

P0174 **Features of clusterization of mass-spectra of *Aspergillus* spp. cellular extracts**

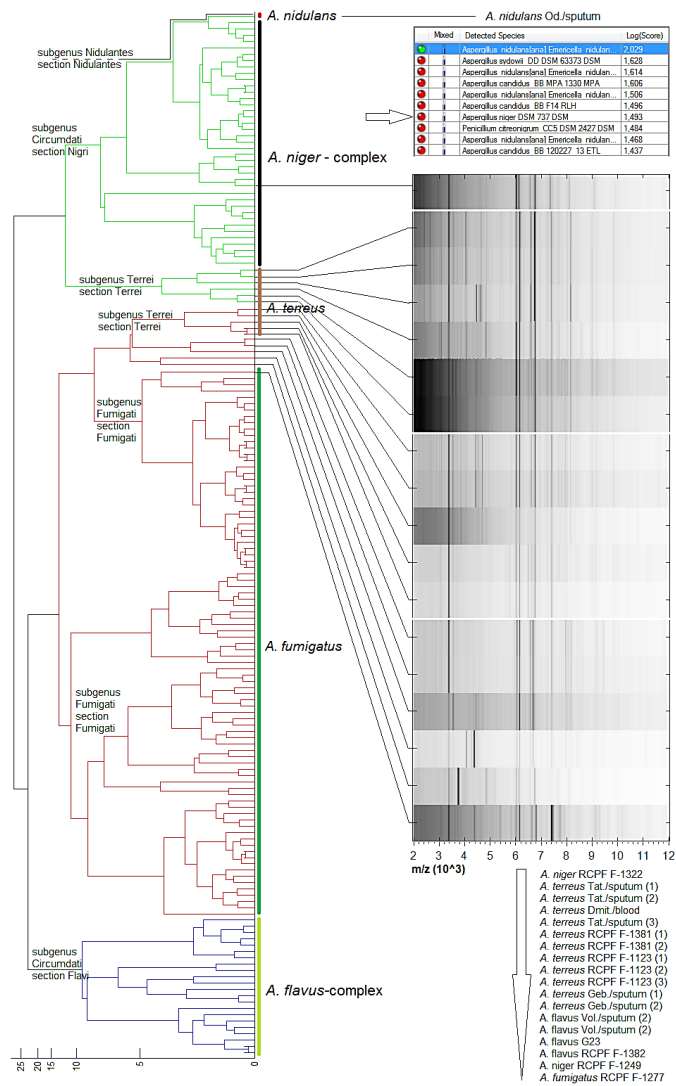
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**Background:** Hierarchical clustering of mass-spectra (MS) obtained by studying the microorganisms using the MALDI-TOF-MS method is a valuable tool for clarifying species identification, intraspecific typing and phylogenetic research. The purpose of the study was to reveal the features of the hierarchical clusterization of the mass-spectra of *Aspergillus* spp. cellular extracts identified with different «Score Values» (SV).

**Materials/methods:** 728 mass-spectra of 19 aspergillus species strains divided into 3 groups (A -  $SV \geq 2.000$ ; B -  $1.999 \geq SV \geq 1.700$ ; C -  $SV \leq 1.699$ ) were included in the study. The mass-spectral bank is collected using the Autoflex speed TOF/TOF with the MALDI Biotyper 3.1 software and the Fungi Library main-spectral-profiles (MSPs) database (Bruker Daltonik GmbH, Germany). The algorithm of hierarchical clustering was applied, as described previously [Riabinin I.A. et al., 7th Advances Against Aspergillosis, 2016].

**Results:** As appeared in group A the mass-spectra are combined mainly in accordance with their belonging to the species, sections and subgenera, except for the mass-spectra of *A. terreus*, the MS of *A. nidulans* which has similarity with MSP of *A. niger*, and for some atypical spectra of *A. flavus* (fig. 1).



**Fig. 1.** Dendrogram illustrated the hierarchical clustering of MS from group A.

The former turned out to be divided into 2 isolated clades located near the MS of the Nigri section aspergilli (1<sup>st</sup>) and MS of *A. fumigatus* (2<sup>nd</sup>). Mass-spectra of these clades differ in intensity of peaks in the ranges of  $m/z$  3-5 and 6-7 kDa. Clustering of group B reveals grouping errors and even a large clade which included the mass-spectra of different *Aspergillus* species. Group C is clustered without conservation of taxonomic order; however, the mass-spectra of individual strains are often grouped together.

**Conclusions:** Selection of high-quality mass-spectra characterized by the highest «Score Values» is necessary to achieve optimal results of the application of hierarchical clustering.