3050 Spruce Street, St. Louis, MO 63103 USA
Tel: (800) 521-8956 (314) 771-5765 Fax: (800) 325-5052 (314) 771-5757
email: techservice@sial.com sigma-aldrich.com

# Product Information

**Large Scale Metabolite Library**
Supplied by IROA Technologies, LLC.

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

## Product Description

LSMLS™ (Large Scale Metabolite Library) 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 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.

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

LSMLS contains over 500 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.

LSMLS includes:

- 7 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.

Plates 6 and 7: These plates contain primarily lipid-like compounds (with the exception of the water soluble sugar compounds in plate 6). 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.

Note: There may be duplicate compounds placed in the set for QC/QA purposes. Duplicate pairs differ in CAS number, salt and/or hydration form.

**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 LSMLS 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.
Note: Plate 6 contains water soluble sugar compounds, which have masses too close in range to inject together.

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 504 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 56 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**


1. Wishart, D.S. et al., HMDB: the Human Metabolome Database. Nucleic Acids Res., 2007, Jan; 35 (Database issue):D521-6. 17202168.
2. Wishart, D.S. et al., HMDB: a knowledge base for the human metabolome. Nucleic Acids Res., 2009, 37 (Database issue):D603-610. 18953024.
3. Wishart, D.S. et al., HMDB 3.0 – The Human Metabolome Database in 2013. Nucleic Acids Res., 2013, Jan 1; 41(D1):D801-7. 23161693
4. Hastings, J. et al., The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Res., 2013.
5. Kanehisa, M., and Goto, S., "KEGG: Kyoto Encyclopedia of Genes and Genomes". Nucleic Acids Res., 2000, 28 (1): 27– 30. doi:10.1093/nar/28.1.27. PMC 102409.PMID 10592173.
6. Tautenhahn, R. et al., An accelerated workflow for untargeted metabolomics using the METLIN database. Nature Biotechnology, 2012, 30: 826–828. doi:10.1038/nbt.2348.
7. Smith, C.A. et al., METLIN: a metabolite mass spectral database. The Drug Monit., 2005, 27 (6): 747–51. doi:10.1097/01.ftd.0000179845.53213.39. PMID 16404815.
8. Bolton, E. et al., PubChem: Integrated Platform of Small Molecules and Biological Activities. Chapter 12 IN Annual Reports in Computational Chemistry, Volume4, American Chemical Society, Washington, DC. 2008, Apr [free author manuscript]


LSMLS and MLSDiscovery are trademarks of IROA Technologies, LLC.
MasterBlock is a registered trademark and VIEWseal is a trademark of Greiner Bio-One GmbH.

SS,KV,AA,MAM 05/19-1