

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: data or information resource, organization portal, 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

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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 108 mentions in open access literature.

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

Liu J, et al. (2026) Synergistic Growth and Metabolic Interactions of *Kluyveromyces marxianus* and *Lactococcus lactis* in Rose-Aroma Fermented Milk Revealed by Integrated Flavoromics and Metabolomics. *Metabolites*, 16(4).

Nguyen TNP, et al. (2026) Composition of Primary Metabolites in Winter Barley Grain as Affected by NPK Fertilization of Reclaimed Land. *Plants (Basel, Switzerland)*, 15(12).

Lieberman HP, et al. (2026) Seasonal Flooding Disrupts Expected Depth-Dependent Patterns of Mineral Associated Carbon, Nitrogen, and Phosphorus Across Land Uses. *Global change biology*, 32(4), e70860.

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

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.

Vaccari ME, et al. (2025) Preparation of a Micronutrient-Enriched Apricot Kernel Oil and Assessment of In Vitro Chemopreventive Properties. *International journal of molecular sciences*, 26(18).

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).

Hu M, et al. (2025) Correlation of volatile flavors with physicochemical properties and microbiota and verification of resultant flavor variation patterns in sauce-braised duck flippers during refrigeration. *Food chemistry: X*, 31, 103101.

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).

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

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

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.

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).

Wu Y, et al. (2025) Microbiome-volatile metabolome analysis reveals aroma regulation driven by microbial niche competition in Jinggang honey pomelo wine. *Frontiers in microbiology*, 16, 1725554.

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

Thapa S, et al. (2025) Phytochemical Profile and α -Amylase Inhibitory Activity of Pomegranate Peel Extract: An In Silico and In Vitro Investigation. *Food science & nutrition*, 13(11), e71191.

Khawaja N, et al. (2025) Detection of organic compounds in freshly ejected ice grains from Enceladus's ocean. *Nature astronomy*, 9(11), 1662.

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*.

Mazzocchi E, et al. (2025) Combination of Exhaust Gas Fermentation Effluent and Dairy Wastewater for Microalgae Production: Effect on Growth and FAME Composition of *Chlorella sorokiniana*. *Microorganisms*, 13(5).