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Product Information

Large Scale Metabolite Library (International)
Supplied by IROA Technologies, LLC.

Catalog Number **LSMLSINT**
Storage Temperature –20 °C

Product Description

LSMLSINT is the international version of LSMLS™ (Large Scale Metabolite Library) - 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 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.

LSMLSINT comes with MLSDiscovery™, a software tool to support the extraction, manipulation, and storage of the data generated when using the LSMLSINT. For further information on the software, to download, and for manual and video links please visit: http://www.sigmaaldrich.com/catalog/product/sigma/lsmls

Components

LSMLSINT contains over 400 unique small molecule metabolites, conveniently provided at 1 mg per well, enough for multiple injections, suitable for manual and automated workflow.

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

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.

LSMLSINT includes:

- 6 polypropylene plates in 96 well format
- 1 mg (dried weight) of each metabolite
- Polypropylene deepwell (1.2 mL, total volume per well) plates (MasterBlock®, Greiner Number 780215) in combination with seals (VIEWseal™, Greiner Number 676070)
- Plate map
- Alphanumeric assigned position
- Descriptors:
  - Name
  - Parent CID
  - KEGG ID where available or ChemSpider ID
  - molecular formula
  - molecular mass
  - CAS
  - 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.

Preparation Instructions

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

Plates 1-5: Add 5% of final volume (up to 20 µL) of high purity methanol (MeOH) to every well of every plate. Add ultrapure water to make up the desired volume. The addition of water ensures the solubilization of the more polar compounds. A final 5% methanol solution is suggested. Pipette liquid up and down in the well 2-3 times to facilitate solubilization.

Note: LSMLSINT does not include plate 6, which comes standard with LSMLS.

Plate 7: This plate contains primarily lipid-like compounds It is recommended to solubilize these compounds using a chloroform:methanol (1:1) mixture.

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.

Storage/Stability
Store the plates at –20 °C.

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.

Procedure
The compounds of the LSMLSINT 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 444 injections, one for each of the unique metabolites (Total volumes for each well of 250 µL–1 mL may be considered).
2. Simple multiplex injections – If the rows of each plate are pooled, then the entire collection may be analyzed with 48 injections of simple mixtures Keep the total volume for each well to 150 µL or less to prevent loss due to dilution and use 5-10 µL of each well for the pooled sample. Then, inject 2, 4, or 6 µL of the pooled material as needed.

References

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