CARDINAL

mass spectrometry imaging tools

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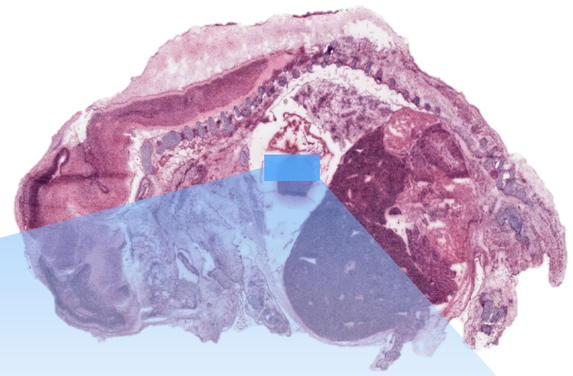
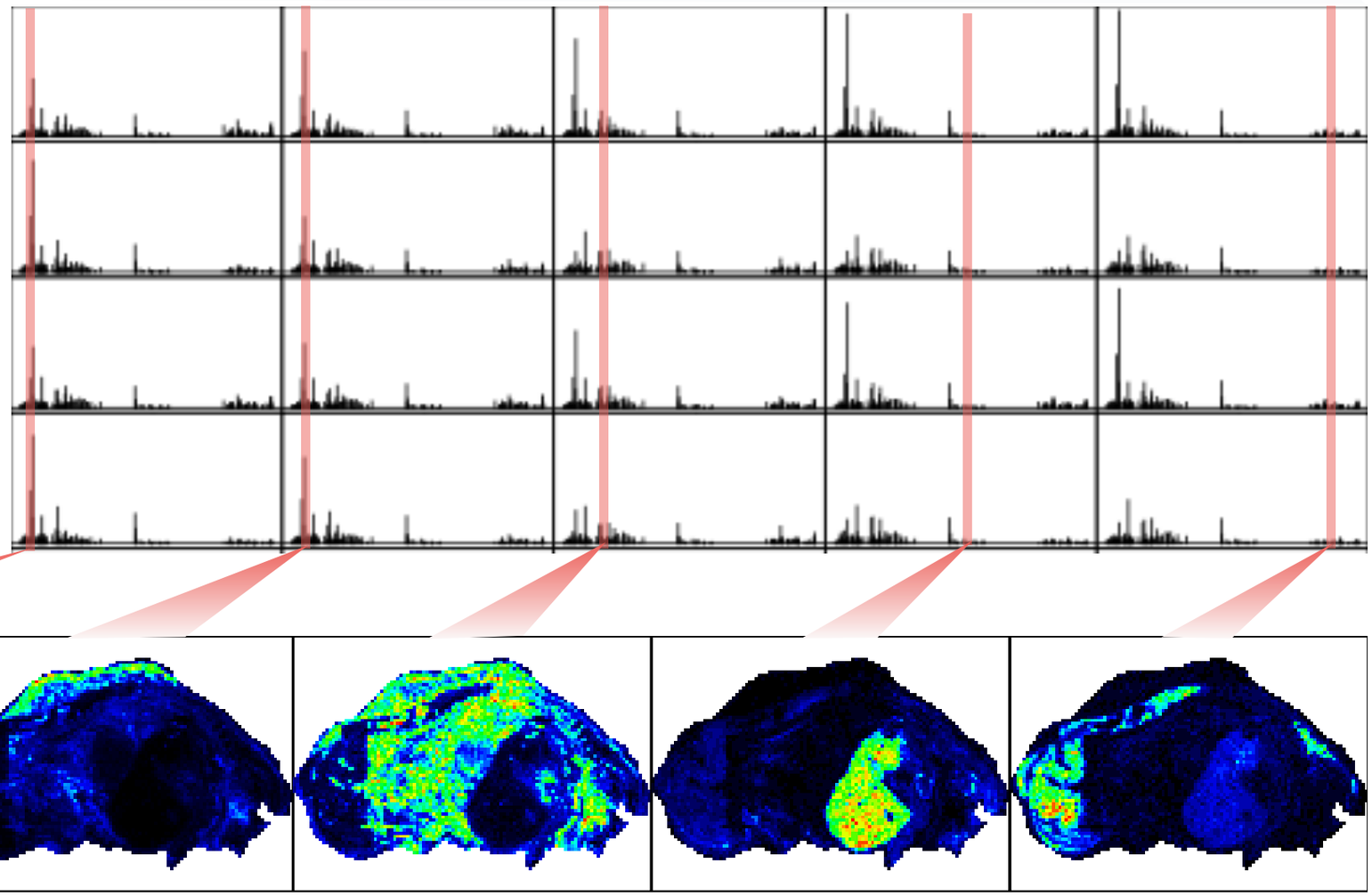
MS imaging

- Scan with laser/spray
- Collect mass spectra
- Reconstruct ion images
- Date "cube"



