

Technical Bulletin

Gut Microbiome Metabolite Library of Standards

Supplied by IROA Technologies

Catalog Number GUTMLS**Product Description**

The **GUTMLS™** Library (Gut Microbiome Metabolite Library of Standards) is a collection of high-quality small biochemicals that the gut microbiome produces and interacts with, including bacterial, dietary, and host xenobiotic metabolites. These are high purity (>95%) compounds supplied in an economical, ready-to-use format.

The library is most commonly used to provide retention times and spectra for key metabolic compounds, help optimize analytical mass spectrometry protocols, and qualify and quantify mass spectrometry sensitivity and limit of detection.

The library is intended to be used for mass spectrometry metabolomics applications and provides a broad representation of primary metabolism.

GUTMLS comes with MLSDiscovery™, a software tool to support the extraction, manipulation, and storage of the data generated when using the GUTMLS.

Components

GUTMLS contains 185 unique small molecule metabolites covering key metabolic pathways, including the following classes of compounds:

- Organic acids and derivatives
- Allyl sulfur compounds
- Steroids and steroid derivatives
- Benzene and substituted derivatives
- Azoles
- Flavonoids and isoflavonoids
- Fatty Acyls
- Lipids and lipid-like molecules
- Indoles and derivatives
- Organonitrogen compounds
- Imidazopyrimidines
- Organooxygen compounds
- Pyridines and derivatives
- Nucleoside and nucleotide analogues

Occasionally the plate map will change due to the availability of compounds. Although we try to make sure the compounds of each row have distinct molecular masses 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. We try to ensure the accuracy of the data, but it may contain errors. We suggest that the information provided is carefully reviewed. To help build a better database, please report any discrepancies.

GUTMLS includes:

- 2 polypropylene plates in 96-well format. The plates are polypropylene deep-well (1.2 mL, total volume per well) plates (MasterBlock®, Greiner Number 780215) in combination with seals (VIEWseal™, Greiner Number 676070)
- 5 µg (dried weight) of each metabolite
- Plate map
- Alphanumeric assigned position

- Descriptors:

- Name
- Parent CID
- KEGG ID where available or ChemSpider ID
- Molecular formula
- Molecular weight
- CAS Registry Number
- ChEBI
- HMDB ID/YMDB ID
- PubChem Compound and Substance ID
- Metlin ID

Precautions and Disclaimer

For R&D Use Only. Not for drug, household, or other uses. Please consult the Safety Data Sheet for information regarding hazards and safe handling practices.

Storage/Stability

Store the plates at -20°C . The product is shipped on dry ice.

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

Preparation Instructions

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

Use high-quality solvents. Compounds in Plate 1 Rows A-F can be solubilized using Ethanol. Compounds in Plate 1 Rows G-H can be solubilized using Methanol. Compounds in Plate 2 (all compounds) are Water soluble. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.

Pool compounds for multiplexing. Be sure to check the plate map to ensure one can adequately separate the compounds using the chromatographic system prior to pooling.

Procedure

The compounds of the GUTMLS library 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. Mixing compounds by row mixtures allows multiple compounds to be analyzed per injection. Again, be sure to check the plate map to ensure one can adequately separate the compounds using the chromatographic system prior to pooling.

The following are only suggestions and depend on user chromatography and instrumentation.

1. Individual Injections – As standards, each well represents a single compound. The entire library may be examined in great detail with several injections, one for each of the unique metabolites (Volumes for each well of $250\ \mu\text{L}$ may be considered).
2. Simple multiplex injections – If the rows of each plate are pooled, then the entire collection may be analyzed with 16 injections of simple mixtures. Keep the total volume for each well to $100\ \mu\text{L}$ or less to prevent loss due to dilution. Take 5-10 μL of each well for the pooled sample, then inject 2, 4, or 6 μL of the pooled material as needed.

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



References

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