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 vailable) 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: web service, database, service resource, data or information resource, data access protocol, software resource

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

Funding:

Resource Name: GMD

Resource ID: SCR_006625

Alternate IDs: nif-0000-21180

Alternate URLs: http://csbdb.mpimp-golm.mpg.de/csbdb/gmd/gmd.html

Record Creation Time: 20220129T080237+0000

Record Last Update: 20250429T055106+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 145 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

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.

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.

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).

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).

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

Stitz M, et al. (2023) TOR acts as a metabolic gatekeeper for auxin-dependent lateral root initiation in Arabidopsis thaliana. The EMBO journal, 42(10), e111273.

Álvarez-Rodríguez S, et al. (2023) Application of Indole-Alkaloid Harmaline Induces Physical Damage to Photosystem II Antenna Complexes in Adult Plants of Arabidopsis thaliana (L.) Heynh. Journal of agricultural and food chemistry, 71(15), 6073.

Fathy WA, et al. (2023) Glycine differentially improved the growth and biochemical composition of Synechocystis sp. PAK13 and Chlorella variabilis DT025. Frontiers in bioengineering and biotechnology, 11, 1161911.

Treves H, et al. (2022) Carbon flux through photosynthesis and central carbon metabolism show distinct patterns between algae, C3 and C4 plants. Nature plants, 8(1), 78.

Bao Y, et al. (2022) Anthocyanin regulatory networks in Solanum tuberosum L. leaves elucidated via integrated metabolomics, transcriptomics, and StAN1 overexpression. BMC plant biology, 22(1), 228.

Kalogeropoulou E, et al. (2022) Combined Transcriptomic and Metabolomic Analysis Reveals Insights into Resistance of Arabidopsis bam3 Mutant against the Phytopathogenic Fungus Fusarium oxysporum. Plants (Basel, Switzerland), 11(24).

Krasteva G, et al. (2022) Metabolite Profiling of Gardenia jasminoides Ellis In Vitro Cultures with Different Levels of Differentiation. Molecules (Basel, Switzerland), 27(24).

Biggio F, et al. (2022) Effects of Chronic Bifidobacteria Administration in Adult Male Rats on Plasma Metabolites: A Preliminary Metabolomic Study. Metabolites, 12(8).

Srinivasan J, et al. (2022) Endophytic Bacteria Colonizing the Petiole of the Desert Plant Zygophyllum dumosum Boiss: Possible Role in Mitigating Stress. Plants (Basel, Switzerland), 11(4).

Knoch D, et al. (2021) Multi-omics-based prediction of hybrid performance in canola. TAG. Theoretical and applied genetics. Theoretische und angewandte Genetik, 134(4), 1147.

Wolf E, et al. (2021) Evolutionary footprints of a cold relic in a rapidly warming world. eLife, 10.

Tedesco S, et al. (2021) The Impact of Metabolic Scion-Rootstock Interactions in Different Grapevine Tissues and Phloem Exudates. Metabolites, 11(6).