- Provides MSI infrastructure
- Website at ***cardinalmsi.org***
- Available on Bioconductor
- *CardinalWorkflows* data pkg
- Google user/help group
- 2015 John M. Chambers Statistical Software Award

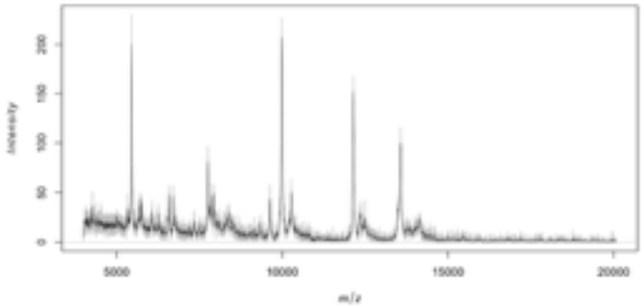


- K. D. Bemis, A. Harry, L. S. Eberlin, C. Ferreira, S. M. van de Ven, P. Mallick, M. Stolowitz, O. Vitek. "Cardinal: an R package for statistical analysis of mass spectrometry-based imaging experiments". Bioinformatics, 31:2418, 2015

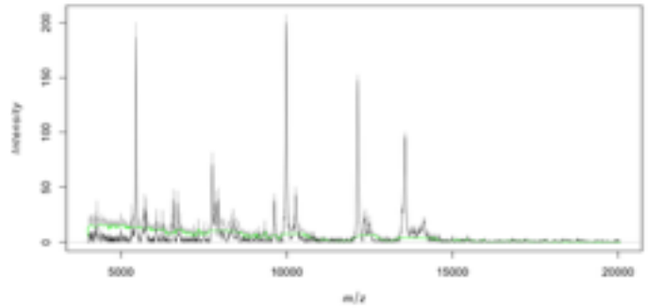
FULL EXPERIMENTAL WORKFLOWS

Spectral processing

`smoothSignal(Brain_1)`



`reduceBaseline(Brain_1)`



`peakPick(Brain_1)`

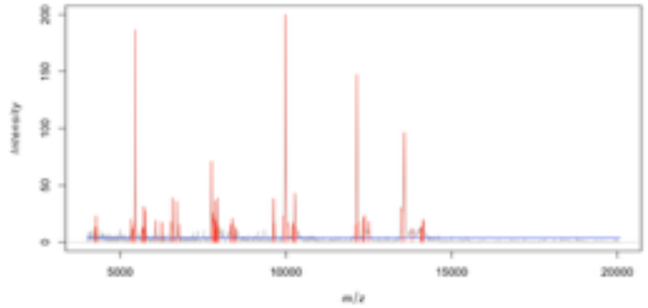
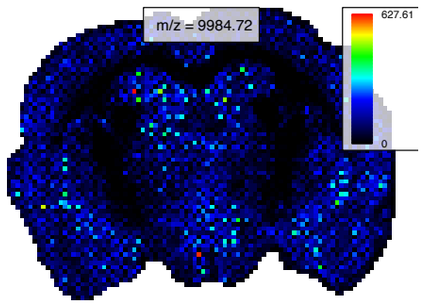
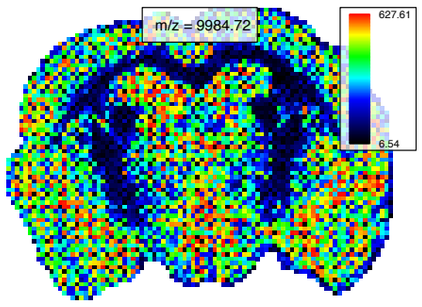


