Resource Summary Report

Generated by dkNET on Apr 15, 2025

NIST Mass Spectrometry Data Center

RRID:SCR_014680
Type: Tool

Proper Citation

NIST Mass Spectrometry Data Center (RRID:SCR_014680)

Resource Information

URL: http://chemdata.nist.gov

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Description: A data center that develops evaluated mass spectral libraries and provides related software tools that assist compound identification by providing reference mass spectra for GC/MS (by electron ionization) and LC-MS/MS (by tandem mass spectrometry). It also provides gas phase retention indices for GC. Resources include the mass spectral library, the peptide library, and a standard refernece material guide.

Synonyms: Mass Spectrometry Data Center, NIST MS Data Center, MS Data Center

Resource Type: portal, organization portal, data or information resource

Keywords: metabolomics, metabolomics tool, peptide, mass spectrometry, compound identification, data center, portal

Funding:

Resource Name: NIST Mass Spectrometry Data Center

Resource ID: SCR_014680

Alternate URLs: https://www.nist.gov/mml/biomolecular-measurement/mass-spectrometry-data-center

Record Creation Time: 20220129T080321+0000

Record Last Update: 20250412T055823+0000

Ratings and Alerts

No rating or validation information has been found for NIST Mass Spectrometry Data Center.

No alerts have been found for NIST Mass Spectrometry Data Center.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 73 mentions in open access literature.

Listed below are recent publications. The full list is available at dkNET.

Pal Mahadevan V, et al. (2025) Preference for and resistance to a toxic sulfur volatile opens up a unique niche in Drosophila busckii. Nature communications, 16(1), 767.

Richard AM, et al. (2025) Analytical Quality Evaluation of the Tox21 Compound Library. Chemical research in toxicology, 38(1), 15.

Brinza I, et al. (2025) Neuroprotective Potential of Origanum majorana L. Essential Oil Against Scopolamine-Induced Memory Deficits and Oxidative Stress in a Zebrafish Model. Biomolecules, 15(1).

Pal Mahadevan V, et al. (2024) Phenolics as ecologically relevant cues for slime flux breeding Drosophila virilis. iScience, 27(11), 111180.

Zubeldia-Varela E, et al. (2024) The impact of high-IgE levels on metabolome and microbiome in experimental allergic enteritis. Allergy, 79(12), 3430.

Mwaheb MA, et al. (2024) Versatile properties of Opuntia ficus-indica (L.) Mill. flowers: In vitro exploration of antioxidant, antimicrobial, and anticancer activities, network pharmacology analysis, and In-silico molecular docking simulation. PloS one, 19(11), e0313064.

Qin Y, et al. (2024) Succession of microbiota and its influence on the dynamics of volatile compounds in the semi-artificial inoculation fermentation of mulberry wine. Food chemistry: X, 21, 101223.

Lecoutre S, et al. (2024) Reduced adipocyte glutaminase activity promotes energy expenditure and metabolic health. Nature metabolism, 6(7), 1329.

Jambrina-Enríquez M, et al. (2024) Microstratigraphic, lipid biomarker and stable isotope study of a middle Palaeolithic combustion feature from Axlor, Spain. iScience, 27(1), 108755.

Warneke R, et al. (2024) Coenzyme A biosynthesis in Bacillus subtilis: discovery of a novel precursor metabolite for salvage and its uptake system. mBio, 15(10), e0177224.

Sandström H, et al. (2024) Data-Driven Compound Identification in Atmospheric Mass Spectrometry. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 11(8), e2306235.

Goecker ZC, et al. (2024) Variation of Site-Specific Glycosylation Profiles of Recombinant Influenza Glycoproteins. Molecular & cellular proteomics : MCP, 23(9), 100827.

Malik S, et al. (2024) Unveiling the Nexus: Cellular Metabolomics Unravels the Impact of Estrogen on Nicotinamide Metabolism in Mitigating Rheumatoid Arthritis Pathogenesis. Metabolites, 14(4).

Luo EK, et al. (2024) Investigating the effects of thermal processing on bitter substances in atemoya (Annona cherimola × Annona squamosa) through sensory-guided separation. Food chemistry: X, 24, 101817.

Tang R, et al. (2024) Tandemly expanded OR17b in Himalaya ghost moth facilitates larval food allocation via olfactory reception of plant-derived tricosane. International journal of biological macromolecules, 268(Pt 1), 131503.

Sarkar B, et al. (2023) Detection of a bibenzyl core scaffold in 28 common mangrove and associate species of the Indian Sundarbans: potential signature molecule for mangrove salinity stress acclimation. Frontiers in plant science, 14, 1291805.

Zhang Y, et al. (2023) The Capsicum terpenoid biosynthetic module is affected by spider-mite herbivory. Plant molecular biology, 113(4-5), 303.

Embarez DH, et al. (2023) Acetaminophen-traces bioremediation with novel phenotypically and genotypically characterized 2 Streptomyces strains using chemo-informatics, in vivo, and in vitro experiments for cytotoxicity and biological activity. Journal, genetic engineering & biotechnology, 21(1), 171.

Marchut-Miko?ajczyk O, et al. (2023) Endophytic bacteria isolated from Urtica dioica L.-preliminary screening for enzyme and polyphenols production. Microbial cell factories, 22(1), 169.

Wiebach V, et al. (2023) "What I wish I had known before starting my PhD". Analytical science advances, 4(1-2), 6.