MALDIquant: Quantitative Analysis of MALDI-TOF Proteomics Data

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MALDI-TOF is a well established technology for mass spectrometric profiling of proteomics data. There are several ongoing efforts to provide open-source analysis software for proteomics studies, such as OpenMS (Kohlbacher et al., 2007) or PROcess (Li, 2005). However, a complete analysis pipeline for MALDI-TOF data for the *R* platform is lacking.

Common tasks and challenges in mass spectrometric analysis are data input, normalization, calibration, peak peaking and other preprocessing task. Due to technological limitations the intensity values of identified peaks cannot be directly compared across multiple spectra. This renders MALDI-TOF data difficult to use for quantitative analysis.

Here we introduce the `MALDIquant` *R* package for analysis of MALDI-TOF proteomics data. Our package provide routines for importing native Bruker *flex binary format, baseline removal, peak picking and, most importantly, procedures for coherent assignment of intensity values across multiple spectra. This approach generalizes the widely used standard procedures that rely on total ion count calibration or 0/1 truncation of peak intensities. The analysis pipeline is illustrated as well as compared with its competitors by classification of cancer proteomics data from the University Hospital Leipzig.

`MALDIquant` and associated *R* packages are available from CRAN.

References

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