FATTY ACID METABOLITE LIBRARY OF STANDARDS (FAMLS)

Product Description

Cat No. FAMLS

FAMLS™ (Fatty Acid Metabolite Library of Standards) is a collection of high-quality fatty acids. These are high purity (>95%) compounds supplied in an economical, ready-to-use format. The library of standards is most commonly used to provide retention times and spectra for these key metabolic compounds, help optimize mass spectrometry analytical protocols, and qualify and quantify mass spectrometry sensitivity and limit of detection. These compounds are involved in a wide range of biological signaling pathways including ecosanoid production and the modulation of neurological pathways. Fatty acids provide fuel and energy and play a critical role in cell membrane formation. They are of great interest in immune, cell membrane, neurobiology and microbiome research and studies involving lipid and energy homeostasis.

FAMLS comes with **MLSDiscovery™**, a software tool to support the extraction, manipulation, and storage of the data generated when using the FAMLS Library and other libraries of authentic metabolite standards supplied by IROA Technologies.

Features and Benefits

Compounds

FAMLS contains 96 unique small molecule fatty acid metabolites.

Key primary metabolites and intermediates covering key metabolic pathways, including the following classes of fatty acids:

- Short chain
- Medium chain
- Long chain
- Very long chain
- Saturated and unsaturated
- Branched

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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 the chemical classes listed above.

Formatted

FAMLS contains 96 unique small molecule metabolites.

- Arrayed in a 96-well plate
  - Greiner MASTERBLOCK® #780215, polypropylene deep-well (total volume per well = 1. 2mL) in combination with seal, 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

MLSDiscovery (AKA as MSMLSDiscovery) software package is distributed with and is tailored to work with FAMLS to help build a physical mass spectral library using the analytical conditions that are normally employed in the user laboratory. MLSDiscovery 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 SCIEX. 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;
4) Data files must be able to be converted to mzXML format.

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

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MSMLS Discovery User Guide video

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

Plate Map

The library compounds are arranged in (1) one 96-well polypropylene rack 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-U** as follows:

A. **Plate number** - total number of plates is one (1).
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. **Other name** – additional common names provided.
F. **C:D or Structure**
G. **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.

H. **Molecular formula** – formula of neutral form without salts (except in cases where compound has an innate positive charge).
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. **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.
K. **Neutral monoisotopic mass**
L. **KEGG ID or ChemSpider ID (CSID)** – KEGG number where available, otherwise CSID provided.
M. **METLIN ID** – Scripps Center for Metabolomics and Mass Spectrometry; KEGG or CAS number used for METLIN lookup.
N. **PC CID** – PubChem Compound Database ID; KEGG or CAS number used for PC CID lookup.
O. **PC SID** – PubChem Substance Database ID; HMBD, KEGG or CAS number used for PC SID lookup.
P. **CHEBI** – Chemical Entities of Biological Interest (ChEBI); KEGG or CAS number used for ChEBI lookup.
Q. **Supplier CAS**
R. **Supplier**
S. **Supplier Cat. No.** – Millipore Sigma (Sigma-Aldrich) or Vendor catalog number
T. **Supplier compound name** – Millipore Sigma (Sigma-Aldrich) or Vendor compound name
U. **Supplier URL** – Millipore Sigma (Sigma-Aldrich) or Vendor URL

Preparation Instructions

FAMLS compounds are conveniently provided at 5 µg per well, enough for multiple injections. The compounds of the FAMLS 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.

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 96 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 8 injections of simple mixtures. (Keep the well volume to 500 µl or lower to prevent loss due to dilution).

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Note: Be sure to check the individual masses across plate rows to ensure these compounds can be separated with the chromatographic system employed.

Solubilization and compound preparation procedure

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

1) Rows A-C: Solubilize in high-quality chloroform. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.
2) Rows D-H: Solubilize in high-quality ethanol. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.
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 FAMLS 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.

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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