

Resource Summary Report

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GMD

RRID:SCR_006625

Type: Tool

Proper Citation

GMD (RRID:SCR_006625)

Resource Information

URL: <http://gmd.mpimp-golm.mpg.de/>

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Description: It facilitates the search for and dissemination of mass spectra from biologically active metabolites quantified using Gas chromatography (GC) coupled to mass spectrometry (MS). Use the Search Page to search for a compound of your interest, using the name, mass, formula, InChI etc. as query input. Additionally, a Library Search service enables the search of user submitted mass spectra within the GMD. In parallel to the library search, a prediction of chemical sub-groups is performed. This approach has reached beta level and a publication is currently under review. Using several sub-group specific Decision Trees (DTs), mass spectra are classified with respect to the presence of the chemical moieties within the linked (unknown) compound. Prediction of functional groups (ms analysis) facilitates the search of metabolites within the GMD by means of user submitted GC-MS spectra consisting of retention index (n-alkanes, if available) and mass intensities ratios. In addition, a functional group prediction will help to characterize those metabolites without available reference mass spectra included in the GMD so far. Instead, the unknown metabolite is characterized by predicted presence or absence of functional groups. For power users this functionality presented here is exposed as soap based web services. Functional group prediction of compounds by means of GC-EI-MS spectra using Microsoft analysis service decision trees All currently available trained decision trees and sub-structure predictions provided by the GMD interface. Table describes the functional group, optional use of an RI system, record date of the trained decision tree, number of MSTs with proportion of MSTs linked to metabolites with the functional group present for each tree. Average and standard deviation of the 50-fold CV error, namely the ratio false over correctly sorted MSTs in the trained DT, are listed. The GMD website offers a range of mass spectral reference libraries to academic users which can be downloaded free of charge in various electronic formats. The libraries are constituted by base peak normalized consensus spectra of single analytes and contain masses in the range 70 to 600 amu, while the ubiquitous mass fragments typically generated from compounds carrying a trimethylsilyl-moiety, namely the fragments at m/z 73, 74, 75, 147, 148, and 149, were excluded.

Abbreviations: GMD

Synonyms: Golm Metabolome Data Base, The Golm Metabolome Database, Golm Metabolome Database

Resource Type: service resource, data access protocol, software resource, web service, data or information resource, database

Defining Citation: [PMID:15613389](#), [PMID:15733837](#), [PMID:18501684](#), [PMID:20526350](#)

Keywords: drug, expression, functional, gas chromatography, gene, general chemistry databases, bioinformatic, biological extract, biology, biotechnology, compound, genomic, herbicide, mass spectra, mass spectrometry, metabolism, metabolite, metabolomics, organism, profiling, protein, spectral, system, FASEB list

Resource Name: GMD

Resource ID: SCR_006625

Alternate IDs: r3d100011046, nif-0000-21180

Alternate URLs: <http://csbdb.mpimp-golm.mpg.de/csbdb/gmd/gmd.html>,
<https://doi.org/10.17616/R3MC9K>

Record Creation Time: 20220129T080237+0000

Record Last Update: 20260731T042727+0000

Ratings and Alerts

No rating or validation information has been found for GMD.

No alerts have been found for GMD.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 157 mentions in open access literature.

Listed below are recent publications. The full list is available at [kravitz2](#) .

Wittemeier L, et al. (2025) Positional ¹³C enrichment analysis of aspartate determines PEPC activity in vivo. The New phytologist, 248(1), 401.

Iglesias-Sanchez A, et al. (2025) Activation of alternative oxidase ensures carbon supply for ethylene and carotenoid biosynthesis during tomato fruit ripening. Plant physiology, 199(3).

Martínez Rivas FJ, et al. (2025) Parallel evolution of salinity tolerance in *Arabidopsis thaliana* accessions from Cape Verde Islands. *Science advances*, 11(28), eadq8210.

