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

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In a nutshell

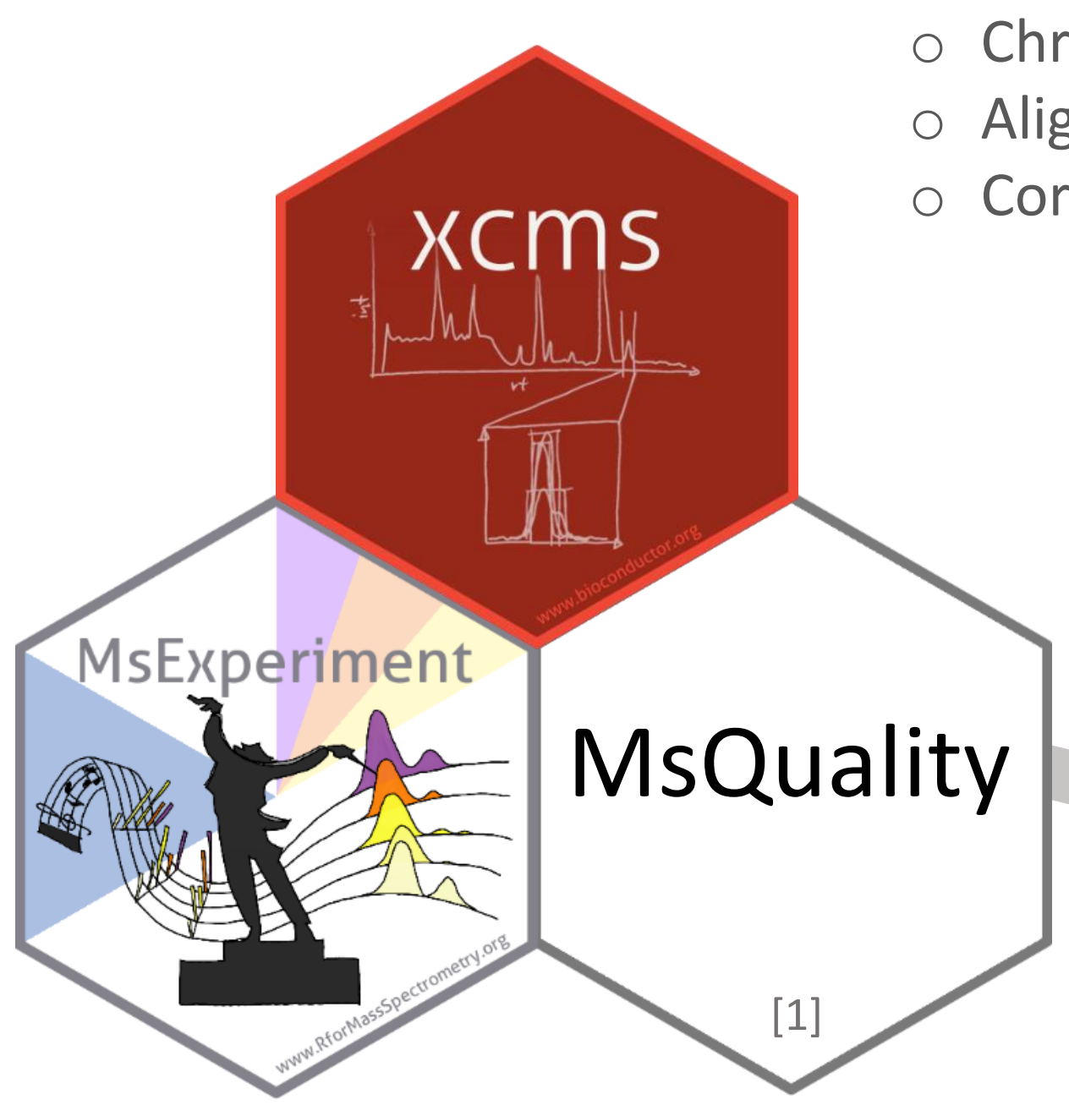
Get in touch/contribute

Poster on Zenodo

… to see it in action

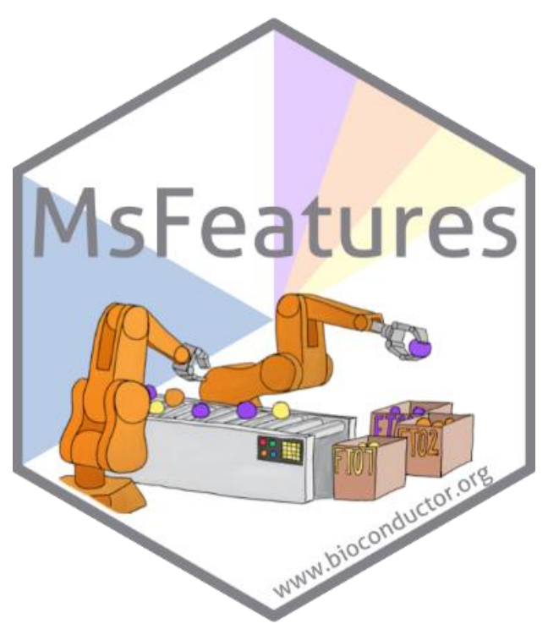
- Powerful and flexible infrastructure for efficient analysis of large-scale MS data
