MASS SPECTROMETRY METABOLITE LIBRARY OF STANDARDS (MSMLS)

Product Description

Cat No. MSMLS

MSMLS™ (Mass Spectrometry Metabolite Library of Standards) is a collection of high quality small biochemical molecules that span a broad range of primary metabolism. These are high purity (>95%) compounds supplied in an economical, ready-to-use format. The library of standards are most commonly used to provide retention times and spectra for key metabolic compounds, help optimize mass spectrometry analytical protocols, and qualify and quantify mass spectrometry sensitivity and limit of detection. MSMLS comes with **MSMLSDiscovery™** is a software tool to support the extraction, manipulation, and storage of the data generated when using the MSMLS Library of authentic metabolite standards.

Features and Benefits

Compounds

MSMLS contains over 600 unique small molecule metabolites

Broad metabolite spectrum, key primary metabolites and intermediates covering key metabolic pathways, including the following classes of compounds:

- Carboxylic acids, amino acids
- Biogenic amines, polyamines
- Nucleotides, coenzymes and vitamins
- Mono- and disaccharides
- Fatty acids, lipids, steroids, and hormones

Note: There are a total of 634 compounds including 33 "duplicate" compounds placed in the set for QC/QA purposes. Some duplicate pairs differ in CAS number, salt and/or hydration form.

Convenient

- High purity metabolites, pre-weighed, supplied dried, 5µg each compound
- The library is intended to be used for mass spectrometry metabolomics applications and provides a broad representation of primary metabolism.

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MSMLs contains over 600 unique small molecule metabolites, a total of 634 compounds.

- Arrayed in 96-well format
- 7 polypropylene racks
    - Greiner MASTERBLOCK® #780215, polypropylene deep-well (total volume per well = 1. 2mL) in combination with seals, Greiner VIEWseal #676070
- Supplied as 5 µg dried weight
- Plate map provided upon purchase
    - Alphanumeric assigned position
    - Descriptors (see Plate Map)
- Suitable for manual and automated work flow

Software

MSMLSDiscovery software package is distributed with and is tailored to work with MSMLS to help build a physical mass spectral library using the conditions that are normally employed in the user laboratory from compounds contained in MSMLS. MSMLSDiscovery collects spectra, retention time, mass and relative intensity information for compounds, fragments and adducts.

The software supports most MS data files including Agilent, Thermo, and Waters. The requirements of the program are that:

1) Java 8 must be installed and callable;
2) The computer should have at least 8 GB of RAM;
3) You are running Windows 7 or higher.

While the MSMLSDiscovery software program is intuitive, to facilitate the use of the program a MSMLSDiscovery User Manual and MSMLS Discovery User Guide video (link below) are provided to help you run through the standard workflow. The MSMLSDiscovery User Manual gives clear instructions on how to load the MSMLSDiscovery software. Once the program is loaded, both the MSMLS User Manual and the Discovery User Guide video can be used as instructional guides to operate the program.

MSMLS Discovery User Guide video

Once libraries are generated using MSMLSDiscovery, the program can also be used to identify these compounds in biological samples. Please see the MSMLSDiscovery User Manual for further information.

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Plate Map

The library compounds are arranged in (7) seven 96-well polypropylene racks with alphanumeric assigned positions. Please refer to plate map excel sheet that comes with the library for product locations and identifiers.

Occasionally the map plate will change due to the availability of compounds. Although we try to make sure that the compounds of each row have distinct molecular weights and can be multiplexed, users should refer to the plate map before proceeding.

The plate map contains descriptors and represents information gathered from multiple databases and therefore may contain errors. We suggest that the information provided is carefully reviewed. To help build a better database, please report any discrepancies.

The excel spreadsheet plate map includes columns **A-R** as follows:

A. **Plate number** - total number of plates is seven, 1-7.
B. **Plate row letter** - rows are marked A-H.
C. **Plate column number** - columns are numbered 1-12.
D. **Primary compound name** – from KEGG or PubChem where available.
E. **SMILES** – from https://pubchem.ncbi.nlm.nih.gov/search/help_search.html#Smiles

SMILES -- **S**implified **M**olecular **I**nput **L**ine **E**ntry **S**ystem, a chemical structure *line notation* (a typographical method using printable characters) for entering and representing molecules. SMILES strings can be imported or exported from many molecular editors.

Note: The formulae and SMILES for nucleotides are represented as neutral forms (N+ and O-).

