Adaptation of the brain tumors classifier, constructed on the direct mass spectrometric profiling data, to MALDI mass spectrometry analysis

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Motivation and Aim: The localization of the exact boundaries of malignant brain neoplasms is an important problem of the modern neurosurgery. One of the promising approaches to intraoperative tumor identification is the determination of the type of tissue based on the information, achieved by molecular profiling of brain tissues. Various mass spectrometric approaches can be used to determine feature ions for tumor tissues: for intraoperative analysis the fastest method is the application of direct ionization methods. In contrast, MALDI mass spectrometry allows not only to obtain molecular profiles, but also to analyze the structure of tissue with a high spatial resolution (less than 100 μm). This method has the ability to identify the different types of tissues in the sample, determine their relative position, relative sizes and the structure of the boundaries between them.

Previously, to complete the database of molecular profiles of neoplasms in the human brain, we developed a method for online extraction of lipids from brain tissues and their subsequent profiling. We constructed a classifier that allows determining the type and degree of malignancy of the tumor according to its molecular profile [1]. However, this classifier was teached to work precisely only with the data received as a result of analyzing the lipid fraction using direct electrospray ionization mass spectrometry.

The purpose of this study is to adjust the existing classifier to analyze spatial molecular profiles obtained by MALDI MS.

Methods and Algorithms: To estimate similarity between the profiles obtained by online extraction method and MALDI MS, a correlation analysis of two sets of molecular profiles for each series of samples was conducted. After optimization of the existing classifier parameters, the samples were classified according to MALDI profiles, and then compared with analyze of profiles obtained during online extraction

Results: We have shown that the classifier, that was teached on the online extraction data, is applicable to molecular profiles, obtained by MALDI mass spectrometry. The analysis of the main features, used in the classifier, allowed optimizing the parameters of mass spectrometric experiment to improve efficiency classification and visualization of the spatial structure of the samples.

References
1. Sorokin A. et al. (2017) Feature selection algorithm for spray-from-tissue mass spectrometry. European Journal Mass Spectrometry. 23(4):237-241.