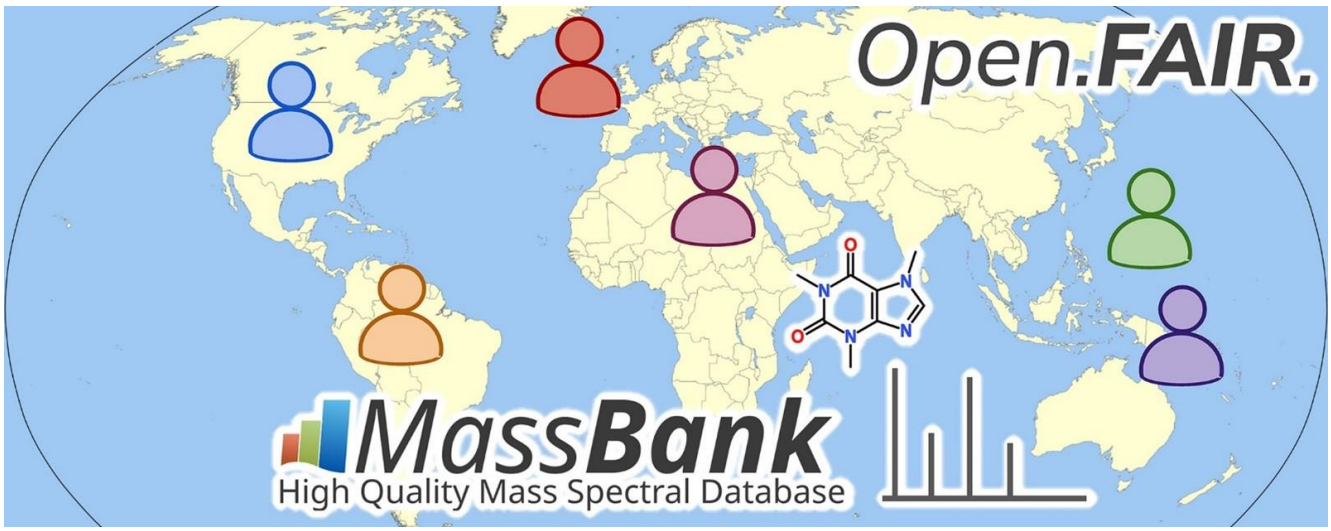
Metabolome database

MassBank

https://massbank.jp/MassBank/

MassBank was established in Japan in 2006 as an open-source, open-access mass spectrum library, supported by the BIRD project of the Institute for Bioinformatics Research and Development, the predecessor of NBDC. Since then, it has been operated with the support of the Mass Spectrometry Society of Japan (MSSJ). In 2011, a dedicated MassBank server was launched in Europe with the support of the NORMAN Society in Germany, and spectra of environmentally related compounds were added. Currently, it provides spectra of 18,529 compounds and a total of 119,845 mass spectrum data entries registered by researchers worldwide.

MassBank integrates with multiple resources, including MassBank of North America, Global Natural Product Social Molecular Networking, PubChem, the US EPA CompTox Dashboard, the NORMAN Database System, and RforMassSpectrometry, and is widely used by researchers worldwide as a metabolome mass spectrum library.



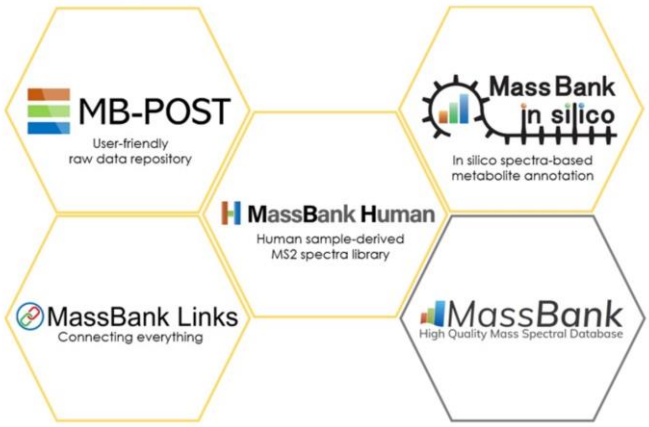
Shin-MassBank Project

Shin-MassBank Project aims to develop a new data processing pipeline for accumulating product ion (MS2) spectra obtained from biological samples.

This pipeline consists of three databases: **MB-POST**, an easy-to-use raw data repository; **MassBank Human**, a library of MS2 spectra derived from human metabolome datasets; and **MassBank in silico**, which provides metabolite annotation using computationally predicted spectra.

