OXFORD

Subject Section

CardinalVis

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Abstract

Motivation: Cardinal is an R package for statistical analysis of mass spectrometry-based imaging (MSI) experiments of biological samples such as tissues. Cardinal allows users to analyse, visualize, and perform statistical analysis on MSI experiments. However, Cardinal is purely a command line tool with no interactive graphical user interface (GUI). Visualization are generated on demand but provide very limited interactivity. Thus motivating CardinalVis, a interactive GUI to act as an interfacet to Cardinal.

Results: CardinalVis is an R "Shiny" dashboard that aims to provide much of the functionality of Cardinal to the user without the need to use the command line, thus enabling researchers to quickly understand their data by enabling rapid exploration of relevant ion images and associate mass spectra.

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Supplementary information: Supplementary data are available at *Bioinformatics* online.

1 Introduction

Mass spectrometry imaging (MSI) is a powerful tool that enables untargeted investigations into the spatial distribution of molecular species in a variety of samples. The combination of information gained from mass spectrometry (MS) and visualization of spatial distributions in thin sample sections makes this a valuable chemical analysis tool for biological specimen characterization.

Recent advancements in technology and research have improved the quality of MSI images collected, allowing for higher acquisition speeds and enhanced spatial resolution, overall improving throughput and depth. But these have made MSI data difficult to process due to large file sizes with high-dimensional spatial data. These are directly reflected in the analysis phase of a study, where expensive proprietary software and hardware are required. In particular, visualization of MSI experiments is a vital part of exploratory analysis, but can be challenging due to the extremely high-dimensional nature of the data, and the need to simultaneously visualize linked mass spectra and associated ion images (Ion images show the relative distribution of molecules at a particular mass-to-charge (m/z) value).

2 Implementation

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Acknowledgements

References