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

**Bile Acid/Carnitine/Sterol Metabolite Library of Standards**
Supplied by IROA Technologies, LLC.

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

## Product Description

BACSMLS™ (Bile Acid/Carnitine/Sterol Metabolite Library of Standards) is a collection of high-quality bile acids, carnitines, and sterols 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.

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

## Components

BACSMLS contains 96 unique small molecule metabolites, conveniently provided at 5 μg per well, enough for multiple injections, suitable for manual and automated workflow.

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

- Bile acids
- Carnitines
- Sterols

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 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. 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.

BACSMLS includes:

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

Most compounds can be solubilized using high-quality methanol. (Exceptions are: A1, B8, B11, B12, C6, C12 – solubilize in high-quality chloroform and B10 – solubilize in high-quality chloroform:methanol (1:1). Pipette 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.

**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 BACSMLS 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. 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; thus the entire library may be examined in great detail in 96 injections for each of the unique compounds. (Total volumes for each well of 250 μL – 1 mL may be considered).
2. Simple multiplex injections – If each row of the plate is pooled, then the entire collection may be analyzed in 8 injections of simple mixtures. (Keep the well volume to 500 μL or less 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.

**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 knowledgebase 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. Jewison, T. et al., YMDB: The Yeast Metabolome Database. Nucleic Acids Res. 2012 Jan;40 (Database Issue): D815-20 PubMed: 22064855.
5. Hastings, J. et al., The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Res. 2013. Jan;41 (Database issue):D456-63. doi: 10.1093/nar/gks1146. Epub 2012 Nov 24.
6. CAS REGISTRY, Division of the American Chemical Society
7. 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.
8. 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.
9. 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.
10. Kim, S. et al., PubChem Substance and Compound databases. Nucleic Acids Res. 2016 Jan 4; 44(D1):D1202-13. Epub 2015 Sep 22 [PubMed PMID: 26400175] doi: 10.1093/nar/gkv951 [Free Full Text at Oxford Journals]




SS,AA,MAM 05/19-1