The Shin-MassBank project is a member of the MassBank Consortium and collaborates with the Spectral Data Division of the Mass Spectrometry Society of Japan.

Shin-MassBank



References

1. Steffen Neumann et al., MassBank: an open and FAIR mass spectral data resource. Nucleic Acids Research (DOI: 10.1093/nar/gkaf1193/8321203)

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(Apr 2026)

Analysis pipeline for metabolome data

Shin-MassBank
Mass spec data processing pipeline

Shin-MassBank

https://shin.massbank.jp/

Shin-MassBank

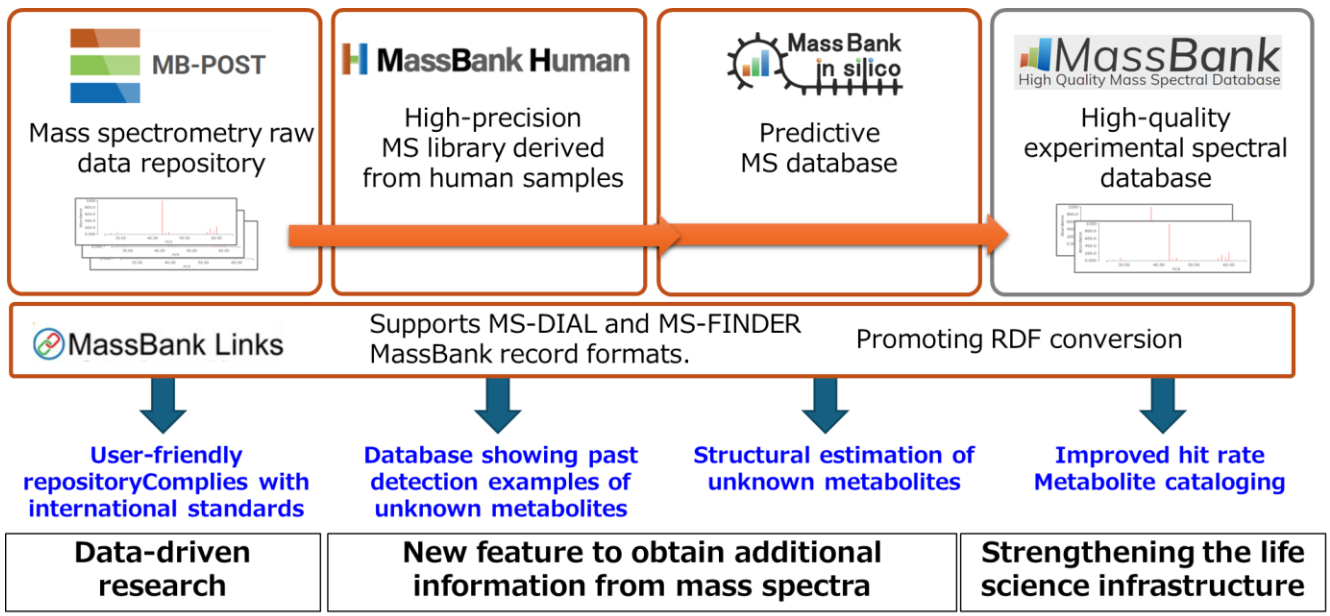
MB-POST
A repository for biospectral data derived from biological samples. It features high-speed file transfer capabilities and a user-friendly interface. Registering data with MB-POST assigns a unique identification number required for journal submission.

MassBank Human (currently beta version)
Reanalyze the mass spectrometry data of metabolites derived from biological samples deposited in MB-POST to compile high-quality spectral data.

MassBank in silico (currently beta version)
A library of mass spectra predicted in silico from compound structures. It generates comprehensive predicted spectra computationally for in vivo metabolites.

MassBank Links
A portal that integrates MB-POST and MassBank and connects to other databases. It converts metabolite tables and mass spectra extracted from MS-DIAL and MS-FINDER into RDF format and makes them available.

MassBank
It is currently operated with the support of the Japanese Society for Mass Spectrometry (MSSJ). In 2011, a dedicated MassBank server began operating in Europe with the support of the German NORMAN Association; spectra of environmental compounds were added, and the database now provides a total of 119,845 mass spectra entries for 18,529 compounds registered by researchers worldwide.



Shin-MassBank is supported under JST Database Integration Coordination Program (DICP), "Development of next generation mass spectra data base, Shin-MassBank" (PI: MATSUDA Fumio Professor, Graduate School of Information Science and Technology, The University of Osaka).

References

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