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Method for mass spectrometry spectrum deisotoping based on fuzzy inference systems

Proteins are very significant molecules that can construct the fingerprint of cancer. When dealing with large molecules, such as proteins, the crucial issue is their trustful and precise identification. In the majority of cases, mass spectrometry is used to identify the protein. Processing of data gathered in mass spectrometry experiment consists of several steps, and one of them is deisotoping. It is an essential part of preprocessing because some peaks in the spectrum are not the unique compound, but they are members of an isotopic envelope. There are several existing methods of deisotoping, but none of them is general and can be used in any experimental settings. To manage this, we propose a new algorithm based on fuzzy inference systems. The method was tested on the data provided by Institute of Oncology in Gliwice, that has been gathered in MALDI experiment in two different settings on head and neck cancer tissue samples. The comparison study, done between the developed fuzzy-based algorithm and mMass method revealed that the proposed method was able to identify more consistent with the expert annotation isotopic envelopes.

References

[1] A. Glodek, J. Polańska, *Method for mass spectrometry spectrum deisotoping based on fuzzy inference systems*, Mathematica Applicanda 46(1) (2018), 77–86, doi=10.14708/ma.v46i1.6384.