- Open collaborative development of software for MS data analysis:
  - Well documented and thoroughly tested
  - Long-term support and maintenance
- Modular package ecosystem to allow creation of custom analysis workflows
- Tightly integrated into Bioconductor

LC-MS(/MS) preprocessing



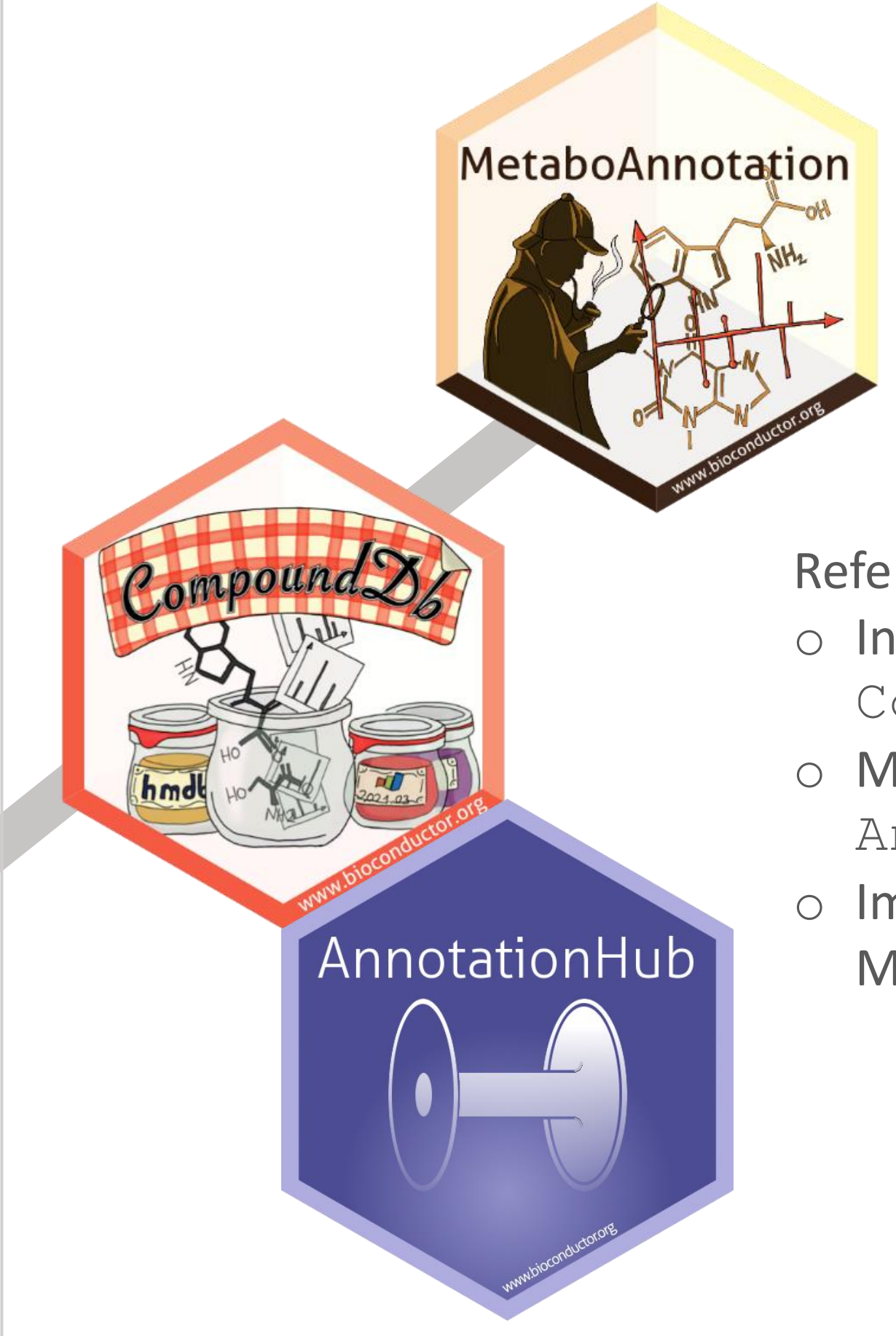
- Quality assessment
- Chromatographic peak detection
- Alignment
- Correspondence

