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Comparison of high- and low-resolution MS data for direct tissue profiling on a way from laboratory to clinic

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Motivation and Aim: It is known that the lipid metabolism reprogramming is one of the new hallmarks of cancer. Over the last decade, great progress was made in the understanding of the role of lipid metabolism in the progression of cancer. High-resolution mass spectrometers are widely used in research facilities but applying mass spectrometry to clinical use requires reproducing the results on the low-resolution instruments, which commonly used in routine applications. For the effective automatic classifications, the spectra of one specific type of sample have to represent the same array of peaks characterizing this type of samples. Nevertheless, in practice high- and low-resolution spectra obtained even by similar instruments from one sample are not as similar as one could expect. In this work, the feature selection approach to determine features that are common for the different resolution spectra demonstrated.
Methods and Algorithms: All experiments performed on Thermo LTQ Orbitrap XL instrument. Mass spectrometry data obtained with the novel direct-spray-from-tissue approach ion source in the negative mode as described in [1]. For registration of high-resolution spectra (resolution 56,000 at 800 Th), we used Orbitrap analyzer. The low-resolution spectra (resolution 1,000 at 800 Th) we obtained using LTQ analyzer of the same instrument. All biological samples collected from dissected brain tumors during neurosurgical operations in the N.N. Burdenko Scientific Research Neurosurgery Institute. Mass-spectrometry data preprocessing and feature selection was performed in R environment by custom script available on request from authors.
Results: Both types of spectra from the same tumor fragment were processed separately through the data analysis pipeline for denoising, aggregation, normalization, peak picking and peak alignment. Two datasets were then aligned to each other and analyzed. The low-resolution spectra contain about one-third of the peaks, detectable in high-resolution spectra; however, all major peaks found in both types of spectra. The vast majority of features distinct in tumor and unmodified brain were found in both types of spectra. More than, we have created mapping schema, which allows using classifier trained on high-resolution spectra with low-resolution spectra.
Conclusion: It is shown that low-resolution spectra preserve distinctive features of brain tumor samples and could be used in sample classification.
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References

1. Kononikhin A., Zhvansky E., Shurkhay V., Popov I., Bormotov D., Kostyukevich Y., Karchugina S., Indeykina M., Bugrova A., Starodubtseva N., Potapov A., Nikolaev E. (2015) A novel direct spray-from-tissue ionization method for mass spectrometric analysis of human brain tumors. Analytical and Bioanalytical Chemistry. 407(25):7797-7805.