

Resource Summary Report

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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 reference material guide.

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

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

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

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: 20260803T040642+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 83 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.

Baars IM, et al. (2025) Exploring the associations between preen oil bacterial, chemical and proteomic profiles of passerines. *Antonie van Leeuwenhoek*, 118(11), 173.

Zhang Y, et al. (2025) The Effects and Mechanisms of Ti-Fu-Kang Decoction in Alleviating Central Fatigue: Insights from Network Pharmacology and Metabolomics. *Pharmaceuticals (Basel, Switzerland)*, 18(10).

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

Kalia A, et al. (2025) JESTR: Joint Embedding Space Technique for Ranking candidate molecules for the annotation of untargeted metabolomics data. *Bioinformatics (Oxford, England)*, 41(7).

Wang Y, et al. (2025) Molecular structure characteristics and pyrolytic volatiles of hydrosoluble colored fractions from three melanoidins. *Scientific reports*, 15(1), 17392.

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

Nguyen TNP, et al. (2025) Primary Metabolic Variations in Maize Plants Affected by Different Levels of Nitrogen Supply. *Metabolites*, 15(8).

Rajarathinam Y, et al. (2025) Dynamic photosynthetic labeling and carbon-positional mass spectrometry monitor in vivo RUBISCO carbon assimilation rates. *Plant physiology*, 197(2).

Fiehn O, et al. (2025) The Metabolome Atlas of 22 Tissues in Aging Mice Reveals a Switch in Thermogenesis from Brown Fat to Skeletal Muscle. *Research square*.

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).

Jeffries KA, et al. (2025) Flavonoid contributors to bitterness in juice from Citrus and Citrus hybrids with/without *Poncirus trifoliata* in their pedigree. *Food chemistry: X*, 26, 102289.

Kong XX, et al. (2025) Identification of compounds from the egg volatiles of Asia corn borer, *Ostrinia furnacalis*, that attract egg parasitoid, *Trichogramma ostrinae*. *Pest management science*.

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.

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.

Jambrina-Enr  quez M, et al. (2024) Microstratigraphic, lipid biomarker and stable isotope study of a middle Palaeolithic combustion feature from Axl  r, Spain. *iScience*, 27(1), 108755.

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.

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.