Compounding



- Group adducts
- Group isotopes

Annotation [2]

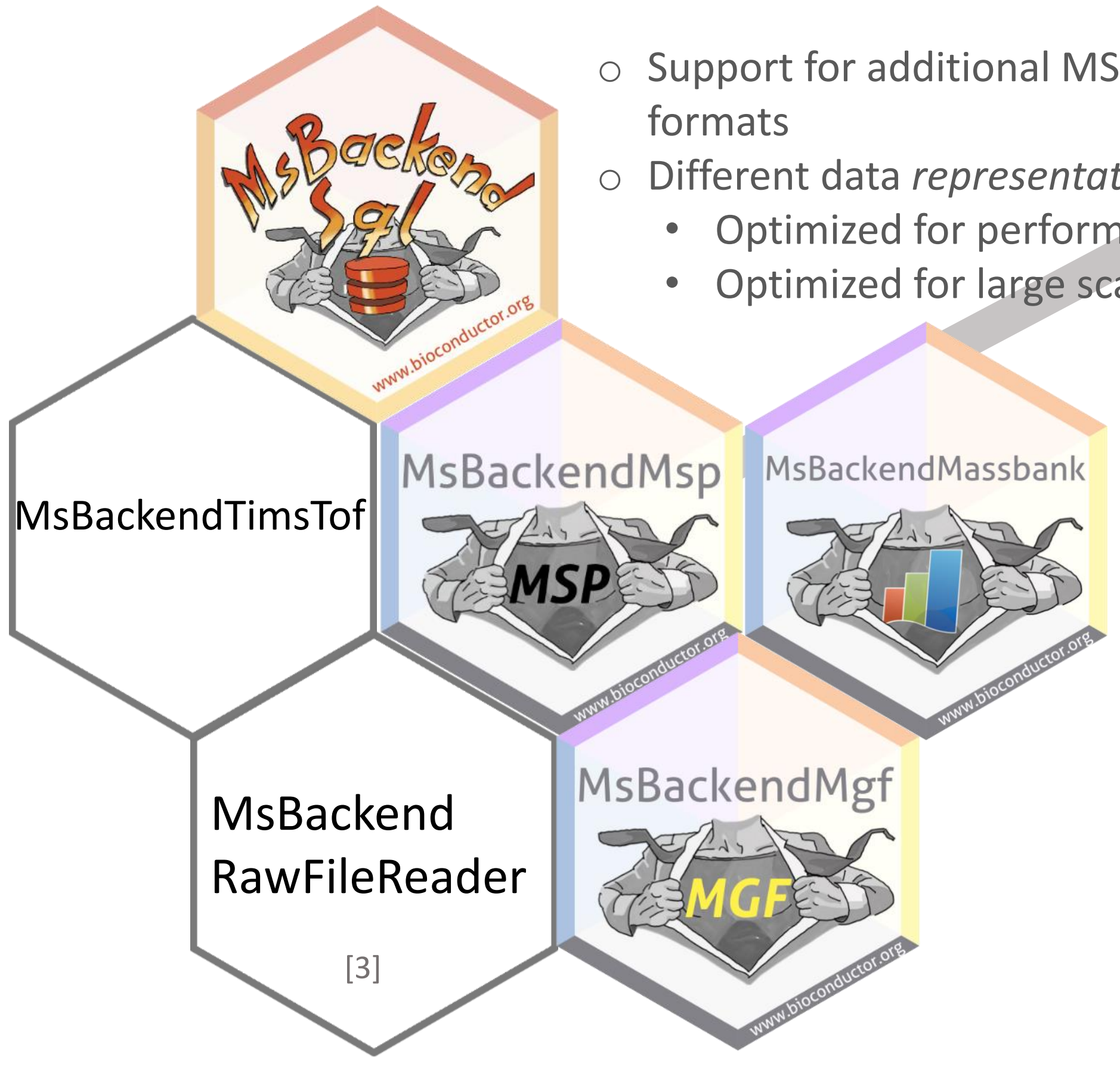


- MS1 and MS2-based annotation
- Fragment spectra matching

Reference libraries

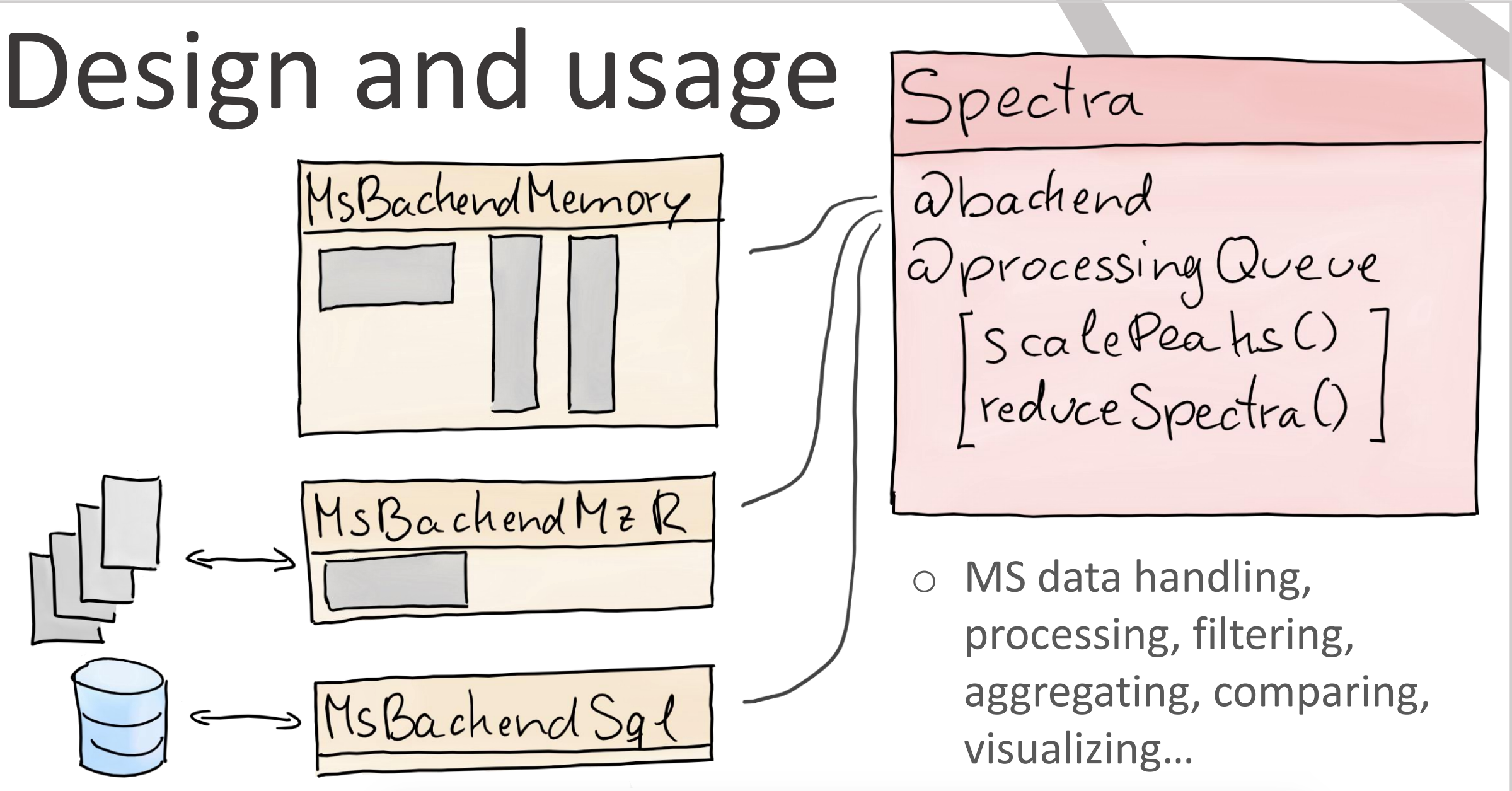
- In-house databases through `CompoundDb`
- MassBank through Bioconductor's `AnnotationHub`
- Import **GNPS** or others from MGF, MSP files.

Data I/O and representation



- Support for additional MS data file formats
- Different data *representations* :
  - Optimized for performance
  - Optimized for large scale data

