

More Information about RMassBank and MassBank

RMassBank is a workflow to enable the creation of [high quality accurate mass MS/MS spectral records](#) for the [MassBank](#) database. The workflow includes automatic recalibration and processing of mass spectra mzML files within [R](#) and the retrieval of compound information via web services to minimise the user efforts in record generation. RMassBank was designed and tested on Orbitrap XL and Q-Exactive (Thermo) data and is now capable of processing data from a range of vendors and acquisition types through collaboration with the [IPB](#), [UFZ](#) and the [NORMAN Network](#). As RMassBank involves automated interpretation of the raw MS and MS/MS data, extensions to alternative formats relies on both the contributions of data and expertise from external parties.

Those directly involved in RMassBank development/maintenance include Michael Stravs & Emma Schymanski (Eawag), Steffen Neumann (IPB), Erik Müller (IPB/UFZ) and Tobias Schulze (UFZ). We also gratefully acknowledge the support of Prof. Nishioka (NAIST, Japan) and Prof. Masanori Arita (NIG, Japan).

The R package "RMassBank" and instructions in the vignette are available from Bioconductor. A demonstration script is available (using RMassBankData) and a prototype of the RMassBankGUI, along with some presentations from the latest [NORMAN MassBank Workshop](#).

- [RMassBank](#) (R package)
- [RMassBankData](#) (raw test data: ~50 MB)
- [RMassBankDemo Script](#)
- [RMassBankDemo Script Lite](#)
- [RMassBankGUI Tutorial](#)
- [RMassBank GUI Video](#)
- Presentations: [RMassBank](#), [RMassBank Demo](#) and [RMassBank with XCMS](#)

Development activities can be followed on github:

- [MassBank Development Team](#)
- [RMassBank](#)
- [RMassBank Extras](#)
- [RMassBankGUI](#)

Example spectra processed with RMassBank can be found on [MassBank.jp](#) and [NORMAN MassBank](#). Tentative, Literature and SI spectra are additionally available on massbank.eu. All MassBank records marked with a "CC" license can also be [downloaded](#).

- Eawag Standard Spectra ([JP](#)), ([EU](#))
- UFZ Standard Spectra ([JP](#)), ([EU](#))
- Eawag Additional Spectra ([EU](#))
- UFZ Additional Spectra ([EU](#))
- Literature Spectra ([EU](#))

Feedback and contributions to RMassBank and MassBank are welcomed. Contact us via:

- MassBank Developer Mailing List
- MassBank User Mailing List
- [Metabolomics-Forum](#)
- Email: massbank {at} massbank.eu (Tobias Schulze, Guido Schramm, Emma Schymanski)
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