

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: software resource, data access protocol, service 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: 20260807T042639+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 192 mentions in open access literature.

Listed below are recent publications. The full list is available at [T1D](#) .

Campana N, et al. (2026) Metabolomic Signatures and Advanced Echocardiography Highlight Clinical Risk and Early Cardiac Changes in Systemic Lupus Erythematosus: Six-Year Follow-Up. *Metabolites*, 16(2).

Studnicka MH, et al. (2026) Morphophysiological disorders and metabolic reprogramming in *Physalis peruviana* infected with the *physalis rugose* mosaic virus. *Scientific reports*, 16(1).

Bilova T, et al. (2026) Analyzing Plant Low-Molecular-Weight Polar Metabolites: A GC-MS Approach. *Plants (Basel, Switzerland)*, 15(3).

Marte DDS, et al. (2026) Development and Characterization of Pasta Enriched with Giant Mealworm (*Zophobas morio*) Powder: An Innovative Nutritional Alternative. *Insects*, 17(2).

Sheteiwiy MS, et al. (2026) Evaluating the beneficial role of bio-inoculants (*Bradyrhizobium* and arbuscular mycorrhizal fungi) in improving the nutritional value and metabolic profile of soybean seeds. *Scientific reports*, 16(1).

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.

Bouزيد M, et al. (2025) Natural variation in *Arabidopsis thaliana* highlights a key role of glyoxalase I;2 in detoxifying glucose-derived reactive carbonyl species. *BMC plant biology*, 25(1), 1288.

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

Staykov N, et al. (2025) Sustainable agriculture through seaweed biostimulants: a two-year study demonstrates yield enhancement in pepper and eggplant. *Frontiers in plant science*, 16, 1655340.

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).

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).

Zrig A, et al. (2025) The biomass and health-enhancing qualities of lettuce are amplified through the inoculation of arbuscular mycorrhizal fungi. *BMC plant biology*, 25(1), 521.

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

Benjamin G, et al. (2025) Nitrogen-fixing symbiosis induces differential accumulation of *Medicago truncatula* leaf defence metabolites in response to pea aphid infestation. *Frontiers in plant science*, 16, 1670344.

Santos ÍVC, et al. (2025) Exploring the Effects of VgPIP1;2 Overexpression in the Roots of Young Rice Plants: Modifications in Root Architecture, Transcriptomic and Metabolomic Profiles. *Plants (Basel, Switzerland)*, 14(23).

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

Osmolovskaya N, et al. (2025) Metabolic Responses of *Amaranthus caudatus* Roots and Leaves to Zinc Stress. *Plants (Basel, Switzerland)*, 14(14).

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