

Resource Summary Report

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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>

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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

Availability: Free, Freely available, Available for download

Resource Name: RMassBank

Resource ID: SCR_002797

Alternate IDs: OMICS_02657

License: Artistic License, v2

Record Creation Time: 20220129T080215+0000

Record Last Update: 20260820T054347+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 9 mentions in open access literature.

Listed below are recent publications. The full list is available at [NIF](#) .

Neumann S, et al. (2026) MassBank: an open and FAIR mass spectral data resource. *Nucleic acids research*, 54(D1), D601.

Schanbacher F, et al. (2026) Curation of Mass Spectrometry Reference Data for Improved Identification and Dereplication of Cyanobacterial Specialized Metabolites. *Journal of natural products*, 89(5), 1499.

Ahlendorf A, et al. (2026) The MassBank contributions of the mFam collaboration. *Metabolomics : Official journal of the Metabolomic Society*, 22(4).

Rypar T, et al. (2025) Targeted Isolation of Prenylated Flavonoids from *Paulownia tomentosa* Fruit Extracts via AI-Guided Workflow Integrating LC-UV-HRMS/MS. *Metabolites*, 15(9).

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.