An Open Software Development-based Ecosystem of R Packages for Metabolomics Data Analysis

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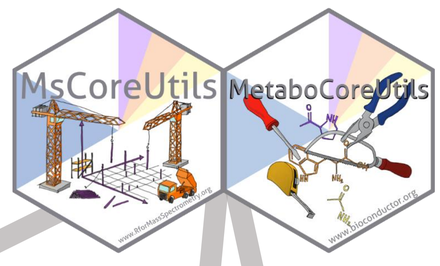
In a nutshell

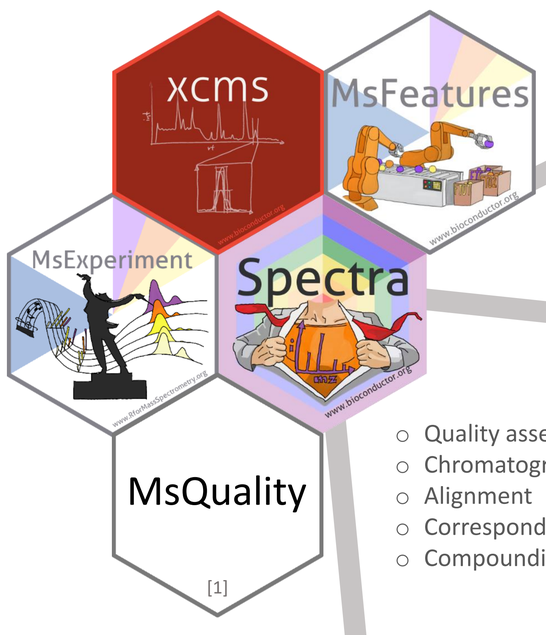
- Open collaborative development of software for MS data analysis:
  - Well documented and thoroughly tested
  - Long-term support and maintenance
- Modular package ecosystem to allow creation of custom analysis workflows
- Access to low-level functions enables *advanced users* and developers to integrate packages into their own projects
- Open for contributions from the community

Core *low-level* functions



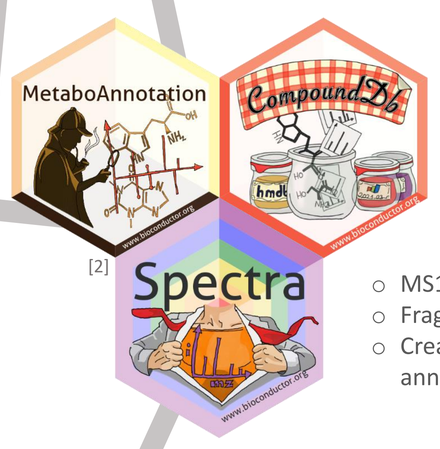
- Spectra similarity scores
- Peak alignment
- Handling chemical formulas
- Isotope peak prediction
- Adduct/exact mass calculations
- …

LC-MS(/MS) analysis



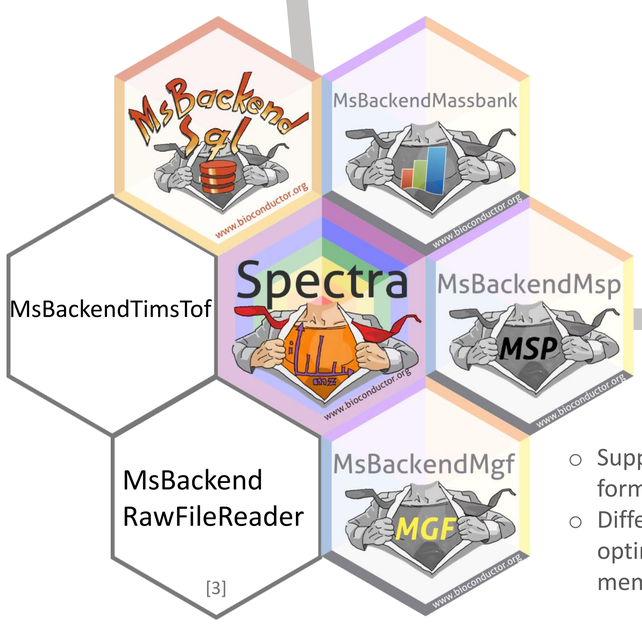
- Quality assessment
- Chromatographic peak detection
- Alignment
- Correspondence
- Compounding

Annotation



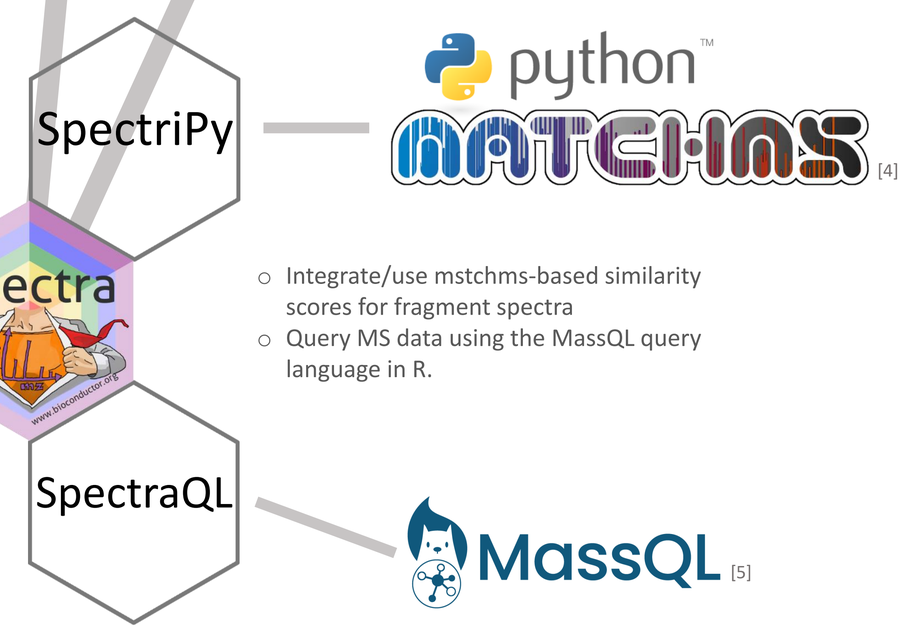
- MS1 and MS2-based annotation
- Fragment spectra matching
- Creating and maintaining annotation libraries

Supported data files/formats



- Support for additional MS data file formats
- Different representations of MS data in R optimized either for performance or low memory footprint.

Integration with external tools



- Integrate/use mstchms-based similarity scores for fragment spectra
- Query MS data using the MassQL query language in R.

Tutorials and documentation

xcms data analysis | MetaboAnnotation | Spectra

References

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