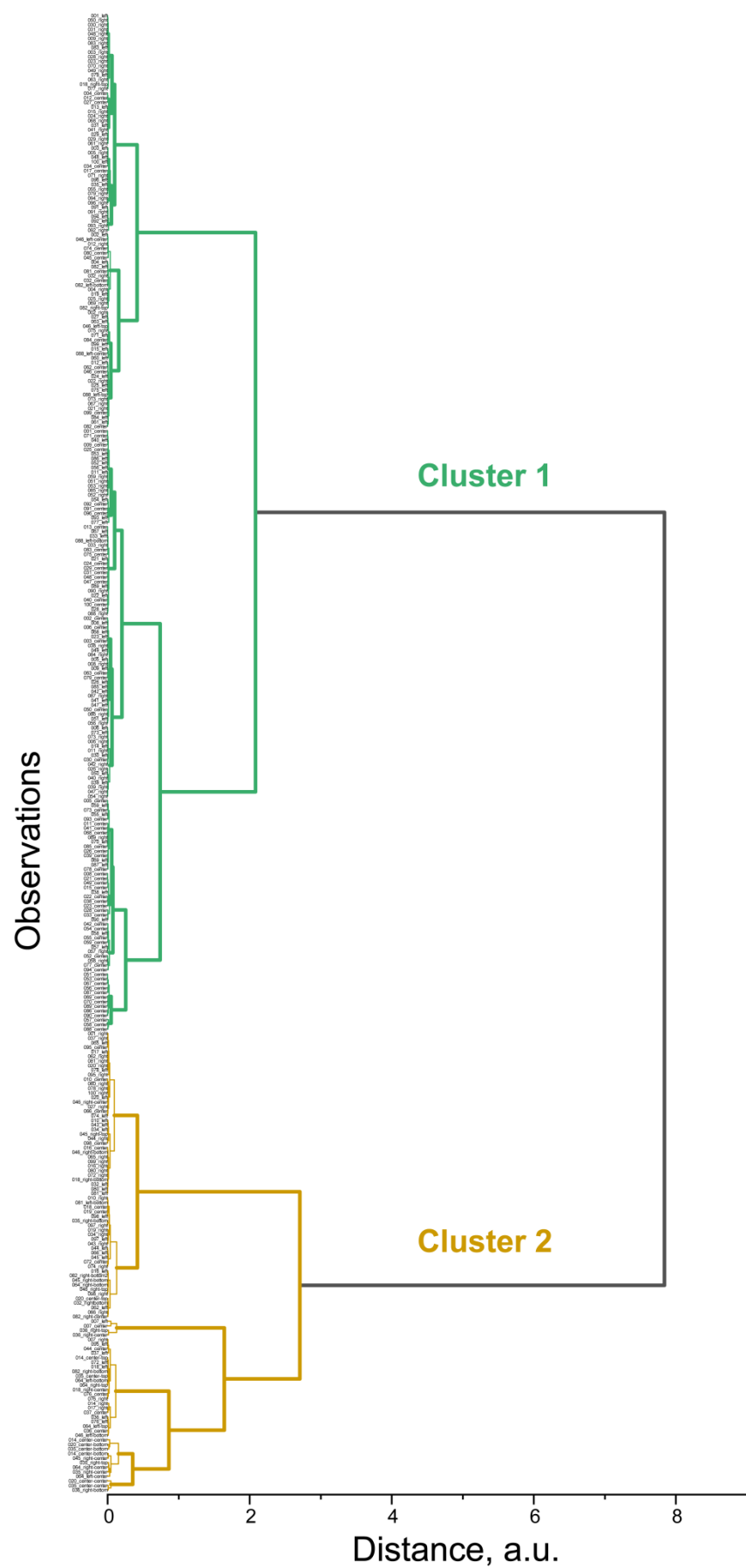


Figure S1. The result of clusterization version 2.

The main idea was the following: the positive result is identification of yellowing and the negative result is absent of yellowing. According to the e.g. [R1,R2] the accuracy, sensitivity, specificity, positive predictive value and negative predictive value are introduced as follows:

$$\text{Accuracy} = N_{\text{corr}}/N_{\text{tot}}.$$

$$\text{Sensitivity} = T_P/(F_N + T_P),$$

$$\text{Specificity} = T_N/(F_P + T_N),$$

$$\text{Positive predictive value} = T_P/(F_P + T_P),$$

$$\text{Negative predictive value} = T_N/(F_N + T_N),$$

where N_{tot} is the total number of areas under investigation, N_{tot} the number of correctly classified areas, T_P is the number of correctly identified positive results, T_N is the number of correctly identified negative results, F_P is the number of false positive results, F_N is the number of false negative results.

Table S1. Accuracy, sensitivity, specificity, positive predictive value and negative predictive value for the case of 3rd degree polynomial kernel and regularization parameter 5 within SVM approach classification.

Definition	Items	Definition	Items
N_{tot}	324	Accuracy	0.99
N_{corr}	321	Sensitivity	0.97
T_P	98	Specificity	1
T_N	223	Positive predictive value	1
F_P	0	Negative predictive value	0.99
F_N	3		

R1. Pankin D, Povolutckaia A, Borisov E, Povolotskiy A, Borzenko S, Gulyaev A, et al. Investigation of Spectroscopic Peculiarities of Ergot-Infected Winter Wheat Grains. *Foods*. 2023;12:3426.

R2. Pankin D, Povolutckaia A, Kalinichev A, Povolotskiy A, Borisov E, Moskovskiy M, et al. Complex Spectroscopic Study for Fusarium Genus Fungi Infection Diagnostics of “Zalp” Cultivar Oat. *Agronomy*. 2021;11:2402.