

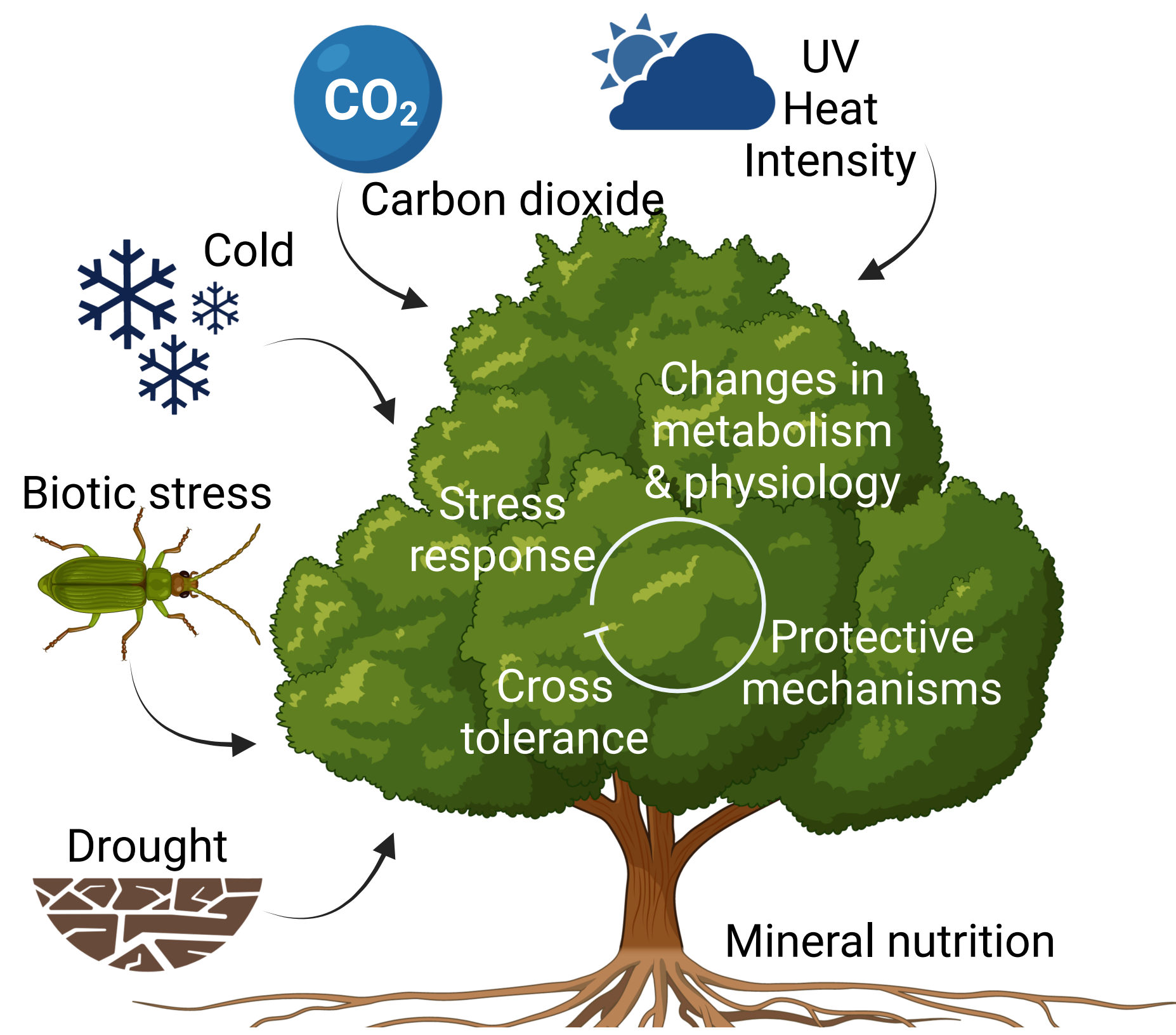
Introducing MetaboPeak: Streamlining Environmental Metabolomics Analysis for Terrestrial Plant Metabolism Modeling



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Supervisor: doc. Mgr. Otmar Urban, Ph.D.

