# **Resource Summary Report**

Generated by NIF on May 16, 2025

## **RMassBank**

RRID:SCR\_002797

Type: Tool

## **Proper Citation**

RMassBank (RRID:SCR\_002797)

#### Resource Information

URL: http://www.bioconductor.org/packages/release/bioc/html/RMassBank.html

**Proper Citation:** RMassBank (RRID:SCR\_002797)

**Description:** Workflow software to process tandem MS files and build MassBank records. Functions include automated extraction of tandem MS spectra, formula assignment to tandem MS fragments, recalibration of tandem MS spectra with assigned fragments, spectrum cleanup, automated retrieval of compound information from Internet databases, and export to MassBank records.

**Resource Type:** software resource, workflow software, software application, data processing software

**Keywords:** standalone software, mac os x, unix/linux, windows, r, mass spectrometry, metabolomics

Funding:

Availability: Artistic License, v2

Resource Name: RMassBank

Resource ID: SCR\_002797

Alternate IDs: OMICS\_02657

**Record Creation Time:** 20220129T080215+0000

Record Last Update: 20250516T053645+0000

## **Ratings and Alerts**

No rating or validation information has been found for RMassBank.

No alerts have been found for RMassBank.

### **Data and Source Information**

Source: SciCrunch Registry

## **Usage and Citation Metrics**

We found 5 mentions in open access literature.

**Listed below are recent publications.** The full list is available at NIF.

Janho Dit Hreich S, et al. (2024) Activation of the P2RX7/IL-18 pathway in immune cells attenuates lung fibrosis. eLife, 12.

Elapavalore A, et al. (2023) Adding open spectral data to MassBank and PubChem using open source tools to support non-targeted exposomics of mixtures. Environmental science. Processes & impacts, 25(11), 1788.

Ruttkies C, et al. (2019) Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. Analytical and bioanalytical chemistry, 411(19), 4683.

Oberacher H, et al. (2018) Annotating Nontargeted LC-HRMS/MS Data with Two Complementary Tandem Mass Spectral Libraries. Metabolites, 9(1).

Schymanski EL, et al. (2017) Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of cheminformatics, 9(1), 22.