The R for Mass Spectrometry Initiative

Laurent Gatto[1], Sebastian Gibb[2] and Johannes Rainer[3]

[1] de Duve Institute, UCLouvain, Brussels, Belgium
[2] Department of Anaesthesiology and Intensive Care, University Medicine Greifswald, Germany
[3] Institute for Biomedicine, Eurac Research, Italy

The aim of the **R for Mass Spectrometry** initiative is to provide efficient, thoroughly documented, tested and flexible R software for the analysis and interpretation of high throughput mass spectrometry assays, including proteomics and metabolomics experiments.

The project formalises the longtime collaborative development efforts of its core members (notably the `mzR`, `MSnbase` and `xcms` packages) under the *RforMassSpectrometry* organisation to facilitate dissemination and accessibility of their work.

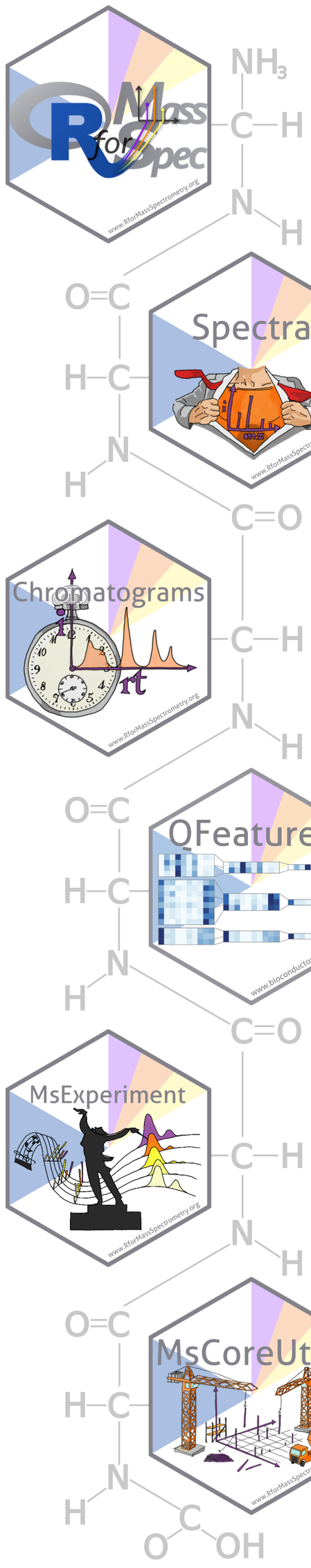
RforMassSpectrometry currently contains a set of packages (some are described on the right), that lay out the infrastructure for the **analysis and interpretation of high throughput mass spectrometry assays**.

Contributions to the initiative are more than welcome, whether under the form of ideas, documentation, code, packages, ...

Find details about contribution guidelines and **code of conduct** on our web page.

To learn more about our work at this conference, see

- Christophe Vanderaa's workshop where he demonstrates *Reproducing a single-cell proteomics data analysis using* **QFeatures** *and* **scp**.
- Johannes Rainer's workshop that shows how to use the **Spectra** package for *Seamless Integration of Mass Spectrometry Data from Different Sources*.
- Meet us at the **Bioconducor Mass Spectrometry** table in the lounge.



RforMassSpectrometry is a meta-package that is used to manage the R for Mass Spectrometry suite of package versions in a coherent way. Users will rely on this package to install and manage the other software.

The **Spectra** package provides base classes and processing methods for raw mass spectrometry data. It is designed with efficiency, both in terms of memory footprint and processing time in mind, and can manage data in different types of formats.

The **Chromatograms** package provides base classes and processing methods for chromatographic data. It is designed with efficiency, both in terms of memory footprint and processing time in mind, and can manage data in different types of formats.

The **QFeatures** package offers the infrastructure to manage and process quantitative features for high-throughput mass spectrometry assays, including proteomics and metabolomics experiments.

The **MsExperiment** package provides the infrastructure to store and manage all aspects related to a complete proteomics or metabolomics mass spectrometry experiment. It relies on the other RforMassSpectrometry core packages for the data crunching.

The **MsCoreUtils** package defines low-level functions for mass spectrometry data processing and is independent of any high-level data structures.

For more details, visit

`https://RforMassSpectrometry.org`

`https://github.io/RforMassSpectrometry`