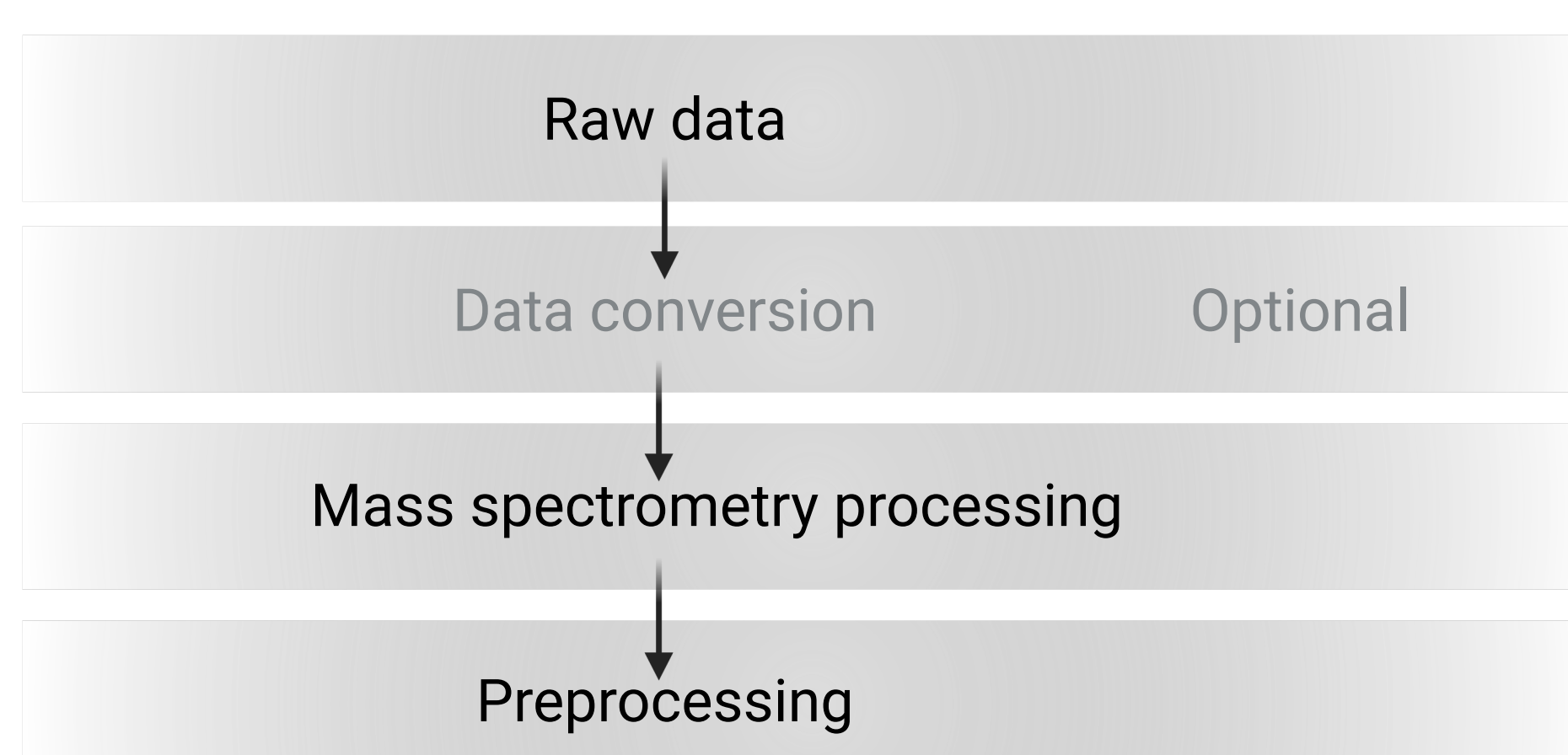
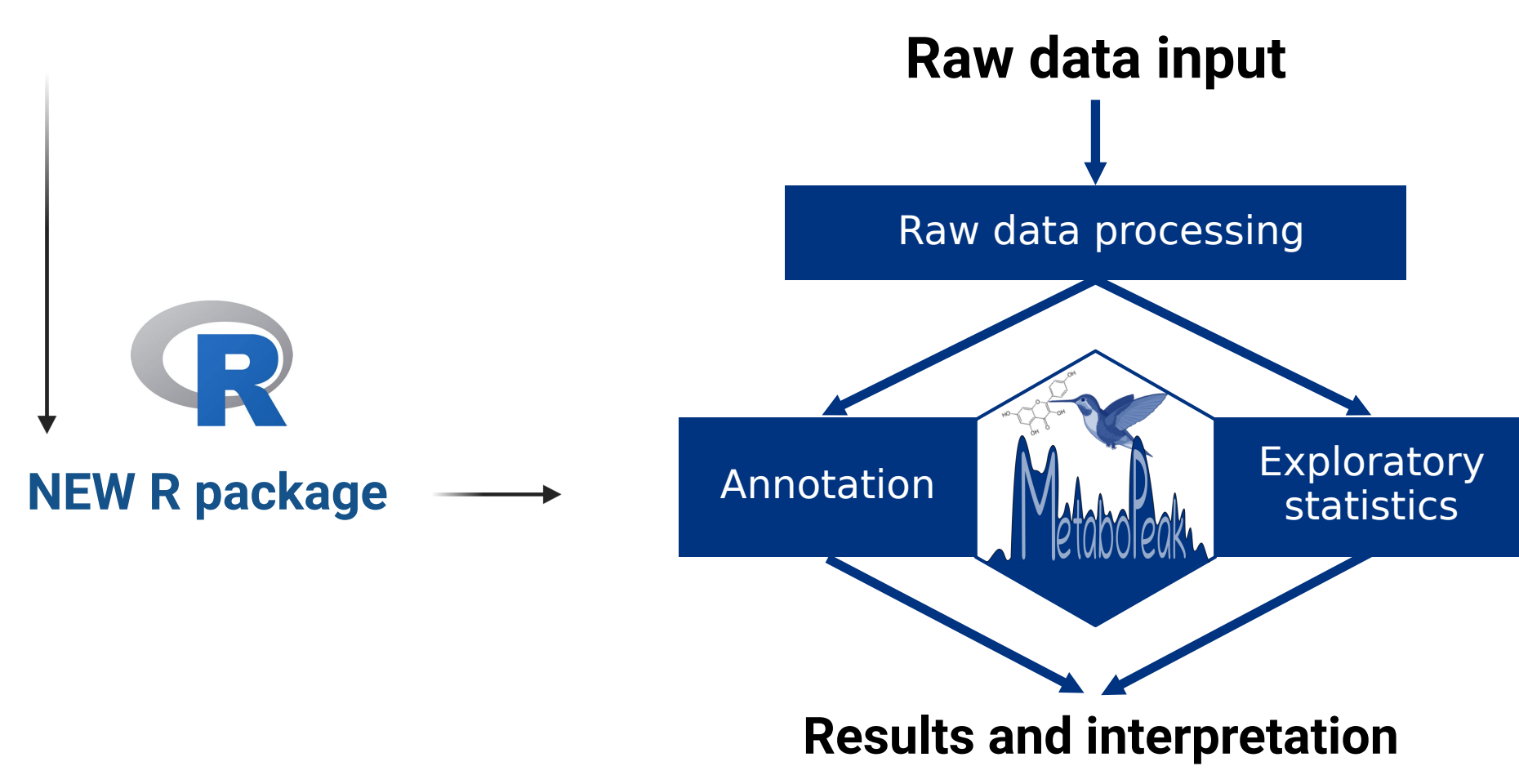
INTRODUCTION