Image processing

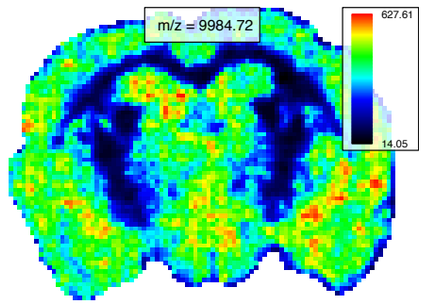
`image(Brain_1, mz=9984.7, …)`



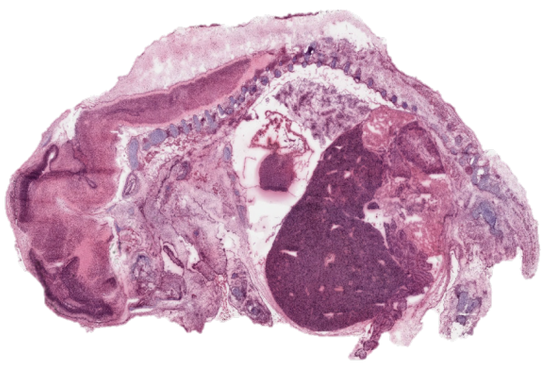
`contrast.enhance="histogram"`

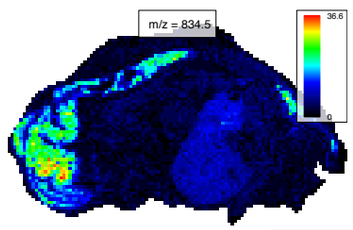


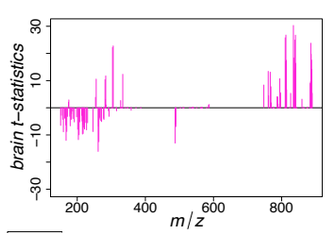
`smooth.image="gaussian"`

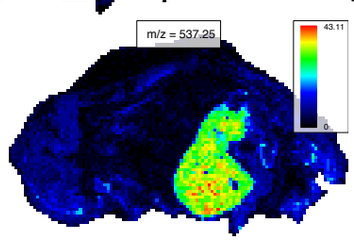


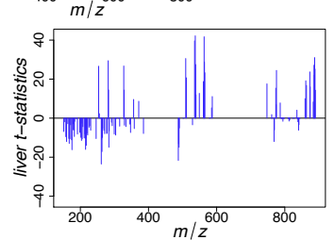
Statistical analysis



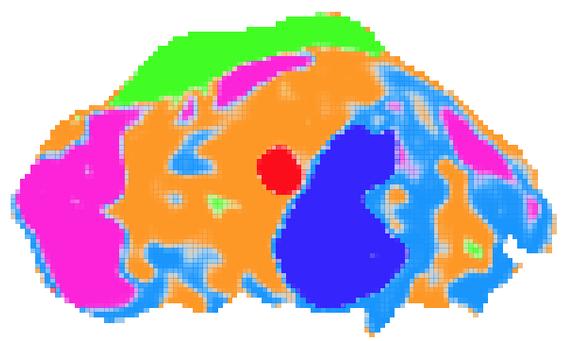








`spatialShrunkenCentroids(pig206, …)`



FUTURE DEVELOPMENT

Cardinal

- More statistical methods needed!!!
- Contribute, or write new packages
- Support for more formats
- Support for large datasets
- Support for 3D experiments
- More infrastructure for developers

(e.g., traverse neighborhoods)

matter

- New package in development at

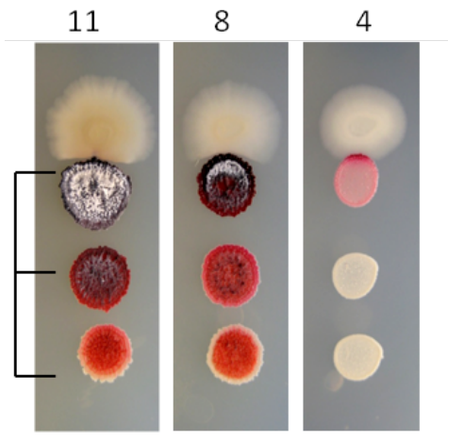
github.com/kuwisdelu/matter

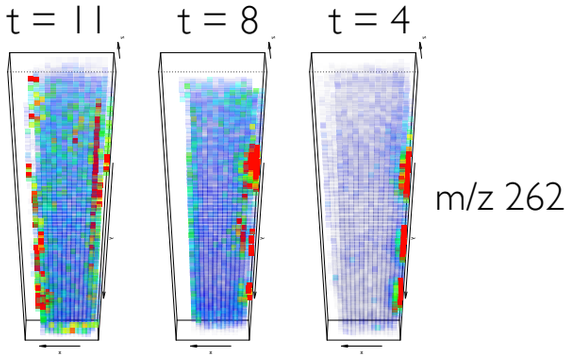
- Disk-based computing similar to

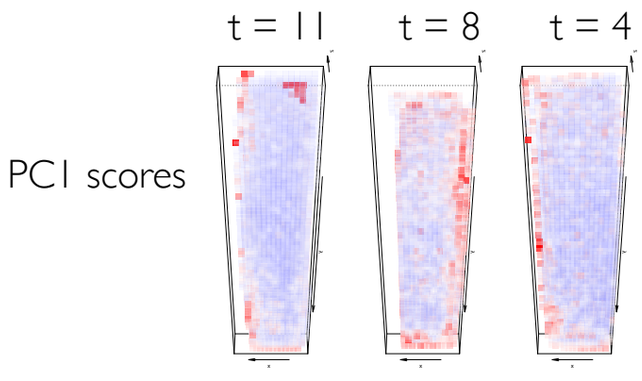
bigmemory, *ff*, and *HDF5Array*

- Focus on flexibility of on-disk data
- Focus on minimal memory
- User-specified file structure
- Future backend for *Cardinal*

Oetjen et al, GigaScience, 2015







- 3D microbial time-course
- 2.85 GB on disk
- 17,672 pixels
- 40,299 features

234 MB to compute 3 PC
79 MB memory overhead