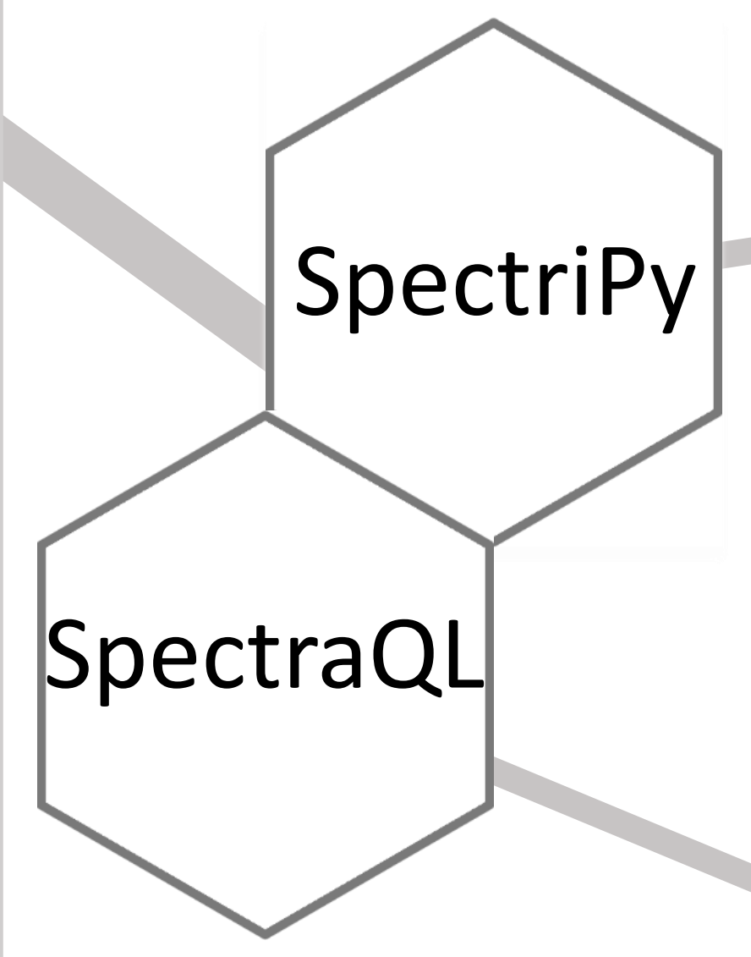
Design and usage



- MS data handling, processing, filtering, aggregating, comparing, visualizing…

```
> filterMsLevel(sps, msLevel = 1L) |>
+     scalePeaks() |>
+     reduceSpectra()
```

Integration with external tools



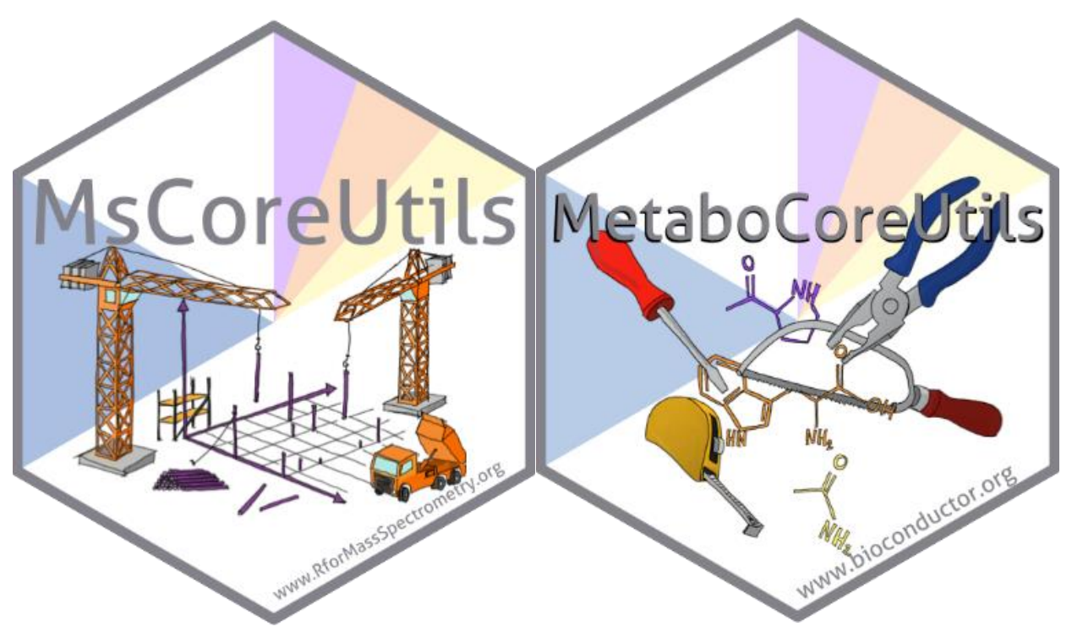
python

MATCHMS [4]

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

MassQL [5]

Core *low-level* functions



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

Outlook

- Continue integration of R/Bioconductor packages and external software
- Emphasis on seamless integration to improve user experience
- Open for contributions from the community -> reach out via github issue or email

References

[1] MsQuality – an interoperable open-source package for the calculation of standardized quality metrics of mass spectrometry data. Naake T et al. Bioinformatics 2023. https://doi.org/10.1093/bioinformatics/btad618
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