Global climate models predict changes in environment conditions → need of understanding how forest ecosystems are affected → environmental metabolomics provides valuable insights into dynamic processes and external stimuli → LC-MS non-target analyses → annotation → exploratory statistics → pathway analyses → metabolite fingerprint

METHODS

- LC-MS data can be overwhelming
- Understanding data leads to better results
- Preprocessing is usually overlooked



| Important feature detection | |
|---|--------------|
| Peak information | peakInfo |
| Peak-fragment correlation | checkCorr |
| Positive and negative mode correspondence | checkCorr |
| Background noise variability check | barPeaks |
| Merging treatment/group information | treatGroup |
| Complete cases in treatment check | treatCases |
| Top sample selection | highestAbund |

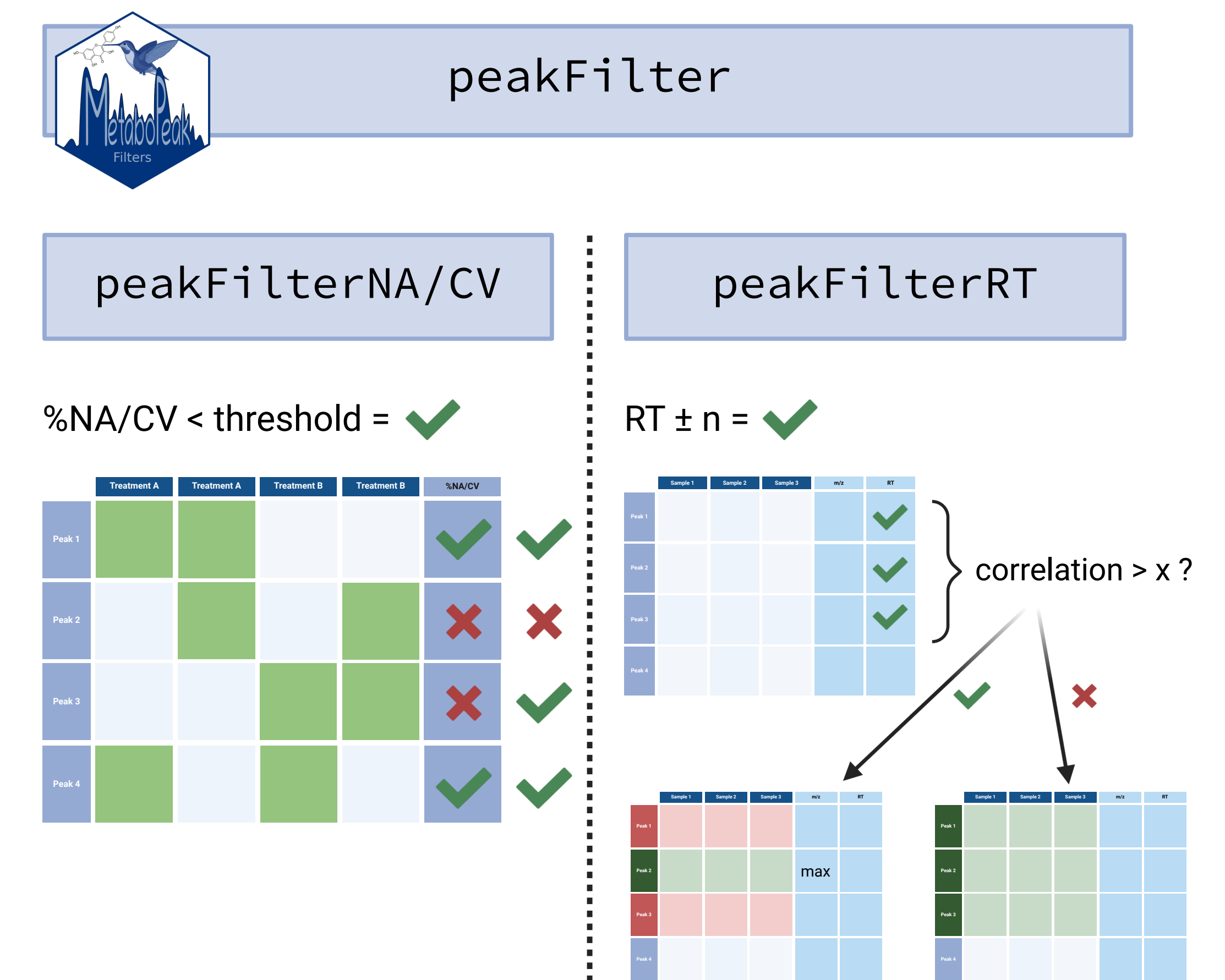
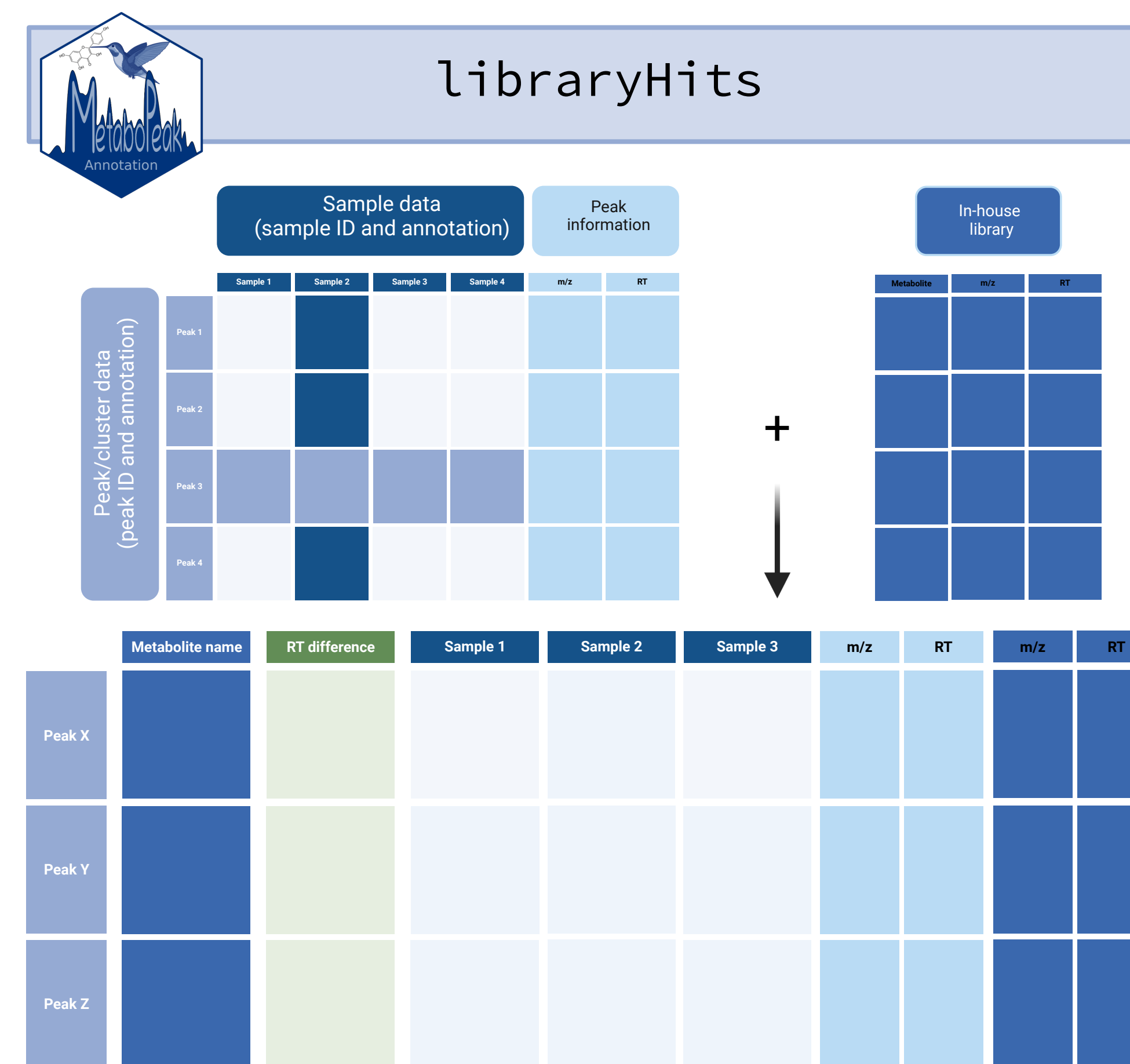
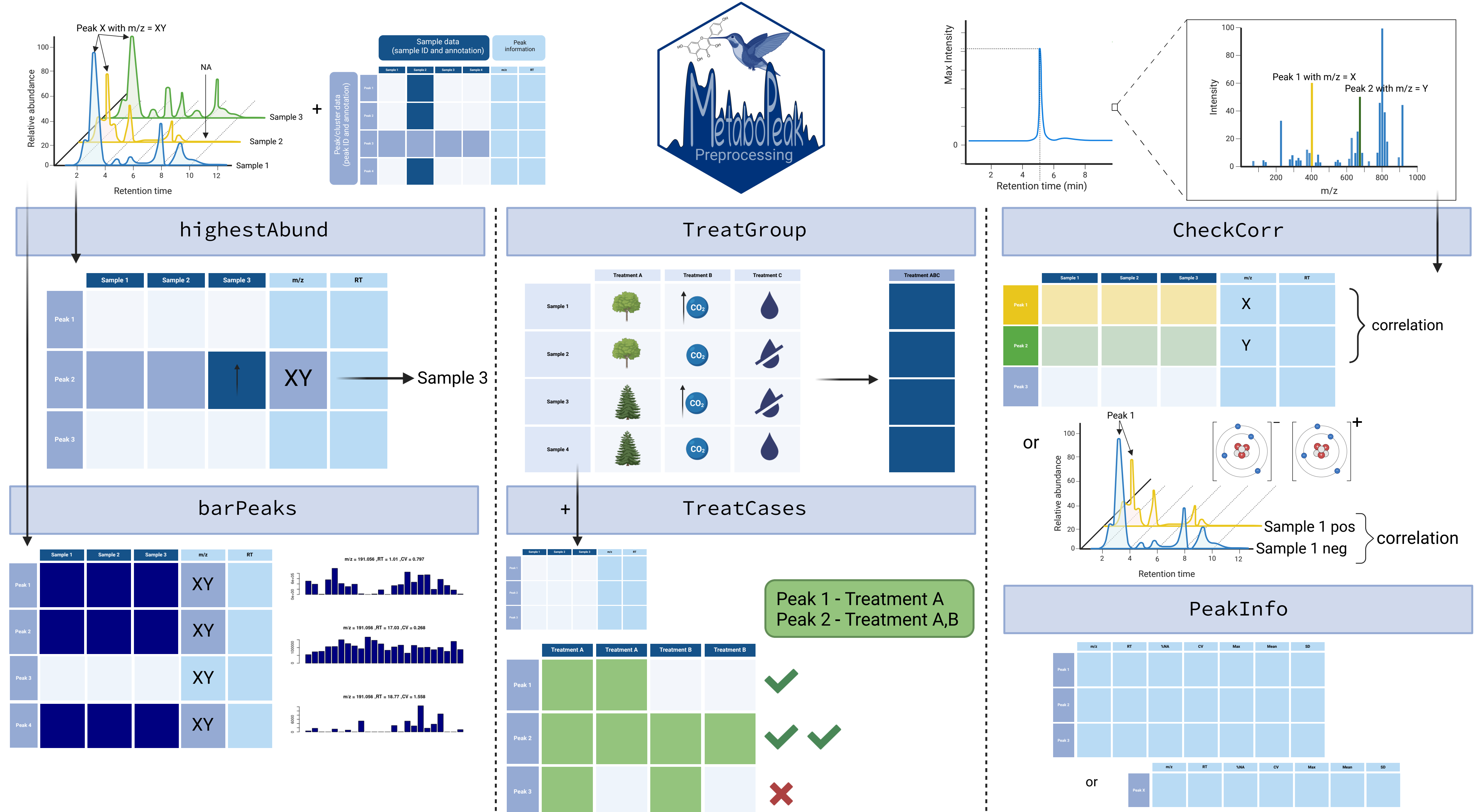
| Annotation | Exploratory statistics |
|-------------------------------|------------------------|
| Merging with in-house library | libraryHits |
| Filters | peakFilter |
| Filter by NA | peakFilterNA |
| Filter by CV | peakFilterCV |
| Filter by RT | peakFilterRT |

