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Success story

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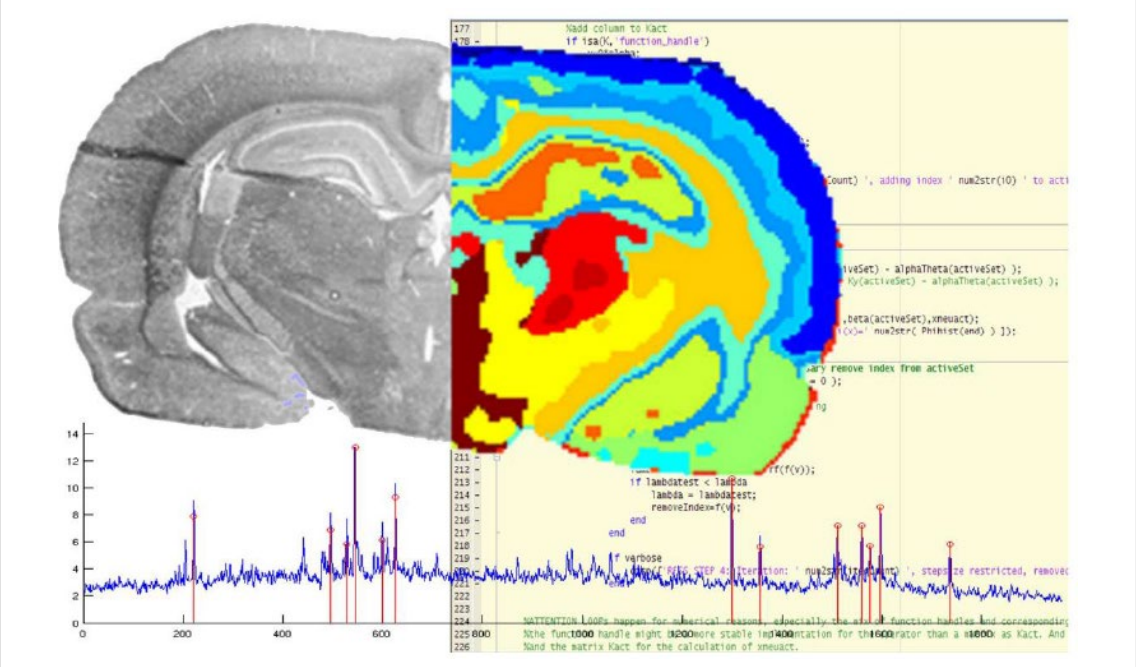
SS_030_2021

MALDI

Imagin exploring the molecular landscape. Machine learning approaches for blind source separation of high dimension mass spectrometry data.



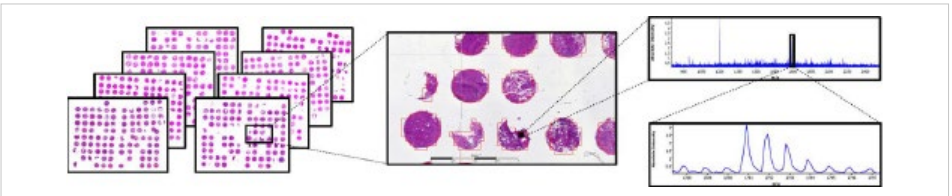
MALDI Imaging overview.

PROBLEM DESCRIPTION

Mass spectrometry imaging (MSI), in particular matrix-assisted laser desorption/ ionization time-of-flight (MALDI-TOF), is a label-free technique for spatially resolved molecular analysis of tissue samples with a broad range of applications in life sciences and biomedical research. It has become a routine technique for applications in drug discovery, biomarker detection or several Omics-methods. MSI, however produces extremely completely data sets, which cannot be evaluated without bioinformatics tools.

CHALLENGES AND GOALS

The success of MSI data analyses is based on a combination of technological hardware developments and the development of novel mathematical theories for extracting meaningful information. Data sets contain mass spectra, which are measured at different locations (pixels) of a tissue section. This yields a hyperspectral data set with thousands of channels (mass-to-charge values) at every pixel.



Schematic data structure. Optical images of hematoxylin/eosin stained TMAs (left), each with multiple core biopsies of lung cancer (middle). For each core several spectra are collected (upper right), close-up of an isotopic pattern for a peptide at m/z 1790.9 (lower right).

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MATHEMATICAL AND COMPUTATIONAL METHODS

The mathematical algorithms used for MSI data analyses are based on theoretical research at the interface of functional analysis (inverse problems) and numerical linear algebra (matrix factorization). One important task is to determine characteristic spectral patterns in the data, which are the building blocks for classification schemes (e.g. in tumor typing) or identification (e.g. for biomarker detection).

RESULTS AND BENEFITS

The challenges and methods described are the core of the research activities of the Center for Industrial Mathematics (ZeTeM), University of Bremen, Germany. ZeTeM provided the mathematical foundations as well as – in collaboration with the national leading pathological service institute Proteopath GmbH in Trier, Germany – prototypical implementations for supporting pathological diagnosis. The resulting publications and patents were the basis for founding the spin-off company SCiLS GmbH, which developed a commercial software for analysing MSI data. This software has a market share of 80% worldwide and was acquired by Bruker Daltonics, the worldwide market leader in mass spectrometry imaging.

MALDI imaging has become a standard bioanalytic procedure in pharmaceutical and medical research.

Present developments aim at implementing MSI based procedures into clinical routine applications particular for supporting tumor diagnostics.

The mathematical methods described are relevant for the sort as well the long-term development of digital pathology.

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