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**FACULTY OF AUTOMATIC CONTROL, ELECTRONICS AND COMPUTER SCIENCE**

**Doctoral Dissertation**

by

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**Deisotoping methods in MALDI ToF Mass Spectrometry Imaging**

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## ABSTRACT

### *“Deisotoping methos in MALDI-ToF Mass Spectrometry Imaging”*

Mass spectrometry is one of the essential steps toward protein identification due to the fact that it provides information on the proteins' structure. Since most chemical elements have isotopes of different masses, the isotopic mass of a molecule observed in a mass spectrum reflects the type and number of atoms in the ion being measured and the distribution of the different isotopes. Depending on the resolution of the mass spectrometer, molecular ions can be represented either by the monoisotopic mass (taking into account only the mass of the most abundant stable isotope of each atom present in the molecule) or by the average mass (taking into account the presence of both light and heavy isotopes). For an atom, the difference between the two masses is insignificant. However, in molecules such as proteins, the difference between them increases with the number of atoms that make up the molecule. Such a discrepancy leads to the misidentification of peptides, which is why it is vital to remove isotope peaks from the mass spectrum by performing a deisotoping procedure. Several existing algorithms include the deisotoping step. However, most of them are dedicated to different mass spectrometry experiments and have limitations depending on the kind of data from those experiments. The MALDI-ToF technique provides high-dimension data. This dissertation introduces a method for isotopic envelopes identification in MALDI-ToF MSI data. It is based on combining the Mamdani-Assilan fuzzy-inference system with analysing the spatial molecular distribution of the peaks (model components). The spatial molecular distribution is evaluated by several image texture metrics. The proposed method was tested on eight MALDI-ToF MSI datasets provided by the National Institute of Oncology in Gliwice from patients who suffered from head and neck cancer. Obtained results were compared with three existing deisotoping algorithms. The method presented in this research is based on the pairwise approach for isotopic envelopes member identification. Such an approach enables the identification of overlapping isotopic envelopes in large MALDI-ToF MSI-driven datasets.