RESULTS

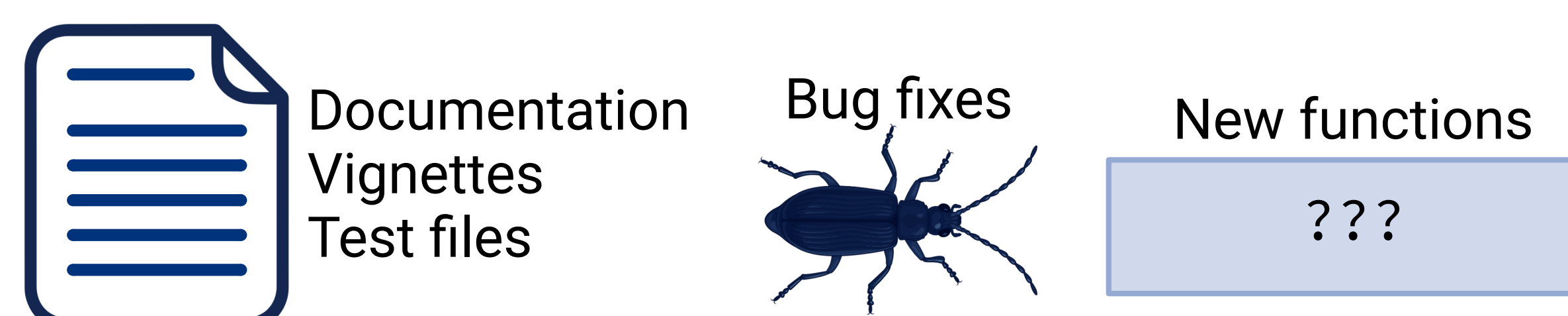
MetaboPeak in short:

- Simplify and automate processes commonly done in Excel
- More in-depth understanding of LC-MS data
- Offers options to link files and filter data

- Designed to work with processed data from a mass spectrometry software (MS-DIAL, MZmine, GeneData etc)



FUTURE PROSPECTS



Looking for collaborators:

- Better efficiency in R code
- Shiny App
- Beta testers



GitHub MetaboPeak



Got interested or an idea? Contact me!

Acknowledgement:

- Saleh Alseekh
- Markéta Macho



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