F. **Molecular formula** – formula of neutral form without salts (except in cases where compound has an innate positive charge).
G. **KEGG ID** – KEGG number where available.
H. **CAS** – a unique numerical identifier assigned by Chemical Abstracts Service, a division of the American Chemical Society, to every chemical substance described in the open scientific literature.
I. **HMDB/YMDB ID** – Human Metabolome Data Base or Yeast Metabolome Data Base ID number. Either the chemical name or the CAS number was used to search for the HMDB/YMDB ID entry.
J. **Neutral monoisotopic mass**
K. **Charge of molecule** – neutral, unless compound cannot be zwitterionic, e.g. choline.

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L. **METLIN ID** – Scripps Center for Metabolomics and Mass Spectrometry; KEGG or CAS number used for METLIN lookup.
M. **PC CID** – PubChem Compound Database ID; KEGG or CAS number used for PC CID lookup.
N. **PC SID** – PubChem Substance Database ID; KEGG or CAS number used for PC SID lookup.
O. **CHEBI** – Chemical Entities of Biological Interest (ChEBI); KEGG or CAS number used for ChEBI lookup.
P. **Sigma-Aldrich Cat No.** – Sigma-Aldrich catalog number, as available.
Q. **Sigma-Aldrich name** – Sigma-Aldrich catalog compound name, as available.
R. **Sigma-Aldrich URL** – web address of Sigma-Aldrich compound, as available.

Preparation Instructions

MSMLS compounds are conveniently provided at 5 µg per well, enough for multiple injections. The compounds of the MSMLS can either be used as standards and injected individually or mixed in such a way that the entire library may be examined with reasonable efficiency. Across all plates the compounds in each row *may* all have unique masses; mixing compounds by row *may* allow multiple compounds to be analyzed per injection.

Note: Plate 6 contains sugar H2O soluble compounds of which have masses too close in range to inject together.

Additional information can be found reading MSMLS Frequently Asked Questions (FAQ).

The following are suggestions and dependent on user chromatography and instrumentation.

1) Individual injections. As standards, each well represents a single compound; thus the entire library may be examined in great detail in 612 injections for each of the unique compounds. (Volumes of 250 µL-1 ml may be considered).
2) Simple multiplex injections. If each row of each plate is pooled, then the entire collection may be analyzed in 56 injections of simple mixtures. (Keep the well volume to 500 µl or lower to prevent loss due to dilution).
   Note: Be sure to check the individual masses across plate rows to ensure these compounds can be separated with the chromatographic system employed.
3) Complex multiplex injections. If the rows across all plates are pooled then the entire library may be analyzed in 8 injections, but the mixtures will be complex and may be dilute. (Keep the well volume to 200 µl or lower to prevent loss due to dilution).

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Solubilization and compound preparation procedure

The following are suggestions and dependent on user chromatography and instrumentation.

1) Plates 1-5: Add 5% of final volume (up to 20 µl) of very clean MeOH to every well of every plate. Add distilled water to make up the desired volume. The addition of water ensures the solubilization of the more polar compounds. We suggest a final 5% methanol solution. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.
2) Plates 6-7: These wells contain mostly lipid-like compounds (with the exception of the sugar H2O soluble compounds in plate 6). We recommend solubilizing these compounds in 1: 1: 0.3 chloroform: methanol: water.
3) Pool compounds for multiplexing. Again, be sure to check the plate map to ensure you can adequately separate the compounds using your chromatographic system prior to pooling.

Precautions and Disclaimer

The MSMLS product is for laboratory research use only. Wear safety glasses and handle with gloves. Avoid contact with skin and eyes. Please consult the Safety Data Sheet for safe handling practices and hazards information.

Storage/Stability

Store plates at -20° C. Once diluted the plates should be resealed and kept at -20° C or -80° C for long-term storage and protected from moisture and light. Avoid repeated freeze/thaw cycles.

Legal Information

Acknowledgements

We gratefully acknowledge usage of the following websites and databases for their publicly accessible information.

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Database	Website
The Human Metabolome Database (HMDB), v 2.5 [1-3]	http://www.hmdb.ca/
The Yeast Metabolome Database [4]	http://www.ymdb.ca/
Chemical Entities of Biological Interest (ChEBI) [5]	https://www.ebi.ac.uk/chebi/
Chemical Abstracts Service (CAS) REGISTRY Database [6]	https://www.cas.org/
Kyoto Encyclopedia of Genes and Genomes (KEGG) [7]	http://www.genome.jp/kegg/
The METLIN Metabolomics Database [8-9]	http://metlin.scripps.edu/index.php
The PubChem Compound and Substance Database [10]	https://pubchem.ncbi.nlm.nih.gov/

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