Turek S, et al. (2025) Multi-omics integration of transcriptome, miRNA, and metabolome uncovers molecular mechanisms of male flower development in cucumber line B10 (*Cucumis sativus* L.). *Scientific reports*, 15(1), 45734.

Liu Z, et al. (2025) Metabolomics Profiling and Advanced Methodologies for Wheat Stress Research. *Metabolites*, 15(2).

Ding G, et al. (2025) Identifications of Genes Involved in ABA and MAPK Signaling Pathways Positively Regulating Cold Tolerance in Rice. *Plants (Basel, Switzerland)*, 14(4).

Derba-Maceluch M, et al. (2025) Glucuronoyl Esterase Expressed in Aspen Xylem Affects ??-Ester Linkages Between Lignin and Glucuronoxylan Reducing Recalcitrance and Accelerating Growth. *Plant biotechnology journal*, 23(12), 5417.

Lee DY, et al. (2025) Profiling of Metabolite Changes in Lettuce Leaves during Fermentation by *Bacillus subtilis*. *Journal of microbiology and biotechnology*, 35, e2501026.

Martinez-Seidel F, et al. (2025) Remodelled ribosomal populations synthesize a specific proteome in proliferating plant tissue during cold. *Philosophical transactions of the Royal Society of London. Series B, Biological sciences*, 380(1921), 20230384.

Samo N, et al. (2025) Polycomb repressive complex 2 facilitates the transition from heterotrophy to photoautotrophy during seedling emergence. *The Plant cell*, 37(7).

Zhao Y, et al. (2025) Combined analysis of proteomics and metabolism reveals critical roles of oxidoreductase activity in mushrooms stimulated by wolfberry and sea buckthorn substrates. *Frontiers in nutrition*, 12, 1543240.

Bahadar H, et al. (2025) Blue light-induced stomatal opening is associated with species-specific changes in primary metabolism but not with starch breakdown in guard cells. *The New phytologist*, 248(5), 2347.

Chai YN, et al. (2024) Root-associated bacterial communities and root metabolite composition are linked to nitrogen use efficiency in sorghum. *mSystems*, 9(1), e0119023.

El-Zairy AH, et al. (2024) Spectroscopic analysis of wild medicinal desert plants from wadi sanor (beni-suef), Egypt, and their antimicrobial and antioxidant activities. *Heliyon*, 10(21), e39612.

Hassan AHA, et al. (2024) Inoculation with *Jeotgalicoccus* sp. improves nutritional quality and biological value of *Eruca sativa* by enhancing amino acid and phenolic metabolism and increasing mineral uptake, unsaturated fatty acids, vitamins, and antioxidants. *Frontiers in plant science*, 15, 1412426.

Nehela Y, et al. (2023) Gamma-Aminobutyric Acid Accumulation Contributes to Citrus *sinensis* Response against 'Candidatus Liberibacter Asiaticus' via Modulation of Multiple Metabolic Pathways and Redox Status. *Plants (Basel, Switzerland)*, 12(21).

Alsherif EA, et al. (2023) Understanding the Active Mechanisms of Plant (Sesuvium portulacastrum L.) against Heavy Metal Toxicity. *Plants* (Basel, Switzerland), 12(3).

Deidda M, et al. (2023) Right Ventricular Subclinical Dysfunction in SLE Patients Correlates with Metabolomic Fingerprint and Organ Damage. *Metabolites*, 13(7).

Fathy WA, et al. (2023) Exploring Exogenous Indole-3-acetic Acid's Effect on the Growth and Biochemical Profiles of *Synechocystis* sp. PAK13 and *Chlorella variabilis*. *Molecules* (Basel, Switzerland), 28(14).

Sikron-Persi N, et al. (2023) Mass spectrometry-based metabolite profiling reveals functional seasonal shifts in the metabolome of *Zygophyllum dumosum* Boiss and its relation to environmental conditions. *Planta*, 258(1), 10.